iCSI

industrial Catalysis Science and Innovation

Annual Report 2021

Centre for Research-based Innovation

NTNU

iCSI Partners

Centre for Research-based Innovation
The Research Council of Norway

NTNU

SINTEF

UiO : University of Oslo

YARA

HALDOR TOPSØE

inovyn

K·A·Rasmussen NORWAY

dynea®

The Research Council of Norway

Cover photo: The capillary setup used for flow through experiments on BM31 at The European Synchrotron Radiation Facility (ESRF) by IIA5. The quarts capillary has an inner diameter of 1.5 mm and a wall thickness of 0.01 mm. The cone below the capillary is a heat blower. Photo by Karoline Kvande.

2021 Summary

Although 2021 started off in a similar manner to what had been the case through most of 2020, iCSI work was able to proceed almost normally with open laboratories all year. The vaccination program gave a boost to the hope of better times. However, travel restrictions and quarantine requirements made international cooperation difficult, and beam times in European laboratories in particular had to be cancelled or postponed.

Educating master's students is important to iCSI. In 2021, eleven graduating master's students were associated with iCSI, of whom two delivered directly into the ongoing projects. The gender balance within iCSI is maintained, with all personnel categories within a 40/60 distribution.

In 2021, iCSI finalized the centre's employment plan by welcoming the three final candidates: Postdoctoral fellow Tina Bergh and PhD candidate Björn Frederik Baumgarten at NTNU, and PhD candidate Bjørn Gading Solemsli at UiO (being respectively the 6th postdoc and the 14th and 15th PhDs within iCSI). Three candidates (Endre Fenes, Hongfei Ma and Stine Lervold) finalized their PhD theses with two defences in March and one in June, respectively. iCSI congratulates them!

The high publishing activity has continued from last year, and 23 reviewed papers were accepted and published in 2021. As in the previous year, Innovation Area 4 (PVC Value Chain: World Class Energy and Raw Material Efficiency for the Production of Chlorine and Vinyl Chloride Monomer) kept going with a high publication rate, but also IIA1, 3, 5 and 6 have published several papers. The publication and presentation lists can be found on pages 65–71.

Once more, lack of travel and conference participation are reflected in the list of conference contributions. Most of the presentations are from the iCSI Annual Seminar, which after two postponements, fortunately could take place at Hovde gård in October. In 2021 a few international digital events took place, however, and some of them had invited lecturers from iCSI.

The science is progressing in all Industrial Innovation Areas, and on page 15 we present this year's highlight. One goal in IIA1 has been to explain why the Pd/Ni net used in the production of nitric acid for fertilizers, transforms into something similar to a porous plate during industrial operation. This change results in a significant pressure drop through the gauze pack, limiting the number of Pd/Ni gauzes which can be installed simultaneously. The answer revealed by Asbjørn Slagtern Fjellvåg was similar to a classical corrosion mechanism; the grain boundaries serve as a rapid transport path for Pd- and Pt-diffusion, causing the grain boundaries to develop porosity and recrystallize the surface. In short, we can simply describe it as corrosion by platination.

In September, iCSI and NTNU made a contribution to the international catalysis society, by hosting the Webinar for the European Federation of Catalysis Societies (EFCATS) 2021 Catalysis Award event. Eight prize winners were presented, and they all gave lectures showing results from their work. iCSI is proud of our former PhD candidate Dimitrios Pappas, who won the Best PhD Thesis Award.

iCSI is also proud to have dedicated and enthusiastic international scientific advisors. This report introduces the readers to one of the advisors, Professor Regius in Chemistry Graham Hutchings from Cardiff University (page 12–14). Hutchings was the 2021 recipient of the Michel Boudart Award in Fundamental Catalysis from EFCATS and NACS, and iCSI congratulates him on this well-deserved honour!

The representation on the iCSI Board has changed for one of the industry partners in 2021, with Camilla Jordal taking over from Marco Piccinini as Inovyn's board representative in January. We thank everyone on the board as well as all the scientists for their efforts for iCSI throughout the year.

While this report was prepared, we were seeing diminishing impacts of the Covid-19 pandemic. The Norwegian society opened up, lectures became physical, and the student social life was back. We started looking forward to an iCSI 2022 Annual Seminar with participation from our International Scientific advisors and to prepare for finalization of our research and innovation efforts in the best possible way.

But before we were able to complete the work, war was waged in Europe. iCSI and its participants express their deepest sympathy with the Ukranian people and condemn the invasion. iCSI is particularly concerned about Ukranian scientists and universities, as well as the open, global scientific and industrial community in general. Conflicts in the 21st century must be resolved through transparency, negotiations, compromise and without the use of violence and military force.

Content

Photo: Anne Hoff

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

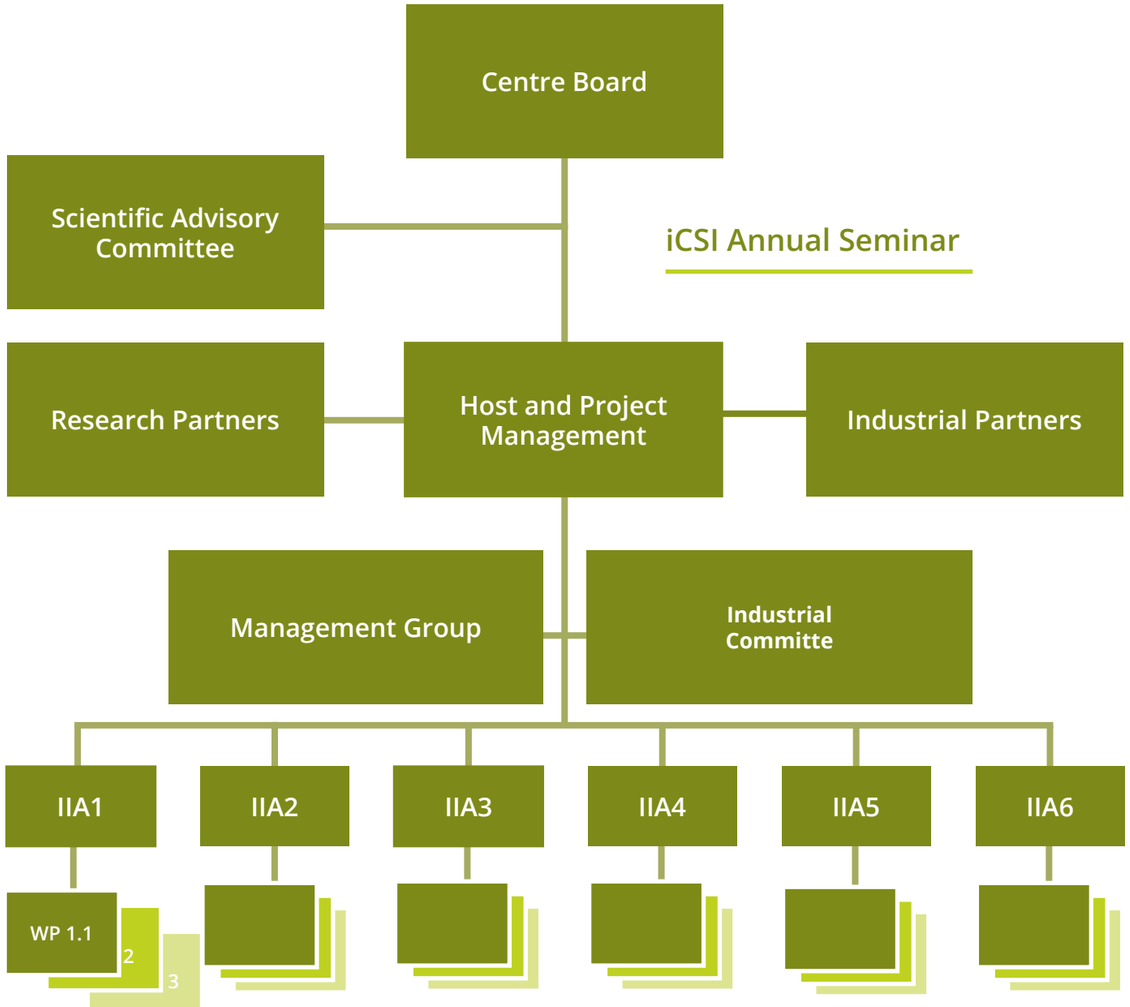
iCSI's main objective is to boost industrial innovation and competitiveness and provide efficient, low-emission processes

This 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 2021. In January 2021, Kamilla Jordal replaced Marco Piccinini 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 & Licensing 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

Kamilla Jordal

Chemical engineer at Inovyn RTE-VCM

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

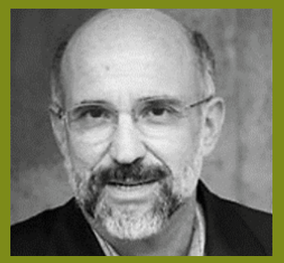
Special advisor RCN, with Responsibility for Nanotechnology and Advanced Materials

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

Ragnhild Aaen

Economy Advisor
iCSI Economy advisor
January–March 2021

Hilde M. Flaathe

Financial Project Advisor
iCSI Economy advisor
April–December 2021

Researchers Portrait: Regius Professor of Chemistry: Graham Hutchings

Photo: University of Cardiff

iCSI is lucky to have top international researchers as scientific advisors, and Graham Hutchings is no exception. The complete list of his awards and accolades is too long to be included here, but a few are mentioned in the fact box. Graham, as the gentle and wonderful man he is, gave us time for a chat to hear how his successful career developed and to get some advice for the younger generation of scientists.

So, Graham's career didn't start with heterogenous catalysis at all. His PhD is in biological chemistry, and he was looking for a job in that industry. After a few offers he didn't like, he reluctantly accepted a job in Imperial Chemical Industries on Teesside. This was a place neither he nor his wife Sally really wanted to go to because it was a very poor, polluted area with few facilities, quite different from London.

—"I decided I would just enjoy coming up for the interview because they were going to put me up at a Country Club, and I really fancied staying in a Country Club"

But the position was well paid, so Graham accepted the job offer and they bought a house and had a baby. And then before he arrived, ICI had changed the job in biochemistry to one with heterogeneous catalysis and vanadium phosphates. That switch changed the course of his life for forever, because ever since then in 1975, he has been doing heterogeneous catalysis.

After a few years in research, he rather wanted to go where the company made money. He became the production support manager and later the plant manager for hydroformylation plasticizer alcohols. "It was a wonderful time, " he said.

"What did I learn during my years in the industry? I did research and I did production, and I liked the mixture of those. I learned that managing people is extremely challenging but also very rewarding. You know, you have to listen to people. It's important and you have to engage them. You have a team, and everybody on that team has a voice. I learned that you don't manage from the top. You're certainly in the front, but you have to get everybody on board and working with you. I also learned to think big and not to take no for an answer."

In 1981 Graham wanted to come back to research, and due to the recession in the UK and difficulties finding a job there, he stayed within ICI and took his family with him to South Africa, where he was a seconded Senior Officer and later Chief Research Officer at AECI in Modderfontein for 3 years. Then he realized he wanted to be "in charge of his own destiny" and decided that he would become an academic, but that wasn't easy. He applied for lots of jobs but nobody at all wanted to employ someone from industry who didn't have any papers, so a number of places turned him down.

—"And you know, at this point I look back and think, well maybe they might have regretted that. Just slightly. At this point"

He finally managed to find an opening at Witwatersrand University in Johannesburg, mainly because his main reference was Max McGlashan – at that time probably the leading thermodynamicist in the world – and the Wits Head of Department was also a thermodynamicist! And there, his academic career started in 1984.

When asked what Graham is most proud of in his professional career, he doesn't have a moment's doubt. "I think people would be surprised if I didn't say it was my discovery of catalysis by gold". For those who don't know, gold was at that time, in 1982–83, considered to be totally inert and not suitable for catalysis. He had earlier contributed to solving some of the AECI plant's operational problems, and through that gained the production peoples' trust. Now, they asked him to find a new catalyst for acetylene hydrochlorination to replace mercury, which was treated in a frighteningly lax manner despite being a serious health hazard. "I hit upon gold by reading some papers and taking the process data from one of these papers and coming up with a correlation for the activity versus the standard electrode potential. And I looked at this and I thought, if that's right, then gold is the best catalyst. And experiments confirmed that. If I hadn't gone to this factory, I would never have dealt with that problem – and I would never have come up with gold as a catalyst for the heterogeneous reaction." In 2013, China signed the Minamata Convention which sought to ban uses of mercury worldwide, and in 2017 it entered into force as international law.

—"I think that discovery, that insight of using gold for this reaction, led to a change in international law. I don't think anything else I've done has had that level of impact"

When it comes to students and young researchers, Graham has observed that times are now tough with hard competition for temporary positions, much tougher than in his young years. His best advice for them is that if you don't enjoy doing science, then choose something else. But if you really love it, you should trust yourself, your own judgement and believe in yourself. Be aware of any unusual observations, because something that you weren't expecting could open up a whole new area of research that you weren't suspecting, so be open minded. You should also pick your advisors and mentors with care and choose ones who tell you when you're doing things wrong.

Many people have influenced his path in his own career, and he is grateful for their guidance and corrections. The first mentor he mentions is Charles Vernon, his PhD supervisor. "He was an exceptionally bright person, who left me alone for long periods, and gave me the freedom to do the project the way I wanted to." Graham has applied these experiences to his own PhD students, who are set up in groups with postdocs as co-supervisors.

The next mentor was Arthur Thomas. "He was my boss at ICI in South Africa, and he challenged me and gave me a lot of opportunities."

Michel Che is another mentor, with whom Graham talked on the phone with regularly when he went to Cardiff. "He questioned why I was doing things." Michel also helped him in a big way because he invited Graham to Paris as a visiting professor. There he could step back, and he realized that he should be doing a lot more with gold. And after that, things really took off.

Ian Smith was someone who helped him when he was a head of school and helped him to understand the context of his science in the wider world.

Graham Hutchings with colleagues and friends at the 2016 CCI Conference, Cardiff, UK. Photo: Michael Hall.

The last person Graham mentions is Richard Catlow, who got the UK catalysis hub going. “I certainly couldn't have done that without Richard.”

Graham has certainly had good advisors and supports but also an inner drive and curiosity to find explanations for observed phenomena. “You don't know when the next big, wonderful discovery is going to be made. Maybe you'll make it. Maybe you won't, but there are always new things out there, and that's what inspires me to ask questions as a researcher and answer them.“

—"Time is the most valuable possession that you have, and you must use it as effectively as you can"

Last year Graham celebrated his 70th birthday, but he doesn’t plan to stop working yet. He has a 50 % appointment at Cardiff University, and he is still the Regius Professor of Chemistry. Whether he will still be at Cardiff when he is 80, he doesn’t know. “I think the next generation has to take over at some point, but not yet. I’ll stop when I don't think I've got any decent ideas anymore.”

Graham’s view for the future is that we now need to find how we can use resources more effectively and how to use carbon in a circular way. “We can't carry on consuming resources and we have to be very innovative. In the very long term, I see direct air capture of carbon dioxide. To me that's the big thing and it's something I want to be part of still. Reactions of CO_2 are not thermodynamically infeasible. They're just energetically uphill. The cost is energy, and energy is expensive, so the cost of what we are going to use in the future will be more expensive than it is now, but hopefully it will be better for the planet.”

Graham claims that chemistry is his hobby. Ever since he saw his first chemistry experiment at the age of 11 he wanted to be a chemist. Chemistry has been a passion for 60 years. “If you don't watch out, it can make you into a very boring person.” His dear Sally shared this concern and once 20 years ago, when the weekends were spent writing papers, she asked him to get himself a life. “So, I joined the wine club. I now have an interest in wine and have become quite knowledgeable on Bordeaux wines and Alsace wines, and I delight in South African wines.” Sally said this was not what she had in mind! But he also reveals that he reads Nordic crime (unlike science, they have an ending), and goes for walks in the beautiful countryside around the small farm and the village where they live in North Yorkshire.

As have most of us, Graham has suffered from the pandemic, and he is now looking forward to travelling again. He especially misses his daughter and grandson in Oregon, and a visit to them is first priority when it becomes advisable to travel abroad again. iCSI wishes him a good trip and also the very best with his wife and family in England and Wales going forward.

Graham Hutchings – CV in short:

Education
1972: BSc in Chemistry with First Class Honours, University College London
1975: PhD in Biological Chemistry, University College London. Supervisor: Prof C. Vernon
2002: DSc (University of London)

Experience
1975–1984: ICI Petrochemicals Division: Researcher, plant manager and production support manager at Teeside, Senior and Chief Research Officer at AECI, Modderfontein, South Africa

1984–1987: University of Witwatersrand, South Africa: Lecturer and Professor

1987–1997: University of Liverpool: Assistant Director of the Leverhulme Centre for Innovative Catalysis, Deputy Director and Professor

1997 – present: Cardiff University: Head of School and Professor of Physical Chemistry, Director of Cardiff Catalysis Institute, Pro Vice-Chancellor Research, Distinguished Research Professor and Regius Professor of Chemistry

- Has supervised around 200 PhDs and 100 Postdocs over his career
- 776 refereed research papers; 54 Patents; 74 Review articles; 21 Edited works, 58 000 citation

Many academic positions entailing trust and awards, of which a few can be mentioned:

- European Federation of Catalysis Societies 2021 Michel Boudart Award in Fundamental Catalysis
- Royal Society of Chemistry 2018 Faraday Lectureship Prize
- ENI Award for Advanced Environmental Solutions 2017
- Royal Society Davy Medal 2013
- Dechema 2012 Alvin Mittasch Award
- International Association of Catalysis Societies 2012 Heinz Heinemann Award
- European Federation of Catalysis Societies 2006 François Gault Lecturer
- American Chemical Society 1996 Langmuir Distinguished Lecturer Award

Scientific Highlight 2021: Platinum catchment

Synthetic nitrogen-based fertilizers are perhaps the most important product of the chemical industry today, because of their vitality for feeding the human population. Without the synthetic binding of nitrogen from the air, approximately 40 % of the human population would likely not be alive today. One of the key constituents in synthetic fertilizers is nitric acid, HNO_3, produced by the Ostwald process. During the ammonia oxidation step (NH_3 →NO; T ≈ 900 °C), significant quantities of Pt (and some Rh) are lost from the Pt/Rh (90/10 wt. %) catalyst in the form of PtO_2 (and RhO_2). To mitigate the Pt-loss, a Pd/Ni (95/5 wt. %) gauze (woven net) is installed downstream to capture the Pt. However, during industrial operation, the Pd/Ni (95/5 wt. %) net transforms into something more similar to a porous plate (Figure 1a), resulting in a significant pressure drop through the gauze pack, limiting the number of Pd/Ni gauzes which can be installed simultaneously.

In the platinum catchment project in iCSI (IIA1, WP1.1), we have shown how only PtO_2 in an air-flow causes a complete reconstruction of the Pd/Ni (95/5 wt. %) net, and that thermal/gas etching causes porosity and a large Pd-loss [1]. To understand the mechanism of grain reconstruction, in situ tomography was performed at the ESRF (ID15A) using the setup illustrated in Figure 1b. Combined with several lab scale techniques, our goal was to unravel how a solid Pd and Pd/Ni wire can transform into a porous wire instead of experiencing grain growth. The answer was similar to a classical corrosion mechanism; the grain boundaries serve as a rapid transport path for Pd- and Pt-diffusion, causing the grain boundaries to develop porosity and recrystallize the surface [2]. In short, we can simply describe it as corrosion by platination (Figure 2).

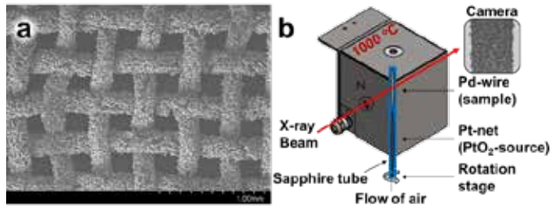


Figure 1. a) Pd/Ni-net after 5 months of industrial operation and b) schematic of the furnace (10x10x12 cm) used for the tomography experiments.

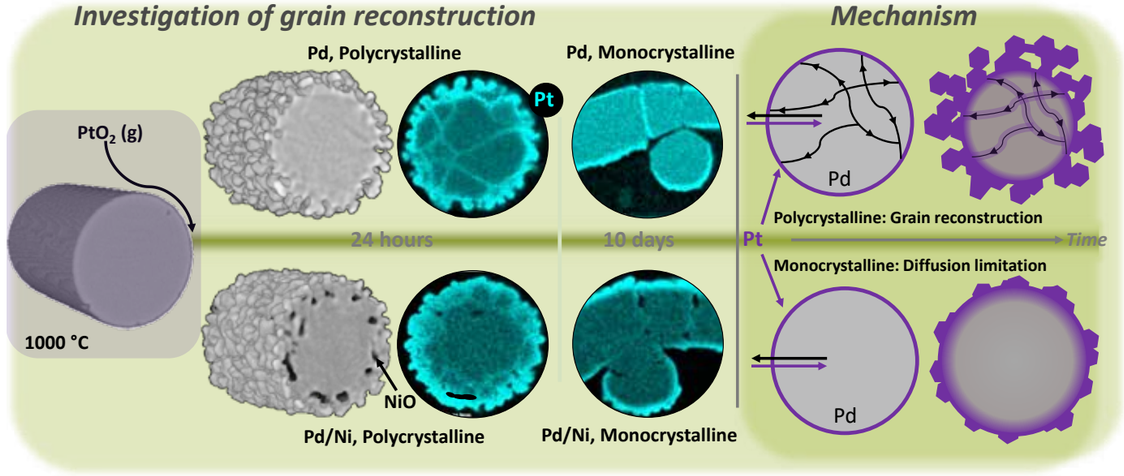


Figure 2. Summary of the results and mechanism for grain reconstruction of the Pd- and Pd/Ni wires.

Publications

1. Fjellvåg, A.S., Sjåstad, A.O., Waller, D., and Skjelstad, J., Grain Reconstruction of Pd and Pd/Ni Alloys for Platinum Catchment. Johnson Matthey Technology Review, 2019. 63(4).

2. Fjellvåg, A.S., Jørgensen, P.S., Waller, D., Wragg, D.S., Michiel, M.D., and Sjåstad, A.O., Mechanism of grain reconstruction of Pd- and Pd/Ni wires during Pt-catchment. Materialia, 2022. 21: p. 101359.

HEGRA Project – Herøya Green Ammonia

2021 marked a milestone year for Yara's electrification efforts for the ammonia plant at Herøya, Porsgrunn. The year started by establishing a dedicated organization, Yara Clean Ammonia, that will develop a portfolio of green and blue ammonia projects across the globe as well as establishing new markets for these products. For the Herøya plant, Yara was granted funding from ENOVA in December for the first phase of the electrification project.

This first phase aims to qualify the necessary technology, but also to mature the market for the final products. This stepwise approach is required as the cost both to build and to operate are higher than using conventional technology.

The technology chosen for this first phase is PEM-electrolysers provided by British manufacturer ITM Power. Linde Engineering was awarded the EPC contract. This will make the ammonia plant a hybrid plant, mixing hydrogen from the electrolysers with feed gas from the current steam methane reformer, into the existing Haber-Bosch process, to synthesize ammonia. The construction has already started, and the plant will become operational in mid-2023, making it one of the first green ammonia projects at this scale since Yara (Norsk Hydro) closed down its old electrolyser plant in Glomfjord in 1993.

The 24 MW project will support roughly 20 000 tonnes of ammonia production per year, or 60–80 000 tonnes of fertilizer equivalents. The electrolyser technology is continuously under development, but further research is required to develop cheaper, even more efficient and more durable stacks to make ready for a full-scale electrified ammonia plant. Together with sufficient access to cheap and reliable renewable energy, this step represents the beginning of decarbonizing an industry emitting ~1.5 % of the global CO_2 emissions. Yara is continuously monitoring the landscape for new commercially available technology to enable us to invest in the right technology at the right time.

For the full-scale electrification of the Porsgrunn plant, Yara has established Hegra. The project is maturing and full-scale electrification will be able to save around 800 000 tonnes of CO_2 per year, eliminating one of the largest emission points in Norway. The project has gained a lot of attention in the last year, and if implemented it will start production in 2026–2027.

Photo: Dag Tore Heiland

Company presentation: K.A.Rasmussen NORWAY

K.A. Rasmussen is a company which produces precious metals. Within this field we cover everything from collecting and buying used precious metals, to producing different products using these scarce and valuable elements: gold (Au), silver (Ag), platinum (Pt), palladium (Pd) and rhodium (Rh).

The company was founded in 1872 and has since evolved from a small goldsmith shop in Oslo to a precious metals company dealing with the recycling and refining of end-of-use products to return the metal to the market.

What all of these elements have in common is that they are highly noble metals and prefer to be in a metallic state. In addition to this, Pt, Pd and Rh, which are three of the six Platinum Group Metals (PGM), are very similar when it comes to chemical behaviour. The result of this effect is that separating them from each other is rather difficult. KAR's greatest expertise is this challenging separation process, and we can extract these elements with a purity of 99,9 % or greater.

Another interesting part of the function of precious metals is that they are highly efficient catalysts for different chemical reactions. For instance, platinum is a great oxidation catalyst. The same goes for silver. Although these expensive metals have been exchanged with other catalyst types in many applications, they are still in use in some areas, most commonly in processes with very harsh environments often involving high temperatures. One such example is the Ostwald process, burning ammonia in air to produce NOx and further downstream, HNO_3. Here, a platinum catalyst is placed in the high temperature zone for the ammonia oxidation, keeping the conversion and yield high.

To provide such a catalyst, KAR can produce wires with diameters down to 60 µm. These wires are then knitted or woven to form a cloth which can be fitted to the chemical reactor of the Ostwald process.

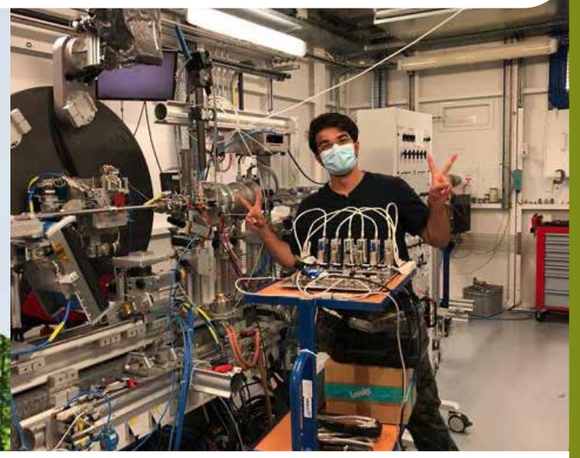
For KAR the goal is to remain the leading Nordic precious metal company. In the practical world, this means our company always needs to have the best available employees, knowledge and methods for recycling metals and producing high-quality products. The products of tomorrow need not be the same as they are today, but we believe there is a place for Precious Metals for both industrial and consumer use.

Photos: K.A Rasmussen

iCSI moments 2021

Another year wearing face masks

Skiing in Bratsberg – March



Visiting ESRF in Grenoble – June

Visiting Yara at Herøya – November

Safety first! – Always

There´s always an excuse for cake! - February & November

New PhDs – March & June

2021 Doctor promotion – November

Lund MAX IV – November

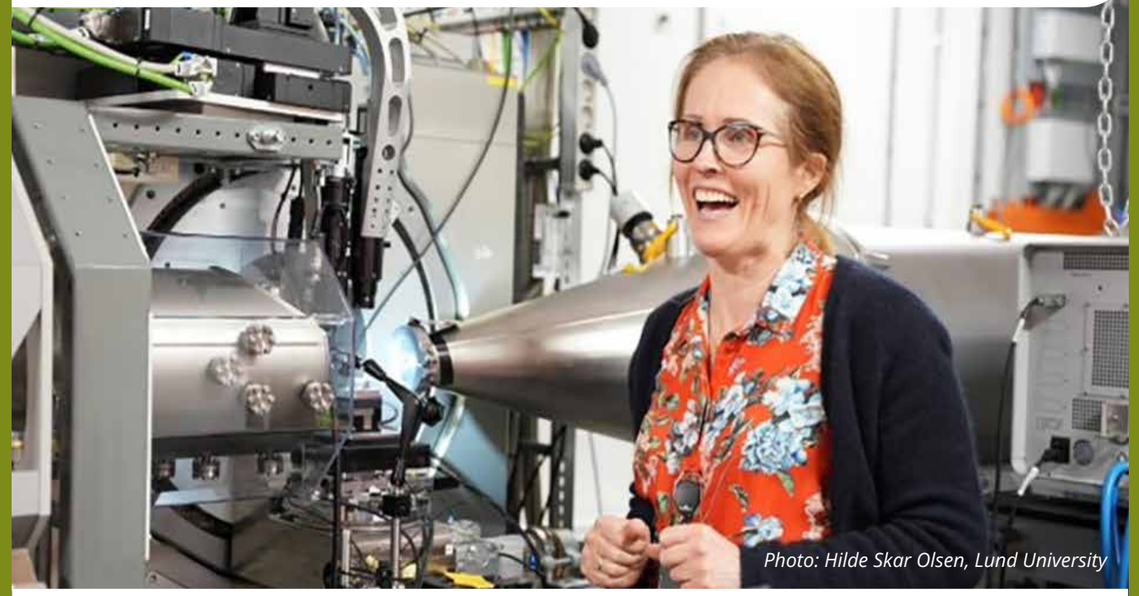


Photo: Hilde Skar Olsen, Lund University

Bortistu in Stordalen – September

Annual Seminar

After two postponements, 49 researchers were finally able to meet at Hovde farm October 18-19. About half came from NTNU, the others were evenly distributed between SINTEF, UiO and the industry partners.

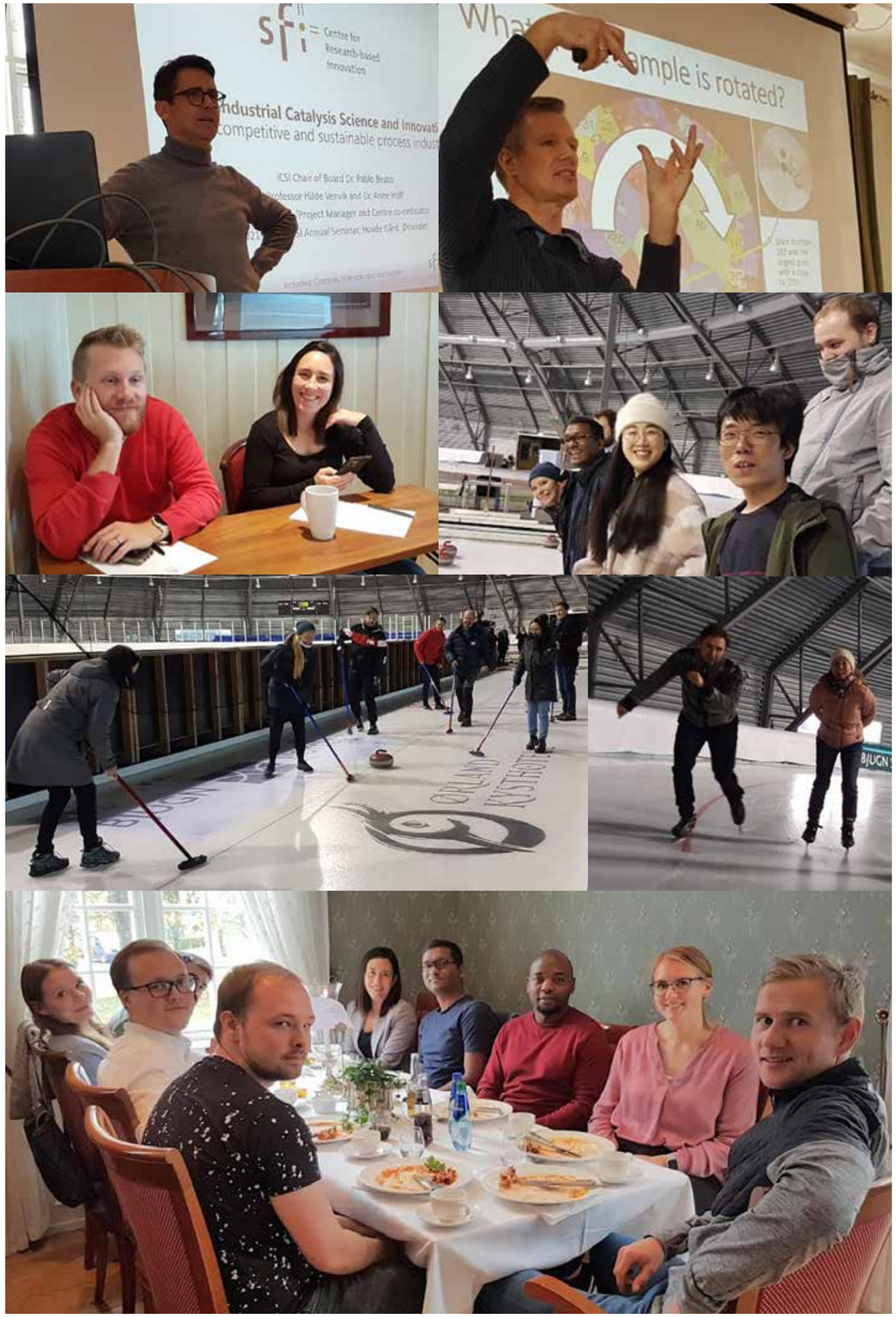
After two years of pandemics, there has been a great longing for conferences and other arenas where PhD students and young researchers can present their results and practice in scientific discussions. Since the pandemic once again prevented the international scientific advisors from coming, we were given more time for our own researchers. All doctoral students and post-docs within iCSI were therefor encouraged, and given the opportunity to present orally. A general comment from the board members was that the presentations were interesting and good. They also thought the level of the discussion of results and the communication skills had increased.

Although the board missed the poster session not on the agenda, they agreed that it was correct to give priority to the young researchers for oral presentations. iCSI promised to come back with a poster session at the 2022 seminar, which will take place June 21–22 in Oslo.

The seminar is also an important place for colleagues from the different institutions to meet, get to know each other and discuss future projects.

Day 1 (Monday October 18)	
09:00-11:30	**Registration/check-in/small talk**
11:30-12:30	**Lunch**
12:30-13:00	Opening remarks (Chair of the Board, Pablo Beato) Status of iCSI (Director, Hilde J. Venvik)
13:00-13:30	IIA2: Silje Fosse Håkonsen & Martin Fleissner Sunding: *Abatement of nitrogen-containing pollutants: Characterisation studies of industrial de-N_2O catalysts*
13:30-14:00	IIA1: Julie Hessevik: *LaNiO3 as a Pt catchment material in the ammonia oxidation process*
14:00-14:30	**Coffee break**
14:30-14:50	IIA1: Jithin Gopakumar: *Catalytic oxidation of NO to NO2 for nitric acid production*
14:50-15:10	IIA1: Børge Holme: *How hard can it be to get a platinum depth profile from a palladium sample by SIMS (Secondary Ion Mass Spectrometry)?*
15:10-15:30	Martin Jensen, UiO: *Generic approach to controlled bimetallic nanoparticle synthesis*
15:30-15:40	IIA3: Jasmina: *Short summary from IIA3 activities*
15:40-15:50	IIA3: Youri van Valen: *Methanol partial oxidation to formaldehyde over silver - continued*
16:00-18:00	**Social activity**
18:15-20:00	**Board meeting** / Break / (IIA internal meetings or IIA6 meets the other IIAs?)
20:00-22:00	**Dinner**

Day 2 (Tuesday October 19)	
08:00-08:45	**Breakfast**
08:45-09:15	IIA6: Oleksii Ivashenko: *Operando APXPS studies of PtRh alloys for ammonia oxidation*
09:15-09:40	IIA4: Yalan Wang: *Promoter effects on CuCl2/γ-Al2O3 catalyzed ethylene oxychlorination by DFT calculations*
09:40-10:00	IIA4: Wei Zhang: *Understanding of K , La and Mg co-promoter effect in ethylene oxychlorination by operando UV–vis-NIR spectroscopy*
10:00-10:30	IIA4: Kumar Rout: *Modelling, Estimation and Optimization of Oxychlorination of Ethylene*
10:30-10:50	**Coffee break**
10:50-11:10	IIA5: Sebastian Prodinger: *Synthesis-Structure-Activity Relationship in Cu-Mordenite for Partial Methane Oxidation: Directing Al Siting via Inorganic Structure Directing Agents*
11:10-11:20	IIA5: Bjørn Gading Solem: *Methylation of lower alkenes thought stepwise reaction with methane*
11:20-11:30	IIA6: Björn Baumgarten: *A new ISMA – Simultaneous deactivation and deposition studies*
11:30-11:40	IIA6: Tina Bergh: *Transmission electron microscopy characterisation at NTNU*
11:40–12:00	IIA6: Moses Mawanga: *Insights into the reaction kinetics and mechanism of industrial relevant reactions*
12:00-13:00	**Lunch**
13:00-13:30	New stratigies for the industry partners
13:30-13:50	Closing remarks



Postdoc Sebastian: Industrial exchange to Haldor Topsøe

Last October I finally had the chance to spend a couple of months at Haldor Topsøe. This had been planned for a long time, however, corona kept interfering with those plans. In October, it finally seemed like the risk was manageable only for me to learn that the housing situation in Copenhagen is a little more dire than back in Oslo. Luckily, at the last minute I succeeded in finding a place – with "hygge" but pricey – on Jægersborggade, a street in the trendy neighbourhood of Nørrebro. From there, the commute to Lyngby took only about an hour via the metro, a bus and a small local train. At work at last, I really did get into it, thoroughly enjoying my stay there and helped of course by the – by Norwegian standards – rich lunch buffet.

I had the chance to work in the Characterization group with iCSI's very own Chair of the Board, Pablo Beato. We wanted to see whether we could improve a well-aged test unit so it could perform methane to methanol reactions relevant to IIA5, which would enable us to compare and benchmark test results across labs. In addition, we also utilized Raman spectroscopy to induce resonance vibrations in copper species of our active materials and finally had the opportunity to probe some of our most exploratory and novel zeolite materials with the highly advanced transmission electron microscope and the support of Topsøe's Ramchandra Tiruvalam.

The time passed much too quickly, owing to the fact that between long hours at work and the commute, I also found time to explore the city and experience non-work related activities. For example, it was great to have been invited by Topsøe's Juan Salvador Martinez Espin to come and join his field hockey team. In the end, the only thing that was amiss with my stay at Haldor Topsøe was the cancelled Julefrokost (Christmas breakfast) due to the surge of Omicron cases in the last few days before the end of my trip. Overall, it was grand time and I am grateful I could partake in this opportunity.

PhD Karoline: Research stay at the University of Turin, Italy

From August 2021 to February 2022, I was on a research stay at the University of Turin, working with Prof. Silvia Bordiga. I found this to be a really great experience where I had the chance to challenge myself, both scientifically and culturally. Living in Turin for six months gave me the opportunity to learn about Italian culture, learn a little bit of Italian and eat and drink a lot of fantastic Italian, and more specifically, Piedmontese food. The group in Turin welcomed me with open arms, providing me with a lot of help in the lab, nice discussions as well as lots of social events like dinners or an "aperitivo" after work.

The group members are experts on spectroscopic characterization techniques, which gave me the chance to learn and work with something new and different to what I usually work with in Oslo. From mostly working on catalytic testing and temperature-programmed reduction (TPR) protocols for the direct activation of lower alkanes, I started my stay in Turin with trouble-shooting and finalizing a setup for operando UV-vis spectroscopy measurements. With this setup, I was able to measure UV-vis on several types of reactions, giving us exciting, new knowledge. Besides UV-vis, I also learned how to operate a specially designed CO-volume-try experimental setup, as well as working a little bit on Raman and CO-IR spectroscopy measurements. At the end, I also had some nice sessions with our expert on spectroscopy, Prof. Elisa Borfecchia, providing me with great help and guidance for analysing XAS data that we collected at a beam time at BM31 at ESRF in November.

All in all, I am so grateful to iCSI for giving me the opportunity to do this exchange, and it is truly an experience I would not want to be without, professionally or personally.

Top left: We were at Prof. Bordiga's beautiful Italian house in the countryside for a team-building trip. Here I am holding a 5 min presentation about myself and my research.

Top right: This picture shows the setup for operando UV-vis experiments. At the time the picture was taken, the Uv-vis fibre was not connected to the oven.

Bottom left: A close-up of the UV-vis fibre.

Bottom right: Karoline at the Truffle Festival in Alba.

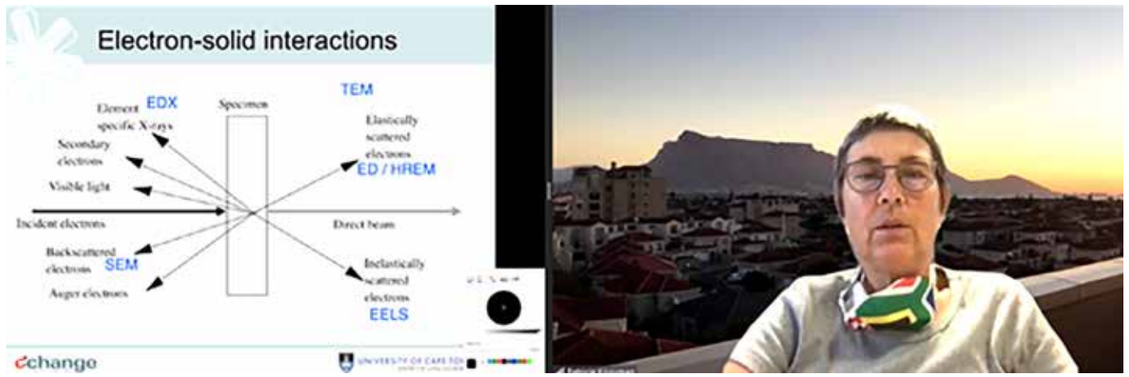
The CATHEX partnership

The CATHEX project, with support from the INTPART programme funded by the Research Council of Norway, is a large network project running from 2020 to 2025. The project 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. The core activity of the network is to strengthen the integration of theory and experiments in catalysis research and education through personnel exchange and shared workshops.

The start-up was a bit delayed due to the pandemic, but in 2021 the travel restriction was overcome by starting a webinar series where the partners contributed with online lectures, open for students and researchers at all the partner universities. Even though the time difference is a challenge (15:00 CET = 22:00 in Shanghai = 8:00 in Madison) 40–50 participants from all over the world typically took part in the webinars. More lectures are planned for 2022.

The webinar on November 12, 2021 was dedicated to Professor Emeritus Anders Holmen, who recently celebrated his 80th birthday. His lecture was an overview of the main knowledge gained from his 40 years doing Fischer-Tropsch research, while Associate Professor Jia Yang continued by showing recently obtained results in Fischer-Tropsch studies using Steady-State Isotopic Transient Kinetic Analysis (SSITKA).

CATHEX supported one professor visit by Patricia Kooyman from the University of Cape Town (UTC) to UiO in 2021, and for 2022 several student and researcher exchanges from UTC to NTNU and UiO are in the planning stages.



Patricia Kooyman, University of Cape Town, was the first professor to give a CATHEX lecture

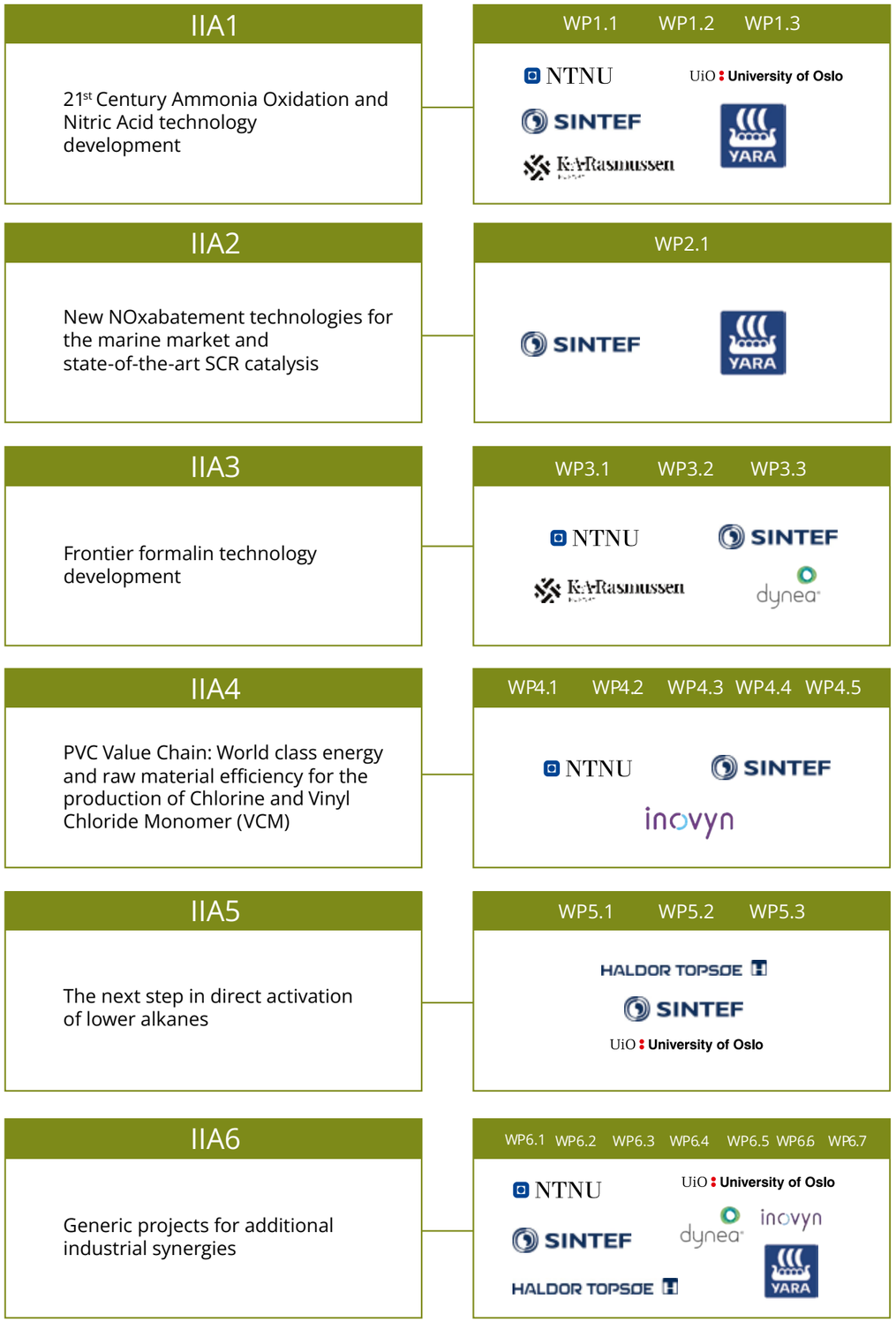
Date	Lecturer	Lecture topic
07.05.2021	Patricia J. Kooyman, UCT	Bridging the pressure gap in transmission electron microscopy
21.05.2021	Xinggui Zhou, ECUST	Regulating the Adsorption Configuration on Metal Catalysts for Semi-Hydrogenation of Acetylene
04.06.2021	Michael Claeys, UCT	Catalyst characterization using in-situ magnetic measurements
24.09.2021	Hilde Johnsen Venvik, NTNU	Methanol partial oxidation to formaldehyde over silver – new kinetic and structural insights
15.10.2021	Magnus Rønning, NTNU	Characterisation of catalysts in chemical processes by combination of operando techniques
12.11.2021	Anders Holmen, NTNU Jia Yang, NTNU	Studies of the Fischer-Tropsch Synthesis Steady-State Isotopic Transient Kinetic Analysis (SSITKA) for investigation of catalysts for Fischer-Tropsch synthesis
10.12.2021	Anja O. Sjåstad, UiO	From model to real catalysts operated at relevant process conditions

Photo: Hilde Skar Olsen, Lund University

Scientific Activities

Scientific Activities

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



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

The IIA1 team 2021

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)
Oskar Iveland	UiO	Master student (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)
Siri-Mette Olsen	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)
Magnus Rønning	NTNU	PhD supervisor, WP responsible (WP1.3)
Jithin Gopakumar	NTNU	PhD candidate (WP1.3)
Sunniva Vold	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-catchment materials

The current technology to mitigate noble metal loss from the Pt-Rh catalyst used in high temperature ammonia oxidation in the Ostwald process is to employ catchment nets of Pd-Ni alloys.[1,2] Although considerable amounts of Pt are captured by such nets and hence are available for recycling, the Pd-based nets show significant losses of Pd at the same time. Earlier we showed that oxides like $LaNiO_3$ are also able to capture Pt at process conditions where the reaction with PtO_2(g) at 900°C yields La_2NiPtO_6 as product.[3] This suggests that oxides may become important catchment materials at reduced costs. Currently, we screen a number of oxide candidate compounds in order to validate and discover essential parameters for an efficient Pt-catchment material at process conditions.

Among the selection criteria, we emphasize that the oxide needs to form a thermodynamically stable Pt-containing phase at relevant temperatures (800–900 °C) when reacting with PtO_2(g). Several ternary and quaternary platinates are mentioned in the literature. On the basis of known or hypothetical crystal structures, we use DFT calculations to better describe enthalpies of formation and possible reaction pathways. The maximum theoretical limit for platinum incorporation into the structure of the oxide obviously depends on the chemical composition of the resultant platinates. In practice, it also depends on the transport of Pt into the oxide pellet material. Consideration of the crystal structures, diffusion pathways and experimental studies of Pt diffusion into oxide single crystals and porous pellets provide insight into the Pt transport into these

materials. We note a strong Pt enrichment in the surface of the catchment pellets after exposure to PtO_2; see the SEM-EDX cross sections in Figures 1 and 2. The candidate oxides must furthermore show chemical stability at process conditions (steam and NO_X gases) and not negatively influence NOX gas species equilibria in the product stream. For instance, catchment pellets based on oxides with a basic cation may possibly decompose in humid and harsh conditions due to pulverization triggered by formation of hydroxides or carbonates.

Our first generation of oxide catchment materials focuses on perovskite and Ruddlesden-Popper type compounds. The second and wider screening covers a number of binary oxides, several of which form colourful platinates (Figure 3). A series of oxides have been tested in dry air with PtO_2 (g) in our in-house 6-zone furnace at 700, 800 and 900 °C, and the same type of oxides are currently being tested at real process conditions in a pilot plant at Yara International in Porsgrunn. Based on all the mentioned factors, we aim to conclude on the most promising Pt-catchment materials for mitigating Pt loss in the nitric acid plant.

References

1. A.S. Fjellvåg, D. Waller, J. Skjelstad, A.O. Sjåstad, Grain Reconstruction of Palladium and Palladium-Nickel Alloys for Platinum Catchment, Johns. Matthey Technol. Rev. 63 (2019) 236–246.

2. A.S. Fjellvåg, P.S. Jørgensen, D. Waller, D.S.Wragg, M.D. Michiel, A.O. Sjåstad, Mechanism of Grain Reconstruction of Pd and Pd/Ni wires during Pt-Catchment, 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., in review.

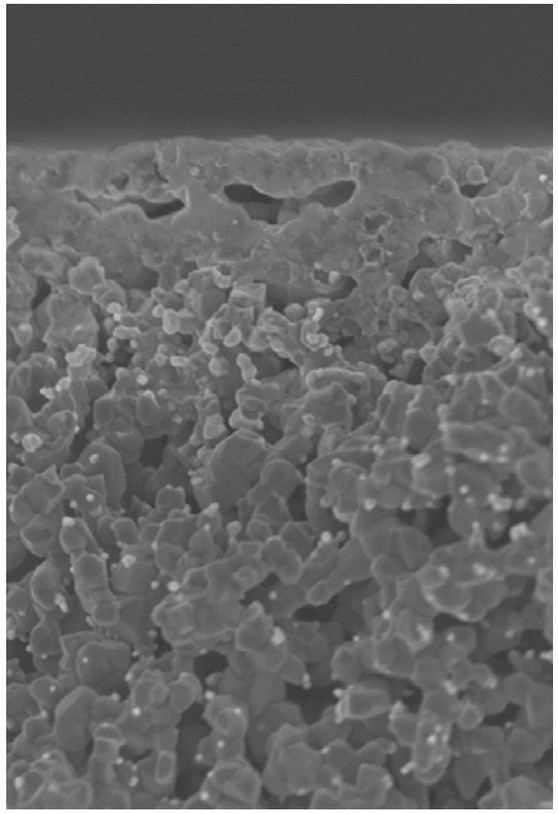


Figure 1. Cross-section SEM of La-Ni-Pt-O system show a dense layer of $La_2Ni_{2-X}Pt_{2X}O_6$ at the top and a number of NiO particles at the boundary to the porous structure.

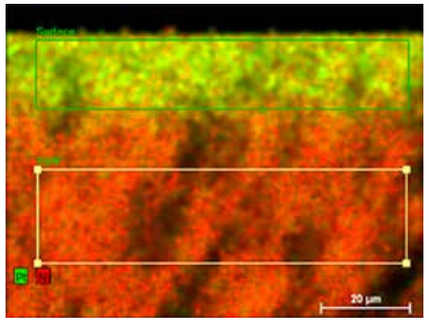


Figure 2. Cross-section SEM-EDX of La-Ni-Pt-O pellet shows Pt enrichment in the surface part but not in the bulk.

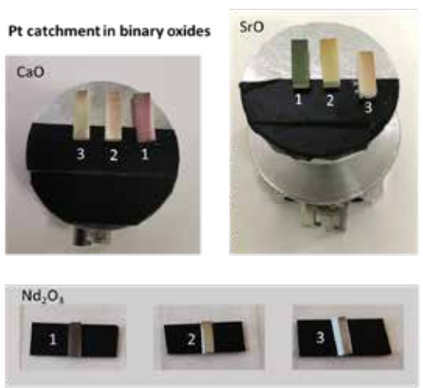


Figure 3. Pellets after exposure to PtO_2 at 1) 900 °C; 2) 800 °C; 3) 700 °C. Original color is white.

Experimental investigations of Pt/PtRh volatilization and catchment

A set of polished Pd and PdPt discs with a diameter of 5–6 mm and 5 different PdPt compositions have been exposed to a flow of different partial pressures of PtO_2 vapor for four hours at 900 °C. The diffusion profile was subsequently analysed using Sputtered Neutral particle Mass Spectrometry (SNMS) and is shown in Figure 1.

Our results show that for the low Pt-containing samples, Pt is captured from the gas and a clear diffusion profile is observed. However, for samples that initially contained high amounts of Pt, we measure the opposite effect, where Pt is actually lost from the catchment sample under these conditions. This behaviour is more pronounced in the catchment samples containing the most Pt. An interesting observation is that with higher PtO_2 partial pressure the more Pt is caught by the discs.

The turning point (with net zero uptake of Pt) also seems to shift to higher Pt containing alloys when increasing the PtO_2 partial pressure in the gas phase.

The conclusions from this work are that:

1. There is a limiting Pt concentration for Pt catchment in Pd. Once a certain Pt concentration has been reached, equilibrium is established, and equal amounts of Pt are caught and lost from the sample (Figure 2).
2. Another limiting factor for Pt catchment is that the higher the partial pressure of PtO_2 in the gas phase, the more Pt will be captured on the Pd.

This work has answered a key question as to why ammonia oxidation plants observe a limitation in how much Pt they are able to capture.

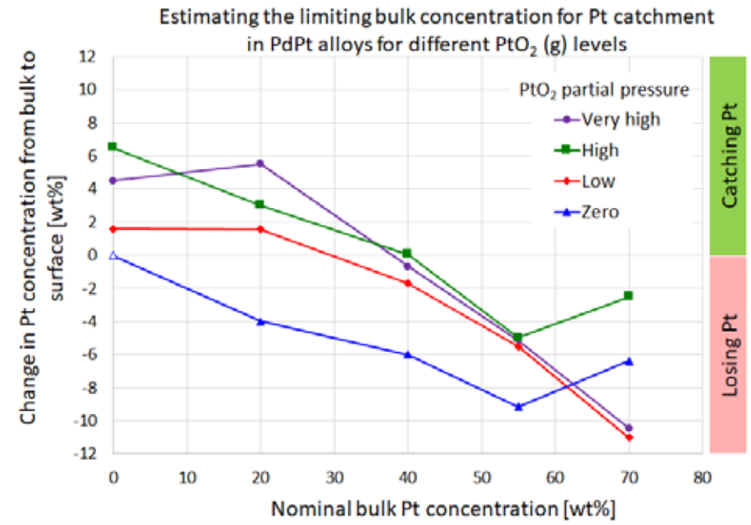


Figure 1. Net Pt uptake in Pd and PdPt binary alloys after 4 hours exposure to different PtO_2 partial pressures.

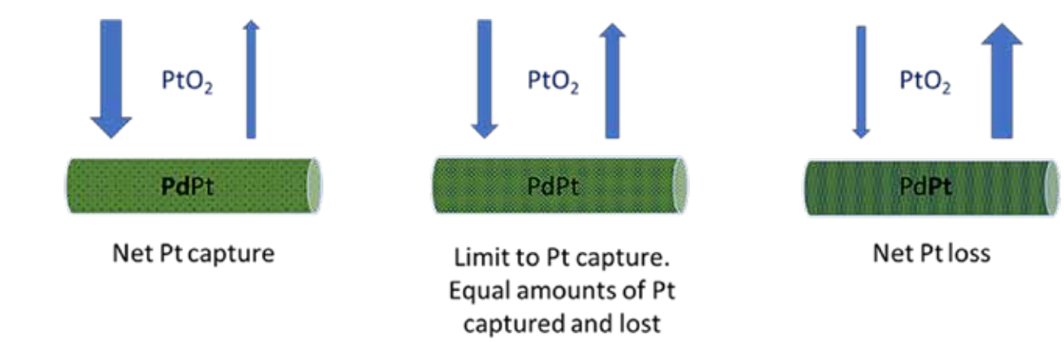


Figure 2. Illustration of PtO_2 catchment in Pd

NO_2 a Product and a Catalyst Inhibitor for Nitric Oxide Oxidation

Nitric acid (HNO_3) is an important chemical building block and 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 to reduce the CAPEX by replacing the bulky homogeneous oxidation process with a much more compact heterogeneously catalysed process. Literature reports on catalytic NO oxidation at high concentrations are scarce.

Catalytic oxidation of NO has, however, been studied extensively in diesel engine exhaust treatment. Here 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 catalysts in the literature so far range from noble metals via supported metal oxides, to ion exchanged zeolites and activated carbon fibres. The thermodynamics of the reaction itself require a low-temperature condition, 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 oxidises 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. But as we move away from the ammonia combustor exit towards the absorption tower, the gas composition changes to a greater percentage of NO_2 in the feed. Hence, any novel catalyst used at this stage in nitric acid plant for NO oxidation should be able to withstand NO_2 and also be inert towards the product.

Manganese is quite widely known to be an excellent low temperature oxidation catalyst. Two 20wt % Manganese on Zirconia support catalysts were prepared using incipient wetness impregnation. One of the catalysts was co-promoted with 1wt % Ag. The current work aims to investigate NO_2 inhibition on a manganese zirconia catalyst for oxidising NO at two operating conditions, (i) 10 % NO, 6 % O_2 and 15 % H_2O and (ii) 5 % NO, 5 % NO_2, 3.5 % O_2 and 15 % H_2O in a packed bed reactor at a space velocity of 24 000 $Ncm^3/h \cdot g_{catalyst}$. A temperature ramp was performed from 120–400 °C. Figure 1 presents the conversion results and a clear inhibition of catalyst performance by NO_2. Clearly the performance of an Ag-promoted catalyst is better at the exit of the ammonia combustor with 10 % NO in the feed, but with 10 % NOx (5 % NO and 5 % NO_2), the performance of both promoted and unpromoted is the same and much lower in conversion. Moreover, both catalysts tend to reach equilibrium faster in the 350–400 °C temperature range with 5 % NO, 5 % NO_2, 3.5 % O_2 and 15 % H_2O as feed in comparison to 10 % NO feed.

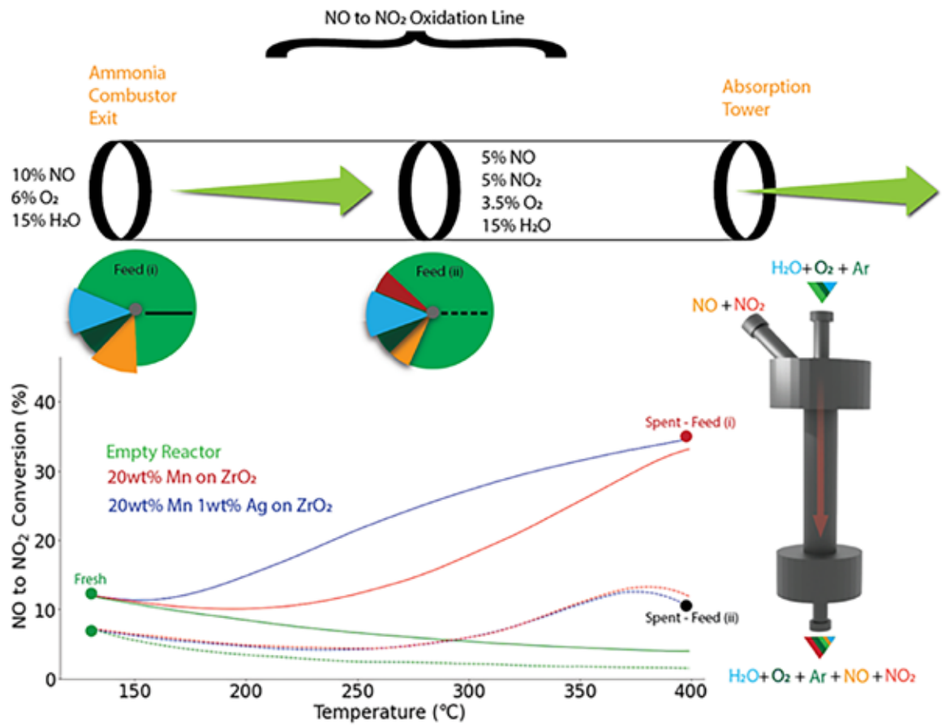


Figure 1. NO to NO_2 conversion with two different feed compositions, Feed (i) and Feed (ii) over two different catalyst systems

What happened to Ag's performance? An ex-situ XANES was collected for 20wt %Mn1wt %Ag on Zirconia Catalyst on Ag K edge at three points as presented in Figures 1 and 2. A linear combination fitting (LCF in Athena, XAS Data Processing Software) was performed on this data at Ag edge with different Ag standards (mainly, Ag^O: Ag_{foil} and Ag^1: $AgNO_2$, $AgNO_3$ and Ag_2O). Fresh 20wt %Mn1wt %Ag on Zirconia Catalyst holds Ag as Ag^O.In the spent catalyst after Feed (i), contributions of Ag^O and Ag^1 ($AgNO_2$) were found and in the spent catalyst after Feed (ii), contributions of Ag^O and Ag^1 ($AgNO_2$ and Ag_2O) were found. With respect to the spent catalyst after co-feeding NO_2, Ag tends to be in Ag^1 (Ag_2O) state, which was not found in the spent catalyst with Feed (i). The experimental results provide further insight to hypothesise how Ag behaves in NO oxidation to NO_2. It can be visualised as in Feed (i) Ag^O goes to Ag^1 ($AgNO_2$) state and back to Ag^O with the release of NO_2 as product. But with Feed (ii), which contains more oxygenated species, Ag^O goes to Ag^1 ($AgNO_2$ % Ag_2O) state. Ag in silver oxide (Ag_2O) form is more stable, and hence has lower catalytic performance. The results also portray an ideal location for this Ag-promoted catalyst bed by comparing the differences in total conversions by unpromoted manganese on zirconia catalyst. The favourable region for catalyst bed operation would be closer to the exit of the ammonia combustor with less or no amount of NO_2 for a manganese-based catalyst.

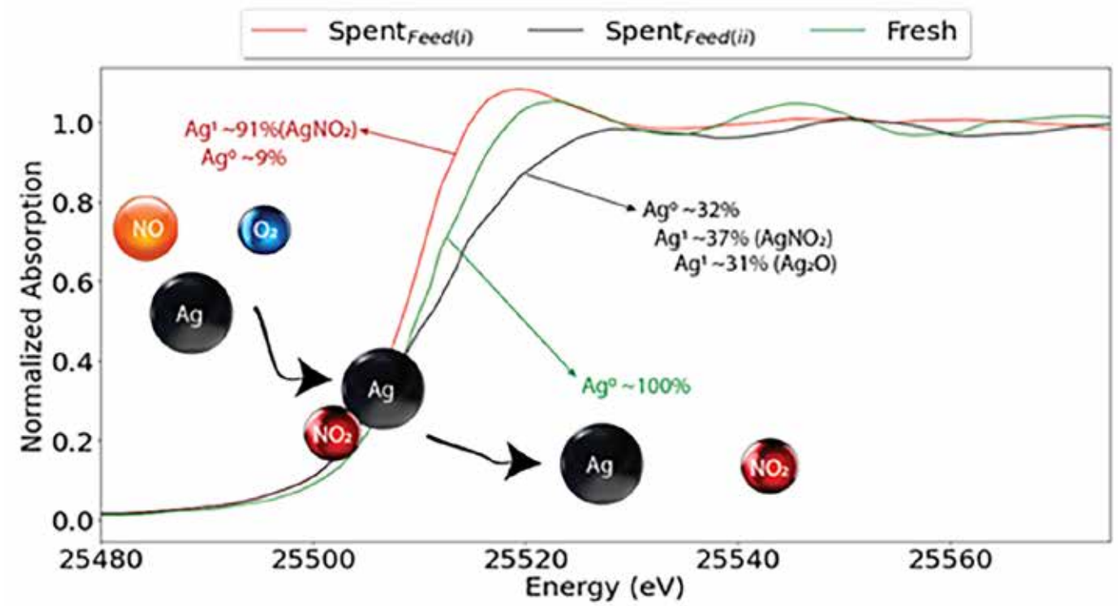


Figure 2. Ex-situ Ag K Edge XANES Measurements for Fresh and Spent (at both Feed (i) and (ii)) 20wt %Mn1wt %Ag on Zirconia Catalyst

Publication

Publications and conference contributions from IIA1 in 2021 are listed on page 65.

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

The IIA2 team 2021

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

Motivation

When ammonia is combusted in a nitric acid plant in the Oswald process to produce NOx, N_2O is an undesired by-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 greater than 95 % abatement with no changes to plant operation. The deN_2O catalysts have proven to be able to perform at a high level in the harsh conditions inside an ammonia burner for over a decade. In this project, aged catalysts are being studied to better understand the transitions in the material with the aim to formulate even more active and stable catalyst.

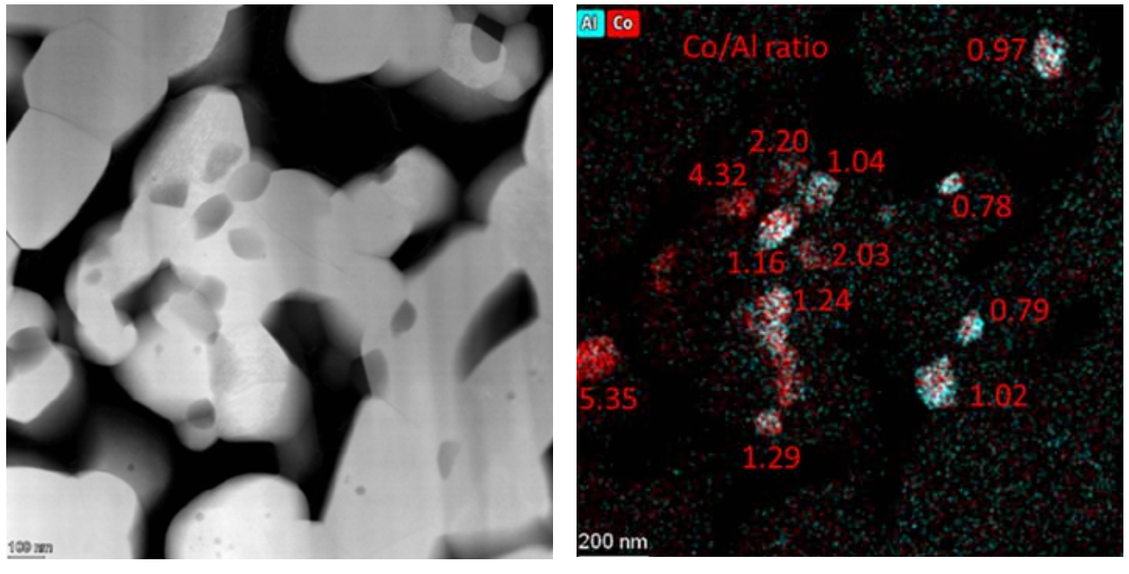


Figure 1. STEM/EDS of interior of catalyst that has been on stream for 6 months. Co:Al ratio of spinel particles.

Research project

Different deN_2O catalyst samples that have been in operation in a commercial nitric acid plant at various times on stream have been investigated by light microscopy, UV-Vis-NIR, XRD and SEM-EDS. 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.

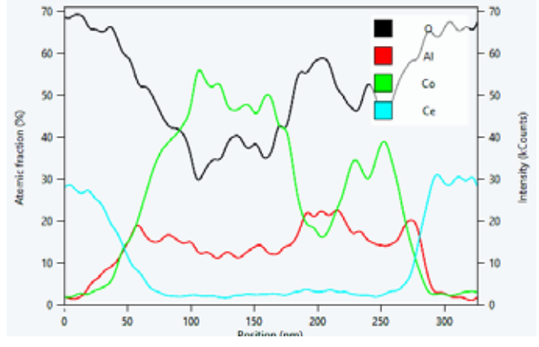
Polished cross-sections of the samples were investigated by light microscopy, dark field illumination. The results showed that the fresh catalyst has a homogeneous green colour through the cross section, while a homogeneous light blueish colour is observed in the sample that has been in the plant for four years. Interestingly, a clear colour change and presence of a core region are observed in the 6-month and 2-year samples.

EDS line scan of the cross section of the sample that has been on stream for six months shows a clear, sharp gradient in the Co level that corresponds to the colour change observed under light microscopy. Uniform concentration of Al was found in the cross section. This sample has a core region with the original Co:Al ratio of 2, while the surface region has lost Co and has a Co:Al ratio similar to the sample that has been on stream for four years.

TEM samples were extracted by FIB from the surface and core area of the catalyst that has been on stream for 6-month. STEM/EDS of the core region showed a large spread in the Co:Al ratio of the spinel particles, ranging from below 1 up to above 5 (Fig. 1). Figure 2 shows overlaid EDS maps of a spinel particle close to the surface, an area where SEM/EDS has shown a depletion of Co compared to the core of the catalyst. Interestingly, the image shows that Co and Al segregate within the particle. Al appears as a shell around the particle, in addition to an area in the centre. A line scan across the particle clearly illustrates the difference in Co and Al content in the particle. Moreover, the Co-rich areas show oxygen depletion, indicating that the Co is partly reduced. This segregation of Co and Al in the spinel is not observed in spinel particles in the core of the catalyst sample.

After studying the catalyst that has been on stream for six months with SEM/EDS, UV-Vis-NIR and XRD it was concluded that the original Co_2AlO_4 spinel phase in the fresh catalyst is transformed to $CoAl_2O_4$. The transition from Co_2AlO_4 to $CoAl_2O_4$ happens gradually and starts at the surface, then moving inward to the core of the catalyst. However, STEM/EDS results of the core region of the 6-month on stream sample show that the spinel particles consist of a range of different spinel phases, and indicate that the results from SEM/EDS, UV-Vis-NIR and XRD are an average of these.

Another interesting result from STEM-EDS is that spinel particles close to the surface show segregation of Co and Al, where Co is partly reduced. This is not observed in spinel particles in the core. It is therefore easy to propose that the segregation of the spinel is related to the spinel transition from high cobalt to low cobalt type, and this relationship will be interesting to explore further.



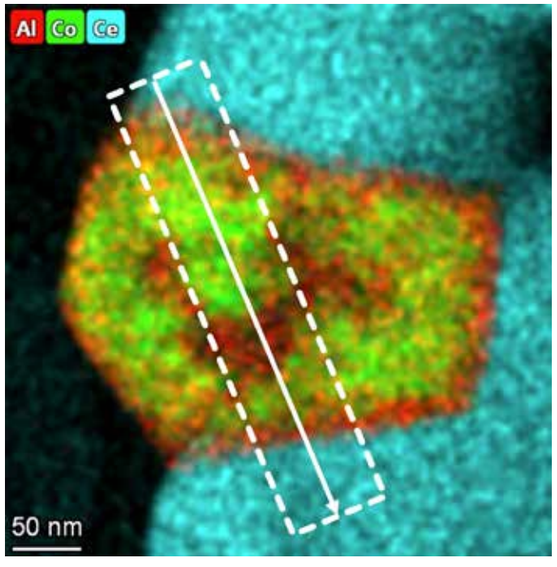


Figure 2. STEM/EDS of surface spinel particle sample that has been on stream for 6 months. The bottom figure shows the composition along the line indicated in the upper picture

IIA3: Frontier formalin technology development

The IIA3 team 2021

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Kari Anne Andreassen	SINTEF	Senior engineer (WP3.3)

An annular reactor design for the methanol to formaldehyde (MTF) reaction

One of the research topics in WP3.1 is extracting kinetic data of the MTF reaction. A new reactor and catalyst design has therefore been developed to aid us in these endeavours. The conventional particle bed design, while true to the industrial reactor, poses some limitation in obtaining such data. Based on previous work on alkane partial oxidation in microstructured reactors, and on work done by iCSI advisor Prof. Beretta, an annular reactor concept has been developed and implemented. Using this reactor design, gas phase reactions can be eliminated, and we are able to perform the MTF reaction at low methanol and oxygen conversion with high formaldehyde selectivity.

The reactor design features a cylindrical silver catalyst with an outer diameter a millimetre smaller than the inner diameter of the quartz reactor. Above and below the catalyst are quartz tubes with similar diameters, thus minimizing the total volume inside the reactor and changes in the flow pattern throughout the reactor. This reactor design allows us to run experiments with a laminar flow, high linear gas velocity, and no pressure drop. Catalyst temperatures are measured inside a quartz duct at the centre of the catalyst cylinder and isothermal conditions are obtained. Figure 1 shows a schematic representation of the catalyst fitted inside the reactor.

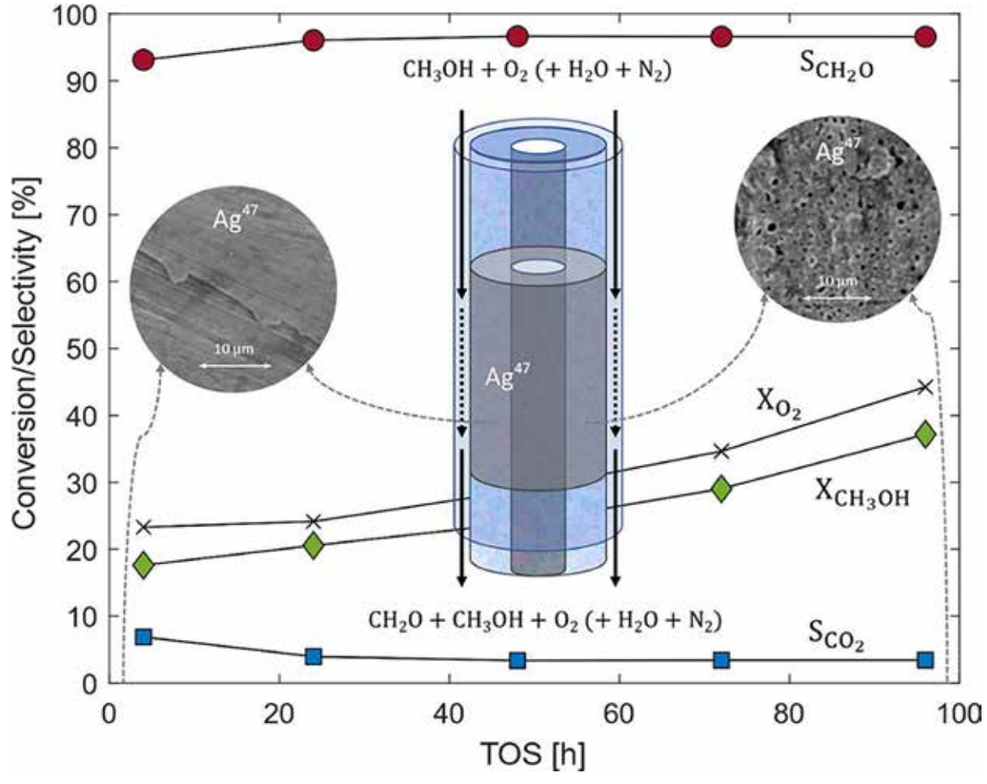
Using this reactor design, various experiments have been conducted in an attempt to extract meaningful kinetic data from the MTF reaction. The state of the restructuring of the catalyst surface must be considered for each experiment, starting with a smooth surface for the fresh silver. Various tests with fresh silver catalyst were run at a range of temperature set points (540–600 °C) for every 20 °C step. During these experiments the influence of residence time and oxygen partial pressure were evaluated over the course of four days on stream. At the end of each experiment the catalyst surface was characterized using SEM. In order to collect kinetic data, separate catalyst tubes were subjected to eight days at 600 °C and steady reaction conditions before a stepwise cooling regime was started. This enabled the collection of kinetic data at what is believed to be a reasonable morphological steady state of the catalyst surface.

The first results from the work were published in Lervold et al. (2021), and the main findings are:

- Using the annular reactor we can run the MTF reaction at partial oxygen conversion at high temperatures (>500 °C), and high formaldehyde selectivity (93–97 %).
- The oxygen partial pressure has a notable influence on the methanol. However, bed temperatures also increased as the oxygen partial pressure was increased. When doubling the oxygen partial pressure the catalyst was a consistent 20 °C warmer compared to the reference conditions, and it proved challenging to adjust the furnace setpoint in such a way as to keep the bed temperature constant. However, an increase in methanol conversion and molar oxygen consumption can be observed with an increasing oxygen partial pressure. While not final, the results indicate a first order dependency on oxygen partial pressure within the range of these experiments.
- Our annular silver catalyst undergoes massive morphological changes on the surface similar to those established for electrolytic silver particles (see “start” and “end” surface structure in Figure 1). But unlike the particles, for which it could be only a matter of hours, this process takes several days until a “dynamic steady-state morphology” is reached at temperatures of >600 °C. With regards to catalyst performance, the extent of the restructuring has a definite effect on the total conversion during the reaction, which increased throughout the extended time on stream.
- When extracting kinetic data, a clear non-linearity is observed between low (<540 °C) and high (>540 °C) bed temperatures for both methanol conversion and the corresponding Arrhenius plot. An activation energy estimate was made for the higher temperatures, which comes out to be 41 kJ/mol. The non-linearity in the plot indicates a difference in mechanism at lower temperatures compared to the higher temperatures.

Publication

Publications and conference contributions from IIA3 are listed on page 66



Graphical abstract of Lervold et al. (2021) showing the conversion plots (marked X) and selectivity plots (marked S), a schematic representation of the annular catalyst fitted in the reactor, and the development of the silver surface over the course of the MTF reaction.

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

The IIA4 team 2021

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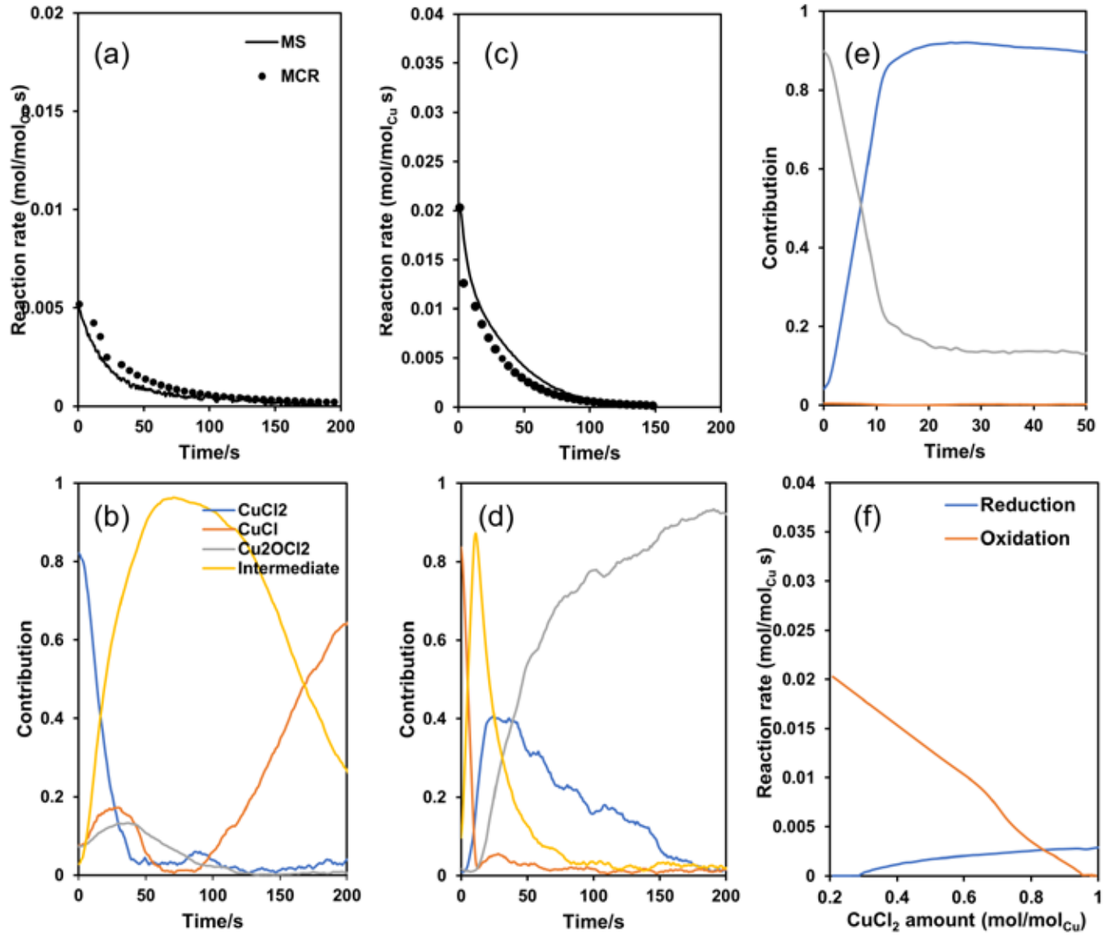
Motivation

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

The $CuCl_2/\gamma\text{-}Al_2O_3$ system is the commonly used catalyst in this process, and it is generally agreed that the oxy-chlorination reaction involves a redox process in which copper cycles between Cu(I) Cu(II) states. The ethylene oxychlorination redox cycle depends on the dynamics of elementary steps that cause the reduction and oxidation of the redox-active metal chlorides. The active sites of the surface $CuCl_2$ layer are highly dynamical, involving Cl and O removal and insertion. The dynamic structure of the active sites, namely the oxidation state of the Cu and Cl vacancy concentration of the catalysts, plays a very important role in determining the properties of molecular species that act as intermediate and transition states, thus the catalyst activity, selectivity and stability.

It remains a challenge to monitor dynamic active sites, these properties in situ, and to provide a principle to tune the Cl vacancy concentration at industrially relevant conditions. The main objectives of the project are to: 1) experimentally and theoretically elucidate the site requirement and mechanisms of surface catalysis of half-reactions such as $CuCl_2$ reduction by ethylene to EDC and CuCl, CuCl oxidation by oxygen to Cu_2OCl_2, and its hydrochlorination as well as the whole redox cycle at an atomic level; 2) provide a predictive kinetic model to accurately describe the dynamics of active sites and their activity; 3) rationally design catalysts to control the redox cycle to achieve high activity, selectivity and stability.

Four working packages were designed in the project of ethylene oxychlorination to 1,2 dichloroethane (EDC) to address the project goals: WP4.1, kinetic investigations and modelling; in-situ characterization; WP4.2, reactor modelling and simulation; WP4.3, deactivation and by-product formation; WP4.4, new development.



Cu species contribution and reaction rate changes with time: (a) C_2H_4 reaction rate as function of reaction time obtained from MS (line) and MCR (symbol), (b) Cu species distribution in the reduction step, (c) O_2 reaction rate as function of reaction time obtained from MS (line) and MCR (symbol), (d) Cu species distribution in the oxidation step, (e) Cu species distribution in the hydrochlorination step, Reaction condition: T = 230 °C, W_{cat}= 0.3 g, F_{tot} = 120 ml/min, P_{tot} = 1 bar, $P(C_2H_4)$= 0.1 bar, $P(O_2)$= 0.1 bar, P(HCl)= 0.1 bar. (f) reaction rates of the reduction and oxidation steps on the $KCuCl_2/Al_2O_3$

Research in 2021

The main achievements of 2021 are as follows:

1. The new method of transient kinetic study was established by combining UV/Vis-NIR and mass spectroscopy. The full spectra of Cu species such as $CuCl_2$, $CuCl_2$ with vacancies, CuCl, and Cu_2OCl_2 were detected and identified for the first time, and their transient changes and contribution in the reduction, oxidation, and hydrochlorination steps as well as in the steady-state operation in the catalytic cycle can be accurately "imaged" by resolving the UV−vis-NIR spectra dataset using the multivariate curve resolution (MCR) analysis.
2. A DFT-assisted microkinetic model was established to predict the steady-state reaction and $CuCl_2$ concentration.

Transient kinetic study of Ethylene Oxychlorination to 1,2 dichloroethane (EDC)

We have demonstrated an effective multivariate curve resolution kinetic approach for analyzing the large UV−vis-NIR spectroscopy dataset to monitor the copper active site dynamics at the real reaction conditions as function of time on stream, see figure. MCR analysis of the time-resolved UV−vis-NIR spectra make it possible to image and quantify all the Cu species involved in the reaction, including the intermediates in the step transient experiments, of the reduction and oxidation, especially for the hydrochlorination steps. In particular, MCR analysis can monitor the evolution of the active site changes at steady-state, which is more complicated due to the highly dynamic nature of the catalyst and multi-active sites playing roles for the different steps. It provides better and deeper insights into the active sites for multifunctionality in ethylene oxychlorination. The Cu species of $CuCl_2$, $CuCl_2$-□ ($CuCl_2$- vacancy), CuCl and Cu_2OCl_2 are active sites involved in the reaction. The active sites on the catalyst are highly dynamic, and their contributions depend on the kinetic balance of reduction, oxidation and hydrochlorination reaction rates. KCl prompted the oxidation reaction significantly and manipulated the active sites at steady-state, making the catalyst more stable. It has been proved that this method is a relatively simple and easy-accessible operando technique compared to synchrotron-based techniques. We gained a better understanding of this important industrial process. This approach corresponds to screening and monitoring of the working catalysts, and it is expected to be applied to other catalytic systems that can be characterized by time-resolved spectroscopy techniques like UV−vis-NIR. We believe the method of MCR to resolve UV−vis-NIR spectra can shed new light on determining the identity and contributions of the surface species or reaction intermediates that belong to part of the reaction and monitor the transition changes of the active sites.

Tailoring active sites of $CuCl_2/Al_2O_3$ at industrially relevant conditions

The structures of $CuCl_2$ clusters on alumina (110) with alkaline and alkaline earth metals as promoters were established, and the electronic properties, charge distributions and energetic profiles of elemental steps of the ethylene oxychlorination were studied by density functional theory (DFT). The effects of the promoter on the activity and stability of the catalysts were studied by DFT-assisted microkinetic modelling. The dependence of the reaction rate and the $CuCl_2$ concentration on the coordinated structure of Cu with Cl, such as the charge of Cl and Cu and Cl-Cl length, and descriptors to describe the reaction rate and $CuCl_2$ concertation at the steady state conditions were identified.

Publication

Publications and conference contributions from IIA4 are listed on page 66.

IIA5: The next step in Direct Activation of Lower Alkanes

The IIA5 team 2021

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Bjørnar Arstad	SINTEF	Senior researcher (WP5.3)

In the iCSI IIA5, we have focused extensive efforts on the study of CH_4-temperature programmed reduction (TPR) (Figure 1a). Our earlier studies have shown CH_4-TPR to be a successful screening tool for finding the optimal CH_4 activation temperature for the direct methane to methanol (DMTM) conversion of varying Cu-loaded zeolite frameworks. This is accomplished by determining the temperature at which CO_2 is produced, or alternatively, the onset of CH_4 consumption across different zeolite frameworks. Initial studies further suggest that the amount of produced CO_2 could be used to determine the most active Cu-zeolite composition when comparing a set of isostructural zeolites. We hypothesized the descriptive potential of the CH_4-TPR technique to be related to the nature of Cu-oxo species in the framework, as well as the Cu reducibility. Consequently, we

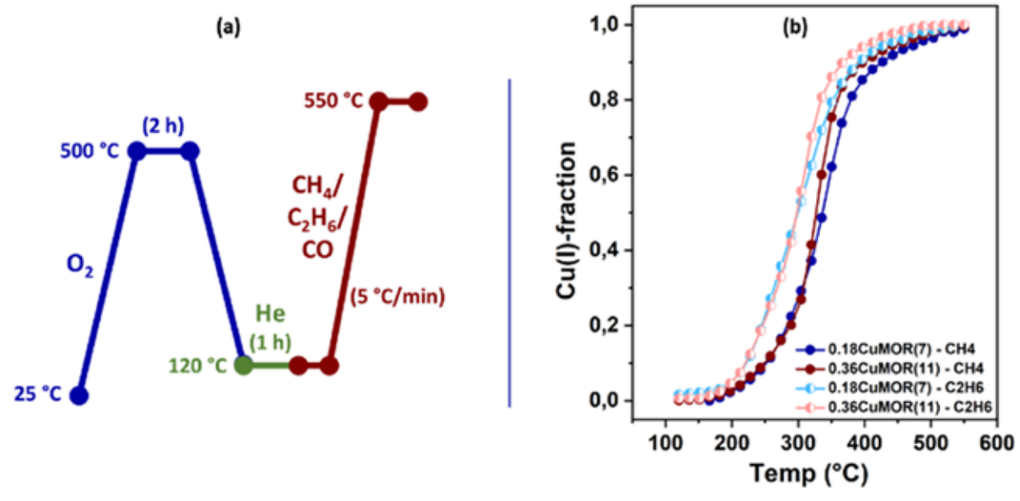

Figure 1. (a) A schematic of the TPR protocol used at BM31. (b) shows the different evolvement of the Cu(I)-fraction throughout CH_4- and C_2H_6-TPR for two different MOR zeolites. The fraction of Cu(I) has been found using LCF analysis.

spent significant efforts on applying for XAS beam time, in order to confirm our hypotheses. With our first trial at MAX IV, we were only partially successful, hampered by complications from the onset of COVID-19. Things were looking better when we received a new beam time at ESRF for spring 2021, however, due to our need to be onsite, the beam time was postponed to the beginning of November. Finally, with a great team from both Oslo and our collaborators in Turin, we were able to get an excellent dataset with a flowthrough capillary setup at BM31 (Figure 2). We performed the experiments on a set of well-characterized Cu-MOR of optimal composition exhibiting high CH_3OH-productivity. Additionally, we performed C_2H_6- and CO-TPR to use as supplementary and comparative measurements, with the aim that these additional datasets will aid us in the search for understanding specific changes to the Cu speciation and oxidation state throughout the protocols. Now we are working on extended analysis of the dataset, using linear combination fitting (LCF) and multivariate curve resolution alternating least square (MCR-ALS) analysis on the X-ray absorption near edge structure (XANES) spectra to separate out the pure Cu components appearing throughout the protocol. The preliminary results from LCF are shown in Figure 1b. In addition, we will do advanced analysis of the extended X-ray absorption fine structure (EXAFS) region, performing wavelet transform (WT) analysis. This is done by creating 2D spectra from interpreting and fitting the R-space and Fourier Transform EXAFS spectra. With this technique we may be able to separate out and decipher the local structure and nuclearity of the Cu species present at different conditions. In total, this study should give us a deeper insight into why and how CH_4-TPR can be used as a descriptor for the DMTM reaction, making it easier to find optimal materials and reaction conditions in the future to optimize the protocol.

Publication

Publications and conference contributions from IIA5 are listed on page 67.

Pictures from the beam time at ESRF in November 2021. The picture on the left shows parts of the team enjoying a nice dinner the first evening. On the right is a picture of the capillary setup used for flow-through experiments. The quarts capillary has a 1.5 mm inner diameter and a wall thickness of 0.01 mm. The cone below the capillary is a heat blower.

IIA 6: Generic projects for additional industrial synergies

The IIA6 team 2021

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Helmer Fjellvåg	UiO	Researcher (WP6.2)
Oleksii Ivashenko	UiO	Funded Researcher (WP 6.2)
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Alexandra Jahr Kolstad	UiO	Master student (WP6.2)
Mathilde Ingeborg V. Nilsen	UiO	Master student (WP6.2)
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Kumar R. Rout	SINTEF	Researcher (WP6.1)
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Shreenath Krishnamurthy	SINTEF	Researcher (WP6.4)
Francesca Lønstad Bleken	SINTEF	Researcher (WP6.4)
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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)
Per-Erik Vullum	SINTEF	Researcher and postdoc supervisor (WP6.7)

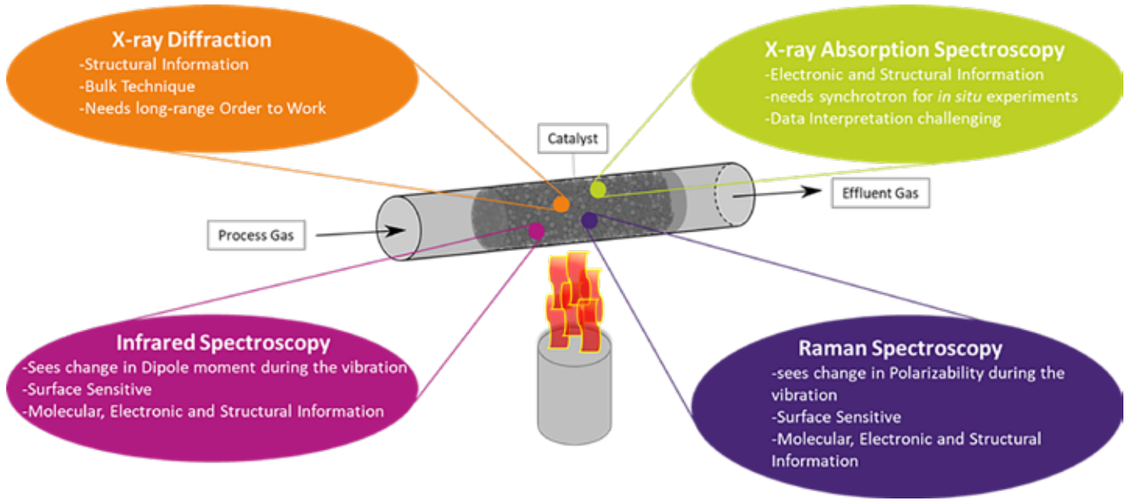
Motivation

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.

Advanced operando characterisation of heterogeneous catalysts for sustainable process industries

We use a multiprobe approach to link structural properties of a catalyst with its activity and selectivity. For this, we apply in situ and operando spectroscopy in-house (Infrared, X-ray, UV-vis) and at synchrotrons (XAFS, PXRD) for combined data acquisition. New insight on the active sites of the catalysts and the respective kinetics of the occurring chemical reactions can guide us towards favourable compositions and conditions, thereby enabling sustainable processes with higher efficiency, lower cost, reduced emissions or by-products and improved lifetime.

The massive datasets associated with such combined studies of catalysts at work call for efficient procedures of data reduction. With the application of multivariate statistical analysis tools, rapid data reduction and analysis enables combined and more complex experiments. We have direct synergies with four out of the five other industrial innovation areas within iCSI and collaborations within the Catalysis Group at NTNU. Several publications were co-authored and made it into or are well underway to publication: Pt-Ni bimetallic nanoclusters in dry reforming,[1] oxychlorination of studied by UV–vis–NIR,[2] carbon supported Fe-based Fischer-Tropsch synthesis to olefins from renewable feedstocks[3] and selective catalytic reduction of NO by ammonia over Cu-based catalysts[4], and with the SUNCAT Group at Stanford University on understanding selectivity in CO_2 hydrogenation to methanol for MoP nanoparticle catalysts using *in situ* techniques.[5]



Comparison between different in situ catalyst charactersation techniques

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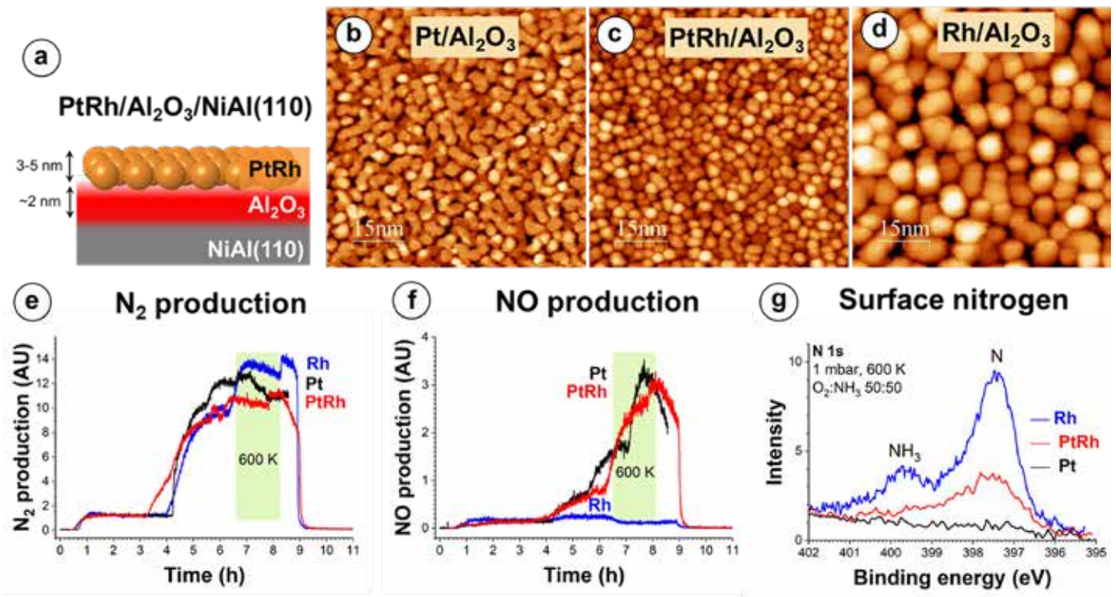
Bridging materials gap in operando NAP XPS study of ammonia oxidation

In this work we focus on explaining the performance of PtRh alloys for ammonia oxidation. PtRh alloys are excellent catalysts for NH_3 oxidation, with relevance to both the production of mineral fertilizers and environmental applications. For these applications, temperature and reactant composition define the two primary regimes: i) high temperature conditions relevant to the Ostwald process with O_2:NH_3 ratio around 65:35, and ii) intermediate temperature (500–700 K) ammonia "slip" abatement by oxidation in high oxygen excess of 99:1. For establishing the catalyst's structure-performance relationship, closing pressure, temperature and materials gaps is necessary. Towards bridging the pressure gap, our previous operando near-ambient pressure (NAP) X-ray photoelectron spectroscopy (XPS) study of PtRh surface alloys on Pt(111) showed how abundancy of surface oxygen (-O) and nitrogen species (-N) dictates product distribution to N_2, NO and N_2O. Here we describe preliminary results from the latest operando NAP XPS measurements (TEMPO 2021, Soleil) of PtRh alloys supported on model Al_2O_3, where we are also aiming to bridge the materials gap.

The model catalyst for bridging the materials gap was prepared by deposition of Pt, Rh and Pt+Rh onto a thin (~2 nm) alumina film, which was grown on NiAl(110) crystal (panel a). Scanning Tunneling Microscopy (STM) images show that formed nanoparticles are ca. 3–5 nm thick (panels b-d) and are stable during annealing at 600 K for 30 min, in which a minor increase in nanoparticle size was found (not shown).

Quadruple Mass spectrometry, when measured simultaneously with NAP XPS, shows that production of N_2 at 600 K is comparable for all compositions (Pt, Rh, PtRh alloy) in 1 mbar with a 50:50 O_2:NH_3 blend (panel e). The proportion of N_2 was above 75 %. The major difference appeared in NO production (panel f), where pure Rh/Al_2O_3 showed a negligible amount of NO and N_2O produced (<2 %). Pt and PtRh alloy behave similarly, producing ~15 % of the oxides.

Preliminary analysis shows that surface nitrogen abundancy is the likely reason for this behaviour (panel g). On pure Pt almost no -N was found on the surface. Pt is the most active from PGM, reaction is fast, and no unreacted NH_3 is present either. Enrichment with Rh results in more atomic -N species at the surface (for PtRh). Pure Rh binds -N the strongest, allowing critical -N coverage to be present at the surface, for N-N to recombine and desorb. These results are consistent with our previous conclusions for PtRh/Pt(111), namely that a critical amount of atomic -N coverage is needed for N_2 to be the preferred product, which can be achieved by using a surface that binds -N more strongly, such as Rh.



Microkinetic modelling with DFT (DFTKIN)

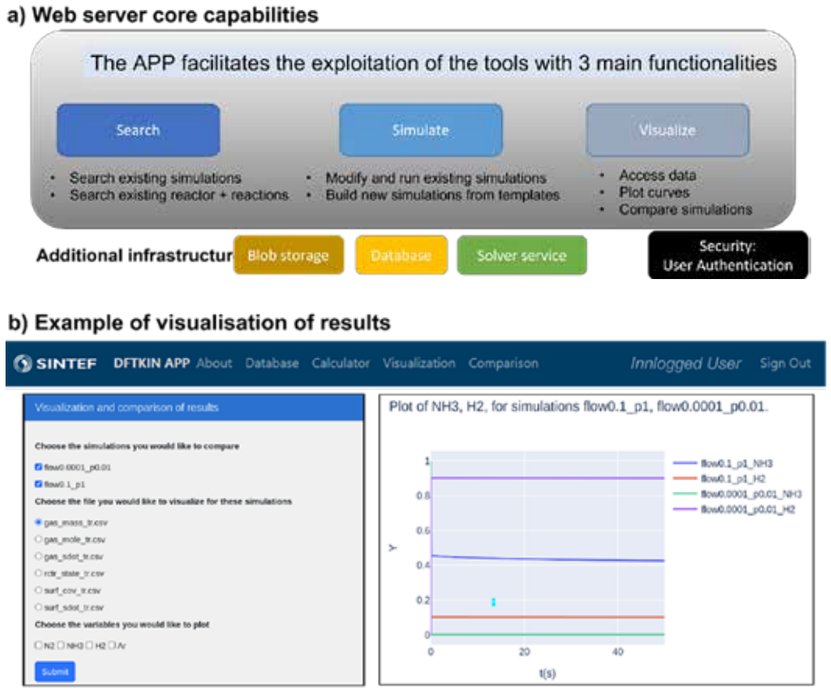
The DFTKIN framework consists of a collection of tools for building, solving and analysing the results of microkinetic models with input from DFT/QM or experimental results. The purpose of the DFTKIN framework is to make microkinetic modelling more readily available in SINTEF as a general, complementary tool for atom scale modellers, with a focus on providing support for surface reactions with and without a changing surface. While the intended applications are primarily surface reactions, gas phase reactions must also be supported for complete descriptions of gas-surface reactions. The focus has been on assembling various available open-source tools and building on these to create a practical workflow. pmutt and openMKM provided by the Vlachos group at MIT were eventually chosen as the basis for the workflows. Time and effort have been invested in making the tools run seamlessly on normal workstations for development, and for setting up interactive systems for presenting results.

Two different use cases were chosen for demonstration: CO_2 adsorption on various systems with amines, and oxidation of a Si surface. Each use case was broken into a ladder with various degree of complication. While this toolbox is primarily intended for use with in-house generated data for reactions, this was not feasible within the project. Thus, literature data has been collected for the use cases.

Si oxidation was investigated in several stages:(1) oxidation at high temperature of the first Si layer by etching, (2) oxidation of several Si-layers at high temperature by etching, (3) oxidation of the first Si layer by oxide growth at lower temperatures (4) oxidation of several Si-layers at lower temperatures by oxide growth and finally (5) competitive oxidation by etching or oxide growth of several layers at intermediate temperatures. Each of the above-mentioned steps represents an increased complication of the model. This use case takes into account a surface that permanently changes during reaction, which is more advanced than pure catalytic surface reactions.

The implementation of the CO_2 case proved to be more cumbersome than expected. Gas phase reactions, while simpler in principle, were not correctly implemented in the chosen software packages. Corrections for this were implemented as part of the project.

In addition to the model development and integration, a web interface has been developed to initially facilitate storage and analysis of data, and then execution of new simulations in 2022. The figure below illustrates how to plot curves from results stored in an online database. The tab indicates the other functionalities available: Search in the database, Prepare and Launch a new simulation, Visualize and Compare results, Upload results and template (description of a reactor system where parameters can be changed).



The DFTKIN web interface allows for storage of data, searching for previously run simulations, performing additional simulations on already defined models by varying reactor parameters and settings, and visualisation of data. The main capabilities are shown in (a), and an example of a visualized result in which several simulations are compared is shown in (b).

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

For many industrial reactions, the formation of coke (or other deposits) is a relevant side reaction which leads to deactivation of the catalyst. With the ISMA, deposition kinetics and deactivation kinetics can be investigated simultaneously. In addition, sorption processes can be investigated.

The ISMA (shown in Figure 1) is a fixed-bed reactor with the added capability to simultaneously measure weight changes of the catalyst bed during reaction. The reactor tube oscillates, and the frequency is directly correlated to mass changes. Thus, the mass changes of the catalyst can be recorded in real time during the reaction with the formula:

$$\Delta m = K_0 [1/f_1^2 - 1/f_0^2].$$

Figure 1. ISMA unit

A direct measurement of the mass of the catalyst is possible, without the need to rely on conventional gravimetric microbalances. However, as the mass inside the reactor is measured, changes in gas density – e.g., caused by pressure or temperature changes – impact the weight signal. The time resolution of the mass signal is about 0.1 s, with a sensitivity of about 1 µg. The reactor itself has a volume of 200 to 900 µl, and the feed section is equipped with a liquid flow controller and 8 mass flow controllers for different gases. The reactor tube (made of quartz) is inside a housing as shown in Figure 2, which can be pressurized up to 62 bar and heated up to 700 °C, hence covering a wide selection of industrial reaction conditions.

After installation of the ISMA, it will first be used to investigate CO_2 sorption, before being used for more challenging processes involving chemical reactions like Fischer-Tropsch synthesis and coupled CO_2 hydrogenation and methanol to olefins. Additionally, depending on the predictability of the influence of changing temperature on the weight signal, thermogravimetric analyses like temperature-programmed reduction and oxidation might be of interest.

The ISMA was developed (improved version of the earlier so-called TEOM, tapered element oscillatory microbalance) and will be provided by SINTEF.

Publication

Publications and conference contributions from IIA6 are listed on page 67

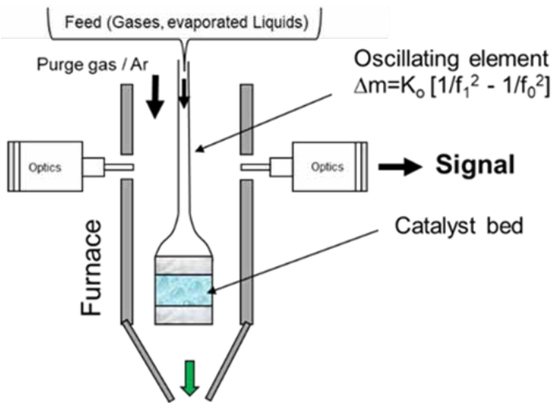


Figure 2. Configuration of the ISMA reactor

Three new PhDs

Candidate:	**Endre Fenes**
Date of defense:	March 17, 2021
Title of thesis:	Ethylene Oxychlorination on $CuCl_2$ based Catalysts: Mechanism and Kinetics
Public trial lecture:	Fixed vs fluidized bed reactors for highly exothermal reactions: Pros and cons
The Committee	
First opponent:	Professor Dmitry Yu. Murzin, Åbo Akademi, Finland
Second opponent:	Professor Alessandra Beretta, Politecnico di Milano, Italy
Administrator:	Professor Kristin Syverud, NTNU
Supervisor:	Professor De Chen, NTNU
Co-supervisors:	Terje Fuglerud, Inovyn and Kumar Ranjan Rout, SINTEF
iCSI Industrial Innovation Area:	PVC Value Chain: World class energy and raw material efficiency for the production of Chlorine and Vinyl Chloride Monomer (VCM).
Industry partner:	Inovyn
Current Position:	Senior Process Engineer at Inovyn, Rafnes

To the left: De Chen, Endre Fenes, Kristin Syverud and Kumar Ranjan Rout To the right: The opponents Dmitry Yu. Murzin and Alessandra Beretta

Candidate:	**Hongfei Ma**
Date of defense:	March 23, 2021
Title of thesis:	Kinetic Studies of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride
Public trial lecture:	Catalysis in E-Hydrogen and Ammonia
The Committee:	
First opponent:	Professor Tapio Salmi, Åbo Akademi University, Finland
Second opponent:	Professor Xiang Feng, China University of Petroleum (Huadong), China
Administrator:	Dr. Li He, NTNU
Supervisor:	Professor De Chen, NTNU
Co-supervisors:	Terje Fuglerud, Inovyn and Kumar Ranjan Rout, SINTEF
iCSI Industrial Innovation Area:	PVC Value Chain: World class energy and raw material efficiency for the production of Chlorine and Vinyl Chloride Monomer (VCM).
Industry partner:	Inovyn
Current Position:	Postdoc at NTNU, Trondheim

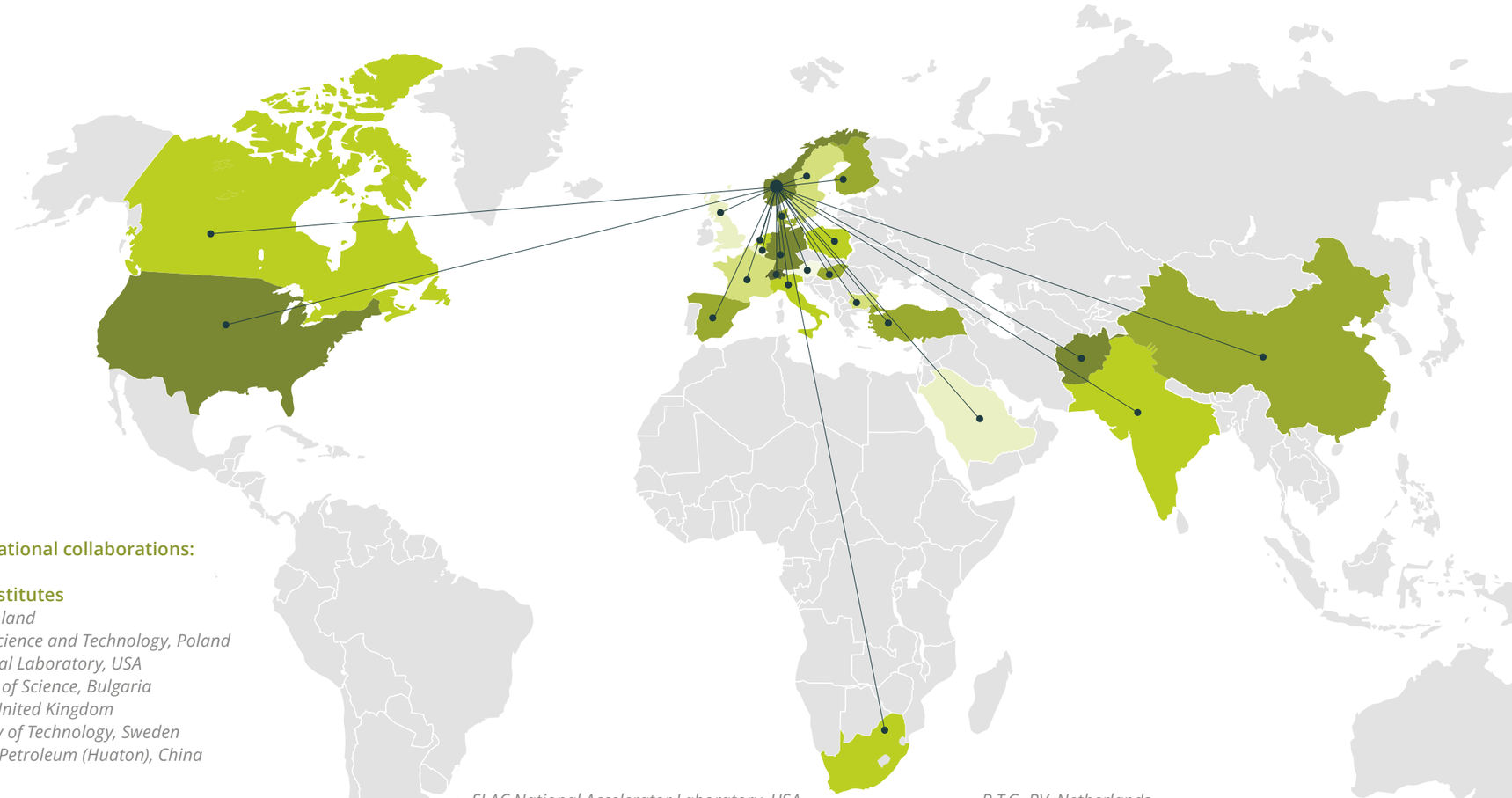
To the left: De Chen, Li He, Hongfei Ma and Kumar Ranjan Rout. To the right: His opponents Tapio Salmi and Xiang Feng on the screen.

Candidate:	**Stine Lervold**
Date of defense:	June 23, 2021
Title of thesis:	Investigations of the methanol to formaldehyde (MTF) reaction over silver
Public trial lecture:	Recent developments in catalyst properties and stability for the methanation of CO_2
The Committee:	
First opponent:	Professor Leon Lefferts, University of Twente, The Netherland
Second opponent:	Professor Hanna Härelind, Chalmers University of Technology, Sweden
Administrator:	Professor (Head of Department) Jens-Petter Andreassen, NTNU
Supervisor:	Professor Hilde Johnsen Venvik, NTNU
Co-supervisors:	Ass. professor Jia Yang, NTNU, and Senior Researcher Rune Lødeng, SINTEF
iCSI Industrial Innovation Area:	Frontier formalin technology development
Industry partners:	K.A. Rasmussen and Dynea
Current Position:	Senior Engineer at Equinor, Trondheim

To the left: Rune Lødeng, Hilde Johsen Venvik, Stine Lervold and Jia Yang.To the right: Stine Lervold with the opponents Leon Lefferts and Hanna Härelind on the screen

Photo: Hilde Skar Olsen, Lund University

Internationalization 2021



iCSI and the affiliated research institutions are attractive for international students and researchers. The 65 master's students, PhD candidates, postdocs and guest researchers within or affiliated with iCSI represent 18 countries. Non-Norwegians make up 50% of this group of employees and students.

In addition, three exchange PhD candidates (from Bulgaria, China and France) visited iCSI in 2021 with stays lasting for 2 and 3 months. Three master's exchange students (from Germany, France and Spain) also did their thesis at NTNU.

Seventy per cent of the 23 scientific publications from 2021 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.

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. See more about the CATHEX project on page 26.

iCSI hosted September 2 a webinar where the European Federation of Catalysis Societies (EFCATS) 2021 Catalysis Award event took place. Nearly 300 hundred participants took part in the announcement of the five awards, followed by the prize winners' lectures. The recorded lectures can be seen from EFCATS' webpage. iCSI is proud to tell that both our scientific advisor Graham Hutchings and our former PhD candidate Dimitrios Pappas were among the prize winners! Graham received the Michel Boudart Award in Fundamental Catalysis, while Dimitrios got the EFCATS Best PhD Thesis Award.

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

4Refinery - Scenarios for integration of bio-liquids in existing REFINERY processes. H2020-LCE-2016-RES-CCS-RIA, iCSI-partner involved: SINTEF. Duration: 2017–2021

CARMOF – New process for efficient CO_2 capture by innovative adsorbents based on modified carbon nano-tubes 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 CO_2 utilization through tri-reforming of methane. H2020-MSCA-IF: iCSI-partner involved: NTNU. Duration: 2020–2023

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

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

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

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

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

MBCL - Moving Bed Carbonate Looping, CLIMIT-supported (Gassnova), Owned by FTG (Fjell Technology Group), iCSI-partners involved: NTNU, SINTEF, International partner: Southeast University, Institute of process technology, Chinese academy, China, Duration 2017–2021

Chemical Looping Desulfurization of Producer Gas from Biomass Gasification by Mn-based Solid Sorbent. RCN - researcher project. iCSI-partners involved: NTNU, SINTEF, Duration: 2017–2021.

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

Bio Fischer-Tropsch- Staging and Multiple Hydrogen Feed of Biomass to Fischer-Tropsch Fuel Synthesis, RCN - researcher project. iCSI-partners involved: NTNU, SINTEF, Duration: 2018–2021

H2MemX - 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

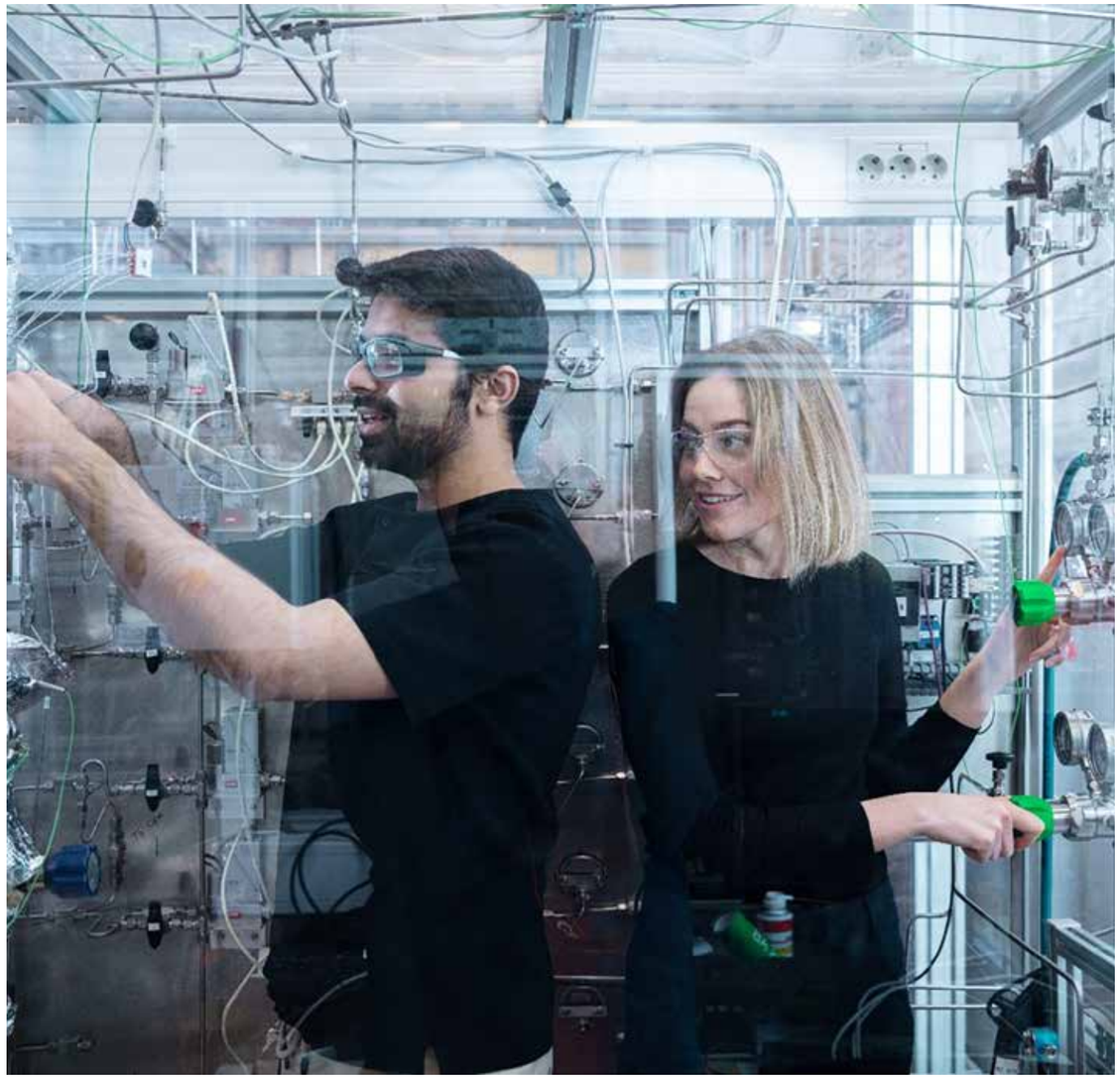
PhotoRed – Photoelectrochemical carbon dioxide reduction. EØS-Poland. iCSI-partner involved: SINTEF Industry. Other Norwegian partners: SINTEF Ocean, University of South Eastern Norway. International partners: West Pomeranian University of Technology. Duration: 2021–2023

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

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

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



Accounts 2021

All cost and budget numbers appear in 1000 Norwegian Kroner (NOK) as of January 2022 NOK100 are equivalent to €10.0.

Table 1: Summarizes the costs in 2021 and the total budget for the period of the Centre after revision in January 2021.
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 2021	2015–2023 Total budget
Payroll and indirect expenses	8 294	58 365
Procurement of R&D services	14 261	93 207
Equipment	2 207	10 565
Other operating expenses	3 722	34 675
Totals	**28 484**	**196 813**

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	2021 Accounts		2015–2023 Total budget	
Partner	Costs	Financing	Costs	Financing
NTNU	11 608	3 814	77 315	29 629
University of Oslo	7 213	1 842	49 622	12 953
SINTEF	7 047	2 163	43 585	7 942
Industrial partners	2 616	5 613	26 290	50 290
Research Council of Norway		15 050		96 000
Totals	**28 484**	**28 484**	**196 813**	**196 813**

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 2021	Costs 2015–2021	2015–2023 Total budget
IIA1 21st century Nitric Acid technology development	5 145	29 155	38 996
IIA2 New NOx abatement technologies	1 511	6 706	8 108
IIA3 Frontier formalin technology development	3 277	189 972	23 996
IIA4 PVC Value Chain	5 047	25 019	32 239
IIA5 The next step in direct activation of methane	5 338	25 737	34 820
IIA6 Generic projects	4 158	30 759	34 317
IIA7 2020 Catalysis	2 022	2 022	8 409
iCSI Management and administration	1 986	11 994	16 022
Totals	**28 484**	**150 269**	**196 813**

Education

David Waller from Yara has been appointed adjunct professor (20%) in Industrial Catalysis at the Department of Chemical Engineering, NTNU. He has many years of experience as an industrial senior researcher, and will contribute with teaching and student supervision at NTNU. Some of his students are a part of iCSI.

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 new postdoctoral fellow was welcomed in IIA6 (Generic projects for additional industrial synergies) in 2021. Tina Bergh joined iCSI in April, after finishing her PhD with the title *Interfacial intermetallic phases in aluminium-steel joints* as part of SFI Manufacturing. Tina has been awarded a 4-year postdoc position, of which two years are with iCSI and the other two years are with the Department of Chemical Engineering and the Department of Mechanical and Industrial Engineering. Her tasks in iCSI are allocated to Transmission Electron Microscopy investigations and methodology development. Her supervisors will be professor Hilde Johnsen Venvik from iCSI, and Professor Randi Holmestad (Department of Physics, NTNU), as well as Adjunct Professor Per-Erik Vullum (SINTEF), from the TEM-group.

PhD candidates with financial support from iCSI

Endre Fenes [1]	NTNU	Norway	2015–2019	M	IIA4
Samuel Regli [2]	NTNU	Switzerland	2016–2019	M	IIA6
Stine Lervold [3]	NTNU	Norway	2016–2020	F	IIA3
Asbjørn Slagtern Fjellvåg	UiO	Norway	2016–2021	M	IIA1
Hongfei Ma [4]	NTNU	China	2017–2021	M	IIA4
Moses Mawanga	NTNU	Uganda	2018–2021	M	IIA6
Karoline Kvande	UiO	Norway	2019–2022	F	IIA5
Julie Hessevik	UiO	Norway	2019–2023	F	IIA1
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) Endre Fenes left iCSI in 2019 for a job in the industry, and his defense took place 17 March 2021.
2) Samuel Regli has held a temporary position as lab engineer at IKP, NTNU since August 2020, and his defense is expected to take place in 2022.
3) Stine Lervold left iCSI in November 2020 for a job in industry, and her defense took place 9 June 2021.
4) Hongfei Ma's defense took place 23 march 2021. He is now a postdoc at Department of Chemical Engireering, NTNU.

Bjørn Gading Solemsli started under the supervision of Stian Svelle as a PhD candidate at the Department of Chemistry at University of Oslo February 15, after finalizing his Master's Thesis for professor Unni Olsbye. In iCSI he will be continuing the work in IIA5 on zeotype catalysts for the methane-to-methanol (MTM) reaction. The working title of his project is "A deeper fundamental understanding of direct CH activation".

Björn Frederik Baumgarten, started, as the last PhD candiate within iCSI, April 1. Björn did his bachelor at the Karlsruher Institute of Technology (KIT), before he did his master's in 2015–2017 at NTNU, with the specialization in Environmental Catalysis and Biofuels. Björn went back to Germany and worked in the biomass combustion group at The Rottenburg University of Applied Forest Sciences from 2018 to 2021. In his PhD project in IIA6, he will use an in-situ mass analyzer (ISMA) in CO_2 Hydrogenation. Associate Professor Jia Yang and Senior Research Scientist Rune Lødeng (SINTEF) will act as Björn's PhD supervisors.

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

Ole H. Bjørkedal	NTNU	Norway	2016–2020	M	Selective catalytic reduction (SCR) of NO_X emissions in maritime transport.
Muhammad Zubair[1]	NTNU	Pakistan	2017–2020	M	Enhanced visible light adsorption TiO_2 based catalysts for photocatalytic H_2 production
Martina Cazzolaro	NTNU	Italy	2017–2020	F	Cu/CNF for selective hydrogenation of hydroxyacetone to 1,2-propanediol
Joakim Tafjord	NTNU	Norway	2017–2021	M	Iron-based Fischer Tropsch synthesis based on renewable feedstocks
Jianyu Ma[2]	NTNU	China	2017–2020	M	Chemical looping desulphurization
Daniel Skodvin	NTNU	Norway	2017–2021	M	Carbon Nanomaterial-Ionic Liquid Hybrid for Ultrahigh Energy Supercapacitor
Jibin Antony	NTNU	India	2018–2021	M	Nanostructured hybrid catalysts for photocatalytic applications
Mario Ernesto Casalegno	NTNU	Spain	2018–2022	M	Catalyst for onboard hydrogen generation from bioethanol
Ask Lysne	NTNU	Norway	2019–2022	M	Staging and Multiple Hydrogen Feed of Biomass to Fischer-Tropsch Fuel Synthesis
Dumitrita Spinu	NTNU	Romania	2019–2022	F	Low temperature CO_2 capture
Junbo Yu	NTNU	China	2019–2022	M	Hydrogen membrane separation technology
Monica Pazos Urrea	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
Mustafa Kømurcu[3]	UiO	Norway	2017–2021	M	Ethene oligomerization
Martin Jensen	UiO	Norway	2018–2022	M	Catalytic Materials
Vladyslav Shostak	UiO	Ukraine	2020–2023	M	Development of comprehensive diffusion/ adsorption models for TAP kinetic experiments
Dag Sannes	UiO	Norway	2020–2023	M	Rational design of MOF catalysts for CO_2 conversion
Nicolai Haaber-Junge	UiO	Denmark	2020–2023	M	Zeolite catalyst deactivation

1) Muhammad Zubair defended his PhD thesis 18 March 2021
2) Jianyu Ma defended his PhD thesis 26 January 2021
3) Mustafa Sæterdal Kømurcu defended his PhD thesis 20 May 2021

International exchange PhD candidates in iCSI, NTNU

Consolato Rosmini	Bulgarian academy of Science	2 months	F	Aqueous phase reforming of Woxygenated compounds
Aldo Lanza	Politecnico de Milan	2 months	M	Production of Chlorine and Vinyl Chloride Monomer (VCM)
Yurou Li	East China University of Science and Technology	3 months	F	Acetylene selective hydrogenation

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

Suresh Balasingam Kannan	NTNU	India	2018–2021	M	Energy storage by high energy supercapacitors
Marie Døvre Strømsheim	NTNU	Norway	2018–2021	F	Surface chemistry and segregation phenomena of Pd-alloy membranes
Katarzyna Swirk	NTNU	Poland	2020–2022	F	MesoSi-CO_2. Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO_2 utilization through tri-reforming of methane
Hongfei Ma	NTNU	China	2021–2023	M	Chemical transformation of enzymatic hydrolysis lignin (EHL) with catalytic solvolysis to fuel commodities under mild conditions (EHLCATHOL)
Nico König	UiO	Germany	2020–2021	M	Catalyst synchrotron studies
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	2019–2021	M	Catalyst deactivation by coke formation
Oskar Iveland	UiO, iCSI	Norway	2019–2021	M	Synthesis and characterization of perovskites and catalytic testing
Odd Reidar Bygdnes	UiO	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-Nafuma, iCSI	Norway	2021–2023	M	In-situ XPS of PtRh NPs for NH_3 oxidation
Vilde Vinnes Jacobsen	NTNU	Norway	2019–2021	F	Production of olefins from waste plastics
Lasse Svendsen Chrobak	NTNU	Norway	2020–2021	M	Carbon formation and catalysis in the conversion of methyl chloride and silicon into dimethyldichlorosilane.
Ida Emilie Malde Jacobsen	NTNU	Norway	2020–2021	F	Carbon formation mechanisms on Co surfaces: A DFT study
Kristin Øxnevad Madsen	NTNU	Norway	2020–2021	F	Catalytic Steam Reforming of Hydrocarbon Impurities from Biomass Gasification
Leo Gosbert Mboyerwa	NTNU	Tanzania	2020–2021	M	Catalytic conversion of ligno-cellulosic biomass to flues
Albert Miró i Rovira	NTNU	Spain	2020–2021	M	Photocatalytic ammonia synthesis
Sunniva Skogheim	NTNU	Norway	2020–2021	F	Catalytic methane abatement for natural gas engines
Sunniva Vold	iCSI, NTNU	Norway	2020–2021	F	Efficient catalysts for attaining NO /NO_2 equilibrium in nitric acid production
Erlend Skjørstad Værnes	NTNU	Norway	2020–2021	M	Low temperature selective hydrogenation using noble metal catalysts
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 CO_2 capture
Karthikai Selvan Sivasamy	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 oxy-chlorination on promoted $CuCl_2$/Al_2O_3 catalysts

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

Isabel Maria Pascual Garcia	Master, NTNU	Spain	6 months	F	Preparation and characterization of pelletized Mn-based sulfur sorbents
Leo Gräber	Master, NTNU	Germany	4 months	M	Photocatalysis
Rémi Lilian Guy Snidaro	Master, NTNU	France	3 months	M	Characterization of hydrocarbon steam reforming catalysts for Syngas conditioning

Specialization students in catalysis group, NTNU, Autumn 2021

Communication and Dissemination 2021

iCSI Invited Plenaries:

Magnus Rønning: Operando XAS in aqueous phase reforming and other energy processes. BIKE Workshop; 2021-01-14–2021-01-15

Olsbye, Unni; Gutterød, Emil Sebastian; Lazzarini, Andrea; Fjermestad, Torstein; Pulumati, S.H.; Nova, Ainara; Skúlason, Egill: Mechanistic studies of CO_2 hydrogenation to methanol, methane and CO over Pt-containing Zr-MOFs. ACS Spring meeting 2021; 2021-04-05–2021-04-09

Unni Olsbye: Site - structure - performance correlations in zeolite- and MOF-based catalysts, FEZA 2021 Virtual, 2021-07-5–2021-07-09

Hilde Johnsen Venvik: Methanol partial oxidation to formaldehyde (MTF) over silver – new kinetic and structural insights, 53rd Annual Polish Conference on Catalysis (digital), 2021-09-22

Hilde Johnsen Venvik: Methanol partial oxidation to formaldehyde (MTF) over silver – new kinetic and structural insights, CATHEX Webinar lecture; 2021-09-24

Magnus Rønning: Characterisation of catalysts in chemical processes by combination of operando techniques. CATHEX Webinar Lecture; 2021-10-15

Hilde Johnsen Venvik: LINXS THEME NEW MATERIALS: Thermal Catalysis. LINXS Catalysis Workshop; 2021-10-28

Anders Holmen: Studies of the Fischer-Tropsch Synthesis. CATHEX Webinar Lecture; 2021-11-12

Jia Yang: Steady-State Isotopic Transient Kinetic Analysis (SSITKA) for investigation of catalysts for Fischer-Tropsch synthesis. CATHEX Webinar Lecture; 2021-11-12

iCSI Publications and conference contributions 2021

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

Journal Publications

Fjellvåg, Asbjørn Slagtern; Fjellvåg, Øystein; Breard, Y.; Sjåstad, Anja Olafsen: Structural disorder and antiferromagnetism in $LaNi_{1-x}Pt_xO_3$. Journal of Solid State Chemistry, 2021, 229, 122181.

Fjellvåg, Asbjørn Slagtern; Fjellvåg, Øystein; Kumar, Susmit; Ruud, Amund; Sjåstad, Anja Olafsen: Interplay of valence states and magnetic interactions in the perovskite system $LaNi_{1-x}Rh_xO_3$. Journal of Solid State Chemistry 2021, 298, 122124

Ivashenko, Oleksii; Johansson, Niclas; Pettersen, Christine; Jensen, Martin; Zheng, Jian; Schnadt, Joachim; Sjåstad, Anja: How surface species drive product distribution during ammonia oxidation: An STM and operando APXPS study, ACS Catal, 2021, 11, 8261–8273

Oskar Iveland: Ammonia Oxidation Based Reactions and their Catalysts, Master thesis, University of Oslo, 2021

Pettersen, Christine; Sjåstad, Anja Olafsen; Ivashenko, Oleksii: Near-Surface Alloys of PtRh on Rh(111) and Pt (111) Characterized by STM. The Journal of Physical Chemistry C, 2021, 125(45), 25140–25147

Oral Presentations

Børge Holme: How hard can it be to get a platinum depth profile from a palladium sample by SIMS (Secondary Ion Mass Spectrometry)? iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

J. Hessevik, A. S. Fjellvåg, O. Iveland, T. By, J. Skjelstad, D. Waller, H. Fjellvåg, A. O. Sjåstad: $LaNiO_3$ as a Pt catchment material in the ammonia oxidation process. iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

Jithin Gopakumar, Magnus Rønning, David Waller: Catalytic Oxidation of Nitric Oxide (NO) to Nitrogen Dioxide (NO_2) for Nitric Acid (HNO_3) Production. iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

Martin Jensen, Bruno Gonano, Walace Kierulf-Vieira, Patricia J. Kooyman, Anja O. Sjåstad: Synthesis of Pt-Rh nanoparticles for in-situ TEM studies. iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

Ivashenko, Oleksii; Pettersen, Christine; Johansson, Niclas; Jensen, Martin; Schnadt, Joachim; Sjåstad, Anja Olafsen: Operando (N) APXPS study of PtRh alloys for NH_3 oxidation. iCSI meeting; 2021-10-18–2021-10-19

Ivashenko, Oleksii; Pettersen, Christine; Johansson, Niclas; Jensen, Martin; Schnadt, Joachim; Sjåstad, Anja Olafsen: How surface species drive product distribution during ammonia oxidation: an operando APXPS Study. Max IV user meeting; 2021-10-25–2021-10-27

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; Hovde Gård, 2021-10-18–2021-10-19

IIA3: Frontier Formalin Technology Development

Journal Publications

Stine Lervold; Rune Lødeng; Jia Yang; Johan Skjelstad; Kristin Bingen; Hilde Johnsen Venvik: Partial oxidation of methanol to formaldehyde in an annular reactor, Chemical Engineering Journal, 2021, 423, 130141

Oral Presentations

Youri van Valen: Methanol partial oxidation to formaldehyde over silver – continued, iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

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

Journal Publications

Bao, Yuxiang; Ma, Hongfei; Tuo, Yongxiao; Qi, Yanying; Feng, Xiang; Yang, Chaohe; Chen, De: Research progress on catalyst for the synthesis of vinyl chloride monomer (VCM). Huagong jinzhan, 2021, Volume 40(4), 2034–2047

Hongfei Ma, Jithin Gopakumar, Wei Zhang, Samuel K. Regli, Yalan Wang, Kumar R. Rout, Terje Fuglerud, Marco Piccinini, Magnus Rønning, and De Chen: Insights of the Dynamic Copper Active Sites in Ethylene Oxychlorination Studied by the Multivariate UV–vis–NIR Resolution Kinetic Approach, Ind. Eng. Chem. Res. 2021, 60, 26, 9437–9447*

Hu, Wenshuo; Selleri, Tommaso; Gramigni, Federica; Fenes, Endre; Rout, Kumar Ranjan; Liu, Shaojun; Nova, Isabella; Chen, De; Gao, Xiang; Tronconi, Enrico: On thered ox mechanism of low-temperature NH_3-SCR over Cu-CHA: A combined experimental and theoretical study of the reduction half cycle. Angewandte Chemie International Edition, 2021, Volume 60(13), 7197–7204

Ma, Hongfei; Sollund, Erling S.; Zhang, Wei; Fenes, Endre; Qi, Yanying; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Piccinini, Marco; Chen, De: Kinetic modeling of dynamic changing active sites in a Mars-van Krevelen type reaction: Ethylene oxychlorination on K-doped $CuCl_2$/Al_2O_3. Chemical Engineering Journal 2021, 407, 128013

Ma, Hongqin; Guan, Yanan; Chen, Wenyao; Sui, Zhijun; Qian, Gang; Chen, De; Zhou, Xinggui; Duan, Xuezhi: Support effects of Cs/Al_2O_3 catalyzed aldol condensation of methyl acetate with formaldehyde. Catalysis Today 2021, Volume 365, 310–317

Oral Presentations

Wang, Yalan; Qi, Yanying; Ma, Hongfei; Zhang, Wei; Fenes, Endre; Rout, Kumar Ranjan; Piccinini, Marco; Fuglerud, Terje; Chen, De: Promoter effects on $CuCl_2$/γ-Al_2O_3 catalyzed ethylene oxychlorination by DFT calculations. iCSI seminar; 2021-10-18–2021-10-19

Wei Zhang: Understanding of K , La and Mg co-promoter effect in ethylene oxychlorination by operando UV–vis-NIR spectroscopy, iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

Kumar Rout: Modelling, Estimation and Optimization of Oxychlorination of Ethylene, iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

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

Journal Publications

Gabriele Deplano, Andrea Martini, Matteo Signorile, Elisa Borfecchia, Valentina Crocellà, Stian Svelle, Silvia Bordiga: Copper pairing in the mordenite framework as a function of the Cu(I)/Cu(II) speciation, Angewandte Chemie International Edition, 2021, Volume 60(49), 25891–25896

Sebastian Prodinger, Pablo Beato & Stian Svelle: From Catalytic Test Reaction to Modern Chemical Descriptors in Zeolite Catalysis Research, Chemie Ingenieur Technik, 2021, Volume 93, 902–915 (part of a special issue In Memory of Prof. Dr.Ing. Jens Weitkamp)

Prodinger, Sebastian; Kvande, Karoline; Arstad, Bjørnar; Borfecchia, Elisa; Beato, Pablo; Svelle, Stian: Synthesis-Structure-Activity Relationship in Cu-MOR for Partial Methane Oxidation: Al Siting via Inorganic Structure Directing Agents, ACS Catalysis, Manuscript ID: cs-2021-05091b.R1

Oral Presentations

Kvande, Karoline; Svelle, Stian; Pappas, Dimitrios K; Borfecchia, Elisa; Martini, Andrea; Bordiga, Silvia; Beato, Pablo: Methane to methanol conversion over Cu-zeolites – structure performance relationships. 8th Conference of the Federation of European Zeolite Associations (FEZA 2021); 2021-07-05–2021-07-09

Prodinger, Sebastian; Svelle, Stian; Beato, Pablo: On the Role of Ions in the Formation of Zeolites. Workshop on Water in Zeolites; 2021-09-19–2021-09-22

Sebastian Prodinger: Synthesis-Structure-Activity Relationship in Cu-Mordenite for Partial Methane Oxidation: Directing Al Siting via Inorganic Structure Directing Agents, iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

Bjørn Gading Solem: Methylation of lower alkenes thought stepwise reaction with methane, iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

IIA6: Generic Projects for Additional Industrial Synergies

Journal Publications

O.H. Bjørkedal, S.K. Regli, R.J.G. Nuguid, P.E. Vullum, D. Ferri, M. Rønning: One-pot synthesis of highly dispersed mesoporous Cu/ZrO_2 catalysts for NH_3-SCR, Catal. Today, 2021, https://doi.org/10.1016/j.cattod. 2021.05.010

Duyar, Melis S.; Gallo, Alessandro; Regli, Samuel K.; Snider, Jonathan L.; Singh, Joseph A.; Valle, Eduardo; McEnaney, Joshua; Bent, Stacey F.; Rønning, Magnus; Jaramillo, Thomas F.: Understanding Selectivity in CO_2 Hydrogenation to Methanol for MoP Nanoparticle Catalysts Using In Situ Techniques. Catalysts 2021, 11(1), 143

Oral Presentations

Björn Baumgarten: A new ISMA – Simultaneous deactivation and deposition studies, iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

Moses Mawanga: Insights into the reaction kinetics and mechanism of industrial relevant reactions, iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

Oleksii Ivashenko: Operando APXPS studies of PtRh alloys for ammonia oxidation, iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

Tina Bergh: Transmission electron microscopy characterisation at NTNU, iCSI annual seminar; Hovde Gård, 2021-10-18–2021-10-19

iCSI associated Publications and conference contributions 2021

Journal Publications

Aunan, Erlend; Affolter, Chris W.; Lillerud, Karl Petter; Olsbye, Unni: Modulation of the Thermochemical Stability and Adsorptive Properties of MOF-808 by the Selection of Non-structural Ligands. Chemistry of Materials, 2021, Volume 33(4), 1471–1476

Bernal, Fabian Leonardo Martinez; Lundvall, Fredrik; Kumar, Susmit; Hansen, Per-Anders S.; Wragg, David S.; Fjellvåg, Helmer; Løvvik, Ole Martin: Jahn-Teller active fluoroperovskites ACrF3 (A=Na+, K+): Magnetic and thermo-optical properties. Phys. Rev. Materials, 2021, 5(6), 064420

Chang, Qing-Yu; Wang, Kai-Qi; Sui, Zhi-Jun; Zhou, Xinggui; Chen, De; Yuan, Wei-Kang; Zhu, Yi-An: Rational design of single-atom-doped Ga_2O_3 catalysts for propane dehydrogenation: Breaking through volcano plot by lewis acid–Base interactions. ACS Catalysis, 2021, Volume 11(9), 5135–5147

Chen, Chen; Tuo, Yongxiao; Lu, Qing; Lu, Han; Zhang, Shengyang; Zhou, Yan; Zhang, Jun; Liu, Zhanning; Kang, Zixi; Feng, Xiang; Chen, De: Hierarchical trimetallic Co-Ni-Fe oxides derived from core-shell structured metal-organic frameworks for highly efficient oxygen evolution reaction. Applied Catalysis B: Environmental, 2021, Volume 287, 119953

Chen, Wenyao; Cao, J.B.; Yang, Jia; Cao, Yueqiang; Zhang, Hao; Jiang, Zheng; Zhang, Jing; Qian, Gang; Zhou, Xinggui; Chen, De; Yuan, Wei-Kang; Duan, Xuezhi: Molecular-level insights into the electronic effects in platinum-catalyzed carbon monoxide oxidation. Nature Communications 2021, Volume 12(1), 6888

Chen, Wenyao; Wang, Jingnan; Zhang, Yanfang; Zhang, Jing; Duan, Xuezhi; Si, Rui; Chen, De; Qian, Gang; Zhou, Xinggui: Kinetics decoupling activity and selectivity of Pt nanocatalyst for enhanced glycerol oxidation performance. AIChE Journal, 2021, Volume 67(10), e17339

Chen, Zhaohui; Mo, Yasi; Lin, Dong; Tuo, Yongxiao; Feng, Xiang; Liu, Yibin; Chen, Xiaobo; Chen, De; Yang, Chaohe: Engineering the efficient three-dimension hollow cubic carbon from vacuum residuum with enhanced mass transfer ability towards H_2O_2 production. Chinese Journal of Chemical Engineering, 2021, Volume 38, 98–105

Cnudde, Pieter; Redekop, Evgeniy; Dai, Weili; Porcaro, Natale G.; Waroquier, Michel; Bordiga, Silvia; Hunger, Michael; Li, Landong; Olsbye, Unni; Van Speybroeck, Veronique: Experimental and theoretical evidence for promotional effect of acid sites on the diffusion of alkenes through small-pore zeolites. Angewandte Chemie International Edition, 2021, 60(18), 10016–10022

Dar, Hassan Jamil; Jakobsen, Hugo Atle; Rout, Kumar Ranjan; Jens, Klaus-Joachim; Chen, De: Autothermal Gas-Phase Oxidative Dehydrogenation of Ethane to Ethylene at Atmospheric Pressure. Industrial & Engineering Chemistry Research, 2021, Volume 60(18), 6784–6802

Du, Juan; Xiao, Jin; Li, Chenyang; Qiao, Jia; Chen, De; Yang, Jianhong; Zhong, Qifan; Luo, Yingtao; Chen, Kaibin; Sun, Lizhen: The preparation of three-dimensional binder-free polyaniline/aligned carbon nanotube on flexible etched Al foil substrate as high-performance pseudocapacitive cathode for nonaqueous lithium-ion capacitor. Journal of Energy Storage, 2021, Volume 33, 102165

Fu, Wenzhao; Wang, Qianhong; Chen, Wenyao; Qian, Gang; Zhang, Jing; Chen, De; Yuan, Wei-Kang; Zhou, Xinggui; Duan, Xuezhi: Engineering Ru atomic structures toward enhanced kinetics of hydrogen generation. Chemical Engineering Science, 2021, Volume 235, 116507

García, R.; Gil, M.V.; Rubiera, F.; Chen, De; Pevida, C.: Renewable hydrogen production from biogas by sorption enhanced steam reforming (SESR): A parametric study. Energy, 2021, Volume 218, 119491

Gerz, Isabelle; Jannuzzi, Sergio Augusto Venturinelli; Hylland, Knut Tormodssønn; Negri, Chiara; Wragg, David Stephen; Øien-Ødegaard, Sigurd; Tilset, Mats; Olsbye, Unni; DeBeer, Serena; Amedjkouh, Mohamed: Structural Elucidation, Aggregation, and Dynamic Behaviour of N,N,N,N-Copper(I) Schiff Base Complexes in Solid and in Solution: A Combined NMR, X-ray Spectroscopic and Crystallographic Investigation. European Journal of Inorganic Chemistry (EurJIC), 2021, Volume 2021(46), 4762–4775

Guo, Xiaoyang; Vullum, Per Erik; Venvik, Hilde Johnsen. Inhibition of metal dusting corrosion on Fe-based alloy by combined near surface severe plastic deformation (NS-SPD) and thermochemical treatment. Corrosion Science 2021, 190(6873):109702

Han, Guangda; Cai, Jihai; Liu, Chuanfu; Ren, Junli; Wang, Xiaohui; Yang, Jia; Wang, Xiaoying: Highly sensitive electrochemical sensor based on xylan-based Ag@CQDs-rGO nanocomposite for dopamine detection. Applied Surface Science, 2021, Volume 541, 148566

Hansen, Per-Anders Stensby; Kumar, Susmit; Meijerink, Andries: Strong self-sensitized green and NIR emission in $NaYS_2$ doped with Pr^{3+} and Yb^{3+} by inducing Laporte allowed and charge transfer transitions. Journal of Luminescence 2021, Volume 235, 118012

Jebasty, Mariyal R.; Sjåstad, Anja Olafsen; Ravindran, Vidya: Prediction of intermediate band in Ti/V doped gamma-In_2S_3. RSC Advances, 2022 ;Volum 12. s. 1331–1340

Karthikeyan, Jayakumar; Fjellvåg, Helmer; Bundli, Silje; Sjåstad, Anja Olafsen: Efficient Exfoliation of Layered Double Hydroxides; Effect of Cationic Ratio, Hydration State, Anions and Their Orientations. Materials, 2021, Volume 14(2), 346

Li, Yahao; Zang, K.; Duan, Xuezhi; Luo, Jing; Chen, De: Boost oxygen reduction reaction performance by tuning the active sites in Fe-N-P-C catalysts. Journal of Energy Chemistry, 2021, Volume 55, 572–579

Lin, Dong; Zhang, Quande; Qin, Zhengxing; Li, Qing; Feng, Xiang; Song, Zhaoning; Cai, Zhenping; Liu, Yibin; Chen, Xiaobo; Chen, De; Mintova, Svetlana; Yang, Chaohe: Reversing Titanium Oligomer Formation towards High-Efficiency and Green Synthesis of Titanium-Containing Molecular Sieves. Angewandte Chemie International Edition, 2021, Volume 60(7), 3443–3448

Ma, Jianyu; Mahmoodinia, Mehdi; Rout, Kumar Ranjan; Blekkan, Edd A.: Regenerable Sorbents for High-Temperature Desulfurization of Syngas from Biomass Gasification. Chemie Ingenieur Technik, 2021, Volume 93(6), 949–958

Ma, Jianyu; Mahmoodinia, Mehdi; Rout, Kumar Ranjan; Blekkan, Edd Anders: The Impact of Operating Parameters on the Gas-Phase Sulfur Concentration after High Temperature Sulfur Sorption on a Supported Mo-Mn Sorbent. Reactions 2021, 2(4), 365–373

Mehandzhiyski, Aleksandar Yordanov; Anquetil-Deck, Candy; Wang, Xuehang; Chen, De; Grimes, Brian Arthur: Microscopic Insight to Nonlinear Voltage Dependence of Charge in Carbon-Ionic Liquid Supercapacitors. Energy Material Advances, 2021, ID 9849202

Mortén, Magnus; Cordero Lanzac, Tomas; Cnudde, Pieter; Redekop, Evgeniy; Svelle, Stian; Van Speybroeck, Veronique; Olsbye, Unni: Acidity effect on benzene methylation kinetics over substituted H-MeAlPO-5 catalysts. Journal of Catalysis, 2021, Volume 404, 594–606

Niu, Juntian; Wang, Yalan; Liland, Shirley Elisabeth Sjø; Regli, Samuel K.; Yang, Jia; Rout, Kumar Ranjan; Luo, Jun; Rønning, Magnus; Ran, Jingyu; Chen, De: Unraveling Enhanced Activity, Selectivity, and Coke Resistance of Pt–Ni Bimetallic Clusters in Dry Reforming. ACS Catalysis 2021, Volume 11(4), 2398–2411

Pandey, Umesh; Runningen, Anders; Gavrilovic, Ljubisa; Jørgensen, Erik Andreas; Putta, Koteswara Rao; Rout, Kumar Ranjan; Rytter, Erling; Blekkan, Edd Anders; Hillestad, Magne: Modeling Fischer–Tropsch kinetics and product distribution over a cobalt catalyst. AIChE Journal 2021, Volume 67(7), e17234

Periyasamy, Manimuthu; Patra, Lokanath; Fjellvåg, Øystein; Ravindran, Ponniah; Sørby, Magnus Helgerud; Kumar, Susmit; Sjåstad, Anja Olafsen; Fjellvåg, Helmer: Effect of electron doping on the crystal structure and physical properties of an n = 3 Ruddlesden-Popper compound $La_4Ni_3O_{10}$. ACS Applied Electronic Materials, 2021, Volume 3(6), 2671–2684

Pham, Thanh Hai; Cao, Junbo; Song, Nan; Cao, Yueqiang; Chen, Bingxu; Qian, Gang; Zhou, Xinggui; Chen, De; Duan, Xuezhi: Mechanistic aspects of facet-dependent CH_4/C^{2+} selectivity over a χ-Fe_5C_2 Fischer–Tropsch catalyst. Green Energy & Environment 2021, https://doi.org/10.1016/j.gee.2020.10.015

Pinilla-Herrero, Irene; Borfecchia, Elisa; Cordero-Lanzac, Tomás; Mentzel, Uffe V.; Joensen, Finn; Lomachenko, Kirill A.; Bordiga, Silvia; Olsbye, Unni; Beato, Pablo; Svelle, Stian: Finding the active species: The conversion of methanol to aromatics over Zn-ZSM-5/alumina shaped catalysts. Journal of Catalysis, 2021 , Volume 394, 416–428

Poissonnier, Jeroen; Ranga, Chanakya; Lødeng, Rune; Thybaut, Joris W.: Oxygen functionality and chain length effects in HDO: Impact of competitive adsorption on reactivity. Fuel, 2022, Volume 308, 121940

Redekop, Evgeniy; Johansson, Niclas; Kokkonen, Esko; Urpelainen, Samuli; Lopes Da Silva, Felipe; Kaipio, Mikko; Nieminen, Heta-Elisa; Rehman, Foqia; Miikkulainen, Ville; Ritala, Mikko; Olsbye, Unni: Synchronizing gas injections and time-resolved data acquisition for perturbation-enhanced APXPS experiments. Review of Scientific Instruments, 2021, Volume 92(4), 044101-1 - 044101-11

Rodríguez, S.; Capa, A.; Garcia, R.; Chen, De; Rubiera, F.; Pevida, C.; Gil, M.V.: Blends of bio-oil/biogas model compounds for high-purity H_2 production by sorption enhanced steam reforming (SESR): Experimental study and energy analysis,. Chemical Engineering Journal, 2021, 134396–

Saha, Dipankar; Kumar, Susmit; Gonano, Bruno Raymond Gino; Sjåstad, Anja Olafsen; Fjellvåg, Helmer: Total Scattering Study of Local Structural Changes in $MnAs_{1-x}P_x$ Influenced by Magnetic Interactions. Chemistry of Materials, 2021, Volume 33, 2576–2584

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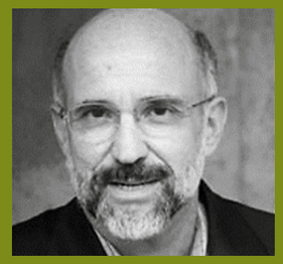

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