iCSI

industrial Catalysis Science and Innovation

Annual Report 2020

sfi Centre for Research-based Innovation

NTNU

iCSI Partners

sfi 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: Education is an important aspect of iCSI's mandate. Photo shows catalysis master`s students at NTNU June 2020 after finalizing their master's thesis. Photo: Jithin Gopakumar

2020 Summary

Looking back to the 2019 Annual Report, the heading was "Time to refresh". Well, 2020 did certainly not turn out to be a refreshing year.

The University of Oslo faced more challenges and delays than NTNU, due to longer closures of the labs and generally more restrictions imposed in our capital area. Despite these limitations, iCSI research as such has suffered only moderately from the pandemic due to fortunate timing. Many of our PhD candidates were near completion in 2020, focusing on writing up their research results. Then some new candidates were recruited, and these have manoeuvred impressively well during their start-up phase with course work and supervision via screen.

Educating master's students is important to the Centre. In 2020, 17 graduating master's students were associated with iCSI, of which two delivered directly into the ongoing projects. The gender balance within iCSI has been maintained in all personnel categories – within a 40/60 distribution.

In March of last year, just before the lockdown, iCSI welcomed Sebastian Prodinger, a new Postdoctoral fellow, to the University of Oslo. In September three new PhD candidates started at NTNU: Youri van Valen, Jithin Gopakumar and Wei Zhang. They come from different parts of the world, and you can get to know them better through the interview on p. 28.

The high publishing activity has continued from last year, and twelve reviewed papers were accepted and published in 2020. At the end of the year, even more articles were submitted for review. Especially Industrial Innovation Area 4 (PVC Value Chain: World Class Energy and Raw Material Efficiency for the Production of Chlorine and Vinyl Chloride Monomer) should be mentioned for the large quantity, as well as the high quality of published articles this year. The publication and presentation lists from the centre can be found on page 65-66.

The lack of traveling and conference participation is reflected in the list of conference contributions. We were fortunate to be able to hold the iCSI Annual Seminar at Oscarsborg in September, and 98% of the presentations and posters are from that event. For most of us, this was the only occasion to present research results and for in-person meetings with iCSI partners at other locations.

Another exception was the Young Researchers Seminar at the end of February, which was lucky timing. Pablo Beato and Haldor Topsøe hosted the event at their locations in Lyngby. The young researchers were also invited to a tour at the Topsøe catalyst plant in Fredrikssund.

iCSI is proud to have dedicated and enthusiastic international scientific advisors. When they were not able to join our seminar due to travel restrictions, they compensated by giving digital guest lectures as well as one-to one meetings with four of iCSI's PhD candidates and postdocs. The lectures were appreciated by the industry partners as well.

The representation on the iCSI Board has changed in 2020, as Thomas By took over from Johan Skjelstad as K.A. Rasmussen's board representative in August. As of January 2021, Kamilla Jordal replaced Marco Piccinini as Inovyn's representative. iCSI thanks everyone for their efforts during their period on the Board.

Content

A different year!

We all know why 2020 was different. In February, we were planning for international projects and collaboration, research exchange and conference participation as usual. Two months later the campuses were partly or completely closed, and we had serious concern about the human and economic consequences of the COVID-19 pandemic. One year later we look back at events and situations we could never have imagined back then.

Norway has had fewer deaths than most countries with a high level of welfare compensations and a sparse population as part of the explanation. But the semi lock-down regime has taken its toll on our campuses and our students. Even if the digital teaching has demonstrated new ways of communication – with room for improvement – it has shown how critical physical interaction is in higher education. And we have seen the impact of a fully internationalized working environment. It has been heartbreaking to see our colleagues from distant countries not being able to care for their near and dear ones in dire situations.

iCSI research as such has suffered only moderately due to fortunate timing. Many of our PhD candidates were near completion in 2020, focusing on writing up their research results. Then some new candidates were recruited, and these have manoeuvred impressively well during their start-up phase with course work and supervision via screen. The University of Oslo has faced more challenges and delays than NTNU, due to longer closures of the labs and generally more restrictions imposed in our capital area. NTNU (Trondheim) and SINTEF (both Trondheim and Oslo) were mostly able to keep lab activities running. What suffers most is team spirit and social arenas. But even there iCSI had some good luck with arranging our Young Researcher seminar at Topsøe in February and our Annual seminar in September, a period where meetings and domestic travel saw relatively light restrictions. International collaboration has also been hampered. Meeting via screen is not the same with respect to creating state-of-the-art research, and the fruitful Oslo-Torino-Lyngby triangle has experienced this in particular.

However, the reports from all iCSI industrial partners have been encouraging, as they have so far kept production going and not experienced reduced revenues. It has been challenging, with measures and restrictions varying between sites. The partners praise their employees' efforts in keeping plants operating. Licensing and development of new projects are also difficult when partners, suppliers and clients cannot meet up and solve new issues. But they have found ways around these difficulties and learnt new ways of communicating and collaborating that will also strengthen the companies in the long run. Despite a general uncertainty about the long-term economic impact, it is reassuring that Yara, KA Rasmussen, Dynea, Inovyn and Haldor Topsøe are keeping up their business and contributing to the global economy and the supply of products necessary to maintain the food and energy supply, healthcare and infrastructure. Even more uplifting is to learn that they have developed and started to implement new strategies for mitigating climate change (see page 12)!

Hilde Johnsen Venvik

Professor
iCSI Centre Director

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, industrial competitiveness, as well as future chemical processing and energy conversion with a minimum 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 allows 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 to the environment. State-of-the-art methodology in synthesis, characterization and technology development is applied in order to obtain a detailed understanding of complex catalysts under industrially relevant conditions, thereby identifying factors critical to their performance. iCSI researchers also develop predictive tools for optimization of materials, chemistries and processes.

Photo: From dynea.com

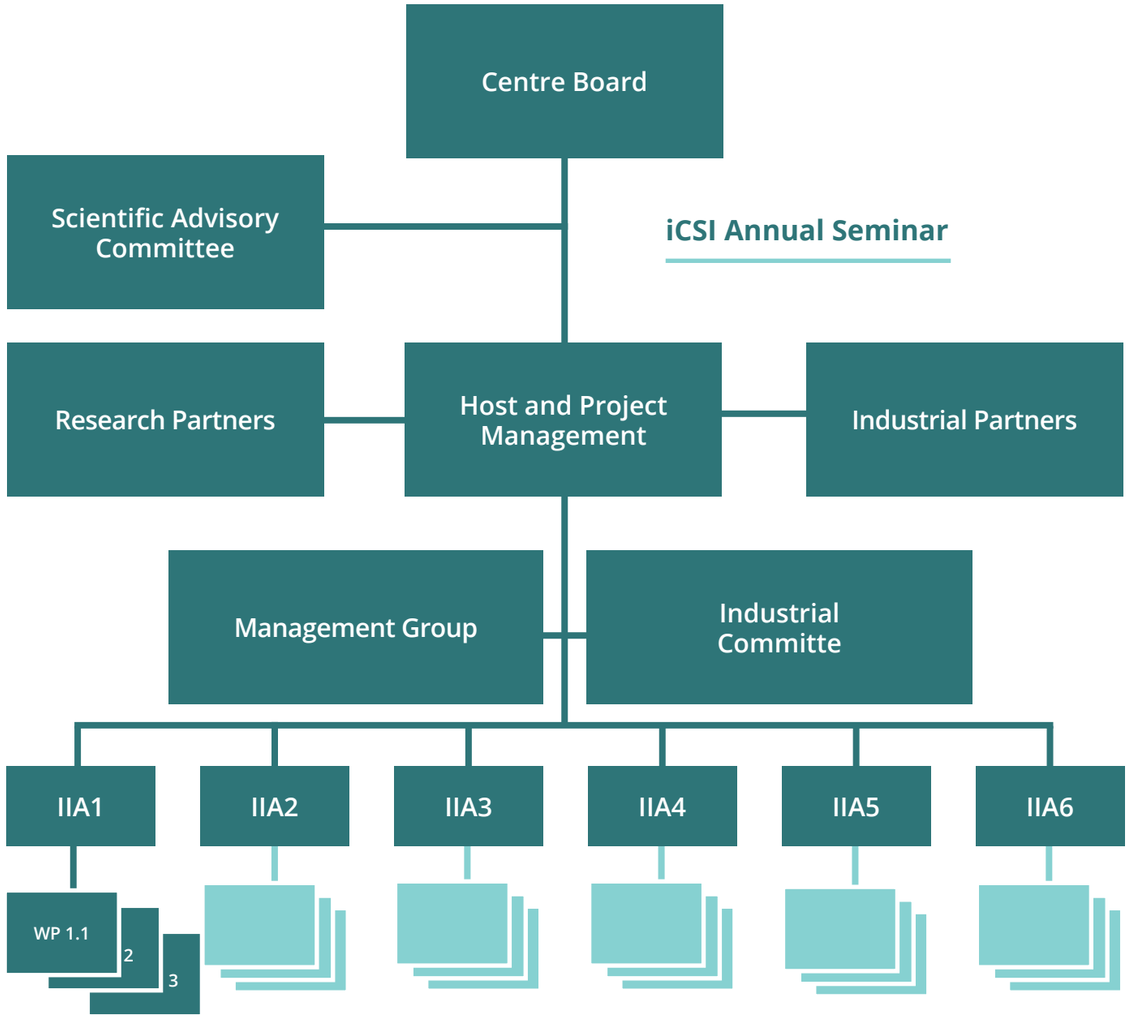
iCSI's main objective is to boost industrial innovation and competitiveness and provide efficient, low-emission processes.

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 Topsoe wants to be the global leader within carbon emission reduction technologies for the chemical and refining industries. By perfecting chemistry for a better world, we enable our customers to succeed in the transition towards renewable energy.

K.A. Rasmussen AS is a refiner of precious metals and supplier of catalysts and products based on precious metals located in Hamar, Norway among other places in Europe. 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 well known Dynea Silver Catalyzed Formaldehyde technology, fasil®. In iCSI, Dynea aims to continue its technological leadership in formalin production for improved plant operations and reduced cost for its fasil® technology.

Centre Board

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

Pablo Beato from Haldor Topsøe has acted as the Chair of the Board in 2020. Thomas By took over from Johan Skjelstad as K.A. Rasmussen's board representative in August. As of January 2021, Kamilla Jordal is replacing 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

Dr. Marco Piccinici

Vinyl Chloride Monomer and Organic Chlorine Derivatives Research Manager at INOVYN

Professor Einar Uggerud

Head of Department of Chemistry at 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

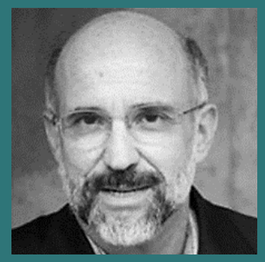
Special advisor RCN, with Responsibility for Nanotechnology and Advanced Materials

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 Adviser (20% position).

Hilde J. Venvik

Professor
iCSI Centre Director

Anne Hoff

Senior advisor
iCSI Coordinator

Torgrim Mathisen

Senior Executive Officer
iCSI Economy advisor

A green deal for the iCSI industrial partners!

On 11 December 2019 the European Commission launched the European Green Deal: a plan to make the EU's economy sustainable. Four of the six actions may be considered highly relevant to iCSI:

- investing in environmentally-friendly technologies
- supporting industry to innovate
- decarbonizing the energy sector
- working with international partners to improve global environmental standards

In April 2018, the Norwegian government established Prosess21, an expert group with the main task of providing strategic advice and recommendations on how Norway can best achieve its goal of sustainable growth whilst minimizing emissions. The representatives were from industry, industry organizations and the academic community, and the final report was launched on 8 February 2021 with the following recommended goals to develop and strengthen the process industry by 2030:

- Reduce emissions corresponding to 2.5 million tons of CO_2 equivalents from known projects in the process industry, resulting in reductions of more than 50 percent in industrial emissions compared with 1990.
- Develop and produce highly specialized green products with relevant accompanying services.
- Establish a new low-emission industry in Norway.
- Develop new innovation projects in the process industry that contribute to further climate cuts, including the establishment of carbon capture on major industrial point emissions beyond what is currently part of the Longship-project.
- Take a leading position globally in realizing the potential for increased value creation from digitization.
- Support lifelong learning with a focus on product and service development, digitization and climate.

iCSI is proud to present how our industrial partners are taking a lead in the transitions emerging to mitigate climate change through recent strategic investment decisions.

Yara has announced plans to establish Europe's first large-scale green ammonia project in Norway by electrifying Yara's existing ammonia facility in Porsgrunn. With partners Statkraft and Aker Horizons they are targeting green hydrogen and green ammonia opportunities within shipping, agriculture and industrial applications.

> "The announcement of the green ammonia project in Porsgrunn and the establishment of Clean Ammonia as a business unit in Yara are exiting news which demonstrates that Yara is committed to be an important player in the green shift and will continue to have a strong focus on technology development in the future"
>
> *Torgeir Lunde, Yara*

INEOS/Inovyn have launched a new Clean Hydrogen Business and announced investments in decarbonization of specific European sites at Tavaux, France and Antwerp, Belgium.

> "INEOS/Inovyn is working on several projects to improve process performances and reduce consumptions of raw materials, to decrease carbon emissions including energy saving and electrification and to develop carbon neutral products as part of its sustainability roadmap."
>
> *Kamilla Jordal, new iCSI Board member from Inovyn*

Haldor Topsøe's new vision is to be recognized as a global leader in carbon emission reduction technologies by 2024. New technologies have been launched within hydrogen, ammonia, biofuels and electrification.

> "During 2020, I have witnessed the largest reorganization of the company during my entire career at Topsøe. It is very clear what we are aiming for. In the renewable fuels area, our role as an early player has already paid off, as some of the catalyst solutions developed to meet the challenges related to new feedstocks and process solutions have become market leaders. With our focus on green hydrogen and other carbon emission reduction technologies, new solutions are on their way, including several of them in collaboration with Norwegian companies",
>
> *Pablo Beato, Chair of the iCSI Board.*

Photo by: Haldor Topsøe AS

Researcher Portrait: Professor Unni Olsbye

She doesn't need to make noise to be heard, our Unni. Her knowledge, personal qualities and skills make her an attractive teacher, advisor, collaborator and research partner, and people listen when she talks in her soft way. Over the last several years Unni Olsbye has received several high-hanging international awards for innovation and her work in the gas conversion field. So of course we are proud to have her available as an advisor and discussion partner at iCSI. In many ways she is the godmother of iCSI, as she was an initiator and managed inGAP, the SFI which was iCSI's predecessor.

In typical fashion, when we talked about what she has achieved Unni started by introducing her long-term collaborating partners. Her own research focus is kinetic and mechanistic investigations of catalytic reactions, and she enjoys systems thinking. Her toolbox consists of catalytic test reactors ranging from vacuum to 30 bar pressure, steady-state and transient experiments, and extensive use of isotopic labelling to elucidate mechanistic details. She collaborates particularly closely with materials scientist Karl Petter Lillerud, and other colleagues in the UiO catalysis group, as a means to investigate the effect of single material parameter variations.

Furthermore, collaboration with spectro-scopist Silvia Bordiga at the University of Turin has been important in unravelling mechanistic details. More recently, she has challenged herself by looking into bio-catalysis, and together with Vincent Eijsink at NMBU, Serena De Beer at the Max Planck Institute and Silvia Bordiga she received prestigious funding from the EU's ERC Synergy grants for the CUBE project "Unravelling the secrets of Cu-based catalysts for C-H activation". They will explore synthetic and enzymatic catalysts side-by-side, aiming to cross-fertilize the development of both fields.

The CUBE team in Brussels, just after the final selection interview for the ERC Synergy grant.

> "Before commencing a new project, always ask yourself: "If I succeed beyond my wildest dreams, will I have advanced my knowledge by an order of magnitude?"
>
> *Prof.Gabor Somorjai (inGAP advisor)*

Generally, Unni strives to build teams with complementary qualities, and to introducing the students to collective problem-solving, where each team member focus on, and contribute with, their own specialty field. One of her recent bachelor's and master's students, Bjørn Solemsli, says she introduced him to big project and group meetings so he could learn how things functioned practically and what people worked on. He further describes how Unni, as a supervisor, helps you to come up with and realize your own thoughts and ideas about the project, so that you arrive at the answer without her telling you. "When teaching General Chemistry, she explains the basic principles in a way that everyone can understand. She is the first professor many students meet, and she shows a real interest in the subject and passes this on to the students," he says.

> "Students, don't cut corners, but do proper scientific work - it will pay off in the long run."

Unni is proud of the achievements of her students and postdocs, and confirms that students and young researchers in the group give her energy and faith in the future". The next generation researchers has a quite different skillset from what we started out with, and this leads to novel approaches and project ideas. That's exactly what we need now, to facilitate the transfer towards a post-fossil era", she says.

As Unni sees it, her role in this work and that of her iCSI colleagues is to develop new and improved processes, and to increase and transfer process expertise (including front-line chemical insight into catalytic processes) to the next generation of chemists and chemical engineers. "We work hard on this, and we see that our candidates are attractive and get good jobs, both nationally and internationally. Where we could probably improve, me included, is in the recruitment of students to our field: Catalysis is an important key to a 'greener' future, both for environmentally friendly

Unni Olsbye – CV in short:

- 1987: Master's in Industrial Chemistry, Norwegian Institute of Technology (NTH), Norway
- 1988-91: PhD in Organic Chemistry, University of Oslo, Norway, after 3 years fellowship from Elf Aquitaine Norge A/S, working in their R&D center in France
- 1991-2000: Researcher and later Senior Scientist and group leader at Department of Hydrocarbon Process Chemistry, SINTEF
- 2000-2001: R&D Manager, NORDOX Industrier AS
- 2001 – : Associate professor, and from 2002 Professor at Department of Chemistry, University of Oslo. Teaching General Chemistry (BSc level) and Catalysis and Industrial Chemistry (BSc/MSc level)
- 195 peer-reviewed articles with 14 346 citations, 3 book chapters, 11 patent applications
- A large number of academic positions entailing trust, board work and editorial duties

> "It took me 10 years to obtain funding for buying a TAP machine, and another 5 before we published our first research paper from it. I am sure it was worth it!"

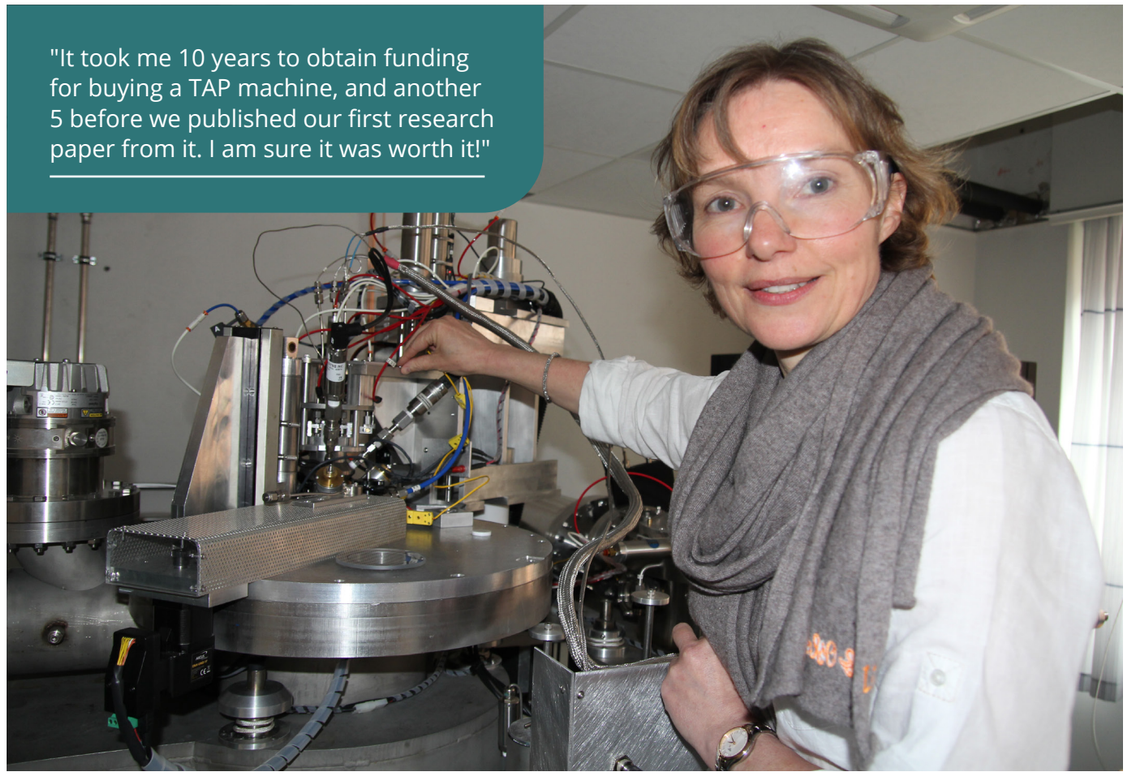


Photo: Gunhild M. Haugnes, UiO.

"An important driving force for me, beside natural curiosity, is the desire to make a small contribution to positive development for the world, first and foremost by producing new knowledge in my field of research, and secondly to apply this knowledge to make the world a 'greener' place through a cleaner and more energy efficient process industry. The education of the next generation of chemists is an essential and very rewarding part of the work."

production of consumer goods and long-term storage of renewable energy. This, we have to tell the outside world!" she says.

To broaden the PhD candidates' perspectives, references and network of contacts, she encourages them to go abroad for a semester in the last part of their studies. Doing so they experience that their knowledge adds value elsewhere, at the same time as they learn something new to bring home. It matures them.

She is also proud of what was achieved through the successful inGAP Centre. Academia and industry worked together for a long time towards a common goal, with mutual respect for each other's competence and strengths. Industry partners increased their revenue by applying new insight from the collaboration, and the input from industry and long-term focus increased the quality of academic research, as reflected in the increased number of citations of published works. (She is now one of Norway's most cited chemists!) One key to inGAP's success, she believes, was her background as an engineer from NTNU and her experience with industrial collaboration in her years with SINTEF. That gave her insight into industry's needs and way of thinking, and they had a common language in planning and executing the project.

Unni says she is inspired by discussions with colleagues, new developments in her scientific topics, knowledge and new methods and techniques that provide opportunities for new answers to old questions. Some people say that research interests go in cycles. She asserts that development goes in a spiral – upwards. You occasionally return to old issues but increased basic understanding and new tools give a boost and new insights.

And who knows – maybe she also gets a boost and a bit of inspiration when skating on the Oslofjord ice or kayaking on a lake nearby?

Scientific Highlight 2020

Polyvinyl chloride (PVC) is the most versatile and useful of all thermoplastics and is the third-highest volume polymer. Vinyl chloride (VCM), the monomer of PVC, is the key building block for PVC production, which is mainly produced from ethylene dichloride (EDC) through thermal cracking. Currently, approximately 90% of VCM production plants worldwide are using a balanced VCM process by first chlorinating ethylene with Cl2 to produce EDC, the EDC is then thermally converted to VCM. The HCl produced in the dehydrochlorination reactor is typically captured and recycled to an oxychlorination reactor to convert C2H4, O2, and HCl to EDC, which is again converted to VCM. EDC dehydrochlorination, also called EDC cracking, is an energy-intensive process that is carried out at high temperatures (500−550°C), high pressures (15−20 bar), at a conversion of approximately 50−60% leading to an overall VCM yield of about 50% in a single pass. The complexity of the process drives the search for simplification. Directly producing VCM from C2H4, O2, and HCl could hence represent significant progress.

In our 2020 publication in Angewandte Chemie International Edition, we have demonstrated a new method for producing VCM in a single-step at relatively low temperature (250˚C) and ambient pressure. A bifunctional catalyst concept combining CuCl2 and N-doped carbon was invented. The metal-free carbon catalyst was demonstrated to contain sites (N functional groups) active in both ethylene oxychlorination and dehydrochlorination in mild conditions. A reaction mechanism of Cl-loop between ethylene oxychlorination and EDC dehydrochlorination was proposed to rationalize the observed synergy effect of the two reactions (Figure 1). We also utilized the dual-bed configuration to produce VCM with a much higher yield (76%) than the current two-step industrial process in a single-pass (Figure 2).

The work suggests a promising alternative process for energy-efficient VCM production via ethylene oxychlorination, in mild conditions and through a single pass reactor.

Ma, Hongfei; Ma, Guoyan; Qi, Yanying; Wang, Yalan; Chen, Qingjun; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De: Nitrogen-Doped Carbon-Assisted One-pot Tandem Reaction for Vinyl Chloride Production via Ethylene Oxychlorination. Angewandte Chemie International Edition 2020, 59 (49), 22080-22085.

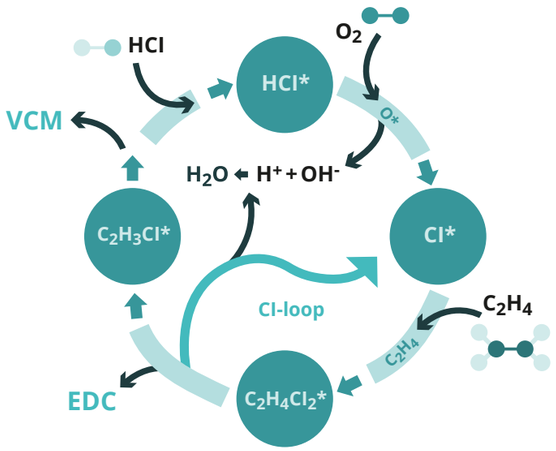


Figure 1. The suggested reaction mechanism, including a Cl-loop between ethylene oxychlorination and EDC dehydrochlorination, for producing VCM in a single-step on a metal-free carbon catalyst.

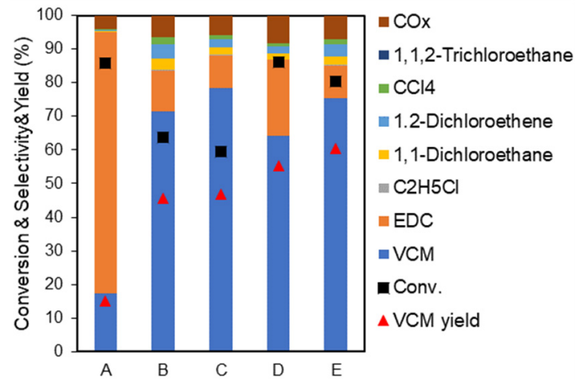


Figure 2. Catalytic results of the dual-bed method (CeCu/ /γ–Al_2O_3 at the top, N0.5 at the bottom) with different mass ratios: (A) 1:1; (B) 1:4; (C) 1:9, (D) 1:2; (E) 1:5, with the total mass of 1 g for A, B, C; 1.2 g for D and E.

The value of knowledge

"Being innovative and presenting a proven technology based on industrial and scientific experience is a key for building customer trust and loyalty in technology licensing. One way to achieve in-depth know-how is through being part of the iCSI Centre."

The statement above belongs to the general manager for Licensing & Projects, Lars Axelsen, at Dynea's Technology Centre in Lillestrøm. They are one of iCSI's industry partners, and he acts as their representative on the iCSI Board.

The history of the Dynea AS company goes back to 1947, when they first started producing formaldehyde and resin, mainly for the wood working industry. Over a period of five decades, the company was the chemical branch of Dyno Industries, once the world's largest producer of explosives.

With Norway and Lillestrøm as their home-base, Dyno, which for the last 20 years has been named Dynea, developed the process technology. They expanded the product range and grew to become a truly international company with production and sales on every continent, based on internal innovations and development.

"The licensing of our process technology has enabled Dynea to continue to develop our own formaldehyde plants and to benefit from the operational and process know-how to build up a separate profit unit for technology licensing within in Dynea," Axelsen says. "Dynea today owns the trademark fasil® for its Silver Catalyst Formaldehyde Technology, used to produce Formaldehyde which we are licensing. Revenues in 2020 for fasil® licensing came to NOK 100 million."

Formaldehyde is a C1 reactive molecule used in several processes as an "intermediate", and it is a building block to make materials and products which are in daily use by most people in the world today. They include paints, synthetics, thermoplastics and all kinds of wood products, which today is a key factor for using wood in a sustainable way.

"The catalyst development is an important part of our innovation work to improve the technology, by reducing raw material consumption (methanol), increasing the yield and reducing the CO_2 emissions, hence we are part of iCSI," he continues.

In addition to having an improved catalyst, Dynea transfers the knowledge from the iCSI research internally, as well as to their customers. A good overview and understanding of process build confidence and make it easier to have a more tailored marketing approach.

Many of Dynea's customers belong to a group of the 10 largest petrochemical companies. They currently have four licensing projects in development, two in the USA, one in Russia and one in Germany.

Dynea's long-term experience in producing formalin for its own use, years in conducting the license projects and efforts used to improve the process and the catalyst have been, are and will be important during the customer selection process. These customers have many skilled and professional engineers with excellent chemical and process know-how which challenge Dynea each day to improve the process and the way they work. Dynea's knowledge in the areas of *process, catalysis and how to work as part of larger project complexes in many different cultures* are important keys to their success.

"All our projects are headed by a relatively small group in Dynea, so the knowledge we gain from the catalyst testing in pilot reactors, kinetic modelling, and PhD research under the supervision of Professor Hilde Johnsen Venvik is of great value both in the sales process and during the realisation of a project," Axelsen concludes.

Catalyst filling in a new process unit. How the reactor is filled is crucial for the process performance. Filling procedures are based on process and catalyst knowledge combined with decades of operational experience.

Lars Axelsen in Dyneas formaldehyde production unit in Lillestrøm.

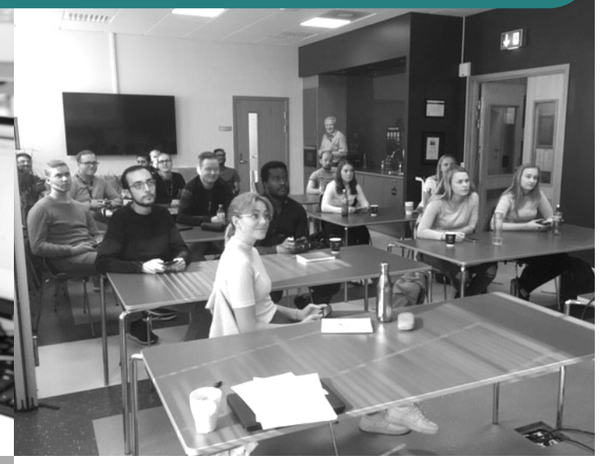
iCSI moments 2020

Summer, sun and soon graduating

Young researchers seminar in February

iCSI associated PhD defense at NTNU

Specialization students: HMS in theory and practice



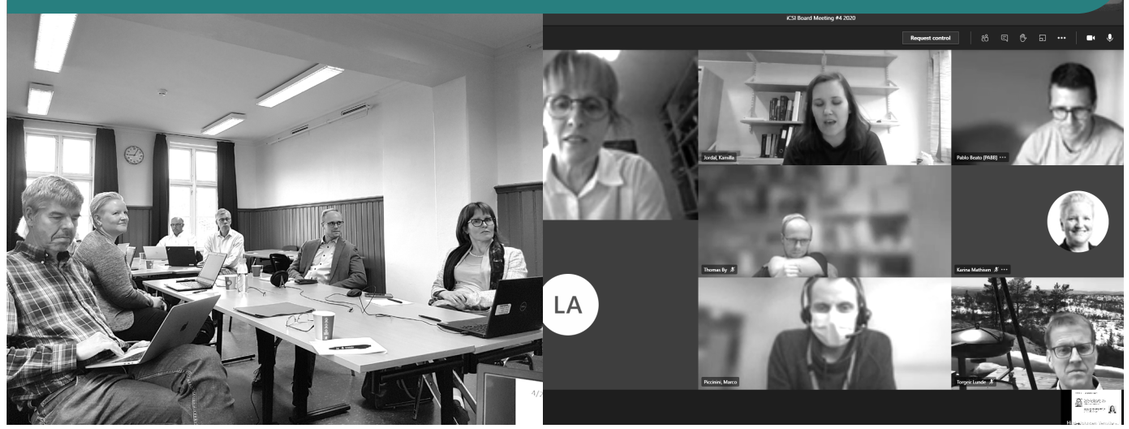
A new friend (finally) arrived from China

Annual seminar in September

Thanks and goodbye Odd-Arne Lorentsen

SAC delivers digitally!

Boardmeeting physically and digitally



Professor free zone

On 26 and 27 February, 14 PhD candidates, postdoctoral fellows and industry researchers gathered at Haldor Topsøe's facilities in Lyngby outside Copenhagen. This was a continuation of the series of "professor-free" workshops for iCSI's young researchers that started in 2018. The idea is to let the researchers meet the "real world" and gain insight into the challenges facing the industry. For the industry, this is an opportunity to meet young people with up-to-date knowledge and potential candidates for their recruiting base.

The first day, experienced researchers from Topsøe and Yara contributed with presentations on "Advanced operando techniques – from atomic scale to industrial reactor", "Nitric acid production – from a catalyst point of view" and "Patenting and IP strategy". The talks by invited speakers were followed by the young scientists from universities and industry giving a brief overview of their own work and then opened up for discussion and input from the group. The first day concluded with socializing over dinner at a nice Copenhagen restaurant.

The second day was spent at the Topsøe catalyst plant in Fredrikssund, showing large scale catalyst production.

iCSI is privileged to have committed industrial partners who see the value of such events, introducing our candidates to industry challenges. Thanks to Haldor Topsøe for hosting the 2020 workshop!

Walk and talk: iCSI Board Chair Pablo Beato from Haldor Topøe (centre) in discussion with young researchers from NTNU

Thomas By from K.A. Rasmussen introducing the scientists to his company's challenges

Digital meetings with SAC

An enthusiastic professor Alessandra Beretta giving an inspiring lecture for about 50 listeners

Due to the travel restrictions in this year of the pandemic, the iCSI Annual Seminar was held without any members from the international Scientific Advisory Committee (SAC) being able to attend. To compensate for the absence of scientific input and corrections from the committee, several digital meetings were arranged where they could contribute their knowledge.

Enrique Iglesia and Alessandra Beretta each gave a digital guest lecture, which drew a large number of participants from the iCSI partners as well as from the two professors' home universities. As shown in the screenshots below, Alessandra's engaging manner goes right through the screen and out to the audience. After the lectures, there was time for questions and good discussions. One of the industry partners commented that this type of lecture should be on the agenda even after the pandemic, due to the easy access for everyone to lectures of high relevance and quality.

In addition to the guest lectures, there were two days of individual discussions between the two professors and young iCSI researchers. On 16 June two PhD candidates well along in their studies met Iglesia and Beretta, while one PhD and one Postdoc met professor Beretta on 4 November. According to the candidates, being challenged by world leading scientists was a unique and highly valued opportunity.

DIGITAL LECTURES

Enrique Iglesia, 18 June:

Redox cycles in oxidation catalysis:

C-H and O=O activation pathways

on metal oxides

Alessandra Beretta, 30 October:

NH3-SCR over V-based catalysts:

Kinetic investigation on the role of NO + O_2 in the reduction and reoxidation steps of V redox cycle

Seminar – lecturers

Annual Seminar

When the pandemic hit us in March, we had to postpone the planned Annual Seminar, and we didn't know if it would be possible at all to gather with people during the year. Luckily for us, there was a period with low infection numbers through the summer, and in September up to 200 people were allowed to gather. Since most people at this time were bored and frustrated and missed getting together to share results and discuss science, we took the opportunity to arrange this year's seminar.

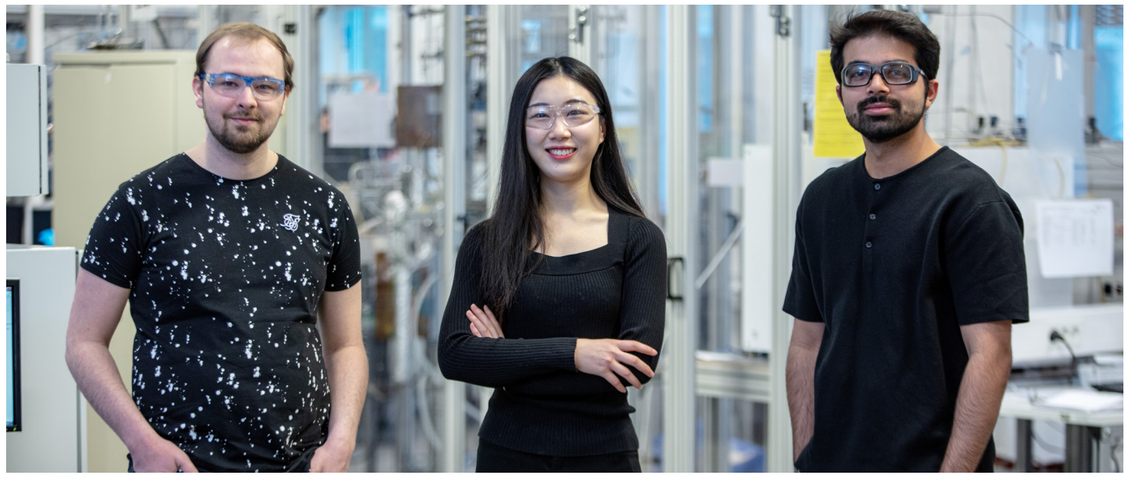
Forty people from the industry partners, UiO, SINTEF and NTNU convened in beautiful surroundings at Oscarsborg Hotel from 14 to 15 September. After the long time spent in isolation at the various locations, it was refreshing to have the chance to meet again in person (though still maintaining one meter distancing and applying a lot of disinfectant). In retrospect, we know that for most of us, this was the only opportunity to meet in this way in 2020.

Several new doctoral candidates and postdocs had the chance to get to know their iCSI colleagues in organizations other than their own. Another 14 people, who did not have the opportunity to travel, attended the seminar via streaming in a Zoom meeting. This was done for the first time, and was appreciated by those who for various reasons had to be at home.

Despite the COVID-19 shutdown, the presentations and posters showed that there has been significant experimental production over the past year. The same can be confirmed by the long list of publications that are already out or have been submitted and are in revision. The project is now characterized by knowledge maturing over several years, and we have gained a more basic understanding of the industrial issues that have been addressed.

Before we departed for home, the next annual seminar was announced: Hovde Gård outside of Trondheim is booked for two days in June 2021 – let's hope it's possible to meet again there.

Researcher corner: Meet the three new PhDs - Youri, Wei and Jithin



We welcomed three new PhD candidates from three different parts of the world who all met iCSI with its projects, people and culture in September 2020: Jithin Gopakumar from India and Dubai, Wei Zhang from China and Youri van Valen from the Netherlands. We sat down with them to have a chat about their backgrounds, expectations and experiences so far with iCSI, and what it's like to be at NTNU and in Trondheim.

We wondered what makes three young people travel such a long way to start a PhD programme in the catalysis group at NTNU. The reasons are many and varied. For Youri, the simple answer is love. He met a Norwegian woman doing her master's degree at NTNU, and wanted to live with her. When looking for jobs in Trondheim, the possibility of starting a PhD within iCSI came up. He found the combination of going in depth academically while collaborating closely with industry partners especially interesting. He had positive experiences with internships in industry in his bachelor's and master's studies in the Netherlands and wanted to have more of the same. NTNU's good reputation made the choice easy, and he was happy to be considered qualified despite some gaps in catalysis knowledge. His long-term career plan is to become a teacher at a college. But Youri's best teachers from his school days were those with hands-on experience in the subject before they started teaching. He wants to achieve this himself before moving to teaching.

> "When discussing with Prof. De Chen, it was my first time I realized there would be someone who really takes a keen interest in science."
>
> *Wei Zhang*

The path to science was quite different for Wei. She did not plan an academic career at all – until 2018 when she met Professor De Chen, who then was a guest researcher at her previous university. "I was totally attracted by his insightful and inspirational comments and motivating discussions. It really motivated my interest in research, and I want to follow in his footsteps," she says.

Jithin was already at NTNU as a student in the international master's programme at the Department of Chemical Engineering, and he wanted to remain in Trondheim and the catalysis group. In fact, he was one of four of last year's master students continuing with a PhD in the same group. Even though he has no clear plans yet, he sees himself in a future career in industry, and preferably in research. Like Youri, he appreciates iCSI's close relationship with industry, and he has never before experienced working so closely with actual

> "The work culture - this is still a big shock to me. People are very free and informal"
>
> *Jithin Gopakumar*

problems. This is something he really enjoys. Jithin tells us that he has moved several times in his life and has no specific place he calls home, other than where his parents live. He might stay in Trondheim and Norway for some years after his defense but is also open to travelling to other places with job opportunities.

We asked if there was anything that has surprised them here in Norway, and what they found different from home. They agreed that the way we collaborate, help and support each other in the catalysis group was unexpected – and they like the way we do it. Using the first name of the professors instead of "Sir" or "Professor" was a bit strange at the start, but now they feel more comfortable with it. They see that respect between people doesn't comes from titles, but rather from what we know, what we do and how we treat each other. Youri was surprised to be invited to the Annual Seminar after only two weeks at iCSI, and was glad for the opportunity to become acquainted with colleagues and industry partners. Wei agreed, and said that for her the seminar was her very first day in iCSI after her arrival and travel quarantine. A very nice start!

> "I went on a "fake stay abroad."
>
> *Wei Zhang, referring to the restrictions due to the pandemic*

They were all warmly welcomed, and different student groups at the university helped them to find new friends. Especially in the pandemic situation it is good to have friends and colleagues that care about you. But of course, the limitations set by the pandemic are frustrating and make the "Norwegian experience" a bit different than planned. That said, they realize there could have been even worse places to be this year.

At work, Jithin does not have a lot of challenges, and everybody is very helpful. "But it's a kind of closed atmosphere at times – an everyone-for-themselves mode," he says. The strict attitude to HSE guidelines and routines in the lab is a bit unfamiliar for all three. That you cannot even gain access to the lab without a

> "What could improve a bit is if the university could offer a little guidance with getting a foreign PhD set up in Norway."
>
> *Youri van Valen about bureaucracy*

completed risk assessment is a new experience. They find most things well organized and facilitated, and they appreciate that they have to do a lot of the practical laboratory work themselves. Through that they are gaining a lot of process knowledge as well as a critical attitude toward analytical results.

Youri has had his run-ins with the administrative side of NTNU, but he doesn't know if it is bad luck or if he doesn't understand the system. It is quite a maze of bureaucracy to navigate, and the order in which to do things isn't always clear.

Wei's largest challenge so far is communication. It is difficult for her to express herself in English with much accuracy, and she feels she needs more time to improve. Jithin misses having more social events with the group. Since he started the PhD during the pandemic he doesn't know how it normally is. What he does know is that things have been quite dull socially since he started. Travelling, which he loves doing, isn't possible, so instead he's spent a lot of his free time indoors with painting, cooking and solving puzzles.

Youri spends much of his free time outdoors. He loves snowboarding and likes the easy access to areas with ski resorts. He and his girlfriend have also gotten quite a taste of the hikes around Trondheim and are exploring the trails in Bymarka. Wei, on the other hand, has stopped running and dancing which she used to do and now prefers to just keep life as simple as possible.

However, regardless of their varied interests and hobbies, they all agree on one thing: "You are the best – and we look forward to going out again, having a beer among good friends and you colleagues!" .

Scientific Activities

Scientific Activities

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

IIA1

21st Century Ammonia Oxidation and Nitric Acid technology development

WP1.1 WP1.2 WP1.3

NTNU · University of Oslo · SINTEF · YARA · KA Rasmussen

IIA2

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

WP2.1

SINTEF · YARA

IIA3

Frontier formalin technology development

WP3.1 WP3.2 WP3.3

NTNU · SINTEF · KA Rasmussen · dynea

IIA4

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

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

NTNU · SINTEF · inovyn

IIA5

The next step in direct activation of lower alkanes

WP5.1 WP5.2 WP5.3

HALDOR TOPSOE · SINTEF · University of Oslo

IIA6

Generic projects for additional industrial synergies

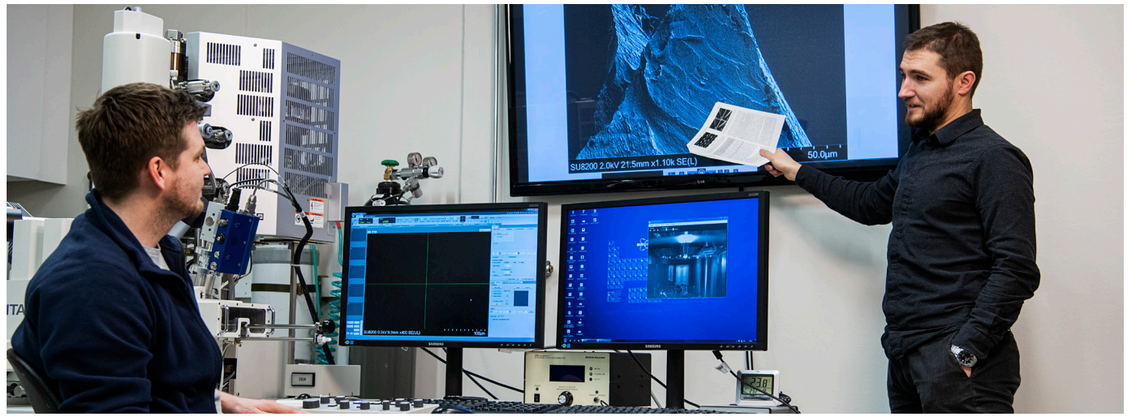
WP6.1 WP6.2 WP6.3 WP6.4 WP6.5

NTNU · University of Oslo · SINTEF · dynea · inovyn · HALDOR TOPSOE · YARA

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

The IIA1 team 2020

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)
Oleksii Ivashenko	UiO	Postdoctoral fellow (WP 1.1)
David Waller	YARA	Industrial senior (Yara), PhD supervisor (WP1.1), industry researcher (WP1.2-1.3)
Ketil Evjedal	YARA	Industry researcher (WP 1.1)
Siri-Mette Olsen	YARA	Industry researcher (WP 1.1)
Torgeir Lunde	YARA	Industry researcher (WP 1.1-1.2)
Sang Baek Shin	YARA	Industry researcher (WP 1.3)
Johan Skjelstad	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Thomas By	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Terje Pedersen	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, researcher (WP1.3)
Bjørn Christian Enger	SINTEF	Researcher (WP1.3)



Publications IIA1
Publications and conference contributions are listed on page 65.

$LaNiO_3$ as Pt catchment material

The exothermic nature of the ammonia oxidation reaction results in loss of platinum from the PtRh catalyst in the form of PtO_2 vapor. Much of the lost platinum is recovered on Pd-Ni catchment gauzes installed downstream of the PtRh catalyst. In the catchment process, PtO_2 is incorporated as Pt to the Pd-Ni alloy. However, this catchment system suffers from severe reconstruction and Pd-loss.[1] Alternative systems, based on noble metal alloys or oxides, are currently under evaluation. In the following, we report on our preliminary findings for the oxide system $LaNiO_3$.

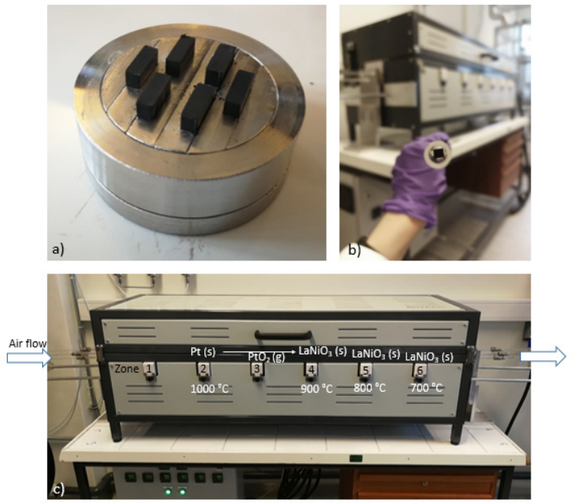


Figure 1. (a) Rectangular pellets of $LaNiO_3$ (b,c) placed upstream of a Pt source in our 6-zone furnace during the catchment experiments.

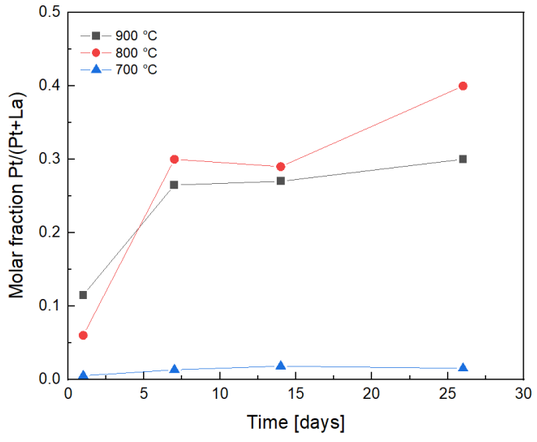


Figure 2. EDX results for the 12 pellets from catchment experiments with duration time 1, 7, 14 and 26 days at 700, 800 and 900°C.

Pt catchment experiments in our 6-zone furnace (Figure 1) proves that $LaNiO_3$ is catching platinum at industrial relevant temperatures (800-900°C). Powder X-ray diffraction (XRD) data proves that La_2NiPtO_6 forms and energy dispersive X-ray (EDX) analysis of the pellet surface after catchment experiments with duration times of 1, 7, 14 and 26 days at 700, 800 and 900°C show the presence of platinum in all samples (Figure 2). The Pt/(Pt+La) molar fraction for the double perovskite La_2NiPtO_6 has a theoretical maximum at 0.33, which the samples at 800 and 900°C approach at longer duration times. For the sample showing a Pt/(Pt+La) molar fraction of 0.40, also pure Pt crystals are observed on the surface (Figure 3).

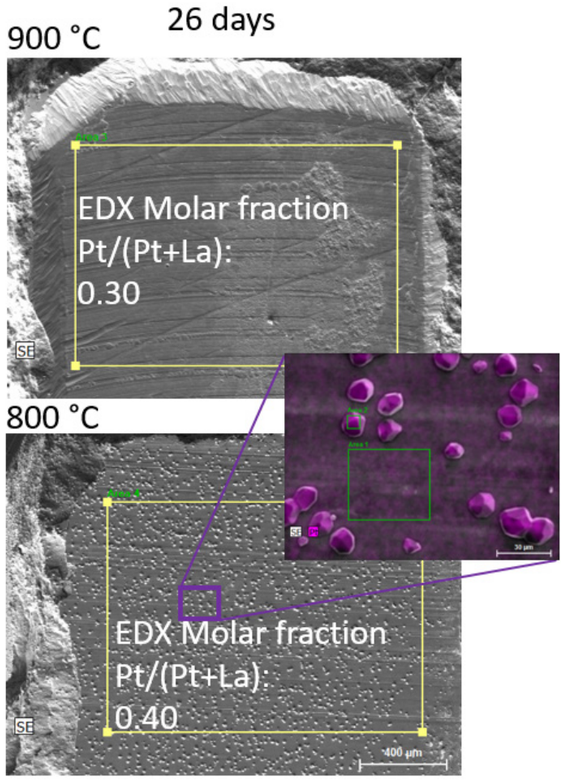


Figure 3 . SEM-EDX maps show pure platinum crystals at the surface for the pellet run at 800°C for 26 days, with a Pt/(Pt+La) molar fraction of 0.40. The sample run at 900°C for 26 days, with a Pt/(Pt+La) molar fraction of 0.30, did not have such crystals at the surface.

References: 1.Fjellvåg, A. S., Waller, D., Skjelstad, J., Sjåstad, A. O. Johnson Matthey Technol. Rev., 2019, 63, (4)

Experimental investigations of Pt/PtRh volatilization and catchment - can SIMS (Secondary Ion Mass Spectrometry) analysis of Pt in Pd be trusted?

Pt catchment is a process where platinum lost from the ammonia combustion gauze in the form of PtO_2 vapor, is caught on a palladium gauze downstream to allow regeneration of platinum. To understand this process there is a need to measure the concentration and diffusion profiles of Pt in a Pd sample. The dynamic SIMS instrument at the University of Oslo seemed to be a good candidate, even though SIMS is known to be a "semi-quantitative" technique since it can be difficult to obtain exact concentrations without reference samples. An annealed sample with 1 wt% Pt in Pd has been studied extensively by SIMS and other techniques. An Electron Back Scatter Diffraction (EBSD) analysis showed that the sample was polycrystalline with many different grain orientations represented (Figure 1; left part). Twenty grains were selected for SIMS analysis where three craters of 100 µm by 100 µm were sputtered in each grain. Later, seventeen more craters were analysed within grain number 183, with the sample rotated 10°degrees between each analysis (Figure 1; right panel)).

Among the twenty grains analysed initially, the count rates of Pt and Pd ions in the SIMS were quite consistent within each grain. But in some grains the Pd count rate was particularly high or low (Figure 2, left panel). In other grains it was the Pt count rate which was different from the other grains (see blue ovals in chart). It is known in SIMS that the so called "channeling effect", where the incoming and outgoing atoms move more easily along close-packed crystal directions, may give sputtering yields that differ with crystal orientation. But these effects are generally small, in the sub-percent range. When calculating the Pt/Pd ratio from the 20 grains, some grains gave four times as high ratios as other grains.

What about the Pt/Pd ratio measured within grains which in the first experiment was quite stable? What if the incoming primary beam entered the grain from a different angle? To test this, the sample was rotated about 10° between analyses inside grain 183 (see top right and bottom right figures). Here the sample had been exposed to PtO_2 vapor, so a Pt concentration gradient had formed from the surface to a depth of about 2 µm. Even inside the same grain, the Pt/Pd ratio curves differ in absolute values by up to 5 times. If such curves were used to extract diffusion coefficients, the coefficients would also differ by a factor of 5. But since diffusion within the same grain is likely to follow one single diffusion coefficient, this study has shown that one needs to be very careful when interpreting SIMS data from PtPd alloys.

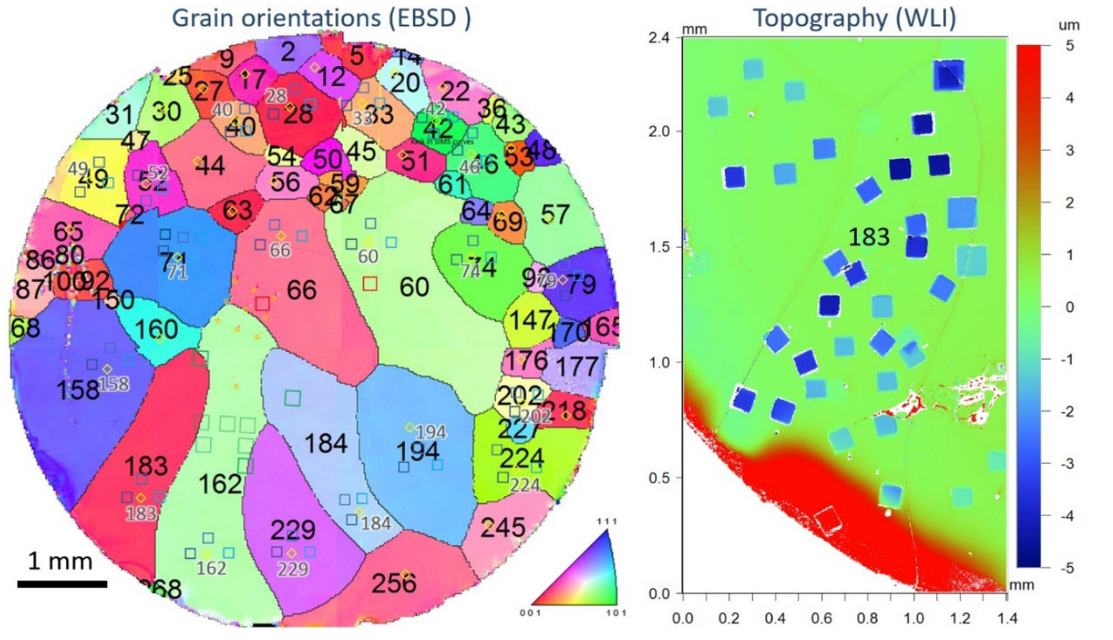


Figure 1 Left side: EBSD grain orientation map where the color coding shows the crystallographic orientation of the grain surface normal. Small squares show the location and size of various SIMS craters. Right side: White Light Interferometry (WLI) topography image of grain 183 after SIMS analyses where the sample was rotated 10° around its surface normal between each run. The sputtering conditions were identical, but the crater depth differed by a factor of 2.

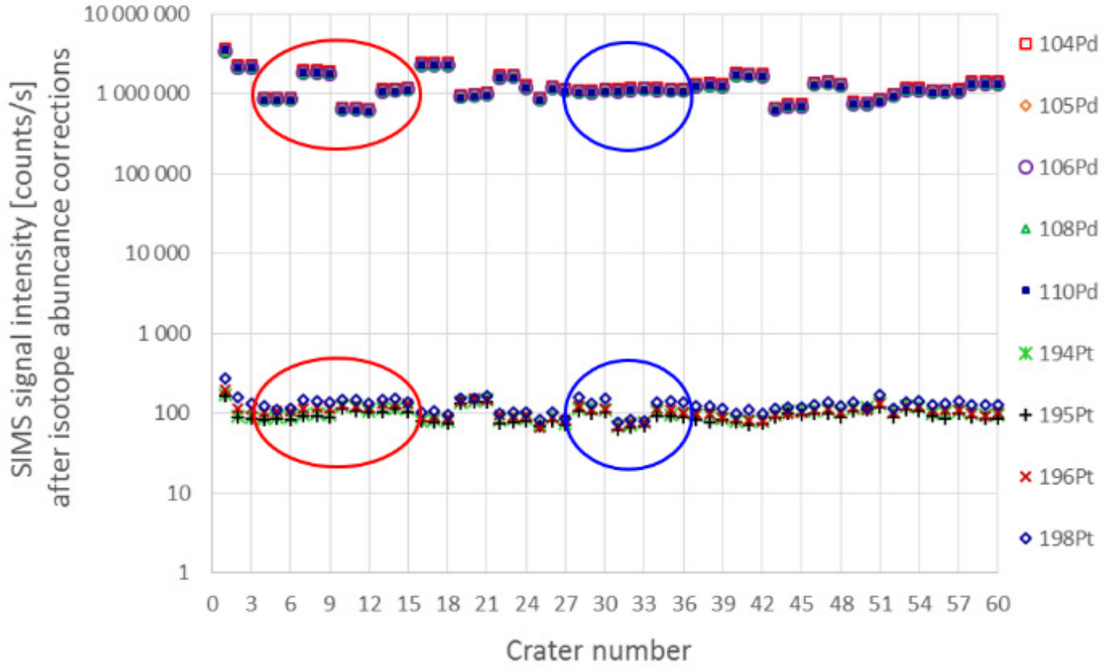


Figure 2 Top: SIMS count rates for five Pd isotopes and four Pt isotopes after abundance correction for three parallels made inside 20 different grains. Bottom: SIMS depth profiles within grain number 183 from the same sample after Pt deposition. The values of the Pt/Pd ratio vary by a factor of 5 in a non-systematic way with incidence angle.

Catalytic oxidation of NO to NO_2 for nitric acid production

Nitric acid is one of the most important industrial chemicals, whose first production dates to the 8th century. Earlier production of nitric acid used potassium nitrates and sulphuric acid as raw materials, which were then replaced by sodium nitrate in the 19th century. The present-day commercial production of nitric acid uses a hundred-year-old process called the Ostwald process. Wilhelm Ostwald patented this three-step or two-stage process in 1902. Several decades of research on this process exist, and it has been the cornerstone of many chemical industries to produce the raw material for fertilizers and other chemical commodities.

The Ostwald process comprises three important chemical steps: (i) oxidation of Ammonia using Pt/Rh gauzes at high temperature to produce nitric oxide, (ii) a homogeneous gas phase oxidation of nitric oxide to nitrogen dioxide, (iii) absorption of nitrogen dioxide with water to produce nitric acid.

Conversion of NO to NO_2 is one of the few known third-order gas phase reactions, with inverse Arrhenius behaviour. Commercially a series of heat exchangers are used to recover heat and produce NO_2 more economically. Converting this homogeneous gas phase reaction to a catalytic reaction is challenging but beneficial, as it leads to (i) significant increase in heat recovery, (ii) accelerated oxidation reaction and (iii) substantial decrease in capital expenditure (CAPEX) for new plants.

The thermodynamics of the reaction is favoured by low temperatures whereas catalytic activity is usually favoured by higher temperatures. Additionally, the high concentration of nitric oxide and presence of water in the feed are the main challenges preventing this reaction from being performed catalytically. Hence, to this date there is no catalyst that can convert NO to an extent where equilibrium is attained at industrial conditions.

The first phase of this project concluded with the manganese on zirconia catalyst being the most promising, and that the catalyst onset temperature had to be same for both NO conversion and catalyst reduction. Literature suggests the manganese (Mn) based catalysts shows good catalytic oxidation for nitric oxide at low temperatures.

The preferred catalyst working conditions are 200-250°C and 4 bar pressure. The current work aims to find an efficient catalyst for oxidizing NO to NO_2 at these operating conditions, and thus enabling significant process intensification of the nitric acid production plant.

A dedicated experimental setup was already built in the first phase of this project, capable of catalytic activity investigation at atmospheric conditions. The major challenge of this project is to reduce the gas phase conversion as much as possible. Hence, the reactor had to be modified initially to dose the NO near the mouth of the reactor so as to mix the gases closer to the catalyst bed than before (Figure 1).

An additional goal of this project is to investigate and understand the reaction kinetics and the mechanism of oxidation of NO over promising catalysts. Manganese on zirconia is a promising catalyst, and promoting it with noble metals will improve its performance. Platinum, which shows good catalytic activity without the presence of water and silver, which is popular for formaldehyde production via oxidative dehydrogenation of methanol, were two promising candidates as promoters Another benefit of silver is the ability to decompose N_2O upstream of NO oxidation in a nitric acid plant.

A total of six zirconia-supported catalysts were made, each with two different loadings of manganese and two promoters (Pt and Ag). The seventh catalyst is 5wt% silver on zirconia, to observe the performance of silver alone in comparison to manganese.

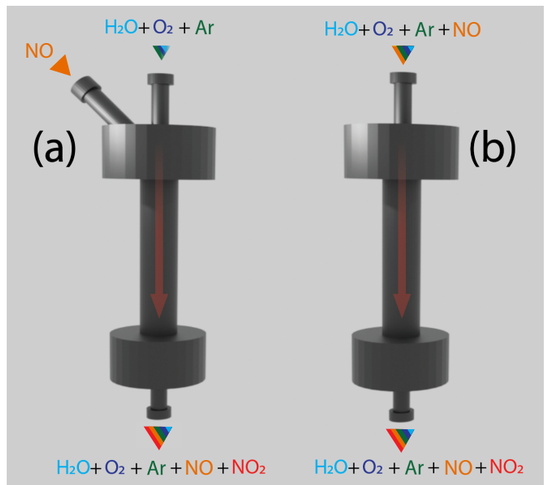


Figure 2 : (a) Modified reactor – Nitric oxide dosed separately; and (b) Old reactor – Nitric oxide mixed with other reactants

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

The IIA2 team 2020

Jasmina Hafizovic Cavka	SINTEF	IIA leader
David Waller	YARA	Industrial senior YARA, industry researcher
Karl Isak Skau	YARA	Industry researcher
Siri-Mette Olsen	YARA	Industry researcher
Bente Furevik	YARA	Industry researcher
Torgeir Lunde	YARA	Industry researcher
Silje F. Håkonsen	SINTEF	Researcher and WP responsible
Martin F. Sunding	SINTEF	Researcher
Patricia Almeida Carvalho	SINTEF	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 biproduct. The levels of N_2O might appear to be low but the high Global Warming Potential (GWP) of N_2O of 298 meant that it used to account for 50% of Yara's Greenhouse Gas (GHG) emissions. Yara developed an abatement catalyst that is located directly below the platinum-based oxidation catalysts. The catalyst consists of a Co and Al spinel phase supported on CeO_2. This catalyst can achieve >95% abatement with no changes to plant operation. The deN_2O catalysts 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 studied to better understand the transitions in the catalyst with the aim to formulate even more active and stable catalysts

Research project

Fresh deN_2O catalysts that have been in operation in a commercial nitric acid plant at various times on stream have been investigated by light microscopy 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 are shown in Figure 2. The fresh catalyst has a homogeneous green colour through the cross section, while a homogeneous light bluish 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 (the blue square indicates the positions analysed with SEM-EDS).

Figure 1. Fresh catalyst pellets of the type investigated in the study. Pellet length 1 inch.

The same samples were investigated using SEM-EDS. An EDS line scan of the cross section of the fresh sample showed uniform levels of Al and Co with a Co:Al ratio of 2. Analysis of the sample that has been on stream for four years also shows uniform Co and Al levels, but with a Co:Al ratio of 0.5. The shift in Co:Al ratio is attributed to loss of Co.

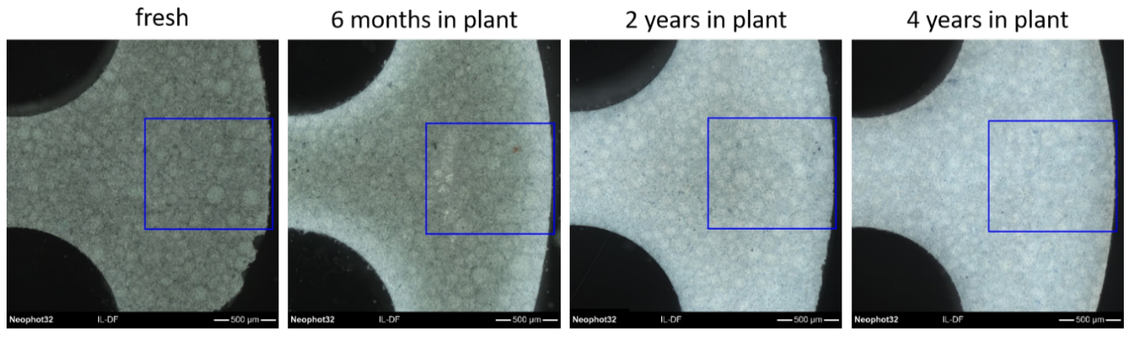


Figure 2. Light microscopy, dark field illumination image of polished cross-sections of catalyst pellets after varying times in plant

An 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 (blue line) that corresponds to the colour change observed under light microscopy. Uniform concentration of Al (red line) 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.

We believe that Co is lost from the sample during operation as evaporative loss of $Co(OH)_2$, until a more stable spinel phase $CoAl_2O_4$ is formed throughout the sample. This loss starts at the surface and moves as a front into the core until the original Co_2AlO_4 spinel phase is transformed to $CoAl_2O_4$. XRD and TEM results support these findings. Calculations on the thermodynamic activity of cobalt in the Co_3O_4-$CoAl_2O_4$ solid solution series indicate that decreases in activity to a very low level when the $CoAl_2O_4$ composition is approached, explaining why little cobalt loss is observed after very long plant exposure times.

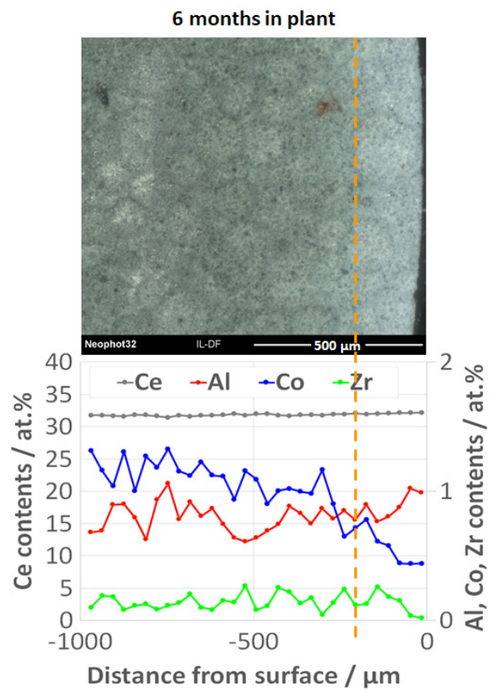


Figure 3. Catalyst sample after 6 months on stream. Top: Light microscopy, dark field illumination image of polished cross-sections (blue squere in Figure 2). Bottom: SEM-EDS line scan of the cross section.

Publications IIA2

Publications and conference contributions are listed on page 65

IIA3: Frontier formalin technology development

The IIA3 team 2020

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Motivation
Formalin is a base chemical that is widely used in adhesives and resins applied in the wood industry. The production proceeds by catalytic oxidation of methanol to formaldehyde, in excess air over a mixed metal oxide catalyst or excess methanol over a silver-based catalyst. Dynea owns both process technologies, and KA Rasmussen is a manufacturer of silver catalysts. The silver process is assumed to have the highest economic improvement potential, due to lower energy consumption and the possibility of increasing the formaldehyde yield beyond 90-92%.

Gas phase chemistry may play an additional role at typical reaction temperatures exceeding 600°C, at which temperature structural changes in the Ag catalyst also occur that are known to affect both the reaction chemistry and the catalyst stability. The lifetime of the catalyst in industrial operation is in the order of months, depending on parameters such as particle morphology, size distribution and the structure of the catalyst bed in addition to the reaction conditions. Further developments are achievable by a more detailed understanding of the reaction conditions and tuning of the silver particle/bed morphology, thus controlling both selectivity and stability.

The main objective of IIA3 is improving the formaldehyde yield of the silver-based process. The fast and exothermic nature of the reactions involved requires control of the heat and mass transfer phenomena as well as the surface chemistry proceeding on the silver surface.

The three work packages are partly integrated through addressing the reaction kinetics and the nature of the Ag species (oxide) affecting the reaction chemistry (WP3.1), the effect of reaction parameters under industrial operation (WP3.2), and further development of mechanistic and reactor models (WP3.3).

Micro-detailing of methanol to formaldehyde (MTF) chemistry on electrolytic Ag

The research activity in IIA3-WP3.3 supported by IIA6 (DFT, Yanying Qi) aims to progress beyond state-of-the-art regarding the silver catalyst, its oxygen dynamics and interplay with the detailed kinetics of the MTF reaction. Microkinetic descriptions have been established and used to test hypotheses and thereby reveal new knowledge.

Topics targeted in WP3 are given as:

- Parameter dependencies (T, P, xi) on the relative and overall contribution of oxygen species (O_2-, α-O and γ-O) to MTF performance.
- Identification of alternative pathways, for example to CO_2 and H_2, to clarify whether these are primary or secondary products, or both.
- Kinetics at surface species level and significance of surface termination, for example Ag(111) and Ag(110).
- Interplay between gas phase and catalytic chemistry.

A fundamental puzzle
The functionality of the silver catalyst is complex. It is well known that several oxygen types are formed upon chemisorption and subsequent steps, including surface and bulk species. Figure 1 shows a principal illustration of main chemistry and oxygen species. The most common principal types in literature are the three surface species, O_2-, α-O, γ-O and then bulk β-O formed by dissolution of α-O in the Ag crystal lattice. It is generally agreed that there is a dynamic cycle from α-O via β-O to γ-O, and that diffusion of O atoms in Ag is important. All surface oxygen types are important to the catalysis, including the reactive O_2-, the α-O and the more stabilized γ-O. The catalyst morphology – and consequently the behaviour – adapts to changes in temperature and feed composition – meaning that the low surface-area, largely non-porous, Ag particles are in a dynamic steady-state without a fixed number of physically pre-defined active sites. The active sites/phases are partly created via the oxygen dynamic oxygen cycle and evolving morphology changes.

Global versus microkinetics
While global kinetic models are highly useful for predicting reaction behaviour on a macro-level (conversion and selectivity) within defined ranges of conditions, they are not based on an in-depth understanding of the underlying chemistry at site and bond level. By introducing adsorbed species, elementary surface steps and reaction intermediates, as well as detailing surface morphology and changes, it is possible to establish a wider perspective and rational hypotheses for optimization strategies with respect to catalyst, bed and reaction conditions. In this way, the microkinetic toolbox constitutes a "theoretical laboratory framework".

A reasonable microkinetic description can only be established if a backbone of knowledge related to pathways, surface state and energetics are available. Energy profiles of candidate reactions with respective activation energies and frequency factors has been established by Yanying Qi (IIA6, DFT). This provided a basis for rational selection of probable intermediates and elementary reactions. It provided refinement of parameters from different types of surface crystallography (Ag(110) and Ag(111)), and elucidated effects of potential adsorbate-adsorbate interactions.

Similarly, kinetic data obtained at low conversion and relevant conditions from WP1 (PhD project Stine Lervold) provided insight into primary product formation, highly useful for assisting pathway selections.

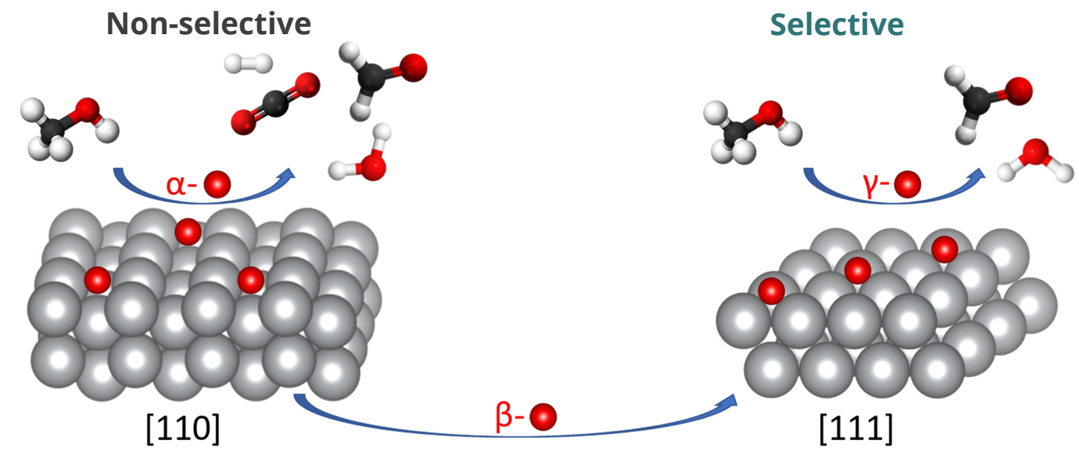

Figure 1: Principal illustration of selective and non-selective reaction pathways over Ag[110] and Ag[111], major oxygen species and their surface/bulk dynamics (Sketched by PhD Youri van Valen]

Main findings

- Pathways and key adsorbed intermediates (HO*, CH_3O*, H_2COO*, H_2CO*, HCO*, H*), and their relative importance for CH_3OH conversion and CH_2O product loss, have been identified and insight to rate-determining chemistries have been obtained. Figure 2 shows examples of conversion – selectivity profiles, while Figure 3 shows the concentrations of molecular components – as a function of time.

- A primary pathway from methanol to CO_2 at low temperature, due to extended lifetime of reactive O_2- on the surface, has been deducted that agrees with experimental observations. Moreover, the selectivity to CO_2 is more prominent on the O_2- and α-O species than on γ-O.

- The coupling with DFT has shed light on the oxygen dynamics of the Ag catalyst: whereas O_2 is very easily activated on open Ag(110), forming α-O, it is much more difficult forming γ-O directly on the more closed Ag(111).

- Dehydrogenation, explaining the significant H_2 formation observed experimentally, is linked to elementary steps involving oxygen and proceeds during both CH_2O and CO_2 formation.

- Catalytic CO formation (HCO*+*↔CO*+H*) is minor, yielding only trace levels (< 1000 ppm).

- There is an interplay: The microkinetic model should be supplemented with gas phase chemistry, for example thermal decomposition of CH_2O, to explain the effect of high temperatures and performance of industrial reactors.

Publications IIA3

Publications and conference contributions are listed on page 65

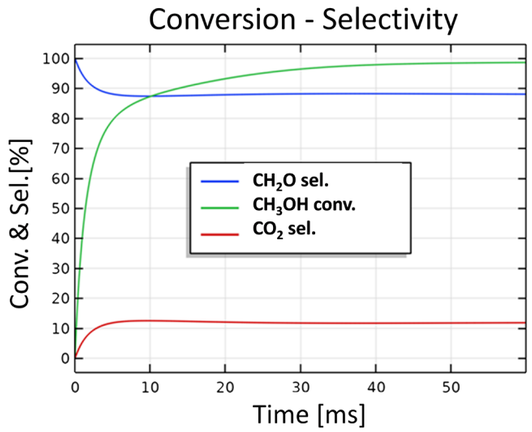

Figure 2. Microkinetic model (923K); CH3OH conversion and selectivity to CH_2O and CO_2 as function of contact time in milliseconds.

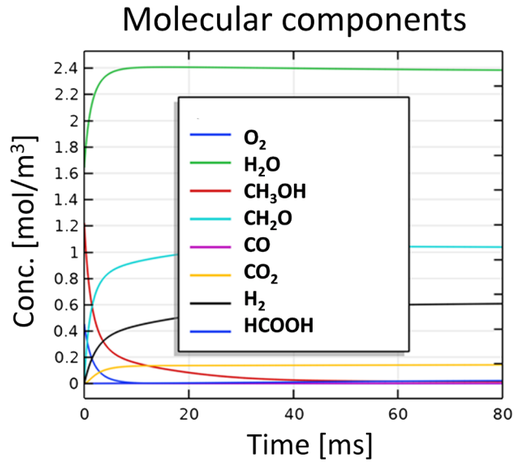

Figure 3. Microkinetic model (923K); Concentrations of molecular components

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

The Team in 2020

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Hongfei Ma	NTNU	PhD candidate (WP4.3 and WP4.4)
Wei Zhang	NTNU	PhD candidate (WP4.3 and WP4.4)
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Kumar R. Rout	SINTEF	Researcher (WP4.1-4.2-4.3)
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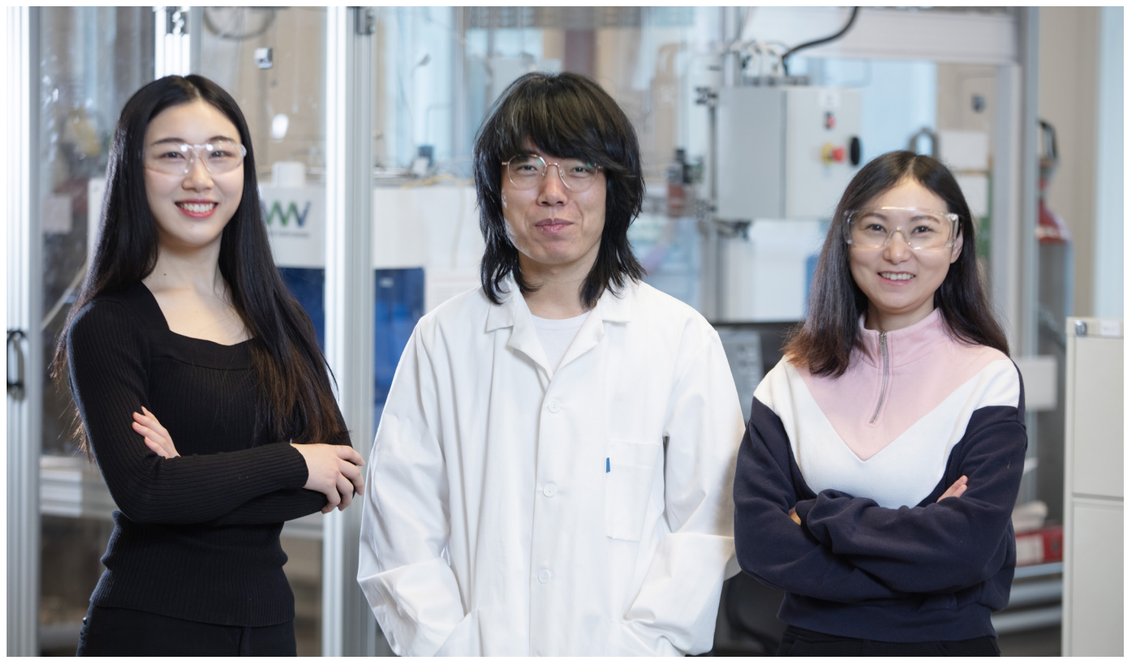


Motivation

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 oxychlorination reaction involves a redox process in which copper cycles between Cu(I) Cu(II) states, as shown in the scheme. 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 intermediates 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:

- 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 $Cu_2O\text{-}Cl_2$, and its hydrochlorination as well as the whole redox cycle at an atomic level.
- Provide a predictive kinetic model to accurately describe for dynamics of active sites and their activity.
- 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 developments.

Dynamic kinetic modeling of Ethylene Oxychlorination to 1,2 dichloroethane (EDC)

The catalytic cycle of ethylene oxychlorination has been studied by a combined experimental and theoretical approach. The activity and selectivity, as well as the evolution of active sites during the reduction, oxidation, hydrochlorination steps, plus at steady-state conditions, were studied experimentally by combined UN-VIS-NIR and MS spectra (Figure 1). The DFT calculation was carried out to get the atomic image of the active site and the catalytic elementary steps in the catalytic cycle.

The kinetic model was also developed for half-reactions of $CuCl_2$ reduction by ethylene and CuCl oxidation by oxygen on the $CuCl_2/Al_2O_3$ and K-doped $CuCl_2/Al_2O_3$ catalysts. By combining the kinetics from two steps, the dynamic kinetic model of the whole cycle was obtained, which accurately describe the evolution of active sites ($CuCl_2$/CuCl ratio) with time at different conditions. By the steady-state approach, the obtained kinetic model

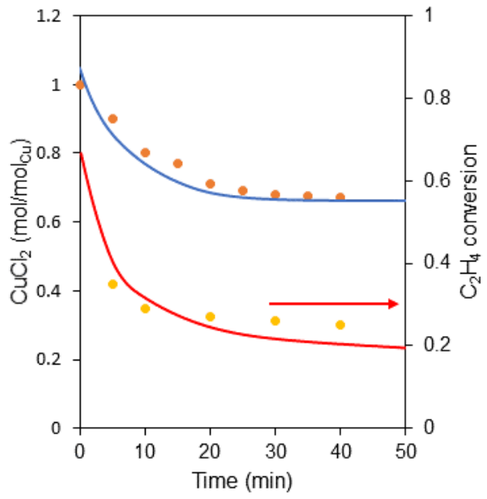
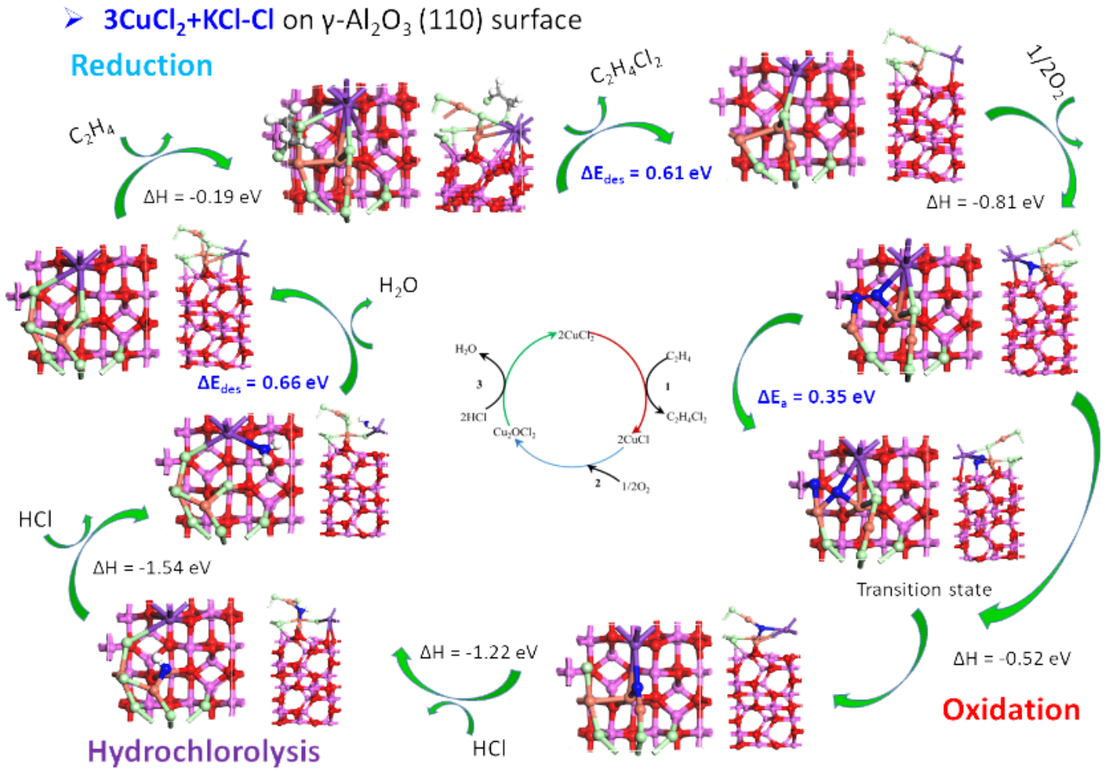


Figure 1. Evolution of $CuCl_2$ fraction in the catalyst (blue line 1.y-axis) and ethylene conversion (redline and 2.y-axis) with time on stream.
Symbols: Experimental data Line: Model prediction



Figur 2. Catalytic redox cycle of 3 $CuCl_2$ + KCl with 1 Cl vacancy

can adequately describe the number of active sites and the steady-state activity at given conditions.

The kinetic model suggests that K promoter lowers the activity of $CuCl_2$ reduction and enhances the activity of CuCl oxidation compared to neat $CuCl_2$ catalysts. A two-dimensional reactor model has been developed to simulate the industrial reactors and accurately predict the temperature, concentration and $CuCl_2$ and CuCl concentrations inside the reactor.

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

The activity and stability of $CuCl_2$ catalysts depend on the coordinated structure of Cu with Cl, where the charge of Cl and Cu and Cl-Cl length were identified as the critical parameters. These parameters can be tailored by promoters. The structure of promoted catalysts on alumina, electronic properties, charge distributions, and energetic profiles of elemental steps were studied by density functional theory (DFT). The structures of the $CuCl_2$ catalysts with alkaline metals and alkaline earth metals with the interface of $\gamma\text{-}Al_2O_3$ were established (Figure 2). The elementary steps in the redox cycle were studied, and the adsorption energies of intermediates and activation energy of elementary steps were calculated and correlated to the surface properties. It provides principles to tailor the surface properties and kinetics of the catalytic cycle.

Publication from IIA4

Publications and conference contributions are listed on page 66

IIA5: The next step in Direct Activation of Lower Alkanes

The IIA4 team 2020

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Sebastian Prodinger	UiO	Postdoctoral fellow (WP5.1-5.2)
Chiara Negri	UiO	Postdoctoral fellow (WP5.3)
Carlo Buono	UiO	Postdoctoral fellow (WP5.3)
Pablo Beato	Haldor Topsøe A/S	Industrial senior and researcher (WP5.1-5.2-5.3)
Bjørnar Arstad	SINTEF	Researcher (WP5.3)

Motivation
Researchers at SINTEF, UiO and Haldor Topsøe AS joined forces to reveal the mechanism of the direct conversion of lower alkanes to chemicals or liquid fuels over copper-doped zeolite catalysts and to develop new nanostructured catalyst materials.

The low temperature activation and transformation of methane – as well as other lower alkanes – directly into valuable chemicals, such as methanol, is commonly considered "a dream reaction" due to its enormous industrial potential. Haldor Topsøe AS supplies essential technology to most existing routes of indirect valorization but is monitoring potential extensions for the current portfolio and the application of zeotype materials.

A different year
The beginning of the second iCSI centre period turned out to be quite different than what we all had expected beforehand.

Within IIA5, the first taste of restriction in 2020 hit us when we went for a scheduled beam time at MAX IV at the end of February. Upon arriving in Lund, we learned that our colleagues from the University of Turin were denied entrance to the facilities. This was a significant bump in the road, and without our collaborator's expertise in X-ray Absorption Spectroscopy (XAS), we did indeed have some difficulties during data collection and data analysis later on. After this trip, it did not take long before we were all placed in lockdown, and all travels, plans and ideas had to be reorganized. It was at this point that a new PostDoc, Dr. Sebastian Prodinger, joined the project and had to spend the first month in lockdown. It is not an understatement to say that it was a tough spring for most of us, with huge changes and uncertainties about the future affecting our days.

That being said, after the first lockdown things slowly started to stabilize into a new normal. We could again enter the labs, and in IIA5, the last half of 2020 has been dedicated to developing new materials and new testing procedures, making us feel very optimistic about the year to come.

2020 Research highlights
In January, we published a paper on the comparison of the nature of active sites in Cu-loaded SAPO-34 and SSZ-13, two isostructural zeolite frameworks. With the use of various spectroscopic characterization techniques, we show that the Cu-siting in the two frameworks is different. And with the use of CH_4- Temperature Programmed Reduction (TPR), we were able to elucidate optimal reaction conditions to significantly improve the methanol yield over the initially inactive Cu-SAPO-34 in the direct methane to methanol conversion.

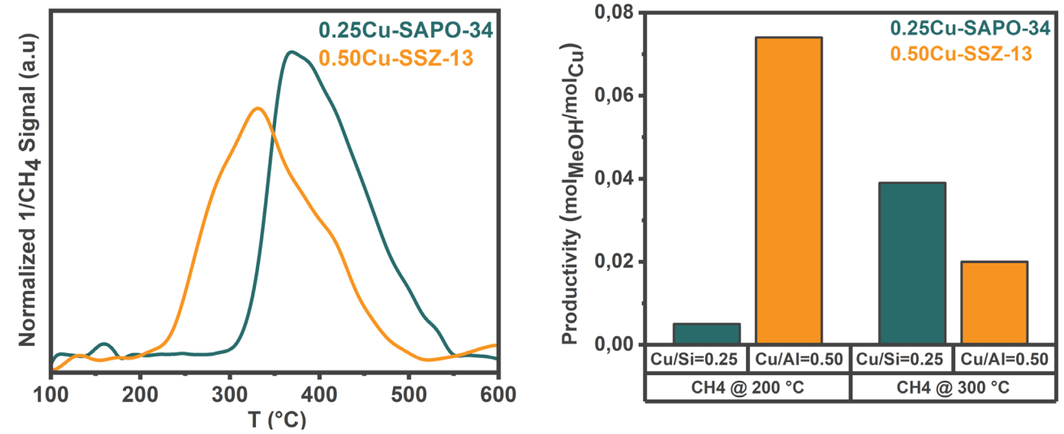

Figure1. On the left, a comparison of CH_4 consumption in SAPO-34 and SSZ-13 collected from CH_4-TPR. On the right, the productivity of Methanol is compared between the two samples, before and after adjusting the CH_4 activation temperature.

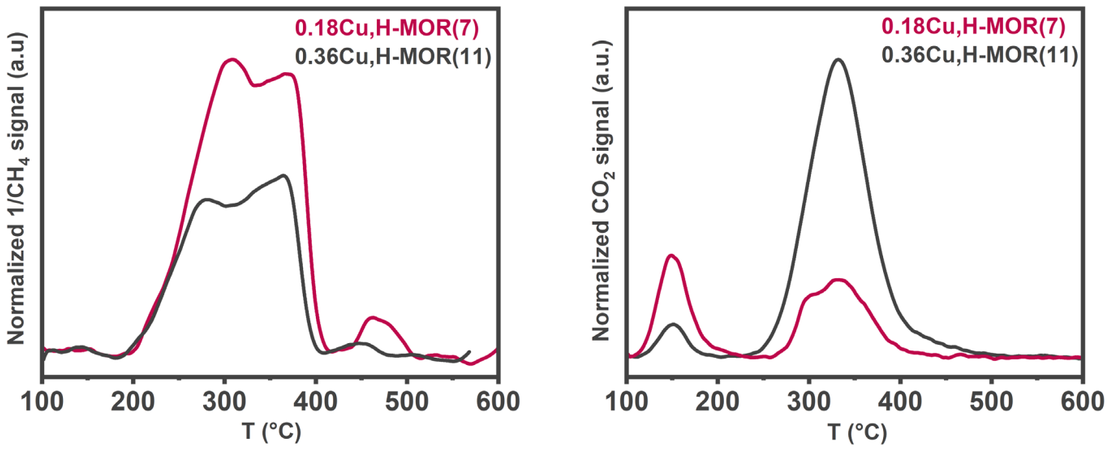

Figure 2. On the left, a comparison of CH_4 consumption in two different MOR zeolites with different Cu-loading, obtained from CH_4-TPR. On the right, the productivity of CO_2 during CH_4-TPR for the two different MOR zeolites are compared.

The beam time at MAX IV, back in February, gave us the opportunity to investigate our well-studied library of Mordenite zeolites with CH_4-TPR, while coupled with X-ray Absorption Near Edge Spectroscopy (XANES). The initial results, indicate that TPR, in addition to aiding in optimizing reaction conditions, can be used as a screening technique to find optimal catalyst materials for the direct activation of lower alkanes. And with a new beam time received at ESRF for the spring of 2021, we look forward to deepening our investigation into the possibilities that this technique can offer. In addition, we aim to see if the new set of XANES spectra enables us to determine how the Cu-speciation changes with temperature in the presence of CH_4.

Exciting new things to come

Building on the excellent knowledge gained on the capabilities of various Cu-loaded zeolites (MOR, FER, CHA) for the oxidation of methane in the first half of the centre period, in 2020 we aimed to delve deeper into the workings of these nanostructure materials. In order to elucidate the structural motifs imparting some of these materials with exceptional activity we spent the last year setting up a new materials library for the subsequent screening in the direct activation of lower alkanes. A new generation of MOR zeolites has been created by fine-tuning the Brønsted site location, using different Al-precursors, and consequently also changing the Cu-speciation inside the frameworks. This enables us to control the number of active Cu sites, a promising strategy towards the development of new nanostructured catalysts in the coming years.

Furthermore, as more and more knowledge has been obtained on the direct methane to methanol conversion, several new questions arise. And with an aim to answer some of these, a new test rig has been constructed and will soon be ready to be put to use for exploring our Cu-loaded zeolites under new and different reaction conditions and pathways.

All in all, we are very much looking forward to embarking on a new year, and are confident that we have some exiting times ahead of us!

Publications IIA6

Publications and conference contributions are listed on page 66.

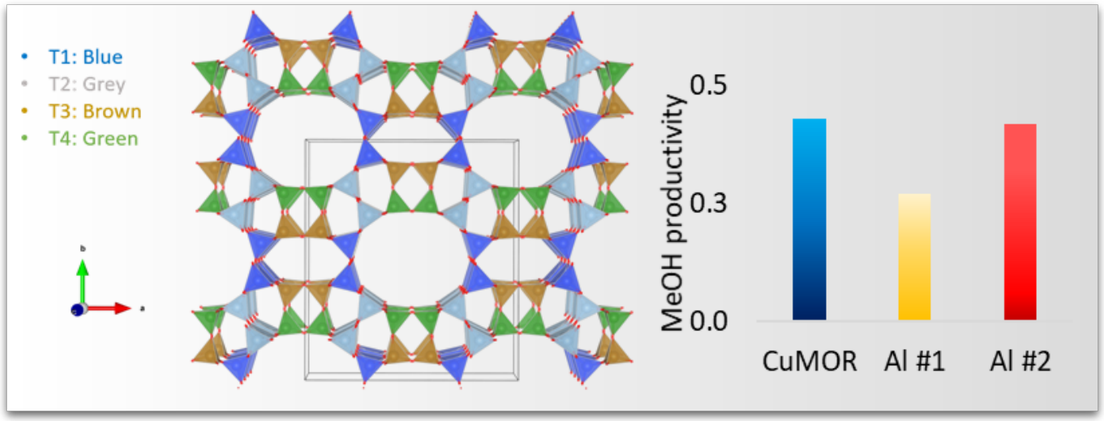

Figure 3. Control over active site location determines methanol productivity of Cu-MOR.

IIA6: Generic projects for additional industrial synergies

The IIA6 team 2020

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Pablo Beato	Haldor Topsøe	Industrial senior researcher (WP6.1)
Terje Fuglerud	INOVYN	Industry senior researcher (WP6.1-WP6.3)
Anja Olafsen Sjåstad	UiO	WP responsible (WP6.2)
Helmer Fjellvåg	UiO	Researcher (WP6.2)
Oleksii Ivashenko	UiO	Postdoctoral fellow (WP 6.2)
Christine Pettersen	UiO	Master student (WP6.2)
Martin Jensen	UiO	PhD candidate, not iCSI (WP6.2)
David Waller	YARA	Industrial senior researcher (WP6.2)
De Chen	NTNU	WP responsible (WP6.3)
Yanying Qi	NTNU	Postdoctoral fellow (WP6.3)
Kumar R. Rout	SINTEF	Researcher (WP6.3)
Kristin Bingen	Dynea	Industry senior researcher (WP6.3)
Marco Piccinini	Inovyn	Industry senior researcher (WP6.3)
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Ingeborg Helene Svenum	SINTEF	Researcher (WP6.4)
Anna Lind	SINTEF	WP responsible and researcher (WP6.4)
Carlos Grande	SINTEF	Researcher (WP6.4)
Martin Fleissner Sunding	SINTEF	Researcher (WP6.4)
Mathieu Grandcolas	SINTEF	Researcher (WP6.4)
Otto Lunder	SINTEF	Researcher (WP6.4)
John Lein	SINTEF	Researcher (WP6.4)
Athanasios Chatzitakis	UiO	Researcher (WP6.4)
Edd A. Blekkan	NTNU	WP responsible and PhD supervisor (WP6.5 and 6.6)
Jia Yang	NTNU	Researcher and PhD supervisor (WP6.5 and 6.6)
Moses Mawanga	NTNU	PhD candidate (WP6.5)
Rune Lødeng	SINTEF	Researcher (WP6.6)

Motivation

With the intention of moving the research forefront and providing methodological tools that can be applied in the industrial innovation areas 1-5, particularly advanced spectroscopic and microscopic investigations under conditions highly relevant to industrial operation are targeted. 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 the material with its catalytic activity. For this, we apply 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 chemical reactions can guide towards favourable compositions and conditions, thereby enabling sustainable processes with higher efficiency, lower cost, reduced emissions or by-products and improved lifetime.

The increasingly larger datasets associated with such combined studies of catalysts at work, call for automated procedures for efficient data reduction prior to any data interpretation. The use of multivariate statistical analysis tools to make full use of the experimental capabilities was explored and was presented at the annual user meeting in an invited talk at the European Synchrotron Radiation Facility[1].

We have direct synergies with four out of the five other industrial innovation areas within iCSI and collaborations within the Catalysis Group at NTNU (Fe-based Fischer-Tropsch synthesis to olefins from renewable feedstocks and selective catalytic reduction of NO by ammonia over Cu-based catalysts)[2], and with the SUNCAT Group at Stanford University.

The work has made strides in finding previously unknown intermediate components in XAS spectra of e.g. oxychlorination catalysts (shown in Figure 1 below). Our aim is to be able to identify the chemical nature of such species and our chemical knowledge of the catalyst system. Current ongoing work is the theoretical calculation of possible chemical compounds and compare those with the resolved spectra from the data reduction.

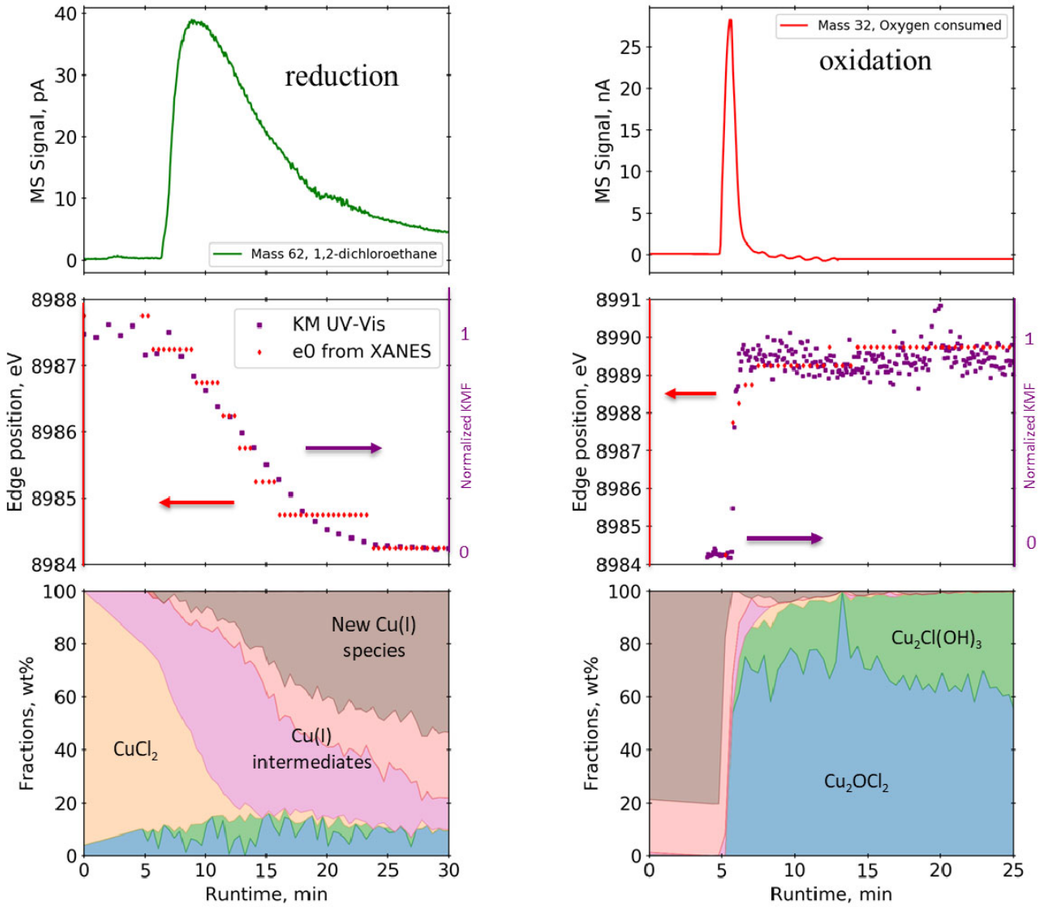


Figure 1. Transients of the reduction and oxidation steps of 0.4 K/Cu mol/mol 5 wt% Cu on γ-Al_2O_3, followed by operando XAFS and UV-Vis. Top row: Product formation (EDC) and oxygen consumption during reduction and oxidation. Middle row: Normalized Kubelka-Munk function of the UV-Vis signal at 796 nm and edge position derived from XANES. Bottom row: Fraction of the Cu species determined with MCR-ALS from XANES.

Advanced Synthesis and Characterization – Novel Thin Film Preparation and Reactor STM

This work focuses on preparation and operando characterization of 2D surfaces used for single-parameter model studies of NH_3 oxidation. PtRh alloys are extensively utilized for catalytic NH_3 oxidation and they are active in the two primary temperature/mixing regimes, high temperature Ostwald process conditions with O_2:NH_3 mixing around 65:35, and intermediate temperature ammonia "slip" oxidation with mixing close to 99:1. To correlate surface composition with catalytic performance, we prepared a range of model PtRh alloys with systematic variation of Pt enrichment at the surface, ranging from pure Rh(111) through mixed PtRh on Rh(111) or Pt(111) and to bare Pt(111). In the ammonia "slip" oxidation regime the gas composition closely resembles that of a pure O_2 environment, and as a first step we explain the oxidation of 2D surface alloys in oxygen.

The corresponding ultra-high vacuum Scanning Tunneling Microscopy (STM) images demonstrate that oxidation of the surfaces at 10^{-3}mbar and 700 K yields results substantially dependent on alloy composition (Figure 1). Based on particular moiré features in STM and Low Energy Electron Diffraction (LEED), we conclude that Rh(111) and Rh-rich surfaces develop an extensive network of O-Rh-O trilayer oxide with maximum O coverage of 1.8 ML. By contrast Pt(111) and Pt-rich surfaces resist oxidation and allow for maximum coverage of 0.25 ML. As we proposed in the recent APXPS study, the coverage of surface -O and -N species are detrimental for the formation of either NO or N_2 respectively[3].

To extend our analysis of (-O, -N) surface species present during NH_3 oxidation and how they lead to formation of NO and N_2, we continue constructing a multidimensional map spanning (O:NH_3 mixing ratio, temperature, alloying) parameter space. In the recent APXPS session at MaxIV (December 2020) we explored the performance of alloys shown in the STM Figure 1 in temperature range of 473-723 K and O_2:NH_3 mixing ratio varying from 99:1 to 65:35. The temperature-dependent APXPS presented in Figure 2 shows catalytic formation of -N in the temperature range 523-673 K at Rh(111) surface. Comparison with similar T-dependencies for Pt(111) and PtRh alloys will enable us to explain how controlling PtRh alloying can lead to development of better PtRh-based catalysts.

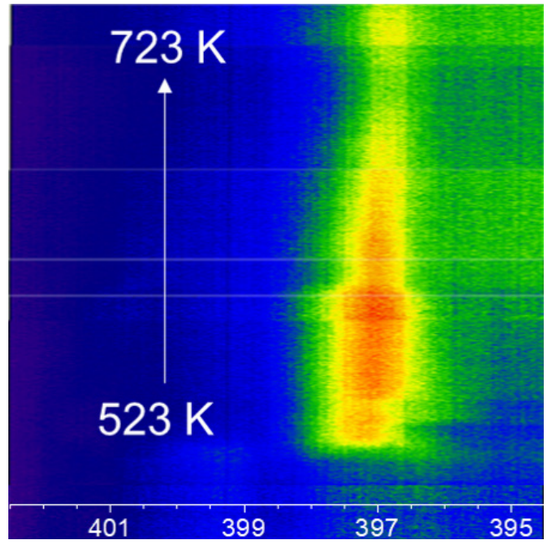


Figure 2. Temperature-dependent APXP spectra of N 1s core level of Rh(111) during NH_3 oxidation at (65:35) mixing.

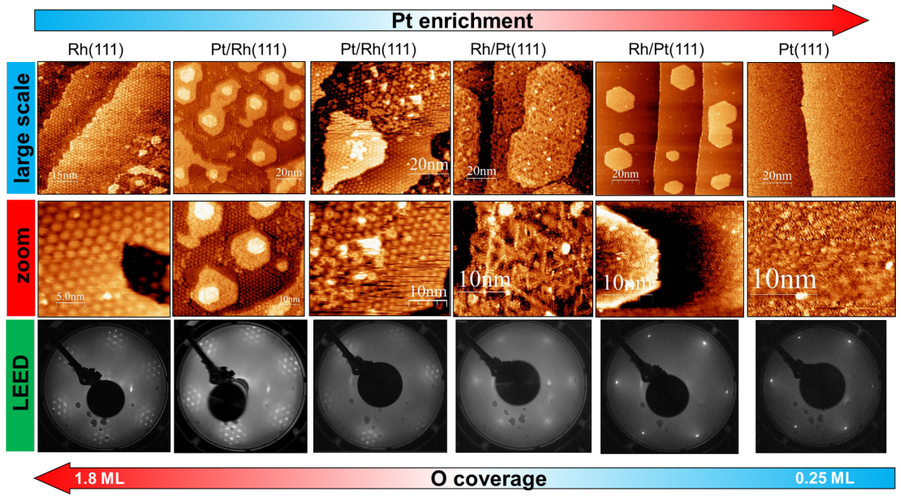


Figure 1. UHV STM morphology and LEED of PtRh alloys after oxidation. Pt enrichment decreases possible coverage of –O species at the surface.

Anodization of 3D printed titanium for photocatalysis (PHOTO-3D)

The main idea of this project is to produce an advanced photocatalyst by combining the concept of 3D-printing and anodization of titanium (Ti), and to prove its activity towards water cleaning and water splitting under solar illumination.

TiO_2 photocatalysts are commercially most commonly available as powder and a post-treatment separation stage is therefore needed. This is a great disadvantage, and it would be highly desirable to have the possibility of supporting the TiO_2 active phase on a structured material. This can be achieved through electrochemical anodization of Ti to TiO_2. Highly ordered, vertically oriented arrays of TiO_2 nanotubes can be prepared on a Ti substrate by anodization. In this project, we have used 3D printed Ti structures as substrates for the anodization. By using 3D structures, we can optimize the photocatalytic reactors to substantially increase the surface area/volume accessible to the light compared to what is possible with conventional reactors, giving an improved efficiency of the photocatalysts. This is a crucial improvement, as low efficiency is one of the challenges with photocatalysts today.

The material showed catalytic activity towards both the water splitting as well as the water cleaning reactions. From the preliminary study, the effect was more prominent with the water cleaning. The water cleaning experiments were performed by studying the degradation of methylene blue in water as a test pollutant under solar illumination. The photocatalytic degradation of methylene blue was measured in a closed system by UV-VIS spectroscopy over time. The photocatalytic activity of the 3D structured catalysts was measured under both static and rotating conditions. With rotation, the samples were rotated in front of the light source to make full use of their 3D structure.

All the prepared 3D structures showed enhanced photocatalytic degradation activity when rotating conditions were applied. This is illustrated in Figure 1, where the photocatalytic activity is plotted as the change in concentration (C/C_0) vs time for the three most promising samples, showing results from both static measurements, and when applying rotation.

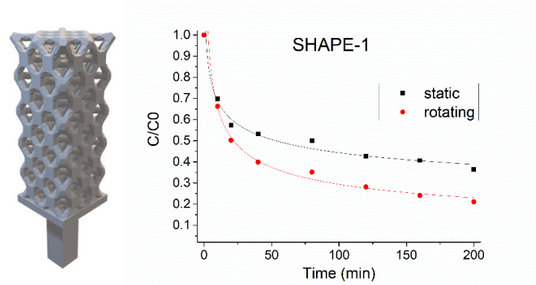


Figure 1. Static vs. rotation photocatalytic activity of the three most promising 3D printed shapes.

Insights into the kinetics and mechanism of selected industrial catalyzed reactions

The first part of the project aims to understand the reaction kinetics and mechanism of the catalysts for the oxidation of nitric oxide at near-industrial conditions. Experiments involve the use of the Steady-State Intrinsic Transient Kinetic Analysis[4] method on 1 wt.% Pt/SiO_2 and 15 wt.% Mn/SiO_2 catalysts prepared by incipient wetness impregnation. Reactant gases constitute 1 mol% NO and 6 mol% O_2 in Argon within 150–500 oC range and atmospheric pressure conditions at a GHSV of 240,000 ml.g-1h-1. Preliminary results using an oxygen-only switch (without NO reactant) has been used to show minimal scrambling of oxygen on the surface of the Mn/SiO_2 catalyst at 400°C. Further studies will involve isotopically labelled gases nitric oxide (^{15}NO) and oxygen ($^{18}O_2$) in the reactant stream. The results will be used to discriminate between the dominant mechanism of reaction: Either a Langmuir-Hinshelwood type or an Eley-Rideal as proposed by Weiss and Iglesia[5] and Salman et al[6] respectively.

The second part of the project involves using the adsorption microcalorimetry to measure the heats of adsorption for catalytic activation and functionalization of light alkanes, such as metal-exchanged zeolites. NH_3 and CH_4 probes are used to study the nature of surface interaction of layered MWW zeolites (Figure 1). Heats of adsorption are indicative of the adsorption energetics and bonding strength of surface species to probe the nature of active sites of the catalyst. With these fundamental experimental data, it will be possible to gain a better understanding of the catalytic reactions and thereby use the data for better catalyst design.

Publications IIA6

Publications and conference contributions are listed on page 66.

References IIA6:

1. *Regli SK, Rønning M. Invited talk "Multivariate statistical analysis of in situ and operando X-ray Absorption Spectroscopy data". ESRF User Meeting 2020, Grenoble, France.*
2. *Bjørkedal, Ole Håvik; Regli, Samuel K.; Rønning, Magnus. (2020) One-Pot Synthesis of Highly Dispersed Mesoporous Fe and Cu Catalysts for NH_3-SCR. International Conference on Environmental Catalysis. University of Manchester; 2020-09-07 - 2020-09-09.*
3. *Ivashenko, O.; Johansson, N.; Pettersen, C.; Jensen, M.; Zheng, J.; Schnadt, J.; Sjåstad, A. O., How surface species drive product distribution during ammonia oxidation, STM and APXPS study. submitted 2021.*
4. *S. Shannon, G. Goodwin Chem. Rev., 1995, 95, 677-695*
5. *Brian. Weiss, E. Iglesia. Journal of Catalysis 2010, 272 74–81*
6. *A.u.R Salman, B.C. Enger, X. Auvray, R. Lødeng, M. Menon, D. Waller, M. Rønning, Applied Catalysis A, 2018, 564 142–146.*

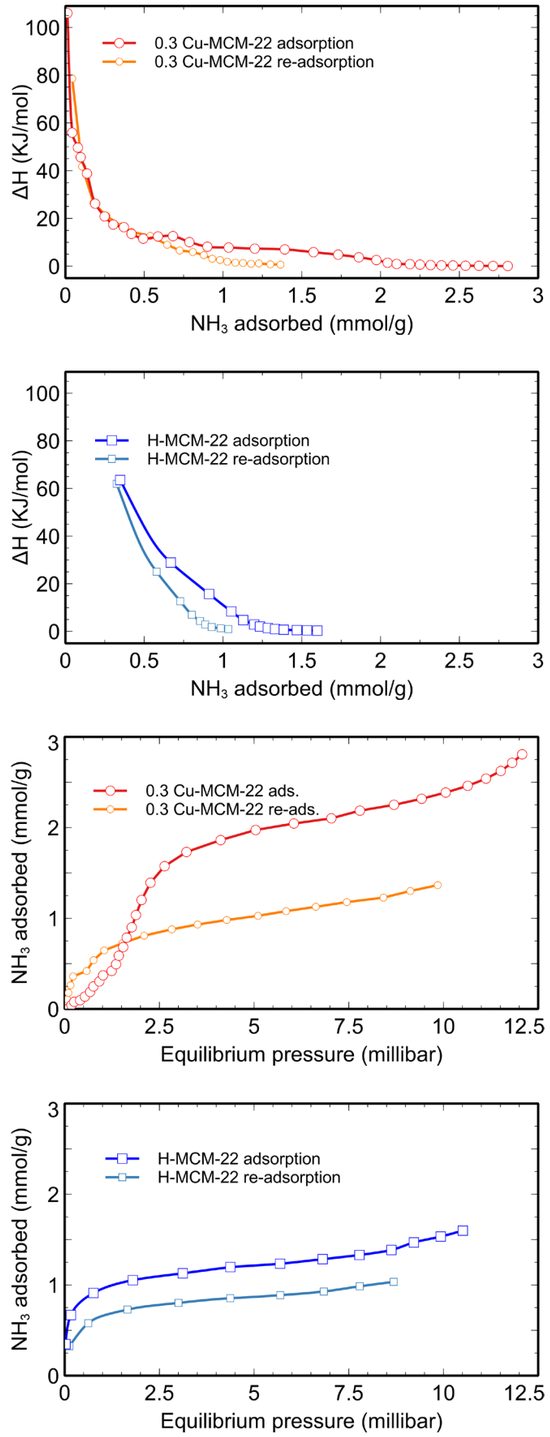
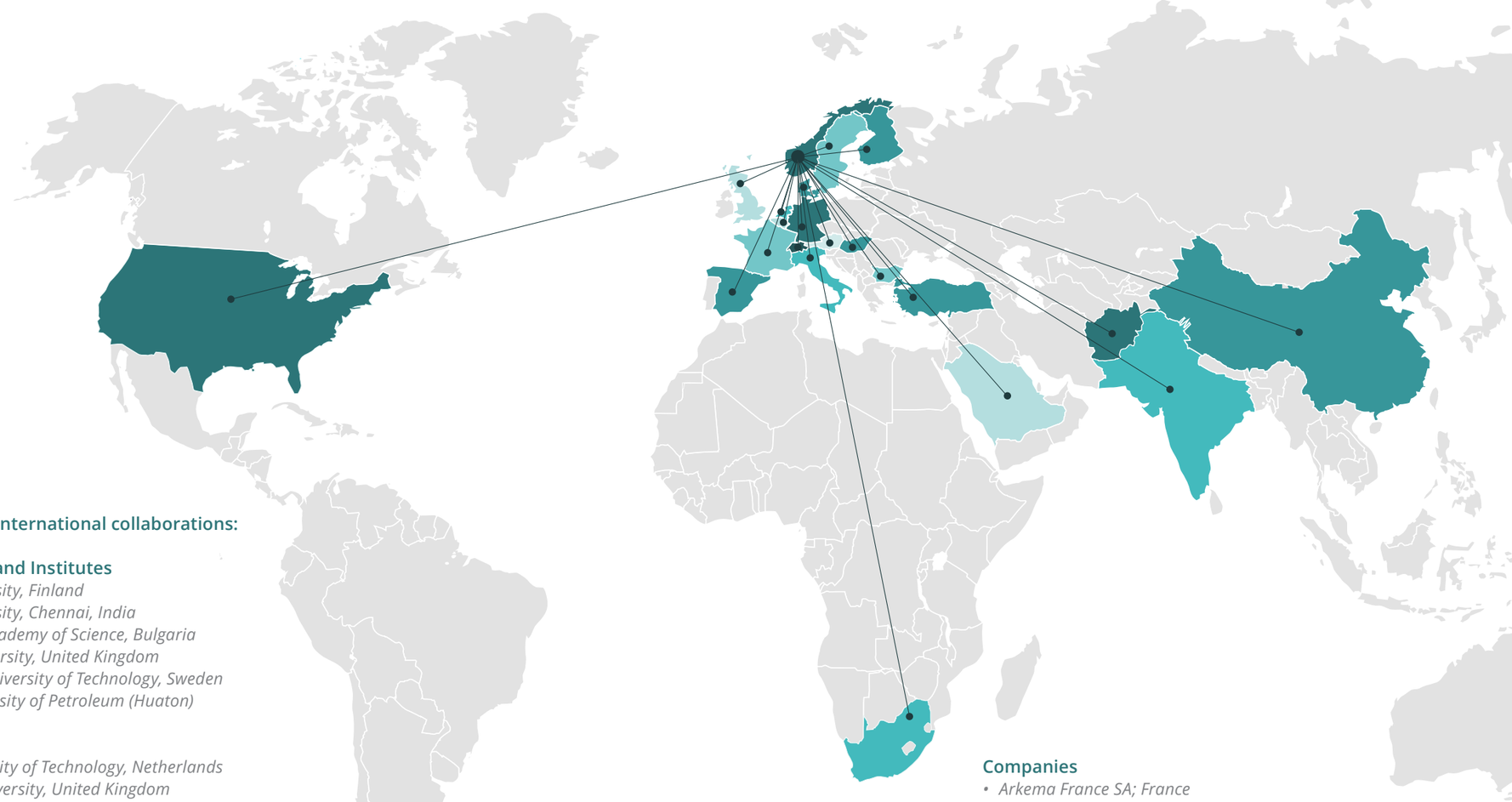


Figure 1. Heats of NH3 adsorption (two top) and adsorption isotherms (two bottom) of Cu-exchanged (yellow/red) and protonated (blue) zeolite MCM-22 at 80°C

Internationalization 2020



iCSI and the affiliated research institutions are attractive for international students and researchers. The 86 master's students, PhD candidates, postdocs and guest researchers within or affiliated with iCSI represent 24 countries. Non-Norwegians make up 58% of this group of employees and students.

In addition, 5 exchange PhD candidates, 4 from China and one from Spain, visited iCSI in 2020 with stays lasting from 4 to 17 months. One bachelor's exchange student from Germany and one from Spain did their thesis at NTNU. One master's exchange student from Italy visited University of Oslo, but had to go home without finishing when the lab was closed down due to COVID-19 in March.

Fifty per cent of the scientific publications from 2020 were published in collaboration with colleagues at international universities.

Hilde Johnsen Venvik has been appointed to the Lise Meitner guest professorship at Lund University's Department of Chemical Engineering in Sweden. The aim of the professorship, created in January 1999, is to offer a distinguished female researcher the opportunity to work at LTH for a period of one to three years, and to be a role model for other women at LTH.

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 2024. It is linking iCSI with four world-leading catalysis environments: 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 will be to strengthen the integration of theory and experiments in catalysis research and education through personnel exchange and shared workshops.

Overview of international collaborations:

Universities and Institutes

- *Aalto University, Finland*
- *Anna University, Chennai, India*
- *Bulgarian academy of Science, Bulgaria*
- *Cardiff University, United Kingdom*
- *Chalmers University of Technology, Sweden*
- *China University of Petroleum (Huaton)*
- *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*
- *Ghent University, Belgium*
- *Institut de Recherches sur la Catalyse et l'Environnement de Lyon, CNRS, France*
- *Institute of Coal Chemistry, Chinese Academy of Sciences, China*
- *Instituto Nacional del Carbón, INCAR-CSIC, Spain*
- *IMDEA Energy Institute, Spain.*
- *Karlsruhe Institute of Technology – KIT, Germany*
- *KAUST, Saudi Arabia*
- *Kemijski Institut (NIC), Slovenia*
- *Leiden University, Netherlands*
- *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*
- *National University of Science and Technology, Pakistan*
- *Paul Sherrer Institut, Schweiz*
- *Polytechnic University of Catalonia, Spain*
- *Politecnico di Milano, Italy*
- *Royal Institute of Technology (KTH), Sweden*
- *School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, China*
- *Shanghai Institute of Applied Physics, China*
- *Shanxi Institute of Coal Chemistry, Chinese Academy of Sciences, (ICC), China*
- *Sorbonne University, France*
- *Stanford University, California, USA*
- *South China University of Technology, China*
- *Swiss-Norwegian Beamlines at ESRF, France*
- *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 Duisburg-Essen, Germany*
- *University of Eastern Finland, Finland*
- *University of Málaga, Spain*
- *University of Sheffield, United Kingdom*
- *University of Strasbourg, France*
- *University of Surrey, United Kingdom*
- *University of Wisconsin-Madison, USA*
- *University of Torino, Italy*
- *Utrecht University, Netherlands*

Companies

- *Arkema France SA; France*
- *Asociacion Espanol de NormalizacionA, Spain*
- *A-V-S, United Kingdom*
- *B.T.G. BV, Netherlands*
- *Borealis, Austria*
- *BTG-BTL, Belgium*
- *C2P2, Lyon (CNRS), France*
- *Compania Espanola de Petroleos, Spain*
- *DOW chemicals, USA*
- *Fundacio EURECAT, Spain*
- *GE Healthcare, Norway*
- *Haldor Topsøe AS, Denmark*
- *ICI Caldaie, Italy*
- *Johnson Matthey, United Kingdom*
- *Linde, Germany*
- *Perstorp AB, Sweden*
- *Processi Innovativi SRL, Italy*
- *ProfMOF AS, Norway*
- *Repsol SA, Spain*
- *ST1, Finland*
- *Steeper, Denmark*
- *Strane Innovations SAS, France*
- *Tata Steel UK Limited, United Kingdom*
- *Turkiye Petrol Rafinerileri Anonim Sirketi (Tüpras),Turkey*
- *UOP LLC, USA*
- *Velocys, USA*
- *VTT, Finland*

European research - Horizon 2020 projects

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 nanotubes and MOF materials. H2020-NMBP-20-2017, iCSI-partner involved: SINTEF. Duration: 2018 –2021

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.

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: 2021-2023.

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.

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

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

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

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

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

Continued membership in the Swiss-Norwegian Beamlines (SNBL) at ESRF. NFR INFRASTRUKTUR. iCSI-partners involved: NTNU, UiO. Other Norwegian partners:w 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.

Accounts 2020

All cost and budget numbers appear in 1000 Norwegian Kroner, NOK.
As of January 2021 NOK 100 are equivalent to €9.7.

Table 1: Summarizes the costs in 2020 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 2020	Total budget 2015-2023
Payroll and indirect expenses	6 875	58 534
Procurement of R&D services	12 760	92 574
Equipment	961	10 955
Other operating expenses	4 508	35 524
Totals:	**25 104**	**197 587**

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

Cost and Financing per partner	Accounts 2020		Total budget 2015-2023	
Partner	Costs	Financing	Costs	Financing
NTNU	8 721	2 006	78 256	30 250
University of Oslo	7 850	1 857	49 073	12 723
SINTEF	4 910	1 191	43 501	7 858
Industrial partners	3 623	6 623	26 756	50 756
Research Council of Norway		13 427		96 000
Totals:	**25 104**	**25 104**	**197 587**	**197 587**

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 2020	Costs 2015-2020	Total budget 2015-2023
IIA1 21st century Nitric Acid technology development	4 207	24 009	37 649
IIA2 New NOx abatement technologies	1 719	5 195	8 026
IIA3 Frontier formalin technology development	2 344	15 695	23 927
IIA4 PVC Value Chain	4 998	19 972	32 858
IIA5 The next step in direct activation of methane	5 154	20 399	34 669
IIA6 Generic projects	5 019	26 601	35 337
IIA7 2020 Catalysis*	0	0	8 699
iCSI Management and administration	1 663	9 914	16 422
Totals:	**25 104**	**121 785**	**197 587**

**No costs in 2020 due to Covid-19-delayed start-up of one PhD and one Postdoc.*

Education

Postdoctoral researchers with financial support from iCSI

Yanying Qi	NTNU	China	2016-2020	F	IIA6
Oleksii Ivashenko	UiO	Ukraine	2016-2021	M	IIA1 / IIA6
Yalan Wang	NTNU	China	2019-2021	F	IIA4
Sebastian Prodinger	UiO	Austria	2020-2022	M	IIA5

One new postdoctoral fellow was welcomed in 2020. Sebastian Prodinger joined iCSI in March, and he came from a position as postdoc at the University of Delaware, Newark DE. There, he explored the possibility of converting glucose to dimethylfuran in a tandem catalytic approach and identified and mitigated challenges in the process.

Postdoc Yanying Qi left iCSI in June, after being an important contributor to the combined DFT calculations and microkinetic modelling performed in IIA6 as well as in other projects since 2016. Her approach has been employed in reaction systems of ethylene oxychlorination and methanol oxidation to formaldehyde.

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	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

1) Endre Fenes left iCSI in 2019 for a job in the industry and his defense will take 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 2021.
3) Stine Lervold left iCSI in November 2020 for a job in industry and her defense will to take place 9 June 2021.

Transfer of experience between experienced and new PhD candidate in IIA4, Hongfei Ma and Wei Zhang

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	NTNU	Pakistan	2017-2020	M	Enhanced visible light adsorption TiO_2 based catalysts for photo-catalytic H_2 production
Martina Cazzolaro	NTNU	Italy	2017-2020	F	Cu/CNF for selective hydrogenation of hydroxyacetone to 1,2-propane-diol
Joakim Tafjord	NTNU	Norway	2017-2020	M	Iron-based Fischer Tropsch synth-esis based on renewable feedstocks
Jianyu Ma	NTNU	China	2017-2020	M	Chemical looping desulphurization
Daniel Skodvin	NTNU	Norway	2017-2020	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
Volodymyr Levchenko	UiO	Ukraine	2016-2020	M	Au-based catalysts for C-C and C-X couplings
Mustafa Kømurcu	UiO	Norway	2017-2020	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

International exchange PhD candidates in iCSI, NTNU

Nianjun Hou	Chemical Engineering and Technology, Tianjin University	17 months	F	Ethanol fuel cells and also the ORR catalysts for fuel cells
Gang Wang	East China Univer-sity of Science and Technology	12 moths	M	Oxidation of propene to propene oxide with gold catalyst
Wenzhao Fu	Shanghai Institute of Applied Physics	12 months	M	Redox catalytic cycle of VOC oxidation and ethylene epox-idation
Hao Zhang	Shanghai Institute of Applied Physics	12 months	M	XAS study of nanoclusters in electrochemical reaction
Javier Torres	Universidad de Málaga	4 months	M	Cr/Ag-oxide fibers in methanol oxidation process

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

Gavrilovic Ljubisa	NTNU	Serbia	2018-2020	M	Bio Fischer-Tropsch (BioFT)-Staging and Multiple Hydrogen Feed of Biomass to Fischer-Tropsch Fuel Synthesis
Ainara Moral Larrasoana	NTNU	Spain	2018-2020	F	MBCL project
Yuanwei Zhang	NTNU	China	2018-2020	M	MBCL project – simulation work
Suresh Balasingam Kannan	NTNU	India	2018- 2020	M	Energy storage by high energy supercapacitors
Marie Døvre Strømsheim	NTNU	Norway	2018-2021	F	surface chemistry and segregation phenomena of Pd-alloy membranes
Mehdi Mahmoodinia	NTNU	Iran	2019-2021	M	Nanoscale Investigation of Co(0001), Co(10-12), and Co(11-20) Single Crystals as Catalyst Model Systems: Insights from Experiment and Theory
Zhenping Cai	NTNU	China	2018-2021	M	Conversion of lignocellulosic wastes into biofuels and bioplastics
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-reform-ing of methane
Jingxiu Xie	UiO	Singapore	2019-2020	F	Catalytic testing, CO_2 conversion
Christian Ahoba-Sam	UiO	Ghana	2019-2020	M	Catalytic testing, CO_2 conversion
Nico König	UiO	Germany	2020-2023	M	Catalyst synchrotron studies

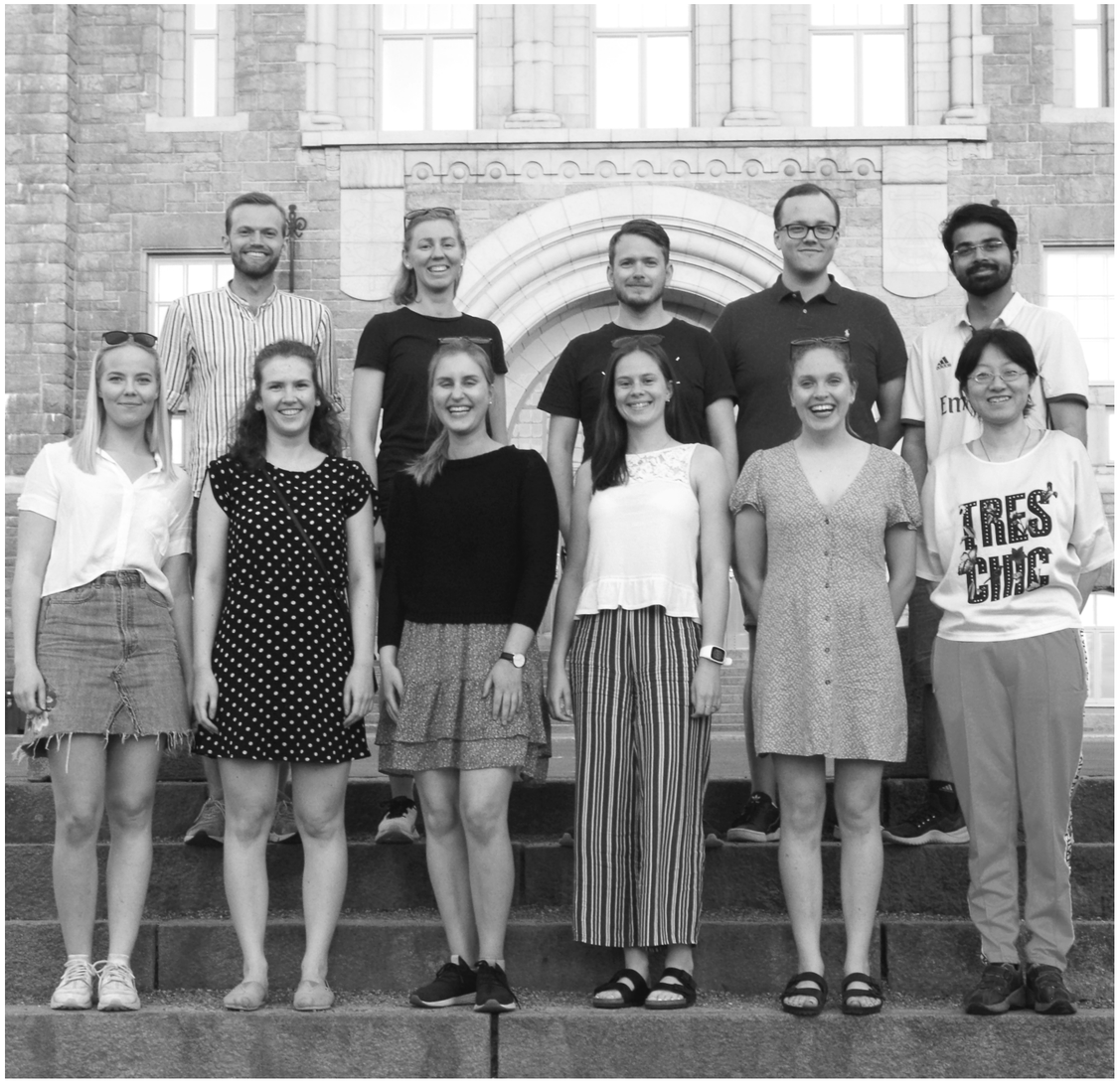
Master's students in Chemical engineering[1)] (NTNU) or Chemistry[2)] (UiO) in iCSI

Johnny Sannes	UiO	Norway	2018-2020	M	CO2 adsorption and character-ization of tailor-made metal-organic frameworks
Bjørn Garding Solemsli	UiO	Norway	2018-2020	M	A Study of Catalytic Pt Nano-particles inside a Nano-porous Functionalized UiO MOF-matrix for CO2-Hydrogenation
Christine Pettersen	iCSI, UiO	Norway	2018-2020	F	Preparation, Characterization and Oxidation of Nanostruc-tured Pt-Rh Surfaces
Kristoffer Flem Grimstvedt	UiO	Norway	2019-2021	M	Catalyst deactivation by coke formation
Oskar Iveland	iCSI, UiO	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	Norway	2020-2022	F	Reactor STM and NAP XPS for ammonia oxidation
Julie Christine Claussen	NTNU	Norway	2019-2020	F	Polymers Assisted Preparation of Iron based Fischer-Tropsch Catalysts for biomass to fuel
Oscar Ivanez Encinas	NTNU	Spain	2019-2020	M	High temperature CO2 capture / combustion - fixed bed
Hammad Farooq	NTNU	Pakistan	2019-2020	M	Carbon formation and catalysis in the conversion of methyl chloride and silicon into dimethyldichlorosilane
Jithin Gopakumar	NTNU	India	2019-2020	M	Ethylene oxychlorination on Cu based catalysts
Jørgen Lausund Grinna	NTNU	Norway	2019-2020	M	Low temperature CO2 capture by solid sorbents
Eirik Søreide Hansen	NTNU	Norway	2019-2020	M	Hydrogen production from biomass derived compounds by sorption enhanced reforming
Maren Wassås Kveinå	NTNU	Norway	2019-2020	F	CO2 emission reduction by CO to carbon / CNF - Fixed bed
Yun Liu	NTNU	South Korea	2019-2020	F	Low temperature CO2 capture / TGA
Kishore Rajendran	NTNU	India	2019-2020	M	Biomass conversion to chemical / Fixed bed reactor, ethanol
Ingvill Andrea Røed	NTNU	Norway	2019-2020	F	Low temperature selective hydrogenation using noble metal catalysts
Jon Arve Selnes	NTNU	Norway	2019-2020	M	Catalytic methane abatement for natural gas engines
Susanne Klungland Stokkevåg	iCSI, NTNU	Norway	2019-2020	F	Oxidation of methanol to formaldehyde (MTF) over Ag catalysts
Petter Tingelstad	NTNU	Norway	2019-2020	M	Biomass conversion to fuels / Oxidation, autoclave, catalyst
Anne Charlotte Gusfre Wold	NTNU	Norway	2019-2020	F	Kinetic study of processes for high temperature CO2 capture by solid sorbents
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 lignocellulosic 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 /NO2 equilibrium in nitric acid production
Erlend Skjørstad Værnes	NTNU	Norway	2020-2021	M	Low temperature selective hydrogenation using noble metal 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 bachelor's and master's students associated with iCSI

Philip Walter Putze	Bachelor NTNU	Germany	5 months	M	Methodology Development for the Characterization of Contact Mass in the Direct Process
Rodrigo Ortiz Sánchez-Ramos	Bachelor NTNU	Spain	6 months	M	Pelletized shaped Mn-based solid-sorbents for chemical looping desulfurization
Elisa Longhin	Master UiO	Italy	2 months	F	Could not finish due to COVID-19



11 of the 14 graduating master's students from the Catalysis group at NTNU, June 2020

Communication and Dissemination 2020

iCSI Plenaries:

Rønning, Magnus: Catalytic oxidation of NO to NO_2 for nitric acid production. Catalysis Seminar; KTH, Stockholm, 2020-02-28 - 2020-02-28 (Invited)

Ingeborg-Helene Svenum: Effect of promotors and inhibitors in Co-based FTS. 2020 iCSI annual seminar; 2020-09-14 - 2020-09-15 (Invited)

iCSI Publications and conference contributions 2020

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

Oral Presentations

Asbjørn Slagtern Fjellvåg; Julie Hessevik; David Waller; P.S. Jørgensen; Thomas By; Johan Skjelstad; Oskar Iveland; Helmer Fjellvåg; Anja Olafsen Sjåstad: Platinum Catchment on Noble Metal Alloys. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Oleksii Ivashenko: Operando NAP XPS and Reactor STM studies of PtRh alloys for NH_3 oxidation. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Silje Fosse Håkonsen: Experimental investigations of Pt/PtRh volatilization and catchment. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Magnus Rønning: Overview: Catalytic oxidation of NO to NO_2 for nitric acid production. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Ivashenko, Oleksii; Johansson, Niclas; Pettersen, Christine; Jensen, Martin; Zheng, Jian; Schnadt, Joachim; Sjåstad, Anja Olafsen: How surface species drive product distribution during ammonia oxidation, STM and APXPS study. 7th Annual Ambient Pressure X-ray Photoemission Spectroscopy workshop; 2020-12-15 - 2020-12-17 (digital)

Poster Presentations

Asbjørn Slagtern Fjellvåg; David Waller, Peter S. Jørgensen, Anja O. Sjåstad: Platinum Catchment on Noble Metal Alloys. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Asbjørn Slagtern Fjellvåg; David Waller, Anja O. Sjåstad: PdAu as industrial Platinum Catchment system. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Julie Hessevik, Asbjørn Slagtern Fjellvåg, Oskar Iveland, Davis Waller, Helmer Fjellvåg, Anja Olafsen Sjåstad: Complex oxide for Pt catchment. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Oskar Iveland, David Waller, Marion Duparc, Helmer Fjellvåg, Anja O. Sjåstad, Karl Isak Skau: Defining test conditions: Screening of catalysts for N-based reactions. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

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

Oral Presentations

Silje Fosse Håkonsen; Karl Isak Skau; David Waller; Martin F. Sunding; Anna Lind; Stephan Kubowicsz; Jasmina H. Cavka: Understanding and control of deactivation in catalysts for abatement of nitrogen-containing pollutants. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

David Waller: Nitrous oxide (N_2O) emissions from Yara's nitric acid plants. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

IIA3: Frontier Formalin Technology Development

Oral Presentations

Kristin Bingen; Rune Lødeng; Roman Tschentscher: MTF reactor development. Background, strategy and updates. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Stine Lervold; Hilde Johnsen Venvik: Methanol to Formaldehyde (MTF) in an Annular Reactor. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

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

Journal Publications

Fenes, Endre; Qi, Yanying; Ma, Hongfei; Zhu, Jun; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Piccinini, Marco; Chen, De: Prediction and Tuning of the Defects in the Redox Catalysts: Ethylene Oxychlorination. ChemCatChem 2021,13(1), 221-226.

Ma, Hongfei; Fenes, Endre; Qi, Yanying; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De: Understanding of K and Mg co-promoter effect in ethylene oxychlorination by operando UV–vis-NIR spectroscopy. Catalysis Today 2020 (in Press) .

Ma, Hongfei; Ma, Guoyan; Qi, Yanying; Wang, Yalan; Chen, Qingjun; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De: Nitrogen-Doped Carbon-Assisted One-pot Tandem Reaction for Vinyl Chloride Production via Ethylene Oxychlorination. Angewandte Chemie International Edition 2020, 59 (49), 22080-22085.

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; Volume 407, 128013.

Ma, Hongfei; Wang, Yalan; Qi, Yanying; Rout, Kumar Ranjan; Chen, De: Critical Review of Catalysis for Ethylene Oxychlorination. ACS Catalysis 2020 ;Volume 10 s. 9299-9319

Qi, Yanying; Fenes, Endre; Ma, Hongfei; Wang, Yalan; Fuglerud, Terje; Marco, Piccinini; Chen, De: Origin of potassium promotion effects on $CuCl_2$/gamma-$Al2O_3$ catalyzed ethylene oxychlorination. Applied Surface Science 2020; Volume 521. s. 146310-.

Qi, Yanying; Fenes, Endre; Ma, Hongfei; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Marco, Piccinini; Chen, De: Cluster-Size-Dependent Interaction between Ethylene and CuCl2 Clusters Supported via gamma-Alumina,. Journal of Physical Chemistry C 2020; Volume 124. s. 10430-10440.

Wang, Yalan; Wang, Xin-Xin; Zhu, Yi-An; Zhu, Ka-Ke; Chen, De; Zhou, Xing-Gui.: Shape selectivity in acidic zeolite catalyzed 2-pentene skeletal isomerization from first principles. Catalysis Today 2020 ;Volum 347. s. 115-123.

Oral Presentations

Hongfei Ma: Production of Vinyl Chloride Monomer. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Yalan Wang: Fundamental understanding of ethylene oxychlorination catalysts by DFT - Effect of different promotors iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

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

Journal Publications

Kvande, Karoline; Pappas, Dimitrios; Dyballa, Michael Martin; Buono, Carlo; Signorile, Matteo; Borfecchia, Elisa; Lomachenko, Kirill A.; Arstad, Bjørnar; Bordiga, Silvia; Berlier, Gloria; Olsbye, Unni; Beato, Pablo; Svelle, Stian: Comparing the Nature of Active Sites in Cu-loaded SAPO-34 and SSZ-13 for the Direct Conversion of Methane to Methanol. Catalysts 2020; Volume 10.(191) s. –.

Martini, Andrea; Signorile, Matteo; Negri, Chiara; Kvande, Karoline; Lomachenko, Kirill A.; Svelle, Stian; Beato, Pablo; Berlier, Gloria; Borfecchia, Elisa; Bordiga, Silvia: EXAFS wavelet transform analysis of Cu-MOR zeolites for the direct methane to methanol conversion. Physical Chemistry, Chemical Physics - PCCP 2020; Volume 22. s. 18950-18963

Pappas, Dimitrios; Kvande, Karoline; Kalyva, Maria Evangelou; Dyballa, Michael Martin; Lomachenko, Kirill A.; Arstad, Bjørnar; Borfecchia, Elisa; Bordiga, Silvia; Olsbye, Unni; Beato, Pablo; Svelle, Stian: Influence of Cu-speciation in mordenite on direct methane to methanol conversion: Multi-Technique characterization and comparison with NH_3 selective catalytic reduction of NOx. Catalysis Today 2020 s. 1-7.

Oral Presentations

Stian Svelle: Future directions – new model material. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Sebastian Prodinger: Evaluation of Reactive Separation Techniques for process Intensification. iCSI Annual Seminar; 2020-09-14 - 2020-09-15.

Karoline Kvande: New paths for "direct activation of lower alkanes". iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15.

Poster Presentations

Karoline Kvande: CH_4-TPR: A good description for optimizing the direct conversion of methane-to-methanol? iCSI Annual Seminar; 2020-09-14 - 2020-09-15.

Sebastian Prodinger, Sigurd Øien-Ødegaard, Karoline Kvande, Pablo Beato, Stian Svelle: Targeted (Cu)-MOR Synthesis for selective CH_4 oxidation. iCSI Annual Seminar; 2020-09-14 - 2020-09-15.

IIA6: Generic Projects for Additional Industrial Synergies

Oral Presentations

Moses Mawanga: Surface Adsorption Energetics of Zeolites for Methane Activation, IKP-day, Department of Chemical engineering, NTNU, 2020-11-23 - 2020-11-24

Samuel Regli; Magnus Rønning: Speciation of Cu. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15

Moses Mawanga; Jia Yang; Edd Anders Blekkan: Insights into the reaction mechanism and Kinetics of Industrial Catalyzed Reactions. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15

Ingeborg-Helene Svenum; Magnus Rønning; Øystein Dahl: Cobalt aluminate formation in supported Co catalysts. iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15

Poster Presentations

Moses Mawanga; Blekkan, Edd Anders; Yang, Jia: Kinetics of NO oxidation over Pt and Mn Catalysts (A prologue to Intrinsic Transient NO oxidation Kinetics). iCSI annual seminar; Oscarsborg, 2020-09-14 - 2020-09-15

iCSI Associated Journal Publications

Ahoba-Sam, Christian; Borfecchia, Elisa; Lazzarini, Andrea; Bugaev, Aram L.; Isah, Abdulrahman Adamu; Taoufik, Mostafa; Bordiga, Silvia; Olsbye, Unni: On the conversion of CO_2 to value added products over composite PdZn and H-ZSM-5 catalysts: excess Zn over Pd, a compromise or a penalty? Catalysis Science & Technology 2020; Volume 10. s. 4373-4385

Acha, E; Chen, De; Cambra, J.: Comparison of novel olivine supported catalysts for high purity hydrogen production by CO_2 sorption enhanced steam reforming. Journal of CO_2 Utilization 2020; Volume 42. s. 101295-

Arstad, Bjornar; Blom, Richard; Hakonsen, Silje F.; Pierchala, Joanna; Cobden, Paul; Lundvall, Fredrik; Kalantzopoulos, Georgios N.; Wragg, David; Fjellvag, Helmer; Sjastad, Anja O.: Synthesis and Evaluation of K-Promoted Co_3-xMgx-Al-Oxides as Solid CO_2 Sorbents in the Sorption-Enhanced Water-Gas Shift (SEWGS) Reaction, Industrial & Engineering Chemistry Research 2020, Volume: 59 Issue: 40 Pages: 17837-17844

Bjørkan, Hilde; Rønning, Magnus; Venvik, Hilde Johnsen; Johannessen, Tue; Holmen, Anders: Water–Gas Shift Activity of Pt Catalysts Prepared by Different Methods. Catalysts 2020 ;Volum 10, 1132

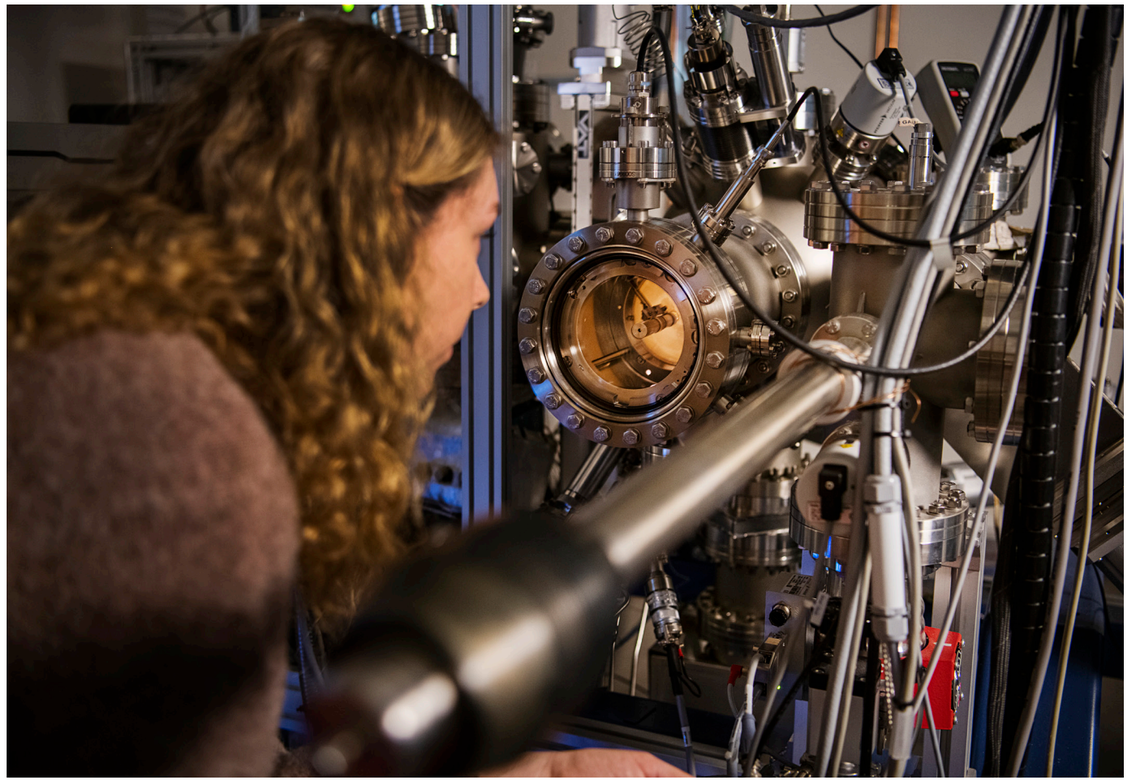
Bratvold, Jon E.; Fjellvåg, Helmer; Nilsen, Ola: Phase and Orientation Control of $NiTiO_3$ Thin Films. Materials 2020 ;Volum 13.(1) s. 1-19

Capa, Alma; García, Roberto; Chen, De; Rubiera, Fernando; Pevida, Covadonga; Gil, Mara Victoria: On the effect of biogas composition on the H2 production by sorption enhanced steam reforming (SESR). Renewable Energy 2020; Volume 160. s. 575-583

Chang, H; Bjorgum, Erlend; Mihai, Oana; Yang, Jia; Lein, H. L.; Grande, T.; Raaen, S.; Zhu, Yi-an; Holmen, Anders; Chen, De: Effects of Oxygen Mobility in La-Fe-Based Perovskites on the Catalytic Activity and Selectivity of Methane Oxidation. ACS Catalysis 2020; Volume 10. s. 3707-3719

Chen, Qingjun; Wang, Siyu; Rout, Kumar Ranjan; Chen, De: Development of Polyethylenimine (PEI)-impregnated mesoporous carbon spheres for low-concentration CO_2 capture. Catalysis Today 2020

Chen, Wenyao; Chen, S. M.; Qian, G.; Song, L.; Chen, De; Zhou, Xinggui; Duan, Xuezhi: On the nature of Pt-carbon interactions for enhanced hydrogen generation. Journal of Catalysis 2020; Volume 389. s. 492-501



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Chen, Wenyao; Zhang, W.Z.; Cao, J.B.; Fu, W.Z.; Qian, G.; Chen, De; Zhou, Xinggui; Duan, Xuezhi: Atomic Insights into Robust Pt-PdO Interfacial Site-Boosted Hydrogen Generation. ACS Catalysis 2020 ;Volum 10. s. 11417-11429

Cheng, Q. Y.; Wang, K. Q.; Hu, P.; Sui, Z. J.; Zhou, Xinggui; Chen, De; Yuan, Wei-kang; Zhu, Yi-an: Dual-function catalysis in propane dehydrogenation over Pt-1-Ga2O_3 catalyst: Insights from a microkinetic analysis. AIChE Journal 2020; Volume 66

Dietzel, Pascal D.C.; Blom, Richard; Fjellvåg, Helmer: Variability in the formation and framework polymorphism of metal-organic frameworks based on yttrium(III) and the bifunctional organic linker 2,5-dihydroxyterephthalic acid. Zeitschrift für Anorganische und Allgemeines Chemie 2020 s. 1-12

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Du, Juan; Kang, Le; Zhong, Qifan; Zhou, Haitao; Yang, Jianhong; Chen, De; Luo, Yingtao; Chen, Kaibin; Li, Wangxing; Xiao, Jin: High Peel Strength and Flexible Aligned Carbon Nanotubes/Etched Al Foil Composites with Boosted Supercapacitor and Thermal Dissipation Performances. Industrial & Engineering Chemistry Research 2020; Volume 59.(4) s. 1549-1558

Duparc, Marion Jeanne Louise; Sønsteby, Henrik Hovde; Nilsen, Ola; Sjåstad, Anja Olafsen; Fjellvåg, Helmer: Atomic Layer Deposition of $GdCoO_3$ and Gd0.9 Ca0.1CoO_3. Materials 2020; Volume 13.(1) s. 1-10

Eleri, Obinna Egwu; Azuatalam, Kingsley Ugochukwu; Minde, Mona Wetrhus; Trindade, Ana Maria; Muthuswamy, Navaneethan; Yu, Zhixin: Towards high-energy-density supercapacitors via less-defects activated carbon from sawdust. Electrochimica Acta 2020 ;Volum 362.

Gao, Hongquan; Yang, Jianhong; Chen, De: Boosting Gravimetric and Volumetric Energy Density of Supercapacitors by 3D Pomegranate-like Porous Carbon Structure Design. Applied Surface Science 2020 s. 147613

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Goodarzi, Farnoosh; Pinilla Herrero, Irene; Kalantzopoulos, Georgios N.; Svelle, Stian; Lazzarini, Andrea; Beato, Pablo; Olsbye, Unni; Kegnæs, Søren: Synthesis of mesoporous ZSM-5 zeolite encapsulated in an ultrathin protective shell of silicalite-1 for MTH conversion. Microporous and Mesoporous Materials 2020; Volume 292. s. 10,97,30

Guo, Xiaoyang; Vanhaecke, Estelle Marie M.; Vullum, Per Erik; Ma, Jianyu; Panditha Vidana, Daham Sanjaya Gunawardana; Walmsley, John; Chen, De; Venvik, Hilde Johnsen: Effects of metal dusting relevant exposures of alloy 601 surfaces on carbon formation and oxide development. Catalysis Today 2020 s. 1-14

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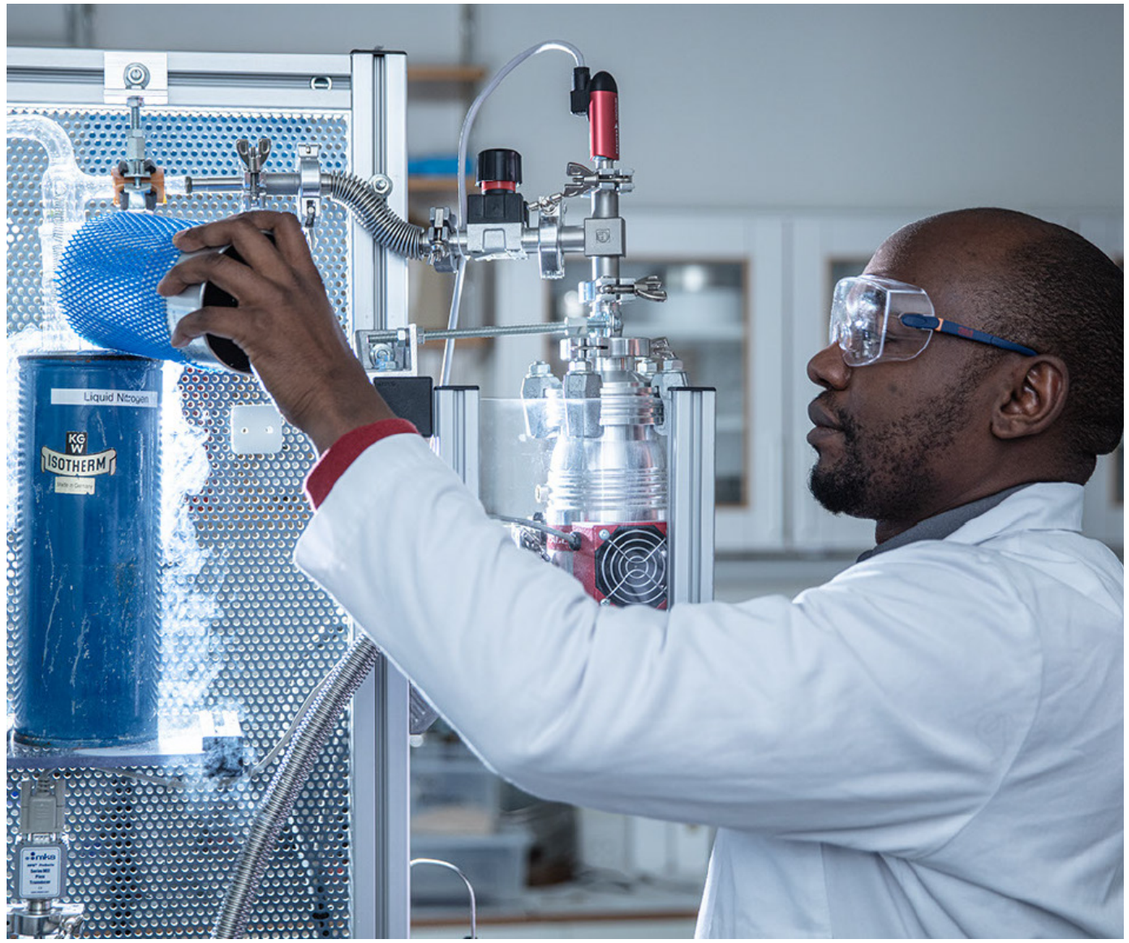

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Rytter, Erling; Yang, Jia; Borg, Øyvind; Holmen, Anders: Significance of C3 Olefin to Paraffin Ratio in Cobalt Fischer–Tropsch Synthesis. Catalysts 2020

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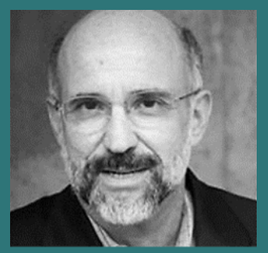

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