iCSI

industrial Catalysis Science and Innovation

Annual Report 2022

Norwegian Centre for Research-based Innovation

NTNU

iCSI Partners

Norwegian Centre for Research-based Innovation

NTNU

SINTEF

UiO : University of Oslo

YARA

HALDOR TOPSØE

inovyn

K·A·Rasmussen NORWAY

dynea®

Funded by The Research Council of Norway

Cover photo: Scanning Electron Microscope- Electron Backscatter Diffraction (SEM-EBSD) map of the cross-section of a Pd net after being exposed to 5% NO in N_2 for 90 minutes at 920°C. The different colors represents different planes in the grain structure. Photo by Martin F. Sunding.

2022 Summary

2022 has been a somewhat more "normal" year, which may sound a bit boring. However, after two highly unconventional years, most of us have learned to appreciate normality.

Thirteen reviewed papers were submitted and accepted for publishing in 2022. The publications were evenly distributed between IIA1, IIA4, IIA5 and IIA6, and most of them were published with international collaboration partners.

Travel and conference participation with international mingling again could once again take place. iCSI was represented at conferences in Wales, Finland, USA, Japan, as well as in international events in Oslo and Stavanger. PhD candidates participated in an international renewable energy summer school in Asker and a catalysis winter school and also a synchotron school in France. A complete list of publications and conference contributions from iCSI and associated researchers in 2022 can be found on pages 55-63.

For the first time iCSI could welcome guest researchers to both UiO and NTNU, funded by our CATHEX INTPART project. The two professors Patricia Kooyman and Michael Claeys with four young scientists/students from University of Cape Town visited us. We also funded a four-month research stay to the University of Wisconsin-Madison for one NTNU-associated candidate.

Educating master's students is important to iCSI. In 2022, nine 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.

One candidate, Asbjørn Slagtern Fjellvåg, finalized his PhD thesis with a defence in September. iCSI congratulates him and his supervisor, Professor Anja Olafsen Sjåstad! We are also proud to announce that Hongfei Ma's PhD thesis from 2021 was named the best PhD thesis of the year at NTNU's Faculty of Natural Sciences.

The science is progressing in all Industrial Innovation Areas, and on page 15 we present this year's highlight. In collaboration with personnel at the MAX IV synchrotron in Lund, Ingeborg-Helene Svenum and Hilde Venvik have utilized in situ near ambient pressure x-ray photoelectron spectroscopy (NAP-XPS) on the HIPPIE beamline. They were able to follow the surface properties of PdAg alloy catalysts and thin film membranes in response to the reaction environment, such as changes in temperature and relative concentrations of the species in the gas phase. The results show how CO_2 formation differs between Pd and PdAg surfaces and how segregation (ratio Pd to (Pd+Ag)) changes with temperature during CO oxidation. Palladium (Pd) membranes alloyed with silver (Ag) are used in hydrogen separation.

Thirty-nine members of the iCSI family gathered at Voksenåsen Hotel in June for our Annual Seminar. This year we were lucky, as the whole Scientific Advisory Committee (SAC) had time and opportunity to join the seminar. All three SAC scientists contributed with high-level lectures, inspiring scientists from iCSI. They actively participated in the scientific discussions by challenging and encouraging iCSI researchers, and they spent time meeting individually with four of our PhD candidates.

Two PhD candidates received the opportunity for industrial exchanges with our industry partners. Jithin Gopakumar spent two months with Yara this summer, while Youri van Valen visited Dynea for one month in November and has plans for another month, this time with K.A. Rasmussen in March 2023. They share their experiences on pages 22-23.

The representation on the iCSI Board has changed for one of the industry partners in 2022, with Tigran Margossian taking over from Camilla Jordal as Inovyn's board representative in April. We thank everyone on the board, as well as all the scientists for their efforts for iCSI throughout the year.

MAX IV Laboratory, Lund University, Sweden (www.maxiv.lu.se/)

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Catalysis remains a key technology
(even when the times are a-changin')!

The energy and commodity markets have seen dramatic changes in 2022. This may be regarded as mainly due to the war in Ukraine, but climate change and the pandemic affect the global trends as well. Increased prices are not necessarily only bad or good for each industrial operation/partner but there is definitely greater uncertainty about the future. An overall result appears to be a stronger push towards renewable energy production and circular economy in Europe. However, while in the US with the *inflation reduction act* (IRA) a large investment package has been launched to provide incentives for investments in the green transition, the necessary efforts and results in the EU this far are insufficient.

For the iCSI team, it is becoming apparent that catalysis is more important than ever. Catalysts:

- enable important chemical transformations that are otherwise difficult to achieve, such as the synthesis of ammonia and splitting of water.
- clean exhaust emissions like NOx and CO.
- reduce energy consumption, greenhouse gas emissions, CAPEX and OPEX of industrial processes.
- generate fewer side-products than non-catalytic alternatives.

These are the very functions that the iCSI industrial partners exploit and strive to improve everyday. Important future applications that have been identified within the European and global initiatives as key to the high ambitions for a sustainable world include:

- production of hydrogen (H_2) from water
- conversion and recycling (reduction) of CO_2
- chemicals and liquid fuels from biomass and waste

These transformations are energy or resource intensive in nature, and their applicability strongly depends on our capability to design efficient catalysts and associated process schemes. We also need completely new catalysts that do not involve scarce resources such as platinum. But there is no way forward without the catalysts.

From iCSI, we therefore urge continued investment in our research, our competence and our education. Catalysts, catalysis knowledge and catalysis people are very much in demand!

iCSI Board

Photo: Åge Hojem

Vision, objectives and strategy

iCSI focuses on Catalysis Science and Innovation related to a range of industrial processes that are key to Norwegian land-based industry and industrial competitiveness, as well as future chemical processing and energy conversion with the smallest possible environmental footprint. The industrial partners involved supply key sectors of the global market (e.g. catalysts, chemicals, fertilizer, plastics, fuels), which are the very products that impact our food supply and standard of living the most. The iCSI consortium represents leading competence and technology, for which the core business relies largely or completely on catalytic processes. iCSI represents significant industrial operations in Norway as well as worldwide. iCSI's basic vision has been to establish an integrated competence and technology platform that promotes world class energy and raw material efficiency and enables spin-off activities in the different directions of prime interest for the industrial partners. Furthermore, iCSI is developing a strong competence base for the Norwegian chemical industry in the long term and to the benefit of society in terms of securing jobs, reducing energy consumption and abating harmful emissions into the environment. State-of-the-art methodology in synthesis, characterization and technology development is applied in order to obtain a detailed understanding of complex catalysts under industrially relevant conditions, thereby identifying factors critical to their performance. iCSI researchers also develop predictive tools for optimization of materials, chemistries and processes.

Photo: Jithin Gopakumar

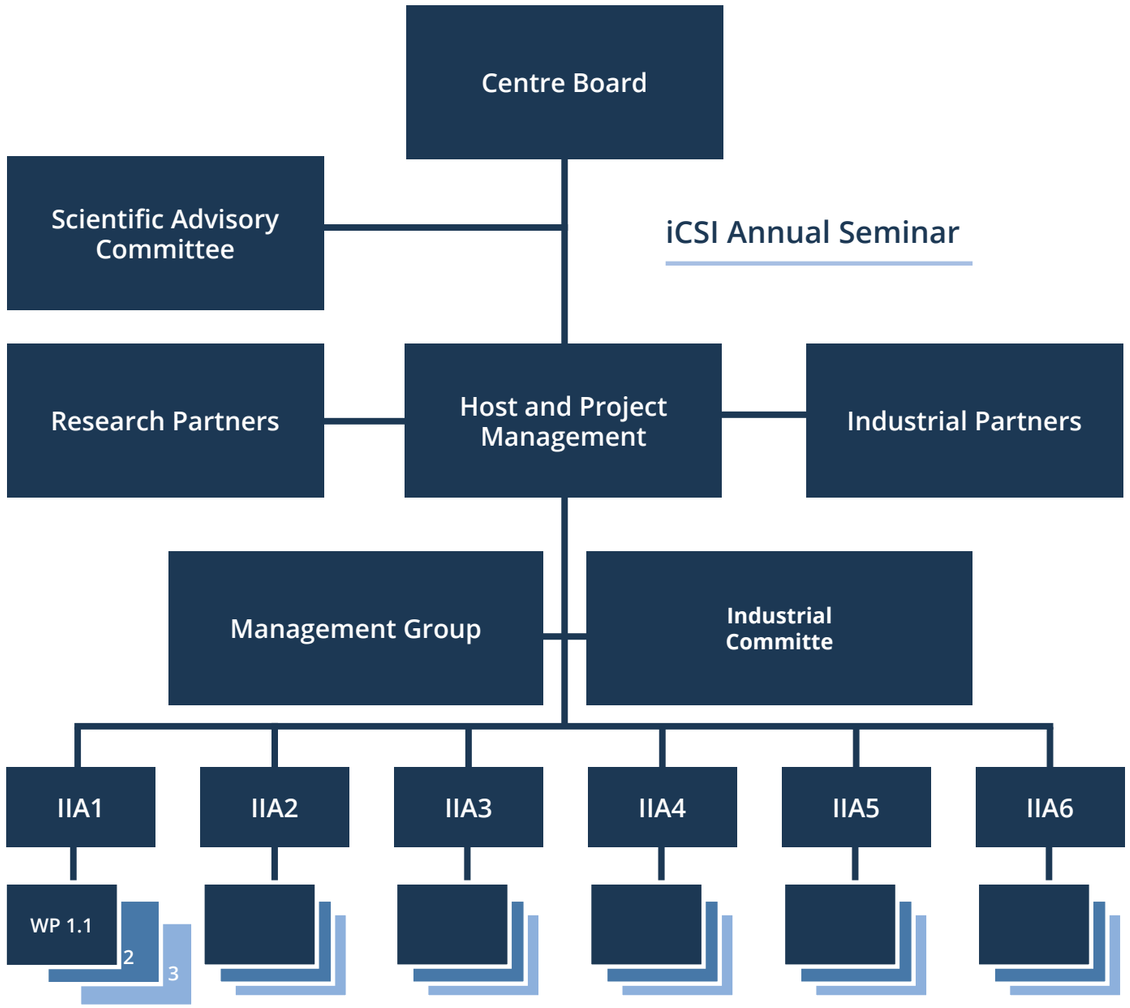
iCSI's main objective is to boost industrial innovation and competitiveness and provide efficient, low-emission processes.

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



Industrial Partners

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

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

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.

Haldor Topsøe AS is a catalyst producer and process plant technology developer based in Denmark. Haldor Topsøe 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. KA Rasmussen has specialized in technology for producing structured catalysts for the Ostwald process and silver particles for the oxidation of methanol. In iCSI, KA Rasmussen wants to expand its catalyst market base, contribute to meeting emissions targets and reduce the net consumption of noble and scarce metals in their product range.

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

Centre Board

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

Pablo Beato from Haldor Topsøe has acted as Chair of the Board in 2022. In April 2022, Tigran Margossian replaced Kamilla Jordal as Inovyn's representative.

Dr. Pablo Beato

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

Lars Axelsen

General Manager of Technology Sales & Li-censing at Dynea.

Torgeir Lunde

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

Thomas By

Head of Research and Development at K.A. Rasmussen

Tigran Margossian

Research and Develop-ment Manager at Inovyn

Professor Einar Uggerud

Head of Department of Chemistry at the University of Oslo

Professor Karina Mathisen

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

Dr. Duncan Akporiaye

Research Director at SINTEF Industry.

Dr. Aase Marie Hundere

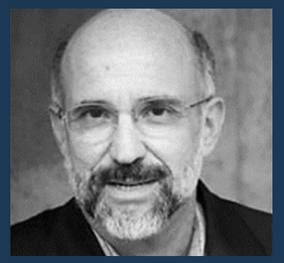
Special advisor RCN, with Responsibility for Nanotechnology and Advanced Materials

Scientific Advisory Committee

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

Professor Alessandra Beretta

Politecnico di Milano, Italy



Professor Enrique Iglesia

University of California, Berkeley, USA

Professor Graham Hutchings

Cardiff University, United Kingdom

Management and Administration

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

Hilde J. Venvik

Professor
iCSI Centre Director

Anne Hoff

Senior advisor
iCSI Coordinator

Hilde M. Flaathe

Financial Project Advisor
iCSI Economy advisor

Researchers Portrait: Professor De Chen

When Stanford University released its latest global list that represents the top 2% of the world's top-cited scientists in various disciplines, Professor De Chen from NTNU's Department of Chemical Engineering was on the list. Colleagues from iCSI are not surprised, as we know he is extremely productive and has over the years contributed to more than 435 published documents with 21 766 citations. He has supervised/co-supervised 70 master's students, 38 PhD candidates, and 25 post docs. Here you have an opportunity to get to know this man a little better.

De Chen was born in 1962 into a family of three children, living on Chongming Island next to the large city of Shanghai in China. This was a very special period of Chinese history, and his entire childhood and youth were dominated by the Cultural Revolution. There was almost no schooling, as all qualified teachers had been sent to the countryside to work, and those who remained had a limited repertoire which they repeated and repeated every year. When China finally opened for university studies again in 1978, De was part of the first cohort to be admitted. They were given half a year to study for the entrance exam, and then they had to catch up on everything they hadn't learned in 10 years. "It was a crash course in self-study," says De.

To illustrate what the level in primary school had been, he relates that when they were questioned on what 3 to the second power was (3^2) on a math test, no one could answer, because they had never heard of this.

Didn't you learn anything useful in those ten years without qualified teachers?
"Oh yes, I learned practical skills, which I have carried with me during my studies and in laboratory work. Assembling instruments and rigs is no problem, and during my PhD work, I built almost all the associated equipment for my project myself."

The incomplete teaching also led to a desire and longing for knowledge, and De's motivation for studies was high when they finally had access to books and competent teachers. The universities mostly had an aging professorial staff, as a whole generation of academics was missing as a result of the Cultural Revolution.

After four years of study, De was ready for a trainee job in Shanghai with SINOPEC (Shanghai Institute of Petrochemical Technology), the state-owned petrochemical giant. "There I received training alongside the process operators, and over three years I visited the vast majority of the various petrochemical processes in the plant. I received good training in reading flowcharts and I made my way through the entire factory with the help of the lines that showed tube streets, heat exchangers, reactors and all other devices found in such facilities.

But De was ready to learn more, and after an application and entrance exam he was one of only a few given the opportunity to start a master's degree. His master's thesis was about process upscaling, and then he got to use everything he had learned about reaction technology, modelling and, not least, identifying key parameters for the process. After completing his education, he was given more responsibility at SINOPEC. He began to teach others, while also doing research and making process improvements, eventually becoming the group leader.

But then, in 1994, his path through life changed direction. He heard about a collaboration agreement between China and Norway, which granted him a five-month exchange stay with Professor Anders Holmen in Trondheim. He arrived here on a day with a doctorate defence, and he was invited to an amazing defence party. He was not easily intimidated, and this made such a strong impression that he applied for a PhD position, which he started in 1995.

It was not easy to stay in Trondheim, far from home. In China he had a wife and a small daughter. This was before video chat apps, and phone calls were expensive. The price increased with the distance between those who spoke. "A private call home cost NOK 70 per minute! However, I discovered that it was cheaper to call from the university, and with a price of "only" NOK 30/min, I could afford a weekly call with my family. I received lists of calls from secretary Lisbeth and had to tick them off and pay for my private calls. In addition, I wrote letters, and I still have a stack of letters that I received from family on the other side of the globe."

After a year and a half, De's family was finally able to reunite in Trondheim, and by then his daughter had turned five. She started at the international school, and when De later completed his PhD, they realized that it would be best for her if she could continue where she had started. He was lucky and received a job offer as associate professor at NTNU and worked as a SINTEF employer-B for 6 months. where he was to work on steam reforming.

However, obtaining a work and residence permit was not as easy as he had hoped. At that time, China was considered a developing country, and scholarship holders were not allowed to stay in Norway after completing their doctorates. It was expected that they would go back to rebuild their homeland. However, De's good friend and mentor Anders Holmen did not give up so easily. He hired a lawyer who explained to the authorities that Norway needed all the good people we could get. He claimed, "We compete with the whole world, and the alternative for the candidates who have been with us is not to go home, but further to the USA, Canada and other countries that happily accept the brightest people." After a tough battle with newspaper notices and a lot of lobbying, De was finally allowed to stay. And, after all this public attention, the law was changed by removing the requirement to return home.

When he was finally allowed to stay, De started to work in the catalysis group as an associate professor. "It was attractive to stay in Norway, because here the funding opportunities were better than in China, and I had more freedom to choose for myself which topics I wanted to delve into. Academia was (and is) interesting as it provides the opportunity to constantly acquire new knowledge, new learning, new challenges. At the same time I have contact with students and am able to pass on what I find out, so that society can in turn benefit from the knowledge.

In 2009/2010 De spent a year with Professor Enrique Iglesia at the University of Berkeley. There he worked in the lab and learned a lot about and from Iglesias' well-established methodology for kinetics and mechanism studies. He also greatly appreciated how Iglesia organized student seminars with varied and deep discussions on academic topics, while at the same time they functioned as social gatherings. The candidates gave long presentations of their own tasks, in addition to giving a review of the latest literature in their field. The professor himself and postdocs also participated and contributed to the discussions when required. "I've brought a lot of what I learned from Professor Iglesia to supervising work with my own students.

Then we challenged the Professor De Chen about his personal achievements and working philosophy. Here are some of his answers:

What are you most proud of?
"A big question, but it must be how we have managed to establish reaction and process models based on a multiscale hierarchical approach, using DFT and theoretical studies. Models with varying degrees of complexity are combined there. The results are attractive to industrial partners and used in industrial projects, both in new processes and for optimizing performance in old and established processes. However, what we have done in the field of carbon-based catalysis is also important, and has contributed to a completely new application of carbon materials. Now, you can design and tune the properties of the materials so that they have a better catalytic effect.

De Chen and Professor Anders Holmen at the 10th Nordic Symposium on Catalysis in Helsingør, Denmark in 2002. They were accompanied by Ingrid Aartun Bøe, Sølvi Storsæter Bjørgum, Erlend Bjørgum and Hilde Johnsen Venvik.

Who has meant the most to you in your career?
"It is undoubtedly Anders Holmen! Ever since he welcomed me in 1994 he has followed my progress and helped me further. In particular, he has been there when I've needed it the most! He has been, and still is, a mentor I value very much. I am so grateful to him and his wife Bjørg. All the other colleagues in the catalysis group are also good to have, without mentioning anyone in particular.

What inspires you?
"Seeing the important challenges in society and industry, and knowing that you possess knowledge and methods that can contribute to solving many of these. It can involve sustainable utilization of biomass, recycling of plastic materials, CO_2 capture. It is important to be able to be at the forefront, so that when society realizes that it has a problem, we already have the basic knowledge and methodology to help solve it. Knowing that you can help save the world by developing industrial processes into something better – in collaboration with the big companies – that's inspiring!

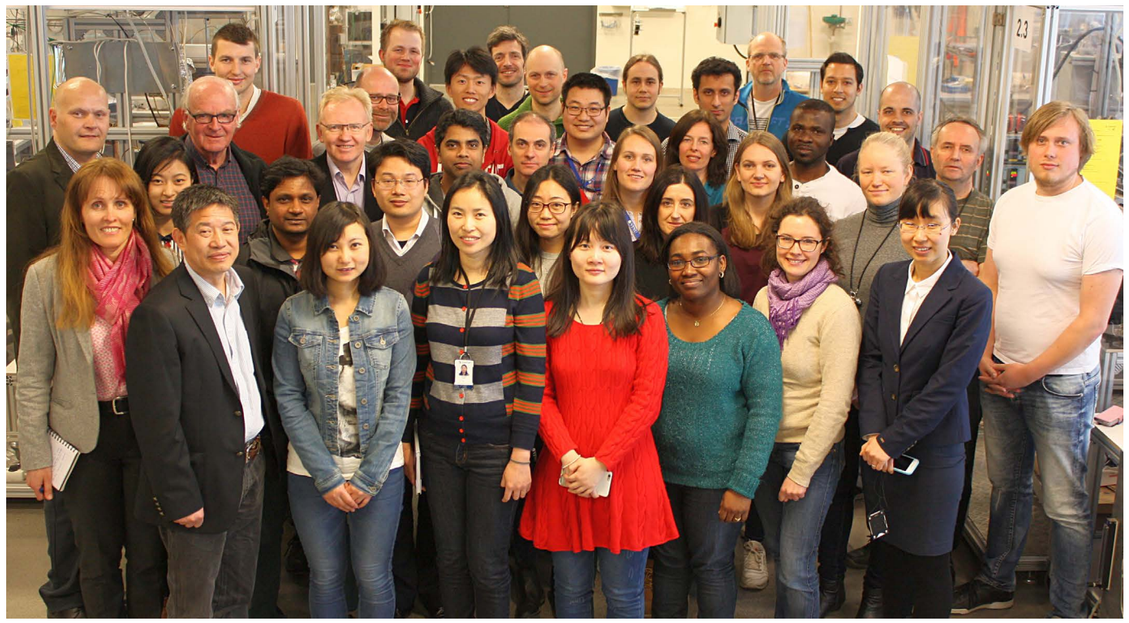
What do you say to all students?
"1. You have to try! Otherwise, you will never know if something works or not.... (have to admit I adopted this from Anders H).

2. You have to bring your knowledge to the industry and out into society! It doesn't help if we produce a lot of knowledge and it's not put to use in useful projects."

How can you and your colleagues contribute to a better world?
"By focusing all our teaching on the major challenges, choosing relevant examples of the application of knowledge, and giving students faith that they can make a difference and be part of the solution.

And finally: To those of us who know him, it may seem like De Chen is always working. But he that's not quite true! He fits in going to his cabin in Oppdal, where he goes for walks in the mountains and enjoys nature. That is relaxing and gives him peace of mind. Have a nice trip, De!

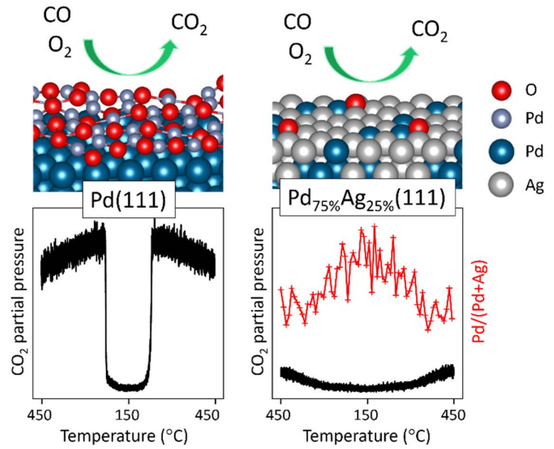
Professor De Chen and his coworkers in project meeting with industry partner Inovyn.



KinCat group 2016

Scientific Highlight 2022: Cyclic alloy segregation during reaction captured by in situ NAP-XPS at the MAX IV synchrotron

We have for some time been interested in the surface segregation of alloy catalysts and thin film membranes in response to the reaction environment, such as changes in temperature and relative concentrations of the species in the gas phase. To which extent will the surface composition attain its thermodynamic minimum? We have encountered this question during our research on 2-10 µm thin palladium (Pd) membranes alloyed with 23wt% of silver (Ag) used in hydrogen separation. Moreover, the effect was also hypothesized and modelled as the cause of a strikingly different hysteresis behaviour during CO oxidation (p = ~0.7 mbar, O_2:CO=10) over the $Pd_{75\%}Ag_{25\%}$(100) surface termination as compared to the pure Pd(111) single crystal surface [1]. We were able to confirm segregation during our first near ambient pressure x-ray photoelectron spectroscopy (NAP-XPS) beamtime at the HIPPIE beamline, MAX IV, but we were not quite satisfied with the experimental protocol and resulting clarity of the data [2]. Basically, each experiment was found to be affected by the previous one when we cycled the temperature from 25 °C to 450 or 600 °C under CO oxidation conditions (p = ~1.1 mbar, O_2:CO = 10).



The figure shows how CO_2 formation differs between Pd and Pd/Ag surfaces and how segregation (ratio Pd to (Pd+Ag)) changes with temperature during CO oxidation.

Proceeding to a different surface termination in our next beamtime at HIPPIE, and comparing the pure noble metal to the alloy, i.e., Pd(111) vs. $Pd_{75\%}Ag_{25\%}$(111), we considerably improved the protocol [3]. Clear, cyclic segregation in the PdAg alloy was achieved by starting each temperature cycle at 450 °C, at which the surface was first oxidized in pure O_2 for 10 min before CO was added (p = ~2 mbar, O_2:CO = 10) and the temperature decreased to 150 °C and then increased. We found that a surface oxide ((√6×√6) Pd_5O_4) is present on Pd(111) when the surface is highly active and the oxidation of CO essentially being limited by diffusion of CO towards the surface. There is a hysteresis in the CO_2 formation profile during temperature cycling that depends on the temperature ramp rate. This behaviour is different for $Pd_{75\%}Ag_{25\%}$(111), with the CO_2 formation rate considerably lower, no diffusion limitation, no surface oxide and only chemisorbed oxygen present at the surface at high temperature, reversible scrambling of the (near) surface Pd/(Pd+Ag) ratio, and no hysteresis behaviour observed. The results suggest that the reactant activation is affected by both surface composition and surface termination, i.e. mechanistically different on $Pd_{75\%}Ag_{25\%}$(111) than Pd(111), and less efficient on (111) as compared to the (100) alloy counterpart.

Publications

1. Fernandes, Vasco R.; Bossche, Maxime Van den; Knudsen, Jan; Farstad, Mari H.; Gustafson, Johan; Venvik, Hilde J.; Grönbeck, Henrik; Borg, Anne. Reversed Hysteresis during CO Oxidation over $Pd_{75\%}Ag_{25\%}$(100). ACS Catalysis (2016), 6(7), 4154-4161. https://doi.org/ 10.1021/acscatal.6b00658

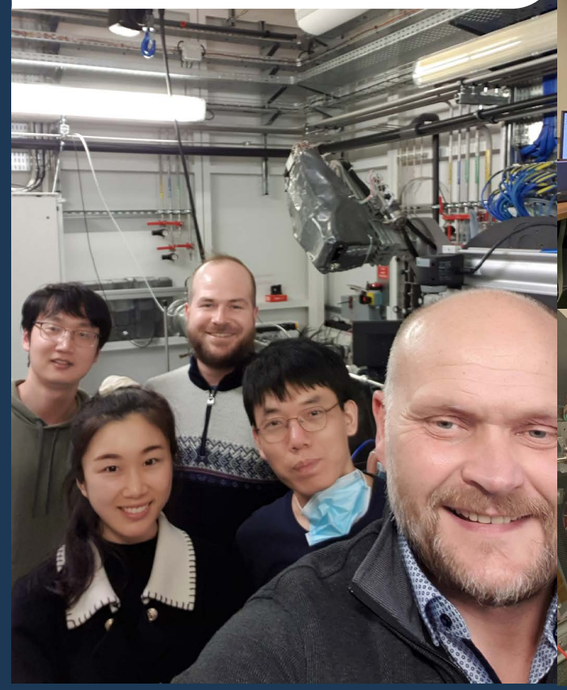
2. Marie D. Strømsheim, Ingeborg-Helene Svenum, Mehdi Mahmoodinia, Virginia Boix, Jan Knudsen, Hilde J. Venvik. Segregation dynamics of a Pd-Ag surface during CO oxidation investigated by APXPS. Catalysis Today, Catalysis Today 384 (2022) 265-273. https://doi.org/ 10.1016/j.cattod.2021.02.007

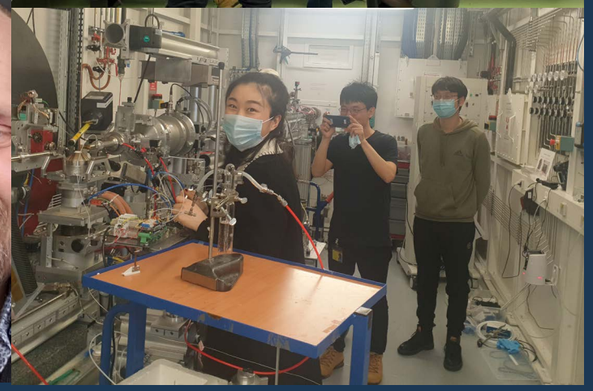
3. Ingeborg-Helene Svenum, Marie D. Strømsheim, Jan Knudsen, Hilde J. Venvik. Activity and segregation behavior of $Pd_{75\%}Ag_{25\%}$(111) during CO oxidation – An in situ NAP-XPS investigation. Journal of Catalysis 417 (2023) 194-201. https://doi.org/10.1016/ j.jcat.2022.11.038

iCSI moments 2022

Asbjørn defends his PhD

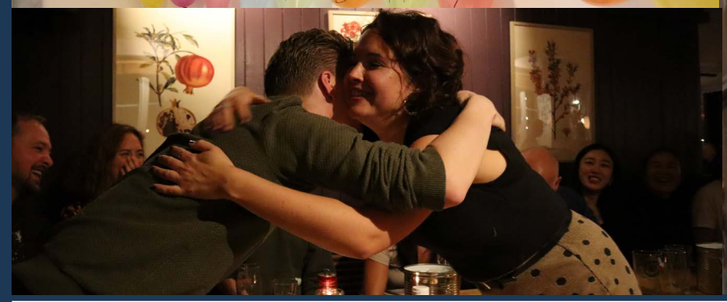
Beamtime SNBL@ESRF, France





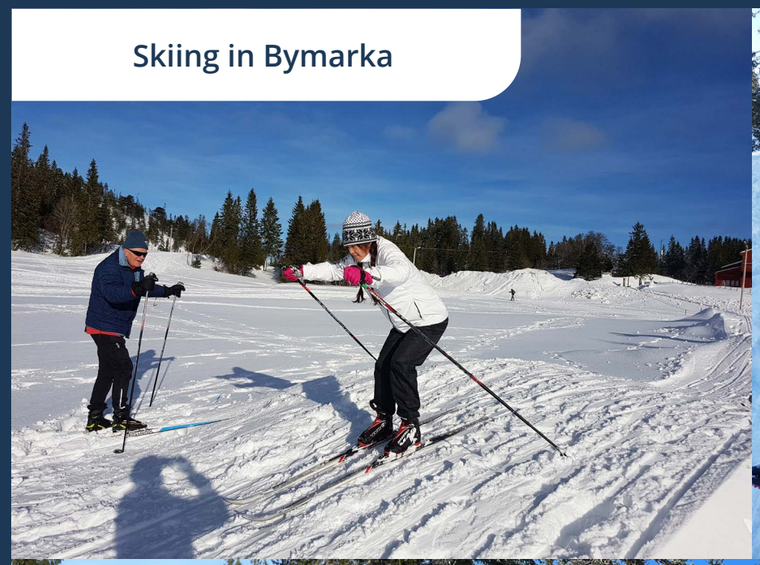
Goodbye to Lin, Yurou and Yalan!

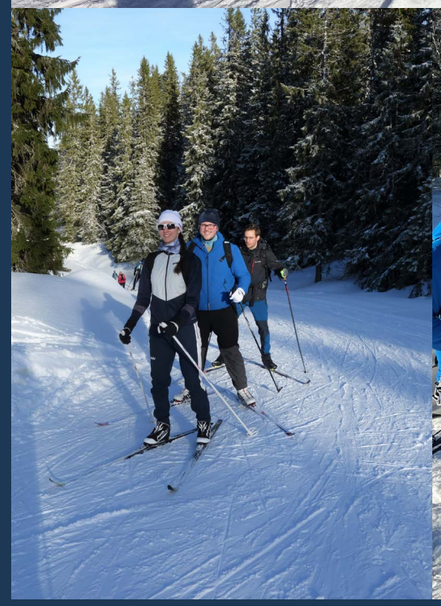
Happy Birthday, Estelle!



A new KinCat group photo 2022

Skiing in Bymarka

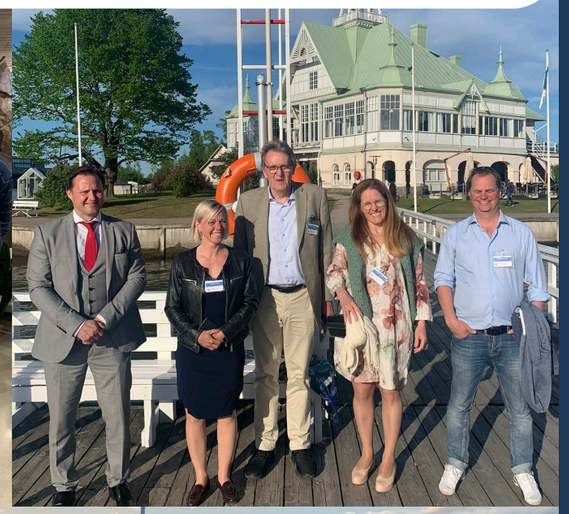




World Congress on Oxidation Catalysis, Wales

IKP Days NTNU

Nordic Symposium on Catalysis, Finland



KinCat in Finnish sunset

Annual Seminar

Hilde Johnsen Venvik between Graham Hutchings from Cardiff University and Alessandra Beretta from Politecnico di Milano.

Enrique Iglesia from University of California, Berkeley

Two suitably warm mid-summer days in Oslo, a fantastic view of the town and three top-ranked international catalysis scientists gathered with iCSI. What could be better? This year we were fortunate that the whole Scientific Advisory Committee (SAC) had the time and opportunity to join our Annual Seminar. All three contributed with high level lectures, inspiring young and not-so-young-anymore scientists from iCSI. They also actively participated in the discussions when the iCSI researchers presented their work, challenging and encouraging them. At the end of day 1, they also spent time in individual meetings with four of our PhD candidates who are about halfway through their coursework. They were given about 20 minutes each to present their own results and received honest feedback from a collective SAC. iCSI is extremely happy with our advisory team, and cannot appreciate their contribution enough.

Thirty-nine iCSI scientists from all the industry partners, SINTEF, UiO and NTNU convened at Voksenåsen Hotel and Culture Centre to share their results from the last year's work in their labs. This was the first real post-pandemic seminar and everybody appreciated the participation from abroad.

At the end of the first day's lectures and scientific discussions, a large group put on hiking/jogging shoes and had a nice walk down to the Holmenkollen ski jump, and back up again via Frognerseteren. With this physical relaxation, we were ready for a good dinner, a good night's sleep and a new day with sharpened attention. We can now look forward to the last iCSI seminar in Trondheim in June 2023, which finalizing the life of the iCSI centre.

Day 1	Tuesday June 21
09:00-10:00	Registration/check-in/small talk /coffee
10:00-10:30	Opening remarks (Chair of the Board, Pablo Beato) Status of iCSI (Director, Hilde J. Venvik)
10:30-11:30	Alessandra Beretta: Intensification and Electrification of Methane Steam Reforming by the use of thermally/electrically conductive catalyst supports
11:30-12:00	IIA3: Frontier formalin technology development: Overview of IIA3 activities, by Hilde J.Venvik Partial oxidation of Methanol to Formaldehyde over Silver, by Youri van Valen
12:00-13:00	Lunch
13:00-14:00	Enrique Iglesia: Mesopores as liquid phase nanoreactors and consequences of outer-sphere solvation effects in surface catalysis
14:00-14:45	IIA1: 21st century Ammonia Oxidation and Nitric Acid technology development Overview of IIA1 activities, by Anja O. Sjåstad How suitable are oxides as alternative Pt catchment materials in the ammonia oxidation process? by Julie Hessevik Catalytic Oxidation of NO to NO2 for Nitric Acid Production, by Jithin Gopakumar
14:45-15:10	Coffee break / Preparations for poster session
15:10-15:30	IIA2: Abatement of nitrogen-containing pollutants – state-of-the-art catalyst technology Characterisation studies of industrial de-N2O catalysts, by Martin F. Sunding
15:30-15:45	IIA5: The next step in Direct Activation of Lower Alkanes Spectroscopic and kinetic studies of the direct activation of lower alkanes over transition metal containing zeolite catalysts, by Bjørn G. Solemsli
15:45-17:00	Poster session
16:45-18:00	New SFI-group meeting / IIA4 project meeting
16:45-18:00	PhD individual meetings with SAC (18 min each: Jithin, Julie, Youri, Bjørn GS)
18:00-19:30	Social activity / A walk in the wood
20:00-22:00	Dinner

Day 2	Wednesday June 22
08:00-08:45	Breakfast
08:45-09:00	Welcome to day 2
09:00-10:00	Graham Hutchings: Catalysis using gold and gold alloys
10:00-10:20	IIA1: 21st century Ammonia Oxidation and Nitric Acid technology development Pd loss and reconstruction under different gas compositions, by Silje F. Håkonsen
10:20-10:50	Coffee break / Checking out
10:50-11:20	IIA6: Generic projects for additional industrial synergies Update from the surface science laboratory in Oslo, by Anja More easily accessible microkinetic modelling with DFT, by Ingeborg-Helene Svenum
11:20-12:15	IIA5: The next step in Direct Activation of Lower Alkanes Overview of IIA5 activities, by Stian Ethane to ethylene over Cu loaded zeolites, by Karoline Kvande Progress in zeolite synthesis for methane to methanol, by Sebastian Prodinger
12:15-13:15	Lunch / Checking out
13:15-14:30	IIA4: PVC Value Chain: World class energy and raw material efficiency for production of Chlorine and Vinyl Chloride Monomer. Overview of IIA4 activities by De Chen Kinetic Study of Byproducts Formation and Optimization of Promoters in Ethylene Oxychlorination, by Wei Zhang Modelling work, by De Chen
14:30	Closing remarks

PhD Exchanges

Two of iCSI's PhD candidates were granted funding for two months industry exchange in 2022.

Jithin Gopakumar, our iCSI PhD candidate from India/ Dubai, spent two months with the industry partner Yara at Herøya in Porsgrunn during summer 2022. Here are some of his experiences:

"At Yara I worked on a second generation single pellet activity tester (SPAT II). The equipment is custom built by engineers at Yara to measure catalytic N_2O abatement.

The machine contains 64 reactors and has a capacity to measure the activity of 64 different pellets. My work was mostly related to aligning the activity results from SPAT II with that of the pilot plant at Yara.

The opportunity was wonderful and provided many insights on industrial research and social dynamics at a workplace such as Yara. This kind of industrial exchange also acts as a platform to use your skills or knowledge and learn more about your strengths and weaknesses. What I loved most was summer in Porsgrunn and the work-life balance I got at Yara compared to that of my PhD, which allowed me to enjoy the city."

Dutch candidate **Youri van Valen** split his exchange with one month at Dynea's Lillestrøm facilities in fall 2022 and one month that he will carry out at K. A. Rasmussen in spring 2023. Here are some experiences from his first stay:

"In November I went for an industrial exchange at Dynea AS. I got to know more about the company involved with my project and the motivation behind their involvement with the iCSI project. The four weeks that I spent there were by no means enough to learn or experience everything the company had to offer, but I did leave with a good taste of what it means to work in the chemical industry. Seeing the formaldehyde production first-hand and learning about all the derivatives they produce was a fascinating experience. During my stay I was tasked with reviewing some work done in other work packages within IIA3. That work combined with regular discussions has helped put the work I do in a broader perspective and in my opinion improved the collaboration between me and Dynea. Overall, it was a great experience and I highly encourage other PhD students to grab this opportunity if they can. In 2023 I will also be visiting KA Rasmussen and I am looking forward to what I will experience there."

Dyneas facilities at Lillestrøm (photo from Dynea.com)

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 WP1.2 WP1.3

NTNU · UiO : University of Oslo · SINTEF · YARA · KA-Rasmussen

IIA2

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

WP2.1

SINTEF · YARA

IIA3

Frontier formalin technology development

WP3.1 WP3.2 WP3.3

NTNU · SINTEF · KA-Rasmussen · dynea

IIA4

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

WP4.1 WP4.2 WP4.3 WP4.4 WP4.5

NTNU · SINTEF · inovyn

IIA5

The next step in direct activation of lower alkanes

WP5.1 WP5.2 WP5.3

HALDOR TOPSØE · SINTEF · UiO : University of Oslo

IIA6

Generic projects for additional industrial synergies

WP6.1 WP6.2 WP6.3 WP6.4 WP6.5 WP6.6 WP6.7

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

IIA1: 21st century Ammonia Oxidation and Nitric Acid technology development

The IIA1 team 2022

Anja Olafsen Sjåstad	UiO	IIA leader, PhD supervisor and WP responsible (WP1.1), advisor (WP1.2)
Helmer Fjellvåg	UiO	Advisor (WP1.1-1.2)
Asbjørn Slagtern Fjellvåg	UiO	PhD candidate (WP1.1)
Julie Hessevik	UiO	PhD candidate (WP1.1)
David Waller	YARA	Industrial senior (Yara), PhD supervisor (WP1.1), industry researcher (WP1.1-1.2-1.3)
Halvor Øien	YARA	Industry researcher (WP 1.1)
Thomas By	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Ann Kristin Lagmannsveen	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Silje Fosse Håkonsen	SINTEF	Researcher WP responsible (WP1.2)
Børge Holme	SINTEF	Researcher (WP1.2)
Martin F. Sunding	SINTEF	Researcher (WP1.2)
Magnus Rønning	NTNU	PhD supervisor, WP responsible (WP1.3)
Jithin Gopakumar	NTNU	PhD candidate (WP1.3)
Pål Martin Benum	NTNU	Master student (WP1.3)
Rune Lødeng	SINTEF	PhD supervisor, senior researcher (WP1.3)
Bjørn Christian Enger	SINTEF	Senior researcher (WP1.3)
Kari Anne Andreassen	SINTEF	Senior Engineer (WP1.2)

Oxides as Pt metal catchment materials – laboratory scale versus pilot plant scale

The present technology to capture Pt metal lost from the Pt-Rh catalyst for the high temperature ammonia oxidation (in the Ostwald process) is based on Pd-Ni catchment gauges.[1,2] Although considerable amounts of Pt are captured by such nets, the Pd-based nets show significant losses of Pd at the same time. In laboratory experiments we have previously documented that the perovskite-based oxide $LaNiO_3$ capture Pt at NH_3 oxidation conditions for fertilizer production. Pt is collected as a result of the chemical reaction between $LaNiO_3$ and $PtO_2(g)$ at 900°C to yield La_2NiPtO_6 as the product.[3] This suggests that such oxides may become important Pt catchment materials with reduced costs relative to the Pd-based alternatives.

Currently, we are in a screening phase where we explore the potential of a series of oxide compounds for Pt catchment. We evaluate the potential oxide materials based on their predicted thermodynamic stability, their capacity to collect Pt, their catalytic activity toward NO decomposition as well as possibilities for subsequent recovery of the noble metal from the catchment oxide.[4] Recently, we decided to expand the list of parameters to evaluate to include the chemical resistance of the oxides at industrial plant conditions. With this mindset, we prepared a series of oxides in pellet form and sewed them into Megapyr gauges for easier handling; see Figure 1. The pellets were subsequently exposed to pilot plant conditions for 12 days (T = 900 °C, P = 5 bara and gas mixture of 10 % NO_x, 15 % H_2O, 5 % O_2 and 1300 ppm N_2O in N_2). Key findings from the experiment were that the oxides in general withstand the severe chemical reaction conditions in the pilot plant. However, we identified a mismatch in observed Pt catchment capacity of the oxides in the pilot plant relative to the systematic experiments carried out in our 6-zone laboratory furnace. We anticipate the main reason for the discrepancy between behavior of the oxides in the pilot plant relative to the laboratory furnace is that the pellets become partly hidden from the process gas when being sewn into the Megapyr gauges for the pilot plant experiments (Figure 1). Likewise, we the discrepancy between experiments is that the observed the Megapyr gauges to chemically react with the oxide pellets, which also is unfortunate. Despite the pilot plant experiments not giving a reliable quantification of the Pt catchment capacity, the results give valuable insight into how the oxides withstand real plant conditions.

Figure 1: Oxide pellet sewn into Megapyr gauge for pilot plant experiment

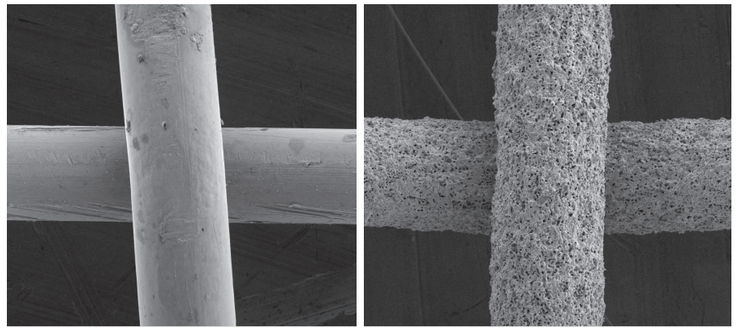


Figure 2: SEM images of Pd net surface before (upper) and after (lower) being exposed to ammonia oxidation product in N_2 for a short time on stream at 920°C

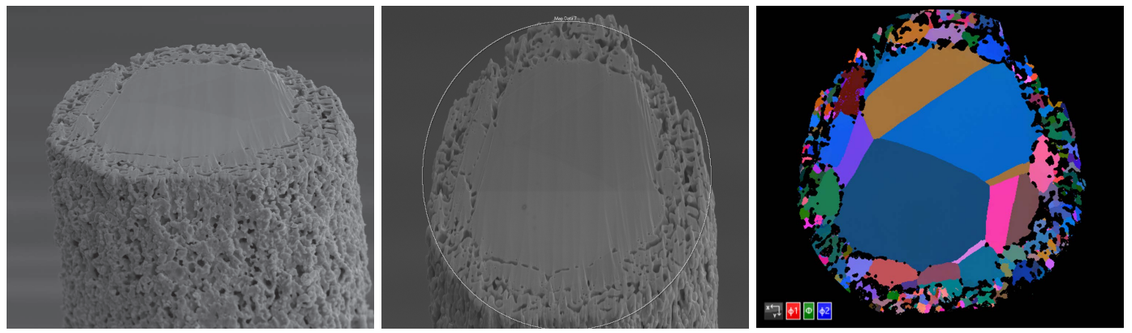


Figure 3: SEM images and EBSD map of the Pd cross-section after being exposed to 5% NO in N_2 for 90 minutes at 920°C

References

1. A.S. Fjellvåg, D. Waller, J. Skjelstad, A.O. Sjåstad, Johns. Matthey Technol. Rev. 63 (2019) 236.

2. A.S. Fjellvåg, P.S. Jørgensen, D. Waller, D.S. Wragg, M.D. Michiel, A.O. Sjåstad, Materialia (2022) 21, 101359.

3. J. Hessevik, A.S. Fjellvåg, O. Iveland, T. By, J. Skjelstad, D. Waller, H. Fjellvåg, A.O. Sjåstad, Mater. Today Commun. 30 (2022) 104084.

4. J. Hessevik et al., manuscript in preparation

Experimental investigations of Pt/PtRh volatilization and catchment

A set of washed woven Pd nets have been exposed to different gas atmosphere at ambient pressure and 920°C for. The degree of reconstruction of the surface and the cross sections of the net wires were subsequently analysed by SEM, and one of the samples was also characterized using electron backscatter diffraction (EBSD) to obtain information on the grain orientation. SEM results of the Pd net surface after being exposed to ammonia oxidation product for a short time on stream at 920°C are shown in Figure 2.

The images clearly show that even after a short time on stream, the Pd surface has been heavily reconstructed. The original smooth surface of the Pd wire is now pitted and sponge-like. Diameter measurements of the fresh and aged wire also reveal that the wire has swollen during this treatment.

Cross-sections of the same sample were then prepared by cutting and subsequent abrading with an Ar ion knife ensuring a deformation-free cross-section surface. SEM images and the EBSD map of the cross-section are shown in Figure 3.

Figure 3 shows a cross-section with an highly porous exterior layer and sub-surface areas with both fine porosity and bands of pores. The core of the wire is still solid. From the EBSD map one can see that the surface layer seems completely re-crystallized.

One can also observe that the core is coarsely grained and that the pore bands typically appear in grain boundaries.

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, and the surface layer seems to completely re-crystallize by first attacking the grain boundaries.

Catalytic Oxidation of NO to NO_2 Using Supported Ru Catalyst at Industrial Nitric Acid Production Conditions

Nitric acid (HNO_3), an important chemical building block, is produced industrially by the Ostwald process involving ammonia oxidation by atmospheric oxygen using Pt-Rh gauze catalysts to yield nitric oxide. The typical NO concentration at the exit of the ammonia combustor is 10%, and nitric oxide is further oxidised in a homogeneous gas phase reaction to NO_2, which is further absorbed in water to yield nitric acid. Using a catalyst to oxidise NO to NO_2 is attractive for reducing the CAPEX by replacing the bulky homogeneous oxidation process with a much more compact heterogeneously catalysed process. There is hardly any literature report on catalytic NO oxidation at high concentrations and pressures.

However, catalytic oxidation of NO has been studied extensively in diesel engine exhaust treatment, where the NO concentration in the feed is normally in the range of 10-1000 ppm, which is very far from nitric acid production conditions. The investigated catalyst in literature so far ranges from noble metals via supported metal oxides, to ion exchanged zeolites and activated carbon fibres. According to Le Chatelier's principle, the forward reaction is favoured by higher pressure and lower temperatures, and catalytic activity is usually favoured by higher temperature. Additionally, the high concentration of nitric oxide, gas-phase conversion, and the presence of water in the feed are the main challenges that hold back this reaction from being catalytic. Hence, to date no catalyst has been found that fully oxidizes nitric oxide to nitrogen dioxide at industrial conditions.

Typical gas composition at the exit of the ammonia combustor mainly contains 10% NO, 6% O_2 and 15%H_2O at 4-7 bar pressures. But as we move away from the ammonia combustor exit towards the NO_2 absorption unit, the concentration of NO_2 increases due to gas phase conversion of NO. Any catalyst that is used at this stage in a nitric acid plant for NO oxidation should be able to withstand NO_2 and also be inert towards the product.

The current work aims to investigate NO to NO_2 activity at partial industrial nitric acid conditions (1 bar) and complete industrial nitric acid conditions (4 bar) with 10% NO, 6% O_2, 15%H_2O and balance Ar in a packed bed reactor at a space velocity of 24,000 $Ncm_3/h{\cdot}g_{catalyst}$. A 0.5wt.% Ru on γ-$Al_2O_3$ was prepared using wet impregnation. A temperature ramp was performed for activity testing from 150-450°C for ambient pressure tests and 150-400°C for 4 bar pressure tests. Figure 4 presents the conversion results between two pressure tests. Even with a significant amount of gas phase conversion present at higher pressure, clearly the performance of Ru catalyst exceeds it to meet equilibrium conversion at a lower temperature than at ambient pressure test. The results mainly portray the benefits of using a low loading ruthenium catalyst that can attain equilibrium at low temperatures in complete nitric acid conditions.

Publication

Publications and conference contributions from IIA1 in 2022 are listed on page 55.

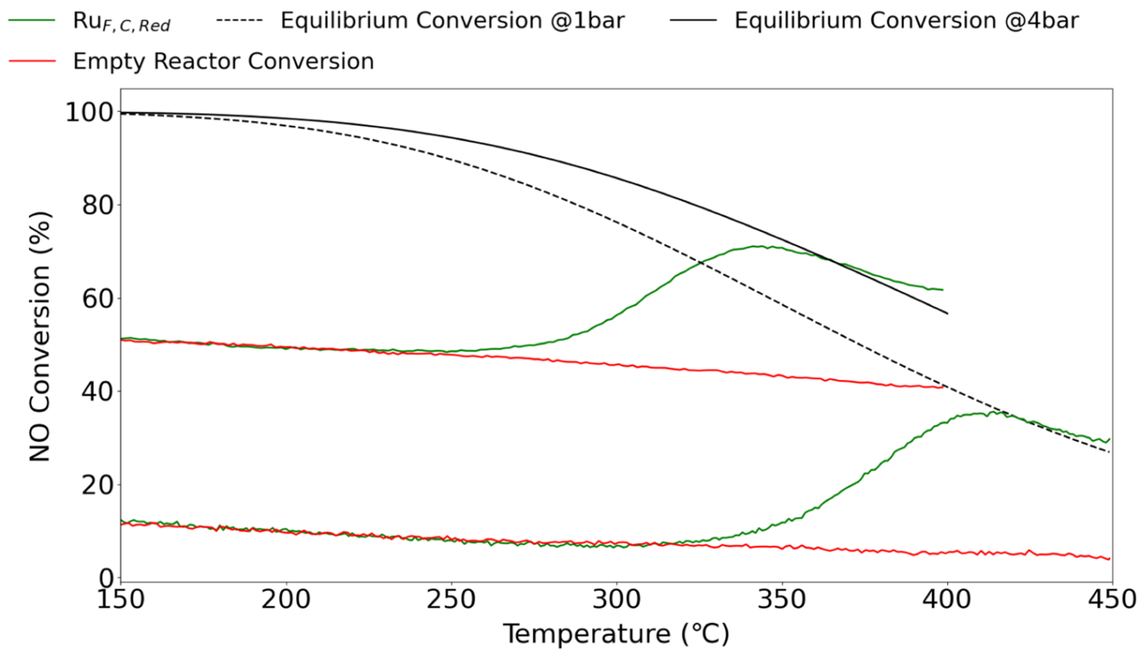


Figure 4: NO to NO_2 conversion using 0.5wt%Ru on γ-Al_2O_3 in 10% NO, 6% O_2, 15% H_2O % and rest inert at ambient and 4 bar of pressure as a function of temperature.

IIA2: Abatement of nitrogen-containing pollutants – state-of-the-art catalyst technology

The IIA2 team 2022

Jasmina Hafizovic Cavka	SINTEF	IIA leader
David Waller	YARA	Industry senior, industry researcher
Karl-Isak Skau	YARA	Industry researcher
Elin Nilsen	YARA	Industry researcher
Torgeir Lunde	YARA	Industry senior
Silje F. Håkonsen	SINTEF	Researcher and WP responsible
Martin F. Sunding	SINTEF	Researcher
Patricia Almeida Carvalho	SINTEF	Senior researcher
Anna Lind	SINTEF	Researcher
Bjørnar Arstad	SINTEF	Researcher

Motivation

When ammonia is combusted in a nitric acid plant in the Oswald process to produce NOx, N_2O is an undesired bi-product. The levels of N_2O might appear to be low but the high Global Warming Potential (GWP) of N_2O of 298 means that it used to account for 50% of Yara's Greenhouse Gas (GHG) emissions. For this reason, Yara developed an abatement catalyst that is located directly below the platinum-based oxidation catalysts. The catalyst consists of a Co and Al spinel phase supported on CeO_2. This catalyst can achieve > 95% abatement with no changes to plant operation. The deN_2O catalysts has 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 fresh deN_2O catalyst that has been in operation in a commercial nitric acid plant for various times on stream have been investigated by light microscopy, SEM-EDS and EPMA. This time series of catalysts is particularly interesting to study as all the catalysts come from the same batch, and have been exposed to the same operating conditions in the plant.

Polished cross-sections of the samples were investigated by 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. The results showed that the fresh catalyst has a homogeneous green colour through the cross section, while a homogeneous light blueish colour is observed in the sample that has been in the plant for more than 3 years. Samples extracted from the plant from between 6 months to about 2 years show a gradual degree of colour change from the surface and into the core of the pellets, clearly showing that the colour change happens quite rapidly close to the surface while there is still a slight green core even after 2 years on stream, as illustrated in Figure 1.

Earlier work has concluded that the original Co_2AlO_4 spinel phase in the fresh catalyst is gradually transformed to $CoAl_2O_4$ which may explain the colour change. We therefore wanted to investigate further how well the colour change in the pellets can be used to correlate to the spinel phase change.

The colour gradients from the light microscopy were compared to element composition gradients obtained from EDS line scan and EPMA of the cross section of samples. Uniform concentration of Al was found in all the samples, but Co is depleted in the used samples starting from the surface and moving towards bulk, before a homogeneous

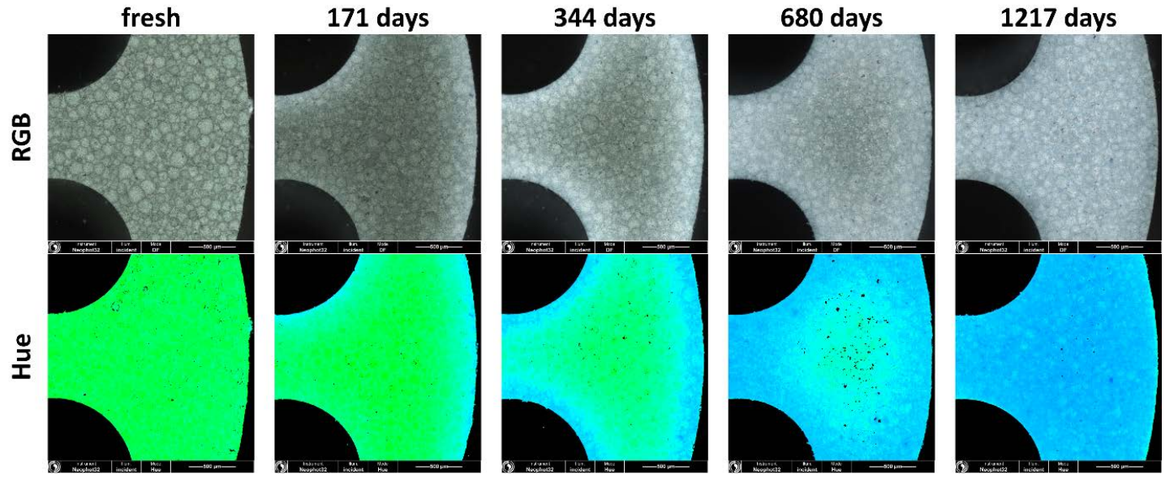


Figure 1: Light microscopy, dark field illumination of polished cross-sections of fresh and used deN_2O samples exposed to ammonia oxidation products for various times on stream. Top row: Standard colours. Bottom row: hue.

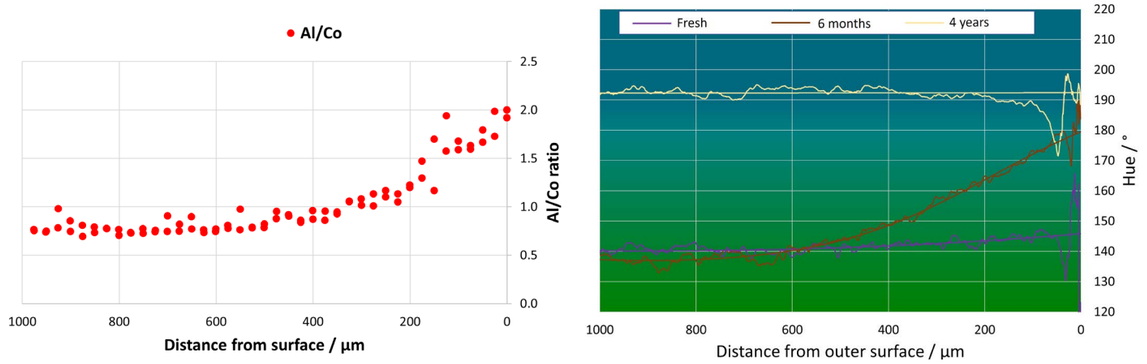


Figure 2: EPMA profile (left) and hue profile (right) of a sample that has been aged for 6 months.

Co concentration was found in the sample aged for more than 3 years. Figure 2 shows a comparison between the hue profile from light microscopy and the Co and Al profile from EPMA.

The results show that the hue profile gives a good indication of the Co:Al ratio in the cross sections. This was also confirmed by SEM-EDS line scans. Light microscopy can thereby be used as a cost effective and quick method to obtain information about the aged state for these deN_2O catalysts. Such a tool can for instance be used to compare sets of time-aged samples run under different conditions, as illustrated in Figure 3.

Characterisation results show that this catalyst is aged at various rates in the two plants run under different conditions, and these results can again be coupled with performance data.

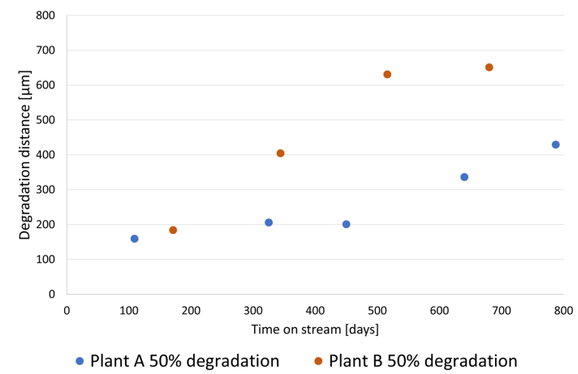


Figure 3: Degradation comparison between deN_2O catalysts aged in two different commercial plants.

IIA3: Frontier formalin technology development

The IIA3 team 2022

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)
Tomasz Skrzydlo	NTNU	Master student (WP3.1)
Thomas By	KA Rasmussen	Industry researcher (WP3.1)
Ann Kristin Lagmannsveen	KA Rasmussen	Industry researcher (WP3.1)
Kristin Bingen	DYNEA	Industry senior researcher (WP3.1-3.2-3.3), WP responsible (WP3.2)
Lars Axelsen	DYNEA	Industry senior (WP3.1-3.2)
Ole H. Bjørkedal	DYNEA	Industry researcher (WP3.2-3.3)
Rune Lødeng	SINTEF	PhD co-supervisor (WP3.1), senior researcher (WP3.2-3.3)
Roman Tschentscher	SINTEF	Senior researcher (WP3.2-3.3)
Kari Anne Andreassen	SINTEF	Senior engineer (WP3.3)

Systematic Scanning Electron Microscopy (SEM) Study of the Annular Silver Catalyst

The evolution of silver (Ag) catalyst surfaces has been a topic of interest throughout the entire duration of the iCSI project at WP3.1. The restructuring is linked to dissolution of oxygen and possibly hydrogen atoms in the Ag crystal lattice, as well as high mobility of surface Ag at temperatures in excess of 500°C. However, some questions remain. We would like to know if there is (1) a significant difference in surface development when using different reactants, and if there is (2) an 'energetic minimum' that the surface wants to settle into. To answer these questions, we would need to perform a more systematic study than we have previously done. This year our master student, Tomasz Skrzydło, was tasked with exactly that.

A series of catalysts were machined and marked with a scratch that would remain visually identifiable. Then the work began of using that scratch as a reference point to identify multiple areas on each catalyst that we could consistently rediscover by using SEM. A series of experiments was conducted where we exposed these catalysts to (A) Inert atmosphere, (B) Air, (C) CO oxidation, and (D) H_2 oxidation. Temperature (620°C) and reaction times were the same for each atmosphere, and pictures of the areas identified on the fresh catalysts were taken after each experiment. Each catalyst was run for 12, 36, and 84 hours, giving a total time on stream for each catalyst of 132 hours. Figure 1 shows how pictures were taken after each stage to follow the development, and because of the markings made we could identify the same spots after each run.

In Figure 2 we can see how the surface developed for a select spot for each atmosphere. These pictures show that there is a significant dependency on the reaction atmosphere. To summarize the main findings:

- Temperature alone causes some degree of Ag surface mobility (Catalyst A). The extent of restructuring was more than we initially expected.
- Addition of oxygen (Catalyst B) is the second driving force of the restructuring process. By adding oxygen, the extent of restructuring is significantly higher than when heating in an inert atmosphere.
- Performing a reaction has significant effect on the surface (Catalyst B and C). Usage of oxygen to oxidise various reactants seems to be another driving force of the restructuring process.

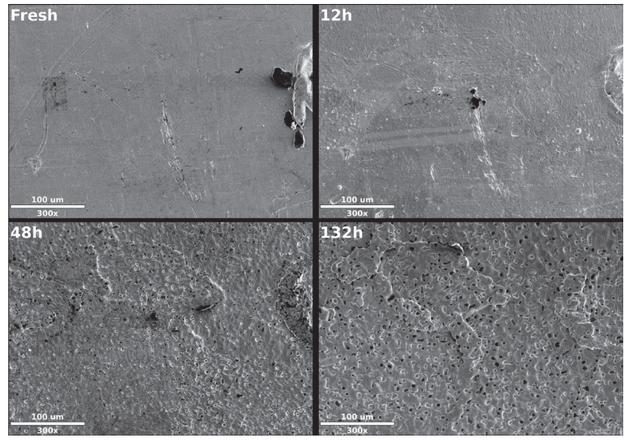


Figure 1: Development of the surface of Catalyst D with different time on stream. Note feature on the right of the picture. This feature was the end of a scratch and used to identify the spot. Reaction conditions: 2% H_2, 6% O_2 in N_2, T_{bed}=620°C.

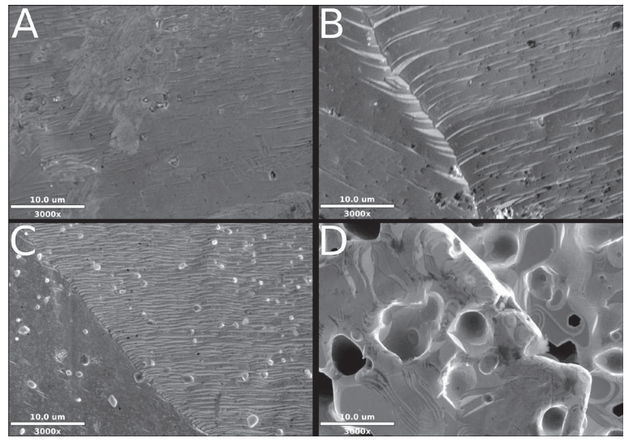


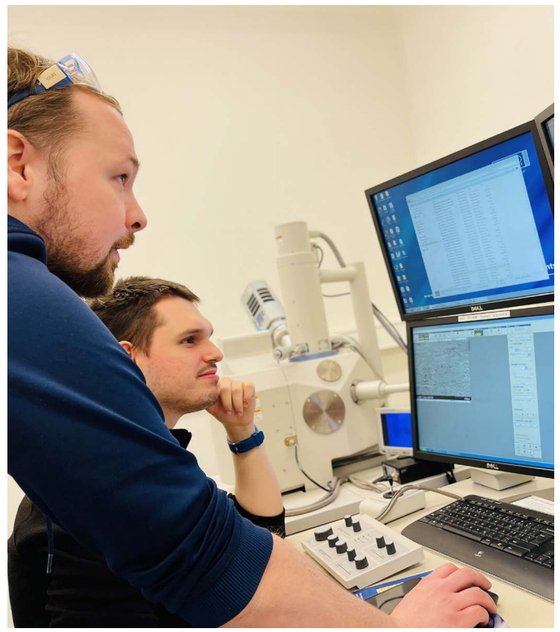
Figure 2: Surface of all catalysts after 132h on stream at T_{bed}=620°C. A: N_2,. B: Air (21% O_2 in N_2), C: 2% CO, 6% O_2 in N_2

- There is a significant difference in the resulting morphology that is dependent on the reactants used in this study The surface resulting from CO oxidation (Catalyst C) shows terracing and some pinhole formation, while H_2 oxidation (Catalyst D) yields a surface with a high density of pinholes and distinct faceting. A possible cause for this difference is the formation of subsurface hydroxyls from lattice dissolved O and H that may recombine to form water within the Ag structure.
- The surface does not seem to reach an 'energetic minimum' during these experiments. Over the course of the total time on stream the surface was never similar to the last.

We want to thank Tomasz Skrzydło for his work during this study and wish him luck with the continuation of his master's degree research project.

Publication

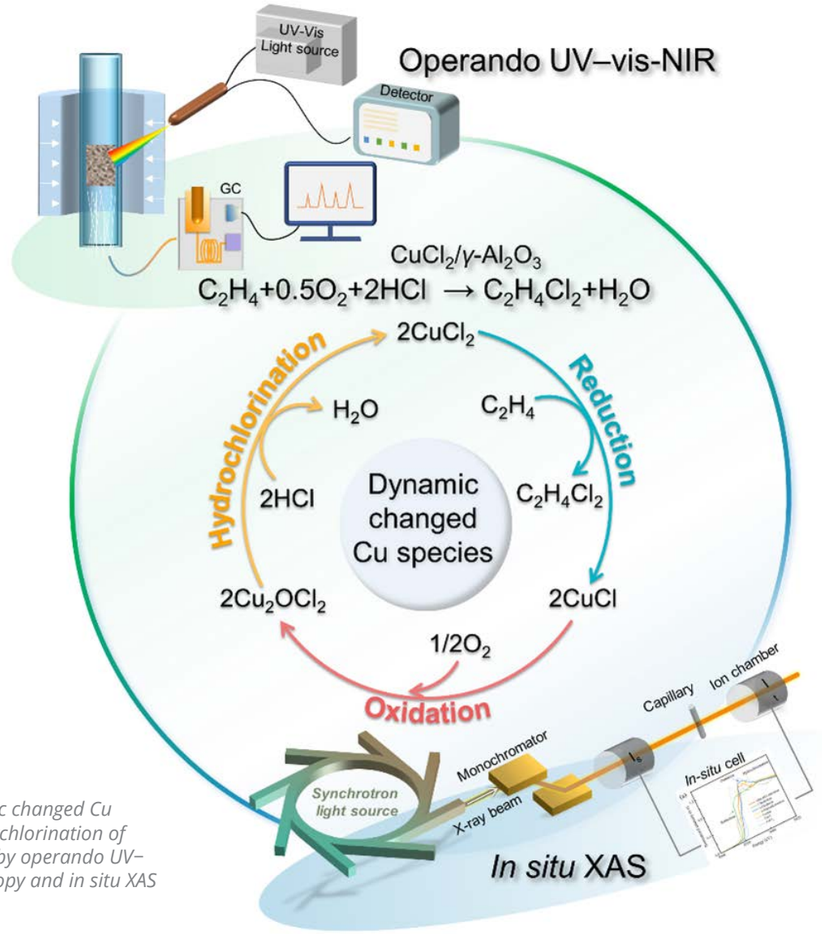
Conference contributions from IIA3 are listed on pages 55-56.



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

The IIA4 team 2022

De Chen	NTNU	IIA leader, PhD supervisor, WP responsible (WP4.1-4.2-4.3)
Yalan Wang	NTNU	Postdoctoral fellow (WP4.1)
Wei Zhang	NTNU	PhD candidate (WP4.3 and WP4.4)
Seyyedeh Roomina F. Motlagh	NTNU	Master student (WP4.3)
Jordal, Kamilla	INOVYN	Industry researcher (WP4.1-4.2-4.3)
Lola Irene Stokstad	INOVYN	Industry researcher (WP4.1-4.2-4.3)
Andrea Marsella	INOVYN	Industry researcher (WP4.1-4.2-4.3)
Sandro Vidotto	INOVYN	Industry researcher (WP4.1-4.2-4.3)
Margherita Macino	INOVYN	Industry researcher (WP4.1-4.2-4.3)
Tigran Margossian	INOVYN	Industry researcher (WP4.1-4.2-4.3)
Dennis Neu	SINTEF	Researcher (WP4.1-4.2-4.3)
Kumar R. Rout	SINTEF	Researcher (WP4.1-4.2-4.3)
Torbjørn Gjervan	SINTEF	Researcher (WP4.2)



Scheme: Dynamic changed Cu species in the oxychlorination of ethylene studied by operando UV–vis-NIR spectroscopy and in situ XAS

Project goals

The main objectives of this project are to experimentally and theoretically elucidate the site requirements and mechanisms of surface catalysis of half-reactions, such as $CuCl_2$ reduction by ethylene to EDC and $CuCl/CuCl_2$ oxidation by oxygen to Cu_2OCl_2, and its hydrochlorination, as well as the entire redox cycle, at an atomic level. Additionally, the project aims to provide a predictive kinetic model to accurately describe the dynamics of active sites and their activity, and to rationally design catalysts to control the redox cycle and achieve high activity, selectivity, and stability. To achieve these goals, the project is divided into four work packages: WP1 for kinetic investigations and modeling; in-situ characterization in WP2; WP3 for deactivation and by-product formation; and WP4 for new development, including reactor modeling and simulation.

Research in 2022

In-situ study of ethylene oxychlorination on La doped CuCl2/Al2O3 catalysts

The oxidation state of Cu species in ethylene oxychlorination is strongly correlated with catalytic performance. $CuCl_2$ and CuCl have been identified as the primary active sites in the reduction and oxidation step, respectively, according to a redox-type mechanism. The distribution of the active sites is governed by the kinetic equilibrium of the reduction, oxidation, and hydrochlorination rates at steady-state. Herein, in situ X-ray absorption spectroscopy (XAS) and operando ultraviolet−visible and near-infrared spectroscopy (UV–vis-NIR) were utilized to quantify the dynamic changes of the Cu active sites over the La-doped $CuCl_2/\gamma\text{-}Al_2O_3$ in transient and steady-state experiments. A higher $CuCl_2$ concentration plays a key role in dominating the higher activity, EDC selectivity, and stability. Moreover, La promoter does not directly participate in the reaction, but both serve as the structure additive to increase the number of active sites, and chemical promoters alters the structure of the Cu active site by influencing the Cl bonded with La and Cu. A deeper understanding of the complex role of the active species and promoter in the $CuCl_2/\gamma\text{-}Al_2O_3$ based-catalysts for ethylene oxychlorination was obtained.

Reaction networks and catalyst active sites for various reaction pathways

The reaction network of ethylene oxychlorination on the K-promoted $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst has been established, comprising 12 species, including the three main reactants: ethylene, oxygen, and hydrochloride, as well as the main product, 1,2-dichloroethane (EDC), and seven by-products: ethyl chloride (EC, C_2H_5Cl), vinyl chloride (VCM, C_2H_3Cl), 1,1,2-trichloroethane (TCA, $C_2H_3Cl_3$), 1,2-dichloroethylene (DCE, $C_2H_2Cl_2$), carbon tetrachloride (CCl_4), CO, and CO_2. It has been found that both $CuCl_2$ and CuCl catalyze the formation of CO and CO_2. The selectivity of the reaction is affected by the spatial distribution of $CuCl_2$ and CuCl in the reactor, with CuCl typically being generated at the outlet of the fixed bed reactor under different conditions.

Kinetic modelling of the reaction network

The kinetic model for the reaction network on K promoted $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst has been developed through a stepwise approach, with the aim of best fitting the experimental data. The model includes 12 species and 13 reactions, covering primary, secondary, and tertiary products. The Power Law approach and Langmuir Hinshelwood approach were studied, and rate constant values were obtained. The kinetic model was able to describe the reactions within a tolerance range of +/-10 % deviation. The Mars-Van Krevelen approach is currently being studied, and the fitting of the kinetic model is still ongoing.

Optimization of product selectivity

In order to optimize the selectivity in the ethylene oxychlorination process, the key is to maintain a high Cu oxidation state throughout the fixed-bed reactor. The strategy to achieve this is to incorporate multiple promoters into the $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst to modify the redox properties and enhance catalytic performance. The multi-promoter doped catalyst, KMgLa- $CuCl_2/\gamma\text{-}Al_2O_3$ / Al_2O_3, was found to exhibit superior ethylene oxychlorination activity, reduce by-product formation, and maintain higher stability by increasing the fraction of active Cu species and remaining in a more stable $CuCl_2$ state. Through transient kinetic and operando studies, the role of each promoter component was investigated to gain a deeper understanding of their effects on the redox properties of the catalyst and to develop a rational catalyst design approach.

Publication

Publications and conference contributions from IIA4 are listed on page 56.

IIA5: The next step in Direct Activation of Lower Alkanes

The IIA5 team 2022

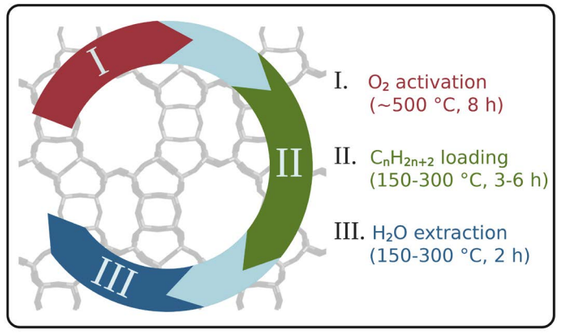
Stian Svelle	UiO	IIA Leader, PhD supervisor, WP responsible (WP5.1-5.2-5.3)
Unni Olsbye	UiO	PhD supervisor (WP5.1-5.2)
Karoline Kvande	UiO	PhD candidate (WP5.1-5.2)
Sebastian Prodinger	UiO	Postdoctoral fellow (WP5.1-5.2-5.3)
Bjørn Gading Solemsli	UiO	PhD candidate (WP5.1-5.2)
Pablo Beato	Haldor Topsøe A/S	Industrial senior and researcher (WP5.1-5.2-5.3)
Lars Fahl Lundegaard	Haldor Topsøe A/S	Industrial researcher (WP5.1-5.2-5.3)
Aino Nielsen	Haldor Topsøe A/S	Industrial researcher (WP5.1-5.2-5.3)
Søren Birk Rasmussen	Haldor Topsøe A/S	Industrial researcher (WP5.1-5.2-5.3)
Jeremy Neil Bum	Haldor Topsøe A/S	Industrial researcher (WP5.1-5.2-5.3)
Catarinja Mokrzyczka	Haldor Topsøe A/S	Industrial researcher (WP5.1-5.2-5.3)
Bjørnar Arstad	SINTEF	Senior researcher (WP5.3)

In the first period of iCSI, our focus was on the development of a stepwise stoichiometric conversion of methane to methanol (MTM) over Cu-exchanged zeolites, studying the structure-activity relationships of this reaction. Over the last few years, however, we have also been exploring the next steps related to how we can utilize the obtained knowledge of the method to develop other reactions based on similar techniques. Additionally, we have been utilizing novel methods and materials to unravel more about the different steps of the reaction. We have, among other things, developed a similar method for converting ethane to ethylene, and created a methylation reaction process for converting benzene into toluene utilizing the methoxy species formed from methane within the Cu zeolites. Some of this research also led to new and intriguing questions, so we decided to apply for an XAS beam time experiment at the Swiss-Norwegian beamline, BM31 at ESRF. Our experiment was allocated at the end of January 2023, and it turned out to be a very successful experiment performed together with our colleagues from the University of Turin. With lots of data to process, master student, Nishant Patel (Figure 1), at the University of Turin, will have a handful this spring.

As the iCSI center is starting to reach the finish line, so are some of the projects we have been working on. We would like to highlight two of these projects. The above-mentioned work on the conversion of other light alkanes led to a novel reaction pathway for the direct activation of ethane to ethylene operating at low temperatures (150°C) and ambient pressure (Figure 2). From a systematic study into the required material properties, we found that akin to the well-tested MTM reaction, Cu-sites confined within nanoporous zeolites were indeed needed for the ethane activation. However, the requirements for the active site appeared to be somewhat different for the two alkanes. We identified a stepwise mechanism via an ethoxy intermediate to be the most likely reaction pathway. Overall, this work discloses some new and interesting questions for the C-H activation research.

Furthermore, we have also had a fruitful collaboration with another iCSIwork package, IIA6. We have had a joint experimental endeavor, where Moses Mawanga, working with Edd Anders Blekkan and Jia Yang at NTNU, performed NH_3- and CH_4-calorimetry experiments on a set of Cu-loaded MCM-22 zeolites that we had tested for the MTM reaction. MCM-22 (Figure 3 (a)) is a hitherto untested material for the reaction, and although it had moderate productivity for methanol, combining calorimetry with NH_3 temperature-programmed desorption experiments led to some interesting findings. Predominantly, we found

Figure 1: A group from the beam time in January 2023.



Figur 2: Illustration of the stepwise reaction mechanism applied for both methane-to-methanol and ethane-to-ethylene. Created with Biorender.com.

that the MCM-22 zeolite topology led to only a small set of homogeneously strong acid sites, subsequently leading to a small number of Cu-sites that could form the active site for methane activation (Figure 3 (b)). Additionally, CH_4-calorimetry experiments showed a very weak interaction between the alkane and the Cu-zeolite, highlighting the need for a high methane partial pressure and a strongly adsorbing Cu-site to form the active methoxy species (Figure 3 (c)). With this study, we have resolved some of the importance behind screening for an optimal zeolite framework, which ideally has a high concentration of homogeneous Cu-exchange sites that can activate methane and stabilize its intermediates.

Publication

Publication and conference contributions from IIA5 are listed on pages 56-57.

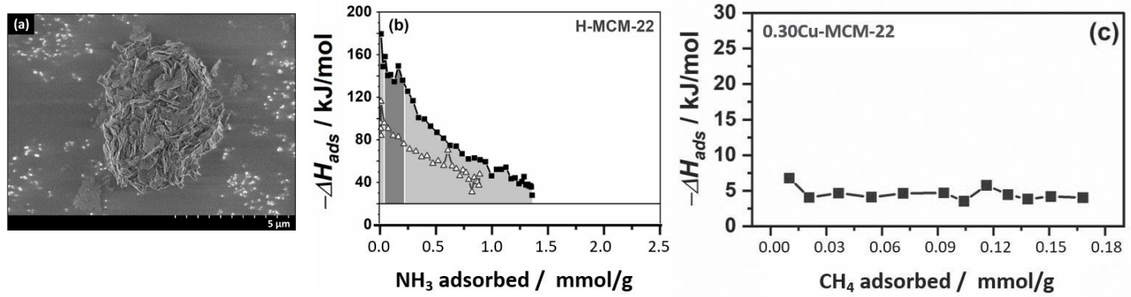


Figure 3: (a): SEM image of an MCM-22 crystal agglomerate. (b): The slope present for the differential heats of adsorption measured during NH_3 adsorption on the H-form of MCM-22 shows very heterogeneous acid sites within the zeolite. (c): The differential heats of adsorption measured during CH_4 adsorption disclosed a very weak interaction of CH_4 with the zeolite.

IIA 6: Generic projects for additional industrial synergies

The IIA6 team 2022

Magnus Rønning	NTNU	IIA leader, PhD supervisor and WP responsible (WP6.1)
Hilde Johnsen Venvik	NTNU	PhD co-supervisor (WP6.1) and postdoc supervisor (WP6.7)
Samuel K. Regli	NTNU	PhD candidate (WP6.1)
Anja Olafsen Sjåstad	UiO	WP responsible (WP6.2)
Martin Jensen	UiO	PhD candidate, associated (WP6.2)
Alexandra Jahr Kolstad	UiO	Master student (WP6.2)
Mathilde Ingeborg V. Nilsen	UiO	Master student (WP6.2)
Walace P. S. Kierulf-Vieira	UiO	Master student (WP6.2)
Evgeniy Redekop	UiO	Researcher (WP6.2)
Oleksii Ivashenko	DNV	Associated (WP 6.2)
David Waller	YARA	Industrial senior researcher (WP6.2)
Bjørn Christian Enger	SINTEF	WP responsible and senior researcher (WP6.4)
Ingeborg-Helene Svenum	SINTEF	Researcher (WP6.4)
Edd A. Blekkan	NTNU	WP responsible (WP6.5) and PhD supervisor (WP6.5) and co-supervidsor (WP6.6)
Jia Yang	NTNU	WP responsible (WP6.6) and PhD supervisor (WP6.6) and co-supervisor (WP6.5)
De Chen	NTNU	PhD co-supervisor (WP6.5 and 6.6)
Moses Mawanga	NTNU	PhD candidate (WP6.5)
Björn Frederik Baumgarten	NTNU	PhD candidate (WP6.6)
Muhammad Arslan Aslam	NTNU	Specialization student (WP6.6)
Rune Lødeng	SINTEF	Senior researcher (WP6.6)
Tina Bergh	NTNU	Postdoc (WP6.7)

Motivation

Advanced spectroscopic and microscopic investigations under conditions highly relevant to industrial operation are being particularly targeted, with the intention of moving the research to the forefront and providing methodological tools that can be applied in the industrial innovation areas 1-5. Other efforts are directed towards advancing atomistic and kinetic modelling of metals and oxides, as well as reactor modelling, with the goal to eventually enable an integrated, multiscale modelling approach.

Specs XPS add-on to our Reactor STM

Since 2016 our Reactor STM (Scanning Tunneling Microscopy), the 5th of its kind worldwide, has been operative at the Department of Chemistry, University of Oslo. The instrument is capable of scanning surfaces in the temperature range from 20 to 300 °C and pressures from ultra-high vacuum (UHV) to 6 bar in presence of reactive gasses such as NH_3, NO, H_2 and CO. The Reactor cell has a volume of 0.5 mL and is equipped with gas inlet and outlet lines. At the outlet, the effluent is analysed by means of QMS, allowing operando studies. The Reactor STM system is equipped with a preparation chamber, hosting a preparation stage that allows annealing up to 1000 ^{o}C, a sputter gun, several leak valves for chemical treatment, 4-pocket electron beam evaporator (EBE) as well as a combined LEED-Auger unit. To supplement STM measurements, the team has focused on carrying out experiments at synchrotron facilities that provide Near Ambient Pressure X-ray Photoelectron Spectroscopy (NAP XPS), e.g., at Hippie, MAXIV and Tempo, SOLEIL. The combined STM and XPS data have provided significant scientific contributions into the development of well-defined model Pt-Rh surfaces for ammonia oxidation, and on the understanding of the implications on morphological surface features and adsorption/ desorption of O- and N-based surface species on product selectivity (NO, N_2O, N_2) at various temperatures and O_2/NH_3 ratios.

In 2021, the team was awarded AVIT funding for integrating a third chamber into the Reactor STM instrument, which accommodates a Specs XPS system equipped with an XR 50M dual X-ray anode (Ag/Al), Focus 500 monochromator, 1D DLD detector, Phoibos 150 hemispherical analyser and a flood gun (FG 22/35); see Figure 1. The sample stage for the XPS chamber can be heated to 1000°C. During 2021, the design phase was accomplished, and the commissioning of the system took place during autumn 2022 and was finalized end of December 2022.

Part of the acceptance test was to follow the effect of post-annealing of an as-deposited ~1 ML Rh/Pt(111) surface prepared at room temperature; see collected XPS spectrum inserted in Figure 2. As-deposited surface (blue curve) was heated to 600°C over a period of 9 mins and allowed to dwell there for some extra few mins (red curve, figure to the right) before cooling down to ambient temperature. XPS data were collected using the monochromatic Al Kα X-ray (1486.6 eV). The analyser pass energy was 10 eV, the energy step was 0.05 eV, and the dwell time was 0.1 s. Approximately 1 spectrum was collected each min of the experiment.

For Rh/Pt(111) as-prepared at 300 K, the Rh 3d5/2 core level was observed at ~307 eV and the Rh 3d3/2 component is also seen, partially overlapping with the Pt 4d5/2 peak at ~314 eV. Upon annealing to 600°C, the Rh/Pt ratio decreased, which can be rationalized either by Rh subsurface movement or by the onset of Pt incorporation into Rh islands and, thus, Pt enrichment at the surface. This observation is in line with our previous findings, based on XPS data collected at Leiden University.[1]

References

1. "Roadmap for Modeling RhPt/Pt(111) Catalytic Surfaces", J. Zheng, O. Ivashenko, H. Fjellvåg, I. M. N. Groot, Anja O. Sjåstad, Journal of Physical Chemistry C 2018 122 (46), 26430-26437.

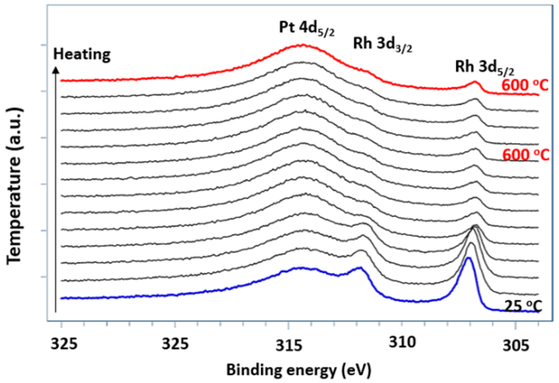


Figure 2: XPS spectrum from acceptance test

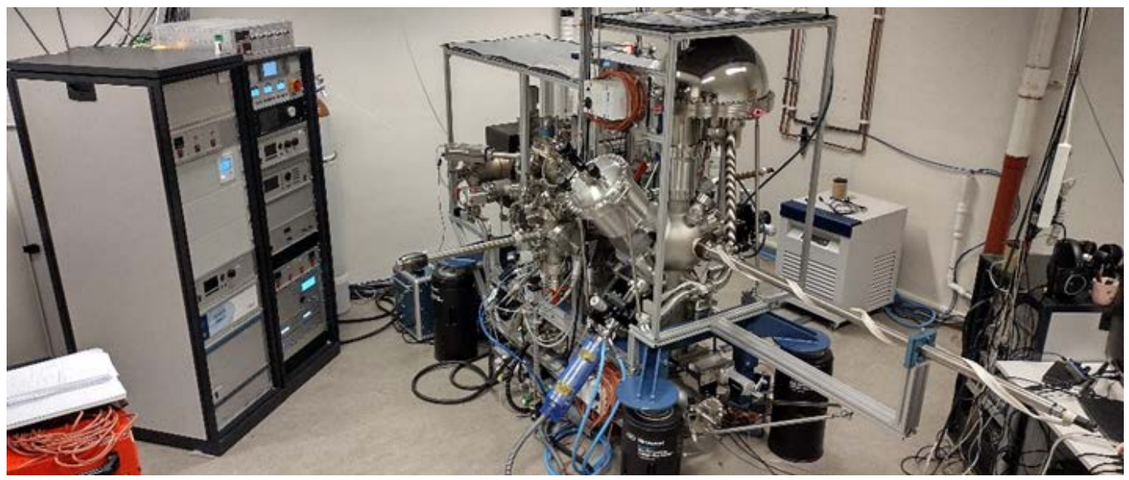


Figure 1: STM instrument with the XPS add-on

Phase and orientation mapping of nanocrystals by scanning precession electron diffraction (SPED)

With electron microscopes it is possible to map the local crystal structure by scanning the electron beam and acquiring a diffraction pattern at each probe position. For scanning transmission electron microscopy (STEM), such techniques are often referred to by the umbrella term four dimensional (4D)-STEM since a resulting dataset is 4D; essentially a 2D image in which each pixel has a corresponding 2D diffraction pattern. One such method that the TEM Gemini Centre, NTNU, is focusing on is scanning precession electron diffraction (SPED). In SPED, a nanometre-sized probe is scanned at the same time as it is precessed, i.e. tilted to an angle called the precession angle, typically ~1°, and rocked around the optical axis. Precession is a great advantage since it typically leads to excitation of more diffraction spots at higher scattering angles and to a reduction of dynamical diffraction effects that often complicate analysis of electron diffraction data. By analysing SPED data from one or more crystalline phases, orientation, phase and strain maps can be obtained.

SPED datasets are typically large (~20 GB) and require (semi-)automatic analysis methods. We have worked on and compared four data analysis approaches for phase mapping that are implemented in or based on the open-source python libraries *hyperspy* [1] and *pyxem* [2]. We applied the four methods to a demonstration dataset from an Al-Cu-Li alloy that contained nanoscale precipitates, namely the hexagonal T1-Al_2CuLi phase and the tetragonal θ'-Al_2Cu phase. Figure 3(a) shows the scanned area, while (b) shows selected diffraction patterns from each of the phases. Phase maps resulting from using each of the four methods are shown in Figure 4, and all four achieved accuracies >98% as compared to the ground truth [3]. Each method has its own pros and cons depending on the application. In general, developing and using such open-source data analysis methods give flexibility and allow us to tailor the approach depending on the material studied.

Further, we use SPED to study surface facets, grain structures and twins in silver catalysts from IIA3. While high resolution (S)TEM images provide direct real space views of the (sub-)surface atomic structure, SPED can provide such information over larger areas (up to a few µm) and is superior when it comes to statistics and lower electron beam dose. Further, the setup at NTNU includes a direct electron detector installed in 2021, which enables higher speed and sensitivity and allows us to also study some beam sensitive materials. 4D-STEM methods, and SPED in particular, are powerful methods that can be applied for detailed characterisation of the crystal structures of catalysts in the future.

References:

1. F. de la Peña et al. (2022). hyperspy/hyperspy: Release v1.7.3 (v1.7.3). Zenodo. https://doi.org/10.5281/ zenodo.7263263

2. D.N. Johnstone et al. (2022). pyxem/pyxem: pyxem 0.14.2 (v0.14.2). Zenodo. https://doi.org/10.5281/ zenodo.6645923

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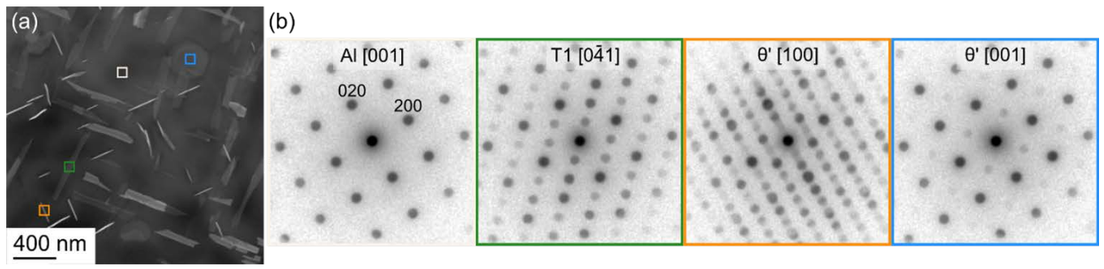


Figure 3: SPED of an Al-Cu-Li alloy with T1-Al_2CuLi and θ'-Al_2Cu precipitates. (a) Virtual annular dark field image. (b) Selected precession electron diffraction patterns from each of the phases.

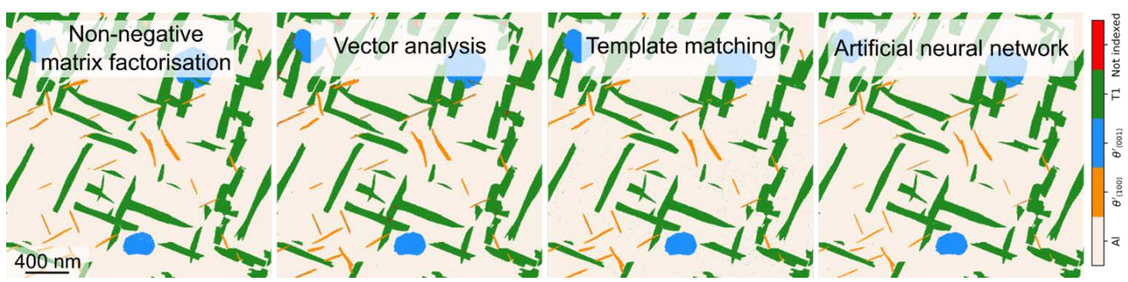


Figure 4: Phase maps created using four different SPED data analysis methods.

Hydrogen dissociation over Co(0001)

In Fischer-Tropsch synthesis cobalt is often used as a catalyst for the formation of long-chain hydrocarbons from CO and hydrogen. In this study we investigate the activation of hydrogen on Co(0001). The Co(0001) surface is modelled with 4 atomic layers, where the two bottom layers are kept fixed. Different coverages were explored by using (3x3) and (2x2) surface unit cells, see Figure 1. In addition, the effect of adsorbed oxygen on the activation of hydrogen was investigated.

The activation of hydrogen on Co(0001) goes through a physisorbed state, before adsorbing dissociatively, see Figure 5, and the behaviour is similar for both surfaces. This agrees with previously reported results [1]. The adsorption energy in the physisorbed state is about -0.3 eV for Co(0001)-(3x3) and Co(0001)-(2x2). Transition into the physisorbed state and dissociative adsorption are both associated with an activation barrier of about 0.05 eV. The presence of oxygen on the surface modifies the activation barrier for hydrogen dissociation. This is currently being explored in more detail.

This study includes Hilde J. Venvik, Ingeborg-Helene Svenum and is part of a collaboration with Ali Can Kizilkaya and Kees-Jan Weststrate.

References:

1. P. van Helden, J-A. van den Berg, and C.J. Weststrate, ACS Catal. 2012, 2, 6, 1097–1107.

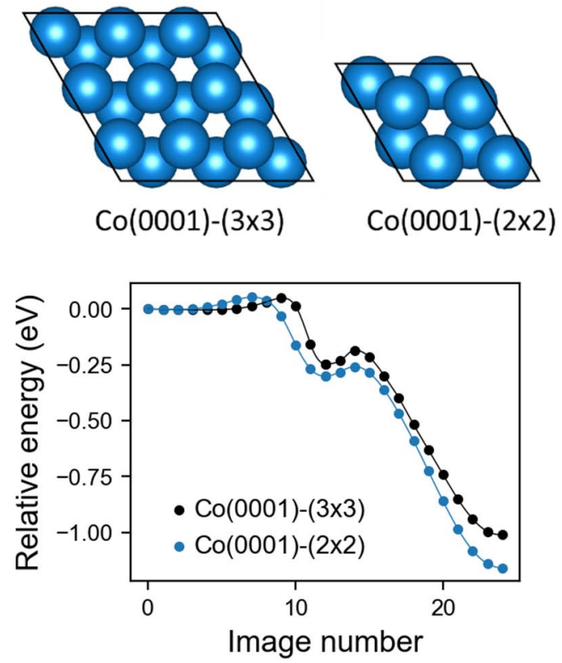


Figure 5: Top: Illustration of the Co(0001) surfaces showing the (3x3) and (2x2) surface unit cells. Bottom: Reaction path for s for H_2 dissociation over Co(0001)-(3x3) and Co(0001)-(2x2).

Publication

Publications and conference contributions from IIA6 are listed on page 57.

Postdoc Tina Bergh operating the TEM at the national infrastructure, NORTEM, NTNU. Photo: Geir Mogen

One new PhD in 2022

Candidate:	**Asbjørn Slagtern Fjellvåg**
Date of defense:	September 30, 2022
Title of thesis:	Platinum Catchment by Noble Metal Alloys and structural studies of Pt- and Rh-containing perovskites
Public trial lecture:	Synchrotron X-ray methods as basis to follow chemical reactions in-situ/ operando - status and perspectives
The Committee	
First opponent:	Professor J Paul Attfield, School of Chemistry, The University of Edinburgh, United Kingdom
Second opponent:	Professor Mari-Ann Einarsrud, Institutt for materialteknologi, NTNU, Norway
Administrator:	Ass. Professor Hanne Røberg-Larsen, Department of Chemistry, UiO, Norway
Supervisor:	Professor Anja Olafsen Sjåstad, UiO
Co-supervisor:	David Waller, Yara
iCSI project:	21st century ammonia oxidation and nitric acid technology development
Industry partner:	Yara, Porsgrunn
Current Position:	Visiting scientist at NIOM (Nordic Institute of Dental Materials)

Main research findings

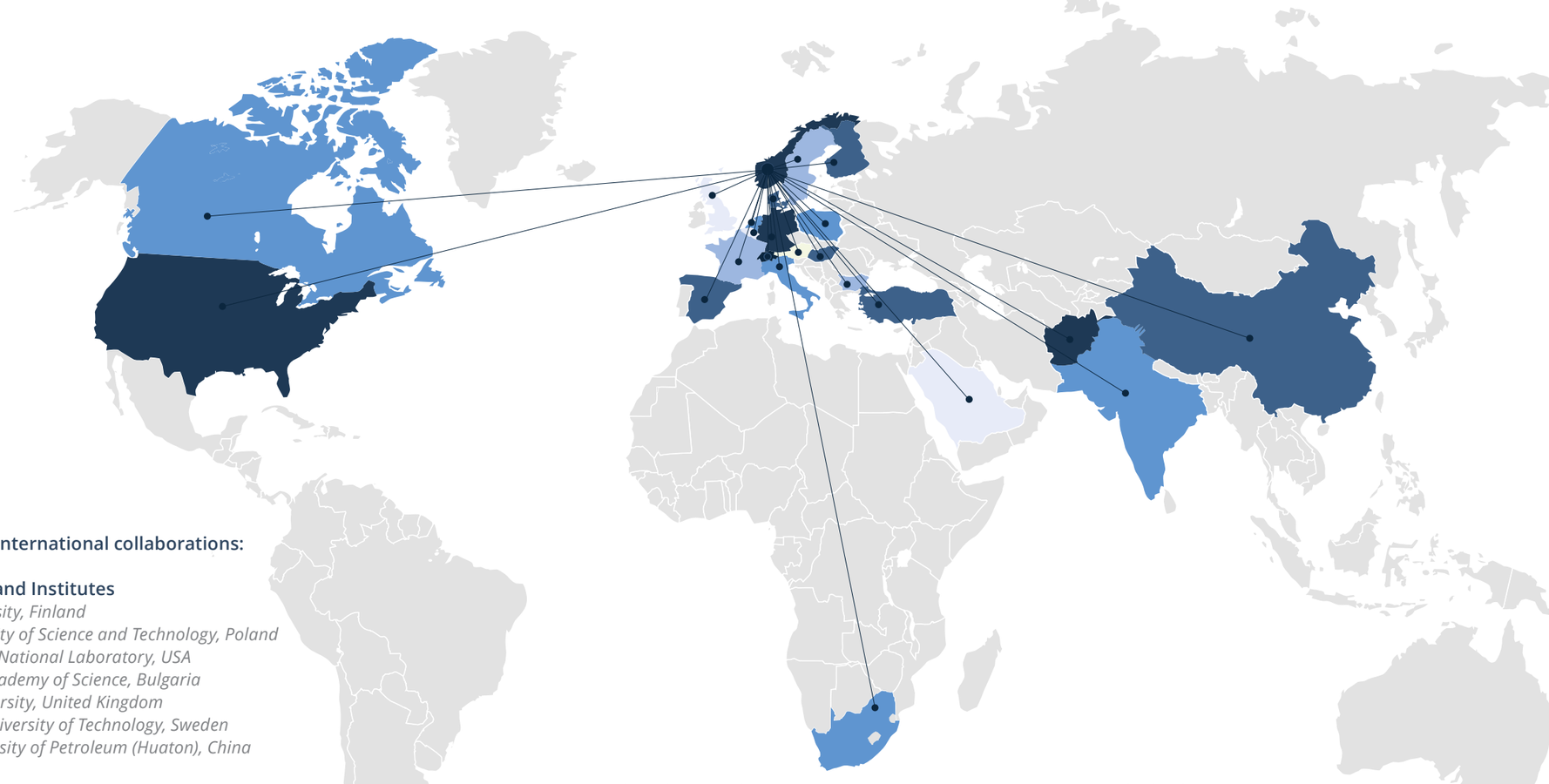
One of the steps in the production of synthetic nitrogen-based fertilizers is the oxidation of ammonia (NH_3) to nitric oxide (NO). In this reaction, Pt/Rh (95/5 wt. %) is used as a catalyst and a significant Pt-loss occurs due to the high temperature and aggressive chemical conditions. The Pt-loss is unavoidable without compromising the catalytic selectivity. Mitigation of the Pt-loss is performed by Pt-catchment, utilizing a Pd/Ni (95/5 wt. %) net placed downstream of the Pt/Rh catalyst, catching the evaporated Pt. A re-alloying process of Pd/Ni with Pt occurs during Pt-catchment, causing the Pd/Ni wires to swell and the net to grow into something more similar to a porous plate. Alloying Pd with Au reduces the swelling, and the nets keep their shape during operation, only at the cost of a small reduction in Pt-catchment.

For the future of industrial chemistry, oxide materials are seen as a cheaper and more environmentally friendly alternative to noble metals. In this mind-set, selected Pt- and Rh-containing perovskite oxides were synthesized for fundamental studies. The stability of the perovskite structure depends strongly on the oxidation states for the present elements and their size, allowing only certain compositions with Pt- and Rh- to be synthesized.

From the left: Prof. J.P.Attfield, Prof. A.O. Sjåstad, Prof. M.-A. Einarsrud,PhD Asbjørn Slagtern Fjellvåg, David Waller, Ass.Prof. H. Røberg-Larsen, Prof. E Uggerud

Photo: Geir Mogen

Internationalization



Hosting a centre like iCSI makes the catalysis community at NTNU and the affiliated research institutions attractive for international students and researchers. The 77 master's students, PhD candidates, postdocs and guest researchers within or affiliated with iCSI represent 19 countries. Non-Norwegians make up 61% of this group of employees and students.

As many as eleven exchange PhD candidates visited iCSI in 2022 with stays lasting from 2 weeks up to 12 months. This is more than twice the numbers from 2020 and 2021, and the increase is most probably a post-pandemic effect. Three master's exchange students were guests of the catalysis group at NTNU.

Nine of the ten scientific publications from 2022 were published in collaboration with colleagues at international universities.

As a Lise Meitner professor, Hilde Johnsen Venvik has visited the Department of Chemical Engineering at Lund University with guest lectures on two occasions. LINKS

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, University of Toronto and University of Wisconsin-Madison. Several researcher and professor exchanges were carried out in 2022: Both UiO and NTNU had several visitors from University of Cape Town, while one PhD candidate from NTNU visited the University of Wisconsin-Madison.

As seen from the project lists below, iCSI researchers are partners in five new Horizon 2020 projects started in 2022, of which two are coordinated by SINTEF.

Overview of international collaborations:

Universities and Institutes

- *Aalto University, Finland*
- *AGH University of Science and Technology, Poland*
- *Brookhaven National Laboratory, USA*
- *Bulgarian academy of Science, Bulgaria*
- *Cardiff University, United Kingdom*
- *Chalmers University of Technology, Sweden*
- *China University of Petroleum (Huaton), China*
- *CNR, Italy*
- *CSIC, Spain*
- *Delft University of Technology, Netherlands*
- *Durham University, United Kingdom*
- *East China University of Science and Technology, China*
- *École Polytechnique Fédérale de Lausanne, Switzerland*
- *French Alternative Energies and Atomic Commission (CEA), France*
- *Ghent University, Belgium*
- *Institut de Recherches sur la Catalyse et l'Environnement de Lyon, CNRS, France*
- *Instituto Nacional del Carbón, INCAR-CSIC, Spain*
- *Karlsruhe Institute of Technology – KIT, Germany*
- *KAUST, Saudi Arabia*
- *Luleå University of Technology, Sweden*
- *Lund University, Sweden*
- *Manchester Metropolitan University, United Kingdom*
- *MAX-IV Laboratory, Lund, Sweden*
- *Max Planck Institute for Energy Conversion, Germany*
- *Norner Research AS (SCG Chemicals), Norway*
- *Paul Sherrer Institut, Schweiz*
- *Polytechnic University of Catalonia, Spain*
- *Politecnico di Milano, Italy*
- *Research Institutes of Sweden (RISE), Sweden*
- *Royal Institute of Technology (KTH), Sweden*
- *School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, China*
- *Shanxi Institute of Coal Chemistry, Chinese Academy of Sciences, (ICC), China*
- *SLAC National Accelerator Laboratory, USA*
- *Sorbonne University, France*
- *South China University of Technology, China*
- *Stanford University, California, USA*
- *Stonybrook University, USA*
- *Swiss-Norwegian Beamlines at ESRF, France*
- *Swedish Environmental Institute (IVL), Sweden*
- *Technical University of Denmark, Denmark*
- *Technische Universiteit Eindhoven; Netherlands*
- *Tianjin University, China*
- *University College London, United Kingdom*
- *University of California, Berkeley, USA*
- *University of Cape Town, South Africa*
- *University of Eastern Finland, Finland*
- *University of Milan, Italy*
- *University of Sheffield, United Kingdom*
- *University of Strasbourg, France*
- *University of Surrey, United Kingdom*
- *University of Toronto, Canada*
- *University of Turin, Italy*
- *University of Virgina, USA*
- *University of Wisconsin-Madison, USA*
- *Utrecht University, Netherlands*

Companies

- *Albemarle, Netherlands*
- *Arkema France SA; France*
- *A-V-S, United Kingdom*
- *B.T.G. BV, Netherlands*
- *Borealis Polyolefine, Austria*
- *BTG-BTL, Belgium*
- *C2P2, Lyon (CNRS), France*
- *CEA – the French Alternative Energies and Atomic Energy Agency, France*
- *Elkem Silicon Materials, USA*
- *Fibre Excellence, France*
- *Firmenich, Swizterland*
- *Fundacio EURECAT, Spain*
- *GE Healthcare, Norway*
- *ICI Caldaie, Italy*
- *Johnson Matthey, United Kingdom*
- *Linde, Germany*
- *NextChem SPA, Italy*
- *OMV, Austria*
- *Process design center B.V. (PDC), Netherland*
- *Ranido, Czeck Republic*
- *Repsol SA, Spain*
- *SOFSID, France*
- *ST1, Finland*
- *Steeper, Denmark*
- *Tata Steel UK Limited, United Kingdom*
- *Technip Energies, France*
- *The Centro Ricerche Fiat (CRF), France*
- *Turkiye Petrol Rafinerileri Anonim Sirketi (Tüpras),Turkey*
- *UOP LLC, USA*
- *VTT, Finland*

European research - Horizon 2020 projects

ELENA - Low energy ELEctron driven chemistry for the advantage of emerging NAno-fabrication methods. H2020-MSCA-ITN-2016 iCSI-partner involved: UiO Duration: 2016-2022

CARMOF – New process for efficient CO_2 capture by innovative adsorbents based on modified carbon nanotubes and MOF materials. H2020-NMBP-20-2017, iCSI-partner involved: SINTEF. Duration: 2018 –2022

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

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

Bizeolcat- Bifunctional zeolite-based catalysts for sustainable hydrocarbon transformation. H2020-CE-NMBP-24-2018, iCSI-partners involved: SINTEF, UiO. Duration: 2019-2022.

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

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

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

MesoSi-CO_2 – Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO2 utilization through tri-reforming of methane. H2020-MSCA-IF: iCSI-partner involved: NTNU. Duration: 2020-2023

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

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

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.

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

EBIO: Turning low value crude bio liquids into sustainable road transport fuels. Grant scheme: H2020-LC-SC3-RES-1-2019-2020. iCSI-partner involved: SINTEF, Duration: 2021-2024

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

TUNEMOF - Metallolinker-Functionalized MOF Catalysts for CO2 Hydrogenation , HORIZON-MSCA-2021-PF-01 , iCSI-partners involved: UiO, Topsøe, Duration: 2022-2025

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

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

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

International collaborations supported by RCN and sources other than EU

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

NanoCat4Fuels - Production of JP-8 Range Fuels and Chemicals from Pyrolysis Bio-Oil using Nanostructured Catalyst, Indo-Norwegian initiative on renewable fuels and chemicals within the Bionœr and EnergiX work program. iCSI-partner involved: SINTEF, International partner: Anna University, Department of Chemistry, Chennai, India Duration: 2018 –2022

H_2MemX - Enabling ultrathin Pd based membranes through surface chemistry diagnostics and control. ENERGIX Researcher project (280903) iCSI-partners involved: NTNU, SINTEF. Duration 2018 – 2022. International partner: Lund University/MAX IV, Sweden.

CATHEX-Advances in heterogeneous catalysis through integrated theoretical and experimental efforts. RCN – INTPART iCSI-partners involved: NTNU, UiO. International partners: University of Cape Town, University of Toronto, University of Wisconsin-Madison, East China University of Sci. & Techn., Duration: 2020-2024

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

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

InnCapPlant – Innovative moving bed adsorption process for CO2 capture in coal-fired power plants operated under variable load. EØS-Poland. iCSI-partners involved: SINTEF, NTNU. International partners: Cracow University of Technology (CUT). Duration: 2021-2023

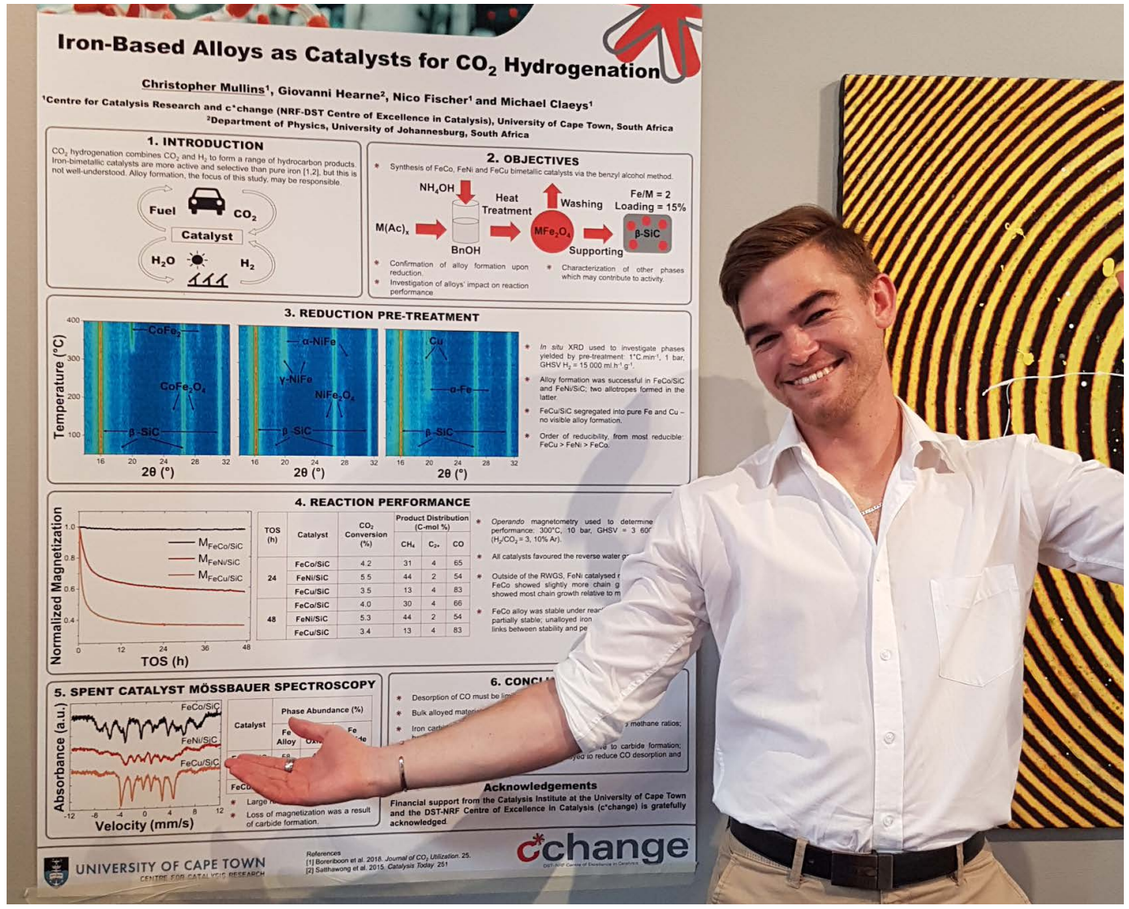
Continued membership in the Swiss-Norwegian Beamlines (SNBL) at ESRF. NFR INFRASTRUKTUR. iCSI-partners involved: NTNU, UiO. Other Norwegian partners: IFE, UiB, UiS. Duration: 2021-2024

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

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

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

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



Christopher Mullins from University of Cape Town, South Africa, was the first CATHEX PhD exchange student to NTNU. Photo from the iCSI Annual seminar in Oslo.

Accounts 2022

All cost and budget numbers appear in 1000 Norwegian Kroner (NOK) as of January 2023 NOK100 are equivalent to €8,9

Table 1: Summarizes the costs in 2022 and the total budget for the period of the Centre after revision in January 2023. The different cost codes concern respectively:

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

Cost code	Costs 2022	2015–2023 Total budget
Payroll and indirect expenses	6 985	58 510
Procurement of R&D services	10 631	94 179
Equipment	1 591	10 570
Other operating expenses	3 148	34 540
Totals	**22 356**	**197 798**

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

Cost and Financing per partner	2022 Accounts		2015–2023 Total budget	
Partner	Costs	Financing	Costs	Financing
NTNU	9 454	3 360	77 329	29 492
University of Oslo	5 411	1 513	50 594	13 924
SINTEF	5 220		43 585	7 942
Industrial partners	2 271	5 271	26 290	50 290
Research Council of Norway		12 212		96 150
Totals	**22 356**	**22 356**	**197 798**	**197 798**

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

Industrial Innovation Area (IIA)	Costs 2022	Costs 2015–2022	2015–2023 Total budget
IIA1 21st century Nitric Acid technology development	5 260	34 415	39 848
IIA2 New NOx abatement technologies	1 041	7 747	8 110
IIA3 Frontier formalin technology development	3 259	22 230	24 117
IIA4 PVC Value Chain	3 485	28 504	32 265
IIA5 The next step in direct activation of methane	3 243	28 980	34 476
IIA6 Generic projects	2 009	32 768	34 720
IIA7 2020 Catalysis	2 316	4 338	8 417
iCSI Management and administration	1 743	13 644	15 846
Totals	**22 356**	**172 626**	**197 798**

Education

Postdoctoral researchers with financial support from iCSI

Yalan Wang	NTNU	China	2019-2022	F	IIA4
Sebastian Prodinger	UiO	Austria	2020-2022	M	IIA5
Tina Bergh	NTNU	Norway	2021-2023	F	IIA6

One postdoc and one researcher left iCSI in 2022. We would like to thank Yalan Wang and Oleksii Ivashenko for their invaluable contributions to iCSI over many years.

PhD candidates with financial support from iCSI

Samuel Regli 1)	NTNU	Switzerland	2016-2019	M	IIA6
Asbjørn Slagtern Fjellvåg2)	UiO	Norway	2016-2021	M	IIA1
Moses Mawanga 3)	NTNU	Uganda	2018-2021	M	IIA6
Karoline Kvande	UiO	Norway	2019-2022	F	IIA5
Julie Hessevik	UiO	Norway	2019-2023	F	IIA1
Jithin Gopakumar	NTNU	India	2020 -2023	M	IIA1
Youri van Valen	NTNU	Netherlands	2020 -2023	M	IIA3
Wei Zhang	NTNU	China	2020 –2023	F	IIA4
Bjørn Gading Solemsli	UiO	Norway	2021-2024	M	IIA5
Björn Frederik Baumgarten	NTNU	Germany	2021-2024	M	IIA6

1) Samuel Regli has held a position as lab engineer at IKP, NTNU since August 2020, and his defense is expected to take place in 2023.
2) Asbjørn Slagtern Fjellvåg's defense took place 30 September 2022.
3) Moses Mawanga left NTNU for a position in industry 31.12.2022, and his defense defense is expected to take place in 2023.

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

Ole H. Bjørkedal	NTNU	Norway	2016-2020	M	Selective catalytic reduction (SCR) of NOx emissions in maritime transport.
Martina Cazzolaro	NTNU	Italy	2017-2020	F	Cu/CNF for selective hydrogenation of hydroxyacetone to 1,2-propanediol
Joakim Tafjord	NTNU	Norway	2017-2021	M	Iron-based Fischer Tropsch synthesis based on renewable feedstocks
Daniel Skodvin	NTNU	Norway	2017-2021	M	Carbon Nanomaterial-Ionic Liquid Hybrid for Ultrahigh Energy Supercapacitor
Jibin Antony	NTNU	India	2018-2022	M	Nanostructured hybrid catalysts for photocatalytic applications
Mario Ernesto Casalegno	NTNU	Mexico	2018-2022	M	Catalyst for onboard hydrogen generation from bioethanol
Ask Lysne	NTNU	Norway	2019-2022	M	Staging and Multiple Hydrogen Feed of Biomass to Fischer-Tropsch Fuel Synthesis
Dumitrita Spinu	NTNU	Romania	2019-2022	F	Low temperature CO2 capture
Junbo Yu	NTNU	China	2019-2022	M	Hydrogen membrane separation technology
Monica Pazos Urrea	NTNU	Columbia	2020-2023	F	Kinetic studies of aqueous phase reforming including deactivation studies
Petter Tingelstad	NTNU	Norway	2020-2023	M	Catalytic upgrading of bio-oil to aviation fuels
Oscar Ivanez Encinas	NTNU	Spain	2020-2023	M	Biofuels production from Biomass
Kishore Rajendran	NTNU	India	2020-2023	M	Development of efficient catalyst for conversion of biomass to aviation fuel
Albert Miró i Rovira	NTNU	Spain	2021-2024	M	Catalytic upgrading of bio-oil to aviation fuels
Zhihui Li	NTNU	China	2021-2024	F	Conversion of biomass and plastic wastes
Erlend Aunan	UiO	Norway	2018-2023	M	Thermochemical Stability and Adsorptive Properties of MOF-808
Martin Jensen	UiO,	Norway	2018-2023	M	Pt-Rh nanoparticles for ammonia oxidation
Vladyslav Shostak	UiO	Ukraine	2020-2023	M	Development of comprehensive diffusion/ adsorption models for TAP kinetic experiments
Dag Sannes	UiO	Norway	2020-2023	M	Rational design of MOF catalysts for CO2 conversion
Mouhammad Abu Rasheed	UiO	Syria	2021-2024	M	Testing of bioinspired catalysts for alkane partial oxidation
Claudia Fabris	UiO	Italy	2022-2025	F	Operando studies of zeolite catalysts
Agnieszka Seremak	UiO	Poland	2022-2025	F	Diffusion, reaction, and entropy in zeolites
Walace Kierulf-Vieira	UiO	Norway	2022-2026	M	Nanoparticles for thermal- and photo catalysis

International exchange PhD candidates in iCSI, NTNU

Yurou Li	East China University of Science and Technology	9 months	F	Acetylene selective hydrogenation
Lin Dong	East China University of Science and Technology	12 months	M	1-hexene epoxidation by metal-incorporated zeolite catalyst
Enrico Tusini	KIT Karlsruhe	2 months	M	BImetallic catalysts Knowledge-based development for Energy applications
Jonatan Duran Martin	Johnson Matthey, United King-dom	2 months	M	BImetallic catalysts Knowledge-based development for Energy applications
Christoper Mullins	Univ. of Cape Town	2 months	M	SSITKA investigation into the activation of CO2 for production of long chain hydrocarbons on iron model catalysts
Miguel Ángel Rodríguez Cano	Univ of Malaga	3 months	M	Efficient fiber catalyst for Fischer-Tropsch synthesis with biomass waste syngas, influence of syngas impurities
Nikhil Kumar	Indian Institute of Technology Madras	7 months	M	Pyrolysis and catalytic upgrading of Biomass
Hari Desai	Indian Institute of Technology Madras	6 months	M	Catalytic Pyrolysis of Plastic
Abdelrahman M. M. Riad Saleh	Politecnico de Milano	3 months	M	Sorption enhanced reforming for hydrogen production, modelling and experimental
Trung Nguyen	SCITEC, Milano	0.5 month	M	BIKE project
Veronica Piazza	Politecnico de Milano	4 months	F	Pyrolysis of biomass and plastic wastes

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

Katarzyna Swirk	NTNU	Poland	2020-2022	F	MesoSi-CO2. Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO2 utilization through tri-reforming of methane
Hongfei Ma	NTNU	China	2021-2023	M	Chemical transformation of enzymatic hydrolysis lignin (EHL) with catalytic solvolysis to fuel commodities under mild conditions (EHLCATHOL)
Ainara Moral	NTNU	Spain	2021-2023	F	Moving Bed Carbonate Looping
Mehdi Mahmoodinia	NTNU	Iran	2019-2022	M	High Efficiency Catalytic system for use in the SIlicone value chain (HECSI)
Felix Herold	NTNU	Germany	2021-2023	M	Carbon materials
Izar Capel Berdiell	UiO	Spain	2021-2023	M	Catalyst deactivation studies

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

Kristoffer Flem Grimstvedt	UiO	Norway	2019-2022	M	Catalyst deactivation by coke formation
Odd Reidar Bygdnes	UiO, iCSI	Norway	2020-2022	M	Methane to methanol - catalyst synthesis
Walace Kierulf-Vieira	UiO	Norway	2020-2022	M	Synthesis and characterization of nanoparticles relevant for catalysis
Alexandra Jahr Kolstad	UiO, iCSI	Norway	2020-2022	F	Reactor STM and NAP XPS for ammonia oxidation
Mathilde Ingeborg Nilsen Verne	UiO, iCSI	Norway	2021-2023	F	In-situ XPS of PtRh NPs for NH3 oxidation
Daniel Levent Arnes	UiO	Norway	2021-2023	M	Methanol-mediated conversion of CO2 and H2 to light hydrocarbons
Cathinka S. Carlsen	UiO	Norway	2022-2024	F	Platinum group metal transport in ammonia combustion and recovery
Phillip A. Mørch	UiO	Norway	2022-2024	M	MOF(UiO-66)-Cu(Ni, Au, Pd) nanoparticle hybrid materials for photo- and thermal catalytic conversion of CO2
Live Bjørnereim Lybekk	UiO	Norway	2022-2024	F	Supported Cu based nanoparticles for thermal- and photo catalysis
Adrian Madsen Lager	NTNU	Norway	2021-2022	M	Fast hydro pyrolysis coupling with catalytic vapor upgrading (CVU)
Anette Synnøve Groven	NTNU	Norway	2021-2022	F	Conversion of synthesis gas from biomass gasification over cobalt catalysts
Eirik Giil Woxholt	NTNU	Norway	2021-2022	M	Synthesis of solid sorbents and kinetic study for CO2 capture
Karthikai Selvan Siv-asamy	NTNU	India	2021-2022	M	Catalytic conversion of biomass-derived oxygenates to biofuel
Muhammad Arslan Aslam	NTNU, iCSI	Pakistan	2021-2022	M	Novel Fe based catalyst for Fischer-Tropsch synthesis
Seyyedeh Roomina Farzaneh Motlagh	NTNU, iCSI	Iran	2021-2022	F	Kinetic study of ethylene oxychlorination on promoted CuCl2/Al2O3 catalysts
Andrea Kjønli	NTNU	Norway	2022-2023	F	Catalytic pyrolysis of waste plastic to liquids
Hammad Ali	NTNU	Pakistan	2022-2023	M	Fast Pyrolysis and upgrading of biomass
Ida Saxrud	NTNU	Norway	2022-2023	F	Catalysts for Syngas Conditioning for Advanced Biofuels
Tomasz Skrzydlo	NTNU, iCSI	Poland	2022-2023	M	Oxidation of methanol to formaldehyde (MTF) over Ag catalyst
Pål Martin Benum	NTNU, iCSI	Norway	2022-2023	M	Catalytic Oxidation of NO to NO2 at Industrial Nitric Acid Conditions
Sahra Louise Guldahl-Ibouder	NTNU	Norway	2022-2023	F	Model catalysts for fundamental insights into the Fischer-Tropsch Synthesis
Robert Lennard Peters	NTNU	The Netherlands	2022-2023	M	Ketonisation of acetic acid
Alicia San Martin Rueda	NTNU	Spain	2022-2023	F	Catalysts for advanced biofuels synthesis via the Fischer-Tropsch process

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

International exchange master's students associated with iCSI

Erdogan Kasisari	Master, NTNU	Germany	5 months	M	Carbon supported iron catalysts for Fischer-Tropsch synthesis
Simon Meilinger	Master NTNU	Germany	6 months	M	Bimetallic catalysts for hydrogen production by aqueous phase reforming of biomass components
Tapiwanashe Dube	Master NTNU	Italy	5 months	M	Hydrogen Production from Biomass - derived compounds by sorption enhanced reforming.

Specialization students in catalysis group, NTNU, Autumn 2022. Photo: Per Henning.

MAX IV Laboratory, Lund University, Sweden (www.maxiv.lu.se/). Photo: Hilde J. Venvik.

Communication and Dissemination 2022

iCSI Invited Plenaries:

Venvik, Hilde Johnsen: In situ NAP-XPS characterization of PdAg hydrogen membranes and catalytic model systems. Norwegian Catalysis Symposium 2022; 2022-12-01 - 2022-12-02

Venvik, Hilde Johnsen: Oxidation reactions over metal surfaces by two different approaches. Guest lecture at Politecnico di Milano; 2022-10-12 - 2022-10-12

iCSI Publications and conference contributions 2022

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

Journal Publications

Fjellvåg, Asbjørn Slagtern; Jørgensen, Peter Stanley; Waller, David; Wragg, David Stephen; Michiel, Marco Di; Sjåstad, Anja Olafsen: Mechanism of grain reconstruction of Pd and Pd/Ni wires during Pt–catchment. Materialia 2022, Volume 21, 101359

Hessevik, Julie; Fjellvåg, Asbjørn Slagtern; Iveland, Oskar; Skjelstad, J.; Waller, David; Fjellvåg, Helmer; Sjåstad, Anja Olafsen:$LaNiO_3$ as a Pt catchment material in the ammonia oxidation process. Materials Today Communications 2022, Volume 33, 104084

Jensen, Martin; Gonano, Bruno Raymond Gino; Kierulf-Vieira, Walace; Kooyman, Patricia J.; Sjåstad, Anja Olafsen: Innovative approach to controlled Pt-Rh bimetallic nanoparticle synthesis. RSC Advances 2022, Volume 12.(31), 19717-19725

Oral Presentations

Gopakumar, Jithin; Waller, David; Enger, Bjørn Christian; Rønning, Magnus: Catalytic Oxidation of NO Using Different Ceria Supported Catalyst for Nitric Acid Production. iCSI Annual Seminar 2022, Oslo 2022-06-21 - 2022-06-22

Hessevik, Julie: How suitable are oxides as alternative Pt catchment materials in the ammonia oxidation process? iCSI Annual Seminar 2022, Oslo 2022-06-21 - 2022-06-22

Silje F. Håkonsen, Børge Holme, David Waller, Martin F. Sunding, Kari Anne Andreassen, Thomas By: Pd loss and reconstruction under different gas compositions, iCSI Annual Seminar 2022, Oslo 2022-06-21 - 2022-06-22

Sjåstad, Anja Olafsen: 21st Century Ammonia Oxidation and Nitric Acid - Technology Development, iCSI Annual Seminar 2022, Oslo 2022-06-21 - 2022-06-22

Gopakumar, Jithin; Miro i Rovira, Albert; Waller, David; Enger, Bjørn Christian; Rønning, Magnus: Catalytic Oxidation of NO to NO_2 for Nitric Acid Production Using Manganese Catalysts. 9th World Congress on Oxidation Catalysis; Cardiff, Wales 2022-09-04 - 2022-09-08

Posters

Gopakumar, Jithin; Rønning, Magnus; Enger, Bjørn Christian; Waller, David: NO_2 An Inhibitor for Catalytic Oxidation of NO at Industrial Nitric Acid Conditions. Catalysis at the Energy-Chemistry Nexus - 2022 Winter School; 2022-03-14 - 2022-03-18

Gopakumar, Jithin; Rønning, Magnus; Swirk Da Costa, Katarzyna; Pazos Urrea, Monica; Enger, Bjørn Christian; Waller, David: Silver-Promoted MnO_2/ZrO_2 Catalyst for Oxidation of NO to NO_2 at Partial Nitric Acid Plant Conditions. NAM 27 - The 27th North American Catalysis Society Meeting; 2022-05-22 - 2022-05-27

Gopakumar, Jithin; Rønning, Magnus; Swirk Da Costa, Katarzyna; Pazos Urrea, Monica; Enger, Bjørn Christian; Waller, David: Silver-Promoted MnO_2/ZrO_2 Catalyst for Oxidation of NO to NO_2 at Partial Nitric Acid Plant Conditions. 19th Nordic Symposium On Catalysis; 2022-06-06 - 2022-06-08

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

Oral Presentations

Silje F. Håkonsen, Karl Isak Skau, David Waller, Martin F. Sunding, Patricia Almeida Carvalho, Anna Lind, Mathieu Grandcolas, Jasmina H. Cavka: Abatement of nitrogen-containing pollutants: Characterisation studies of industrial de-N_2O catalysts. iCSI annual seminar; Oslo 2022-06-21 - 2022-06-22

IIA3: Frontier Formalin Technology Development

Oral Presentations

van Valen, Youri: Influence of Catalyst History on the Oxidation of CO over Silver, iCSI annual seminar; Oslo 2022-06-21 - 2022-06-22

Venvik, Hilde: Methanol partial oxidation to formaldehyde (MTF) over silver – new kinetic and structural insights, iCSI annual seminar; Oslo 2022-06-21 - 2022-06-22

Bergh, Tina; Fyhn, Hursanay; Sandnes, Lise; Blindheim, Jørgen; Grong, Øystein; Holmestad, Randi; Berto, Filippo; Vullum, Per Erik: Hybrid metal extrusion & bonding for multi-material welding of aluminium alloys to copper, steel, and titanium. 18th International Conference on Aluminium Alloys; Toyama, Japan 2022-09-04 - 2022-09-08

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

Journal Publications

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Ma, Hongfei; Wang, Yalan; Zhang, Hao; Ma, Guoyan; Zhang, Wei; Qi, Yanying; Fuglerud, Terje; Jiang, Zheng; Ding, Weiping; Chen, De: Facet-Induced Strong Metal Chloride−Support Interaction over $CuCl_2$/γ-Al_2O_3 Catalyst to Enhance Ethylene Oxychlorination Performance. ACS Catalysis 2022 ;Volum 12.(13) s. 8027-8037

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Zhang, Wei; Ma, Hongfei; Chen, De: Multi-Promoter Effect of K, La and Mg in Ethylene Oxychlorination Studied by Operando UV–vis-NIR Spectroscopy. 19th Nordic Symposium on Catalysis; 2022-06-06 - 2022-06-08

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

Journal Publications

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IIA6: Generic Projects for Additional Industrial Synergies

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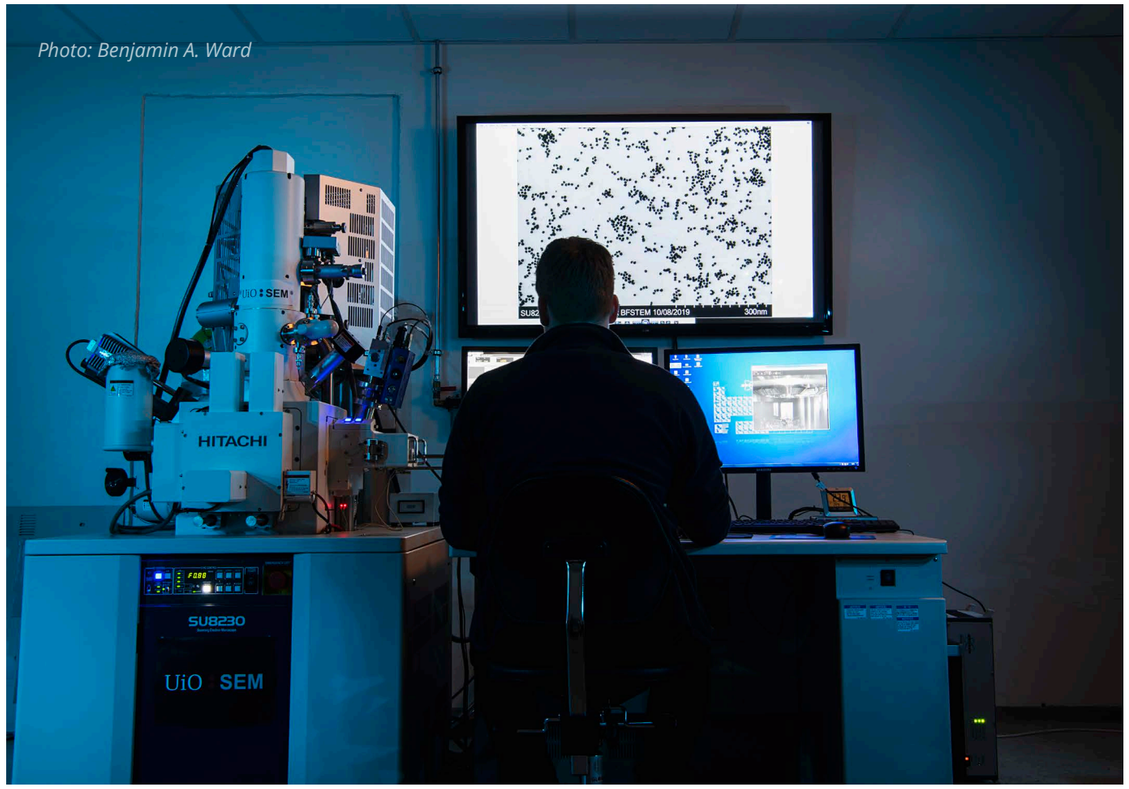

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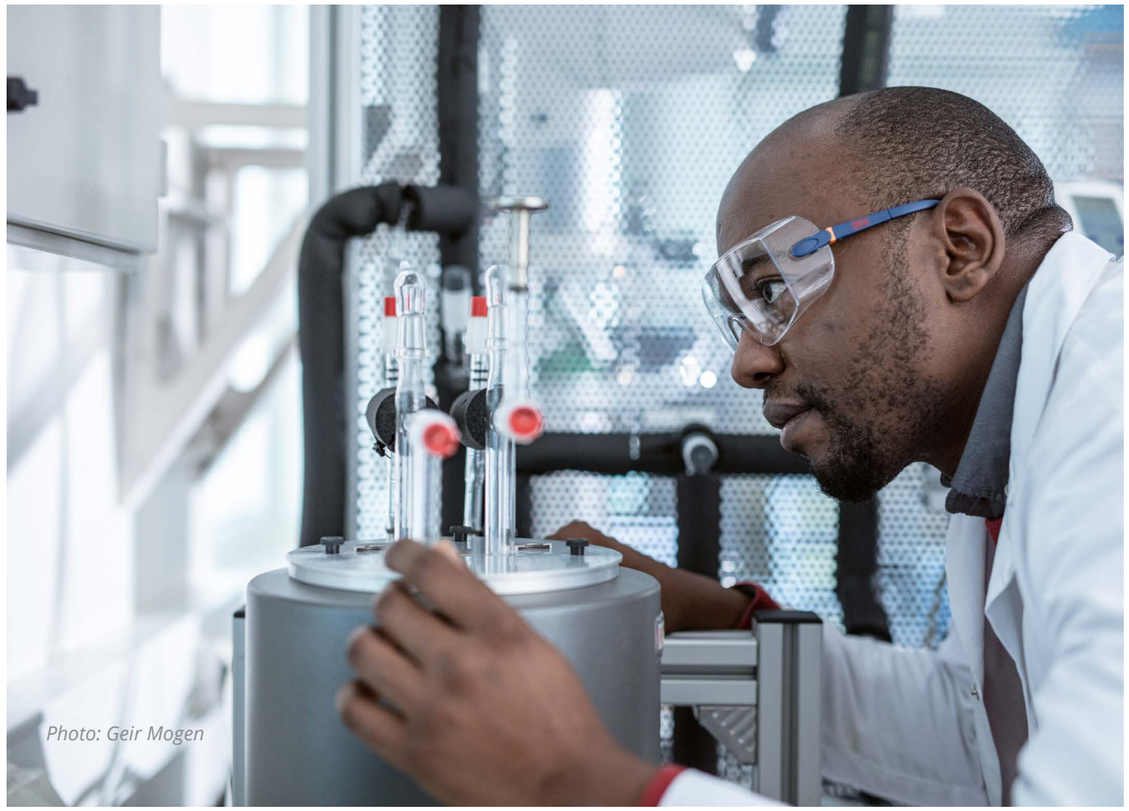

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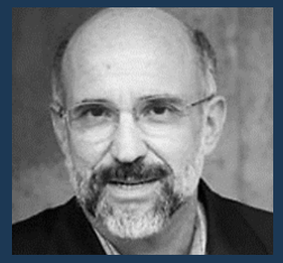

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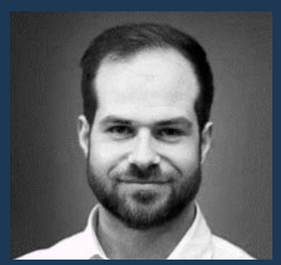

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