iCSI 2015–2023

industrial Catalysis Science and Innovation

Norwegian Centre for Research-based Innovation

NTNU

RESEARCH PARTNERS

NTNU · SINTEF · UiO : University of Oslo

INDUSTRY PARTNERS

YARA · TOPSOE · dynea

INEOS Inovyn · K·A·Rasmussen NORWAY

Funded by
The Research
Council of Norway

Front page photo: Moses Mawanga at the NTNU laboratory, 2021.
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Tor Grande

Rector NTNU

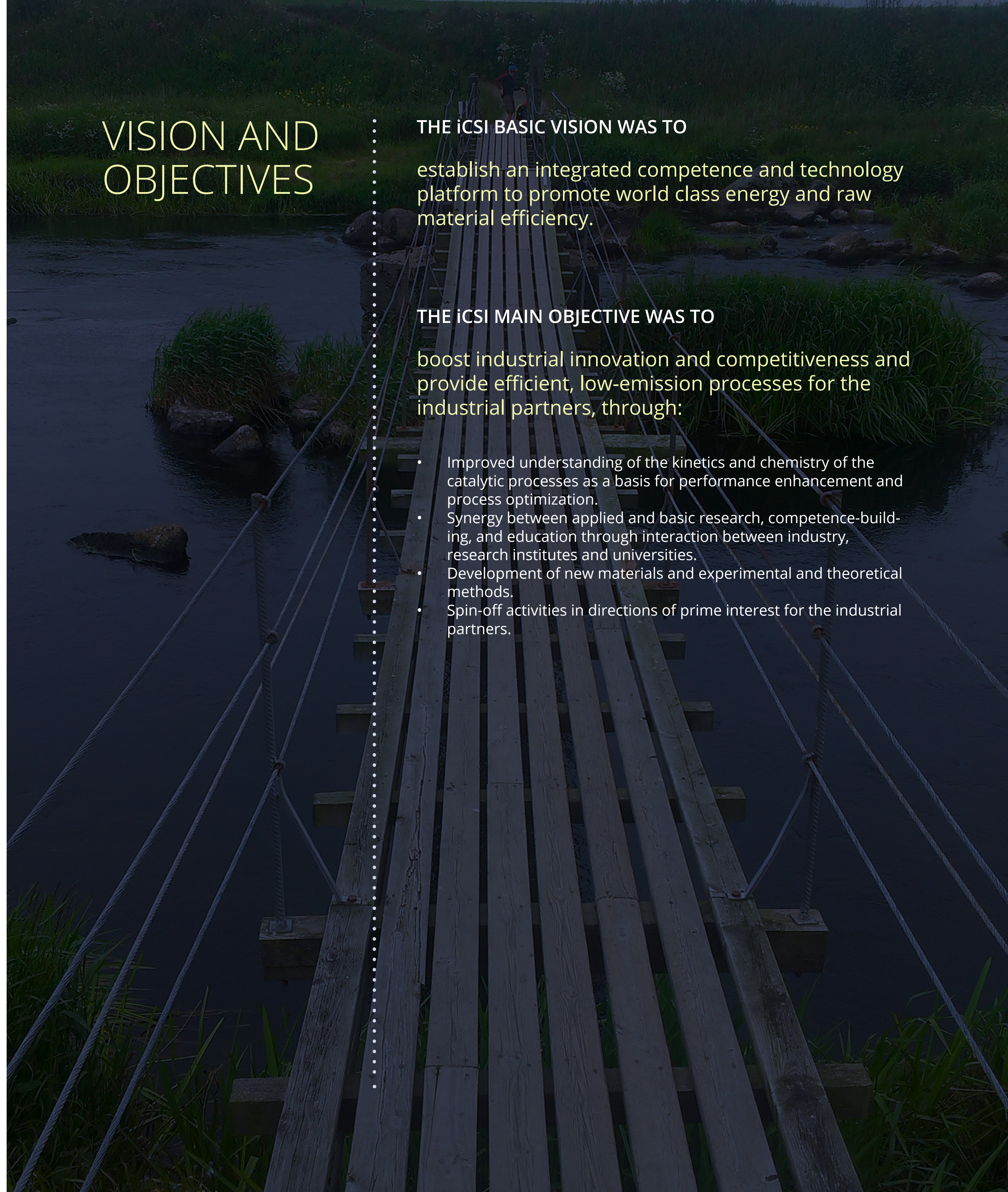
FOREWORD

Catalysis is of paramount importance for the process industry, and it is a prerequisite for most industrial and chemical processes. It is also crucial to the transition towards a greener and more sustainable future. Catalysis makes industrial processes more energy efficient, it reduces waste, reduces use of toxic and hazardous materials, and increases the utilisation of raw materials. But to succeed in developing better catalysts, we need a bridge between the research institutions and the industry. The Centre of Research-based Innovation (SFI) industrial Catalysis Science and Innovation (iCSI) has offered us that.

When iCSI was established, it was based on a long existing partnership between research institutions, catalyst producers and the chemical process industry. At the time, the University of Oslo had already hosted the inGap SFI for eight years. iCSI benefited from the long-term strategic development of a professional field, stretching over more than 30 years.

This is why I so strongly believe in the SFI scheme. It is important for long-term quality research, education and innovation, and it offers continuity and stability. The SFIs help us bring research from our labs to society, through industry partners. The partners are important to the SFIs, but the SFIs are also important to the partners. Through the SFIs, world-leading scientists are doing research on topics and areas that are central to the industry. The SFIs also train students and young scientists who bring with them new knowledge to the industry. The iCSI Centre has trained many attractive master's and PhD candidates who have found relevant jobs in the industry. The partners Yara, INEOS Inovyn, Dynea, K. A. Rasmussen and Topsoe have all recruited candidates who help transfer and utilise knowledge from the centre.

Even though the SFI iCSI now comes to an end, I am sure the strong collaboration between the partners will continue. I am looking forward to new partnerships and innovations within the interdisciplinary field of catalysis in the years to come.



VISION AND OBJECTIVES

THE iCSI BASIC VISION WAS TO

establish an integrated competence and technology platform to promote world class energy and raw material efficiency.

THE iCSI MAIN OBJECTIVE WAS TO

boost industrial innovation and competitiveness and provide efficient, low-emission processes for the industrial partners, 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.
- Spin-off activities in directions of prime interest for the industrial partners.

SUMMARY

The 2015-23 industrial Catalysis Science and Innovation (iCSI) Centre for Research based innovation (SFI) has promoted the technological lead of its industrial partners with respect to selected catalysts and process operations and enabled them to further reduce their environmental footprint, thereby securing and developing certain Norwegian industrial operations and industrial core competences.

The centre has consisted of the three research partners NTNU, University of Oslo (UiO) and SINTEF Industry, and five partners from the chemical process industry: Dynea, K. A. Rasmussen, INEOS Inovyn, Topsoe and Yara. NTNU Department of Chemical Engineering has hosted the centre with Professor Hilde Johnsen Venvik as the Centre Director. All the industrial partners have shown a strong commitment to the scientific challenges and have contributed to development with their own research and in collaboration with the research partners.

At the time of writing, the iCSI scientists have published 100 scientific papers, and among these are three in Angewandte Chemie and two in the Journal of the American Chemical Society (JACS), considered among the most prestigious chemistry journals. The remaining output has also appeared in high-quality, peer-reviewed journals, and even more papers are expected to come as a result of PhD research throughout 2024 and 2025. Another 11 dissemination measures for the general public have also been made. Thus, we will reach the goal set when we started in 2015 - 100 scientific papers - by a good margin.
A characteristic of iCSI has been our academically strong and dedicated candidates and researchers, which is confirmed by one of our PhD candidates, Dimitrios K. Pappas receiving the award for Best European Catalysis PhD in 2021 from the European Federation of Catalysis Societies (EFCATS). In 2019, Professor Unni Olsbye at UiO received the Award for Excellence in Natural Gas Conversion, which is the most prestigious international recognition in this field.

Well trained and educated candidates for both the private and public sectors is another important outcome from the SFI. 42 MSc candidates have finished their theses related to the centre's research areas and with supervisors from the centre staff. 9 PhDs have been completed between the 16 that were started, and the remaining are expected to defend their theses in 2024 or 2025. We are thrilled to see that the candidates find relevant jobs in Norwegian industry and academia. The industrial partners have employed some of the MScs and PhDs from iCSI, and also some of the 21 other PhDs that have been associated with the centre but linked to other projects.
iCSI is internationally oriented, and 30 different countries have been represented in the centre through students, employees and industry partners in the period 2015-2023. All the industrial partners are international players, three of them with headquarters in Norway, one in Denmark and one in Brussels. The international orientation is also demonstrated by the fact that 60% of the scientific publications are co-authored with international collaborators. The senior researchers in iCSI are well recognised and have performed around 60 invited plenaries, keynote and guest lectures internationally in the lifetime of the centre.

The CATHEX (RCN INTPART project) collaboration with University of Oslo, University of Cape Town, University of Wisconsin Madison, University of Toronto, East China University of Science and Technology and NTNU was initiated by the centre. In June 2023, a combined iCSI-CATHEX seminar lasting for four days gathered 70 catalysis researchers from all over the world.

The iCSI community is tremendously grateful to the Scientific Advisory Committee, which has consisted of three renowned researchers from prominent institutions who have excelled in iCSI-relevant areas of heterogeneous catalysis. Alessandra, Enrique and Graham (see p 16) have participated with great commitment, interacted with and challenged the young researchers in one-to-one meetings, and served as inspiration for the whole iCSI community at the iCSI Annual Seminars.

Organising the collaborating groups' long-term research activities as a centre has added significant value in numerous ways. Within iCSI, the collaboration between the universities and the institute sector, as well as between the two universities has been further strengthened. The expertise unique to each research group has been utilised and developed through joint ownership of scientific challenges. Joint effort on the development of advanced methods and equipment has been essential in reaching the goals.

Towards the end, we can see piloting of results, and a spin-off of the teamwork in the form of hosting and organising the EuropaCat 2025 congress in collaboration with the other Nordic catalysis societies. This is based on quality in the research, trust and a good collaborative climate between the partners that has developed over the years with a joint SFI.

For the industry partners, the long-term access to competent personnel and advanced research infrastructure has been one of the major values from being part of the SFI. This has strengthened the platform of knowledge for their companies, and puts them in a position to make better decisions and improve their competitiveness. Many of them also value the improved network to the other industry partners in the SFI.

Associated with the centre activities, there are more than 20 ongoing international projects in 2024 with the research partners, supported by Horizon 2020, Horizon Europe, RCN, and sources other than EU. The catalysis group at NTNU and the NAFUMA group at UiO are involved with the Centre for Environment-friendly Energy Research (FME) HYDROGENi, which started in 2022.

In the recently published National report, *Evaluation of Natural Sciences in Norway 2022-2024* (EvalNat), iCSI is highlighted as one of three impact cases within chemistry that contribute to the development and transfer of more sustainable technologies to industry, rapid uptake of results from basic research, and helps to tackle decarbonisation of the energy system. So even if the eye of the needle becomes narrower, we believe that catalysis science is so important for solving future challenges that the Research Council of Norway will support our application for a new SFI to ensure a continuation of the knowledge development and infrastructure acquired. There, an even stronger focus will be placed on the changes required by the industry to be able to fulfil its ambitions on reaching the UN Sustainable Development Goals. Most of the industrial partners from iCSI are ready to continue the collaboration and new partners will join.

SAMMENDRAG

Fra oppstarten var det et overordnet mål for senteret industrial Catalysis Science and Innovation (iCSI) å styrke konkurranseevnen til industripartnerne gjennom å sikre teknologiforsprang for utvalgte katalysatorer og kjemiske prosesser samtidig som miljøkonsekvensene av den industrielle virksomheten reduseres. Senteret har lyktes godt med å utvikle forskningsmetodikk og kompetanse som kan ta norsk industri gjennom det grønne skiftet.

Senteret for forskningsdrevet innovasjon (SFI) har bestått av tre forskningspartnere: NTNU, Universitetet i Oslo (UiO) og SINTEF Industry og fem partnere fra kjemisk prosessindustri: Dynea, KA Rasmussen, INEOS Inovyn, Topsoe og Yara. Institutt for kjemisk prosessteknologi ved NTNU har vært vertskap for senteret med professor Hilde Johnsen Venvik som senterdirektør. Alle industripartnerne har vist sterkt engasjement i de vitenskapelige utfordringene og bidratt til utvikling, både med egen forskning og i samarbeid med forskningspartnerne.

Per mai 2024 har iCSI-forskerne publisert 100 vitenskapelige artikler. Blant disse er tre i Angewandte Chemie og to i Journal of the American Chemical Society (JACS), regnet blant de mest prestisjefylte vitenskapelige tidsskriftene innenfor kjemi. Resten av produksjonen har også vært i fagfellevurderte tidsskrifter av høy kvalitet, og enda flere artikler forventes å komme som et resultat av doktorgrader som blir ferdige i 2024 og 2025.

Ytterligere 11 formidlinger av populærvitenskapelig karakter er også utført. Vi vil nå målet som ble satt da vi startet i 2015 – 100 vitenskapelige artikler – med god margin.

Et kjennetegn ved iCSI har vært akademisk sterke og dedikerte kandidater og forskere. Dette bekreftes av at en av dem, Dimitrios K. Pappas, mottok pris for beste europeiske katalyse-PhD i 2021 fra European Federation of Catalysis Societies (EFCATS). Professor Unni Olsbye ved UiO mottok i 2019 prisen for fremragende forskning innen naturgasskonvertering, den mest prestisjefylte internasjonale anerkjennelsen på dette feltet.

Kompetente kandidater for både privat og offentlig sektor er et annet viktig resultat fra SFI'en. 42 masteroppgaver har vært knyttet til senterets forskningsområder med veiledning fra senterets professorer. 9 av de 16 påbegynte doktorgradene er så langt fullført, og de resterende forventes å disputere i 2024 eller 2025. Vi er glade for at alle kandidatene går til relevante jobber i norsk industri og akademia. Industripartnerne har ansatt master- og PhD-kandidater både fra iCSI, og fra noen av de 21 andre PhDene som har vært assosiert til senteret, men knyttet til andre prosjekter.

iCSI har vært et internasjonalt senter med 30 ulike land representert gjennom studenter, ansatte og industripartnere i løpet av 2015-2023. Alle industripartnerne er dessuten internasjonale aktører, tre av dem med hovedkontor i Norge, en i Danmark og en i Brussel. Senterets internasjonalisering vises også ved at 60 % av de vitenskapelige publikasjonene er skrevet sammen med internasjonale samarbeidspartnere. Seniorforskerne i iCSI er godt anerkjent og har holdt rundt 60 inviterte foredrag internasjonalt i senterets levetid.

CATHEX-samarbeidet (NFR INTPART-prosjekt) med UiO, University of Cape Town, University of Wisconsin Madison, University of Toronto, East China University of Science and Technology og NTNU ble initiert av senteret. I juni 2023 samlet vårt felles iCSI-CATHEX-seminar 70 katalyseforskere fra hele verden over fire dager.

iCSIs studenter og forskere er særdeles takknemlig for innsatsen til Scientific Advisory Committee, som har bestått av tre anerkjente forskere fra fremtredende institusjoner som har utmerket seg innen iCSI-relevante områder av heterogen katalyse. Alessandra, Enrique og Graham har deltatt med stort engasjement, samhandlet med og utfordret de unge forskerne i en-til-en møter, og fungert som inspirasjon for alle forskerne på iCSI Annual Seminars.

Å organisere samarbeidsgruppenes langsiktige forskningsaktiviteter som et senter har tilført betydelig verdi. Innen iCSI er samarbeidet mellom universitetene og instituttsektoren, samt mellom de to universitetene ytterligere styrket. Spesialkompetansen i de ulike forskningsgruppene er synergisk utnyttet og utviklet gjennom felles eierskap til vitenskapelige utfordringer. Samarbeid om utvikling av avanserte metoder og utstyr har vært avgjørende for å nå målene.

Mot slutten av senterperioden kan vi se pilotering av resultater, og en spin-off av samarbeidet i form av at vi kommer til å arrangere EuropaCat 2025-kongressen i samarbeid med de andre nordiske katalysemiljøene. Dette er gjort mulig gjennom tilliten og samarbeidsklimaet vi har utviklet i løpet av årene med en felles SFI.

For industripartnerne har langsiktig tilgang til kompetent personell og avansert forskningsinfrastruktur vært en av de store verdiene ved å være en del av en SFI. Dette har styrket kunnskapsbasen for bedriftene og satt dem i posisjon til å ta bedre beslutninger og forbedre konkurranseevnen. De verdsetter også et styrket nettverk til de andre industripartnerne i iCSI.

Hos forskningspartnerne i senteret pågår det i 2024 mer enn 20 internasjonale prosjekter støttet av Horizon 2020, Horizon Europe, Forskningsrådet og andre kilder. Både katalysegruppen ved NTNU og NAFUMA-gruppen ved UiO er involvert i det nye Forskningssenteret for miljøvennlig energi, HYDROGENi, som startet i 2022.

I den nylig offentliggjorte evalueringen av naturvitenskapelig forskning i Norge 2022-2024 (EvalNat) blir iCSI løftet fram som ett av tre eksempler på kjemisk forskning som bidrar til utvikling og overføring av mer bærekraftige teknologier til industrien, rask implementering av resultater fra grunnleggende forskning, samt hjelp til å takle dekarbonisering av energisystemet. Så selv om nåløyet blir trangere, vil vi tro at katalysevitenskap er så viktig for å løse fremtidens utfordringer at Norges forskningsråd vil støtte vår søknad om en ny SFI for å sikre videreføring av kunnskapen og bruk av infrastrukturen. Nå skal fokuset rettes enda sterkere mot endringene som kreves av industrien for å kunne oppfylle FNs bærekraftsmål. Flere av industripartnerne fra iCSI er klare til å fortsette samarbeidet, og nye vil komme til.

Hilde Johnsen Venvik

Centre director

CONCLUSION AND OUTLOOK

iCSI has formally concluded and here we stand...

...proud of the achievements – the published research results, the PhD and Master candidates educated and the impact on the industrial partners. The interface between the Research Council of Norway and the research institutions is such that not all candidates have graduated at the point of final reporting due to teaching duties, parental leave, etc. but we are confident that most will complete their studies during 2024-25.

...a bit shaken from the ride – most importantly due to external events that can be summarised as a pandemic and the outbreak of war in Europe and the Middle East, on top of an emerging environmental crisis. Each has affected the iCSI consortium; the work, our organisations, the industrial operations, the market and the regulations, in ways that we were unable to predict at start-up. From this, we have learned that helping and supporting each other, looking out for democracy and academic freedom, and preserving humanity, security and the planet is of outmost importance.

...looking forward. We have developed fruitful collaborations, new methods and new equipment that we are ready to apply to new challenges. We need to educate more scientists with knowledge of chemistry and chemical engineering to enable continued competitiveness alongside circularity and environmentally friendly fuels and chemicals. We also foresee that artificial intelligence (AI) will revolutionise the field of theoretical chemistry and the way we store, curate and analyse experimental data, and not least how these will be combined into new interpretations and insights in the years to come. The quality and precision of experimental data will be as important as ever, however, so we aim to maintain our edge in that field while taking on the AI challenge.

It only remains to say thanks to everyone! iCSI is not just its Board or its Director, but all the people who have made an effort in the laboratories and behind their computers and the research that has resulted. We wish to continue and develop our collaborations in catalysis in a new centre as well as through other instruments, and we are open to new collaborations based on our core values – commitment to fact and scientific principles, and knowledge and technology for a better society.

ABOUT iCSI

PARTNERS

All partners have been part of iCSI from start-up in 2015 to its conclusion in 2023. NTNU has been the host of iCSI, with SINTEF Industry and University of Oslo as research partners

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. Yara operates two industrial sites in Norway: Porsgrunn and Glomfjord

Topsoe AS is a catalyst producer and process plant technology developer based in Denmark. Topsoe wants to be the global leader within carbon emission reduction technologies for the chemical and refining industries.

Dynea AS is a Norwegian-owned specialty chemical company for sustainable wood adhesives, industrial coatings, specialty adhesives and polymers and surfacing solutions. They have production sites in Norway, Denmark and Hungary, and are licensing the Dynea Silver Catalyzed Formaldehyde technology, fasil®.

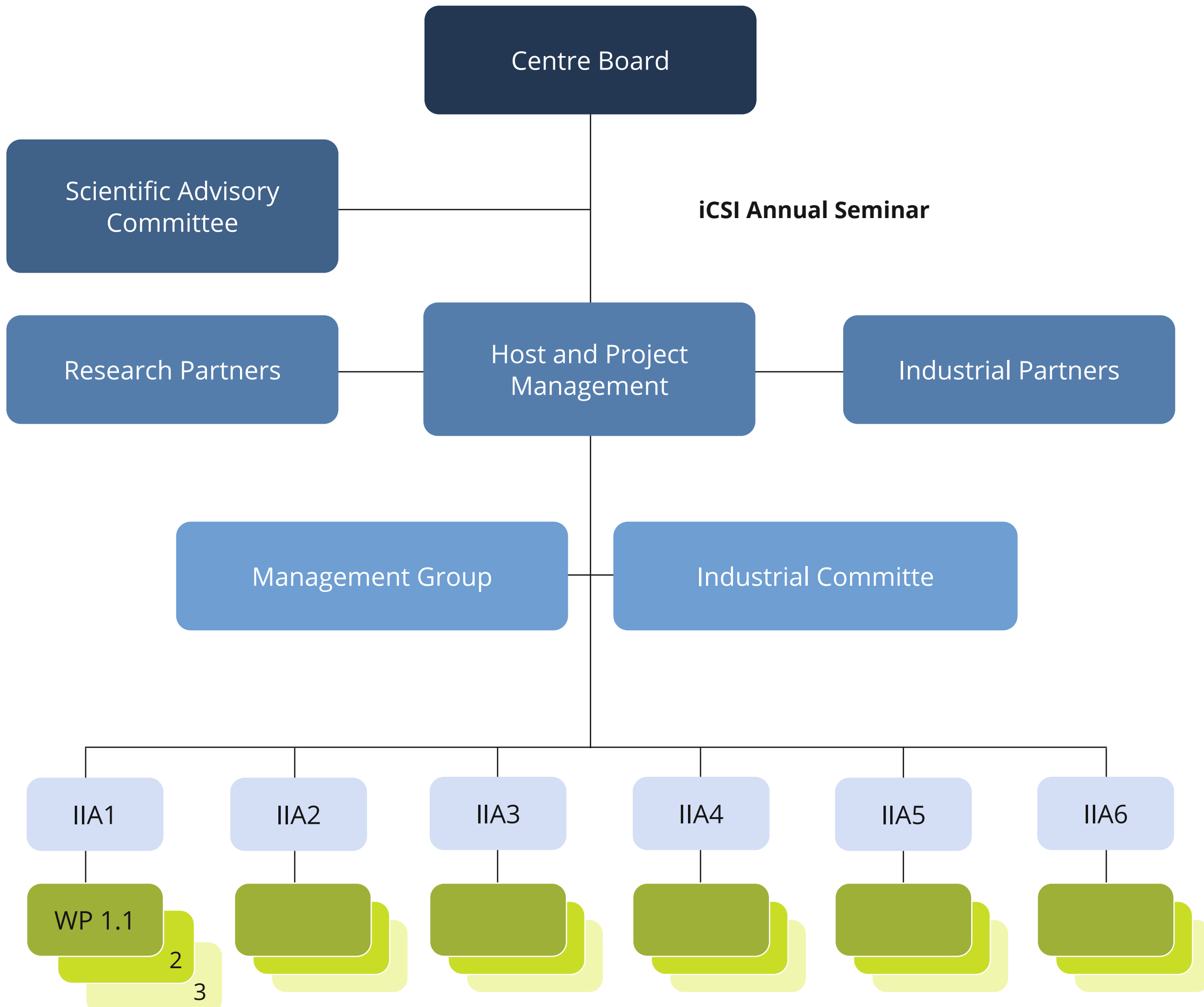
K.A. Rasmussen AS is a refiner of precious metals and supplier of catalysts and products based on precious metals located in Hamar, Norway. They specialise in technology for producing structured catalysts for the Ostwald process and silver particles for the oxidation of methanol.

INEOS Inovyn Ltd. is a leading producer of chlorvinyls and associated products, wholly owned by INEOS. INEOS Inovyn Norway AS constitutes about 300 employees at two sites: The chlorine/ VCM production at Rafnes and the PVC plant at Herøya.

Photo: Topsoe

ORGANISATION

The Norwegian University of Science and Technology (NTNU) has served as the Host institution for the iCSI Centre, with centre management and administration at the Department of Chemical Engineering The research was organized into 6 Industrial Innovation Areas (IIA1–6), each with 1–6 work packages.



THE iCSI BOARD

Each industry and research partner had one representative on the Board and the Chair of the Board has been from the industry. The Research Council of Norway was present with an observer. The following persons have represented their companies on the iCSI Board:

Yara:
Odd Arne Lorentsen, (chair 2015-2019)
Torgeir Lunde (2019-2024)

Topsoe:
Pablo Beato (2015 – 2024, chair 2019-2024)

Dynea:
Lars Axelsen (2015 – 2023)

K.A. Rasmussen:
Terje Pedersen (2015-2017)
Johan Skjelstad (2018-2020)
Thomas By (2020-2023)
Ann Kristin Lagmannsveen (2023-2024)

INEOS Inovyn:
Steinar Kvisle (2015-2017)
Terje Fuglerud (2017 – 2019)
Marco Piccinini (2019-2020)
Kamilla Jordal (2021-2022)
Tigran Margossian (2022-2024)

SINTEF Industry:
Duncan Akporiaye (2015–2024)

University of Oslo:
Vebjørn Bakken (2015-2018)
Kristin Vinje (2018-2019)
Einar Uggerud (2019-2024)

NTNU:
Tor Grande (2015–2017)
Karina Mathisen (2017-2024)

The Research Council of Norway:
Aase Marie Hundere (observer, 2015-2024)


Pablo Beato


Lars Axelsen


Torgeir Lunde


Ann Kristin Lagmannsveen


Tigran Margossian


Einar Uggerud


Duncan Akporiaye


Karina Mathisen


Aase Marie Hundere

SCIENTIFIC ADVISORY COMMITTEE 2015–2024

Alessandra Beretta
Politecnico de Milano

Enrique Iglesia
University of California
at Berkeley

Graham Hutchings
Cardiff University

iCSI MANAGEMENT AND ADMINISTRATION

Hilde Johnsen Venvik
Centre Director
(2015-2023)

Torgrim Mathisen
Economy Advisor
(2015–2020)

Ragnhild Aaen
Economy Advisor
(2021)

Hilde Mogård Flaathe
Economy Advisor
(2021–2024)

Estelle Marie Vanhaecke
Coordinator
(2015–2019)

Nikolas Tsakoumis
Coordinator
(2019)

Anne Hoff
Coordinator
(2018–2023)

Beretta: *"The iCSI consortium is addressing both topical challenges of the chemical process industry and an entirely novel process. Advancements in these fields may have a dramatic impact on the economy of scale of several production processes and major economic returns for the industrial partners."*

Iglesia: *"I am certain that the iCSI Centre is becoming an excellent model for academic-industry collaborations, as well as a place that will be remembered for having grown the talent that will populate catalysis research for decades to come."*

Hutchings: *"You don't know when the next big, wonderful discovery is going to be made. Maybe you'll make it. Maybe you won't, but there are always new things out there."*

SENIOR RESEARCHERS

DEPARTMENT OF CHEMICAL ENGINEERING, NTNU:


De Chen
2015-2023


Edd A. Blekkan
2015-2023


Hilde J. Venvik
2015-2023


Jia Yang
2015-2023


Magnus Rønning
2015-2023

DEPARTMENT OF CHEMISTRY, UNIVERSITY OF OSLO:


Anja O. Sjåstad
2015-2023


Helmer Fjellvåg
2015-2023


Karl Petter Lillerud
2015-2022


Stian Svelle
2015-2023


Unni Olsbye
2015-2023

SINTEF INDUSTRY:


Arne Karlsson
2015-2018


Bjørn Chr. Enger
2015-2023


Bjørnar Arstad
2015-2023


Børge Holme
2015-2021


Francesca Bleken
2021-2023


Ingeborg-H. Svenum
2019-2023


Jasmina Cavka
2015-2023


Kumar R. Rout
2015-2021


Patricia Carvalho
2015-2023


Roman Tschentscher
2015-2023


Rune Lødeng
2015-2023


Silje Håkonsen
2015-2023


Torbjørn Gjervan
2015-2023

iCSI FINANCING AND COSTS 2015-23

Summary sheet for the main categories of partners (NOK million)

Contributor	Cash	In-kind	Total
Host		28.9	28.9
Research partners		21.2	21.2
Industry partners	24.0	26.5	50.5
RCN	96.2	-	96.2
Sum			**196.8**

Distribution of resources (NOK million)

Type of activity	NOK million
IIA1 21st century nitric acid technology development	39.1
IIA2 New NOx abatement technologies	8.7
IIA3 Frontier formalin technology development	24.4
IIA4 PVC value chain	32.3
IIA5 The next step in direct activation of methane	34.2
IIA6 Generic projects	42.0
Projects	**180.7**
Management and administration	12.1
Common centre activities	4.0
Totals	**196.8**

RESULTS

iCSI KEY FIGURES 2015-2024

100 scientific publications (peer reviewed)

>200 presentations at seminars and conferences

11 popular disseminations

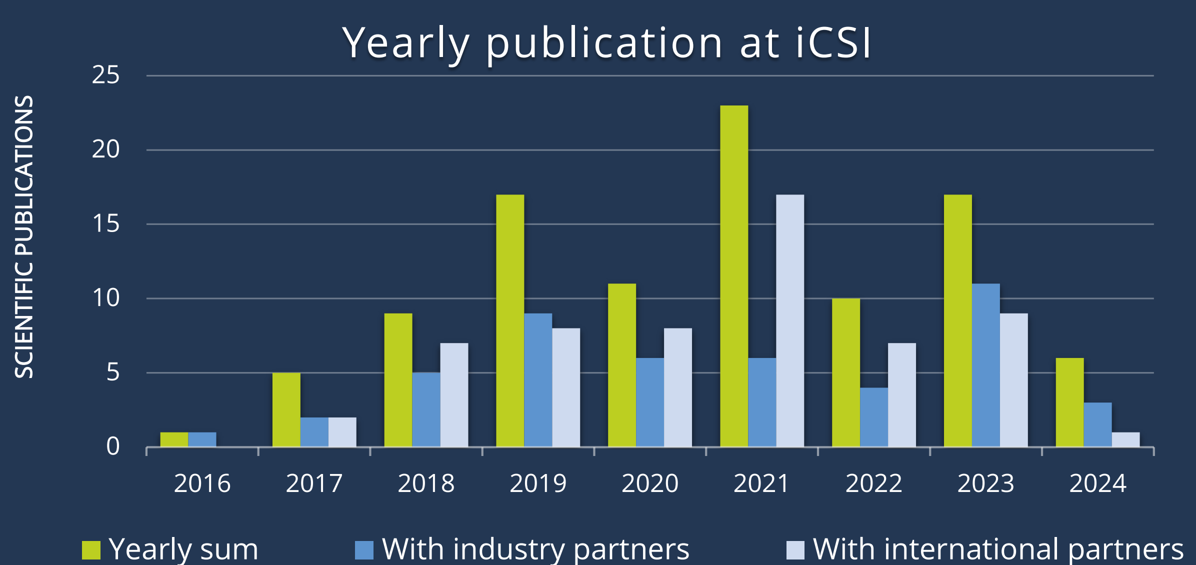
4 patent applications

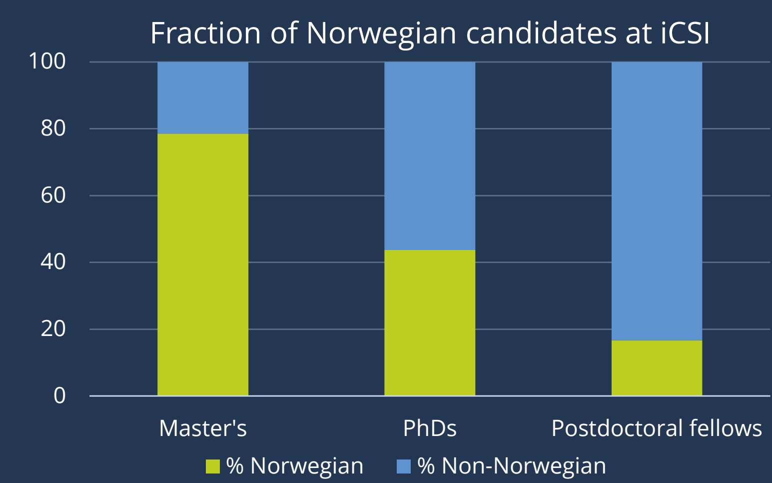
16 PhD — iCSI funded candidates, graduated or in progress

6 iCSI postdoctoral fellows

42 MSc — Theses on iCSI topics

21 PhD — iCSI associated with other funding, graduated





iCSI OUTREACH

IMPACT

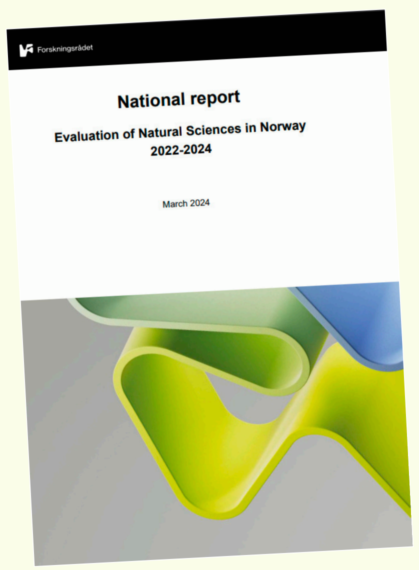
Photo: INEOS Inovyn

iCSI EFFECTS FOR THE INDUSTRY PARTNERS

Overall, the industry partners are very satisfied with their involvement in iCSI. The most important proof of this is their committment to a new SFI grant application. When asked what they consider the most important effects of participating in iCSI, it varies with the industry partners' market, size, and location of own research activities and other factors. The statements below may be summarized as the most important. They are all relevant to the partners, though to varying degrees:

- The long-term horizon of the SFI
- Synergistic cooperation and access to world-class expertise
- Very interesting collaboration with talented people and institutions
- Fundamental knowledge that provides opportunity for improvement of "mature processes".
- Improved theoretical insight into the kinetics and chemistry of important reaction systems
- Recruitment of competent candidates on PhD and Master level
- Such research collaborations help smaller companies with limited R&D resources stay up-to-date and curious about new possibilities
- Networking and visibility on the map of catalysis.

When it comes to assessing the significance of iCSI in a wider perspective, we quote from the recently published report, Evaluation of Sciences in Norway 2022-2024, commissioned by the Research Council of Norway. Here, iCSI was characterised as a very strong research environment and selected as one out of three impact cases within chemistry in Norway. Besides iCSI, our research partners in the Catalysis group at the University of Oslo represented another of the three impact cases due to their research on zeolites and innovation related to the metalorganic framework material UiO-66.



"A small selection of the impact cases submitted to the evaluation is provided here and illustrates the breadth of the research as well as its often significant impact. The cases include development and transfer of more sustainable technologies to industry, rapid uptake of results from fundamental research (………), and helping tackle decarbonisation of the energy system."

"Case: SFI iCSI: During 2015-16, the centre started research to deepen understanding of catalysis in the production of PVC, nitric acid and formaldehyde – bulk chemicals for which there are large markets and many industrial uses, and of which members of the industrial consortium are major producers. iCSI developed new methods and protocols which were used by the industrial partners to increase yields, reduce energy consumption, develop new process technologies and reduce the risk of environmental pollution. The 4 PhD and 18 master's graduates associated with the projects up to 2023 now work in the chemicals industry or universities, and are using their education to significantly reduce the climatic and environmental impacts of chemical processes, and form part of a much bigger cohort of graduates and postgraduates from the centre taking similar skills with them to industry."

EvalNat report 2024

INDUSTRY PARTNERS ABOUT THE OUTCOME FROM iCSI:

Yara:
- Several internal development projects come out of learning from iCSI -

Dynea:
- Regarding competitiveness, participation in the centre proves that we take development and innovation seriously and cooperate with academia. This has been very well received by our customers -

KA Rasmussen:
- In addition to the value of all the new knowledge about the current use of the catalysts, there have been some ideas for new products born from iCSI research that have the potential of commercialisation -

Dynea:
- Extracting "practical" results from the PhDs has given us better insights and guided the company in its innovation work for the future. The macrokinetic model will be used in optimalisation work and future operator training –

Topsoe:
- The very fundamental nature of the project requires a long-term commitment, and it is exactly that what is usually difficult to cover by other types of funding

INEOS Inovyn:
- Achieved research results:
Strengthened understanding of fundamental aspects of the industrial reactions via operando analytic and calculation approaches. This includes different kinetic mechanisms and effect of general parameters on reaction kinetics

KA Rasmussen:
- For us, the most interesting work done has been the characterisation studies of catalysts after exposure to different conditions (temperature, atmosphere, time etc.). We now know more about the mechanisms at play in both reactions, which we are certain will be helpful for future development -

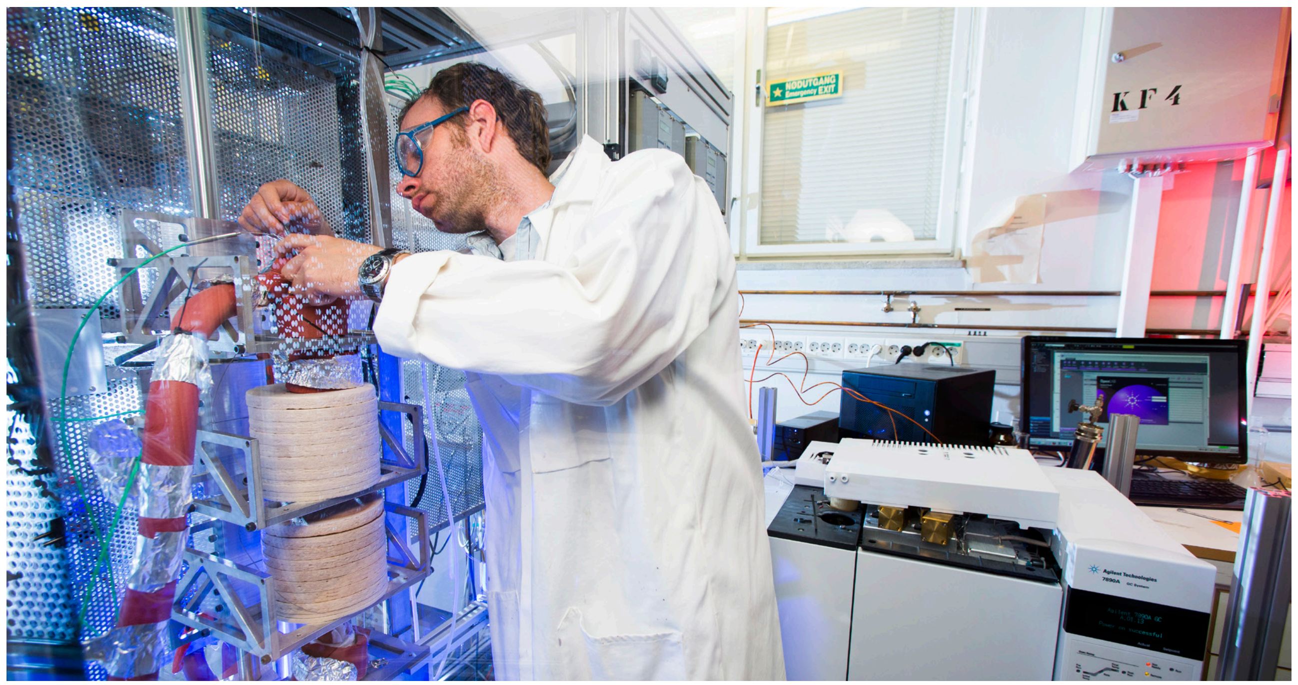
Yara:
- We have achieved new insight in our de-N_2O catalyst system which is a large contributor to GHG reduction (~25 MT CO_2eq/y)

iCSI EFFECTS AT UIO, SINTEF AND NTNU

Stian Svelle, Head of Department of Chemistry, UiO:
Through our participation in iCSI, researchers at UiO have substantially boosted their research portfolio. Through IIA5, we have essentially established a new line of research on low temperature direct methane activation where we now take part at the very edge of the international research front. Secondly, through iCSI we have established lasting links between researchers at UiO, NTNU and SINTEF Industry. Thirdly, we have substantially increased our capabilities and capacity to carry out cutting edge research at major international research facilities such as MAXIV in Lund, Sweden, and the Swiss-Norwegian Beamlines at ESRF, Grenoble, France.

Torbjørn Gjervan, Research Manager, SINTEF Industry:
iCSI has provided SINTEF with a crucial platform for engaging with key national stakeholders in catalysis and process technology. The center has facilitated long-term research focus on topics relevant to several key sectors of Norway's process industry and has created a collaborative environment with industry and research partners. The national infrastructures for advanced characterization NORTEM and NICE have played particularly significant roles. In IIA2 and IIA3, we have developed innovative characterisation methods customized for the respective industries involved, enabling quicker and more accurate analysis of their catalysts. This, in turn, has provided deeper insights into catalyst deactivation mechanisms and triggered new research questions for the potential follow-up activities that could enable further improvement of the industrial processes.

Edd A. Blekkan, Catalysis Group leader, NTNU:
Hosting and being an active part of a centre like iCSI has been incredibly important to the work in the Catalysis group at NTNU over the last 8 years. First and foremost, the long-term commitment invites a deeper and more ambitious approach to the research, each new student building on the experience of the previous candidates. Furthermore, the close interaction with the industrial partners provides exciting challenges, and the fast transfer of knowledge is inspirational to an educational environment like ours. I would also like to mention that the networks developed through the centre are extremely useful and important.



Senior researcher Roman Tschentscher at the SINTEF Industry lab. Photo: Werner Juvik

RESEARCH ACHIEVEMENTS

IIA1

21^{st} Century Ammonia Oxidation and Nitric Acid Technology Development

Anja Olafsen Sjåstad, UiO

Nitric acid is a key industrial chemical with global annual production in 2024 expected to exceed 67 million tons and more than 78 million tons by 2029. 70% of nitric acid is used in the production of fertilisers, which today helps feed more than 45% of the world's 8 billion population. Nitrate-based fertilisers produced from nitric acid are the most efficient means of supplying the key nitrogen nutrient to crops.

Today, Yara is the world's largest producer of nitric acid; combusting ammonia over highly selective platinum-alloy catalyst gauzes to produce NO in the first step (Ostwald process). K.A. Rasmussen is a noble metals refiner and Yara's preferred supplier of combustion gauze platinum-rhodium (Pt-Rh) catalysts. The second step in the process is the homogeneous and exothermic oxidation of NO to NO_2. In modern plants, we recover energy from the ammonia oxidation step, but not from the oxidation of NO. Two long-standing focus areas of Yara have been the optimal use of the precious metals used to combust ammonia and improving the overall energy efficiency of our plants. These have both been addressed in IIA1.

To reduce the evaporative losses of Pt from the combustion gauzes, plants install palladium (Pd) based gauzes directly downstream. These alloy with volatile PtO_2, capturing approximately 70% of the volatilised Pt but lead to new problems: The catchment gauzes swell to develop an undesired flow resistance and palladium is now lost in this process. Prior to iCSI, little was understood about the fundamentals of Pt recovery on Pd. We therefore set out to understand the fundamentals of Pt catchment on Pd/Ni and to improve capture by Pd and other oxide-based systems.

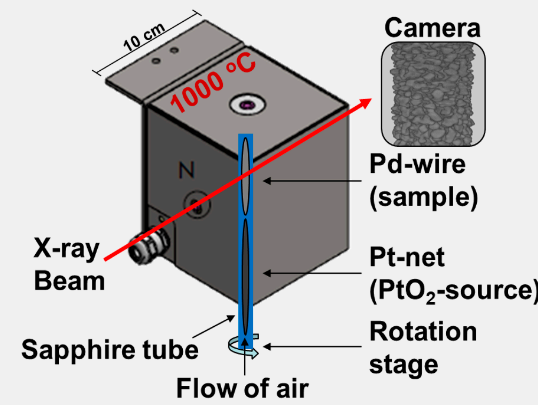
The development of a catalyst to oxidise NO to NO_2 under realistic plant conditions became another goal. In current nitric acid plants, this is carried out by cooling the gas and giving sufficient residence time for the homogeneous gas phase oxidation, and the heat released is mostly lost through pipework walls without energy recovery. By localising the oxidation in a catalytic bed, we identified a potential to increase energy recovery by approximately 15%.

Advancing platinum (Pt) catchment technology

Palladium (Pd) based catchment

Despite the fact that the ammonia oxidation technology in use today is more than 50 years old, many of the basic explanations were still lacking at the start. Questions related to nickel (Ni) and Pd loss, reconstruction and wire swelling of the Pd-Ni (91/9 at. %) gauzes were first addressed by PhD candidate Asbjørn Slagtern Fjellvåg (UiO), his co-supervisor David Waller from Yara and the SINTEF Industry researchers Børge Holme and Silje Fosse Håkonsen. They also wanted to understand why there was an apparent Pt-saturation at ~35 at. % for the resulting Pt-Pd-Ni alloy. The experimental facilities at UiO, SINTEF and Yara, with access to both bench- and pilot plant scale laboratories as well as synchrotron beamtimes at ESRF became indispensable for the investigations.

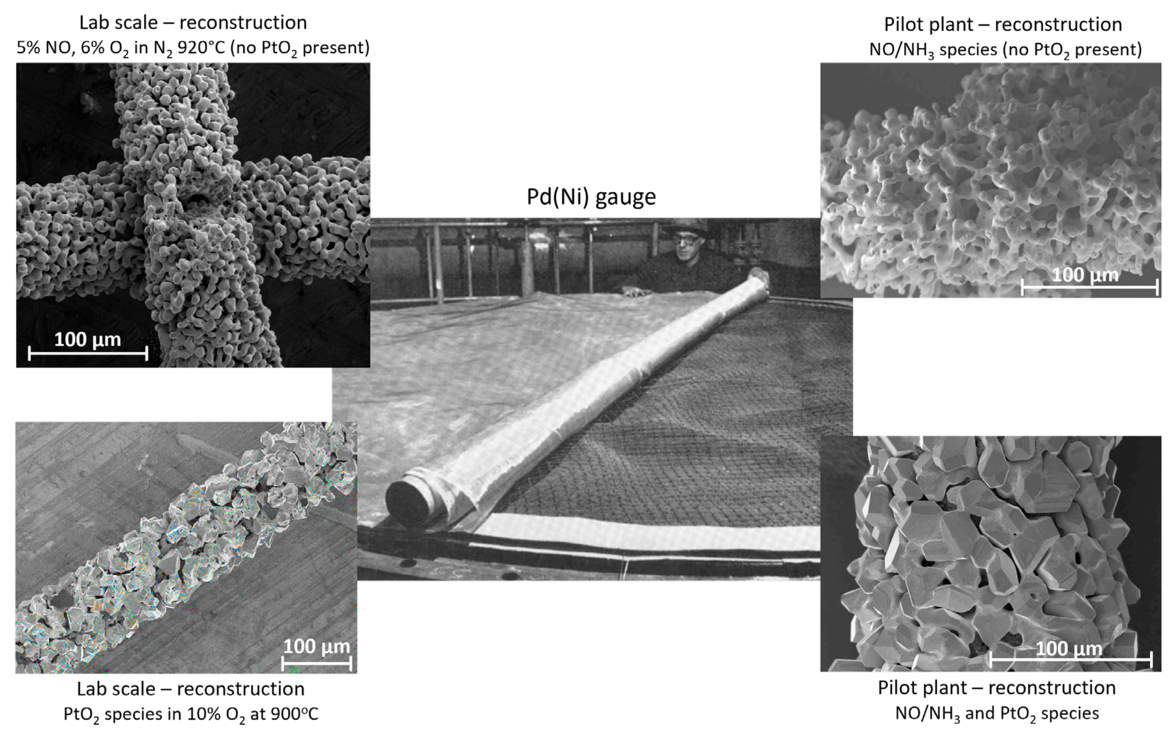
UiO developed furnace system for *in-situ* absorption tomography (ID15A, ESRF)



From the results, it could be concluded that oxygen from the NH_3 oxidation gas stream oxidises Ni in the Pd-Ni catchment material to NiO, which subsequently reacts to form volatile $Ni(OH)_2$. Pd remains in the metallic state, and the Ni loss has no effect on the Pd reconstruction. It was also found that Pd metal from the catchment gauze is lost through formation of Pd complexes with species such as NO and NH_3 as ligands. The Pd loss is accompanied by wire reconstruction. The findings were consistent through bench scale and pilot plant experiments (Figure below).

Another interesting finding was that the transport of Pt inwards to the core of the wire and Pd outward to the surface causes severe reconstruction of the Pd-Ni wires. Slow Pt diffusion in the grains versus the grain boundaries is one explanation for the reconstruction and swelling since similar reconstruction is not observed in quasi-single crystal Pd wires that do not contain grain boundaries.

Systematic studies further demonstrate that the quantity of Pt that can dissolve in the Pd-Ni catchment material is dictated by the equilibrium between gaseous PtO_2 and the Pt-Pd-Ni alloy. Thus, the maximum attainable Pt concentration in the alloy is limited by the partial pressure of gaseous PtO_2 and the process temperature.

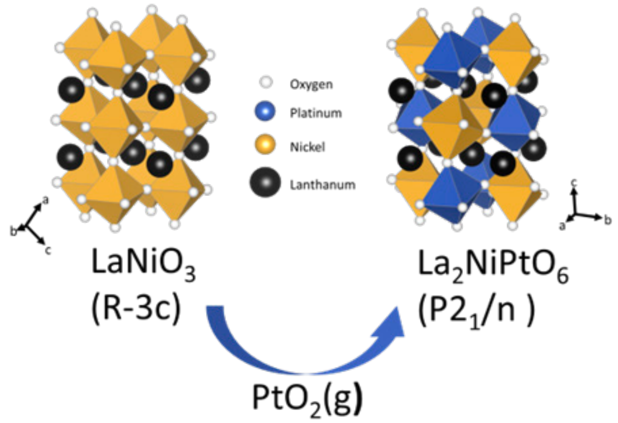


Overall, the studies on the Pd-Ni gauzes gave valuable insight into the current technology that allowed us to conclude that both the detrimental wire reconstruction and the Pd loss are intrinsic effects, which cannot be mitigated. Instead, alternative catchment materials should be explored.

Alternative catchment technologies
The pursuit for better catchment materials was divided into other metallic gauzes and oxides. Pd alloyed with gold (Au) was explored as an alternative to Pd-Ni, and a systematic study covering the pure metals and selected Pd/Au ratios was conducted. The mechanism for grain reconstruction was investigated in detail as well as seen in perspective of the established reconstruction mechanism for the Pd-Ni system. We found that alloy reconstruction induced by Pt catchment can be suppressed if the bulk mobility is comparable to the grain boundary mobility. Alloying Pd with Au enhanced the bulk Pt mobility due to the considerably lower melting point of Au. An optimal Pd/Au alloy composition was proposed, which balances reconstruction and Pd loss against Pt-catchment.

PhD candidate Julie Hessevik joined iCSI in the second centre period with Professor Helmer Fjellvåg and senior researcher David Waller from Yara as co-supervisors besides Professor Anja Sjåstad. Her work has dealt with identifying the potential of replacing the classic Pd-based catchment with an oxide material. In a proof-of-concept study, she explored the reactivity of gaseous PtO_2 toward $LaNiO_3$ and the subsequent formation of the Pt-containing double perovskite La_2NiPtO_6. Beyond this, she conducted a fundamental study to understand features in the Pt catchment process using atomic layer deposition (ALD) thin film grown $LaNiO_3$ in combination with atomic force microscopy (AFM), scanning electron microscopy (SEM) and depth profile X-ray photo electron spectroscopy (XPS) analyses

The experiments demonstrated substantial Pt catchment and transformation of $LaNiO_3$ into La_2NiPtO_6 at 800-900 ºC. The documentation of Pt incorporation was facilitated by the key findings from X-ray diffraction studies on Pt and Rh substituted $LaNiO_3$ reported by Asbjørn Slagtern Fjellvåg. The Pt could also be conveniently recovered from the oxide by a wet chemical approach. Moreover, it was verified that $LaNiO_3$ will not catalyse NO_x decomposition at the relevant process conditions whereas La_2NiPtO_6 exhibits slight activity



toward this reaction, which would be an unwanted product loss in NH_3 oxidation. Finally, both oxides were found to fully decompose the greenhouse gas N_2O at 900°C.

Julie continued to explore a series of different oxides for Pt catchment. This has resulted in innovative findings as well as the discovery of a new compound with a complex crystal structure.

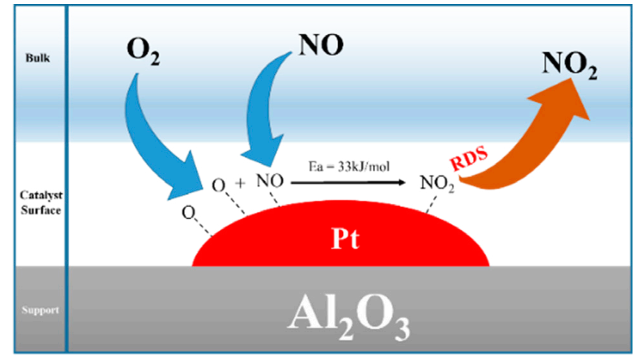
Catalysts for oxidation NO to NO_2

The main target has been to enable increased nitric acid output and heat recovery, as well as reduced plant CAPEX of the 3 nitric acid factories Yara operates in Porsgrunn, and at several plants elsewhere.

Ata ul Rauf Salman was the first PhD candidate working on finding suitable catalysts for oxidation of NO to NO_2. He was supervised by Magnus Rønning at NTNU, and the work was performed in close collaboration with Yara and SINTEF Industry. He designed and built a dedicated experimental setup, able to work at the demanding conditions a catalyst will face in a nitric acid plant and not common to any experimental lab worldwide. Ata studied a range of catalysts such as platinum, manganese oxides, and perovskites.

An important milestone was reached in 2018 by publishing the first paper on catalytic oxidation of NO to NO_2 for nitric acid production over an alumina supported platinum catalyst. We reported for the first time the kinetics of NO oxidation over Pt/Al_2O_3 under conditions relevant to industrial nitric acid production.

It was found that platinum exhibits significant catalytic activity above 300 °C for a feed comprising of 10%



NO and 6% O_2, partially simulating nitric acid plant conditions. The addition of 15% H_2O to the reactant stream had insignificant effect on the catalyst activity. Investigation on reaction kinetics yielded an apparent activation energy of 33 kJ/mol. The proposed reaction mechanism consists of dissociative adsorption of oxygen, associative adsorption of nitric oxide with desorption of nitrogen dioxide as the rate limiting step. Supported Ru catalysts shows promising activity and stability at industrial nitric acid production conditions. Through experiments performed at the Swiss-Norwegian Beamlines (SNBL) by Jithin Gopakumar, the next PhD candidate in this field, at the European Synchrotron Radiation Facility (ESRF), we have decoded the behaviour of the ruthenium catalyst's capacity to oxidise nitric oxide at industrially relevant conditions.

The oxidation state of a fraction of the Ru in the catalyst oscillates between slightly oxidised and completely reduced. Extended X-ray absorption fine structure (EXAFS) and X-ray photoelectron spectroscopy (XPS) analyses were combined to identify the oscillating behaviour as surface Ru oxidation-reduction cycles. The results allowed us to understand and explain the mechanism behind NO oxidation at industrial nitric acid production conditions over γ-Al_2O_3 -supported ruthenium catalysts.

The IIA1 Team at UiO with industry partners 2020: *Front row: David Waller, Julie Hessevik, Oleksii Ivashenko, Anja Olafsen Sjåstad, Oskar Iveland, Johan Skjelstad. Back row: Helmer Fjelvåg, Asbjørn Slagtern Fjellvåg, Thomas By, Børge Holme*

IIA2

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

Silje Fosse Håkonsen, SINTEF Industry

DeNOx

Nitrogen oxides (NOx) are harmful gas phase species that are produced by reaction between nitrogen and oxygen when fuels are combusted, and the temperature gets high. NOx contributes to smog and acid rain, and strict regulations for NOx emissions apply. Selective Catalytic Reduction (SCR) is a core technology in removing NOx from various sources, and new applications are emerging due to stricter regulations for NOx emissions and circular economy. In the SCR technology, a catalyst is used to reduce NOx with ammonia to form harmless nitrogen and water. Commercial catalysts are mainly based on vanadium oxide (V_2O_5) supported on titanium oxide (TiO_2) in the anatase structure. Catalyst lifetimes may be as long as 5 years but vary due to differences in their exposure to catalyst poisons, dust and soot.

The iCSI partners SINTEF and Yara have studied used catalysts from different industrial sources using advanced characterisation techniques. The goal has been to understand how dust, soot and different poisons affect their lifetime and to develop a suitable characterisation toolbox. At SINTEF Industry, Martin Fleissner Sunding has been a key researcher throughout the entire race together with activity leader Silje.

We found that catalysts installed in the exhaust treatment system of coal power plants and ships were heavily polluted by alkali metals, vanadium, sulphur, soot and dust. However, their performance was not dramatically affected. On the other hand, catalysts that had been installed in the exhaust gas treatment of a waste biomass incinerator deactivated heavily. Our studies revealed that these catalysts contained phosphorous, indicating that the performance of SCR catalysts is sensitive towards phosphorous poisoning. Detailed characterisation showed that phosphorous affects the active phase of the catalyst directly, thereby gradually making the catalyst unable to convert NOx. From a wider perspective, our results suggest that unexpected results can occur when deploying the commercial SCR catalyst for treatment of gas streams that contain other species than fossil fuel exhaust. This is particularly relevant in a time where replacing fossil fuels with more sustainable fuels is desirable.

Another study concerned a catalyst previously installed on a ship running on low sulphur fuels. Characterisation of the heavily deactivated catalyst showed that a thick silicon layer (> 1 micrometre) had deposited onto the surface, blocking the active catalyst surface. A change in the fuel production route to obtain the ultra-low sulphur fuel had most probably led to silicon leaching into the fuel, ultimately leading to problems in the exhaust gas treatment in ships.

Fresh deN$_2$O catalysts

DeN$_2$O

The Global Warming Potential (GWP) is a measure of how much energy the emissions of 1 ton of a gas will absorb over a given period of time, relative to the emissions of 1 ton of CO_2. For N_2O, which is an undesired biproduct from ammonia oxidation to obtain NOx and subsequently nitric acid (Ostwald process), the GWP is 298. This means that even with very small emissions of N_2O, this gas used to account for 50% of Yara's Greenhouse Gas (GHG) emissions. For this reason, Yara developed an abatement catalyst that is located directly below the platinum-based NH_3 oxidation catalysts.

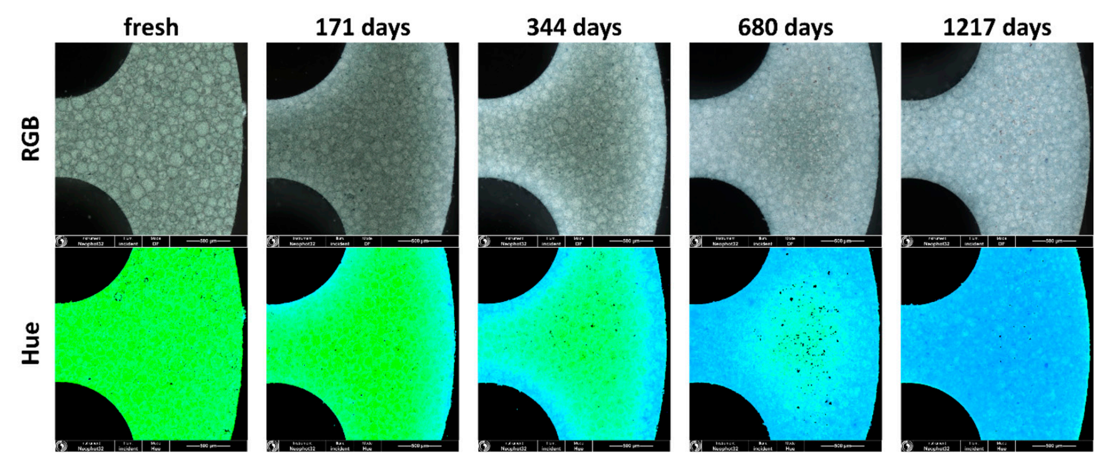
The N_2O decomposition catalyst consists of a cobalt (Co) and aluminium (Al) spinel phase supported on cerium oxide (CeO_2) and extruded into mini-monoliths. This catalyst can achieve > 95% abatement with no changes to plant operation. The N_2O abatement catalysts have proven to be able to perform at a high level in the harsh conditions inside an ammonia burner for over a decade. We have studied used/aged catalysts to better understand the material changes in them, with the aim of formulating even more active and stable catalyst.

An extensive characterisation toolbox has been used to investigate the transitions in this catalyst during its lifetime in different commercial nitric acid plants. We determined the most active phase as Co_2AlO_4, but Co is gradually lost from the catalyst via the gas phase while Al is not. Due to this loss, the Co_2AlO_4 spinel converts to $CoAl_2O_4$, with a different activity level for N_2O decomposition.

We also uncovered that the Co loss, and associated spinel conversion, starts at the surface of the monolith and gradually extends into the core until the whole monolith consists of $CoAl_2O_4$ supported on CeO_2. The rate of spinel conversion depends on plant operation conditions.

Based on this, we developed an easy and accessible method to determine where a catalyst is in its lifetime. Conveniently, the colours in the hue profile from light microscopy of a monolith cross-section can be directly translated into the presence of either spinel phase (figure below). The method can be used to compare the effect of different plants' operating conditions, or to pick up any abnormalities once a plant's catalyst lifetime curve has been established.

Transmission electron microscopy (TEM) was used to investigate fresh catalysts. While the average Co/Al ratio of a fresh catalyst is 2, detailed TEM images showed that there is a large spread in Co/Al ratio between spinel particles. In addition, the spinel particle size in a fresh catalyst varies.



Crossections of a series of spent deN$_2$O catalysts from the same nitric acid plant. Top row: RGB colour profile. Bottom row: Hue colour profile

IIA3

Frontier formalin technology development

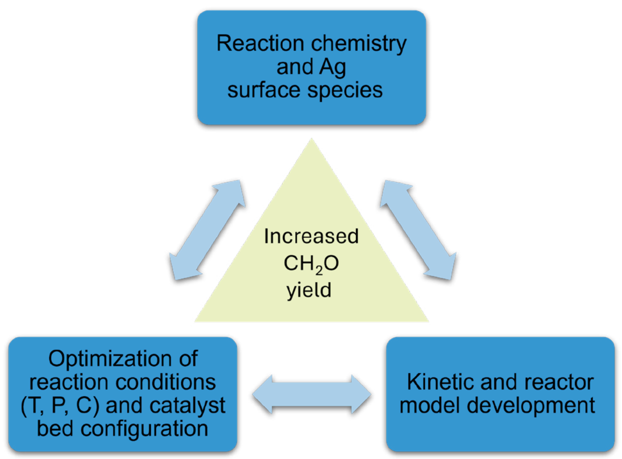
Jasmina Hafizovic Cavka, SINTEF Industry

Formaldehyde (CH_2O) is an important chemical widely used in the production of resins, which are essential in manufacturing of wood products as well as in coatings, adhesives, and insulation. The formaldehyde is usually dissolved in water to stabilise the product and reduce the HSE risks, and this aqueous solution is called formalin.

Production technology for formaldehyde involves oxidation of methanol (CH_3OH) in excess air over a mixed metal oxide catalyst or excess methanol over a silver-based catalyst. Dynea owns both technologies but has identified the highest economic potential for the silver process due to lower energy consumption and possibilities for increasing the CH_2O yield beyond 90 %. K.A. Rasmussen is a noble metals refiner and silver catalyst supplier for the formaldehyde process. In IIA3, Dynea, K.A. Rasmussen, NTNU, and SINTEF have collaborated with the main aim of finding ways that can increase the fraction of formaldehyde produced to methanol fed to the process (=yield) and decrease the fraction of methanol feedstock lost to CO2 and other by-products.

To realise the goal, the team applied various experimental and theoretical strategies to:

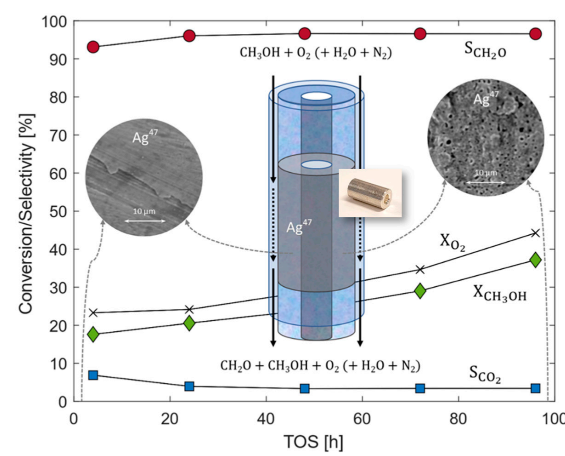
- Gain deeper insights into the reaction mechanism to promote the desired reaction and suppress side reactions.
- Increase the understanding of how catalyst restructuring and oxygen dissolution dynamics impact catalyst performance (activity and selectivity).
- Optimise the silver surface area and catalyst bed geometry.
- Optimise reaction parameters such as temperature, reactant concentration, and residence time.
- Develop a predictive reactor model that can be an important process control tool and guide future process developments.



Reaction mechanisms and surface Ag species in catalytic oxidation of methanol to formaldehyde

The two consecutive PhD projects of Stine Lervold and Youri van Valen have constituted the main effort in this work. Their supervisor team included Professor Hilde Venvik, Associate Professor Jia Yang and Dr. Rune Lødeng. We have also collaborated with researchers from Lund University, MAXIV laboratory (Sweden) and Karslruhe Institute of Technology (Germany) and post-doctoral fellow Dr. Tina Bergh in IIA6.

Stine defended her thesis in June 2021. Her main achievement was to implement an annular reactor concept to partial oxidation of methanol over silver catalyst. This enabled reaction data at low conversion of both methanol and oxygen (kinetic regime) for industrially relevant temperatures and reactant composition, and with minimised impact of mass transfer limitations and (homogeneous) reactions in the gas phase (figure below). This has never before been presented in the research literature! The work showed that when only the surface chemistry plays a role, very high formaldehyde selectivity is possible (up to 97%), and the main by-product formation pathway is direct formation of CO_2. It led to a new problem, however, since at incomplete conversion it becomes clear that the catalyst restructuring and oxygen dissolution dynamics continuously impact the reaction and in response to changes in the conditions – there is rarely a steady state with this silver catalyst.



Very high formaldehyde selectivity can be obtained while running at incomplete conversion of oxygen by applying an annular reactor concept. Lervold et al, Chem. Eng. J. 2021, 423, 130141

Youri proceeded to explore what we can learn from the annular reactor concept. He has studied the sub-reactions hydrogen (H_2) oxidation and carbon monoxide (CO) oxidation in addition to the main reaction (figure below). Through this, he has been able to further elucidate the reaction mechanism and the effect of various side-products and co-reactants (H_2, CO, CO_2, H_2O). Through careful experimental protocols and Tina's expertise on advanced electron microscopy and diffraction methods, he can also show how the silver restructuring and oxygen dissolution dynamics differ between the different reaction atmospheres. The work has uncovered somewhat unexpected and complex findings on catalyst structure and performance (activity and selectivity) that will now be published, and Youri will thereafter defend his PhD.

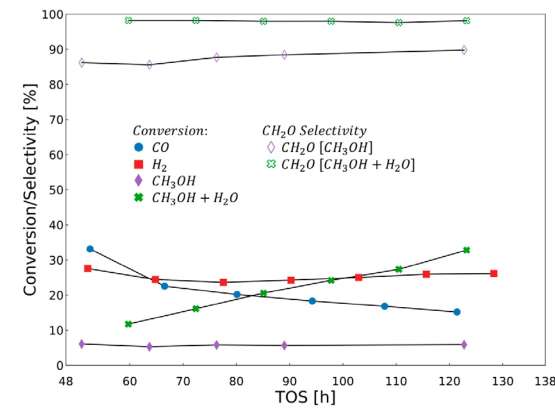
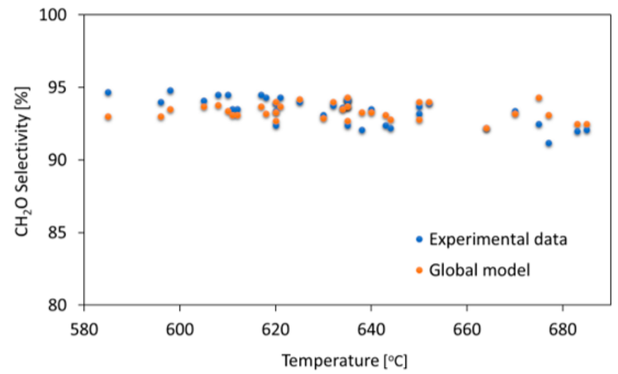
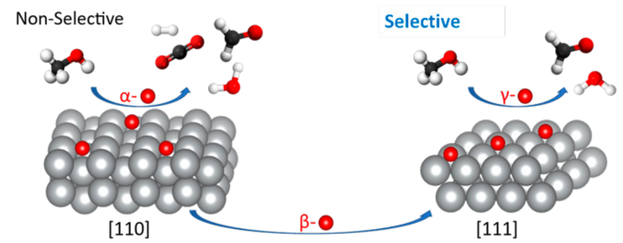


Figure showing how the conversion changes with time on stream for H_2, CO and methanol oxidation over silver, and how the methanol oxidation is impacted by the presence of H_2O.

Finally, through the abovementioned international collaboration, the gas dissolution (O, H, He) and silver restructuring dynamics could be further explored via in situ X-ray imaging. Captivating phenomena were revealed through synchrotron beam times at MAXIV (Sweden) and DESY (Germany) that will soon be published jointly with the collaborators.

To the industry, the work has suggested that it is possible - but not at all straightforward - to further develop the silver catalyst and enhance the formaldehyde yield beyond today's "best industrial performance". Meanwhile, the understanding of the catalyst and the reaction has significantly deepened to the benefit of their unique technologies.





Methanol oxidation to formaldehyde – controlling the selectivity of Ag-based catalysts

We also wanted to examine how the geometry of the catalyst bed and various operational parameters in industrial processes influence the formaldehyde yield. To achieve this, Roman Tschentscher (SINTEF) and his team utilised a small-scale pilot unit capable of handling gas feed rates of up to 20 L/min, which we further refined for optimisation. The catalyst was tested under conditions closely resembling industrial operation. Through several test campaigns, we evaluated different factors including feed composition, process conditions, and catalyst bed geometry. The tests encompassed both existing industrial practices and novel operational approaches.

From our experimental investigations, we found that the height and structural properties of the catalyst bed primarily impact operational costs due to pressure drop. Also, the catalyst ignition behaviour correlates strongly with the tendency for sintering during operation. Initial catalytic reactions predominantly occur within the top catalyst layer, with lower sections contributing to heat distribution and structural stability.

From the results, we also recommend that catalyst design should prioritise achieving plug flow to minimise back mixing of reaction products. Introducing water into the process enhances safety and appears essential, even in small quantities, to promote formaldehyde production.

The ratio of oxygen to methanol feed is a critical parameter in the process, which influences both operating temperature and conversion efficiency. Like in other partial oxidation reactions, higher formaldehyde selectivity is achieved at lower conversion rates, albeit resulting in lower overall yields. Finally, we found that improved formaldehyde yields are attained with longer contact times between the reacting gas and catalyst.

Kinetics and reactor model development for the methanol oxidation to formaldehyde process

Rune Lødeng (SINTEF Industry) has, in collaboration with Dynea, developed mathematical descriptions for predicting formaldehyde yield and for better understanding the details of the chemistry. Data for tuning the models have been obtained from the lab reactors (PhD students) and in the small-scale pilot reactor applied for performance testing by SINTEF. In addition, data from industrial plants were made available for the modelling work. Fundamental theory related to the energies of chemical bonds on surfaces has been used (Yanying Qi, IIA6) for assisting in selecting the right reactions and for calculating required parameters for describing rates and responses to temperature and feed composition. The models have been used to evaluate ways of increasing formaldehyde yield in the industrial perspective, either via changing the way plants are operated or via reactor and catalyst tuning. The best way of utilising the oxygen in the feed has been the aim, i.e. how to avoid side products and excessive temperatures. In addition, improved knowledge about the nature of the silver surface has been established via the detailed chemistry modelling.

Throughout the whole project, the experimental planning and data interpretation have benefited greatly from discussions with the industry partners K.A. Rasmussen (Terje Pedersen, Johan Skjelstad, Thomas By, Ann-Kristin Lagmanssveen, Federica Mudu) and Dynea (Lars Axelsen, Kristin Bingen, Herdis Petterson, Alma Engelbrecht, Mads Lid, Ole H. Bjørkedal). Also, each master and exchange student contributed with unique pieces to the puzzle (Appendix 2).

De Chen, NTNU

IIA4

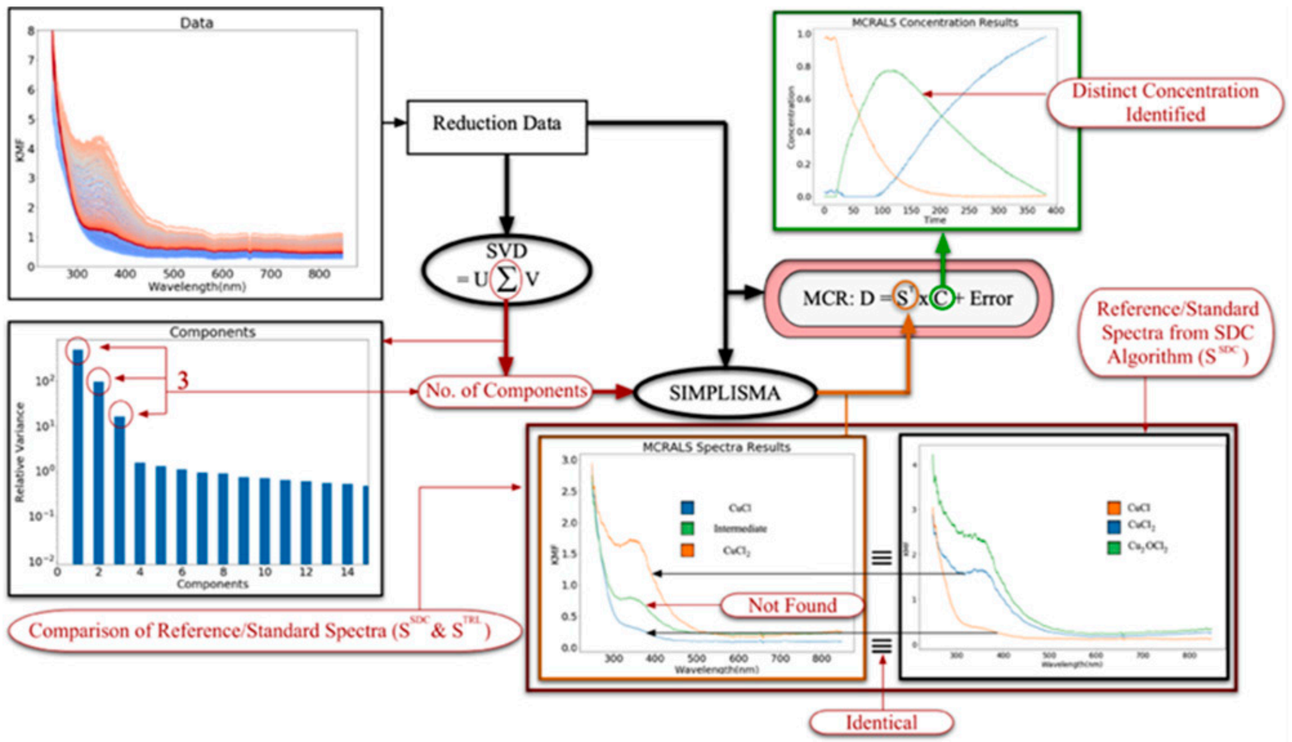
PVC value chain: world class energy and raw material efficiency to produce chlorine and vinyl chloride monomer (VCM)

The advancement in polyvinyl chloride (PVC) production technology, specifically the synthesis of vinyl chloride monomer (VCM) from ethylene, has seen significant scientific progress since its introduction in the 1950s. This evolution has emphasised plant reliability, as well as energy and raw material efficiency. Central to the process is the oxychlorination reaction of ethylene (C_2H_4) to 1,2-dichloroethane (EDC) using a copper chloride-based ($CuCl_2$/γ-Al_2O_3) catalyst system. This reaction is of redox nature, where copper cycles between Cu^{2+} and Cu^{+} states, and the dynamic behaviour of surface $CuCl_2$ layers play a pivotal role in the catalyst's performance.

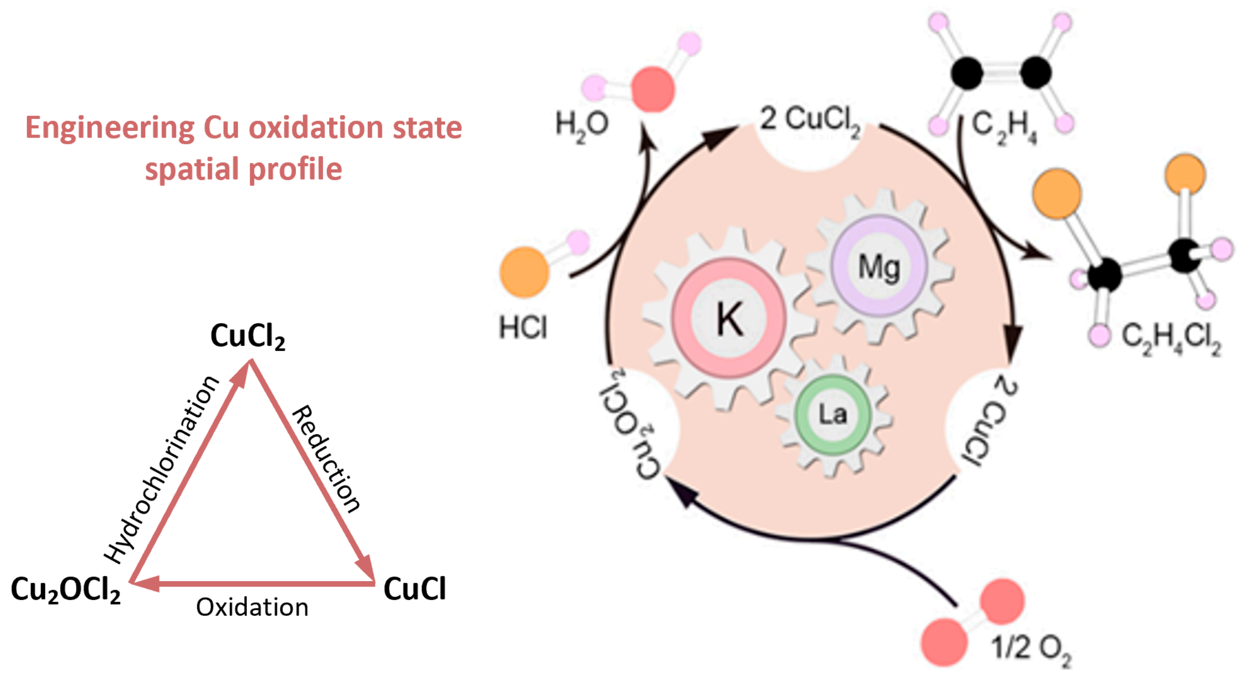
The IIA4 research aimed at obtaining world-class energy and raw material efficiency through atomic-level understanding of surface catalysis mechanisms, specifically the half-reactions in the ethylene oxychlorination redox cycle. This could then be translated into a predictive kinetic model for the dynamic behaviour of active sites, and design of catalysts that optimise the redox cycle for improved activity, selectivity, and stability. The research activities ranged from kinetic investigations to in-situ characterisation, understanding deactivation and by-product formation, and finally, exploration of new catalysts and VCM production methods.

The IIA4 team was led by Professor De Chen at NTNU, with support from Dr. Kumar Rout, SINTEF Industry. Postdoctoral fellows Dr. Yanying Qi and Dr. Yalan Wang made significant theoretical contributions to the research. Many INEOS Inovyn researchers were also involved along the way, especially Terje Fuglerud, Marco Piccinini and Tigran Margossian. And most important: Endre Fenes, Hongfei Ma and Wei Zhang received their PhD degrees having performed challenging experiments to obtain results published with high visibility and presented at several international conferences.

The team's first achievement was a method for predicting the steady-state rate and Cu oxidation state during ethylene oxychlorination through a reaction rate diagram. The rate diagram can predict the steady-state rate and corresponding Cu^{2+} and Cu^{+} concentration based on the transient kinetic data of the separate half-reactions, namely reduction and oxidation. This approach revealed insights into the catalytic behaviour under various conditions and led to the identification of cerium as an effective promoter, significantly enhancing catalyst performance. The results establish that the Cu^{2+} and Cu^{1+} concentration, the number of active sites, and their activity are highly dynamic, depending on the catalyst composition and the operating conditions.



Deep data analysis algorithm with the dataset of reduction step



Toward fully selective ethylene oxychlorination through engineering the Cu oxidation state spatial profile.

Cutting-edge characterisation employed operando UV–vis–NIR spectrometry and multivariate curve resolution analysis to unravel the dynamics of the active sites and their influence on catalytic performance. Mapping the changes in Cu^{2+}, Cu^{2+} with Cl vacancy, and Cu^{+1} concentration with time on stream under different conditions provided a deeper understanding of the role of promoter elements, and the dynamic nature of copper correlates with increased activity, EDC selectivity, and stability.

The study proceeded to underscore the impact of $CuCl_2$ and γ-Al_2O_3 interactions in ethylene oxychlorination. Superior catalytic activity, selectivity, and stability can be obtained utilising the γ-Al_2O_3 (110) facet. In contrast, catalysts with the (111) surface termination rapidly deactivate. This highlights the crucial role of metal-optimising catalyst design for improved redox reaction efficiencies, including stability support interactions, particularly the γ-Al_2O_3 properties, in optimising catalyst design for improved redox reaction efficiencies, including stability.

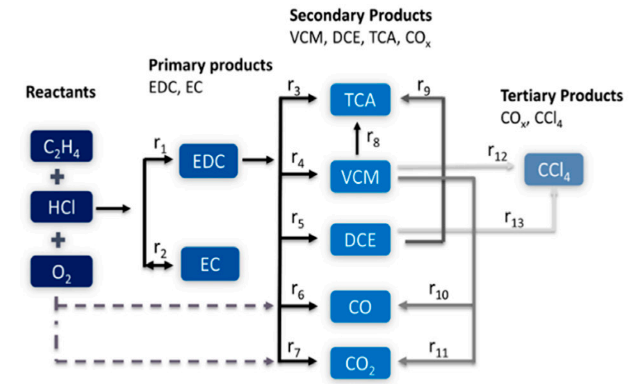
A comprehensive reaction network was also developed to better understand the intricacies of ethylene oxychlorination and its by-product formation, offering insights into improving selectivity.

Emphasising improved selectivity at high conversions, we employed spatial-time resolved UV–vis–NIR analysis to reveal spatially distributed $CuCl_2$ concentrations as being key to catalyst performance. A higher $CuCl_2$ concentration correlates with increased activity, EDC selectivity, and stability.

Innovative use of promoters allows fine-tuning of the oxidation state of copper, leading to a KMgLa-$CuCl_2$/Al_2O_3 catalyst that achieves complete conversion with nearly 100% selectivity towards EDC.

Finally, efforts were devoted to new developments in catalyst design and VCM production routes, including the introduction of carbon-based single-atom catalysts (SACs). This novel bifunctional catalyst design concept demonstrates a promising one-pot ethylene oxychlorination route that surpasses traditional methods in yield and efficiency.

Our comprehensive study not only advances our understanding of the oxychlorination process at an atomic level but also paves the way for the development of more efficient, selective, and stable catalysts



Reaction network of ethylene oxychlorination over K-doped $CuCl_2$/γ-Al_2O_3 catalyst.

for PVC production. Through our multidisciplinary approach, combining theoretical and experimental techniques, the research bridges fundamental understanding and practical application, setting the stage for the next generation of catalysis in VCM production with implications for the sustainability and efficiency of PVC manufacturing processes.

AWARDS:

Kumar R. Rout: Gianni Astarita Young Investigator Award, which recognises "a young researcher for his/her outstanding research in Chemical Reaction Engineering". International Conference on Chemical Reaction Engineering (ISCRE 25), Florence, Italy, 2018

De Chen: The Innovation Award, Faculty of Natural Sciences, NTNU, 2019

Stian Svelle, UiO

Pablo Beato, Topsoe

IIA5

The next step in direct activation of lower alkanes

As all current routes for exploitation of natural gas (methane, CH_4) for chemicals production rely on synthesis gas (CO and H_2) as an intermediate, a low temperature activation and transformation of methane into valuable chemicals is commonly considered a *dream reaction* due to its enormous industrial potential. This is the chemical process that researchers at Topsoe, the University of Oslo and SINTEF Industry decided to investigate together in iCSI.

In a 2005 key publication in *JACS (M. H. Groothaert et al., J Am Chem Soc. 2005, 127(5), 1394.)*, the use of Cu loaded zeolites (ZSM-5 and mordenite) for low temperature conversion of methane to methanol was demonstrated. The catalyst was pre-oxidised, and the product methanol had to be extracted from the catalyst using a protic solvent, which constitutes a serious obstacle from a process point of view.

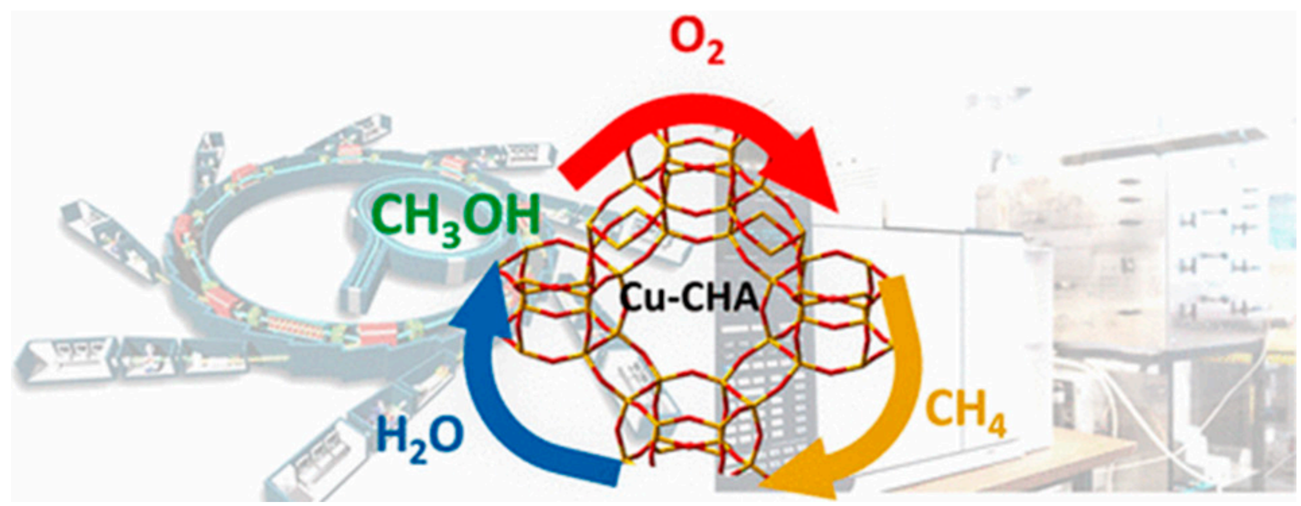
Thus, it was clear at the onset that metal loaded zeolites hold remarkable promise as catalysts for direct conversion of methane. However, several key challenges existed; to maintain high selectivity, to increase turnover rates and to design a proper, closed catalytic cycle. This translated into a need for rational design of zeolite materials with systematic properties, advanced *operando* characterisation of the active site, and process engineering. Within iCSI, all the competences required to successfully deal with these challenges and progress towards a viable low temperature process for the activation of methane were assembled.

During the first phase, our focus was on developing reaction protocols and methodology that allowed us to understand and optimise the underlying chemistry - essentially catching up with the research frontier. This was achieved primarily through the efforts of postdoctoral fellow Michael Dyballa and PhD candidate Dimitrios Pappas.

The focus of Dimitrios' thesis was to study the direct methane to methanol conversion over Cu-exchanged zeolites, to investigate Cu speciation as well as the mechanistic aspects of conversion. Activity measurements were coupled with spectroscopic techniques such as X-Ray Absorption Spectroscopy (XAS), Fourier Transform Infrared (FTIR) and Raman to provide insights into the Cu speciation. The establishment of reliable activity measurements in house and an advanced characterisation platform, based largely on synchrotron methods, was a major breakthrough of this initial work. As a result, Dimitrios received the EFCATS (European Federation of Catalysis Societies) Best PhD Thesis Award within the field of catalysis in 2021!

Dr. Michael Dyballa focused on materials synthesis and rational design of novel and improved zeolite materials. Through systematic efforts, it was possible to develop a zeolite material with unprecedented performance in the methane to methanol reaction. This allowed a careful performance evaluation of the materials comprising different zeolite topologies and different compositional characteristics, employing a wide range of different reaction conditions. We braided the performance data with results from IR spectroscopy as well as XAS coupled with Multivariate Curve Resolution to establish structure-activity correlations. Our data demonstrated that the Cu-MOR active sites are dimeric; a major breakthrough published in the high impact journal JACS (Journal of the American Chemical Society). Michael is now Group Leader at the University of Stuttgart.

Karoline Kvande was recruited as a PhD candidate after completing a master's degree in the Catalysis Group at UiO. She extended on the already established findings and experimental platform. Among other things, Karoline developed a similar method for the conversion of ethane to ethylene, thus unravelling completely new chemistry. From a systematic study into the required material properties, we found that akin to the well-tested methane to methanol reaction , Cu-sites confined within nanoporous zeolites were indeed crucial in ethane activation. . However, the requirements for the active site appeared to be somewhat different for the two alkanes. We identified a stepwise mechanism via an ethoxy intermediate to be the most likely reaction pathway for ethane.



In IIA5, we have investigated the reactivity of Cu-loaded zeolites in the stepwise conversion of methane to methanol using a combination of on purpose material synthesis (middle), advanced characterisation (left), and detailed reactivity investigations (right).

Dr. Sebastian Prodinger continued the all-important synthesis work that is required to establish structure–performance relationships for complex chemical processes. Through his efforts, it was possible to conclude a decade long scientific discussion on the origin of so-called "small port" and "large port" mordenite zeolites. Small port mordenite is characterised by low accessibility, despite having crystal structure seemingly identical to the large port variant. We were able to prove that it is the location of aluminum (Al) that lies behind the mysterious behaviour of mordenite port-size variation, with more Al in the 12-ring leading to a small-port material. Achieving control of aluminium siting and thus active site location in aluminosilicate zeolite constitutes a massive step forward in rational design of functional materials.

Bjørn Gading Solemsli was the final PhD candidate of IIA5. His research has been directed towards pinpointing the elusive reaction intermediate in the methane to methanol conversion. Through meticulous experimentation and analysis, he replaced the third reaction step in the cyclic process, i.e. steam extraction, by using ethylene, propylene, and benzene for extracting methoxy intermediate species. Bjørn's results show that benzene reacts with the hypothesised surface methoxy intermediate and undergoes successful methylation, yielding toluene as the sole product, whereas ethylene and propylene reactions are dominated by the oligomerisation-cracking pathway. Furthermore, reactions with benzene reveal that only a fraction of the methoxy species is available to react with benzene, thus providing an indicator of the accessibility of and the nature of methoxy species.

Many others have made substantial contributions to IIA5. Professor Unni Olsbye has been a key contributor at UiO, and Karl Petter Lillerud must also be mentioned. The activities at SINTEF Industry, led by Senior Scientist Dr. Bjørnar Arstad, have been essential. Through iCSI, we have collaborated extensively with researchers at the University of Torino, in particular Silvia Bordiga, Elisa Borfecchia, and Carlo Lamberti. Carlo sadly passed away in 2019, but his impact on IIA5 has been profound. Several postdoctoral fellows were also partly funded through iCSI; Carlo Buono, Izar Capel Berdiell, Torstein Fjermestad, and Chiara Negri.

The IIA5 Team with the centre director at NTNU 2023, from the left: Stian Svelle, Dimitrios Pappas, Hilde Johnsen Venvik, Karoline Kvande, Izar Capel Berdiell, Pablo Beato and Bjørn Gading Solemsli.

IIA6

Generic projects for additional industrial synergies

Magnus Rønning, NTNU

A selection of iCSI work packages are allocated to research with the intention of moving the research forefront and providing methodological tools to be applied in the industrial innovation areas IIA1-5. Advanced spectroscopic and microscopic investigations under conditions highly relevant to industrial operation have been targeted. Another effort is directed towards advancing atomistic and kinetic modelling of metals and oxides, as well as reactor modelling, to eventually enable an integrated, multiscale modelling approach.

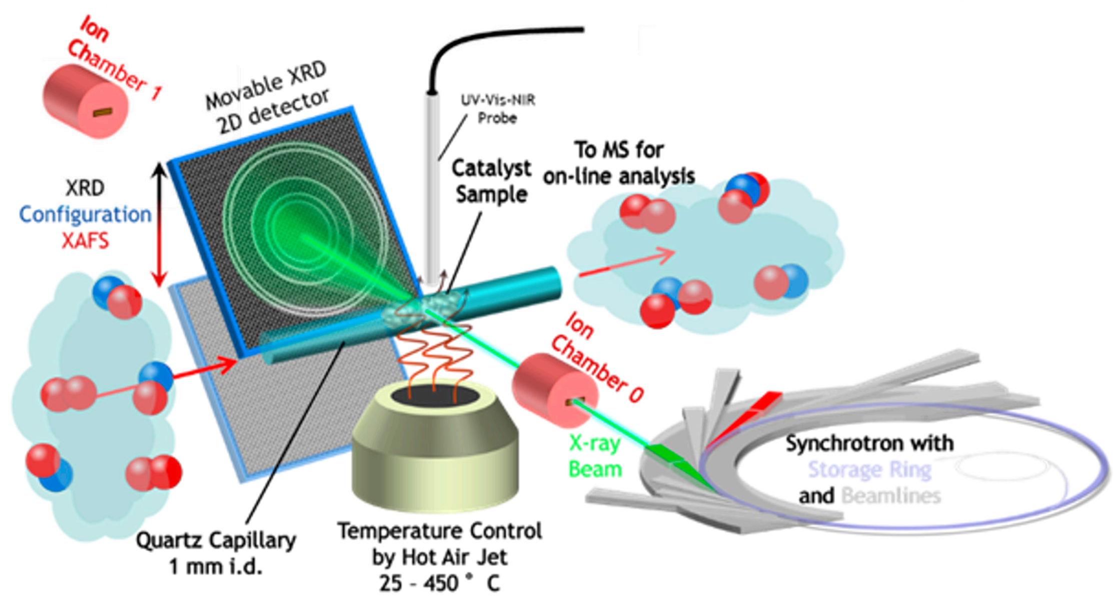
The generic projects include application of microcalorimetry. NH_3 adsorption was used to characterise Cu-exchanged zeolites (IIA5) and steady state isotopic transient kinetic analysis (SSITKA) to elucidate and compare the mechanisms of the catalytic oxidation of NO over Pt-based or Mn-based oxidation catalysts (IIA1). Surface science tools such as reactor STM has been established to allow for atomic scale investigation of catalyst surfaces when exposed to reaction environment (IIA1). Electron microscopy and diffraction tools have been developed in several work packages, serving most of the industrial innovation areas. New techniques and sample treatments can extend our understanding of the catalytic processes to an unprecedented level of detail. Some of the main activities are briefly described in the following section.

Advanced operando characterisation of industrial catalysts

Heterogeneous catalytic systems are complex, and simplification is often not adequate to describe industrial conditions. The PhD project of Samuel K. Regli targeted acquisition of kinetic and structural information in the same setup (operando). The key characterisation techniques employed were X-ray absorption spectroscopy with synchrotron radiation, X-ray diffraction, Fourier-transform infrared spectroscopy and UV-vis spectroscopy. The combination of these techniques provides information on both the bulk and the surface of the catalyst. If combined with exposure to industrial reaction conditions as well as quantification of reactant consumption and product formation, the resulting insight on the active sites of the catalysts can be directly coupled to the respective kinetics (rate) of the chemical reaction. This again can guide towards favourable catalyst design and process conditions, enabling higher efficiency, lower energy consumption and emissions, and lower operational costs in the industry.

In the setup developed and shown in the figure next page, we combined synchrotron X-ray absorption spectroscopy, X-ray diffraction, and UV-Vis spectroscopy during exposure to industrially relevant reactants, pressures and temperatures. However, the increasingly larger datasets associated with such studies of

Process conditions:
Flow: 7-15 NmL/min
Mass of catalyst: 20-50 mg
Concentrations: 2% Ethylene, 1% O_2, 4% HCl, balance He



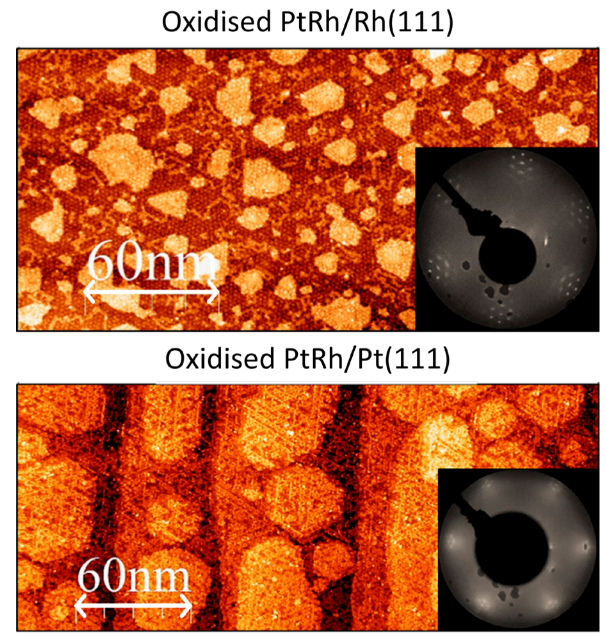
Experimental setup for combined operando powder X-ray diffraction and X-ray absorption spectroscopy as well as UV-vis spectroscopy with simultaneous product gas analysis by mass spectrometer at the Swiss-Norwegian Beamlines BM31 at the European Synchrotron Radiation Facility in France

catalysts at work call for automated procedures for analysing a large number of spectra. We therefore also focused on developing multivariate statistical analysis of in situ and operando X-ray absorption spectroscopy data. This work made strides in identifying previously unknown intermediate components in XAS spectra of oxychlorination catalysts (collaboration with IIA4), and revealed oscillating redox cycles in ruthenium catalysts during oxidation of NO to NO_2 (collaboration with IIA1).

Novel catalytic thin film preparation and reactor STM

Professor Anja Olafsen Sjåstad and Dr. Oleksii Ivashenko at the University of Oslo established a reactor-scanning tunnelling microscopy-X-Ray photoelectron spectroscopy (rSTM-XPS) system - the 5 of its type in the world. The instrument is capable of scanning surfaces in the temperature interval from 20 to 300 °C and pressures from ultra-high vacuum to 6 bar in presence of reactive gases such as NH_3, NO, H_2 and CO. Atomistic insight into catalytic reactions can then be achieved through understanding of the surface phenomena, where reactant molecules interact with the surface atoms to form products via elementary reaction steps at the solid/gas or solid/liquid interface. The team successfully complemented the rSTM work with near-ambient pressure x-ray photoelectron spectroscopy, NAP XPS, carried out at the synchrotron facilities MAXIV (HIPPIE Beamline) and SOLEIL (Tempo beamline).

This research generated significant scientific contributions to the development of well-defined model Pt-Rh surfaces (figure) for ammonia oxidation, relevant to nitrogen-based fertiliser production and ammonia (NH_3) slip catalysis. Key findings are that the product selectivity towards N_2 or NO is driven by the surface population of N and O, which in turn is dictated by the Pt-Rh surface alloying, O_2/NH_3 mixing ratio, pressure, and temperature. Associated PhD candidate Martin Myhre Jensen and three MSc students have been trained in and contributed to the project, and the work has resulted in a series of publications.



STM of oxidized PtRh alloy prepared on Rh(111) and Pt(111) surfaces. Low energy electron diffraction images in the insets show long and short range ordered structures observed in each case.

Reaction Mechanism Investigation by Combined DFT Calculations and Microkinetic Modelling

Developing new catalysts or improving existing ones depend on a better understanding of the reaction mechanism on the catalyst surface and its relationship to the basic catalyst properties. Density Functional Theory (DFT) calculations were carried out to describe surface reactions, provide parameters, and develop so-called descriptors of catalytic activity and selectivity. Microkinetic modelling was then utilised to investigate the reaction mechanism and predict information about surface coverages and relative rates of various elementary steps under reaction conditions. Through this methodology, we can bridge the gap from the atomic level to kinetic analysis at the macro-scale, with an aim to tailor catalysts atom by atom.

The approach was employed by postdoc Yanying Qi to gain atomic insight into active sites and elementary steps of the reaction systems of ethylene oxychlorination and methanol oxidation to formaldehyde. An understanding of mechanisms and processes on many levels has been gained, for example details of the atomic structure of the active sites of $CuCl_2$ and the interaction between the $CuCl_2$ and the alumina surfaces, as well as the effects of alkali and/or rare earth promoters on the $CuCl_2$ reduction and CuCl oxidation in ethylene oxychlorination.

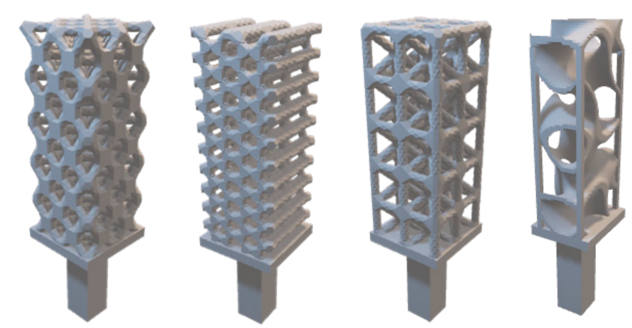
Anodisation of 3D printed titanium for photocatalysis (PHOTO-3D)

Titanium dioxide (TiO_2) is a common material for photocatalysis due to its high efficiency, low cost, chemical inertness and high photostability. Highly ordered, vertically oriented arrays of TiO_2 nanotubes can be prepared on a Ti substrate by electrochemical anodisation. The use of TiO_2 nanotubes generally offers a larger surface area compared to nanoparticles, as well as channels for enhanced electron transfer, and the material gives low efficiency loss.

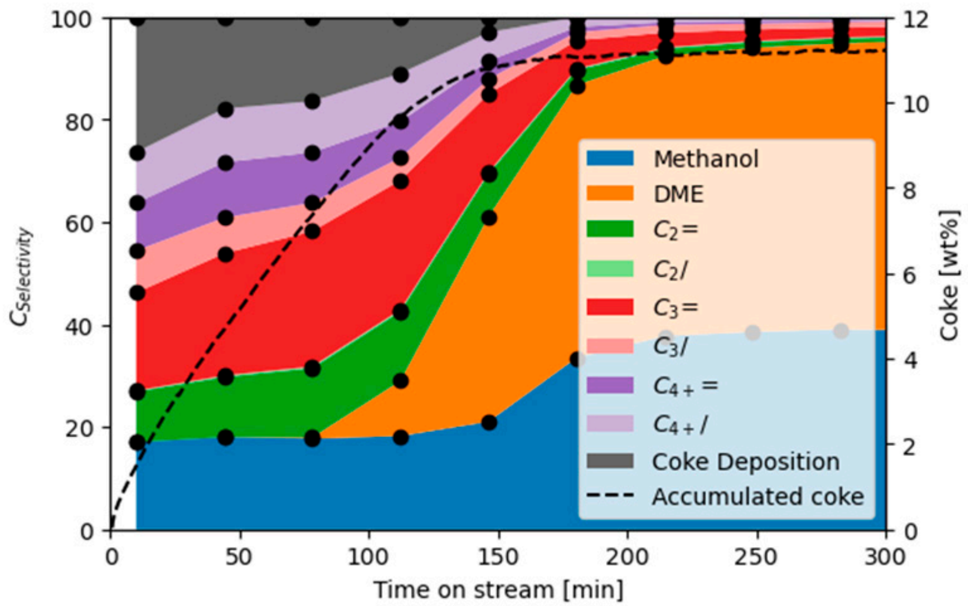
The main idea of this project was to produce an advanced photocatalyst by combining the concept of 3D printing and anodisation of titanium (Ti), and to prove its activity towards water cleaning and water splitting under solar illumination.

When working with 3D printed materials, factors such as material roughness and alloying elements, as well as the lower accessibility of the surface to be anodised, affect the anodisation process. This requires the development of new photocatalyst preparation methodologies.

Researcher Anna Lind and the team at SINTEF Industry found that the material made showed catalytic activity towards both water splitting and water cleaning reactions, but most prominently for the latter. When the samples were rotated in front of the light source to make full use of their 3D structure, the photocatalytic degradation activity was enhanced. Static samples, not rotating, appeared to be better.



Differnt designs of 3D-printed titanium structures



Example ISMA results from the MTO (methanol-to-olefins) reaction over a SAPO-34 catalyst. Coloured segments represent unconverted methanol (blue), DME (orange) and hydrocarbon C-product distribution, dotted line is the corresponding mass change of the catalyst (accumulated coke).

Fundamental microcalorimetry and transient kinetics study

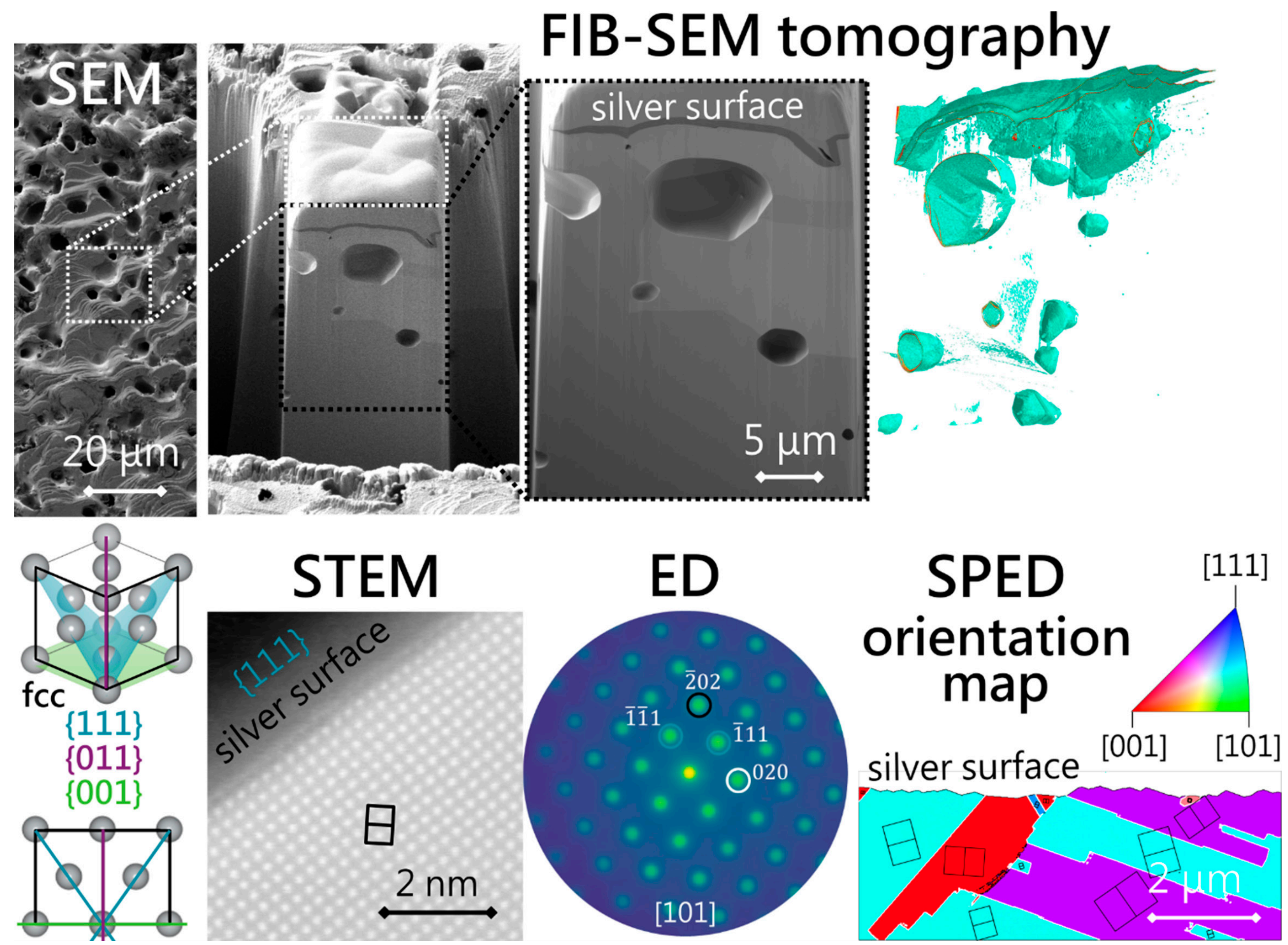
When developing rate equations, access to fundamental, high precision data is beneficial. PhD candidate Moses Mawanga has worked on this using two approaches: microcalorimetry and transient kinetics. His supervisors were Professor Edd Blekkan and Associated Professor Jia Yang.

Moses utilised a sensitive Tian-Calvet calorimeter with a catalytic cell and a vacuum-rig for dosing adsorbent gases in controlled amounts. The activation of methane on zeolitic materials was studied in collaboration with the team at UiO (IIA5). NH_3 adsorption was used to characterise Cu-exchanged zeolites, allowing the identification of adsorption sites. The interaction between the activated, Cu-exchanged catalysts and methane was also studied, but the interaction with the activated Cu-species was weak at the low pressures allowed in the test device.

The transient kinetics work was performed in tandem with conventional catalytic experiments to elucidate and compare the reaction mechanisms of the catalytic oxidation of NO over Pt-based or Mn-based oxidation catalysts (IIA1). Data from SSITKA (Steady State Isotopic Transient Kinetic Analysis), using isotopically marked NO and O_2, helped in the selection of relevant pathways in the detailed kinetic expressions developed. The work has shown how very fundamental investigations can give useful input to catalyst development

Applications of the In Situ Mass Analyser (ISMA) for industrially relevant processes

PhD candidate Bjørn Baumgarten has worked on applying the In Situ Mass Analyser instrument recently acquired from SINTEF Industry. The method is an extension of the TEOM (Tapered Element Oscillating Microbalance) technology that was available for a period from the early 1990s. The instrument is now operational and allows operando measurement of weight changes of a material in a controlled flow (fixed bed) reactor. This is in contrast to conventional balances, where the gas contact with the material is always controlled by diffusion rates. Coke formation, solid state reactions and sorption processes are among the phenomena that can be studied and directly correlated to the material performance. Initial results show the potential of the method (figure below) in a reaction for which the carbon formation (coke) is critical. The unit will also be used to study the reaction where CO_2 is first hydrogenated to methanol, which is then further converted to hydrocarbons in the same reactor. The activities have included two master's students, Ingrid Johanne Paulsen and Kristin Haukaas Hagen, both of whom have learnt to master the ISMA set-up.



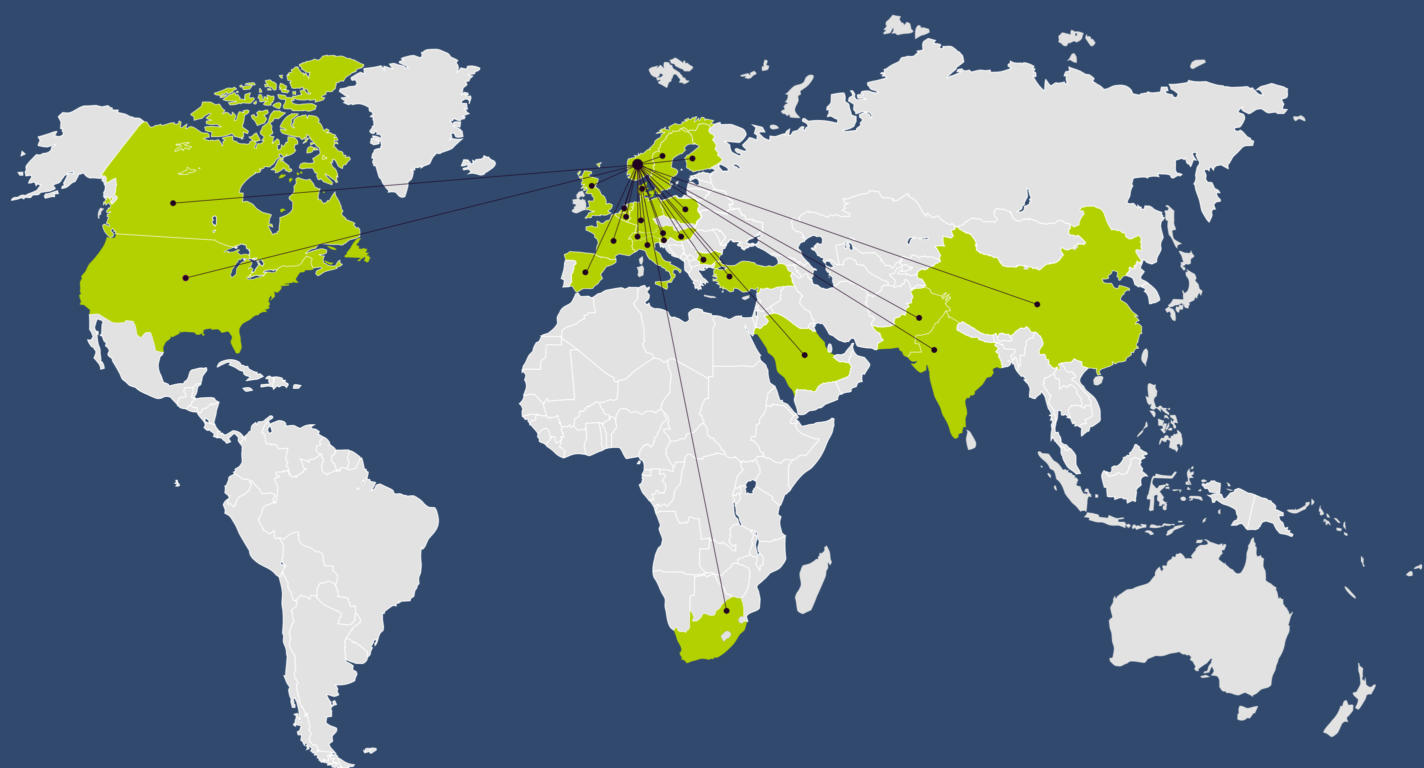
Examples of outcomes from the different electron microscopy methods for a silver catalyst used in methanol oxidation to formaldehyde

New electron microscopy methods for nanoscale characterisation of catalysts

Electron microscopy makes it possible to describe the morphology, chemical composition, and crystal structure of a catalyst at the nanoscale, which is important in understanding its catalytic performance. The objective of the (still ongoing) work of postdoctoral fellow Tina Bergh is to develop and utilise advanced experimental protocols and data analysis workflows for various catalysts. Silver catalysts from IIA3 have been the centre of attention since they change drastically after catalysing oxidation reactions. We image silver in 3D using the tomography method slice-and-view, in which thin slices (~50 nm) are removed using a focused ion beam (FIB) and imaged using scanning electron microscopy (SEM).

By combining FIB-SEM with scanning transmission electron microscopy (STEM), we document the changes in grain structure, faceting, and (sub-)surface cavities. We also scrutinise other catalysts using STEM techniques, such as supported nanoparticles. When it comes to method developments, we concentrate on electron diffraction (ED) and how to combine in situ heating with STEM and ED. We develop workflows for analysing scanning precession ED (SPED) data, to be used for phase and orientation mapping. Further, we seek to establish 3D ED at NTNU together with international collaborators, to be able to determine and refine crystal structures. Another sub-project looks into how to avoid air exposure prior to STEM characterisation.

INTERNATIONALISATION



iCSI researchers have international collaboration partners from academia and industry in 25 different countries

All three research partners in iCSI have several long term internationall collaborators, which are visible through the many joint publications. 62% of all scientific articles from iCSI have recognised international researchers as co-authors. Some of these publications are with the international industry partners in the centre, but research groups at international universities are also important contributors.

In IIA5, researchers at UiO have teamed up with industry partner Topsoe and internationally leading groups at the University of Torino, Italy. In doing so, we have cemented an already existing collaboration within the field of fundamental heterogeneous catalysis and advanced material characterisation. This has been invaluable for the research carried out within iCSI, but also resulted in significant spillover to other projects.

iCSI received funds from the Research Council of Norway for the CATHEX networking project (Advances in heterogeneous catalysis through integrated theoretical and experimental efforts), which is running from 2020 to 2025. It links iCSI with four world-leading catalysis communities: The University of Cape Town, East China University of Science and Technology (ECUST), University of Toronto and University of Wisconsin-Madison. The project supports exchange visits for professors and PhD candidates from the CATHEX partners to NTNU and UiO, or from Norway to the foreign partners. Several of the partners were present at the combined iCSI/CATHEX seminar in Trondheim in June 2023, contributing with inspiring lectures and posters. Joint scientific articles based on this collaboration are in the pipeline.

Teaching of PhDs in a garden outside Torino, Italy. From Karoline Kvande's international exchange stay at University of Torino

The centre's Scientific Advisory Committee has consisted of three internationally recognised experts in catalysis from prominent institutions abroad. They have challenged and raised the scientific ambitions of the iCSI partners, especially the young researchers. iCSI researchers contribute in the joint international catalysis community by taking on voluntary roles in their organisations. Centre Director Hilde Johnsen Venvik has for several years been a part of the Officers of the Board of the European Federation of Catalysis Societies, EFCATS, and is now the Vice-President.

It is with pride and excitement that we invite the European catalysis community to the 16th European Congress on Catalysis, EuropaCat 2025, to Trondheim in September next year. The congress, which takes place biennially will be organised as a joint effort of the Nordic Catalysis Societies. It has been the largest and most important catalysis conference in Europe since 1993 and we expect 1000 – 1500 participants.

Access to advanced instrumentation is necessary to be at the forefront of research, and we have an extensive collaboration with MAX IV Laboratory in Lund and the European Synchrotron (ERSF) with the Swiss-Norwegian Beamline in Grenoble. Both laboratories deliver high-quality X-ray light for research in materials, and groups from iCSI have visited several times per year.

iCSI researchers are recognized internationally. In 2019, Unni Olsbye received the Award for Excellence in Natural Gas Conversion at the 12th Natural Gas Conversion Symposium in San Antonio, USA. She has also given many keynote and plenary lectures at international conferences over the last decade. In 2020, Hilde Johnsen Venvik was appointed as a Lise Meitner-professor for a three-year period at the Department of Chemical Engineering at Lund University. These professorships are granted to leading researchers of the underrepresented gender who are nominated to work at the faculty as a visiting professor and act as a role model for young researchers, teachers, and students.

EXAMPLES OF KEY EU-PROJECTS:

The TomoCAT project is a researcher project funded by Research Council of Norway (RCN) as part of the NANO2021 programme. Partners are UiO, Topsoe, and U. Torino. The overarching objective of TomoCAT is to provide insights that might pave the way for a more efficient utilisation of these catalyst materials. Then, less material will be consumed every year, but it also gives smaller chemical reactors with less process downtime.

The CuBE project is an synergy grant from the European Research Council comprising four partners, UiO, NMBU, UniTo, and the Max Planck institute. The purpose of CuBE is to synergistically disclose the secrets of Cu-containing biological and synthetic catalysts for selective C-H bond activation. The acquired knowledge will be translated into rationally designed new catalysts with unprecedented properties.

The COZMOS project is a large effort linked to Horizon Europe, which aims to provide breakthrough technology for the conversion of CO_2 to fuels and chemical-building blocks, which will decrease CO_2 emissions by 1.9 tons CO_2 for every ton of C_3 product produced.

The Interregional project ESS & MAX IV is a cross border science and society project with international collaboration on *In-situ* X-ray absorption tomography together with Technical University of Denmark/ESRF and with operando near ambient pressure X-ray photoelectron spectroscopy together with Lund University/MAX IV.

In C123 - Methane Oxidative Conversion and Hydroformy-lation to Propylene - SINTEF has collaborated with Ghent University (Belgium) and Johnson Matthey (UK), to develop and validate a novel catalyst for the hydroformylation of ethane to propanal, thereby enriching the knowledge base of iCSI.

The BIKE project dealing with sustainable hydrogen production by aqueous phase reforming of biomass components also allowed iCSI staff at NTNU to have close collaboration and extended staff exchange with Karlsruhe Institute of Technology (Germany) and Johnson Matthey (UK).

The Swiss-Norwegian Beamlines (SNBL, RCN grant) at ESRF has provided iCSI researchers at NTNU and UiO reliable access to state-of-the-art X-ray beamlines at the largest synchrotron radiation facility in Europe. SNBL is an excellent training facility for PhD candidates and postdocs at Norwegian universities and a unique gateway to direct collaboration with international universities such as Eidgenössische Technische Hochschule Zürich (ETH) and École Polytechnique Fédérale de Lausanne (EPFL).

Training well qualified master's and PhD candidates for academia and Norwegian industry is one of the main deliverables from iCSI. We are proud of presenting a list of 41 MSc candidates with theses related to the centre research agenda and a supervisor from the centre staff at University of Oslo and NTNU (Appendix 2). In addition, 16 PhD candidates and 6 postdoctoral fellows have contributed an invaluable effort to the research at the centre.

iCSI has been attractive for international students, and 17 countries from 4 continents are represented by the young scientists. Among the master's students, 21% were international, while among the postdocs and PhDs, 65% came from outside Norway.

The candidates from iCSI are attractive for the industry, as approximately two out of three of the PhD candidates from the centre (funded by the centre or funded by other sources) go to Norwegian companies which offer positions highly relevant to their knowledge. Master's and PhD students and postdocs have all been employed by the industry partners in iCSI, which confirms that the partners consider participation in the SFI important for the recruitment of new employees.

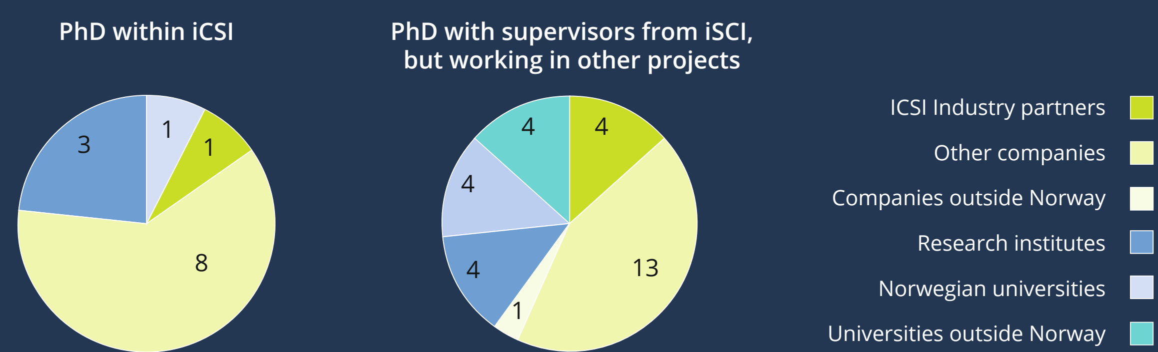
Nine of the iCSI PhD candidates and postdocs have participated in an Industrial Exchange Programme, which offered them a two-month stay with one or two of the industrial partners. There, they had the opportunity experience everyday industrial life and contribute to the hosts' problem-solving with up-to-date knowledge. The two months were added to their granted three-year PhD period.

iCSI has also supported our PhD candidates and postdocs by funding exchange stays at collaborating international universities, such as University of Torino, Denmark Technical University, and the Paul Scherrer Institute (PSI) in Switzerland.

Our Industry partner Yara also opened its doors to demonstrate a new catalyst in a nitric acid pilot plant at the Yara industrial site at Herøya, Norway. This was the last part of Jithin Gopakumar's doctoral work. In addition to the scientific results, it also gave him invaluable insight into industrial development work.

Another arena for the young iCSI scientists was the so-called "Professor-free zone seminars" that were organized twice during the SFI period. The idea was to let the young researchers meet the "real world" and gain insight into the challenges facing the industry. For the industry, this was an opportunity to meet young people with up-to-date knowledge and potential candidates for their recruiting. In 2018, they were gathered at Langesund Hotel before they had a tour at INEOS Inovyn's expanding vinyl chloride monomer (VCM) production facilities at Rafnes - a highly integrated plant with units that are balanced in a marriage of organic and inorganic chemistry. In 2020, 16 PhD candidates, postdoctoral fellows and industry researchers accepted the invitation to Topsoe's facilities in Lyngby on the outskirts of Copenhagen. On the first day, experienced researchers from Topsoe and Yara contributed with presentations of "Advanced operando techniques – from atomic scale to industrial reactor", "Nitric acid production – from a catalyst point of view" and "Patenting and IP strategy". They were followed by the young scientists giving a brief overview of their work. The second day in Denmark was spent at the Topsoe catalyst plant in Fredrikssund, showing large-scale catalyst production.

WHERE DID THEY GO – NEW POSITIONS FOR THE PHDS



"I did my exchange at K.A. Rasmussen and Dynea. I got to experience the industrial aspect of formaldehyde production, but also the origin of the silver catalyst. Having the opportunity to see the processes first-hand broadened my perspective beyond the lab and gave me a better understanding of the importance of my PhD work. While experiencing parts of the industry relevant for the MTF process, I was also challenged with other tasks that industry typically encounters". Stine Lervold, PhD 2019

Jithin Gopakumar proudly displaying his pilot plant reactor setup at Yara, Herøya. He will graduate in June 2024.

Young researchers from academia and industry gathered at the Topsøe facilities in Lyngby, February 2020.

PHD CANDIDATES AT iCSI:

Ata ul Rauf Salman, IIA1

PhD thesis: *Catalytic oxidation of NO to NO2 for nitric acid production*

Period at iCSI: 2016-2019
Supervisor: Magnus Rønning
Current position: Process Engineer, Equinor, Oslo

Asbjørn Slagtern Fjellvåg, IIA1

PhD thesis: *Platinum Catchment by Noble Metal Alloys and structural studies of Pt- and Rh-containing perovskites*

Period at iCSI: 2016-2022
Supervisor: Anja Olafsen Sjåstad
Current position: R&D Scientist Scandi Energy AS, Asker

Julie Hessevik, IIA1

PhD thesis: *Noble metal catchment*

Period at iCSI: 2019-2024
Supervisor: Anja Olafsen Sjåstad
Current position: PhD candidate, UiO, Oslo

Jithin Gopakumar, IIA1

PhD thesis: *Catalytic Oxidation of NO to NO2 For Nitric Acid Production*

Period at iCSI: 2020-2024
Supervisor: Magnus Rønning
Current position: PhD candidate, NTNU, Trondheim

Stine Lervold, IIA3

PhD thesis: *Investigations of the methanol to formaldehyde (MTF) reaction over silver*

Period at iCSI: 2016-2020
Supervisor: Hilde Johnsen Venvik
Current position: Senior Engineer, Equinor, Trondheim

Youri van Valen, IIA3

PhD thesis: *Partial oxidation of methanol to formaldehyde over silver*

Period at iCSI: 2020-2024
Supervisor: Hilde Johnsen Venvik
Current position: PhD candidate, NTNU, Trondheim

Endre Fenes, IIA4

PhD thesis: *Ethylene Oxychlorination on CuCl2 based Catalysts: Mechanism and Kinetics*

Period at iCSI: 2015-2019
Supervisor: De Chen
Current position: Senior Process Engineer, INEOS Inovyn, Larvik

Hongfei Ma, IIA4

PhD thesis: *Kinetic Studies of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride*

Period at iCSI: 2017-2021
Supervisor: De Chen
Current position: Postdoctoral fellow, NTNU, Trondheim

Wei Zhang, IIA4

PhD thesis: *Catalyst Development of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride*

Period at iCSI: 2020-2023
Supervisor: De Chen
Current position: Researcher, NTNU, Trondheim

Dimitrios Pappas, IIA5

PhD thesis: *Direct methane to methanol conversion over Cu-exchanged zeolites: Building structure - activity relationships*

Period at iCSI: 2016-2019
Supervisor: Stian Svelle
Current position: Research Scientist, CoorsTek Membrane Science, Oslo

Karoline Kvande, IIA5

PhD thesis: *Compositional and Mechanistic Studies of Cu-zeolites for the Direct Activation of Lower Alkanes*

Period at iCSI: 2019-2023
Supervisor: Stian Svelle
Current position: Postdoc at University of Berkeley, CA, USA

Bjørn Gading Solemsli, IIA5

PhD thesis: *Compositional and Mechanistic Studies of Cu-zeolites for the Direct Activation of Lower Alkanes*

Period at iCSI: 2021-2024
Supervisor: Stian Svelle
Current position: Application Specialist, LayerOne Advanced Materials, Oslo

Samuel K. Regli, IIA6

PhD thesis: *Advanced in situ characterization of heterogeneous catalysts for sustainable process industries*

Period at iCSI: 2016-2019
Supervisor: Magnus Rønning
Current position: Senior Engineer, NTNU, Trondheim

Moses Mawanga, IIA6

PhD thesis: *Insights into the kinetics and mechanism of selected industrial catalysed reactions*

Period at iCSI: 2018-2022
Supervisor: Edd A. Blekkan
Current position: Process Engineer, Freyr Battery, Mo i Rana

Martin Myhre Jensen, IIA6

PhD thesis: *Synthesis, Characterisation, and In situ / Operando Studies of Pt-Rh Model Catalysts for the NH3 Oxidation Reaction*

Period at iCSI: 2018-2023 (associated, not funded by iCSI)
Supervisor: Anja Olafsen Sjåstad
Current position: Senior Development Engineer, CondAlign, Oslo

Björn Frederik Baumgarten, IIA6

PhD thesis: *Applications of the In-Situ Mass Analyzer (ISMA) for industrially relevant processes*

Period at iCSI: 2021-2024
Supervisor: Jia Yang/Edd A. Blekkan
Current position: Senior Engineer, Equinor, Trondheim (from Oct. 2024)

POSTDOCTORAL FELLOWS AT iCSI:

Oleksii Ivashenko,
IIA1/6

Topic of research: *Advanced synthesis and characterization - novel thin film preparation, NAP XPS and reactor STM. Model reaction – ammonia oxidation at NH3 slip conditions*

Period at iCSI: 2016-2022
Current position: Team Leader, Zero Carbon Fuels Group, DNV

Yalan Wang,
IIA4

Research topic: *First principle based kinetic and promoter effect study of ethylene oxychlorination*

Period at iCSI: 2019-2022
Current position: Process Engineer, Aker Solutions, Trondheim

Michael Dyballa,
IIA5

Research topic: *Materials synthesis and rational design of novel and improved zeolite materials for direct activation of lower alkanes*

Period at iCSI: 2016-2018
Current position: Group leader, University of Stuttgart, Germany

Sebastian Prodinger,
IIA5

Research topic: Unravelling the origin of small port and large port mordenite zeolite used for direct activation of lower alkanes

Period at iCSI: 2020-2023
Current position: Principal Scientist, Topsoe, Denmark

Yanying Qi,
IIA6

Research topic: Advanced reactor modeling – new methodology and multiscale approaches

Period at iCSI: 2016-2020
Current position: Business Data Analyst, Appear, Oslo

Tina Bergh,
IIA6

Research topic: *State-of-the-art developments in Transmission Electron Microscopy (TEM)*

Period at iCSI: 2021-2023
Current position: Postdoctoral fellow, NTNU, Trondheim

AWARDS:

Dimitrios Pappas received the award for the best PhD thesis 2021 from the European Federation of Catalysis Societies.

Hongfei Ma received Best PhD Thesis Award 2021 at the NTNU Faculty of Natural Science, NTNU and Best poster award 14th EuropaCat 2019 Congress, Germany.

Stine Lervold received Best Poster Award at 18th Nordic Symposium on Catalysis, Denmark

Samuel Regli received a Poster Award in recognition of outstanding poster presentation at XAFS2018, Poland

APPENDICES

APPENDIX 1

Detailed statement of accounts for the complete period of centre financing (2015-2023).

FUNDING:

Activity/Item	RCN	NTNU (Host)	UiO	SINTEF	Dynea	K.A. Rasmussen	Ineos	Topsoe	Yara	Total
IIA1: 21st century nitric acid technology development	15 828	4 033	7 684	48		3 644			7 852	39 089
IIA2: New NOx abatement technologies for the marine market and state-of-the-art SCR catalysis	4 300			154					4 213	8 667
IIA3: Frontier formalin technology development	11 396	3 462		439	6 816	2 314				24 427
IIA4: PVC value chain: world class energy and raw material efficiency	15 087	3 945		17			12 820			31 869
IIA5: The next step in direct activation of methane	17 722		4 505	44				11 975		34 246
IIA6: Generic projects for additional industrial synergies	25 480	8 566	1 025	7 239					28	42 338
Administration/ Management	6 337	8 949			357	219	61	72	130	16 125
Sum	**96 150**	**28 955**	**13 214**	**7 941**	**7 173**	**6 177**	**12 881**	**12 047**	**12 223**	**196 761**

COST:

Activity/Item	RCN	NTNU (Host)	UiO	SINTEF	Dynea	K.A. Rasmussen	Ineos	Topsoe	Yara	Total
IIA1: 21st century nitric acid technology development		10 712	13 184	9 770		1 743			3 680	39 089
IIA2: New NOx abatement technologies for the marine market and state-of-the-art SCR catalysis				6 241					2 426	8 667
IIA3: Frontier formalin technology development		9 961		9 315	3 879	1 272				24 427
IIA4: PVC value chain: world class energy and raw material efficiency		18 179		6 850			6 840			31 869
IIA5: The next step in direct activation of methane			24 594	3 647				6 005		34 246
IIA6: Generic projects for additional industrial synergies		22 825	11 686	7 799					28	42 338
Administration/ Management		15 495			294	164	41	41	90	16 125
Sum		**77 172**	**49 464**	**43 622**	**4 173**	**3 179**	**6 881**	**6 046**	**6 224**	**196 761**

APPENDIX 2

List of Post-docs, Candidates for PhD and MSc degrees during the full period of the centre

Postdoctoral researchers with financial support from the centre budget

Name	M/F	Nationality	Years/period in the centre	Scientific topic	Main contact
Michael Dyballa	M	Germany	2016-2019	Direct activation of lower alkanes	Stian Svelle
Yanying Qi	F	China	2016-2020	Advanced reactor modelling – new methodology and multiscale approaches	De Chen
Oleksii Ivashenko	M	Ukraine	2016-2022	NH_3 chemistry fundamentals and *operando* experiments	Anja O. Sjåstad
Yalan Wang	F	China	2019-2022	Ethylene oxychlorination to 1,2 dichloroethane, first principles and kinetic modelling	De Chen
Sebastian Prodinger	M	Austria	2020-2023	Direct activation of lower alkanes	Stian Svelle
Tina Bergh	F	Norway	2021-2023	State-of-the-art developments in transmission electron microscopy (TEM)	Hilde J. Venvik
Torstein Fjermestad	M	Norway	2023	Direct activation of lower alkanes	Stian Svelle

Post-doctoral researchers working on projects in the centre with financial support from other sources

Name	M/F	Nationality	Source of funding	Years/period in the centre	Scientific topic	Main contact
Andrea Cognigni	M	Italy	RCN-SYNKNØYT	2013-2016	Development of X-ray modulation-enhanced techniques to study surface reactions at industrially relevant conditions	Magnus Rønning
Daham Gunawardana	M	Sri Lanka	RCN-inGAP	2013-2016	Metal dusting corrosion initiation on the surface of INCONEL® 601 alloy	Hilde J. Venvik
Diego Alexander Pena Zapata	M	Venezuela	European FP7 FASTCARD	2014-2017	In situ and ex situ characterisation of iron-based catalysts during CO_2-rich Fischer-Tropsch synthesis	Magnus Rønning
Xavier Auvray	M	France	NTNU	2015-2016	NO oxidation at high pressure and high NO and water concentration.	Magnus Rønning
Maria Victoria Gil Matellanes	F	Spain	RCN- ENERGIX	2015-2016	Integrated H_2BioOil process for efficient biofuel production	De Chen
Eleni Patanou	F	Greece	RCN-GASSMAKS	2015-2016	Co-based supports and catalysts for conversion of natural gas into synthetic diesel	Edd Blekkan

Name	M/F	Nationality	Source of funding	Years/period in the centre	Scientific topic	Main contact
Qingjun Chen	M	China	RCN- ENERGIX	2015-2018	Co-based Fischer–Tropsch synthesis mechanism studied by density functional theory (DFT) using K adsorption as a probe	Edd Blekkan
Mari Helene Farstad	F	Norway	NV & IKP, NTNU	2015-2018	Advanced characterisation of catalytic model systems	Hilde J. Venvik
Nikolaos Tsakoumis	M	Greece	RCN-inGAP	2015-2016	Structure - performance relations of Co-based Fischer – Tropsch synthesis catalysts	Magnus Rønning
			NTNU-Energy	2018-2021	Bio-ethanol steam reforming for on board high purity H_2 generation system	De Chen
Evgeniy Redekop	M	Russia, Norway	NFR/Horizon 2020/other sources	2015-	Kinetic studies using TAP instrument	Unni Olsbye
Li He	F	Norway	GASNOVA	2016-2018	CO_2 capture by solid sorbents	De Chen
Susmit Kumar	M	India, Norway	NFR/other sources	2016-2022	Diffusion studies in alloys	Helmer Fjellvåg
Jørgen Svendby	M	Norway	NanoElMem, M-ERA.NET (EU)	2017-2019	Catalysts for alkaline ethanol fuel cell	De Chen
Marie Døvre Strømsheim	F	Norway	H2MemX, RCN-ENERGIX	2017-2021	Advanced characterisation of Pd-based membrane model systems	Hilde J. Venvik
Xiang Feng	M	China	NFP	2017-2019	Futurepack - olefin generation from woody biomass using catalytic pyroysis reaction	De Chen
Andrea Lazzarini	M	Italy	RCN	2017-2019	Detailed characterisation of complexes and nanostructured materials	Unni Olsbye
Irene Pinilla Herrero	F	Spain	Innovations-fonden	2017-2020	Production of aromatics from methanol via metal-exchanged zeolites	Stian Svell
Ljubisa Gavrilovic	M	Serbia	RCN	2018-2020	Advanced biofuels via synthesis gas	Edd Blekkan
Zhenping Cai	M	China	RCN-INNO INDIGO	2018-2020	Conversion of lignocellulosic waste into biofuels and bioplastics	De Chen
Xiaoyang Guo	M	China	RCN, IKP-NTNU, Lyng Drilling & Schlumberger	2018-2021	Low cost drill bit for geothermal applications	Jia Yang (Hilde J. Venvik)
Yuanwei Zhang	M	China	Fjell, CLIMIT, GASSNOVA	2019-2020	Moving bed carbonate looping (MBCL), phase I and II	De Chen
Mehdi Mahdmoodinia	M	Iran	IKP NTNU, RCN	2019-2020	Nanoscale investigation of Co(0001), Co(10-12), and Co(11-20) single crystals as catalyst model systems: insights from experiment and theory	Hilde J. Venvik

Name	M/F	Nationality	Source of funding	Years/period in the centre	Scientific topic	Main contact
Jingxiu Xie	F	Singapore	Horizon 2020 COZMOZ	2019-2020	Catalytic testing, CO_2 conversion	Unni Olsbye
Christian Ahoba-Sam	M	Ghana	RCN	2019-2020	Catalytic testing, CO_2 conversion	Unni Olsbye
Chiara Negri (50%)	F	Italy	EU	2019-2020	Characterisation and FTIR spectroscopy	Unni Olsbye
Sigurd Øien-Ødegaard	M	Norway	NFR/EU/other sources	2019-2021	Zeolite and MOF synthesis	Unni Olsbye
Balasingam Suresh Kannan	M	India	RCN-EmX 2025	2019-2021	Energy storage by high energy supercapacitors	De Chen
Ainara Moral Larrasoana	F	Spain	Fjell, CLIMIT, GASSNOVA	2019-2023	Moving bed carbonate looping (MBCL), phase I and II	De Chen
Nico König	M	Germany	RCN	2020-2021	Catalyst synchrotron studies	Stian Svelle
Katarzyna Swirk	F	Poland	Horizon 2020: Marie Skłodowska-Curie	2020-2023	MesoSi-CO_2. Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO_2 utilisation through tri-reforming of methane	Magnus Rønning
Hongfei Ma	M	China	EU	2021-2023	Chemical transformation of enzymatic hydrolysis lignin (EHL) with catalytic solvolysis to fuel commodities under mild conditions (EHLCATHOL)	De Chen
Izar Capel Berdiell	M	Spain	RCN	2021-2023	Catalyst deactivation studies	Stian Svelle
Abdulla Bin Afif	M	India	UiO	2023	Operando/in-situ Reactor STM and TEM for catalyst development for reactions as ammonia slip and CO_2 utilisation	Anja O. Sjåstad
Tomas Cordero-Lanzac	M	Spain	RCN /EU - Horizon 2020	2020-2024	Catalytic testing, CO_2 conversion	Unni Olsbye
Juan Ignacio Mirena Seguias	M	Venezuela	Academy of Finland	2022-2024	Transient kinetic analysis of zeolite-catalysed reactions	Evgeniy Redekop
Torstein Fjermestad	M	Norway	RCN	2022-2024	Multiscale modelling of zeolite catalysts	Stian Svelle
Jayakumar Karthikeyan	M	India	RCN	2022-2024	Green H_2CHem	Anja O. Sjåstad

PhD candidates who have graduated with financial support from the centre budget

Name	M/F	Nationality	Years/period in the centre	Thesis title	Supervisor
Dimitrios Pappas	M	Greece	2016-2019	Direct methane to methanol conversion over Cu-exchanged zeolites: Building structure – activity relationships	Stian Svelle
Endre Fenes	M	Norway	2015-2021	Ethylene oxychlorination on $CuCl_2$-based catalysts: Mechanism and kinetics	De Chen
Stine Lervold	F	Norway	2016-2021	Investigations of the methanol to formaldehyde (MTF) reaction over silver	Hilde J. Venvik
Asbjørn Slagtern Fjellvåg	M	Norway	2016-2022	Platinum catchment by noble metal alloys and structural studies of Pt- and Rh-containing perovskites	Anja O. Sjåstad
Ata Al Rauf Salman	M	Pakistan	2015-2019	Catalytic oxidation of NO to NO_2 for nitric acid production	Magnus Rønning
Hongfei Ma	M	China	2017-2021	Kinetic studies of ethylene oxychlorination to ethylene dichloride and vinyl chloride	De Chen
Karoline Kvande	F	Norway	2019-2023	Compositional and mechanistic studies of Cu-zeolites for the direct activation of lower alkanes	Stian Svelle
Wei Zhang	F	China	2020-2023	Mechanism and kinetics of byproducts formation in ethylene oxychlorination	De Chen

PhD students with financial support from the centre budget who are still in the process of finishing studies

Name	M/F	Nationality	Years in the centre	Thesis topic	Supervisor
Samuel K. Regli[1)]	M	Switzerland	2016-2023	Advanced in situ characterisation of heterogeneous catalysts for sustainable process industries	Magnus Rønning
Moses Mawanga[2)]	M	Uganda	2018-2022	Insights into the kinetics and mechanism of selected industrial catalysed reactions	Edd Blekkan
Julie Hessevik[3)]	F	Norway	2019-2023	Noble metal catchment	Anja O. Sjåstad
Jithin Gopakumar3)	M	India/UAE	2020-2023	Catalytic oxidation of NO to NO_2 for nitric acid production	Magnus Rønning
Bjørn Gading Solemsli[3)]	M	Norway	2021-2023	Spectroscopic and mechanistic studies of the direct activation of lower alkanes over Cu-containing nano-porous catalysts	Stian Svelle
Youri van Valen[3)]	M	The Netherlands	2020-2023	Partial oxidation of methanol to formaldehyde over silver	Hilde J. Venvik
Bjørn Baumgarten[3)]	M	Germany	2021-2023	Applications of the in-situ mass analyzer (ISMA) for industrially relevant processes	Jia Yang/ Edd Blekkan

[1)] Samuel Regli has held a position as lab engineer at IKP, NTNU since August 2020, and his defence is expected to take place in 2024.
[2)] Moses Mawanga left NTNU for a position in industry 31.12.2022, and his defence is expected to take place in 2024.
[3)] Julie Hessevik, Jithin Gopakumar, Bjørn Gading Solemsli, Youri van Valen and Björn Frederik Baumgarten are expected to defend their theses in 2024.

PhD candidates who have graduated with other financial support, but associated with the centre

Name	M/F	Nationality	Source of funding	Years in the centre	Thesis title	Supervisor
Yanying Qi	F	China	RCN -ISP	2015-2016	Mechanistic insights into cobalt-based Fischer-Tropsch synthesis	De Chen
Farbod Dadgar	M	Iran	RCN-GASSMAKS	2015-2016	Direct synthesis of dimethyl ether in microstructured reactors; the interactions between methanol synthesis and methanol dehydration	Hilde Venvik
Xuehang Wang	F	China	NTNU, RCN	2015-2016	Porous carbon prepared by chemical activation for high-energy supercapacitors in ionic liquid electrolyte	De Chen
Marthe Emelie Melandsø Buan	F	Norway	NTNU, EU-FREECATS	2015-2017	Nitrogen-doped carbon nanofibers for the oxygen reduction reaction	Magnus Rønning
Ida Hjort	F	Norway	NTNU	2015-2017	Catalysis for electrochemical conversion of CO_2 in aqueous solutions.	De Chen
Marie Døvre Strømsheim	F	Norway	RCN -InGAP	2015-2017	Co{11-20} and Pd3Au{100} single crystals as catalyst model system	Hilde Venvik
Yahao Li	M	China	Chinese Scholarship Council	2015-2018	Sustainable electrocatalysts for oxygen reduction reaction. M-N-P (M: transition metals) doped mesoporous carbon from biomass	De Chen
Ljubisa Gavrilovic	M	Serbia	RCN-ENERGIX	2015-2018	Fischer-Tropsch synthesis – influence of aerosol – deposited potassium salts on activity and selectivity of Co-based catalysts.	Edd A. Blekkan
Erik Østbye Pedersen	M	Norway	RCN-GASSMAKS	2015-2018	Mn promotion effects in Co-based Fischer-Tropsch production of light olefins	Edd A. Blekkan
Isaac Yeboah	M	Ghana	RCN-ENERGIX	2015-2019	Integrated H_2 biooil process for efficient biofuel production	De Chen
Yalan Wang	F	China	Notur/ NorStore NN4685K	2015-2019	Model-aided catalyst prediction through descriptor-based hybrid semi-empirical approach	De Chen
Xiaoyang Guo	M	China	RCN-GASSMAKS	2015-2020	Inhibiting carbon growth at the initial stage of metal dusting corrosion of high temperature alloys	Hilde Johnsen Venvik
Emil S. Gutterød	M	Norway	RCN-FRINATEK	2016-2020	On the hydrogenation of CO_2 over Pt-functionalised UiO-67 metal-organic frameworks	Unni Olsbye
Volodymyr Levchenko	M	Ukraine	RCN	2016-2020	Synthesis of cyclometalated Au (III) complexes for catalysis and MOF functionalisation	Mats Tilset
Giuseppe Rotunno	M	Italy	RCN	2016-2022	Vapour-solid interactions for SMSB and asymmetric amplification of pyrimidine and pyridine aldehydes	Mohamed Amedjkouh

Name	M/F	Nationality	Source of funding	Years in the centre	Thesis title	Supervisor
Mustafa Sæterdal Kømurcu	M	Norway	RCN-CONFINE	2017-2021	Tailoring solid catalysts for the ethene oligomerisation reaction	Unni Olsbye
Muhammad Zubair	M	Pakistan	NTNU-NV	2017-2021	Enhanced visible light adsorption TiO_2- based catalysts for photocatalytic H_2 production	Jia Yang
Jianyu Ma	M	China	RCN	2017-2021	High-temperature desulfurisation of biomass-derived synthesis gas using solid sorbents	Edd A. Blekkan
Joakim Tafjord	M	Norway	NTNU-NV	2017-2021	Novel alginate complex-derived Fe catalysts for sustainable lower olefin production: Fischer-Tropsch synthesis based on renewable feedstocks	Jia Yang
Martin Myhre Jensen[1)]	M	Norway	UiO, Inorganic chemistry and materials chemistry	2018-2024	Synthesis, characterisation, and In-situ/ operando studies of Pt-Rh model catalysts for the NH_3 oxidation reaction	Anja O. Sjåstad
Monica Pazos Urrea	F	Colombia	EU-MSCA-ITN	2020-2023	Exploring metal-metal and metal-support interactions in Pt-based catalysts for aqueous phase reforming	Magnus Rønning

1) Martin Myhre Jensen defended his thesis 01.03.2024. His work has been a part of WP6.2 in IIA6.

MSc candidates with theses related to the centre research agenda and a supervisor from the centre staff

IIA	Name	M/F	Nationality	Year(s) in the centre	Thesis title	Supervisor
IIA1	Mads Alexander Lid	M	Norway	2015-2016	Efficient catalysts for achieving NO /NO_2 equilibrium	Magnus Rønning
	Ole H. Bjørkedal	M	Norway	2015-2016	New catalysts for low-temperature selective catalytic reduction (SCR)	Magnus Rønning
	Martin Myhre Jensen	M	Norway	2015-2017	Synthesis and characterisation of Pt(1-x)Pdx nanoparticles and their suitability for NH_3 oxidation catalysis	Anja O. Sjåstad
	Signe Marit Hyrve	F	Norway	2017-2018	Tuning of perovskite composition for NO oxidation	Magnus Rønning
	Henrik Jenssen Gremmetsen	M	Norway	2017-2018	NO oxidation catalysed by high surface area perovskites	Magnus Rønning
	Beate Meisland Østrådt	F	Norway	2017-2018	Supported manganese oxide catalysts for NO oxidation in nitric acid production	Magnus Rønning
	Galina Tenkova Yavasheva	F	Bulgaria	2017-2019	Synthesis and characterisation of bimetallic nanoparticles for selective catalytic conversion of ammonia	Anja O. Sjåstad
	Minadir Saracevic	M	Norway	2018-2019	NO to NO_2 oxidation over supported cobalt oxides catalysts	Magnus Rønning

IIA	Name	M/F	Nationality	Year(s) in the centre	Thesis title	Supervisor
IIA1	Martin Meuche	M	Norway	2018-2019	Advanced characterisation of flame spray pyrolysis prepared catalysts for NO to NO_2 oxidation	Magnus Rønning
	Oskar Iveland	M	Norway	2019-2021	Ammonia oxidation-based reactions and their catalysts	Anja O. Sjåstad
	Sunniva Vold	F	Norway	2020-2021	Efficient catalysts for attaining NO /NO_2 equilibrium in nitric acid production	Magnus Rønning
	Walace P.S. Kierulf-Vieira	M	USA	2020-2022	Solid solution PtxRh1–x nanoparticles synthesis, characterisation, catalyst preparation and thermal stability evaluations	Anja O. Sjåstad
	Mathilde Ingeborg Nilsen Verne	F	Norway	2021-2023	In-situ XPS of PtRh NPs for NH_3 oxidation	Anja O. Sjåstad
	Pål Martin Benum	M	Norway	2022-2023	Catalytic oxidation of NO to NO_2 at industrial nitric acid conditions	Magnus Rønning
	Cathinka S. Carlsen	F	Norway	2022-2024	Platinum group metal transport in ammonia combustion and recovery	Anja O. Sjåstad
IIA3	Stine Lervold	F	Norway	2015-2016	Characterisation of Ag catalysts for formalin production	Hilde J. Venvik
	Vegard Andreas Naustdal	M	Norway	2015-2016	Characterisation of Ag catalysts for formalin production	Hilde J. Venvik
	Rakel Johanne Ekholt	F	Norway	2016-2017	Oxidation of methanol to formaldehyde over Ag – kinetic modelling using comsol	Hilde J. Venvik
	Kamilla Arnesen	F	Norway	2017-2018	Oxidation of methanol to formaldehyde over Ag catalysts	Hilde J. Venvik
	Susanne Klungland Stokkevåg	F	Norway	2019-2020	Oxidation of methanol to formaldehyde (MTF) over Ag catalysts	Hilde J. Venvik
	Tomasz Skrzydlo	M	Poland	2022-2023	Oxidation of methanol to formaldehyde (MTF) over Ag catalyst	Hilde J. Venvik
IIA4	Ellinor Sofie Smith Wiker	F	Norway	2015-2016	Reactor model for oxychlorination of ethylene in multi-tubular fixed bed reactors	De Chen
	Erling Olav Sollund	M	Norway	2017-2018	Kinetic study and reactor modelling of ethylene oxychlorination	De Chen
	Tho Ba Tran	M	Norway	2018-2019	One-pot catalytic vinyl chloride (VCM) production	De Chen
	Jithin Gopakumar	M	India/ UAE	2019-2020	Ethylene oxychrolination on Cu-based catalysts	De Chen
	Seyyedeh Roomina Farzaneh Motlagh	F	Iran	2021-2022	Kinetic study of ethylene oxychlorination on promoted $CuCl_2$/ Al_2O_3 catalysts	De Chen
IIA5	Karoline Kvande	F	Norway	2017-2019	A Study of Cu-loaded SAPO-34 for the direct conversion of methane to methanol	Stian Svelle
	Mia Bodenhoff	F	Denmark	2017-2019	Combined experimental, spectroscopic, and theoretical mechanistic investigations	Pablo Beato, Topsoe
	Odd Reidar Bygdnes	M	Norway	2020-2022	Methane to methanol – catalyst synthesis	Stian Svelle

IIA	Name	M/F	Nationality	Year(s) in the centre	Thesis title	Supervisor
IIA6	Hanna Marie Storvik	F	Norway	2015-2016	Catalysts for control of methane slip in marine machinery using platinum-based catalysts	Hilde J. Venvik
	Helene Sandvik	F	Norway	2015-2016	Catalysts for control of methane slip in marine machinery using palladium-based catalyst	Hilde J. Venvik
	Ragnhild Brokstad Lund-Johansen	F	Norway	2016-2017	Catalysis for control of methane slip in marine machinery over a nickel cobalt spinel.	Hilde J. Venvik
	My Nhung Thi Tran	F	Norway	2017-2018	In situ characterisation of industrial catalysts	Magnus Rønning
	Jane Eiane Aarsland	F	Norway	2017-2018	Operando FTIR study of the NH_3-SCR reaction over Cu/Al_2O_3 and Fe/Al_2O_3 catalysts	Magnus Rønning
	Helene Marie Eng Granlund	F	Norway	2017-2018	Catalytic methane abatement for natural gas engines	Hilde J. Venvik
	Gaute Osaland Hådem	M	Norway	2017-2018	Nanoscale investigations and modifications of catalysts and catalytic model systems	Hilde J. Venvik
	Christine Pettersen	F	Norway	2018-2020	Preparation, characterisation and oxidation of nanostructured Pt-Rh surfaces	Anja O. Sjåstad
	Alexandra Jahr Kolstad	F	Norway	2020-2022	Reactor STM and NAP XPS for ammonia oxidation	Anja O. Sjåstad
	Muhammad Arslan Aslam	M	Pakistan	2021-2022	Novel Fe-based catalyst for Fischer-Tropsch synthesis	Jia Yang
	Ingrid Johanne Paulsen	F	Norway	2023-2024	Indium-enhanced Iron catalysts for CO_2 Hydrogenation	Edd Blekkan
	Kristin Haukaas Hagen	F	Norway	2023-2024	Carbon combustion synthesis of a CO_2 to Methanol catalyst	Edd Blekkan

MSc candidates with theses related to the centre research agenda and a supervisor from the centre staff

Name	M/F	Nationality	Year(s) in the centre	Thesis title	Supervisor
Nicolas Beck	M	Germany	2017	Oxidation of methanol to formaldehyde over Ag catalysts	KIT, Hilde J. Venvik
Matilde Emanuelli	M	Italy	2023	Characterisation of silver catalysts surfaces	Univ.of Bologna Hilde J. Venvik

APPENDIX 3

The Industry Innovation Area Teams

Industry Innovation Area 1 Team
University of Oslo
Anja O. Sjåstad
Asbjørn Slagtern Fjellvåg
Helmer Fjellvåg
Julie Hessevik
Oleksii Ivashenko
SINTEF Industry
Arne Karlsson
Bjørn Christian Enger
Børge Holme
Joanna Pierchala
Kari Anne Andreassen
Martin Fleissner Sunding
Silje F. Haakonsen
NTNU
Ata ul Raud Salman
Jithin Gopakumar
Magnus Rønning
Yara International
Daniela Farmer
David Waller
Halvor Øien
Ketil Evjedal
Marianne S. Grønvold
K.A. Rasmussen
Ann-Kristin Lagmannsveen
Johan Skjelstad
Terje Pedersen
Thomas By

Industry Innovation Area 2 Team
SINTEF Industry
Anna Lind
Bjørnar Arstad
Jasmina H. Cavka
Martin Fleissner Sunding
Patricia Almeida
Silje Fosse Håkonsen
Yara International
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APPENDIX 4

List of Publications from iCSI

2024

Bjørn Gading Solemsli, Izar Capel Berdiell, Sebastian Prodinger, Karoline Kvande, Gabriele Deplano, Unni Olsbye, Pablo Beato, Silvia Bordiga, Stian Svelle: Reactivity of Methoxy species towards Methylation and Oligomerization in Cu-Zeolite systems, 2024 (Submitted)

Holme B, Håkonsen SF, Waller D.: Challenges in quantifying Pt concentrations in Pd alloys by using secondary ion mass spectrometry: Strong grain orientation effects. Surf Interface Anal. 2024;1-12.

J. Gopakumar, A. Miro i Rovira, B.C. Enger, D. Waller, M. Rønning: Comparison of Ceria-Supported Catalysts for Attaining NO - NO_2 Equilibrium at Industrial Nitric Acid Plant Conditions, 2024 (submitted)

J. Gopakumar, R. Myrstad, R. Børresen Anda, H. Øien, B.C. Enger, D. Waller, M. Rønning: Ostwald Process Intensification by Catalytic Oxidation of Nitric Oxide, 2024 (submitted)

Moses Mawanga, Jia Yang, Edd A. Blekkan: Steady-State and transient kinetic investigations of the oxidation of NO over Pt/SiO_2, Journal of Catalysis, 2024, Volume 433, 115483

S. Muthukrishnan, R. Vidya, A. O. Sjåstad: Illustrating the Surface chemistry of Nitrogen Oxides (NOx) adsorbed on Rutile TiO_2 (110) with the aid of STM and AIMD simulation, 2024 (submitted)

Thronsen, Elisabeth; Bergh, Tina; Thorsen, Tor Inge; Christiansen, Emil; Frafjord, Jonas; Crout, Philip; Van Helvoort, Antonius Theodorus Johannes; Midgley, Paul A.; Holmestad, Randi: Scanning precession electron diffraction data analysis approaches for phase mapping of precipitates in aluminium alloys. Ultramicroscopy 2024, Volume 255, 113861

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Ingeborg-Helene Svenum, Marie D. Strømsheim, Jan Knudsen, Hilde J. Venvik: Activity and segregation behaviour of Pd75%Ag25%(111) during CO oxidation – An in-situ NAP-XPS investigation, Journal of Catalysis, 2023, Volume 417, 194-201

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Bjørn Gading Solemsli from UiO was presenting iCSI research at the EuropaCat 2023 Congress in Prague.

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