iCSI

industrial Catalysis Science and Innovation

for a competitive and sustainable process industry

Annual Report 2018

Centre for Research-based Innovation

The Research Council of Norway

NTNU

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

- **Improved understanding** of the kinetics and the chemistry
- **Synergy** between **applied and basic** research
- Development of **new materials and methods**

22 Master students

8 PhD candidates

2 Postdoctoral fellows

10 Professors

17 Research Scientists from SINTEF

14 Scientists from industry

NTNU

UiO : University of Oslo

SINTEF

YARA

dynea

inovyn

K.A.Rasmussen Norway

HALDOR TOPSØE

Cover art: 3D rendering of elevation lines of the Alps resembling *in situ* spectroscopic data, by *Samuel Regli*

2018 Summary

2018 was a year of recognition for iCSi, during which our young scientists and seniors showed their innovation potential by disseminating high quality research from the Centre. iCSI researchers gave **22 *presentations*** at national and international conferences. Furthermore, iCSI partners acquired **6 national and European grants**.

Some iCSI team members had particularly ***high international visibility*** during 2018. Three of the iCSI young scientists received best poster awards in different events, and 2 seniors were recognized for their contribution to catalysis and chemical reaction engineering. An absolute highlight was the announcement of the ***Awardee for Excellence in Natural Gas Conversion 2019*****,** who is no other than iCSI professor Unni Olsbye; becoming the first woman included to the hall of fame of natural gas conversion.

iCSI researchers publish their findings and perspectives in **high impact journals** such as *Journal of the American Chemical Society* and *Chemical Society Reviews*. While the IIA 4 and IIA 5 are leading the way, it is nice to see that high-quality research results and publications are out or in the pipeline for all Industrial Innovation Areas (IIAs). The publication and presentations lists can be found in p. 57-60.

In the same fashion as previous years, the iCSI team had the opportunity to gather in an idyllic lake location for the **Annual Seminar,** this time Selbusjøen. Students, academics, researchers, industrial partners and scientific advisory committee members (52 participants) had the opportunity to spend two days together and exchange experiences, knowledge and ideas.

In addition, a workshop on "*Challenges in Catalysis Research"* was organized from iCSI, were students and industrial researchers working on catalysis had the opportunity to gather and discuss their challenges. The excellent talks from two industrial seniors on real-world catalysis puzzles that they have tackled during their carrier at Topsøe and Yara were the apogee of a purposely professor-free event with a lot of social interaction.

Three iCSI PhD candidates did **industrial exchanges** in 2018, to Herøya (Yara), Lillestrøm (Dynea)/Hamar (KA Rasmussen), and Lyngby (Haldor Topsøe). They returned noticeably wiser while also having contributed with new perspectives and skills at the industrial site.

Once more the representation at **iCSI Board** has changed. UiO representative Vebjørn Bakken changed role to become director of UiO: Energy. UiO is now represented by Kristin Vinje, Vice Dean at the Faculty of Mathematics and Natural Sciences at UiO. While Vebjørn made indispensable contributions in establishing the iCSI research and collaboration, Kristin brings new perspectives with her background from politics as well as research and innovation.

Finally, a big part of 2018 was devoted to preparations for the **Midway evaluation** that will be finalized in 2019. The administrative team was strengthened with experienced staff for tackling the reporting and coordination required (p. 8). This exhaustive team effort is now almost complete, and we hope that we will have the opportunity to continue working in the fascinating world of industrial catalysis with impact to our societies for many years to come!

iCSI moments

Poster awards for three of young iCSI researchers; **Gianni Astarita Young Investigator Award** recognition of Dr. Kumar R. Rout a SINTEF affiliated iCSI Research scientist; Prestigious **Award for Excellence in Natural Gas Conversion 2019** goes to iCSI professor Unni Olsbye.

Contents

Mid-way & Evaluation

Hilde Johnsen Venvik iCSI Director, in action at MAXIV!

iCSI has reached its Midway – although in some way it feels like we have just started! Strictly speaking, if referring to starting up the first iCSI research activities from September 2015, we are mid-way in September 2019. Given that it also took some more months to complete the Consortium Agreement and the recruiting, it is possibly not so strange that it does not feel quite mid-way. Nevertheless, the submission of documentation for the Research Council of Norway Midway Evaluation of the Centres for Research-based Innovation generation III (SFI-III) is just completed. We are looking forward to the evaluation and the final decision of the Board of the Research Council *"about whether to continue the individual centre for the remainder of the overall eight-year term, or to wind it up after five years"*.

In iCSI, we are reasonably confident about our continuation but have as a team made the best effort possible to show how we fulfil the SFI Success Criteria. This has been a demanding but educational journey. When challenged as to our achievements, it is easy to boast about our *JACS* publications and invited lectures. Equally important is, however, the iCSI industrial partners putting down in words and numbers why they are in iCSI and what they expect from the remaining period of the Centre.

Measuring Innovation - what our industrial partners say:

Yara *"Participation in iCSI allows Yara to increase our knowledge of our catalysts and related processes. The development of an improved platinum catchment system has the potential to reduce platinum losses, with a value in excess of 35MNOK per annum. The development of a system to recover the energy from the oxidation of NO to NO_2, if implemented in all Yara plants, would generate steam with a value of 440MNOK per annum*".

KA Rasmussen "*We have gained completely new knowledge about the catalyst surface chemistry and physical changes, which may lead to improvement of our metal products***"**

Dynea "*iCSI enables Dynea to continue our successful way forward to reduce running cost, emissions and increase our competitiveness in licensing our world leading formaldehyde technology by making our research more effective and allowing us to test out ideas with higher risk, and with a high potential*".

INOVYN "*We have through our engagement in ICSI gained knowledge that is and will be used to improve our catalysts, risk reduction and improve operation of our oxychlorination reactors*".

Haldor Topsøe "*The project is internally regarded as a strategic long-term activity, in order to keep track of the developments in the field of direct methane conversion and look out for opportunities to obtain IP, and the development of breakthrough technologies".*

Is the Centre (iCSI) performing research of high international standard?

Enrique Iglesia: "*The tools and skills in iCSI are appropriate for the objectives and are being applied at the level of the state-of-the-art. Some of the projects would benefit from an approach that brings them closer to the fundamental questions and to experiments that can be more closely coupled with the remarkable recent advances in theoretical treatments. This may well require some "detachment" from materials and conditions that seem closest and most relevant to current industrial practice and needs*".

Will the results achieved generate innovation or potential for innovation and enhanced competitiveness among the industrial partners?

Alessandra Beretta: "*Definitely yes! 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".*

The Research Council also emphasizes the opportunity to obtain *"advice on how to improve and further develop the Centres"*. Our prominent SAC advisors have taken the effort to assess our strengths and weaknesses, as well as our position and importance in an international perspective. We will work hard to improve where necessary. An important issue is the interaction between fundamental research questions and the demand for immediate results and value-creation. There is no optimum recipe or balance in this; it is rather something that needs frequent revisiting and consideration.

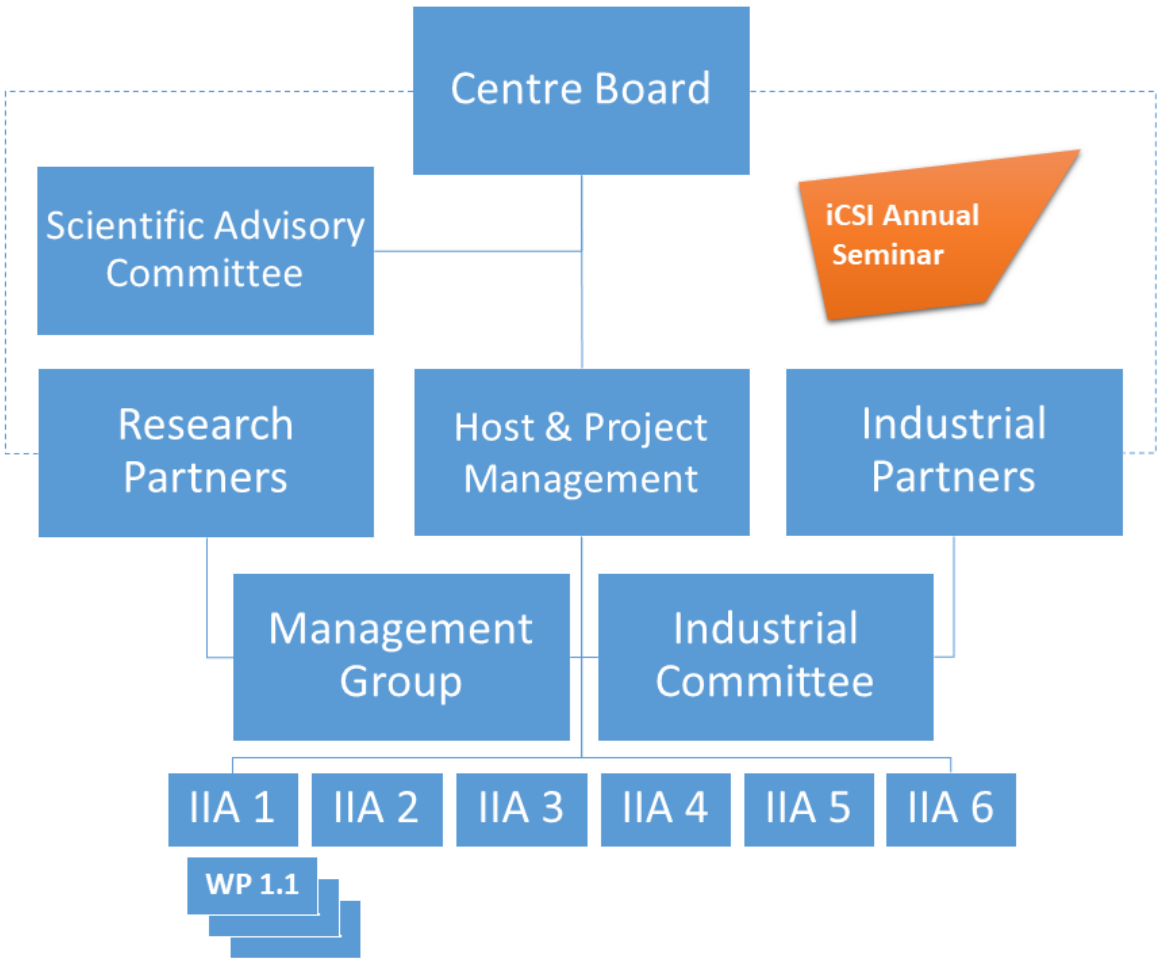
What probably inspires professors and senior researchers the most, is to see our young researchers grow with the challenge and the pressure. They have really started to deliver publications and create value for the partners in 2018. In 2019, the first candidates will defend their PhD theses, the most important milestone in iCSI. One of the postdoctoral fellowships have also ended. We thank Dr. Michael Dyballa for his important contributions in iCSI, and wish him success in his career at the University of Stuttgart (see also p. 44).

iCSI acknowledges the effort put down by postdoctoral fellow Dr. Oleksii Ivashenko and Professor Anja O. Sjåstad in preparing the Operando Surface Catalysis (OPSCAT) meeting in Oslo in January 2019. The meeting gathers a range of international experts within in situ/operando investigations using different techniques and approaches to exchange experience and ideas – thereby providing additional momentum to the Centre in this important area. Finally, Dr. Estelle Vanhaecke will terminate her coordinator function to concentrate on her permanent position as senior engineer at NTNU. Thanks for the enthusiasm and hard work in coordinating the iCSI team, we are glad to keep you around, Estelle! We also say welcome to our new coordinator, Anne Hoff.

Hilde J. Venvik, iCSI Centre Director

Organization

The Norwegian University of Science and Technology (NTNU) is serving as **Host** institution for the **iCSI Centre**. The iCSI **research partners**, NTNU, SINTEF Industry and the University of Oslo (UiO) represent the main research groups involved in heterogeneous catalysis research in Norway, located in Trondheim (NTNU and SINTEF) and Oslo (UiO and SINTEF). The **industrial partners,** Yara, KA Rasmussen AS, Dynea, INOVYN and Haldor Topsøe A/S, also conduct significant own R&D. The collaboration enables optimized use of complementary competence and a shared, highly advanced, experimental infrastructure that is being utilized, expanded and developed within iCSI. The research is organized in **6 Industrial Innovation Areas** (IIA1-6), each with 1-4 work packages. Each IIA has 2-3 research partners and 1-2 industrial partners, IIA6 is generic and involves all partners.



Centre Board

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

Odd-Arne Lorentsen, Yara (Chair)

Pablo Beato, Haldor Topsøe (Vice-Chair)

Lars Axelsen, Dynea

Terje Fuglerud, INOVYN

Johan Skjelstad, KA Rasmussen

Duncan Akporiaye, SINTEF

Karina Mathisen, NTNU

Kristin Vinje, UiO

Aase Marie Hundere, RCN (Observer)

Dr. Odd-Arne Lorentsen is Head of New Front-End Technologies at Yara Technology Centre, Yara International. Odd-Arne has more than 20 years of experience in industrial R&D, mainly primary aluminium production, but recently catalysts for fertilizer production and sustainable technologies.

Dr. Pablo Beato is Lead Scientist at Haldor Topsøe, directing the Atomic-Scale Analysis department.

Lars Axelsen is General Manager of Licensing & Projects in the Technology Centre of Dynea.

Terje Fuglerud, is Chief Engineer at INOVYN.

Johan Skjelstad is Technology Manager at KA Rasmussen.

Dr. Duncan Akporiaye, holds a position as Research Director at SINTEF Industry.

Professor Karina Mathisen is Vice Dean for Education and Dissemination at the Faculty of Natural Sciences, NTNU.

Dr. Kristin Vinje, is Vice Dean for Innovation and External Relations at The Faculty of Mathematics and Natural Sciences, UiO

Dr. Aase Marie Hundere is Special advisor at the Research Council of Norway with Responsibility for Nanotechnology and Advanced Materials

Scientific Advisory Committee

Prof. Alessandra Beretta

Prof. Enrique Iglesia

Prof. Graham Hutchings

POLITECNICO MILANO 1863

Berkeley UNIVERSITY OF CALIFORNIA

CARDIFF UNIVERSITY
PRIFYSGOL CAERDYDD

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

Management and Administration

Hilde Johnsen Venvik,
Professor
iCSI *Centre Director*

Estelle Vanhaecke
Senior Engineer
iCSI *Coordinator*

Anne Hoff
Senior Engineer
iCSI *Coordinator*

Nikolaos Tsakoumis
Researcher
iCSI *Coordinator*

Torgrim Mathisen,
Senior Executive Officer,
iCSI *economy advisor*

The Centre is hosted by the **Department** of **Chemical Engineering,** NTNU. The administration team consists of a **Centre Director,** a **Coordinator**/Vice Director and an **Economy advisor**. In 2018 the increased administrative responsibilities that follow the ongoing *Midway Evaluation of the Centre's for Research-based Innovation generation III (SFI-III)* led to a temporary extension of the coordinator team, counting altogether three members with experience from academic and industrial research, laboratory operations, project management and dissemination from August 2018 to May 2019.

Industrial Partners

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

Yara International ASA is a Norwegian-based chemical company with fertilizer as its largest business area, but with industrial gases, catalyst production and NOx abatement solutions for industrial plants, vehicles and vessels also in its product portfolio. In addition to being present in more than 51 countries, Yara operates 2 industrial production sites in Norway, Porsgrunn and Glomfjord, with approx. 700 employees. In iCSI, Yara aims to further strengthen its global competitiveness through innovation.

KA Rasmussen AS is a refiner of precious metals and supplier of catalysts and products based on precious metals located in Hamar, Norway among other places in Europe. KA Rasmussen has specialized in technology for producing structured catalysts for the Ostwald process, and silver particles for oxidation of methanol. In iCSI, KA Rasmussen wants to expand its catalyst market base, contribute to meeting emissions targets, and reduce the net consumption of noble and scarce metals in their product range.

Dynea AS is a Norwegian-owned company for wood adhesives production, industrial coatings and licensing of Silver Formaldehyde plants with productions sites in Norway, Denmark and Hungary. Dynea holds several unique technologies for licensing, and its further technology R&D is based in Norway. In iCSI, Dynea aims to continue its technological leadership in formalin production for improved plant operations and reduced cost, as well as increase its licensing.

INOVYN Ltd. is a leading producer of chlorvinyls and associated products, wholly owned by INEOS. INOVYN has 8 European production sites and 4300 employees, of which INOVYN Norway AS constitutes about 300 employees in two sites; the chlorine/VCM production at Rafnes and the PVC plant at Herøya. Through iCSI, INOVYN wants to further improve the VCM technology to achieve world class energy and raw material efficiency.

Haldor Topsøe AS is a catalyst producer and process plants technology developer based in Denmark. Topsøe is known for its emphasis on research and scientific excellence as a basis for its business. In iCSI, Topsøe aims to explore new, direct routes from lower alkanes to bulk chemicals, thereby expanding their technology range and potentially reducing the energy consumption and emissions associated with such production.

SAC portrait: Professor Enrique Iglesia

Professor Enrique Iglesia holds the Theodore Vermeulen Chair in Chemical Engineering at the University of California at Berkeley and also a position as Faculty Senior Scientist at the Lawrence Berkeley National Laboratory. He is the former (and founding) Director of the Berkeley Catalysis Center.

Berkeley
UNIVERSITY OF CALIFORNIA

A diverse background

Enrique Iglesia's path to Berkeley was neither straightforward nor predictable. His family is originally from Spain. His parents and grandparents left Europe during difficult times in the early 20th century to seek refuge in Cuba, where he was born. They emigrated to the U.S., once again a refugee family, in 1969. Between his native Spanish and his poor English language skills, mathematics and chemistry provided the language-neutral bridge that ultimately led him to a lifelong career in chemical engineering. Influential mentors in secondary school ignored his language barrier and noted a talent and an intensity that made them encourage him to apply for top universities in the U.S. Princeton offered him a chance and he received his chemical engineering degree as the top-ranked graduating senior in the College of Engineering. Summer internships at Exxon gave him a taste of industrially relevant problems and they also exposed him to the "magic" of catalysis. He was torn between a career in industry and the opportunity to sharpen his skills through graduate studies. Coached by his Princeton mentors, he decided to enter the Ph.D. program in chemical engineering at Stanford University. There, Professor Michel Boudart became not only his mentor but his lifelong teacher and friend. A few weeks ago, Professor Iglesia received the Michel Boudart Award for the Advancement of Catalysis. This is the most prestigious award given by the North American Catalysis Society and the European Federation of Catalysis Societies, and a recognition that he describes as "*the most meaningful in my career*".

The practical challenges then won over academic ambitions and he accepted a position at the Corporate Research Lab of Exxon after graduating from Stanford. From 1982 to 1993, he rose through the managerial ranks without losing sight of research and contributed to the development of some of the enabling concepts for technology developments in natural gas conversion and in catalysis for the upgrading of hydrocarbons to fuels and petrochemicals. His rapid climb through the ranks at Exxon

Enrique Iglesia emphasizes that fundamental understanding is key: "*Industry often proceeds with the illusion of solving the problems without understanding them and one needs to understand the problem in order to solve it*". Academia has a strong advantage on understanding and that is ***time***.

Picture: Lama encounter in Peru and corresponding artwork

did not completely fulfill his inquisitive traits; he found himself missing *"the molecules and the equations that seemed so much more logical than the humans*" that he was leading. After seeking the advice of his mentor, he made the decision to leave the *"comfort of industry for the uncertainties and economic challenges of academia"*. This brought him back to California where he and his wife had started their married life together, and where he cherished the cool and dry weather and the hills and open spaces for hiking and climbing. This time he found the University of California at Berkeley, the prime historic sports rival of his graduate alma mater, to fit best with his diverse background and his love of teaching and mentoring. He started a group that has become known for its alumni, who have gone on to join some of the top chemical engineering and chemistry departments worldwide. This is a legacy that continues from his graduate advisor and one about which Professor Iglesia is particularly proud.

Today, he stands as one of the most recognized academics in the field of catalysis and chemical engineering, and as one who eminently bridges the fundamentals with the practice of catalysis. He has been described upon induction into the American Academy of Arts and Sciences as a role model for the inseparable nature of teaching, research and scholarship. His research accomplishments have been recognized with numerous honors and awards, including election to several national academies and several honorary professorships and doctoral degrees, as well as awards for more relevant practical contributions, such as the ENI Prize, the Tanabe Prize, and the Award for Excellence in Natural Gas Conversion. But given that Professor Iglesia left industry for academia to teach and mentor, he is, not surprisingly, most proud of his many teaching and mentoring awards and of the cadre of students that continue his tradition of excellence in industry and in academia. He has selflessly served the catalysis community as Editor-in-Chief of Journal of Catalysis, as President of the North American Catalysis Society, and as Vice President and President-Elect of the International Association of Catalysis Societies. His publications have been cited more than 30,000 times and his patents have provided some of the enabling features for several technologies in current practice.

***Typical recurring phrases, often posed as challenges and admonitions to Enrique's research group**:*
"thinking Is harder than doing, but more productive"
"the impact of our work is known after 20 years, the rest is glamour, hype, h-index, and salesmanship"
"if it does not have a number, it is not data"
"if it seems truly novel and useful, which law of thermodynamics does it violate? "

Life beyond research:

Enrique tells us of his activities outside science: *"Terry and I were high school sweethearts and have been married for 40 years. We have three children, some of them close to middle age by now (gulp!), but still children to us. We also have four grandchildren between the ages of 18 and 30 months. In contrast with the typical U.S. family, every one of them lives within 20 km of our home. They keep us quite busy and serve as excellent signposts to remind us where we are needed most."*

Picture: Hiking in India with Johannes Lercher

I keep my sanity, and some semblance of physical stamina and shape, by running the quiet hills near our home and by occasionally stretching my spirit of adventure and my aging muscles and joints with exotic and age-inappropriate treks. Recent ones took us to Ladakh in Northern India with my close friend Professor Johannes Lercher (Technical University of Munich) and to the Sacred Valley and Lares in Peru with Terry; there, I bonded with a friendly llama and a painting was made to record the moment for posterity".

Enrique on iCSI and the future of catalysis research:

"It is at the junction between knowledge and its useful practice where concepts driven by ideas and usage driven by market needs and, more recently, sustainability meet, to address the problems that humans face. This boundary often resists, but with good intentions and spectacular successes, all efforts to manage it. The iCSI Centre addresses these challenges with a thoughtful structure that brings together talent and experience in diverse disciplines, a group of engaged industry stakeholders, and a set of problems and techniques at the state-of-the-art in our catalysis discipline. In doing so, it seeks to develop the technologies of the future in areas of interest to the stakeholders. Irrespective of its ultimate success, the work and the people will go on to develop solutions that we do not yet envision as part of the on-going work. It will develop as its most important accomplishment the human talent, competencies, and skills that will go on to train others in industry or academia. This is the multiplicative effect of academic research when its emphasis is to teach and the technological contributions merely the side benefits of a well-crafted academic mission. Society's benefits are both immediate and long-term, even if the current strategies seek to address problems with much shorter horizons. My journey has placed me at the two sides of joint industry-academia efforts and ***I find the structure and the objectives of iCSI to be balanced and enlightened and the execution of this mission to be on target and well-planned****."*

Tips to young scientists *garnered from those with whom I have shared my scientific journey in industry and academia:*

- *Your work will seldom "save the world" or make you famous, but when it creates "recyclable knowledge" it will build upon that of many others, and together it will solve problems that are different and more important than those you initially sought to solve.*
- *To see our ideas come to practice, we often must let others own them and take credit for them.*
- *The value of our work is that part of it will still matter and be read and used after a few decades of scrutiny.*
- *Be skeptical of that which seems too novel or too useful until you check and check again.*
- *Confusion forces you to change your hypotheses and your assumptions and channels your path; this is how science works.*
- "*Lectures must be spontaneous, but spontaneity must be carefully rehearsed*" a paraphrase of a quote attributed to Professor Joel Hildebrand.
- *Talent and tools are seldom enough, without the time to think and the persistence to outlast and to appreciate those precious moments of complete confusion along the journey; they show the way.*

"The iCSI Centre has a well-balanced portfolio of projects and the tools required to address the fundamental questions that such projects ask. Their competence in materials synthesis and characterization complement those in spectroscopy and in reaction studies. I have very much enjoyed the interactions and the intellectual intensity of the iCSI Annual Seminars and I am certain that the Centre will become 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.

I view the future of catalysis research as one with a greater focus on the rules of reactivity and selectivity at the level of bond-making and bond-breaking and on the intrinsic relations between the energetic descriptors of materials and the ability of their surfaces to stabilize transition states for specific reaction channels. This will require that the right level of theory and the structural models most faithful to the reality of relevant catalytic solids be brought much closer to the experimental work. ***We are entering an era in which the synchrony of experiment and theory will become an unavoidable and powerful feature of each project****; I encourage my own group to grow along that path and I give the same advice to the iCSI research team."*

Picture: Lecturing at the iCSI Annual Seminar.

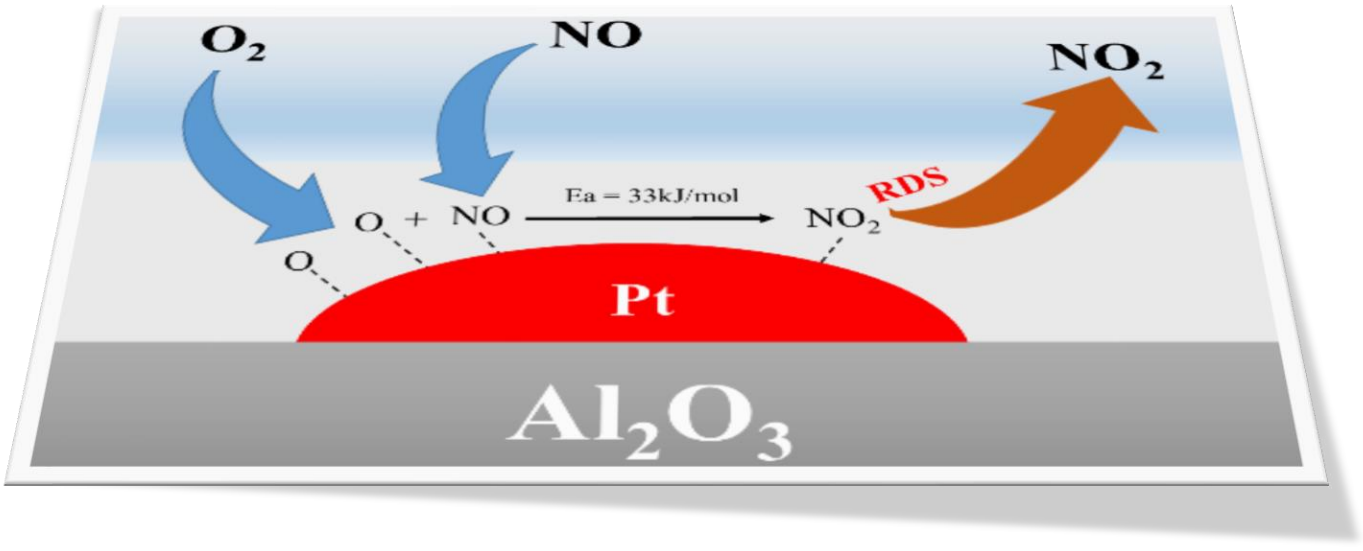
Highlight 2018

iCSI Industrial innovation area 1 (IIA1) "21st century Ammonia Oxidation and Nitric Acid technology development" focusses on developing technology for next generation nitric acid plants. In nitric acid production plants based on the Ostwald process, oxidation of nitric oxide (NO) to nitrogen dioxide (NO_2) is an essential step that proceeds as a homogeneous process without the use of a catalyst. Work package 1.3 targets development of heterogeneous catalysts for oxidation of nitric oxide. With success, 15% additional heat recovery and more rapid oxidation will be enabled, and thereby significant reduction in capital expenditure. This is a challenge in heterogeneous catalysis that hardly has been tackled before and researchers from Yara, SINTEF and NTNU therefore collaborate to find good solutions.

In 2018, an important milestone was reached by publishing the journal paper **"Catalytic oxidation of NO to NO_2 for nitric acid production over a Pt/Al_2O_3 catalyst",** which reports for the first time the kinetics of nitric oxide oxidation under conditions relevant to industrial nitric acid production. Experimental investigations at such conditions is challenging due to corrosion, gas phase conversion, and product analysis, but critical with respect to industrial implementation.

In the study, a supported platinum catalyst (1 wt. % Pt/Al_2O_3) was used with two different concentrations of NO; 400 ppm (representative of diesel engine exhaust aftertreatment) and 10% (nitric acid plant conditions). It was found that platinum exhibits significant catalytic activity above 300 °C for a feed comprised of 10% NO and 6% O_2. Kinetic investigations revealed 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. The addition of 15% H_2O to the feed stream had no significant influence on the catalyst activity. Since water tolerance is crucial to the application, this is very promising.

Reference**: Ata ul Rauf Salman, Bjørn Christian Enger, Xavier Auvray, Rune Lødeng, Mohan Menon, David Waller and Magnus Rønning, Applied Catalysis A: General, 564* ***(2018) *142-146.*



iCSI Seminar 2018

For once more, an idyllic location next to a lake was chosen for hosting our annual meeting. The 2018 iCSI Seminar was held in the outskirts of Trondheim, next to the lake Selbu and at the historic venue of ***Selbusjøen Hotel***. During 19th to 20th of November ***52 delegates*** from industry and academia were mixed to share scientific experiences and ideas. A small reception was arranged before the start of the main event on the occasion of the announcement of the ***2019 Award for Excellence in Natural Gas Conversion*** to Professor Unni Olsbye, and indeed we had the honor to gather no less than three recipients of this prestigious recognition (Enrique Iglesia, Anders Holmen and Unni Olsbye). Two members of the ***Scientific Advisory Committee (SAC)*** were present, with a busy schedule that included plenary lectures on state-of-the-art approaches to catalysis, face-to-face interaction with students in personalized meetings and discussions with the iCSI board. Apart from shorter updates on recent developments in each Industrial Innovation Area (IIA), the **most advanced iCSI research** was highlighted through comprehensive lectures by PhD student Dimitrios Pappas **(IIA5)** and Professor De Chen **(IIA4)**. Social interaction through common dining, chatting at the lounge and team building competitions at the local farm secured a successful meeting.

2018 iCSI Annual Seminar program

Date: 19-20 November 2018.

Venue: Selbusjøen Hotell (http://selbusjoenhotell.no/)
(25-30 min from Trondheim airport, 60 min. from Trondheim)

Day 0 (Sunday Nov 18)	
Afternoon:	SAC/Board arrival and dinner
Day 1 (Monday Nov 19)	
09:00-11:00	*Board meeting*
~11:00	Registration/check-in
11:30	**Lunch**
12:30-13:00	Opening remarks (Chair of the Board, Odd-Arne Lorentsen) Status of iCSI (Director, Hilde J. Venvik
13:00-14:00	SAC presentation 1, Professor Enrique Iglesia, UC Berkeley : *Synthetic strategies for the encapsulation of metal, alloy, and oxide clusters within crystalline aluminosilicates* (abstract appended)
14:00-14:30	**Coffee break**
14:30-15:00 (25 min + discussion)	iCSI Highlight 1, IIA4 PhD candidate Dimitrios Pappas *Cu-Zeolites for the Direct Methane to Methanol Conversion - Unraveling the Nature of Cu Species* (abstract appended)
15:00-15:45 (15 min) (10 min) (15 min)	IIA1-3 update w/focus on innovation and value-creation IIA1: Anja O.Sjåstad/YARA/KA Rasmussen IIA2: Jasmina Hafizovic Cavka/YARA IIA3: Jasmina Hafizovic Cavka/ KA Rasmussen/Dynea
16:00-17:00	Poster session with contributions from iCSI and related projects
17:00-18:00	Poster session, cont. — Parallel: 3-4 SAC-young researcher meetings
18:00-19:30	**Break or social activity**
19:30-22:00	**Dinner**

Day 2 (Tuesday Nov 20)		
09:00-10:00	SAC presentation 2, Professor Alessandra Beretta, Politecnico de Milano: *Intensification of H_2 production by CPO of light and liquid hydrocarbons: analysis of the reactor performance by combined in-situ spatially resolved measurements and modelling* (abstract appended)	
10:00-10:30	**Coffee break**	
10:30-11:00	IIA 6 update (Magnus Rønning)	Parallel SAC-researcher meetings (3-4)
11:00-12:00 (15 + 5min) (15 + 5min) (15 + 5min)	Recent advances and iCSI opportunities in: 1 SSITKA(Jia Yang) 2 TEOM/ISMA (Lødeng/Karlsson) 3 TAP(Olsbye/Redekop et al)	Parallel SAC-researcher meetings (3-4)
12:00-13:00	**Lunch** *(w/SAC-Board meeting)*	
13:00-13:40 (30 min + discussion)	iCSI Highlight 2, IIA5 manager Professor De Chen: *Kinetic modeling, analysis and design of catalytic redox cycles*	
13:40-14:30	Innovation from iCSI (Chair of the Board, OAL/discussion panel) Closing remarks (Director, HJV)	
14:30-15:00	**Coffee**/departure/excursion Bus to Trondheim Airport Værnes and Trondheim city center at approx. 1515	

Welcome!

The iCSI Management and administration team

Hilde, Estelle, Anne & Nikos

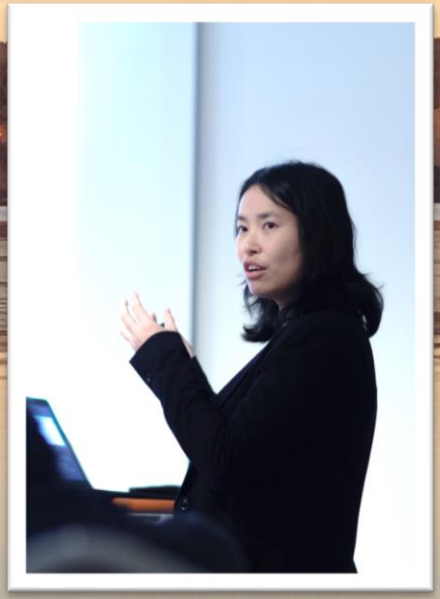
iCSI Seminar 2018

Professor Enrique Iglesia, UC Berkeley:
"Synthetic strategies for the encapsulation of metal, alloy, and oxide clusters within crystalline aluminosilicates"

Professor Alessandra Beretta, Politecnico de Milano:
"Intensification of H_2 production by CPO of light and liquid hydrocarbons: analysis of the reactor performance by combined in-situ spatially resolved measurements and modelling."

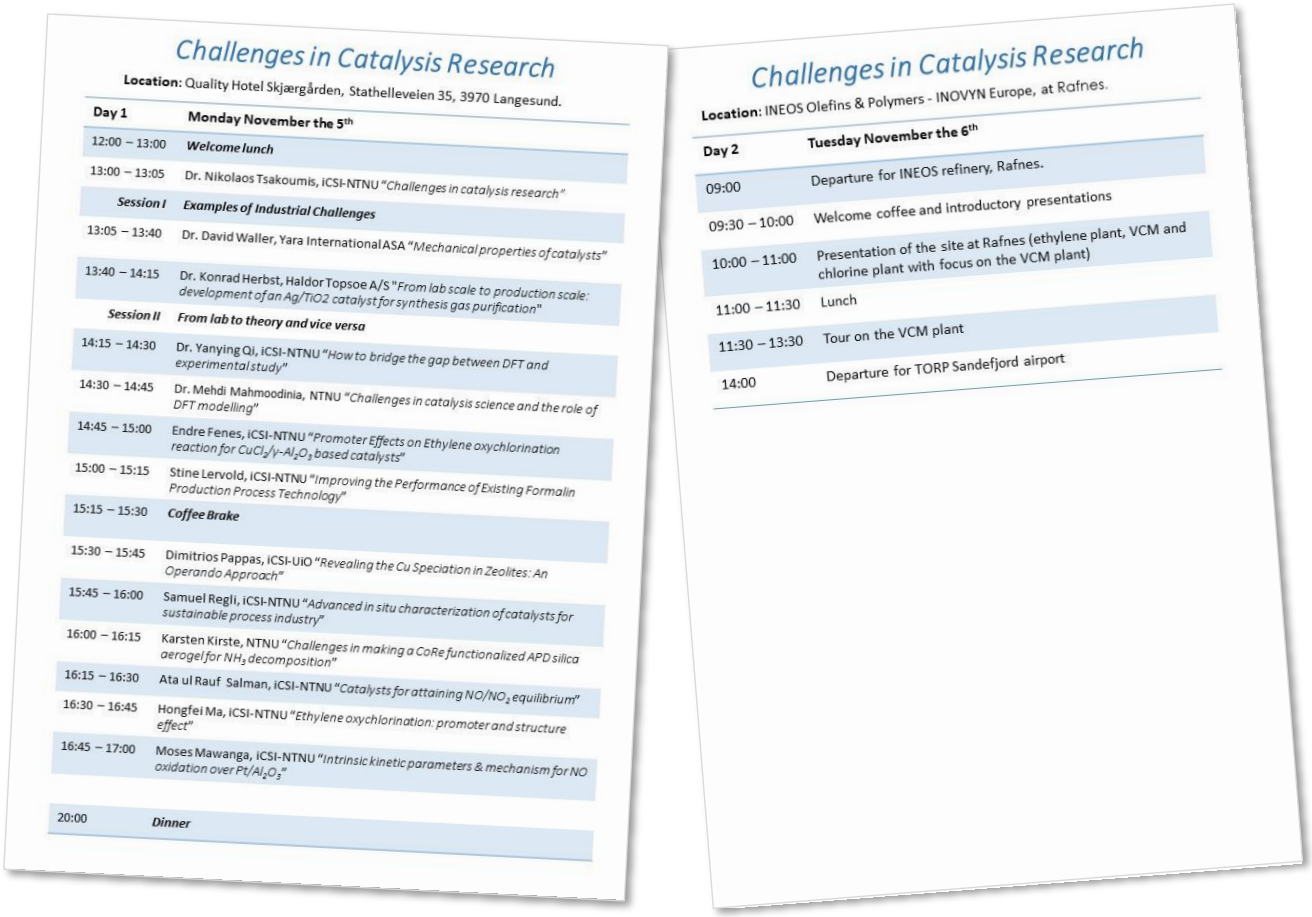
Members of the **Scientific Advisory Committee** (SAC) with the Centre director (above). Gathered recipients of the **Award for Excellence in Natural Gas Conversion** (2009) Anders Holmen, (2019) Unni Olsbye and (2004) Enrique Iglesia (left).

iCSI @Selbusjøen 2018



iCSI Workshop 2018

On the 4th and 5th of November 2018, the majority of **iCSI's young researchers** assembled to meet with representatives from iCSI industrial partners for a workshop on "***Challenges in Catalysis Research***". The event took place in Langesund at the Quality Hotel Skjærgården and included invited lectures on catalysis research from **renowned industrial scientists**. Senior catalyst expert Dr. David Waller from Yara International ASA and senior principal scientist Dr. Konrad Herbst from Haldor Topsøe A/S presented their experiences on "*real world*" catalysis problems that they have had to resolve during their career. The invited talks were followed by presentations on challenges faced by young iCSI researchers in their projects and the first day concluded with social activities at the bathing facilities and a dinner at the venue restaurant. On the second day, thanks to the iCSI board member Terje Fuglerud, participants were invited by **Inovyn** for a tour of the expanding vinyl chloride monomer (VCM) production facilities at Rafnes - a highly integrated plant with units that balance in a marriage of organic and inorganic chemistry. The outcome of the workshop was some new collaborations for overcoming future challenges!



Challenges in Catalysis Research

Location: Quality Hotel Skjærgården, Stathelleveien 35, 3970 Langesund.

Day 1	**Monday November the 5th**
12:00 – 13:00	***Welcome lunch***
13:00 – 13:05	Dr. Nikolaos Tsakoumis, iCSI-NTNU *"Challenges in catalysis research"*
Session I	***Examples of Industrial Challenges***
13:05 – 13:40	Dr. David Waller, Yara International ASA *"Mechanical properties of catalysts"*
13:40 – 14:15	Dr. Konrad Herbst, Haldor Topsoe A/S *"From lab scale to production scale: development of an Ag/TiO2 catalyst for synthesis gas purification"*
Session II	***From lab to theory and vice versa***
14:15 – 14:30	Dr. Yanying Qi, iCSI-NTNU *"How to bridge the gap between DFT and experimental study"*
14:30 – 14:45	Dr. Mehdi Mahmoodinia, NTNU *"Challenges in catalysis science and the role of DFT modelling"*
14:45 – 15:00	Endre Fenes, iCSI-NTNU *"Promoter Effects on Ethylene oxychlorination reaction for $CuCl_2/\gamma$-Al_2O_3 based catalysts"*
15:00 – 15:15	Stine Lervold, iCSI-NTNU *"Improving the Performance of Existing Formalin Production Process Technology"*
15:15 – 15:30	***Coffee Brake***
15:30 – 15:45	Dimitrios Pappas, iCSI-UiO *"Revealing the Cu Speciation in Zeolites: An Operando Approach"*
15:45 – 16:00	Samuel Regli, iCSI-NTNU *"Advanced in situ characterization of catalysts for sustainable process industry"*
16:00 – 16:15	Karsten Kirste, NTNU *"Challenges in making a CoRe functionalized APD silica aerogel for NH_3 decomposition"*
16:15 – 16:30	Ata ul Rauf Salman, iCSI-NTNU *"Catalysts for attaining NO/NO_2 equilibrium"*
16:30 – 16:45	Hongfei Ma, iCSI-NTNU *"Ethylene oxychlorination: promoter and structure effect"*
16:45 – 17:00	Moses Mawanga, iCSI-NTNU *"Intrinsic kinetic parameters & mechanism for NO oxidation over Pt/Al_2O_3"*
20:00	***Dinner***

Challenges in Catalysis Research

Location: INEOS Olefins & Polymers - INOVYN Europe, at Rafnes.

Day 2	**Tuesday November the 6th**
09:00	Departure for INEOS refinery, Rafnes.
09:30 – 10:00	Welcome coffee and introductory presentations
10:00 – 11:00	Presentation of the site at Rafnes (ethylene plant, VCM and chlorine plant with focus on the VCM plant)
11:00 – 11:30	Lunch
11:30 – 13:30	Tour on the VCM plant
14:00	Departure for TORP Sandefjord airport


ICSI
Challenges in Catalysis Research

Researchers' corner

The University of Oslo, SINTEF and Haldor Topsøe have long collaborated in zeolite-based chemistry. In iCSI, they are continuing this fruitful collaboration in Industrial Innovation Area 5 (IIA5). We have asked the principal investigators involved to present their job and their perspectives and ambitions for iCSI.

Blue-sky research on CH_4 activation

The direct conversion of methane to methanol is an exciting research field despite the big challenges that it holds. Our approach involves the synthesis of Cu-exchanged zeolites that mimic the methanotrophic enzymes found in bacteria that feed on methane, which through a stepwise process can facilitate the transformation of methane. The novelty of this approach makes it attractive while it challenges our fundamental understanding.

UiO : University of Oslo SINTEF HALDOR TOPSØE

IIA5 team at the iCSI seminar: Karl Petter Lillerud, Unni Olsbye, Stian Svelle, Bjørnar Arstad, Dimitrios Pappas and Pablo Beato.

Who is in the team?

Stian Svelle has been a Professor at the University of Oslo since 2013. He received his PhD from the same institution in 2004. He has had research visits to the Humboldt Universität zu Berlin with Prof. Joachim Sauer, and has collaborated extensively with Haldor Topsøe. His main research focus is on fundamental studies of zeolite catalysis, especially the conversion of methanol to hydrocarbons, and more recently the direct conversion of methane to methanol. He combines kinetic, quantum chemical, and *operando* studies of individual reaction steps and deactivation phenomena occurring within zeolite catalysts. Another activity is related to the influence of zeolite catalyst crystal morphology and the development of nanostructured zeolites, in both cases aiming for improved performance.

Unni Olsbye has been a Professor at the Chemistry Department of the University of Oslo (UiO) since 2001. She holds an MSc in Chemical Engineering from NTNU (1987), and a PhD in chemistry from UiO (1991). Before joining UiO, she worked in the institute sector (SINTEF) and in industry (Elf Aquitaine, Nordox Industries). During 2007–2015, she was the Managing Director of the inGAP (Innovative Natural Gas Processes and Products) Centre of for Research-Based Innovation. She is the founding advisor of ProfMOF A/S. Her research focus is on heterogeneous catalysis with an emphasis on structure–composition–function correlations and mechanistic studies, in particular single parameter variation studies of zeolitic materials. Her current research is devoted to conversion of small molecules (CH_4, CO_2, CH_3OH, light alkanes and alkenes) over microporous catalysts (zeolites, MOFs).

Pablo Beato obtained his Chemistry degree from Philipps University Marburg, Germany. For PhD he went to the Fritz-Haber-Institute in Berlin, to complete his thesis in 2005 under the supervision of Prof. Robert Schlögl. He thereafter joined Haldor Topsøe A/S, where he currently holds the position of Lead Scientist, working as a project manager mainly in zeolites and synfuel technologies. He is heading the optical spectroscopy laboratories of Haldor Topsøe's R&D and dedicates much time to the development of spectroscopic tools for obtaining fundamental understanding of the synthesis and the working principles of heterogeneous catalysts. His technical experiences cover refinery catalysts for hydrotreating and hydrocracking, syngas catalysts for reforming and methanation, catalysts for the synthesis of sulfuric acid and environmental catalysts, i.e. metal containing zeolites for selective catalytic reduction of NOx and nanoporous materials for conversion of methanol to hydrocarbons.

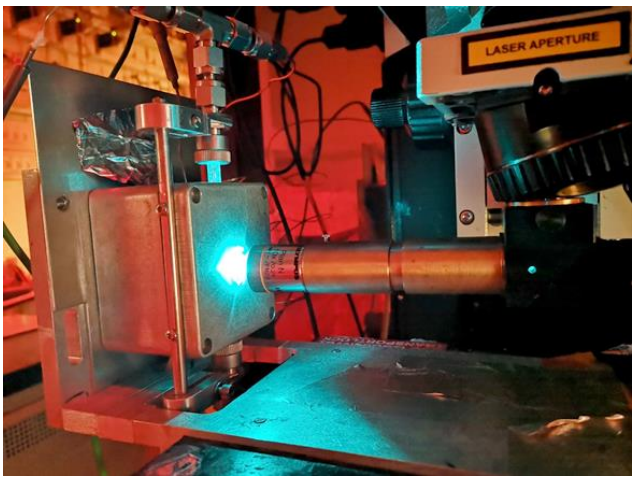
Karl Petter Lillerud has worked as a Professor at the University of Oslo (UiO) since 1996. He earned his PhD in Chemistry from the same institution in 1983. During his career he has functioned as a visiting professor at several universities around the world; Materials Research Lab - University of Illinois, University of California at Santa Barbara, the University of Versailles and more. His main research interest is synthesis and characterization of new crystalline nanoporous materials, potential applications for such materials, and their mechanism and formation. This has resulted in a large number of new developed materials such as: OSI, OSO, OWE, and OBW as well as the recent MOF-materials like the Zr-based UiO-66.

Bjørnar Arstad is Senior Research scientist at the Department of Process technology, SINTEF Industry, where he is presently head of the NMR lab. He graduated as a PhD from the University of Oslo in 2004, and his research interests cover topics such as zeolite- and supported-metal catalysis, solid sorbents for CO_2 capture, reactor technology (fluidized beds, moving beds, membrane), quantum chemical modelling and Nuclear Magnetic Resonance (NMR) Spectroscopy. Topics covered by NMR investigations include structure and dynamics of catalysts, solid sorbents, advanced polymers, energy storage materials, solid state electrolytes, and fundamental properties of CO_2 solvents.

Pablo thinks the challenge is exciting: *"We are dealing with one of the most challenging reactions within the chemical industry; rightly termed "the holy grail" of heterogeneous catalysis. The impact of a potential breakthrough in direct methane conversion cannot be exaggerated, so it is very natural that Topsøe as a major player in the catalyst business is interested. Even though we are far away from any industrial application, I am absolutely fascinated by the underlying chemistry".*
Stian is very enthusiastic: "*Within a short time, the team has been able to reach the absolute edge of the research frontier. The large number of publications, some in very high impact scientific journals, and their rapidly increasing citation numbers testify to this. I consider this to be a remarkable feat of the IIA5 team. We have combined systematic materials synthesis, state of the art characterization, advanced operando measurements, and precise performance measurements to really take our understanding a step forward".*

Our approach

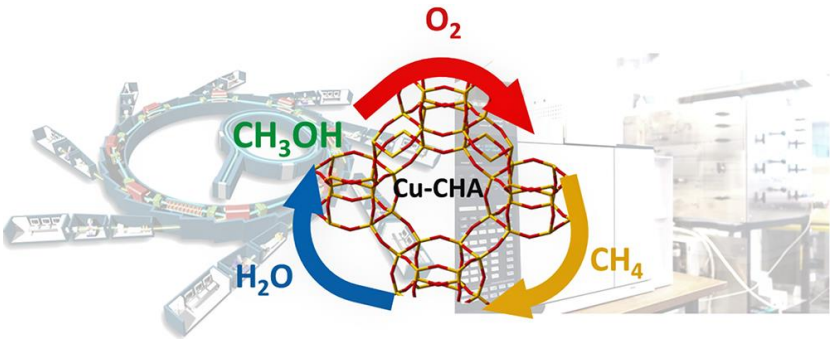
Even though basic characterization can provide meaningful information, the extraction of mechanistic insights as well as structure-activity relationships requires techniques that are more advanced. We therefore developed *operando*/*in situ* methods to tackle the latter, using mostly synchrotron radiation for X-Ray Absorption Spectroscopy (ESRF) along with FT-IR (UiO) and Raman (Haldor Topsøe) spectroscopies, and solid-state NMR (SINTEF). A key component to our approach has been to develop a library of model materials with well-defined properties, covering a wide range of compositions and structures through a dedicated and meticulous synthesis effort. This far, we have gained significant knowledge on what makes a good catalyst and how the reaction proceeds. Our greatest challenge is nevertheless to progress towards commercial realization.



Raman set-up for operando experiments at Haldor Topsøe A/S.

Worldwide interest

Small yields per reaction cycle make the product analysis troublesome. But the high selectivity towards methanol and the mild reaction conditions still makes the approach highly compelling. At the start of iCSI, 17 scientific publications on the topic existed dating from 2005. This gave us the space to improve the fundamental understanding of materials, reaction conditions and reaction mechanisms. During iCSI, a spike in the research took place and the global count of publications is now more than 70. These numbers put the direct conversion of methane to methanol over Cu-exchanged zeolites to the front of academic as well as industrial interests worldwide.



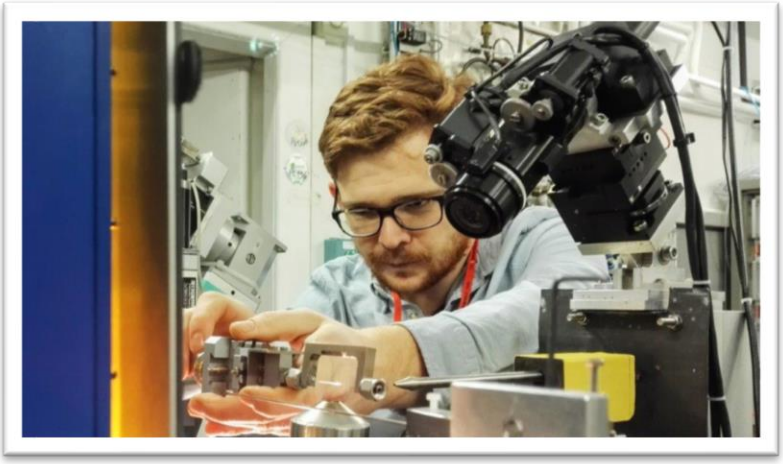
The passing of a great scientist and a dear friend - Carlo Lamberti (1964-2019)

During the preparation of this report, our friend and colleague Carlo Lamberti from the University of Turin unexpectedly and suddenly passed away. Carlo has been strongly involved in the decade's long collaboration between the University of Turin, Haldor Topsøe and UiO. His main field of research was the use of synchrotron radiation to study materials and catalysts. The competence built up through Carlo's work has been of great benefit to iCSI's research, in particular for *operando* X-ray absorption spectroscopy. Carlo was a fantastic scientist with more than 500 publications, he was an inspired and enthusiastic lecturer, and a close friend to many in the team. Our thoughts are with Carlo's wife Silvia and their two sons.

Exchange program 2018

During 2018 three iCSI PhD students had the opportunity to visit our industrial partners. Dimitrios Pappas from UiO spent three months at Haldor Topsøe A/S in Lyngby, while Ata ul Rauf Salman and Stine Lervold from NTNU visited Yara and Dynea (Lillestrøm)/KA Rasmussen (Hamar), respectively. Stine will make additional visits to the two partners in 2019.

From UiO to Haldor Topsøe by Dimitrios Pappas.



I did my industrial visit at Haldor Tospøe from August until November 2018. There I worked at the Atomic-Scale Analysis Department under the supervision of Dr. Pablo Beato. My research was mostly focused on in situ/operando Raman experiments over Cu-exchanged Zeolites for CH_4 activation. Apart from having the opportunity to work at the well-equipped and advanced laboratories I also became more familiar with an industrial R&D department as well as the Topsøe spirit. Finally, I had the chance to meet, interact and exchange ideas with a lot of inspiring people dedicated to catalysis-related research. The whole experience will definitely have an impact in my development as a scientist.

From NTNU to Yara by Ata ul Rauf Salman.

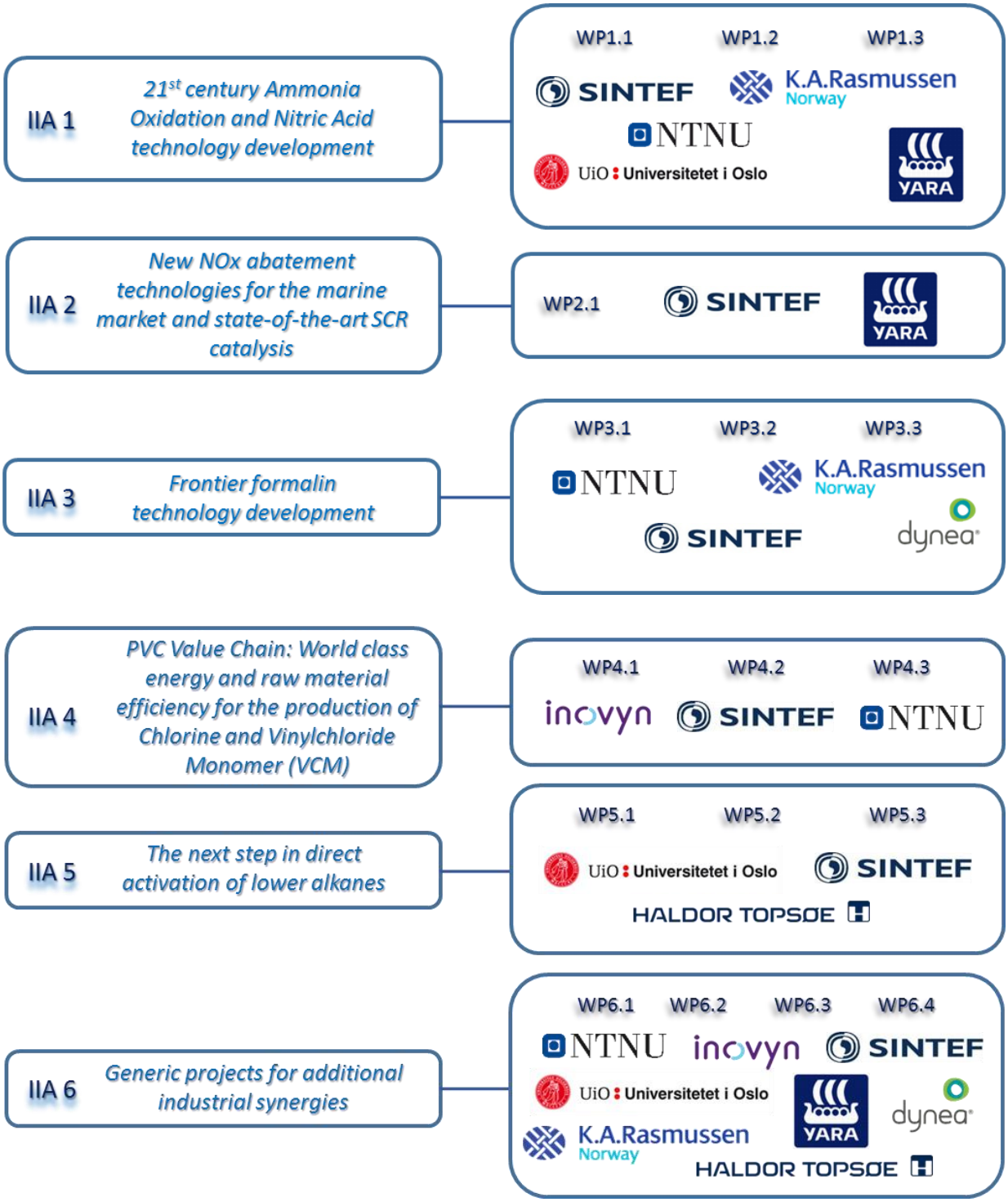
Ata is a PhD candidate in iCSI focusing on the oxidation of nitric oxide by heterogeneous catalysis to enable process intensification of nitric acid plants (WP 1.3). During August to September 2018 complete a two-months internship at Yara ASA through the iCSI industrial exchange program.

"During this period, I had the opportunity to actively participate in the pre-commissioning, commissioning and operation of the pilot plant, working on the oxidation of nitric oxide (NO) to NO_2 by 3D printed catalyst supports. It was a steep learning curve to shift from laboratory reactors to pilot scale and familiarize myself with industrial R&D procedures. Except of the knowledge gain, I had the privilege to meet and work with a lot of nice people at Yara and experience life in the beautiful town of Porsgrunn. I highly encourage other iCSI researchers to benefit from the opportunity to exchange to industry".

iCSI moments

Scientific activities

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



IIA 1 21st century Ammonia Oxidation and Nitric Acid technology development

The Team in 2018

Anja Olafsen Sjåstad	UiO	IIA leader, PhD supervisor and WP responsible (WP1.1), advisor (WP1.2)
David Waller	YARA	Industrial senior (Yara), PhD supervisor (WP1.1), industry researcher (WP1.2-1.3)
Terje Pedersen	KA Rasmussen	Industrial senior, industry researcher (WP1.1-1.2)
Helmer Fjellvåg	UiO	Advisor (WP1.1-1.2)
Asbjørn Slagtern Fjellvåg	UiO	PhD candidate (WP1.1)
Galina Tenkova Yavasheva	UiO	Master student (WP1.1)
Susmit Kumar	UiO	Researcher (WP1.1)
Prasanta Dhak	UiO	Researcher (WP1.1)
Oleksii Ivashenko	UiO	Postdoctoral fellow (WP 1.1)
Ketil Evjedal	YARA	Industry researcher (WP 1.1)
Bente Furevik	YARA	Industry researcher (WP 1.1-1.2)
Van Giau Nguyen	YARA	Industry researcher (WP 1.1)
Arne Hallvard Øygarden	YARA	Industry researcher (WP 1.1-1.2)
Torgeir Lunde	YARA	Industry researcher (WP 1.1-1.2)
Johan Skjelstad	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Thomas By	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Arne Karlsson	SINTEF	Researcher, WP responsible (WP1.2)
Silje F. Håkonsen	SINTEF	Researcher (WP1.2)
Børge Holme	SINTEF	Researcher (WP1.2)
Magnus Rønning	NTNU	PhD supervisor, WP responsible (WP1.3)
Rune Lødeng	SINTEF	PhD supervisor, researcher (WP1.3)
Ata Al Rauf Salman	NTNU	PhD candidate (WP1.3)
Henrik Jenssen	NTNU	Master student (WP1.3)
Beate Meisland Østrådt	NTNU	Master student (WP1.3)
Signe Marit Hyrve	NTNU	Master student (WP1.3)
Mohan Menon	YARA	Industry researcher (WP1.3)
Bjørn Christian Enger	SINTEF	Researcher (WP1.3)

Publications

S. Bundli, P. Dhak, M. Jensen, A. E. Gunnæs, P.D. Nguyen, H. Fjellvåg, A. O. Sjåstad *Controlled alloying of Pt-Rh nanoparticles by the polyol approach*, Journal of Alloys and Compounds 779, 2019, 879-885.

Salman, Ata ul Rauf, Bjørn Christian Enger, Xavier Auvray, Rune Lødeng, Mohan Menon, David Waller, and Magnus Rønning. *Catalytic Oxidation of NO to NO_2 for Nitric Acid Production over a Pt/Al_2O_3 Catalyst*, Applied Catalysis A: General 564, 2018, 142–46.

Motivation

Nitric acid production is a three-step process on the industrial scale. NH_3 is first oxidized to NO over a Pt-Rh gauze catalyst at high temperature, and this is followed by a homogeneous gas phase oxidation of NO to NO_2 at moderate temperatures. Finally, the nitric acid is obtained by absorption of NO_2 in water. A major technological challenge is loss of Pt and Rh in the highly exothermic first step. To avoid permanent loss and costly noble metal recovery, an optimized catchment (recovery) system is required. This is targeted in WP1.1 and WP1.2 through investigating fundamental aspects of PGM species volatilization and transport, as well as surface reaction and reconstruction, gas absorption and diffusion into the solid phase catchment system. WP1.3 concerns the development of new catalyst technology for oxidation of NO to NO_2, which would reduce future capital investments and increase the energy recovery if the bulky homogeneous oxidation system could be replaced by a compact, heterogeneously catalyzed process.

Reconstruction of Pd-Ni catchment gauzes during high temperature ammonia oxidation - PhD project (WP1.1)

Significant quantities of platinum leave the Pt-Rh catalyst as PtO_2 vapor during ammonia oxidation. The currently used industrial catchment system is a pack of Pd-Ni gauzes, capable absorbing Pt up to a concentration of ~50 wt. % Pt. However, the Pd-Ni gauze becomes porous and swells in size during this process (Figure a-d, below), due to two different processes; 1) catchment of Pt, and 2) pore-formation. The Pt-catchment is most prominent for the first gauze in the pack and causes formation of faceted crystallites (Fig. c). The pore-formation is more prominent in the lower layers of the pack and is recognized by a rounded crystallite shape (Fig. d). Moreover, a significant loss of Pd occurs during operation due to the demanding operational conditions, that appears linked to the pore-formation (Fig. d). The mechanisms behind the phenomena are currently not established. To understand Pt-catchment and grain reconstruction, we have performed in-situ X-ray absorption tomography to follow the development of grain reconstruction over time (Fig. e). Our current understanding is that the Pd-Ni gauze reconstruction associated with Pt catchment is rapid, the Pt gradually penetrates inwards in the gauze wire, saturating the outer regions.

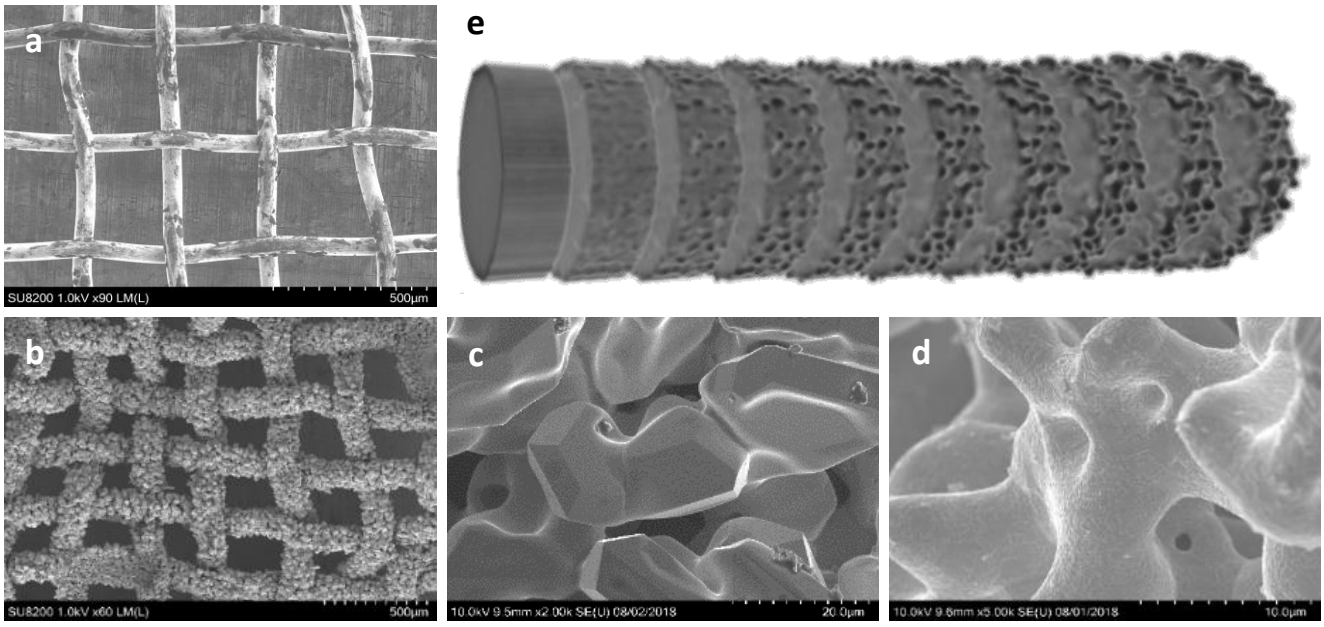


Figure: *SEM-images of 76 um Pd/Ni wires; a) fresh, b) after 20 days at industrial operation, c) close-up image on Pt-rich surface crystals after grain reconstruction (process 1), and d) close up image of porosity caused by the demanding process conditions. e) Tomogram of 20 slices of the Pd/Ni wire investigated by in situ tomography at ESRF, Grenoble.*

Experimental investigations of Pt and PtRh volatilization and catchment (WP1.2)

A dedicated six-zone reactor system is used to generate PtO_2 vapor in dry air and subsequent catchment on pure Pd and Pd-Pt binary alloys. The furnace is optimized to provide temperature gradients in the range 800-1200 °C, representative of those occurring between the location of the Pt volatilization in the ammonia oxidation step and the Pd-Ni catchment gauze in the industrial process.

A set of polished Pd and Pd-Pt discs (Fig. below left panel) with diameter of 5-6 mm and different Pd-Pt compositions have been exposed to a flow of PtO_2 vapor for four hours at 900°C. The diffusion profiles were subsequently obtained using Sputtered Neutral particle Mass Spectrometry (SNMS).
Our results show that, for the low Pt-content samples, Pt is picked up from the gas and a clear diffusion profile can be observed. However, for samples containing 40 wt. % Pt and more we measure an opposite effect where Pt is actually lost from the catchment sample under the conditions applied. This behavior is more pronounced as the Pt content in the Pd-Pt catchment samples increases. Future research will include experiments with varying PtO_2 partial pressure.

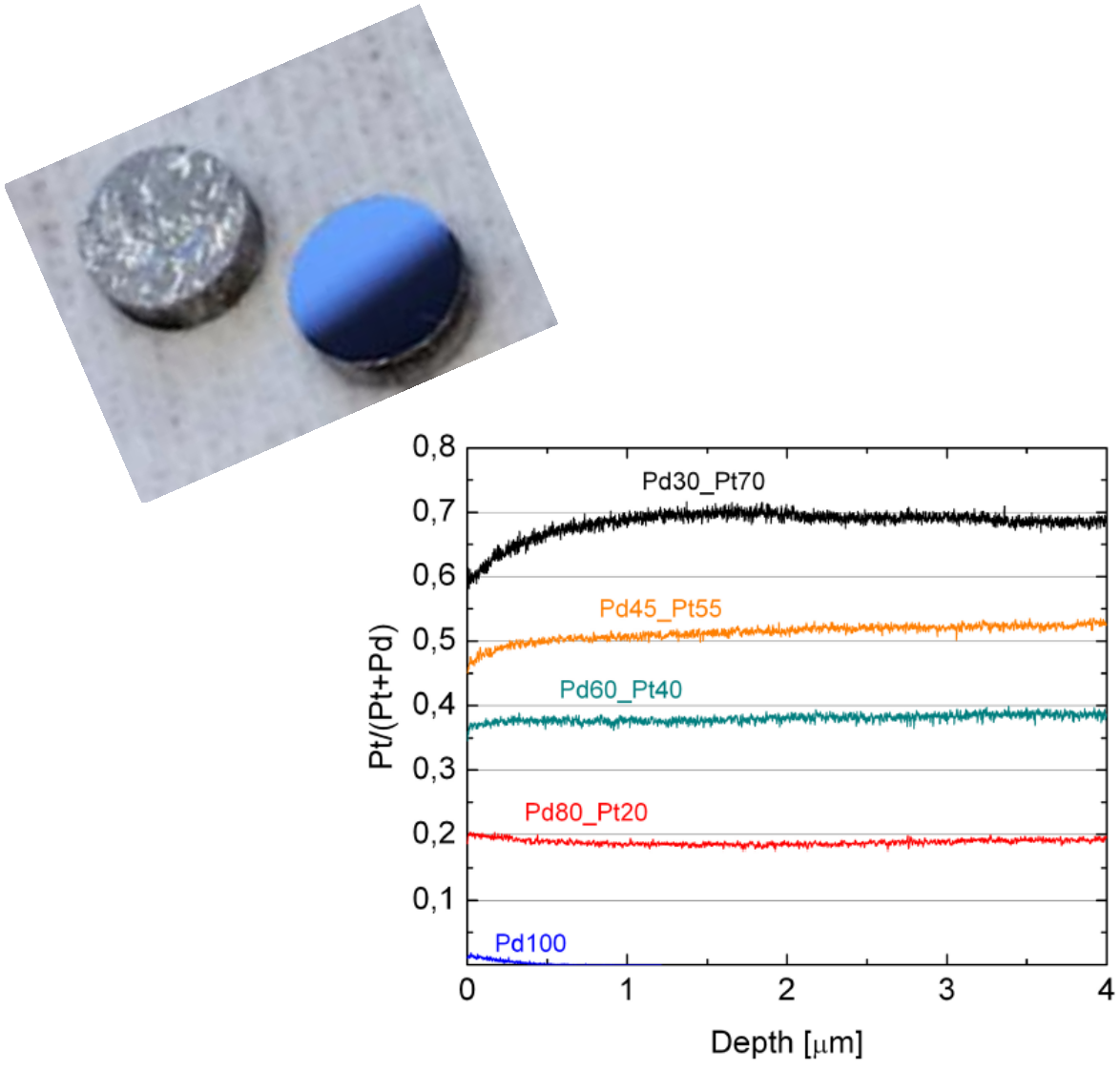


Figure: *The picture shows Pd discs before (right) and after (left) PtO_2 exposure tests; the plot shows diffusion profiles for Pt in Pd and PdPt binary alloys after 4 hours exposure to PtO_2 vapor at 900°C.*

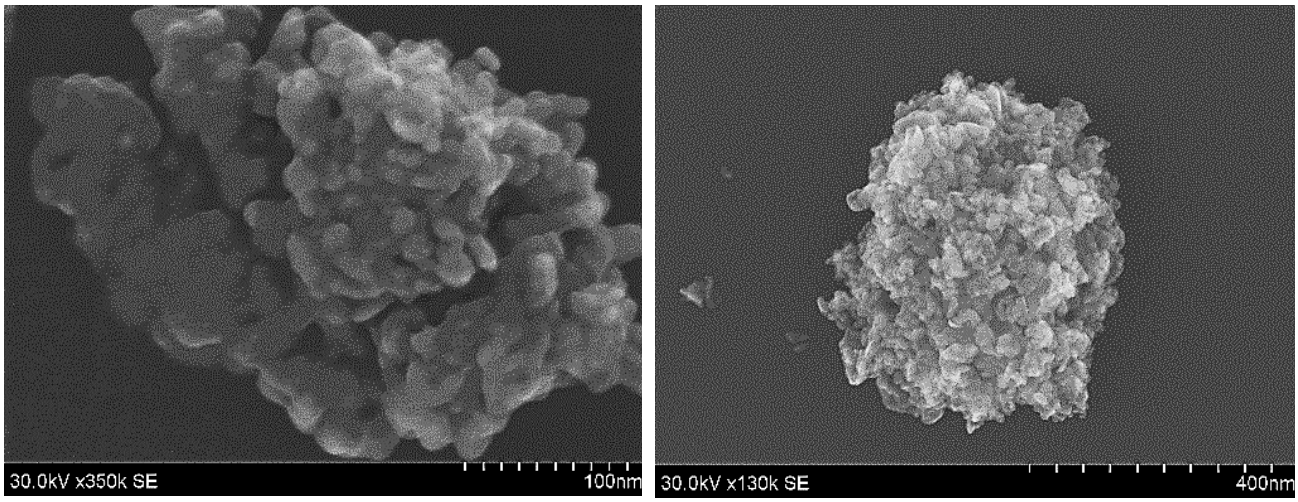
Catalysts for attaining NO/NO_2 equilibrium – PhD project (WP1.3)

As described on page 28, a key chemical step in nitric acid production is the oxidation of nitric oxide into nitrogen dioxide that proceeds as a homogeneous gas phase reaction requiring removal of heat and long residence time. The aim of iCSI is to replace the homogeneous process with a heterogeneously catalyzed process coupled with heat exchangers, permitting significant intensification of the nitric acid plant in terms of the following multiple advantages: a) the oxidation process will be accelerated b) reduction in capital costs and c) additional heat recovery.

Replicating the demanding conditions of industrial NO oxidation in a laboratory reactor is extremely challenging due to the high concentrations of NO/NO_2 in mixture with steam. The researchers from NTNU, SINTEF, and Yara therefore collaborate to tackle this demanding research effort.

Catalytic oxidation of nitric oxide over supported platinum catalysts under industrial conditions have been investigated. Summarized results from the kinetics over Pt/Al_2O_3 including reaction order, apparent activation energy, and proposed reaction mechanism were published in 2018 (see the iCSI 2018 Highlight on p. 14). For an in-depth understanding of the evolution of chemical and structural changes of platinum nanoparticles during oxidation of NO, operando XAS and XRD experiments were performed at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, and the results are currently under analysis.

Another major focus of the project is to identify potential replacement of platinum group metal catalysts, exhibiting superior or comparable catalytic activity. Several transition metal oxides on different supports as well as perovskites have therefore been synthesized and investigated (see figure below).



(a) (b)

***Figure**: SEM images of supported cobalt oxide catalyst (a) Co/ Al_2O_3 (b) Co/ZrO_2*

IIA 2 New NO_x abatement technologies for the marine market and state-of-the-art SCR catalysis

The Team in 2018

Jasmina Hafizovic Cavka	SINTEF	IIA leader
David Waller	YARA	Industrial senior Yara, industry researcher (WP2.1)
Silje F. Håkonsen	SINTEF	Researcher and WP responsible (WP2.1)
Karl Isak Skau	YARA	Industry researcher (WP2.1)
Knut Thorshaug	SINTEF	Researcher (WP2.1)
Martin F. Sunding	SINTEF	Researcher (WP2.1)

Motivation

Selective Catalytic Reduction (SCR) is a core technology in the treatment of exhaust gases (NOx) from stationary power generation (coal, oil and gas), waste incinerators, nitric acid production, and diesel-fueled propulsion. The applications in marine machinery and biomass waste incinerators are emerging markets due to stricter emission regulations and circular economy, respectively. The most common SCR catalyst technology for power and marine applications is based on vanadium and typically supported on monolithic structures (see figure) to allow high throughput and minimum pressure drop for the reduction of NOx with ammonia (NH_3).

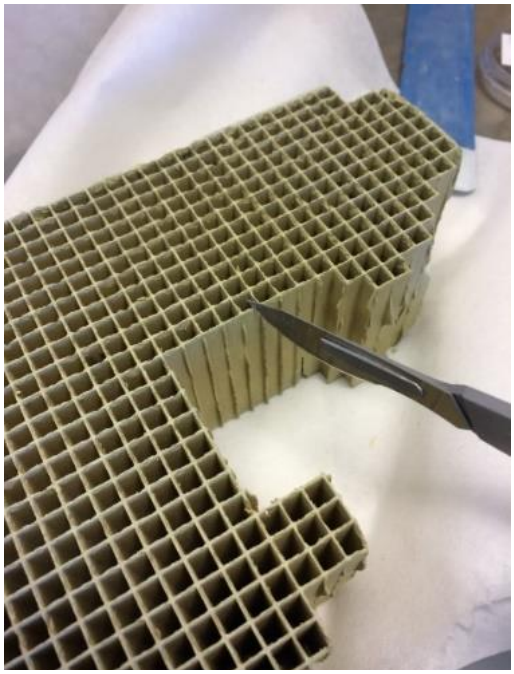


***Figure**: Picture of SCR monolith sample preparation*

Commercial vanadium oxide catalysts are mainly based on V_2O_5 supported on TiO_2 (anatase). The total V_2O_5 loading is 1–5 wt.%, depending on the specific application. WO_3 and MoO_3 are also added to improve the chemical and physical properties of the catalyst. The SCR catalysts' lifetime is dependent on the application, and the catalyst normally deactivates due to fouling, sintering, poisoning, or a combination of these.

Catalyst lifetimes may be as long as 5 years but vary due to differences in their exposure to poisons, dust and soot. It is therefore desirable to be able to rejuvenate or regenerate the SCR catalysts. The former typically involves dust removal and washing to remove surface particulates and soluble deposits but implies difficulties with respect obtaining full recovery of the activity. Regeneration, instead, may involve the addition of an active phase to recover the original activity. It would be highly beneficial if the catalyst activity could be recovered in a simpler way. This is targeted in WP2.1 through first gaining a deeper understanding of the mechanisms causing the catalyst deactivation. The knowledge obtained through thorough characterization of the catalyst at different stages of its lifetime will be translated into new measures.

Research results

Commercial vanadia-based SCR monoliths were used to treat flue gases from a biomass waste incinerator. The catalyst showed rapid deactivation and had to be replaced after relatively short time on stream. To understand the cause of deactivation the characterization tool-box developed in the project was applied.

Powder XRD of fresh and spent catalyst could not confirm significant changes, i.e. the support TiO_2 phase remained in its anatase form. The BET analysis showed a 26% decrease in the available surface area and SEM investigations showed deposition of dust and phosphorus species on the catalyst surface. Although deactivation of vanadia-based SCR catalysts by phosphorous is little reported in the literature, reports indicate that polyphosphoric acids are susceptible to deactivate the catalyst. The deactivation can take place either through interaction with vanadia sites and/or blocking the catalyst pores.

During the SCR process, vanadium sites undergo V(V)-V(IV) redox cycles that govern the reduction of NOx to N_2. The polyphosphoric acids can form stable complexes with V(IV) sites, inhibiting the redox cycle and thus deactivating the catalyst. The high boiling point polyphosphoric acids can also condensate in the pores of the catalyst and reduce the available surface area through deposition. The figure below shows x-ray photoelectron spectra (XPS) of the V 2p core level from fresh and deactivated samples. The fresh sample shows mainly presence of V(V) species with a peak shift to lower binding energies representing V(IV) (left). A thorough examination revealed that this is caused by the X-ray beam during analysis. However, the XPS spectra of the deactivated sample (right) from the incinerator did not indicate presence of V(V) even in the first scan, suggesting complete chemical modification of the active sites of the catalyst.

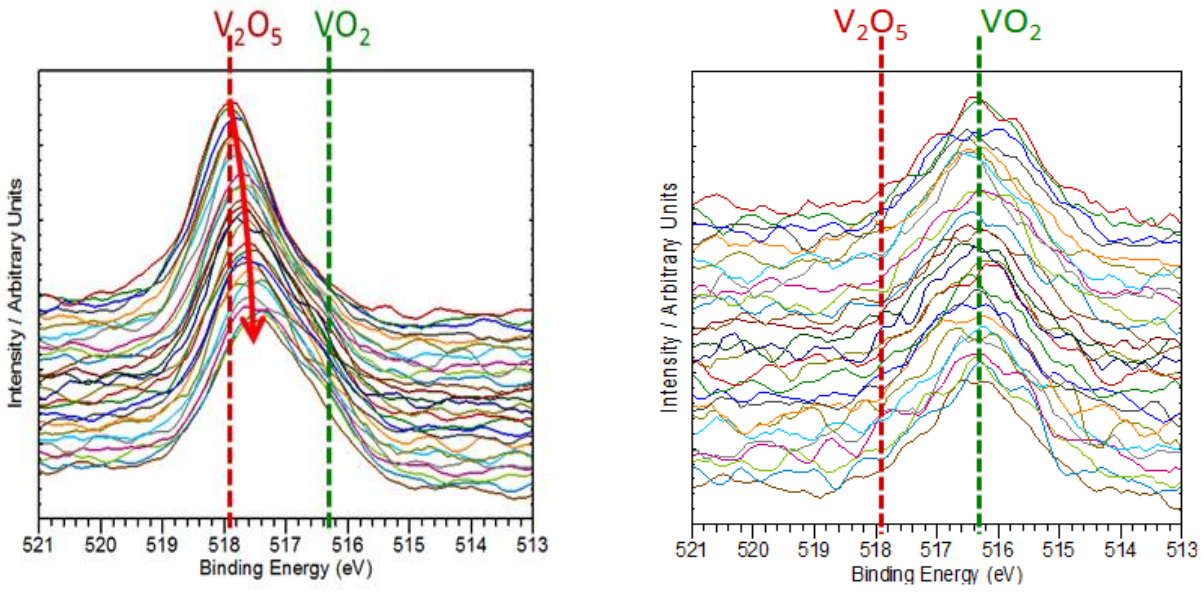


***Figure**: V 2p photoelectron spectra from of a vanadia-based catalyst before and after selective catalytic reduction (SCR) of NOx in biomass waste incinerator exhaust.*

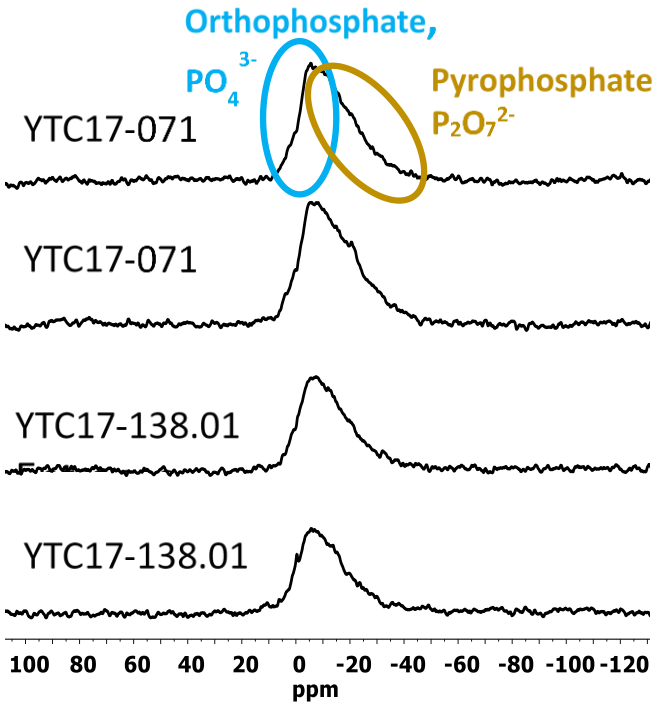


***Figure**: 31P NMR of two deactivated SCR catalysts from an incinerator. YTC17-071 has been longer on stream than YTC17-138.01.*

^{31}P NMR results (above) of the SCR catalyst used after the incinerator clearly show that phosphorous is bonded directly to oxygen atoms both as orthophophates and pyrophosphates. Phosphorous is found both inside the catalyst walls and as deposits on the wall. It is thus believed that phosphorous is first deposited onto the external surface before migrating onto and into the catalyst wall where it interacts to reduce the vanadium from V(V) to V(IV). The binding of V to the phosphorous species results in a termination of the catalyst redox cycle and decreased catalytic activity.

Our own studies hence point in same direction as the research literature, since we observe both physical (reduction in BET area) and chemical effects (interaction with the phosphorous). Deactivated samples that were exposed to marine machinery exhaust did not show the same V oxidation state as the sample rich in phosphorous. The next step of our study will focus on a deeper understanding of the mechanism of phosphorous deactivation and why the phosphorous in the biomass waste incinerator exhaust causes such dramatic decrease in catalytic activity. Methods for regeneration and rejuvenation of phosphorous poisoned catalysts will be explored based on these results.

In addition, will we study vanadia based SCR catalysts installed on ships running on low S fuels. Experience from the industry indicate that, albeit generally advantageous to the catalyst as well as the environment, lowering the sulphur content in the fuel can cause new and unexpected problems to the catalyst, such as increased deposits of Si.

IIA 3 Frontier formalin technology development

The Team in 2018

Jasmina Hafizovic Cavka	SINTEF	IIA leader
Kristin Bingen	DYNEA	Industrial senior, industry researcher (WP3.1-3.2-3.3), WP responsible (3.2)
Mads Lid	DYNEA	Industry researcher (WP3.2-3.3)
Johan Skjelstad	KA Rasmussen	Industrial senior, industry researcher (WP 3.1)
Thomas By	KA Rasmussen	Industry researcher (WP3.1)
Hilde Venvik	NTNU	PhD supervisor, WP responsible (WP3.1), advisor (WP3.3)
Stine Lervold	NTNU	PhD student (WP3.1)
Rune Lødeng	SINTEF	PhD supervisor (WP3.1), researcher (WP3.2-3.3)
Roman Tschentscher	SINTEF	Researcher (WP3.2-3.3)

Publications

Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. *Morphology and Activity of Electrolytic Silver Catalyst for Partial Oxidation of Methanol to Formaldehyde Under Different Exposures and Oxidation Reactions,* Topics in Catalysis, 2019, *in press (10.1007/s11244-019-01159-0)*

Oral presentation

Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. *Investigations of the methanol to formaldehyde (MTF) reaction over silver.* Challenges in Catalysis – iCSI workshop, Langesund, Norway.

Poster contributions

Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. *Morphology study of electrolytic silver catalyst for partial oxidation of methanol to formaldehyde (MTF).* 18th Nordic Symposium on Catalysis, Copenhagen, Denmark.

Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. *Morphology study of electrolytic silver catalyst for partial oxidation of methanol to formaldehyde (MTF).* iCSI Annual Seminar, Selbusjøen, Norway.

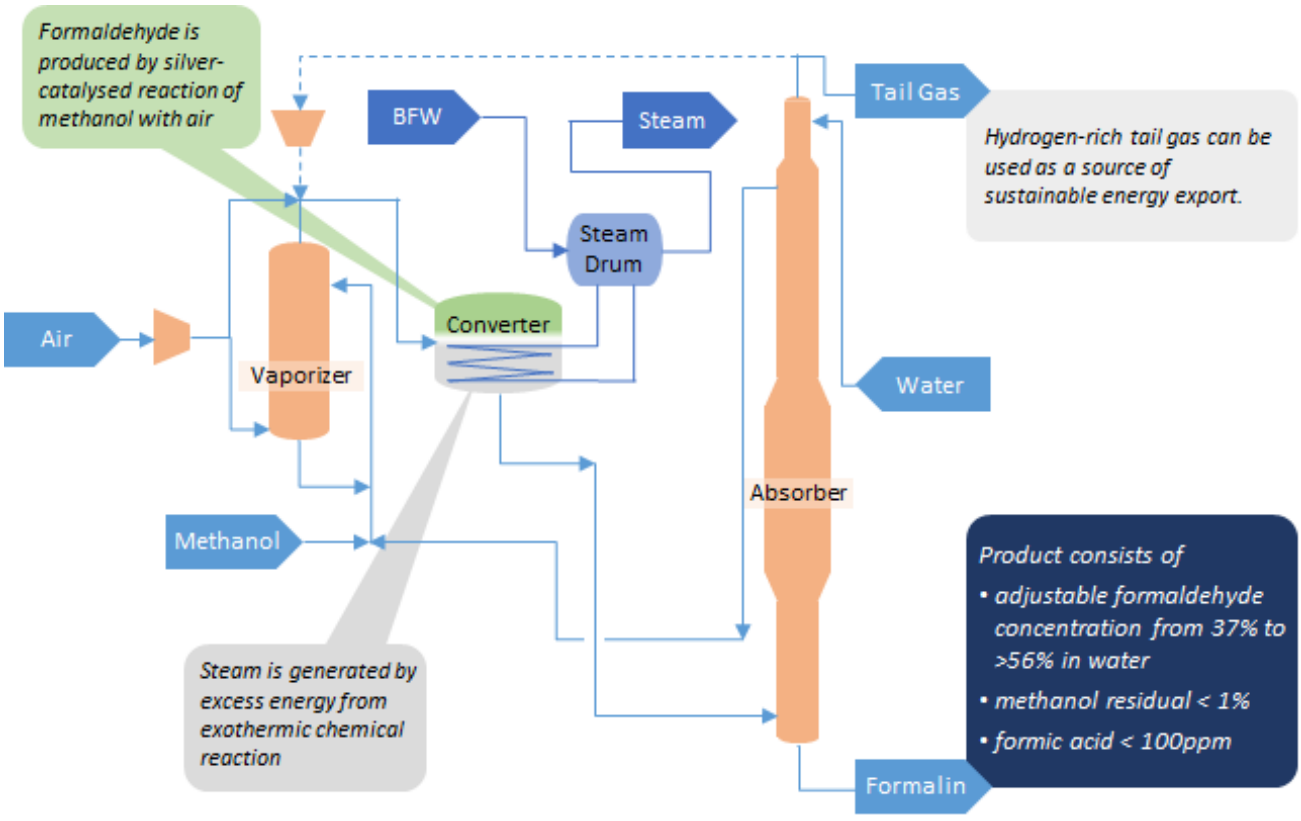
Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. *Morphology study of electrolytic silver catalyst for partial oxidation of methanol to formaldehyde (MTF).* Department-day, Department of Chemical Engineering, NTNU, Trondheim, Norway.

Motivation

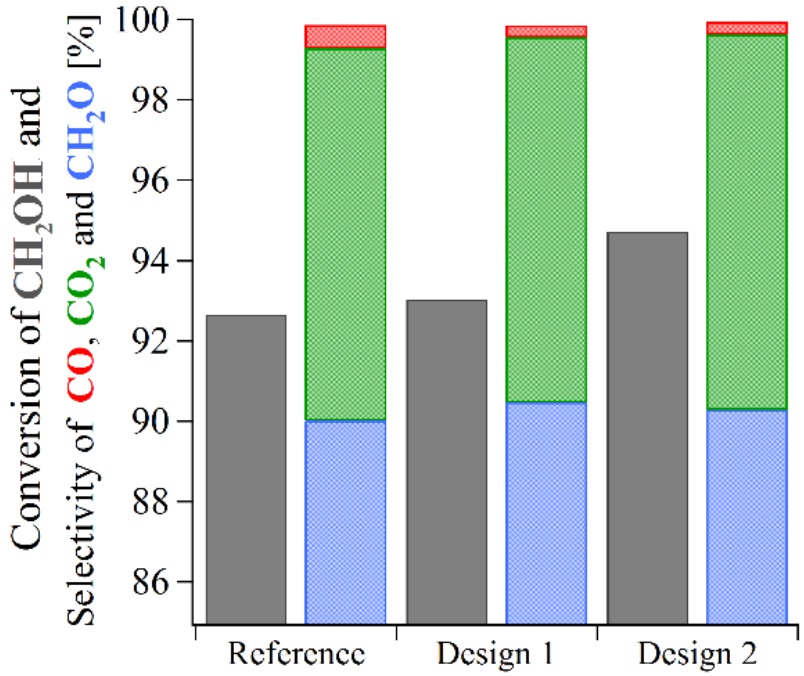
Formalin is a base chemical that is widely used in adhesives and resins applied in the wood industry. The production proceeds by catalytic oxidation of methanol to formaldehyde, in excess air over a mixed metal oxide catalyst or excess methanol over a silver-based catalyst. K.A Rasmussen is a manufacturer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

The main objective of IIA3 is improving selectivity of the silver-based formaldehyde process. The fast and exothermic nature of the reactions involved requires control of the heat and mass transfer phenomena as well as the surface chemistry proceeding on the silver surface. Gas phase chemistry may play an additional role at the typical reaction temperatures exceeding 600°C, at which also structural changes in the Ag catalyst occur that are known to affect both the reaction chemistry and the catalyst stability. The lifetime of the catalyst in industrial operation is in the order of months, depending on parameters such as particle morphology, size distribution, and structure of the catalyst bed in addition to the reaction conditions. Further developments are achievable by detailed understanding of the reaction conditions and tuning of the silver particle/bed morphology, thus controlling both selectivity and stability.

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



Main Findings and Conclusions



The methanol-to-formaldehyde test rig at SINTEF Oslo has been gradually upgraded. The reactor design was adapted to enable reaction conditions that are as close as possible to the industrially relevant conditions. This optimization was based on idealized reactor models for describing the local bed geometry, including mass and heat transfer combined with a simplified reaction mechanism. At the same time, the online analysis had to meet the previously established requirements for high stability. The set-up now allows to test catalysts samples at conditions comparable to industrial reactors. The measured temperature is only 5 °C below the expected adiabatic temperature.

The next objective was then to test and optimize various catalyst beds. Catalyst activation and accelerated aging protocols were developed for this purpose, which make tedious catalyst stabilization unnecessary. The focus of 2018 was to screen catalyst bed thickness with respect to formation of formaldehyde and selectivity to the byproducts CO_2 and CO. This has provided valuable information for the definition of the geometry of an ideal catalyst bed design as well as the effect of steam and inert gasses. While keeping the methanol/oxygen feed molar ratio constant, we managed to gradually increase the experimental formaldehyde yield. The optimized catalyst bed facilitates an increase of the methanol conversion, while the formaldehyde selectivity remains constant (see figure).

In following tests, the feedstock composition will be varied to establish a broad understanding of the effect of different process parameters.

IIA 4 PVC Value Chain: World class energy and raw material efficiency for the production of Chlorine and Vinylchloride Monomer (VCM)

The Team in 2018

De Chen	NTNU	IIA leader, PhD supervisor, WP responsible (WP4.1-4.2-4.3)
Terje Fuglerud	INOVYN	Industrial senior, industry researcher (WP4.1-4.2-4.3), PhD supervisor (WP4.1)
Endre Fenes	NTNU	PhD student NTNU (WP4.1)
Hongfei Ma	NTNU	PhD student NTNU (WP4.3)
Tho Ba Tran	NTNU	Master student (WP4.1)
Erling Olav Sollund	NTNU	Master student (WP4.1)
Kumar R. Rout	SINTEF	Researcher (WP4.2), advisor (WP4.1-4.3)

Publications

Baidoo, M. F., Fenes, E., Rout, K. R., Fuglerud, T., Chen, D. *On the effects of K and La co-promotion on $CuCl_2/\gamma$-Al_2O_3 catalysts for the oxychlorination of ethylene* Catalysis Today, 2018, 299, 164.

Oral contribution

Fenes, Endre; Ma, Hongfei; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De., *Calcined Al-Mg Hydrotalcite as Support in $CuCl_2$ Based Oxychlorination Catalysts* 18th Nordic Symposium on Catalysis; 26-28 August, Copenhagen, Denmark.

De Chen, *Kinetic Aspects in Designing Catalytic Redox Cycles*, 11th National Congress of Environmental Catalysis and Environmental Materials, 19-24 July, Shen Yang, China.

De Chen, Kumar R. Rout, Endre Fenes, Martina F. Baidoo, Terje Fuglerud, *Kinetic Analysis and Design of Catalytic Redox Cycles*, 10th International Conference on Environmental Catalysis, 22-26 September, Tianjin, China.

De Chen, Kumar R. Rout, Endre Fenes, Martina F. Baidoo, Terje Fuglerud, *Kinetic analysis of redox cycle reaction and catalyst development*. 4th International Conference on Advanced Complex Inorganic Nanomaterials (ACIN 2018) 16-19 July, Namur, Belgium.

De Chen, Endre Fenes, Kumar R. Rout, Martina F. Baidoo, Terje Fuglerud, *Kinetic Analysis and Design of Catalytic Redox Cycles*, 25th International Conference on Chemical Reaction Engineering (ISCRE 25), 20-23 May, Florence, Italy.

Poster contribution

Fenes, Endre; Baidoo, Martina Francisca; Ma, Hongfei; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De, *Descriptors for Alkali Metal Promotion in Redox Catalysis: Ethylene Oxychlorination,* 25th International Conference on Chemical Reaction Engineering ISCRE 25; 2018-05-20 - 2018-05-23, Florence, Italy.

Kumar R. Rout, Endre Fenes, Martina F. Baidoo, Terje Fuglerud, De Chen*, New Approach of Kinetic Modelling and Analysis of Catalytic Cycle: Evolution of Production and Catalyst Composition in Ethylene Oxychlorination* 25th International Conference on Chemical Reaction Engineering; 2018-05-20 - 2018-05-23, Florence, Italy.

Ma, Hongfei; Fenes, Endre; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De, *Mg and K effects on the $CuCl_2/\gamma$-Al_2O_3 catalyst in ethylene oxychlorination* 18th Nordic Symposium on Catalysis; 2018-08-26 - 2018-08-28, Copenhagen, Denmark.

Motivation

Direct chlorination and oxychlorination are both used in making of 1,2-dichloroethane, which is then converted into vinyl chloride. As can be seen from the following reactions, oxychlorination is of special importance since 1,2-dichloroethane is cracked, and HCl from this cracking process is recycled by oxychlorination in order to avoid HCl as a byproduct:

$$ClCH_2CH_2Cl \rightarrow CH_2{=}CHCl + HCl$$

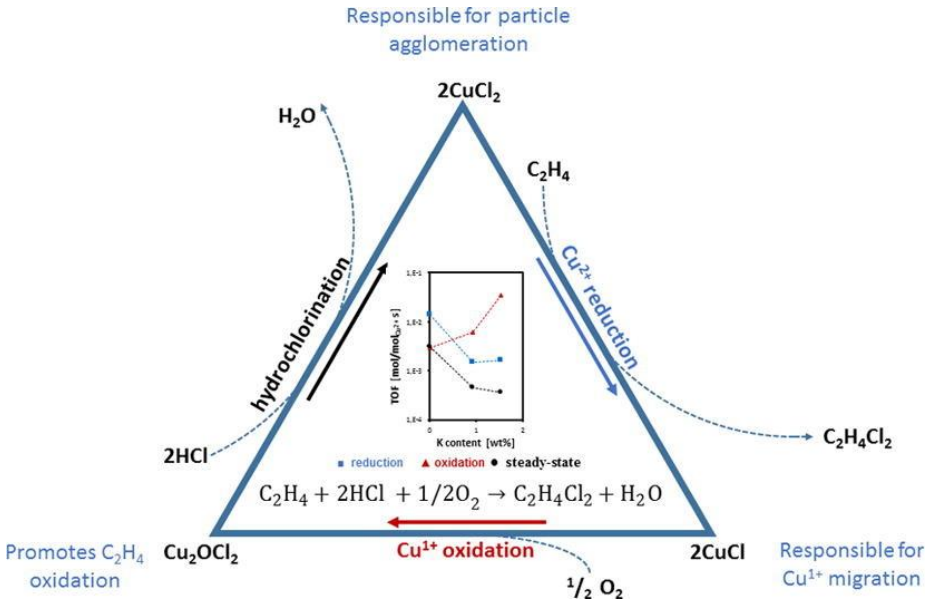
$$2\ HCl + CH_2{=}CH_2 + ½\ O_2 \rightarrow ClCH_2CH_2Cl + H_2O$$

A $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst is commonly used in the oxychlorination process. It is generally agreed that the oxychlorination involves a redox process in which copper cycles between Cu^{I}- and Cu^{II} states. A better fundamental understanding of the oxychlorination process is highly desired for improving the catalyst and further optimizing the process. IIA5 focusses on the study of elementary steps and full catalytic cycle by combined first principles calculation, advanced characterization, transient and steady-state operando kinetic investigation to better understand the reaction at an atomic level and thereby achieve rational catalyst design.

The oxidation state of the Cu catalyst at steady-state depends on the kinetic balance between the rates of reduction and oxidation in the catalytic cycle. A main challenge is that Cu^{I}, due to its low melting temperature and volatility, causes aggregation and loss of active surface. Compounds of alkali metals (K and Na) and/or rare earth metals (La and Ce) are often used as promoters to increase the activity, selectivity and stability of the Cu-based system. For the Cu based fixed bed catalysts, KCl is always present to improve the stability, while other alkali and alkali-metal chlorides may be used as co-promoters.

An operando fixed bed reactor set-up combined with UV/Vis- and mass spectroscopy has been established at NTNU to measure space- and time quantitative kinetics of the reaction while characterizing the active catalyst component involved. A strategy of combined transient- and steady-state kinetic investigations is used to obtain kinetic models for prediction of the reaction rate and the copper oxidation state under steady state conditions.

Another aim is to develop one- and two-dimensional non-isothermal models to predict the impact of reactor parameters on temperature profiles and product formation. The rate expressions can be used herein to predict the profile of Cu oxidation state. Equations and parameters for heat and mass transfer, as well as pressure drop, were evaluated and integrated to the reactor model.



Ethylene Oxychlorination to 1,2 dichloroethane (EDC), kinetic investigations, modeling and in-situ characterization - PhD project (WP4.1)

The work package has focused mainly on fundamental understanding of the redox cycles of ethylene oxychlorination on $CuCl_2/\gamma\text{-}Al_2O_3$ based catalysts. An operando kinetic study was performed in a fixed bed reactor coupled with a corrosion resistant gas chromatograph and a mass spectrometer for product analysis and UV-Vis-NIR spectrometry for determining the oxidation state of the catalyst. A method of kinetic analysis of the redox cycle to predict the steady-state reaction rate and Cu oxidation state by means of a rate diagram through integration of reduction and oxidation rates. The catalysts were characterized by the temperature programmed reduction (TPR), infrared-, Raman- and x-ray photoelectron spectroscopy.

By this methodology, the promoting effects of alkali, alkali earth and lanthanide elements on turnover frequency, catalytic activity, selectivity and stability of the $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst was investigated. The bond gap of the promoted $CuCl_2$ and Cu_2OCl_2 were identified as the descriptors for the reduction and oxidation reaction steps. The Cu^{II}/Cu^{I} ratios of the oxychlorination catalysts were also mapped by operando investigations using combined XAS techniques (XANES and EXAFS) and UV-VI-NIR spectroscopy at ESRF, confirming the cogency of the approach. The method was aslo applied to analyse industrial catalysts.

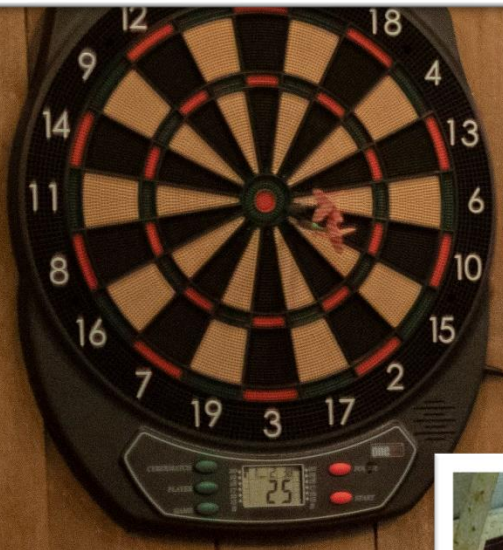
Reactor Modelling (WP4.2):

A master student worked with SINTEF on kinetic- and multi-scale reactor modelling based on laboratory kinetic data. The kinetic modelling was performed on different promoted catalysts. The kinetic model was established on the K promoted catalyst. We have developed a 1D heterogeneous reactor model to predict temperature, concentration and Cu oxidation state profiles. Through comparison to the experimental results available from the industrial reactors, further tuning of the model is enabled. The model predicts well the temperature profiles and conversion of an industrial reactor.

Ethylene Oxychlorination to 1,2 dichloroethane (EDC), deactivation and by-product formation- PhD project (WP4.3)

The WP targets on understanding of deactivation mechanisms and kinetics of by product formation of Cu based catalysts. A new setup has been designed and a method was established to study the copper mobility and fixation on the support by in-situ measurement using UV-Vis spectrometers. Furthermore, the effects of promoters such as K, Li, Ce, Mg and La on the Cu migration and carbon and byproduct formation have been investigated.

iCSI moments

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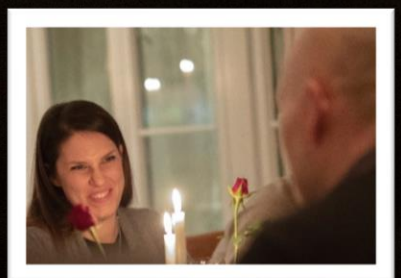


IIA 5 The next step in direct activation of lower alkanes

The Team in 2018

Stian Svelle	UiO	IIA Leader, PhD supervisor, WP responsible (WP5.1-5.2-5.3)
Pablo Beato	Haldor Topsøe A/S	Industrial senior, Industry researcher (WP5.1-5.2-5.3), PhD supervisor (WP4.1)
Unni Olsbye	UiO	PhD supervisor (WP5.1-5.2)
Dimitrios Pappas	UiO	PhD student (WP5.1-5.2)
Michael Dyballa	UiO	Postdoctoral fellow (WP5.1-5.2-5.3)
Karoline Kvande	UiO	Master student (WP5.1-5.2)
Lars Fahl Lundegaard	Haldor Topsøe A/S	Industry researcher (WP5.1)
Bjørnar Arstad	SINTEF	Researcher (WP5.3)

Publications

Michael Dyballa,* Dimitrios K. Pappas, Karoline Kvande, Elisa Borfecchia, Bjørnar Arstad, Pablo Beato,* Unni Olsbye, and Stian Svelle* *On How Copper Mordenite Properties Govern the Framework Stability and Activity in the Methane-to-Methanol Conversion* ACS Catalysis 2019, 9, 365−37.

Dimitrios K. Pappas, Andrea Martini, Michael Dyballa, Karoline Kvande, Shewangizaw Teketel, Kirill A. Lomachenko, Rafal Baran, Pieter Glatzel, Bjørnar Arstad, Gloria Berlier, Carlo Lamberti, Silvia Bordiga, Unni Olsbye, Stian Svelle,* Pablo Beato,* and Elisa Borfecchia* *The Nuclearity of the Active Site for Methane to Methanol Conversion in Cu-Mordenite: A Quantitative Assessment* Journal of American Chemical Society 2018, 140, 15270−15278

Elisa Borfecchia, Dimitrios K. Pappas, Michael Dyballa, Kirill A. Lomachenko, Chiara Negri, Matteo Signorile, Gloria Berlier* *Evolution of active sites during selective oxidation of methane to methanol over Cu-CHA and Cu-MOR zeolites as monitored by operando XAS* Catalysis Today (*10.1016/j.cattod.2018.07.028*)

Kirill A. Lomachenko, Andrea Martini, Dimitrios Pappas, Chiara Negri, Michael Dyballa, G Berlier, Silvia Bordiga, Carlo Lamberti, Unni Olsbye, Stian Svelle, Pablo Beato, Elisa Borfecchia*, *The impact of reaction conditions and material composition on the stepwise methane to methanol conversion over Cu-MOR: an operando XAS study* Catalysis Today (*10.1016/j.cattod.2019.01.040*)

Dimitrios K. Pappas,* Elisa Borfecchia, Michael Dyballa, Kirill A. Lomachenko, Andrea Martini, Gloria Berlier, Bjørnar Arstad, Carlo Lamberti, Silvia Bordiga,* Unni Olsbye, Stian Svelle, and Pablo Beato*, *Understanding and Optimizing the Performance of Cu-FER for The Direct CH_4 to CH_3OH Conversion*, ChemCatChem, 11, 2019, 621-627.

C. Buono , A. Martini, I. A. Pankin, D. K. Pappas, C. Negri, K. Kvande, K. A. Lomachenko, E. Borfecchia* *Local structure of Cu(I) ions in the MOR zeolite: a DFT-assisted XAS study Radiation Physics and Chemistry* (*10.1016/j.radphyschem.2018.12.031*)

Poster contributions

D. K. Pappas, E. Borfecchia, M. Dyballa, G. Berlier, S. Bordiga, U. Olsbye, P. Beato, S. Svelle, *Following O_2-activation of Cu-Zeolites with Time-Resolved XAS Time Work Function Workshop*, Oslo, Norway, 13-15/06/2018.

Karoline Kvande *Selective Oxidation of Methane to Methanol Over Cu-loaded SAPO-34 Catalysts*, Det 21. Landsmøte i Kjemi, Lillestrøm, Norway, 16-18/10/2018.

Oral presentations

Dimitrios K. Pappas *Reducibility of Cu-zeolites: A Descriptor for the Activity in the Methane to Methanol Conversion. NIS Colloquium Cu-based zeolites Versatile materials for redox catalysis*. Torino, Italy, 20/07/2018.

Dimitrios K. Pappas, Elisa Borfecchia, Gloria Berlier, Pablo Beato, Stian Svelle. *Methane to Methanol over Cu-Zeolites: Establishing Structure-Activity Relationships* 18th Nordic Symposium on Catalysis, Copenhagen, Denmark, 26-28/08/2018.

E. Borfecchia*, D. K. Pappas, M. Dyballa, A. Martini, K. A. Lomachenko, G. Berlier, P. Beato, C. Lamberti, S. Bordiga, U. Olsbye, S. Svelle, *Methane to methanol conversion over Cu-zeolites – the XAS view* Det 21. Landsmøte i Kjemi, Lillestrøm, Norway, 16-18/10/2018.

E. Borfecchia*, A. Martini, K. A. Lomachenko, D. K. Pappas, G. Berlier, S. Svelle, P. Beato, C. Lamberti, S. Bordiga *Composition-driven reducibility in Cu-CHA: potential of XAS MCR analysis and implications for methane to methanol conversion 6th International Congress on Operando Spectroscopy*, Estepona, Spain, 16-19/04/2018.

E. Borfecchia, A. Martini, I. A. Pankin, K. A. Lomachenko, G. Berlier, P. Beato, D. K. Pappas, M. Dyballa, S. Svelle, C. Lamberti, S. Bordiga, *XAS reveals structure-activity relationships for the methane to methanol conversion over Cu-SSZ-13 zeolites* 17th International Conference on X-Ray Absorption Fine Structure, Kraków, Poland, 22-27/07/2018.

E. Borfecchia, A. Martini, K. A. Lomachenko, P. Beato, S. Svelle, U. Olsbye, D. K. Pappas, M. Dyballa, G. Berlier, C. Lamberti, S. Bordiga, *Structural Dynamics of Cu Ions in Zeolite Catalysts from Multivariate Analysis of Time-Resolved XAS,* Time Work Function Workshop, Oslo, Norway, 13-115/06/2018.

Motivation

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

Researchers at UiO, SINTEF, and Haldor Topsøe A/S join forces for the fundamental understanding of the direct conversion of lower alkanes to chemicals or liquid fuels over copper loaded zeolite materials. This effort is directed towards enhanced fundamental understanding of the materials and their active sites as well as the mechanism of the reactions with the ultimate goal of commercial realization.

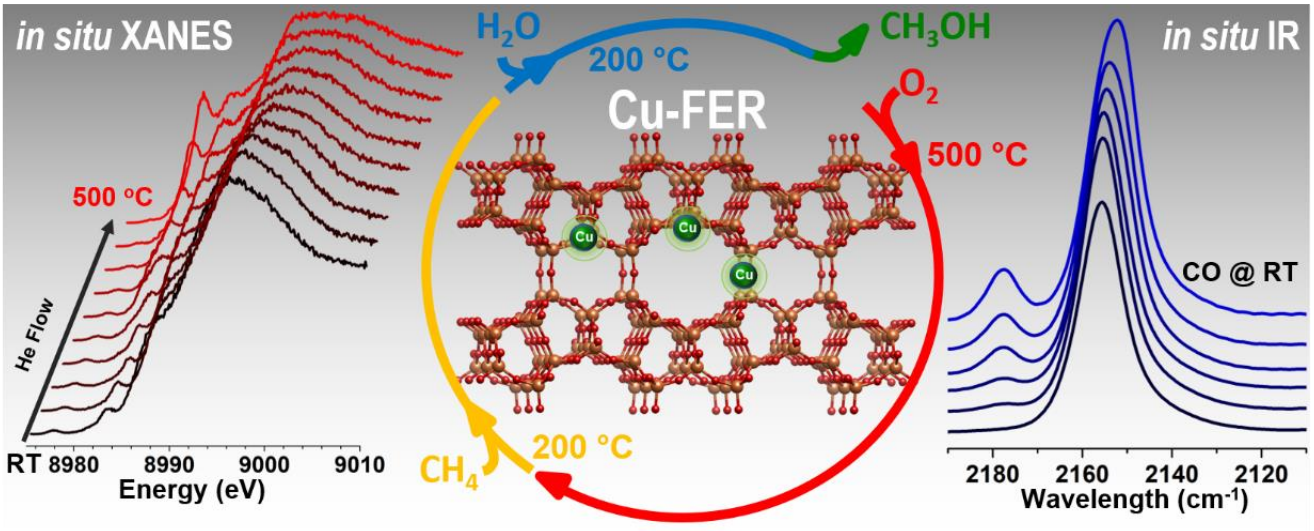


***Figure**: Experimental methodology for investigating Cu-FER zeolites for the methane to methanol conversion.*

Synthesis of new zeolite materials – Postdoctoral fellowship

As a follow-up of previous work, we have in 2018 gained valuable insights on the catalyst library that has been developed and evaluated for the reaction. This derives from studying the materials with MAS NMR (Magic Angle Spinning Nuclear Magnetic Resonance) spectroscopy in the laboratories of SINTEF. The work mostly concentrated on the differences observed in performance and in MAS NMR as well as the effect of multiple reaction cycles on the framework and Cu speciation. A particular achievement has been the development of a protocol that allows ex-situ activation and pretreatment of samples prior to NMR investigations.

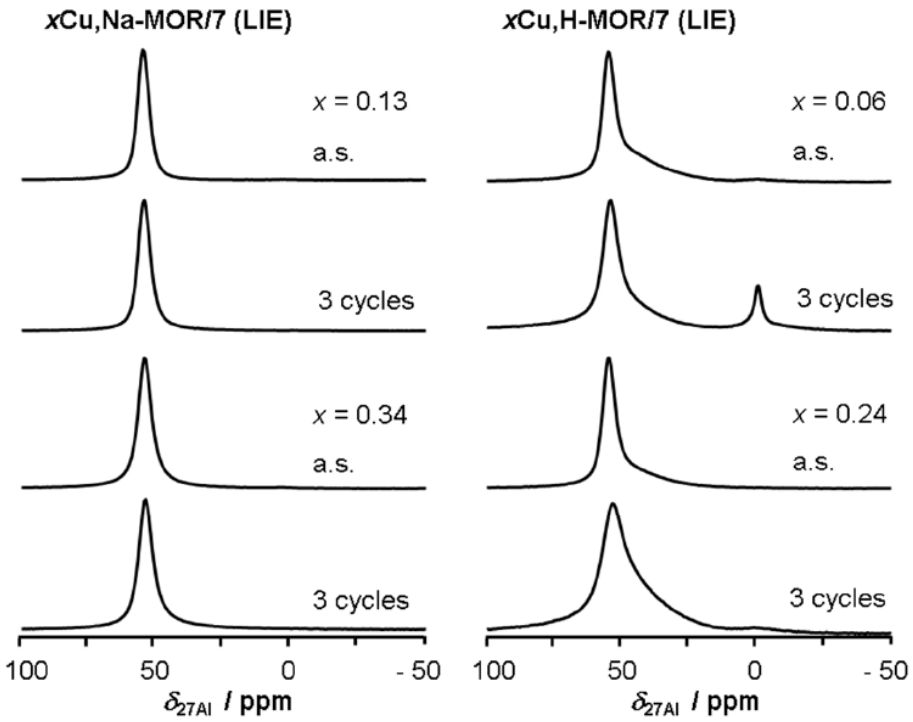


Figure: ^{27}Al MAS NMR spectroscopy performed at SINTEF, Oslo, NO. Copper containing MOR materials were investigated before and after up to three reaction cycles.

Dr. Michael Dyballa completed his postdoctoral fellowship with iCSI in 2018 and will continue his scientific career at the Institute of Chemical Technology, University of Stuttgart, Germany. During his time in the Centre, Dr. Dyballa contributed significantly to the IIA5 and coauthored several publications in *JACS, ChemCatChem, Microporous and Mesoporous Materials and Catalysis Today.* We thank him and wish him success in his future research!

Catalyst performance – PhD project

We have performed a careful evaluation of the catalytic performance of the materials included in the library, comprising different zeolite topologies with different compositional characteristics, employing a wide range of different reaction conditions. We braided the performance of the materials with results from infrared (IR) as well as X-Ray Absorption Spectroscopy (XAS) coupled with Multivariate Curve Resolution (MCR) in order to establish structure-activity correlations. Our results on the nuclearity of Cu-MOR as well as its comparison to the Cu-SSZ-13 have both been published in 2018. Our data demonstrate that for Cu-MOR, the active sites are dimeric. In addition, a detailed reaction condition optimization as well as comprehensive understanding of Cu loading in Cu-FER materials were published. A major lesson from 2018 has been that carrying out laboratory activity measurements at the same conditions as those employed during advanced characterization at the synchrotron is prerequisite for developing accurate structure-performance relationships. In 2019, we plan to compare Cu-SSZ-13 with Cu-SAPO-34, both materials of the same Chabazite topology. In addition, we are developing tools for understanding the reaction pathway utilizing Raman and IR spectroscopies.

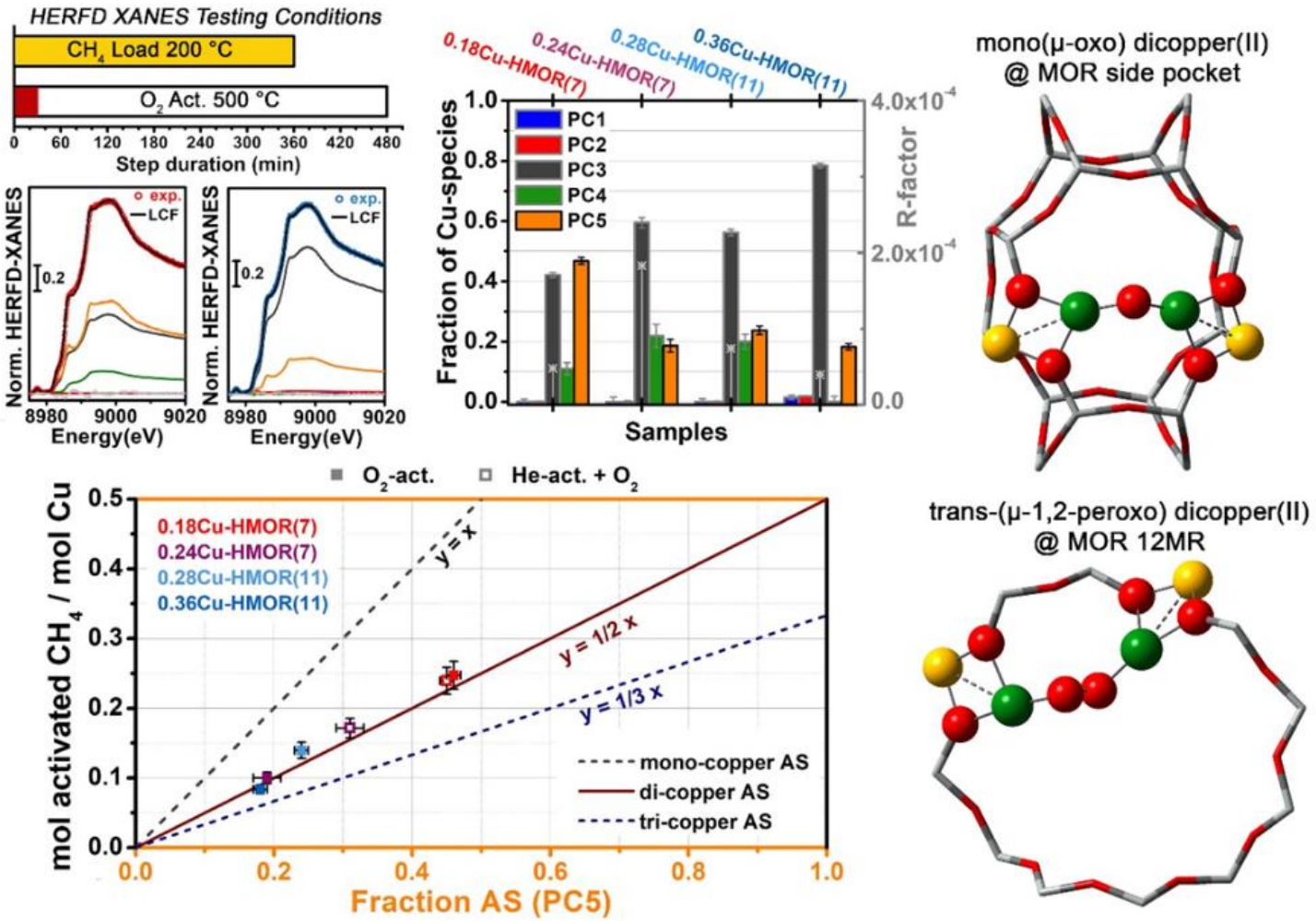


Figure: *Experimental methodology used to derive results on the nuclearity of active site in Cu-MOR zeolites.*

IIA 6 Generic projects for additional industrial synergies.

The Team in 2018

Magnus Rønning	NTNU	IIA leader, PhD supervisor and WP responsible (WP6.1)
Anja Olafsen Sjåstad	UiO	WP responsible (WP6.2)
De Chen	NTNU	WP responsible (WP6.3)
Spyros Diplas	SINTEF	WP responsible, researcher (WP6.4)
Torbjørn Gjervan	SINTEF	WP responsible, researcher (WP6.4)
Samuel K. Regli	NTNU	PhD candidate (WP6.1)
My Nhung Thi Tran	NTNU	Master student (WP6.1)
Jane Eiane Aarsland	NTNU	Master student (WP6.1)
Hilde J. Venvik	NTNU	PhD supervisor (WP6.1)
Oleksii Ivashenko	UiO	Postdoctoral fellow (WP 6.2)
David Waller	YARA	Industrial senior, industry researcher (WP6.2)
Helmer Fjellvåg	UiO	Researcher (WP6.2)
Yanying Qi	NTNU	Postdoctoral fellow (WP6.3)
Terje Fuglerud	INOVYN	Industry researcher (WP6.3)
Kumar R. Rout	SINTEF	Researcher (WP6.3)
Rune Lødeng	SINTEF	Researcher (WP6.4)
John Walmsleyq	SINTEF	Researcher (WP6.1-6.4)
Patricia Almeida Carvalho	SINTEF	Researcher (WP6.4)
Martin F. Sunding	SINTEF	Researcher (WP6.4)
Ragnhild Brokstad Lund-Johansen	NTNU	Master student (WP6.4)
Helene Marie Eng Granlund	NTNU	Master student (WP6.4)

Publications

Mom, R. V.; Ivashenko, O.; Frenken, J. W. M.; Groot, I. M. N.; Sjåstad, A. O., *Nucleation, Alloying, and Stability of Co–Re Bimetallic Nanoparticles on Al_2O_3/NiAl(110). J. Phys. Chem., C* 2018, 122, 8967-8975.

Zheng, J.; Ivashenko, O.; Fjellvåg, H.; Groot, I. M. N.; Sjåstad, A. O., *Roadmap for Modeling RhPt/Pt(111) Catalytic Surfaces J. Phys. Chem., C* 2018, 122, 26430-26437.

Poster contributions:

Regli SK, Salman AuR, Rønning M. *In situ study of NO oxidation over Pt-based catalysts for nitric acid production, 6th International Congress on Operando Spectroscopy* in Estepona, Málaga, Spain, April 2018.

Regli SK, Rønning M. *Operando XRD and XAS study of nitric oxide oxidation over supported Pt catalysts, XAFS2018*. Kraków, Poland, July 2018.

Summer school participation

Regli SK, EXAFS 2018, SSRL Summer School on Synchrotron X-Ray Absorption Spectroscopy at Stanford University (SLAC), USA, August 2018.

Motivation

The IIA6 iCSI work packages are allocated to research with the intention of moving the research forefront and providing methodological tools that can be applied in the industrial innovation areas IIA1-5. In particular, advanced spectroscopic and microscopic investigations under conditions highly relevant to industrial operation is 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.

Advanced *operando* characterization of heterogeneous catalysts for sustainable process industries – PhD project (WP6.1)

In this work package, we are investigating heterogeneous catalysts during operation at industrially relevant conditions and develop data analysis tools as needed. In order to link structural properties of the material with catalytic activity during reaction, we apply spectroscopy (Infrared, X-ray, UV-Vis) in-house and at synchrotrons. We have synergies with four out of the six work packages within iCSI and collaborations also outside of iCSI within KinCat (Fischer-Tropsch synthesis and selective catalytic reduction) and also with SUNCAT at Stanford University (hydrogenation of CO and CO_2 to methanol).

With our setup shown in the figure below, we can combine several techniques for simultaneous characterization of the bulk and the surface of the catalyst during reaction at industrially relevant temperatures (473-723 K) and pressures (up to 20 bar). New insight on the active sites of the catalysts and the respective kinetics of the chemical reactions can guide towards favorable compositions and conditions, thereby enabling processes with higher efficiency, lower cost and reduced emissions or by-products.

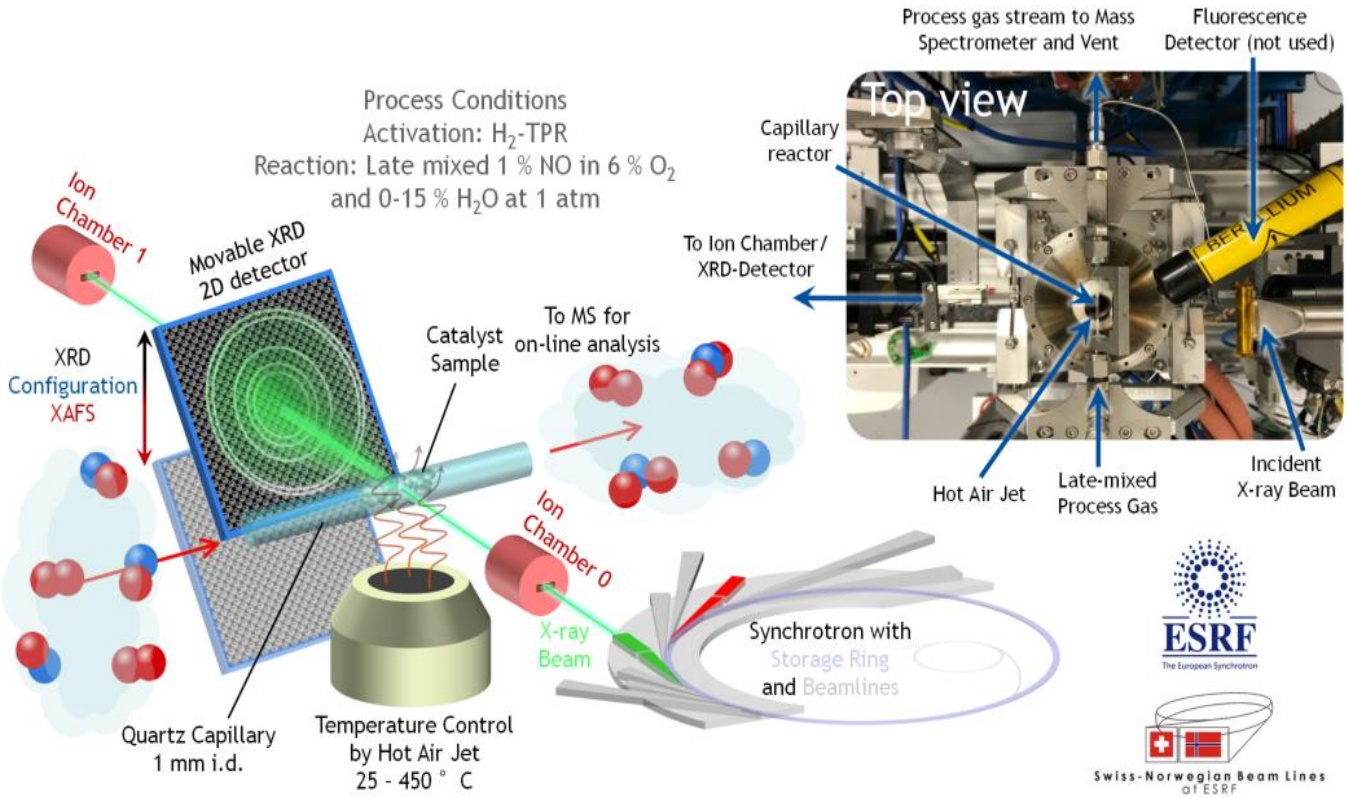


Figure: *Experimental Setup for combined operando powder X-ray diffraction and X-ray absorption spectroscopy with simultaneous product gas analysis by mass spectrometer at the Swiss Norwegian Beamlines BM31 at the European Synchrotron Radiation Facility, Grenoble, France*

Advanced synthesis and characterization – novel thin film preparation and reactor STM – Postdoctoral fellowship (WP6.2)

In this work package we are developing nanostructured surfaces, that mimic catalysts relevant for industrial processes. The obtained model catalysts are utilized in surface sensitive operando studies by means of Reactor Scanning Tunnelling Microscopy (STM) and Near Ambient-Pressure X-ray Photoelectron Spectroscopy (NAP XPS). The two reactions being investigated are the Fischer-Tropsch synthesis and intermediate temperature ammonia oxidation. The recipes for preparation of well-defined bimetallic Co-Re nanoparticles supported on Al_2O_3/NiAl(110) for Fischer-Tropsch synthesis were recently published in Journal of Physical Chemistry C.

Thereafter, efforts have been directed towards the preparation of PtRh surfaces for exploring the role of Rh in intermediate temperature ammonia oxidation over PtRh alloys. The following milestones were achieved:

- Development of a roadmap for preparation of bimetallic alloyed Pt-Rh surfaces on Pt(111) using Reactor STM and UHV XPS (University of Leiden), see Figure below.

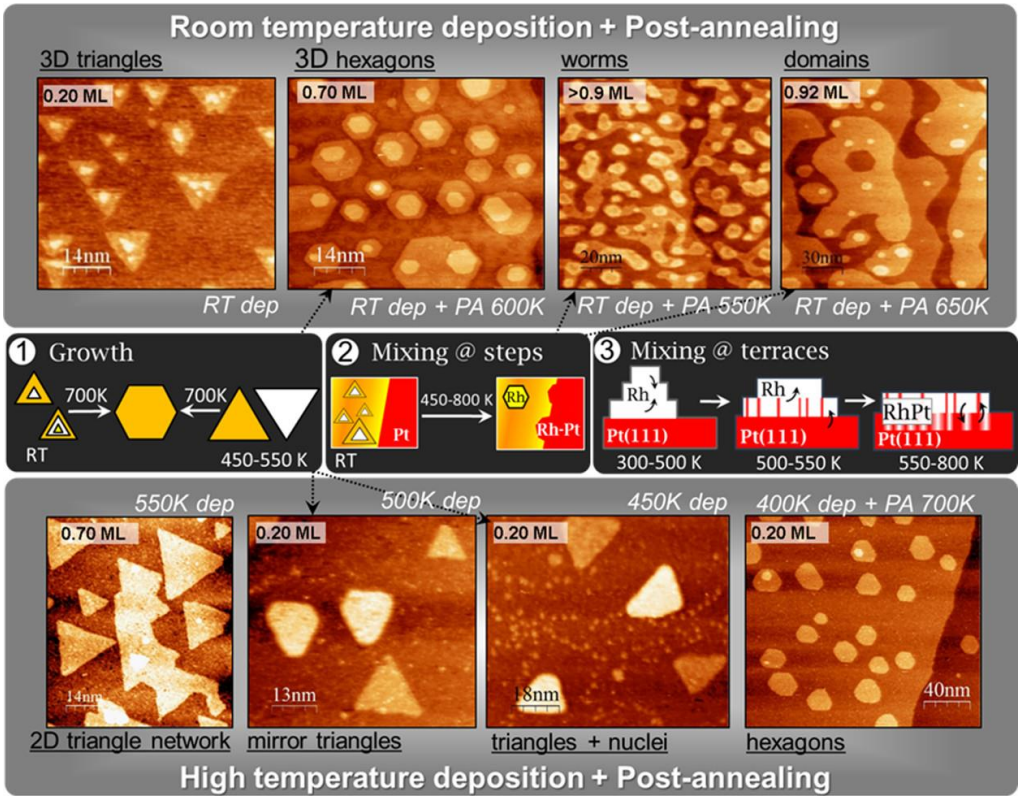


Figure: Roadmap for achieving distinct alloyed RhPt morphologies on Pt(111) using post-annealing (top panel) and deposition at higher temperatures (bottom panel). Structures like three-dimensional triangles and hexagons, worms, domains, two-dimensional networks, opposing triangles, small nuclei, and two-dimensional hexagons can be prepared at the indicated conditions (white font). The starting Rh coverage as estimated by STM is indicated for each surface.(adapted from J. Phys. Chem. C 2018, 122, 26430−26437)

- The PtRh/Pt(111) model surfaces were studied using NAP XPS at the Advanced Light Source at Berkley, USA, and at the MAXIV synchrotron in Lund, Sweden, in collaboration with partners at Lund University and MAXIV. Preliminary analysis of obtained results shows different amount of adsorbed species on Pt(111), Rh/Pt(111) and PtRh/Pt(111) .
- Finally, to represent the industrial PtRh catalyst more accurately, bimetallic PtRh nanoparticles were prepared on Al_2O_3/NiAl(110) and studied during dosing of O_2/NH_3/Ar gas mixtures using operando NAP-XPS at the beamline TEMPO at SOLEIL (Italy).

Fundamental study of ethylene oxychlorination and methanol oxidation– Postdoctoral fellowship (WP6.3)

In the study of ethylene oxychlorination, we built a new model to represent $CuCl_2$ particles supported on γ-Al_2O_3. The model includes the contribution of the support, which is closer to the industrial catalyst compared with the previous model (i.e., bulk $CuCl_2$ surface). The adsorption behavior of ethylene at different Cu loadings were investigated. Distinct adsorption modes at high and low loadings were obversed and the undelying reason was revealed through analysis of the electronic properties, such as Bader charge analysis.

We also built a model with $CuCl_2$ and KCl molecules on a γ-Al_2O_3 surface to study the promoter effect of potassium (Figure 1, below). KCl binds with $CuCl_2$, indicating that a $K_xCu_yCl_z$ salt is formed. The effect of KCl on ethylene adsorption depends on the Cl/Cu ratio. It weakens the ethylene heat of adsorption and thus increases the Cu reduction barrier at high Cl/Cu ratio, while it has negligible effect on the ethylene adsorption energy at relatively low Cl/Cu ratios. Moreover, KCl increases the adsorption strength of oxygen and decreases the barrier of oxygen dissociation compared to the neat Cu^+ catalyst.

Finally, from microkinetic modeling of methanol oxidation to formaldehyde, we found that both O-assisted and OH-assisted reaction pathways could decrease the reaction barrier and thus improve the activity compared to the direct methanol decomposition (Figure 2, below). O-assisted methanol dissociation is suggested to be the most favorable reaction pathway. Moreover, analysis of the free energy profiles suggest that oxygen dissociation is the rate determining step in this mechanism. We will search alternative reaction mechanisms that may reduce the barrier of this step.

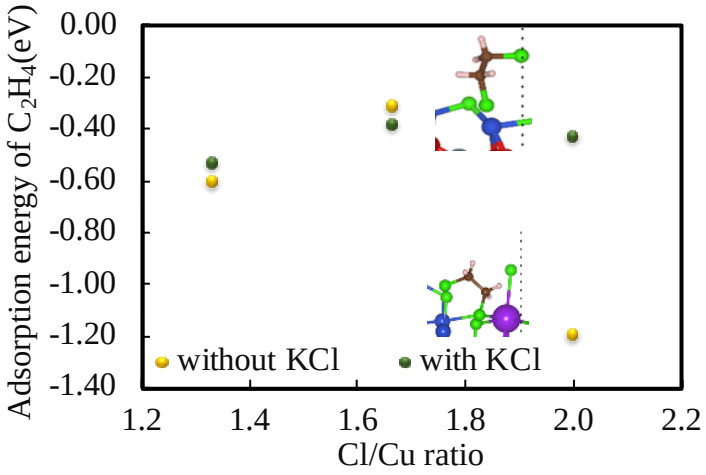
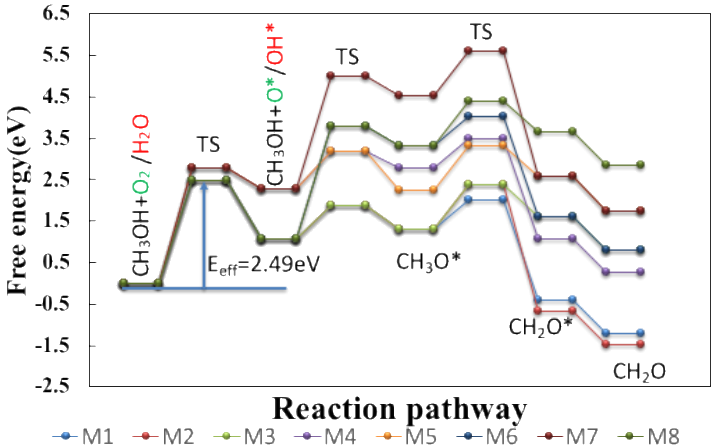


Figure on the left: *Adsorption energy of ethylene on the surface with various Cl/Cu ratios. The inserted picture in (a) is the adsorption configuration of ethylene on neat $CuCl_2$ surface(top) and $CuCl_2$+KCl surface (bottom). Green balls are Cl, blue balls are Cu, the purple ball is K, brown balls are C and pink balls are H atoms.*

Figure on the right*: Analysis of free energy profiles for different reaction mechanisms in methanol oxidation reaction*



SINTEF Fundamental Catalyst Investigations (WP6.4)

The main objective of this project is to develop and demonstrate competence, methods, and procedures for operation and analysis using the electron spectroscopy facilities available at SINTEF and NTNU. The project makes use of Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS). These techniques are complementary and provide detailed surface sensitive information. One major advantage of AES is its high lateral resolution, down to about 10 nm.

During 2018 we have implemented analysis of layer thicknesses for non-destructive estimation of overlayer thickness. An example is shown in the Figure below, with a comparison of sputter depth profiling and estimated remaining oxide thickness during the sputtering. The method allows for determination of spatially resolved overlayer thicknesses in the nm region from AES measurements without sputtering. The use of a focused electron beam makes it applicable for investigations of core-shell particles as well as regular thin film surfaces. We are currently working on a stronger integration of AES and XPS for improved spatial resolution of chemical inhomogeneities.

For 2019 we are planning investigations that include analysis of reduced catalysts and material subjected to reaction conditions. The XPS system has a reaction cell attached making it possible to analyze catalyst sample exposed to realistic conditions without being altered by subjection to ambient conditions. Materials to be studied include Pd based alloys, supported Co particles and Ag catalyst.

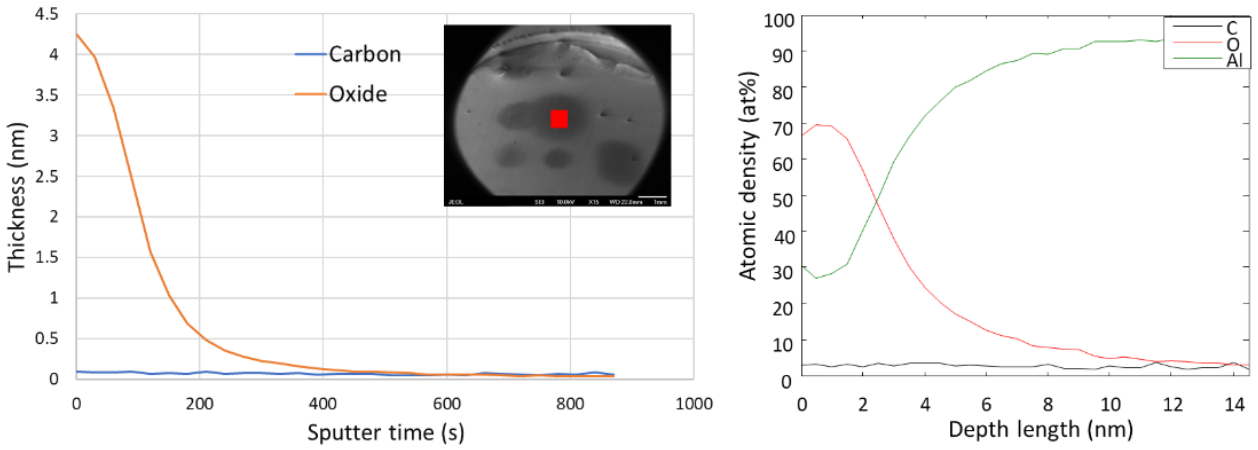


Figure: *Overlayer thickness vs. sputter time (left). The insert shows an SEM images of the analysed area. AES sputter depth profile (right).*

Internationalization 2018

Sabbatical leave

Professor De Chen (NTNU), Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai, China until July 2018.

Overview of international collaborations (institutes and companies)

- Ghent University, Belgium
- School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, China
- East China University of Science and Technology, China
- Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China
- Technical University of Denmark, Denmark
- University of Helsinki, Finland
- Swiss-Norwegian Beamlines at ESRF, France
- Karlsruhe Institute of Technology – KIT, Germany
- University of Torino, Italy
- Utrecht University, the Netherlands
- Instituto Nacional del Carbón, INCAR-CSIC, IMDEA Energy Institute, Spain.
- Lund University, Sweden
- Chalmers University of Technology, Sweden
- Linné University, Sweden
- University of Manchester, UK
- Washington University in St-Louis, USA
- Boreskov Institute of Catalysis, Russian Academy of Sciences
- University of Stuttgart, Germany
- CNRS, France,
- ECN, the Netherlands
- University of St Andrews, Scotland
- University of Porto, Portugal
- Leiden University, the Netherlands
- University of Cape Town, South Africa
- Saint Gobain, France
- ENI S.p.a., Italy
- Johnson Matthey, UK
- Repsol SA, Spain
- Process Design Centre BV, Netherlands
- B.T.G. BV, Netherlands
- Arkema France SA; France
- Biosynthis, France
- Fraunhofer, Germany
- ICN2, Spain,
- Axcel One, France
- Engie Lab, France
- SICAT Sarl, France
- ACM GmbH, Germany
- Linde, Germany
- Borealis
- Endurance Technologies, Canada
- SABIC
- UOP LLC
- DOW chemicals
- LOGE AB, Denmark
- Novozymes, Denmark
- NeoZeo, Sweden
- BTG-BTL, Belgium
- Steeper, Denmark
- Unilever, India

European research projects:

FASTCARD - ***FAST industrialisation by CAtalysts Research and Development***,
FP7-NMP-2017-LARGE-7, iCSI Partners involved: SINTEF/NTNU. Duration: 2014-2018

PrintCr3dit - Process Intensification through Adaptable Catalytic Reactors made by 3D Printing.
H2020-EU.2.1.5.3. iCSI Partners involved: SINTEF, Yara. Duration: 2015-2018

ProDIA - Demonstrating the industrial relevance of hybrid nanoporous materials.
H2020-EU.2.1.2.4, H2020-EU.2.1.2.5. iCSI Partners involved: SINTEF, Yara. Duration: 2015-2018

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

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

Bizeolcat **-** Bifunctional zeolite-based catalysts for sustainable hydrocarbon transformation
Horizon 2020 CE-NMBP-24-2018 - iCSI Partners involved: SINTEF, UiO. Duration: 2019-2022.

BIKE **- BImetallic Catalysts Knowledge-based development for Energy applications**
Horizon 2020 MSCA-ITN: iCSI Partners involved: NTNU. Duration: 2019-2023.

C123 - Methane oxidative conversion and hydroformylation to propylene. (Coordinator)***.***
Horizon 2020 CE-NMBP-24-2018. iCSI Partners involved: SINTEF. Status: granted.

COZMOS **- CO2 hydrogenation to light hydrocarbons (UiO coordinator)**
H2020-LC-SC3-RIA & H2020-LC-SC3-2018- NZE-CC: UiO, SINTEF, Topsøe: Status: granted.

Research Council of Norway (RCN) projects with international collaborations:

FutureFeed - Carbon Dioxide as a Future Feedstock for Chemicals, Polymers.
NANO 2021 Researcher project (228157). iCSI Partners involved: SINTEF, UiO. Duration: 2013 - 18

Development of Catalysts and Materials for Compact Steam Reformer. GASSMAKS Researcher project (233869). iCSI Partners involved: NTNU, SINTEF. Duration: 2014 – 18.

EmX 2025 - an R&D base for reduced exhaust emissions in the Norwegian marine transportation sector.
TRANSPORT 2025 Researcher project (246862). iCSI Partners involved: NTNU/ SINTEF. Duration 2015-19. International partner: Chalmers University of Technology, Sweden.

GAFT Gasification and FT-Synthesis of Lignocellulosic Feedstocks, ENERGIX Knowledge-Building Project for Industry (280903). iCSI Partner involved: SINTEF. Duration: 2015-19.

H_2MemX - Enabling ultrathin Pd based membranes through surface chemistry diagnostics and control.
ENERGIX Researcher project (280903). iCSI Partners involved: NTNU, SINTEF. Duration 2018 – 21. International partner: Lund University/MAX IV, Sweden.

Bio4Fuels - Norwegian Centre for Sustainable Bio-based Fuels and Energy. Centre for Environment-friendly Energy Research (FME, 257622), iCSI Partners involved: SINTEF/ NTNU. Duration: 2016 - 24

TomoCAT - Tracking the deactivation of shaped zeolite catalysts in time and space using X-ray diffraction tomography. NANO 2021 Researcher project (granted), iCSI Partners involved: *UiO, Topsøe.* Duration: 2019-2023.

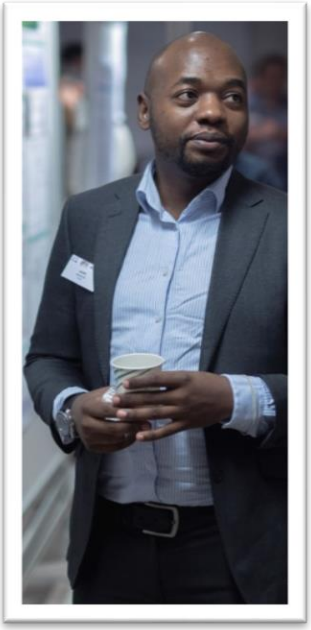
Education

Postdoctoral fellows in 2018

Name	Institution /Group	Country	IIA	Contract duration
Yanying Qi	NTNU	China	IIA6	2016-18
Oleksii Ivashenko	UiO/Nafuma	Ukraine	IIA6	2016-18

PhD candidates in 2018

Name	Institution/Group	Country	IIA	Contract duration
Endre Fenes	NTNU	Norway	IIA4	2015-18
Ata ul Rauf Salman	NTNU	Pakistan	IIA1	2015-18
Dimitrios Pappas	UiO/Catalysis	Greece	IIA5	2016-19
Samuel K. Regli	NTNU	Switzerland	IIA6	2016-19
Stine Lervold	NTNU	Norway	IIA3	2016-20
Asbjørn Slagtern Fjellvåg	UiO/Nafuma	Norway	IIA1	2016-20
Hongfei Ma	NTNU	China	IIA4	2017-20
Moses Mawanga	NTNU	Uganda	IIA6	2018-21



iCSI welcomes PhD candidate Moses Mawanga. Moses comes from Uganda in East Africa and holds a BSc in Industrial Chemistry from Makerere University (Uganda) and a MSc in Chemical Engineering from NTNU. His thesis for the fulfilment of the International Master Program was completed in 2017 and dealt with “Dolomite-based Sorbents for High Temperature Carbon dioxide capture” under the supervision of Prof. De Chen. He was recruited for IIA6 WP6.3 in September 2018. His iCSI research targets development of experimental tools for providing insights into the kinetics and reaction mechanisms of selected industrial catalyzed reactions. The main techniques are measurements of heats of adsorption by microcalorimetry and transient kinetic studies providing intrinsic kinetic data (SSITKA).

2018 Master theses **in Chemical Engineering (NTNU), Nanotechnology (NTNU) or Chemistry (UiO) affiliated or associated with iCSI**

Galina T. Yavasheva	Synthesis and characterization of bimetallic nanoparticles for selective catalytic conversion of ammonia (UiO-Nafuma)
Karoline Kvande	Selective oxidation of methane to methanol over Cu loaded SAPO-34 catalysts (UiO-Katalyse)
Kamilla Arnesen	Oxidation of methanol to formaldehyde over Ag catalyst - A study of reaction pathways and Ag catalyst restructuring during MTF
Erling Olav Sollund	Kinetic study and reactor modeling of ethylene oxychlorination
Henrik Jenssen	Efficient catalysts for achieving NO/NO_2 equilibrium
Beate M. Østrådt	Efficient catalysts for achieving NO/NO_2 equilibrium
Signe Marit Hyrve	Tuning of perovskite composition for NO oxidation
My Nhung Thi Tran	In situ characterization of industrial catalysts with Raman spectroscopy
Jane Eiane Aarsland	Operando FTIR study of the NH_3-SCR reaction over Cu/Al_2O_3 and Fe/Al_2O_3 catalysts
Amalie Tysseland	Carbon Formation and Catalysis in the Conversion of Methyl Chloride and Silicon into Dimethyldichlorosilane
Ane Sofie Lilleng	Synthesis of high-temperature solid sorbents for CO_2 capture
Dani Espevik	Rhodium doped strontium titanate for photocatalytic hydrogen evolution with carbon quantum dots
Eline Nesdal Sundli	Catalytic conversion of biomass derived oxygenates to fuel and chemicals
Gaute O. Hådem	Investigations of Pd_3Au (100) as a catalytic model system
Helene M. E. Granlund	Catalytic methane abatement for natural gas engines
Jonas Save	The Effect of Potassium on Cobalt-based Fischer-Tropsch Catalysts of Small and Medium Cobalt Particle Sizes
Kin Hui	CeO_2-ZrO_2-WO_3-based catalysts for Selective Catalytic Reduction of Nitrogen Oxides by Ammonia
Maria Olsvik	Synthesis of solid sorbents and kinetic study for CO_2 capture
Marit Harneshaug	Biopolymers assister preparation of Fe-based Fischer-Tropsch catalysts
Najma Ali Abdullahi	Effect of lanthanum on cobalt nickel catalysts for catalytic combustion of CH_4
Siri Stavnes	Sorbents for Sulfur Removal from Biomass-derived Syngas
John Helms	Initial Stages of Metal Dusting Corrosion - Surface and subsurface investigation using SEM, Raman spectroscopy, and STEM

Master students at NTNU 2017-2018 *(from left to right) (first raw standing: Kin Hui, Erling Olav Sollund, Eline Nesdal Sundli, Kamilla Arnesen, Marit Harneshaug, Helene Marie Eng Granlund, Jane Eiane Aarsland, Siri Stavnes, Gaute Osaland Hådem; second raw sitting: Amalie Tysseland, Henrik Jenssen, My Nhung Thi Tran, Beate Meisland Østrådt, Ane Sofie Lilleng, Maria Olsvik, Najma Ali Abdullahi, Karin Wiggen Dragsten (laboratory engineer)***. Photo: Estelle Vanhaecke, NTNU**

2018: Specialization Projects in Chemical Engineering (NTNU) or Nanotechnology (NTNU) affiliated or associated with iCSI

Abdulrahman Toutounji	Carbon formation and catalysis in the conversion of methyl chloride and silicon into dimethyldichlorosilane
Dumitrita Spinu	Production of Fuels from Lignin by Fast Hydropyrolysis with Coupled Catalytic Upgrading
Erik Andreas Jørgensen	Fischer-Tropsch Synthesis: Conversion of Bio-Syngas to Hydrocarbons
Fatemeh Khodadady	process design and evaluation of CO_2 capture on solid sorbents
Kristiane Søvde Oftebro	Photocatalytic Ammonia Synthesis
Lisa Leganger Landfall	New catalysts for low-temperature selective catalytic reduction (SCR)
Martin Meuche	Efficient catalysts for achieving NO /NO_2 equilibrium
Minadir Saracevic	Efficient catalysts for achieving NO /NO_2 equilibrium
Siyu Wang	Synthesis of low temperature sorbents for CO2 capture
Tho Ba Tran	Kinetic study of ethylene oxychlorination on promoted CuCl2/Al2O3 catalysts

International exchange students 2018 at NTNU

Iker Hurtado Lopez	Universidad Autónoma de Madrid (UAM), Spain	Biopolymers assisted preparation of cobalt based Fischer-Tropsch catalysts
Johannes Nerb	Chemical Technology I, TU München, Germany	
Maximilian Sauer	Chemical Technology I, TU München, Germany	Investigation of Manganese-based sorbents for hydrogen sulfide capture in a medium to high-temperature process
Dominik Rudolf	Chemical Process Tehcnology, KIT Karlsruhe, Germany	Effect of activation conditions on Fischer-Tropsch synthesis
Christian Maier	Chemical Technology I, TU München, Germany	Catalytic Methane Abatement for Natural Gas Engines

International exchange PhD candidates 2018 at NTNU

Niu Juntian *2016-09-01 to 2018-07-31*	College of Power Engineering, Chongqing University, China	Dry (CO_2) reforming of methane on Ni and Ni-Pt surface alloy catalysts studied by experiment and DFT.
Bingxu Chen *2017-12-01 to 2018-11-30*	State Key Laboratory of Chemical Engineering, East China University of Science and Technology, China	Mechanistic insights into iron-based Fischer-Tropsch catalysts for direct conversion of syngas to lower olefins
Xiaoli Yang *2018-09-07 to 2019-09-06*	Dalian Institute of chemical physics, Chinese Academy of Science	The conversion of syngas to liquid hydrocarbons with OX-ZEO process
Weixin Qian *2018-08-28 to 2019-08-27*	East China University of Science and Technology, Shanghai	The mechanistic and kinetic study of CO and CO_2 hydrogenation to chemicals and fuel
Nianju Hou *2018-11-28 to 2020-11-27*	Chemical Engineering and Technology, Tianjin University	Ethanol fuel cells and also the ORR catalysts for fuel cells.

Accounts 2018

Table 1 summarizes the costs in 2018 and the total budget for the period of the Centre after revision in January 2019. The different cost codes concern respectively:

- NTNU costs in Payroll and indirect expenses
- Other research partners, i.e. SINTEF and UiO in Procurement of R&D services
- Equipment code includes rent of research equipment acquired to serve needs for the SFI
- Other operating expenses regroups mainly research at industrial partners

Cost code	Costs 2018	2015-2023 Total budget
Payroll and indirect expenses	8 731	59 067
Procurement of R&D services	10 278	92 333
Equipment	1 108	7 160
Other operating expenses	4 751	33 517
Totals	24 867	192 078

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

Cost and Financing per partner	2018 Accounts		2015-2023 Total budget	
Partner	Costs	Financing	Costs	Financing
NTNU	11 225	5 090	75 744	27 532
University of Oslo	5 723	1 859	49 036	12 688
SINTEF	4 555	1 113	43 298	7 858
Industrial partners	3 364	6 364	24 000	48 000
Research Council of Norway	-	10 441	-	96 000
Totals	24 867	24 867	192 078	192 078

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

Industrial Innovation Area (IIA)	Costs 2018	2015-2023 Total budget
IIA1 21st century Nitric Acid technology development	5 176	38 035
IIA2 New NOx abatement technologies	657	7 571
IIA3 Frontier formalin technology development	3 233	21 188
IIA4 PVC Value Chain	4 410	30 830
IIA5 The next step in direct activation of methane	3 275	34 229
IIA6 Generic projects	6 004	34 285
IIA7 2020 Catalysis	-	7 432
iCSI Management and administration	2 112	18 508
Totals	24 867	192 078

**In all tables above values appear in 1000 Nok (as per January 2019 10 Nok are equivalent to 1 €)*

Communication and Dissemination

iCSI Plenaries

Chen De: **Catalyst Development from Rational Design and Multidimensional Taming of Electrons**. In: 7th CAS-TWAS Symposium on Green Technology (GT2018), July 23-25, 2018. Beijing, China.

Chen De: **Kinetic Aspects in Designing Catalytic Redox Cycles.** In**:** 11th National Congress of Environmental Catalysis and Environmental Materials, July 19-24, 2018, Shen Yang, China.

Olsbye U: **Understanding the selectivity of the Methanol to Hydrocarbons process at the molecular level**. In: *5th international school-conference on catalysis for young scientists "Catalyst design: From molecular to industrial level": 2018-05-20 - 2018-05-23; Moscow, Russia*.

iCSI Keynote lectures

De Chen, Kumar R. Rout, Endre Fenes, Martina F. Baidoo, Terje Fuglerud: **Kinetic Analysis and Design of Catalytic Redox Cycles**. In: 10th International Conference on Environmental Catalysis, September 22-26 Tianjin, China.

De Chen, Kumar R. Rout, Endre Fenes, Martina F. Baidoo, Terje Fuglerud: **Kinetic analysis of redox cycle reaction and catalyst development**. In: 4th International Conference on Advanced Complex Inorganic Nanomaterials (ACIN 2018), July 16-19th, Namur, Belgium.

De Chen, Endre Fenes, Kumar R. Rout, Martina F. Baidoo, Terje Fuglerud: **Kinetic Analysis and Design of Catalytic Redox Cycles**. In: 25th International Conference on Chemical Reaction Engineering (ISCRE 25), May 20-23, Florence, Italy.

Rønning M: **Synchrotron radiation in catalysis research**. In: *NorScatt Annual Meeting, May 22, Oslo, Norway*.

Yang J: **Isotopic labeling for kinetic and mechanistic investigation in Fischer-Tropsch synthesis.** In: *Nordic Catalysis Symposium, August 26 – 28, København, Denmark*.

iCSI associated invited lectures

Beato P.: **Cu-CHA catalysts for environmental applications** Keynote In: *4th International Symposium on the Catalysis for Clean Energy and Sustainable Chemistry: 2018-07-09 - 2018-07-11; Bilbao, Spain*.

Beato P.: **Operando goes industry** Plenary In: *6th International Congress on Operando Spectroscopy, 2018-04-15 2018-04-19, Estepona, Màlaga.*

Chen D: **Fundamental issues in controlling carbon supported catalyst performance**. Keynote In: *Carbon for catalysis 2018 China: 2018-03-20 - 2018-03-25; Guangzhou*, China.

Olsbye U: **CO_2 hydrogenation over Zr-MOF based catalysts**. Keynote In: *KAUST Research Conference: New Challenges in Heterogeneous Catalysis: 2018-01-29 - 2018-01-31; Thuwal*, Saudi Arabia.

Olsbye U: **CO_2 hydrogenation over Zr-MOF based catalysts (II)**. Keynote In: *EuCheMS Chemistry Congress: Molecular frontiers and global challenges: 2018-08-26 - 2018-08-30; Liverpool*, UK.

Olsbye U: **Tailoring MOFs for CO_2 hydrogenation reactions (II).** Keynote In: *8th Tokyo Conference on Advanced Catalytic Science and Technology TOCAT-8: 2018-08-05 - 2018-08-10; Yokohama, Japan.*

Rønning M: **Carbon-based (Fe-Nx-C) ORR catalysts: What are the requirements for application in PEM fuel cells?** Keynote In: *8th International Symposium on Carbon for Catalysis, CarboCat–VIII: 2018-06-25 - 2018-06-29; Porto, Portugal*.

Publications

iCSI Publications for 2018

1. Baidoo, M. F., Fenes, E., Rout, K. R., Fuglerud, T., Chen, D. "**On the effects of K and La co-promotion on $CuCl_2/\gamma$-Al_2O_3 catalysts for the oxychlorination of ethylene**" *Catalysis Today*, 2018, 299, 164.
2. Borfecchia, Elisa; Beato, Pablo; Svelle, Stian; Olsbye, Unni; Lamberti, Carlo and Bordiga**,** Silvia **Cu-CHA – a model system for applied selective redox catalysis,** *Chem. Soc. Rev.*, 2018, 47, 8097-8133.
3. Borfecchia, Elisa; Pappas, Dimitrios K.; Dyballa, Michael; Lomachenko, Kirill A.; Negri, Chiara; Signorile, Matteo; Berlier, Gloria, **Evolution of active sites during selective oxidation of methane to methanol over Cu-CHA and Cu-MOR zeolites as monitored by operando XAS**, *Catalysis Today*, *In Press. DOI: 10.1016/j.cattod.2018.07.028.*
4. Bundli, S., P. Dhak, M. Jensen, A.E. Gunnæs, P.D. Nguyen, H. Fjellvåg, and A.O. Sjåstad. "**Controlled Alloying of Pt-Rh Nanoparticles by the Polyol Approach."** Journal of Alloys and Compounds 779, 2019, 879–85.
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Authors

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