iCSI

industrial Catalysis Science and Innovation for a competitive and sustainable process industry

Annual Report 2017

sfi 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**

11 Master students

7 PhD candidates

3 Postdoctoral fellows

11 Professors

17 Research Scientists from SINTEF

14 Scientists from industry

...and more to come!

NTNU

UiO : Universitetet i Oslo

SINTEF

YARA

dynea

inovyn

K.A.Rasmussen Norway

HALDOR TOPSØE

2017 Summary

2017 was a year of ***increased visibility and innovation*** from iCSI research efforts. We have published in ***high impact catalysis journals*** such as **Journal of Catalysis** and **ACS Catalysis,** as well as more generic chemistry journals including the prestigious **Journal of the American Chemical Society**. The Industrial Innovation Areas (IIAs) 4 and 5 are leading the way, but high-quality research results and publications are in the pipeline for all IIAs (1-6). Even more important, is that new directions for future innovation developments for the industrial partners are emerging. Our industrial partner Inovyn is already taking selected results to implementation.

The whole iCSI team had the opportunity to meet and interact during ***the 2017 Annual iCSI Seminar*** in November, this time at a venue next to the idyllic lake of Hurdalsjøen. Students, academics, researchers and industrial partners (49 participants) were mixed in a two-day, hard-working scientific and social event. For the first time, all three members of the ***Scientific Advisory Committee*** were present, sharing their experience and ideas with the iCSI members.

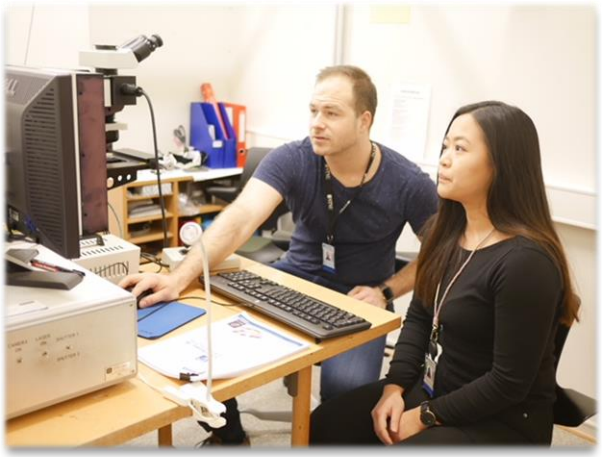
iCSI recruited ***a large number of MSc students in 2017***. 11 completed their Master thesis in 2017, with another 25 in progress. The family of young iCSI scientists was also increased by one new PhD candidate at NTNU, Hongfei Ma, who will work on catalyst deactivation and by-product formation in the oxychlorination process. We also had the pleasure to welcome our ***1st iCSI exchange student***. Master student Luca Altavilla from University of Torino (Italy) spent two months at Haldor Topsøe in Lyngby to perform ***operando*** **Raman experiments** in the Optical spectroscopy laboratories, under the supervision of Dr. Pablo Beato. Industrial exchanges for iCSI PhD students will take place in 2018!

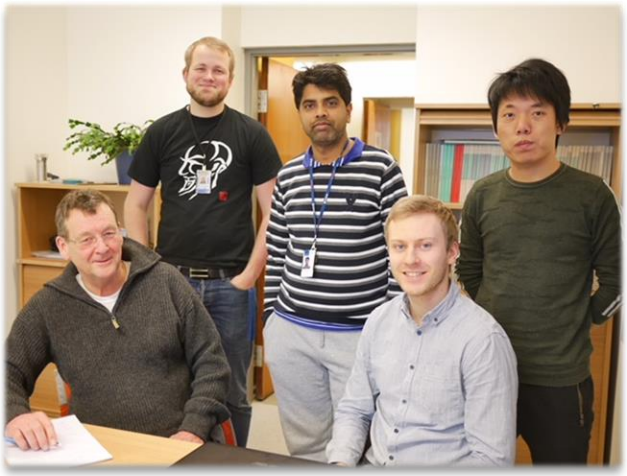
The iCSI researchers have given ***49 presentations*** at national and international conferences in 2017. See the publication and presentations lists on p. 48-55 for a full overview over iCSI researchers' dissemination, including co-publications with many of the institutions mentioned as international partners (p.42). Some iCSI principal investigators had ***particularly high international visibility*** during 2017. Prof. Unni Olsbye (UiO) was invited for the SUNCAT Summer Institute at Stanford University, the Gordon Research Conference on Nanoporous Materials and their Applications, and the Catalysis for Fuels Faraday Discussion. Prof De Chen (NTNU) has established a major networking and research collaboration arena between Norway and China during his sabbatical at the Key Laboratory of Chemical Engineering, East China University of Science and Technology, with invited lectures at many of the key Chinese research institutions and events.

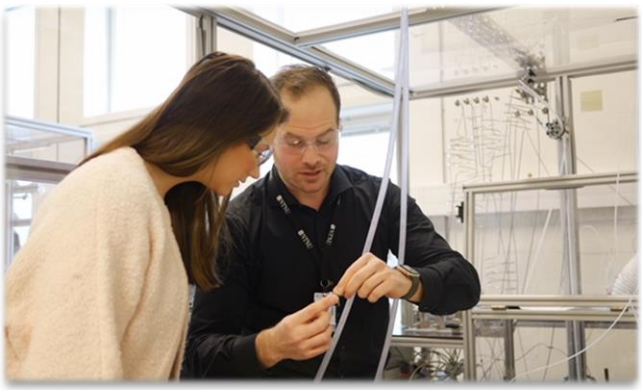
Steinar Kvisle and the GASSMAKS program board at TOTAL/UOP MTO demo plant @ Feluy, Belgium, Fall 2011

Finally, the ***iCSI Board*** has seen some changes. Karina Mathisen has replaced Tor Grande for NTNU, and we thank Tor for his valuable involvement at the iCSI Board. Terje Fuglerud is the new representative from Inovyn. ***Steinar Kvisle*** retired from Inovyn after several decades of significant contributions and active involvement in Norwegian and international research projects, collaborations, and technology developments. Steinar was instrumental to establishing iCSI, and we wish him all the best in the years to come!

Master students from UiO and NTNU together with iCSI PhD students and Scientists. More information available on page 44-46!







Contents

Towards Innovation!

Another year has passed in iCSI. The research activities are starting to produce really interesting results and publications are coming out. The PhD students are experiencing a steep learning curve, and are about to go from unexperienced to experts in their fields. In other words – everything is as it should!

Odd-Arne Lorentsen (iCSI Chair, Yara), Henrik Jenssen Gremmetsen (Master student, NTNU), Svein Tore Holsæther (CEO Yara), Signe Marit Hyrve (Master student, NTNU)

In an academic world, people always find interesting things to study. Some go deep into theory, others scrutinize every detail of a topic. A risk is, however, that at you end up "knowing everything about nothing". Explaining complicated theory and scientific results to someone less skilled is also difficult, and there may be a tendency to over-simplify things to make it easier to grasp. As a student and a teacher it is important to maintain scientifically correct when presenting research, but in a way that the recipients see relevance for themselves. Gaining knowledge and insight is a cornerstone of the iCSI research, but it is still only a tool to get further.

Value-creation is about putting theory into practice, and to make business out of it. As a student it may seem difficult to see the path from fundamental to applied science, but the aspect of innovation should not be forgotten. The PhD students may not experience it within the duration of their project, but should be challenged to discuss their new knowledge in a context of industrial application as well as environmental footprint. In order to obtain results that can be applied in the end, it is extremely important to keep a tight link between the academia and the industry. In iCSI, the industrial partners have invested significant effort and time to develop relevant topics to explore, and all have frequent and good contact with both the academic staff and the students.

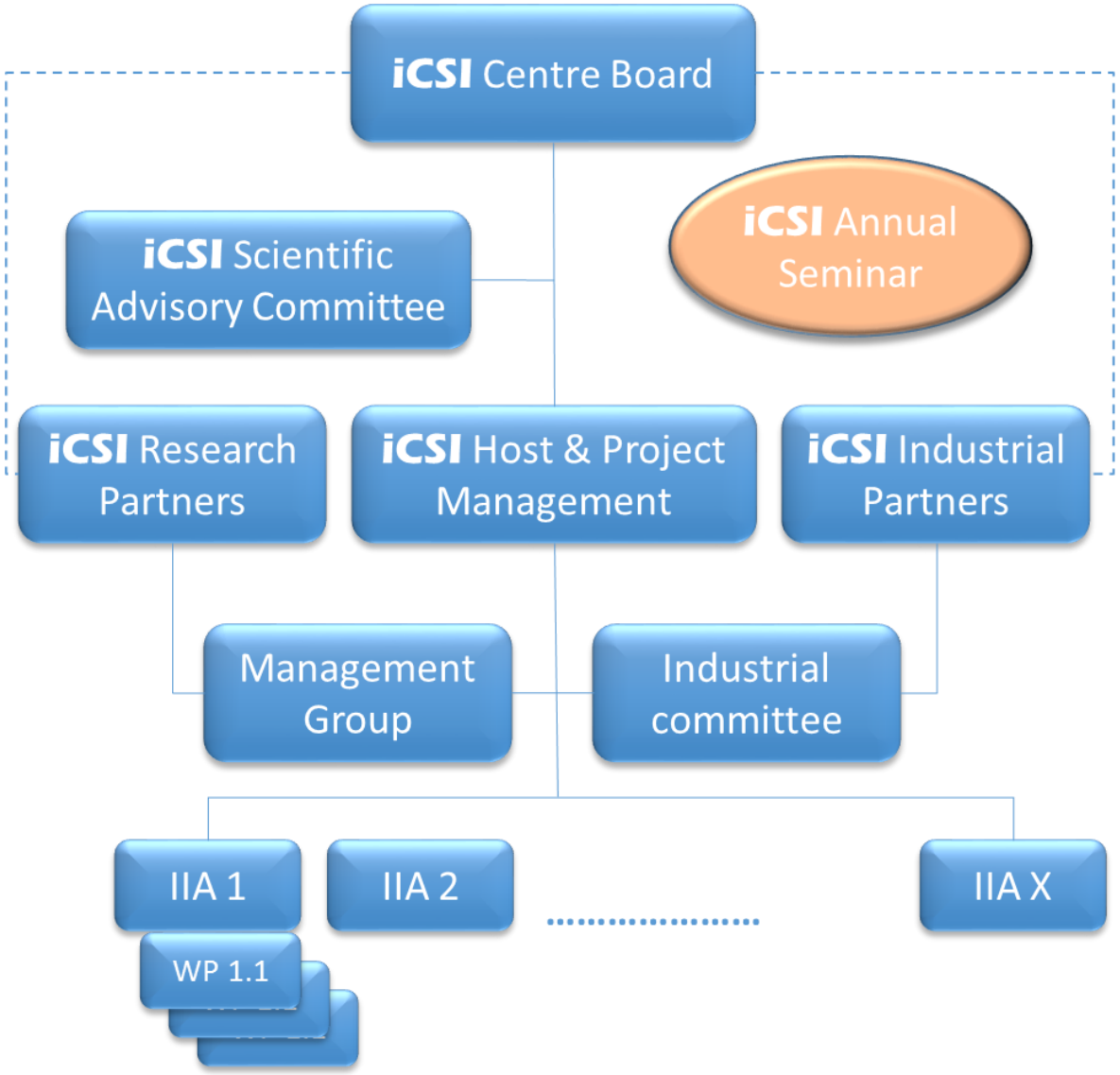
In order to ensure international scientific standard of the work, the Board has established a Scientific Advisory Committee (SAC) with 3 professors from Politecnico Milano, University of California, Berkley and Cardiff University. They all participated in the gathering held at Hurdalsjøen last November with valuable insight and questions as well as suggestions for further work. There is no doubt that the SAC can and will contribute to improve the outcome of the work in iCSI even more in the future. The Board will facilitate good interactions between them and the young researchers.

To summarise, the iCSI Centre now has everything it needs in order to ensure high quality work for the industrial partners as well as educating skilled MSc and PhD candidates suitable for careers both in academia and in the industry. Through the Centre they will also establish important networks across disciplines and industries that will be valuable also in the future. I'm looking forward to seeing how the iCSI research results may lead to valuable insight and innovation, both for the industry in Norway as well as for the students involved! The slogan for Yara is worth citing as the final punchline: "Knowledge Grows"!

Odd-Arne Lorentsen, iCSI Board Chair

Organization

The **Norwegian University of Science and Technology** (NTNU) is the **Centre Host and Manager of iCSI**. 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 AS**, 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.



iCSI Centre Board

Odd-Arne Lorentsen
Yara
(Chair)

Pablo Beato
Haldor Topsøe
(Vice-Chair)

Lars Axelsen
Dynea

Terje Fuglerud
INOVYN

Johan Skjelstad
KA Rasmussen AS

Duncan Akporiaye
SINTEF

Karina Mathisen
NTNU

Vebjørn Bakken
UiO

Aase Marie Hundere
(RCN Observer)

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 working 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.

ICSI Management and Administration

Hilde J. Venvik
Professor
Dept. Chem. Eng. NTNU
iCSI *Centre Director*

Dr. Estelle Vanhaecke
Senior Engineer
Dept. Chem. Eng. NTNU
Coordinator **iCSI**

Torgrim Mathisen
Senior Executive Officer
Dept. Chem. Eng. NTNU
iCSI *economy advisor*

The Scientific Advisory Committee

Prof. Alessandra Beretta

Prof. Enrique Iglesia

Prof. Graham Hutchings

POLITECNICO MILANO 1863

Berkeley UNIVERSITY OF CALIFORNIA

CARDIFF UNIVERSITY
PRIFYSGOL CAERDYDD

The appointment to the iCSI Scientific Advisory Committee (SAC) was finalized in 2017. 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.

The Board and whole iCSI team had the privilege to meet the SAC members at the ***iCSI Annual Seminar*** in November 6-7 at Hurdalsjøen, Norway. They gave their first advice and critics during the seminar, and gave very inspirational presentations:

Towards more accurate descriptions of reactivity in acid and oxidation catalysis on metal oxides, by Professor Enrique Iglesia.

Catalysis using Gold, by Professor Graham Hutchings.

New challenges in the SCR technology for stationary applications: a focus on Hg oxidation, by Professor Alessandra Beretta.

More information on the seminar is available on pages 13-14.

The 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 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 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 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.

Highlight 2017

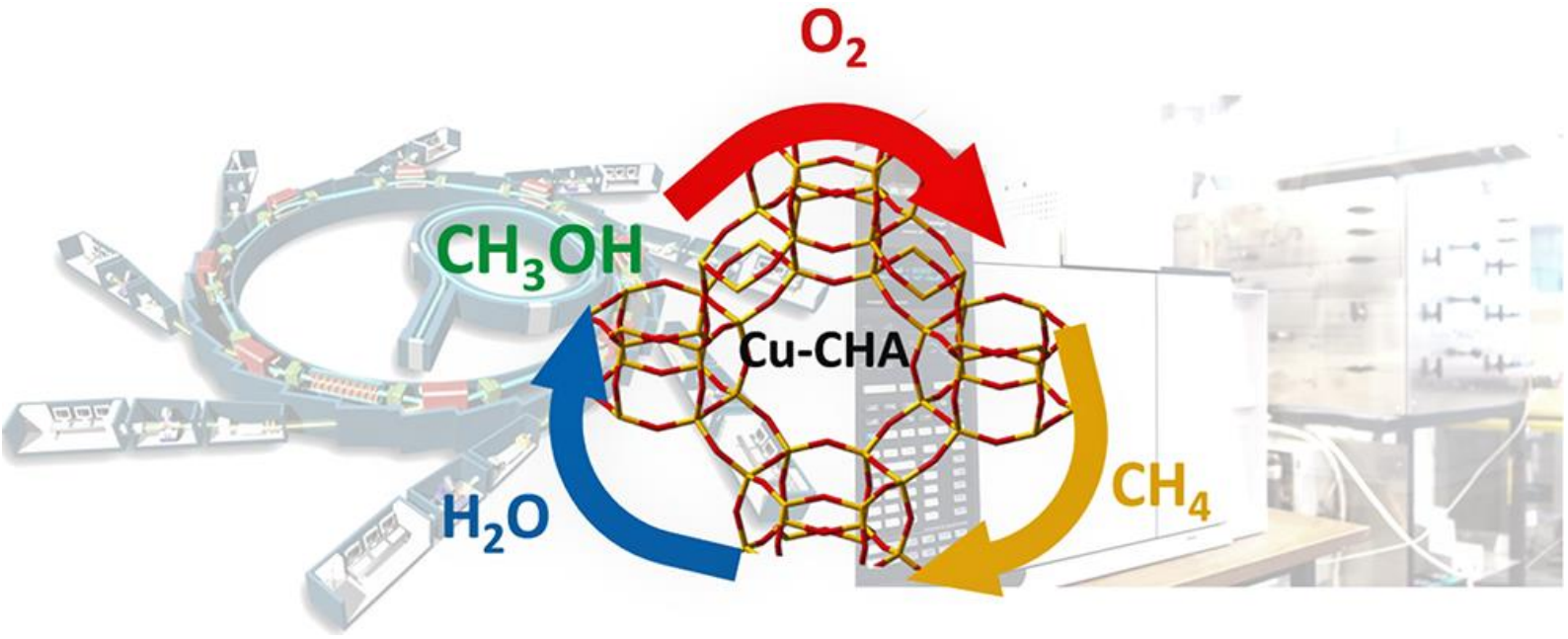
An important iCSI achievement in 2017, was the paper from Industrial Innovation Area 5 released in Journal of the American Chemical Society (JACS); "***Methane to Methanol: Structure-Activity Relationships for Cu-CHA***" by Dimitrios K. Pappas, Elisa Borfecchia, Michael Dyballa, Illia A. Pankin, Kirill A. Lomachenko, Andrea Martini, Matteo Signorile, Shewangizaw Teketel, Bjørnar Arstad, Gloria Berlier, Carlo Lamberti, Silvia Bordiga, Unni Olsbye, Karl Petter Lillerud, Stian Svelle and Pablo Beato.

In this study, Cu-exchanged SSZ-13 zeolites were used to cleave the C-H bond of methane at temperatures ≤200°C, enabling its selective partial oxidation to methanol. Researchers from UiO, Haldor Topsøe, SINTEF and the University of Torino combined activity tests and X-ray absorption spectroscopy (XAS) to investigate the influence of reaction parameters and material elemental composition on the productivity and Cu speciation during the key process steps.

It was found that the active Cu^{II} moieties* are formed in O_2 preferably at high temperature and at prolonged activation time. The reducibility of the materials and their methanol productivity correlate linearly. By optimizing the process conditions and material composition, a methanol productivity as high as 0.2 mol CH_3OH/mol Cu (125 μm/g) was reached, the highest value reported to date for Cu-SSZ-13. Cu^{II} is preferably located in 2Al sites in 6r at low values of both Si:Al and Cu:Al ratios and is inactive for the conversion of methane. $Z[Cu^{II}OH]$ are identified as the precursors to the methane converting active sites. A critical examination of the reported catalytic and spectroscopic data enabled the proposal of adifferent route for the active-site formation.

*parts or functional groups

Reference: J. Am. Chem. Soc., ***2017****, 139, 14961−14975*



UiO : Universitetet i Oslo HALDOR TOPSØE SINTEF

SAC portrait:

Professor Alessandra Beretta

Professor Alessandra Beretta works at the Laboratory of Catalysis and Catalytic Processes at Politecnico di Milano. Since June 2016, she is also one of our three prominent iCSI Scientific Advisors. We had the privilege to meet her during our Kick-off meeting in November 2016 and the iCSI seminar 2017. Here, she gives us the chance to know her better, both as a person and a scientist.

"Well, I have dense days…

Inevitably a large part of my time and energy is devoted to research or to my job in general (many time-consuming activities at the university are not necessarily "research" and growing in age and responsibility brings more of them).

My family occupies a large part of my heart and my thoughts. I have a husband, Aldo, an environmental engineer working in the field of soil remediation (there is a lot to do in this field in Italy - not necessarily new chemistry, but very important). He loves skiing and hiking the mountain, and this tends to affect our weekends and vacations. But we met on a boat while sailing in the Mediterranean. We have two kids, Emanuele (14) and Marta (11). Kids are "systems of infinite capacity" - you keep pouring in energy, feelings, and effort….but they are never full!!

As Catholics we are well integrated in our church community, which means time for being together while giving help and support to others. My hobbies? I don't have time! No, I am joking. I had a classic education in sports and music and, although I cannot play my guitar any longer, from time to time I am able to join a polyphonic choir and sing. I do love it. And of course I love cooking. Hilde once told me that in Norway bread is a staple food: impossible! How can you live happily? A lot of my time is related to the choice of raw material, the recipes, the preparation… I strongly believe in the healing power of food: For me, since cooking is therapy, for whom it is prepared, since food is an excellent vector of love and health."

*I never recommend enough to **study the research literature**. I myself suffer from having less and less time to do it. For the specific case of the iCSI, considering the richness of stimuli to which the students are exposed, I would recommend **to grasp them and squeeze from this experience as much as they can, from the own and other advisors, the various laboratories, the industrial partners, the advisory board members!***

"The most exciting thing in catalysis is understanding what is going on, more properly which surface mechanisms and physical factors that can explain the observables. Then translating this understanding into engineering correlations that describe mathematically the phenomena, and eventually to apply the knowledge to design new improved solutions: a different reactor design, a change of operating conditions, a new experiment that demonstrates a concept or a systematic trend.
In my daily work, also, I feel motivated by the relationship with the students and the colleagues.

The research group is a second family."

iCSI *Scientific Advisory Committee member*

Alessandra gives us her point of view about iCSI and her "*privileged position as a SAC member*":

The first time I learned of iCSI, I was struck by the field and objectives of the research projects: industrial chemistry with specific improvement goals! This is somewhat unique in the present European context. The Centre has the courage to reexamine "textbook" industrial processes, in the acknowledgement of their pivotal role in the economy of the company and thus of the country, calling for new ideas that can improve the efficiency and lower the costs. Well, this has been the topical driving force for the chemical engineering since ever. iCSI has also room for a dream-reaction, like methane selective oxidation, but again starting from the recognition of its industrial potential. iCSI has the potential of a formidable example for Europe, also considering the attention that Norway and its approach to industrial innovation attracts.

I observe the progress of the research activities that engage the forces of several individuals with different competences and background (the PhD student, the WP leader and senior reseachers, the industrial partner, the iCSI board). A very comprehensive picture, where so many aspects and approaches are involved. I can learn a lot.

I feel honored by having this privilege and committed to give my contribution, where my competence and previous experience permit. I must also admit, that being in the SAC together with the two "big" colleagues makes the whole thing even more exiting! But again, it's a fantastic occasion to learn.

The risk? Well, I hope that the industrial partners will be able to be courageous to the very end; industrial implementation of new ideas has an incredibly high activation energy.

The iCSI Seminar closed 2017 under the best auspices; for the first time ***the three members of the Scientific Advisory Committee (SAC)*** were present with the students, researchers, academics and industrial partners. In total ***49 participants*** shared their experience and ideas at a venue next to the idyllic lake of Hurdalsjøen.

It was co-organized with the ***Norwegian Catalysis Symposium*** (NKS) with parallel sessions, making the seminar as an outreach to other research groups in Norway. Dr. Nikolas Tsakoumis and Prof. Hilde Johnsen Venvik were the organizers of this event.

The SAC members gave excellent lectures to the inspiration of every researcher and provided high valuable input during the seminar. Their ability to quickly understand and go to the core of each research activity was striking, and as such, they are already clear assets to iCSI. They also proved themselves as hands-on scientists, preferring direct interaction on the science and with the researchers.

iCSI annual meeting and Norwegian Catalysis Symposium 2017

Monday November, 6

09:15-10:45	Arrival at **K.A. Rasmussen** – plant tour
10:45-11:00	**iCSI / NKS registration** opens in Hurdalsjøen Hotel
12:00	Lunch
13:00	iCSI welcome
13:10-15:10	**IIA presentations** by: Prof. Anja Olafsen Sjåstad (UiO) Dr. Karl Isak Skau (Yara) Dr. Jasmina Hafizovic Cavka (SINTEF) Dr. Kumar R. Rout (SINTEF) Prof. Stian Svelle (UiO) Prof. Magnus Rønning (NTNU)
15:10	Coffee break
16:50	NKS welcome
17:00	**Plenary Lecture**: Prof. Enrique Iglesia (University of California, Berkeley) ***"Towards More Accurate Descriptions of Reactivity in Acid and Oxidation Catalysis on Metal Oxides"***
18:00	Poster session (Common for iCSI and NKS)
19:30	Dinner

Tuesday, November 7

8:30	**Plenary Lecture:** Prof. Graham Hutchings (Cardiff Catalysis Institute) ***"Catalysis using gold"***		
9:30			
9:50	iCSI IIA1: **Ata ul Rauf Salman** (NTNU)	Coffee break	
10:05	iCSI IIA2: **Silje Fosse-Håkonsen** (SINTEF)	9:50	NKS: **Carlos A. Grande** (SINTEF)
10:20	iCSI IIA3: **Stine Lervold** (NTNU)	10:10	NKS: **Kun Guo** (UiS)
10:35	iCSI IIA4: **Endre Fenes** (NTNU)	10:30	NKS: **Isaac Yeboah** (NTNU)
10:50	iCSI IIA5: **Michael Dyballa** (UiO)	10:50	NKS: **Sondre Eliasson** (UiB)
11:05	iCSI IIA6: **Samuel Regli** (NTNU)	11:10	NKS: **Ingeborg-Helene Svenum** (SINTEF)
11:20	iCSI IIA6: **Annett Thøgersen** (SINTEF)	11:30	NKS: **Mari Helene Farstad** (NTNU)
11:35	iCSI IIA6: **Oleksii Ivashenko** (UiO)	11:50	NKS: **Irene Pinilla-Herrero** (UiO)
12:00			
13:00	Lunch		
14:00	**Plenary Lecture:** Prof. Alessandra Beretta (Polytecnico di Milano) ***"New challenges in the SCR technology for stationary applications: a focus on Hg oxidation"***		
14:20-16:20	**iCSI** Board meeting *(for only board members and SAC)*	Coffee break	
		14:20	NKS: **Sigurd Øien-Ødegaard** (UiO) ***NKS award lecture for best PhD thesis***
		15:00	NKS: **Ljubiša Gavrilović** (NTNU)
		15:20	NKS: **Marco Foscato** (UiB)
		15:40	NKS: **Dimitrios K. Pappas** (UiO)
		16:00	NKS: **Shirley E. Liland** (NTNU)
		16:20	NKS closing
		16:30	


The feedback from all the participants was very positive with respect to the venue, the organization and the seminar content. There is still room for improvements and already some input will be taken into account in the next seminar edition!

The SAC members judged the Centre as running well, with potential for lifting the research from “good” to “excellent” while at the same time remaining loyal to the actual, industrial challenges.

To sum up, the iCSI seminar 2017 was a success and contributed to more efficient communication between iCSI members!

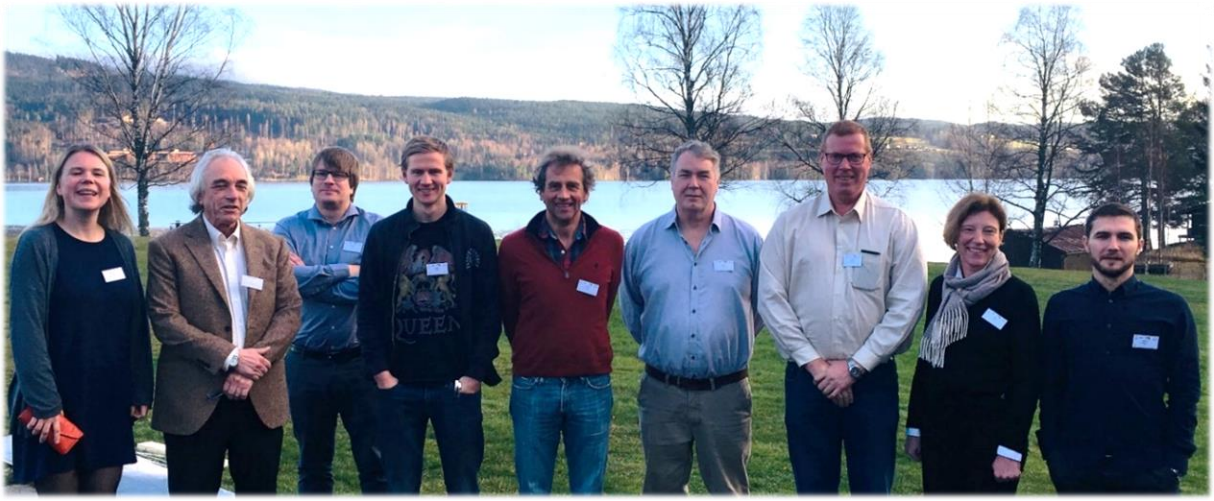


Researchers' corner

This year, we challenged some of the researchers involved to present their job, their collaboration and their perspectives and ambitions for iCSI. The first team consists of Yara, KA Rasmussen, the University of Oslo, SINTEF and NTNU working together in Industrial Innovation Area 1 (IIA1). The second team works within IIA3 to improve the silver based formalin technology and involves researchers from K.A. Rasmussen, Dynea, NTNU and SINTEF.

Nitric Acid world

YARA UiO : Universitetet i Oslo K.A.Rasmussen Norway SINTEF NTNU



UiO-SINTEF-Yara-KA Rasmussen team during the iCSI seminar in Nov 2017: Silje Fosse Håkonsen, Arne Karlsson, Karl-Isak Skau, Asbjørn Slagtern Fjellvåg, Helmer Fjellvåg, David Waller, Johan Skjelstad, Anja Olafsen Sjåstad, Oleksii Ivashenko

Anja Olafsen Sjåstad is Professor at the University of Oslo in the Inorganic materials chemistry section of the Department of Chemistry. Her research is directed towards synthesis and characterization of inorganic solids, in-situ studies of metal-on-support catalysts and surfaces, with emphasis on developing improved catalysts. She is also the leader of IIA1, where the researchers from industry and academia work on "*understanding how we can improve catchment of noble metals lost during high temperature ammonia oxidation,* and recent and exciting results from this activity can be found on page 21.

"To understand the potential we should be aware that in a medium pressure HNO_3 (Nitric Acid) plant, about 0.2 g of platinum (Pt) is released from the catalyst per ton HNO_3 produced. In the current Pt catchment technology, palladium (Pd)-nickel (Ni) gauzes are capable of recovering about 70% of this. During Pt *catchment, however, significant quantities of Pd is also released. So, if we understand the mechanism of the catchment of the PtO_2 (platinum oxide) species and the associated Pd loss* ***we may come in position to significantly improve the cost and efficiency of precious metals recovery****."* (Anja Olafsen Sjåstad).

Anja obtained her PhD in solid state chemistry from the University of Oslo. Her PhD work was on "Structure and stability of rare earth oxide carbonates - Properties of Nd based Ruddlesden-Popper type oxides". Thereafter, she joined SINTEF in 1999. *"In SINTEF, I worked on projects spanning from catalyst development to production of silanes and poly-crystalline silicon. My keen interest in silane-silicon production resulted in that I joined REC Silicon in 2006. In REC, one of my most important duties was the start-up of the new silane plants in the US and the "de-bottle necking" of some important chemistry issues connected to the production units. Returning to academia was not a planned carrier move, but I have not regretted it and I enjoy interacting with young people and collaborating with industry and other research groups, nationally and internationally."*

Yara team: Mohan Menon, David Waller

David Waller was born and educated in the United Kingdom with a B.Sc. in Chemistry at University College, Cardiff, a M.Sc. in Surface chemistry at the University of Bristol, and a Ph.D. at the University of Bath. "*My Ph.D. work, on methanol synthesis catalysts, was in collaboration with the catalyst group of Imperial Chemical Industries (ICI) Agri Division, which was subsequently spun-off and then purchased by Johnson-Matthey. I then undertook a number of postdoctoral fellowships; at University College, London, in the Davy-Faraday Research laboratory of the Royal Institution, at Imperial College. These positions involved the development of light-based computer circuits, in-situ X-ray diffraction and absorption spectroscopy of catalysts, and ion-conducting membranes for solid oxide fuel cell and gas separation applications. These periods of study and research led to my interest in the synthesis and characterization of materials, catalysis, ion-conducting materials and materials transport (solid-state and vapour).*

I have had various positions in industry including the production of paint with ICI, the production of super-hard metal-ceramic composites at Sandvik Hard Materials AB, and research into ion-conducting membranes and catalysts with Norsk Hydro (Yara prior to 2004). Now, at Yara Technology Centre in Porsgrunn, I am employed as Senior Catalyst Expert and based in a newly established group called New Front-End Technology & Process Intensification. The remit of this group is to evaluate and develop new processes for the production of ammonia and nitric acid; with time perspectives of ~5 and ~25 years".

Anja thinks the catchment challenge is exciting: *"Through experiments in six-zone furnace systems we are able to mimic plant conditions and reproduce the reconstruction and material degradation of Pd-Ni gauzes, as well as studying the deposition of PtO_2 onto these.* ***We obtain Pt diffusion profiles in the catchment alloys*** *(see also p 24)* ***and combine various ex-situ and operando analysis methods, to image morphology and to map compositional gradients and phases present.*** *We are convinced that this systematic approach, developed jointly with our industry partners, will bring new insight - information may in the next step be cleverly used to optimize materials properties of the catchment technology."*

David is also very enthusiastic: "***This subject is little studied; with less than 20 academic articles published in the last 40 years.*** *The Yara facilities (laboratory and pilot), along with plant data and knowledge complement those of the University of Oslo, the Process Chemistry and Functional Materials group of SINTEF in Oslo and our other industry partner in this task, K. A. Rasmussen."*

Mohan Menon studied Ceramics materials for his Bachelor Tech in IIT, Varanasi in India and took his PhD in Materials Science at the University of Michigan, Ann Arbor, USA. "*I have worked with processing and characterization of materials to enhance their performance. I have worked with structural materials, electrochemical devices, catalysts, Si wafers for solar power, exhaust cleaning and other environmental technologies*". His job in Yara Technology Centre includes "*product development for Yara Industrial that sells environmental solutions, optimizing processes in Yara Production to minimize emissions, map and assess status of emissions from various Yara plants and to help achieve Yara its environmental commitments and goals*."

David Waller and Mohan Menon work with NTNU and SINTEF in Trondheim on developing a heterogeneous catalyst for the oxidation of NO to NO_2. Professor Magnus Rønning leads a WP team of one PhD student and two SINTEF senior researchers, with several specialization and master students engaged.

Yara-NTNU-SINTEF meeting at NTNU (left to right) Bjørn-Christian Enger, Rune Lødeng, Magnus Rønning, David Waller, Arne Øygarden, Mohan Menon, Ata al Rauf Salman

"*This is a key step in the production of nitric acid via the combustion of ammonia",* explains David. *"The aim is to replace a homogeneous oxidation process, which requires heat removal and a long residence time, with a catalyzed process coupled with heat exchangers. This will yield a more intensified process, with the added bonus of additional energy recovery. In this activity, Yara has provided PhD student Ata ul Rauf Salman at NTNU with information on the NO oxidation reaction from an industrial perspective, along with information on our experiences in the analysis of nitrogen oxides".*

Both Yara researchers are confident in the continuation and the development of this project. Mohan emphasizes that in order to succeed in iCSI we need to "*strike the right balance between basic research and industrial application of catalytic processes. In my opinion, we are dealing with the challenge very well and we should keep this focus."*

*"**The greatest challenge for us in iCSI** is to ensure that fundamental knowledge gained through our academic partners is translated to a real world solution that can be implemented in our plants. Often in an industrial research environment, a task is completed using the minimum level of information or data required to complete the task. We often ask ourselves, "how little do we need to know" to complete the job in a safe and reliable manner. This "quick and dirty" approach - justifiable in a commercial environment - is quite different from academia where knowledge itself is a product with high value. **Collaborations, such as iCSI, give the industrial partners an opportunity to gain more in-depth knowledge** from our skilled and well-equipped academic partners."* (David Waller)

Silver at its best

dynea SINTEF K.A.Rasmussen Norway NTNU

IIA 3 team meeting: (from top left to down right) Stine Lervold, Hilde J. Venvik, Rune Lødeng, Thomas By, Jasmina Hafizovic Cavka, Johan Skjelstad, Kamilla Jenssen, Kristin Bingen, Herdis Petersson, Roman Tschenscher

Who is in the team?

Jasmina Hafizovic Cavka holds a PhD from the Department of Chemistry, University of Oslo. Her thesis, defended in 2008, was about "*synthesis, characterization and testing of metal-organic frameworks (MOFs) for applications within catalysis and gas separation*." She has since been working at SINTEF, first "as *a research scientist within development of catalysts and adsorbents for various reactions and processes, then I got promoted to Research Manager in 2013. For the time being, our research group "Process Chemistry and Functional Materials" consists of 20 people, and we cover broad range of competences with the aim to serve both national and international industry.*" Jasmina also leads Industrial Innovation Area 3, in which the partners collaborate to improve the silver base formalin process. "*Since iCSI gathers the main industrial and academic partners within catalysis in Norway, I think it is time to leverage further. By that I mean that that we should generate more industrially relevant spin-off activities. In a busy daily life this may easily be forgotten".*

Thomas By holds a Master degree in Materials Science and Engineering from NTNU. As a student, he was actively engaged through the student organization for Material Science, Petroleum and Geology at NTNU ("Bergstuderendes forening") to ensure a good social environment for the students, newcomers in particular. His job at K.A. Rasmussen is "*my first fulltime job, where I work on the challenges within the hydro- and pyrometallurgy fields, and also on the finished product side*".

Kristin Bingen obtained her Master degree in Mechanical Engineering from the Department of Thermal Energy and Hydropower at NTNU. She worked five years with application support in simulation of chemical systems at COMSOL, before joining Dynea eleven years ago. Kristin has two main responsibilities as a Senior Engineer in Process Development at Dynea: "*I work to improve the Dynea Silver Formaldehyde process, where the iCSI project for improvement of the silver catalyst is an important part. In addition, I do process and energy optimization, and investment projects for Dynea's plant at Lillestrøm.*"

Rune Lødeng holds a PhD from Department of Industrial Chemistry, NTH (now NTNU). His PhD research was on "a kinetic model for converting methane directly to methanol", involving gas phase reactions and model building. He was recruited to SINTEF by Professor Anders Holmen and has been working there since. "*I have been climbing the horizontal career ladder in SINTEF and am now Senior Scientist in the Kinetics and Catalysis group, now part of the Process Technology department at SINTEF Industry. I contribute to building strategic competence, deliver project research results and solving value-adding problems for the industry. I try to keep up practical work in the laboratory as often as possible! A challenge for SINTEF is to stick to its main role – technology – and maintain strong strategic relations with national industry. It is also a responsibility to give the best (realistic) advice to society. We can become even better than today!*"

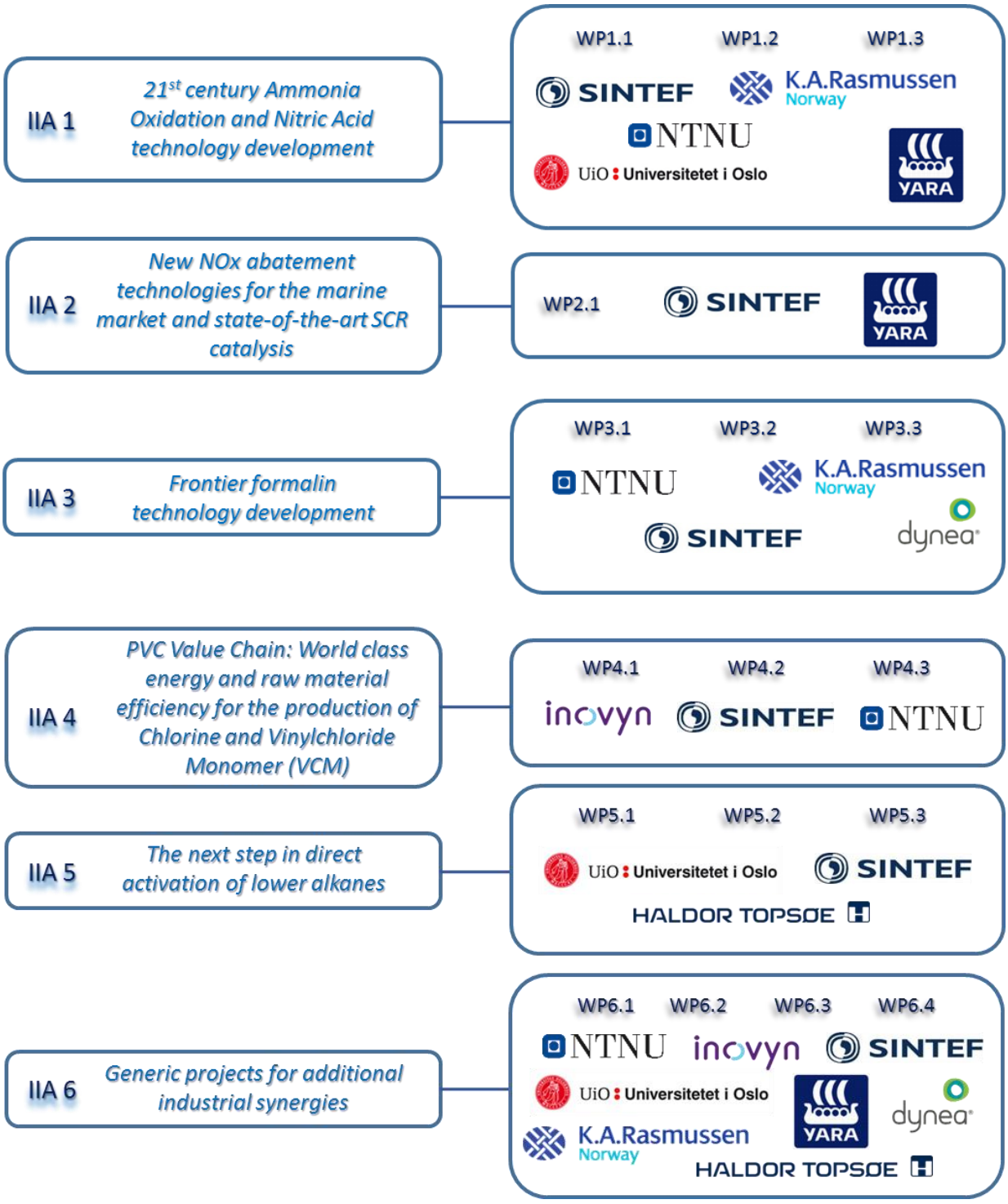
Challenges at each side

IIA3 involves two industrial partners, **Dynea and K.A. Rasmussen**, and two research partners, **NTNU and SINTEF**. **Jasmina** consider her task as "*making sure that we have smooth collaboration between all partners and that we pursue the goals we have set. "Through **iCSI** we have learned to know each other and to better understand the industrial challenges. Moreover, we have been lucky to have several NTNU students involved in this project, both master, PhD and Postdocs. This has been a very positive experience that resulted in several interesting scientific findings and discussions."* 3-4 meetings are held every year, "*but there are frequent email and telephone discussions whenever questions or problems arise, and everyone is contributing!*"

The industrial partners know each other since long as Dynea is a customer of K. A. Rasmussen, and they have been collaborating on the refining and regeneration of the silver catalyst by electrolysis. Both have high expectations: "*The greatest challenge will always be to **deliver the best possible catalyst products**. This is the reason we joined iCSI, for us to be able to innovate further"* says **Thomas**. In Dynea's view, "the *Dynea Formaldehyde Silver technology is today the preferred formalin technology due to lower operational cost with respect to energy and catalyst. To **stay competitive,** it is important that we also reduce the raw material consumption of methanol. **With iCSI we aim to deliver the best catalyst and process technology** with respect to yield."* says Kristin.

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 2017

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)
Martin Jensen	UiO	Master student (WP1.1)
Galina Tenkova Yavasheva	UiO	Master student (WP1.1)
Oleksii Ivashenko	UiO	Postdoctoral fellow (WP 1.1)
Maximilian Warner	YARA	Industry researcher (WP 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)
Spyros Diplas	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)

Oral contribution

Salman, Ata ul Rauf; Enger, Bjørn Christian; Lødeng, Rune; Menon, Mohan; Waller, David; Rønning, Magnus, **Catalysts for attaining NO/NO_2 equilibrium**, iCSI seminar, November 6-7, Hurdalsjøen, Norway

Poster contribution

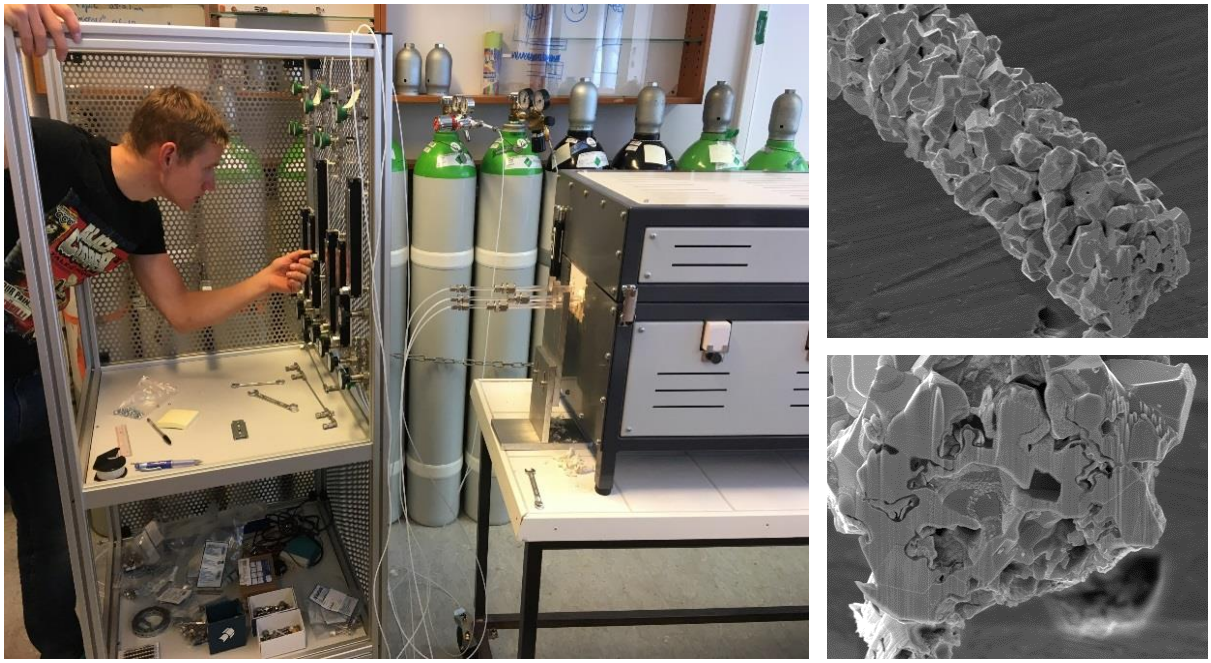
Fjellvåg, Asbjørn Slagtern; Waller, David; Warner, Maximilian; Sjåstad, Anja Olafsen, **Reconstruction of Pd-Ni catchment gauze during high temperature ammonia oxidation**, iCSI seminar, November 6-7, Hurdalsjøen, Norway

Motivation

Nitric acid production is a three-step process at 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 or costly recovery, an optimized recovery system is required. This is targeted in WP1.1 and WP1.2 through investigating the fundamental aspects of PGM species volatilization and transport, as well as the surface decomposition, 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 the capital investment and increase the energy recovery by replacing the bulky homogeneous oxidation by a compact, heterogeneously catalyzed process.

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

The exothermic nature of the ammonia oxidation reaction results in large quantities of platinum loss in form of PtO_2 vapor. Evaporated PtO_2 is transported downstream before capture by a Pd-Ni catchment gauze. In ex-situ lab scale experiments, performed in our new six-zone furnace system, we are re-creating plant conditions with the aim to understand the underlying mechanisms for the reconstruction of the Pd-Ni catchment gauze. Preliminary results indicate fast oxidation of Ni to NiO, mainly along grain boundaries. Furthermore, in presence of steam, the Pd-Ni wire is depleted in NiO, probably leaving the wire as volatile $Ni(OH)_2$. Notably, reconstruction of grains and pore formation is observed only when PtO_2 is present in the gas stream (see images below). The present results show that we through these simple lab scale ex-situ experiments now are able to reproduce the reconstruction observed in the industrial Pd-Ni catchment gauzes. We are thus in position to harvest data that provide us with key information on the reconstruction mechanism.

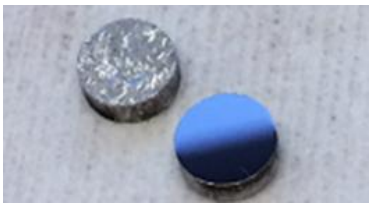


Left panel, six-zone furnace system suited for re-creating relevant plant conditions. Right panel, electron microscopy samples images (overview and cross-section close-up) obtained by focused ion beam sample preparation from a Pd-Ni wire treated for 1 month with Pt upstream in a wet oxidizing gas.

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

A dedicated six-zone reactor system is used for generating volatile PtO_2 species and subsequent catchment on pure Pd and Pd-Pt alloy materials. The furnace is optimized to provide temperature gradients in the range 800-1200 °C, representative of those that may prevail between the location of Pt volatilization in the ammonia oxidation and the catchment gauze in the industrial process.

An analysis "tool box" including EBSD, SIMS, WLI and SEM* was established and put into operation by evaluating a series of polycrystalline Pd and Pt-Pd alloy model samples. The methodology developed is currently utilized for evaluation of Pt-diffusion profiles in these model catchment materials. The surface crystallographic orientation of fresh samples is first mapped by EBSD. Catchment experiments are thereafter performed, and diffusion profiles are obtained on grains with different crystallographic orientation. Recent results show overall consistent Pt-diffusion profiles for the Pd and 60Pd40Pt (wt.%) model samples. Improved methodology for studying high Pt content Pt-Pd alloys is in progress.

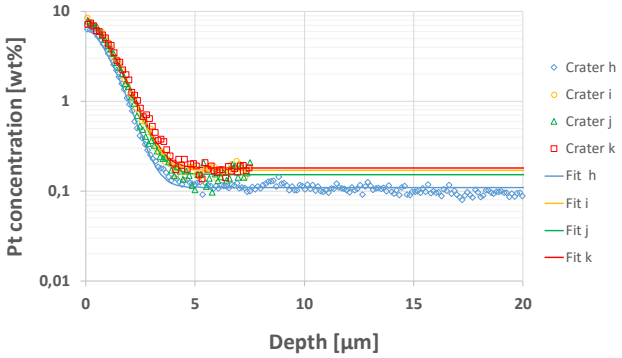


Averages for grain 4 (95% confidence intervals):

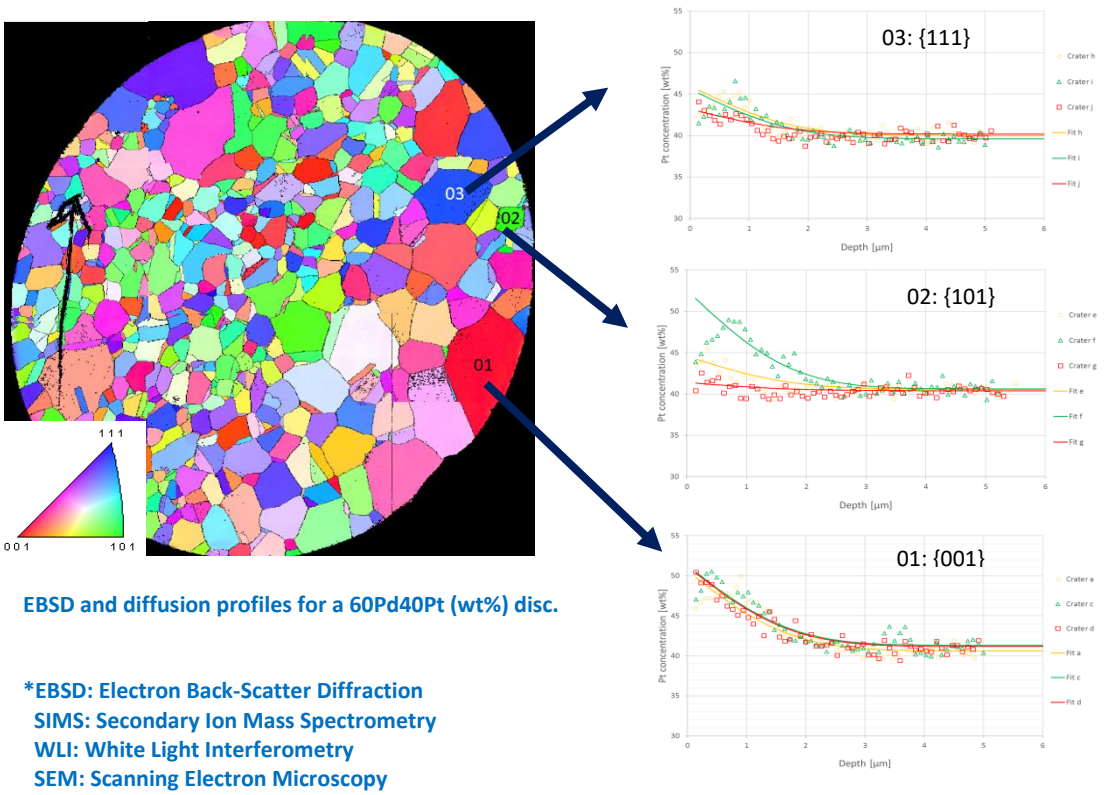
Bulk concentration: (0.15 ± 0.03) wt%

Surface concentration: (8.4 ± 0.6) wt%

Diffusion coefficient: (1.1 ± 0.1)·10^{-5} µm²/s



Diffusion profiles obtained for one grain of a 100% Pd disc. 24 hours exposure time.



EBSD and diffusion profiles for a 60Pd40Pt (wt%) disc.

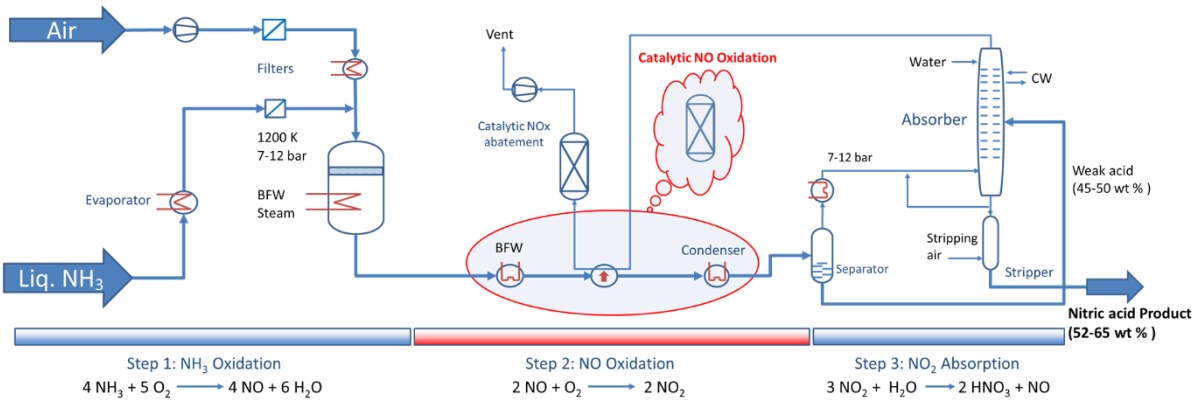
***EBSD: Electron Back-Scatter Diffraction**
SIMS: Secondary Ion Mass Spectrometry
WLI: White Light Interferometry
SEM: Scanning Electron Microscopy

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

Replicating the demanding conditions of industrial NO oxidation in a laboratory reactor is challenging. NO oxidation is a homogenous gas phase reaction favored by high concentration of NO. In order to study the kinetics of the catalytic reaction, minimizing contributions from gas phase reaction is crucial. An experimental setup capable of investigating catalysts for NO oxidation under both engine exhaust and industrial conditions has been designed and validated.

Catalytic oxidation of nitric oxide over supported platinum catalysts using a dry feed (10% NO, 6% O_2) was studied. A kinetic model has been established, and apparent activation energies and reaction orders were determined. A reaction mechanism is proposed based on observed experimental results and the rate expression.

Several catalytic materials are currently under investigation for NO oxidation. Transition metal oxides and perovskites are being explored and compared to noble metal catalysts. The most promising catalysts are currently being tested in presence of water (15% H_2O).



Process flow diagram of a single pressure nitric acid plant indicating substitution of gas phase NO oxidation with a compact catalytic converter.

Manuscript in preparation

Salman, Ata ul Rauf; Enger, Bjørn Christian; Auvray, Xavier; Lødeng, Rune; Menon, Mohan; Waller, David; Rønning, Magnus, **Catalytic oxidation of NO to NO_2 for nitric acid production over a Pt/Al_2O_3 catalyst**

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

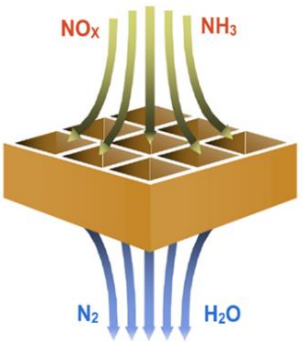
The Team in 2017

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)
Roman Tschentscher	SINTEF	Researcher (WP2.1)
Arne Karlsson	SINTEF	Researcher (WP2.1)
Knut Thorshaug	SINTEF	Researcher (WP2.1)
Patricia Almeida Carvalho	SINTEF	Researcher (WP2.1)
Joachim Graff	SINTEF	Researcher (WP2.1)
Martin F. Sunding	SINTEF	Researcher (WP2.1)
Karl Isak Skau	YARA	Industry researcher (WP2.1)

Oral contribution

Håkonsen, Silje F.; Skau, Karl Isak; Waller, David; Arstad, Bjørnar; Sunding, Martin F.; Graff, Joachim S.; Tschentscher, Roman; Diplas, Spyros; Karlsson, Arne; Cavka, Jasmina; **Poisoning of vanadia-based catalysts for selective catalytic reduction (SCR) of NOx,** ICSI seminar, November 6-7, Hurdalsjøen, Norway

Motivation



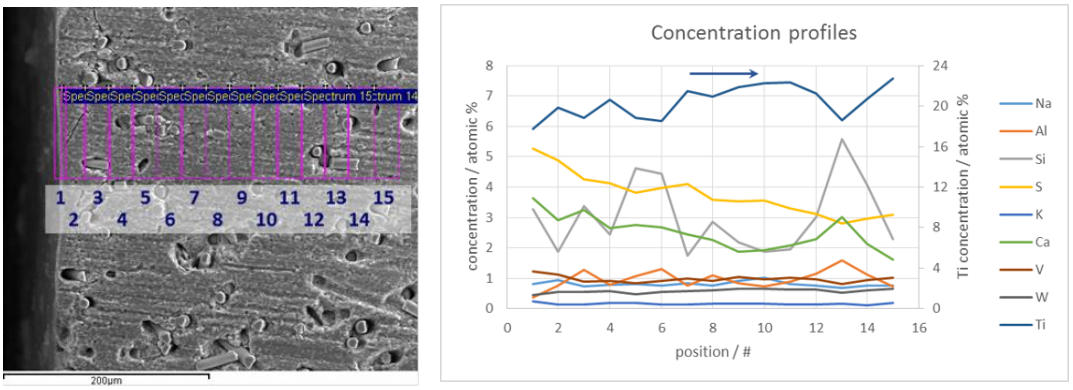
Selective catalytic reduction (SCR) is a core technology in the treatment of Nitrogen oxides (NOx) in exhaust from stationary power generation (coal, oil and gas), nitric acid production, and heavy-road vehicles. The application in marine machinery is an emerging market due to stricter emission regulations. The most common SCR catalyst technology for power and marine applications is based on vanadium oxides combined with other oxides; typically supported on monolithic structures to allow high throughput and minimum pressure drop for the reduction of NOx with ammonia (NH_3). Catalyst lifetimes may be as long as 5 years, but vary due to differences in their exposure to poisons, dust and soot. In oil and marine applications, sulphur levels may be high (up to 5%), increasing the risk of degradation of the catalyst's performance.

It is therefore desirable 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 may instead involve the addition of an active phase to recover more of 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 catalyst deactivation mechanisms by thorough characterization of the catalyst at different stages of the its lifetime, and then translating this knowledge into new measures.

Results and conclusions

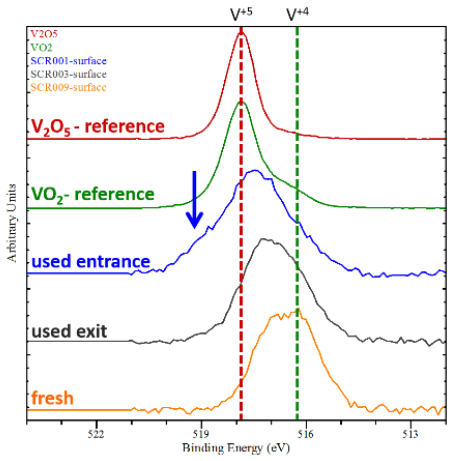
The studied SCR catalyst consists of anatase TiO_2 as a support material, WO_3 as a promoter for activity and stability, and V_2O_5 as the active redox species. The monolith itself also contains significant amounts of binder materials used in the extrusion process of the structured catalyst. A toolbox consisting of a range of different characterization techniques has been developed in order to gain better understanding of the structural and chemical changes in marine SCR catalysts during operation. These changes will in the next step be linked to the performance of the catalyst.

The spent SCR catalysts have been studied by using electron microscopy (EM) combined with Energy-dispersive X-ray spectroscopy (EDS) on a cross-section of the monolith wall. The results from a SCR catalyst used in a marine application are presented below. EDS analysis from different areas of the cross-section reveals that the concentration profile through the wall is relatively uniform for most of the elements present. An exception is Ca and S, which display enrichment towards the surface. Both scanning (SEM-EDS) and transmission (TEM-EDS) electron microscopy analysis show that these two elements are associated, and x-ray diffraction (XRD) confirms the presence of $CaSO_4$. The catalyst also showed some enrichment of vanadium (V) at the surface that most likely originates from the fuel.



Concentration profile through the monolith wall.

X-ray photoelectron spectroscopy (XPS) was performed on a spent SCR catalyst from a marine application. Analyses were made of both the entrance side and exit side of the monolith to see if there were any differences in the vanadium oxidation state relative to how heavily the catalyst has been poisoned. The $V2p_{3/2}$ spectra were then compared to the corresponding spectrum of a fresh catalyst and the spectra from two vanadium oxide references. The results show that all three catalyst samples contain a mixture of V^{+5} and V^{+4}. A surprising result is that the fresh catalyst sample contains a higher amount of V^{+4} than the used samples. The used entrance sample also displays an additional contribution (shoulder) on the high binding energy side (marked with a blue arrow). This indicates formation of vanadium species other than V_2O_5 and V_2O_4.



XPS $V2p_{3/2}$ spectra

IIA 3 Frontier formalin technology development

The Team in 2017

Jasmina Hafizovic Cavka	SINTEF	IIA leader
Kristin Bingen	DYNEA	Industrial senior, industry researcher (WP3.1-3.2-3.3), WP responsible (3.2)
Hilde Venvik	NTNU	PhD supervisor, WP responsible (WP3.1), advisor (WP3.3)
Terje Pedersen	KA Rasmussen	Industrial senior, industry researcher (WP3.1)
Johan Skjelstad	KA Rasmussen	Industrial senior, industry researcher (WP 3.1)
Thomas By	KA Rasmussen	Industry researcher (WP3.1)
Herdis Petersson	DYNEA	Industry researcher (WP3.2-3.3)
Jia Yang	NTNU	PhD co-advisor (WP3.1),
Stine Lervold	NTNU	PhD student (WP3.1)
Rakel Johanne Ekholt	NTNU	Master student (WP3.1)
Nicolas Beck	KIT/NTNU	Master student (WP3.1)
Kamilla Arnesen	NTNU	Master student (WP3.1)
Rune Lødeng	SINTEF	PhD supervisor (WP3.1), researcher (WP3.2-3.3)
Roman Tschentscher	SINTEF	Researcher (WP3.2-3.3)

Oral contribution

Lervold, Stine; Beck, Nikolas; Yang, Jia; Lødeng, Rune; Bingen, Kristin; Pedersen, Terje; Venvik Hilde Johnsen, **Reactor for investigation of the Ag based MTF process,** iCSI seminar, November 6-7, Hurdalsjøen, Norway

Poster contribution

Lødeng, Rune; Yang, Jia; Lervold, Stine; Bingen, K.; Venvik, Hilde Johnsen, **Global models for predicting methanol to formaldehyde (MTF) performance,** iCSI seminar, November 6-7, Hurdalsjøen, Norway

"The reaction data illustrate that we can run methanol partial oxidation experiments at low conversion (kinetic regime) while maintaining a formaldehyde selectivity >90%!"

(PhD student, Stine Lervold).

Motivation

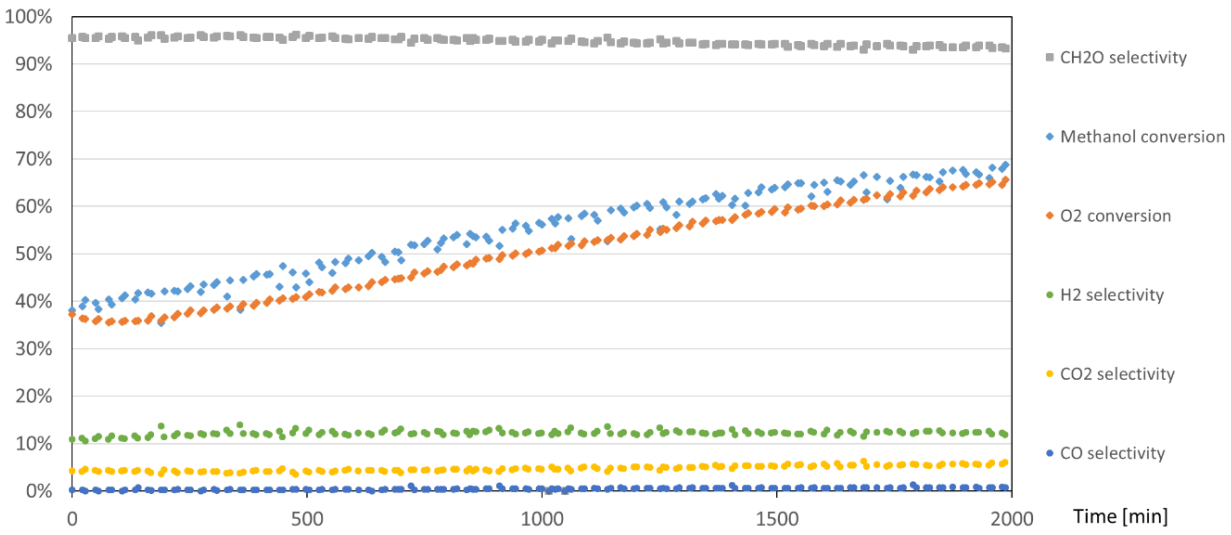
Formalin is a base chemical that is widely used for adhesives and resins applied in the wood industry and as an important intermediate for several specialty chemicals. Production proceeds by catalytic oxidation of methanol to formaldehyde, in excess air over a mixed metal oxide catalyst or excess methanol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

Improving selectivity is the main target, and because of the fast and exothermic nature of the reactions involved, it requires control of the heat and mass transfer phenomena as well as the surface chemistry proceeding on the silver. Gas phase chemistry also plays a role at operation temperatures typically exceeding 600°C, where also structural changes occur in the Ag catalyst 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, and depends 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 environment and tuning of the silver particle/bed morphology, thus controlling both selectivity and stability.

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

Results and conclusions

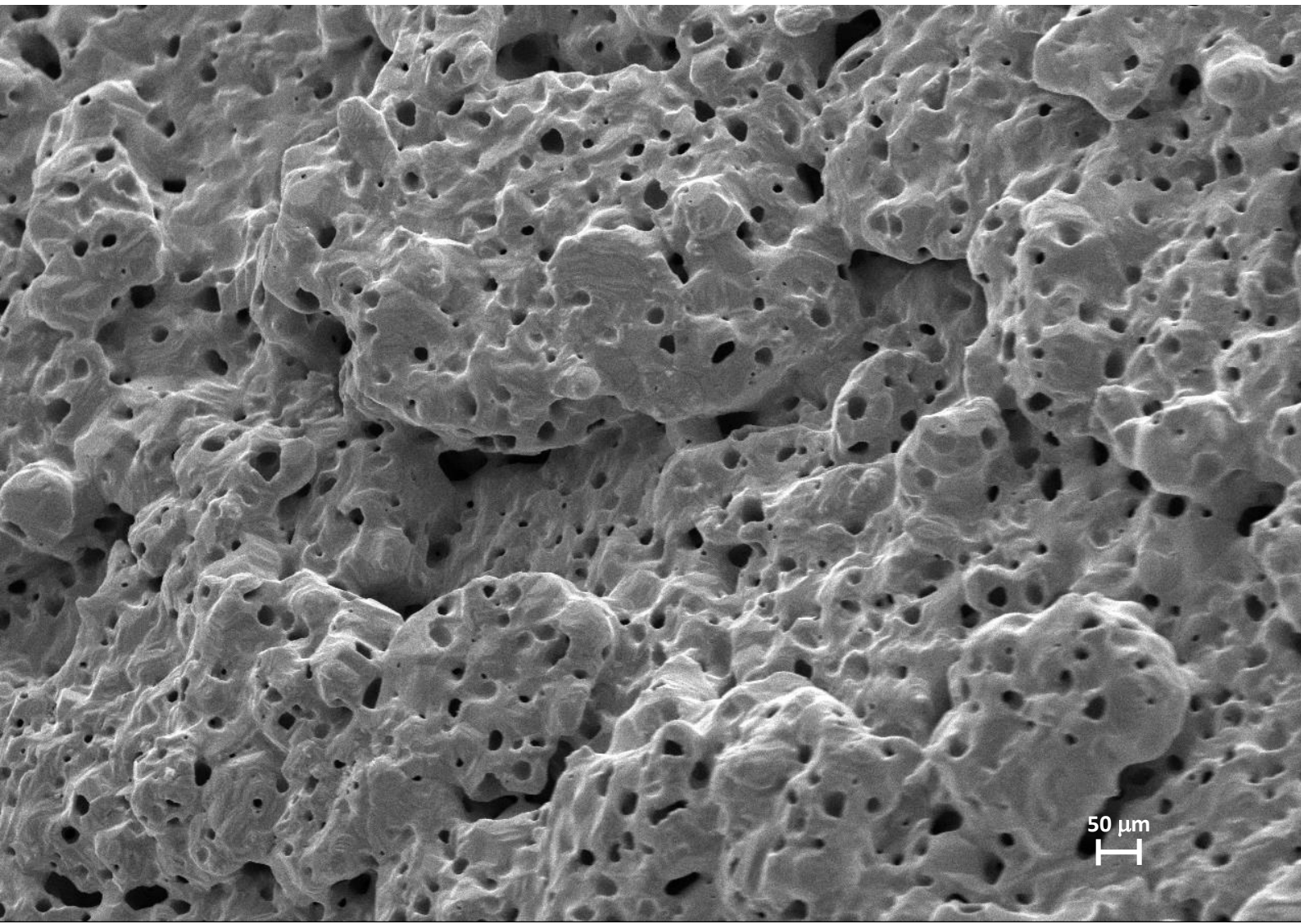
Two complementary experimental set-ups have been established for acquiring high precision data. One is optimized for kinetic studies at laboratory scale (reactor 1) and targets close control of the heat and mass transfer, while the other is designed for screening of parameters at industrial conditions (reactor 2). The figure below shows the conversion and selectivity obtained in reactor 1 as a function of time on stream in a selected period upon reacting methanol with oxygen at ~625°C.



The reaction data illustrate that the Reactor 1 concept can be operated at low conversion (kinetic regime) while maintaining a high selectivity to formaldehyde. The formation of CO is suppressed and the continuous restructuring of the Ag catalyst at pseudo steady-state is also captured.

Systematic investigations of structural changes in the silver catalyst due to the reaction conditions have also been performed. These changes can be linked to catalyst performance and reaction mechanisms taking place on the silver surface. A scanning electron microscope (SEM) image of the silver surface after 15 days under reaction conditions is shown at the bottom of the page, illustrating a high degree of material restructuring and pin-hole formation.

Reactor 2 was optimized to give high precision data at most demanding industrial conditions. The effect of various process parameters was studied, as for instance reactant molar ratio, bed geometry and gas velocity. Finally own data in combination with literature data were used to establish global models for predicting methanol to formaldehyde performance. These initial models will be refined and improved as more data are being generated. The results are of high value for the industrial partner Dynea and will be used for fine-tuning of formaldehyde process plants.



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

The Team in 2017

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)
André Urke Kvamme	INOVYN	Industry researcher (WP4.1-4.2-4.3)
Endre Fenes	NTNU	PhD student NTNU (WP4.1)
Hongfei Ma	NTNU	PhD student NTNU (WP4.3)
Erling Olav Sollund	NTNU	Master student (WP4.1)
Kumar R. Rout	SINTEF	Researcher (WP4.2), advisor (WP4.1-4.3)

Published papers:

1) Baidoo, Martina Francisca; Fenes, Endre; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De, **On the effects of K and La co-promotion on $CuCl_2/\gamma\text{-}Al_2O_3$ catalysts for the oxychlorination of ethylene**, *Catalysis Today*, 2017, 299, 164-171
2) Rout, Kumar Ranjan; Baidoo, Martina Francisca; Fenes, Endre; Zhu, Jun; Fuglerud, Terje; Chen, De, **Understanding of potassium promoter effects on oxychlorination of ethylene by operando spatial-time resolved UV–vis–NIR spectrometry**, *Journal of Catalysis*, 2017, 352, 218-228

Oral contributions:

1) Fenes, Endre; Baidoo, Martina Francisca; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De, **Rational Design of $CuCl_2/Al_2O_3$ based Oxychlorination Catalysts**, NAM25 | North American Catalysis Society Meeting, 2017, June 4-9, Denver, USA
2) Fenes, Endre; Baidoo, Martina Francisca; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De, **First Ionization Energy as a Descriptor of Alkali Metals promoted Oxychlorination Cu-based Catalyst,** 13th Europacat 2017, August 27-31, Florence, Italy

Motivation

The $CuCl_2/\gamma\text{-}Al_2O_3$ 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.

The oxidation state of the Cu catalysts at steady-state depends on the kinetic balance between the rates of reduction and oxidation. A main challenges in this process is that Cu^{I}, due to its low melting temperature and volatility, causes aggregation and loss of active surface. Compounds of alkali metals like K and Na and/or rare earth metals like 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-

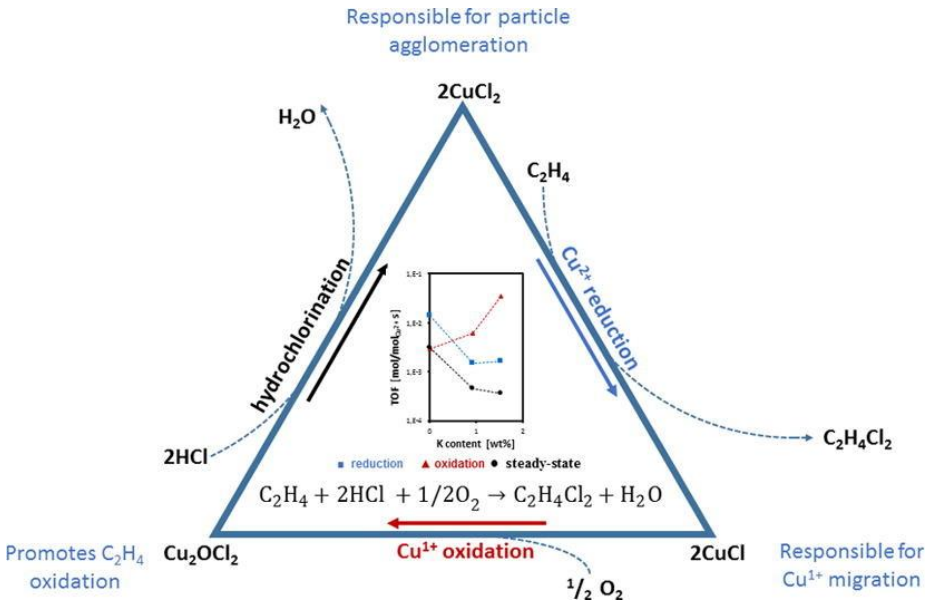
state kinetic investigations is used to obtain kinetic models for prediction of the reaction rate and the copper oxidation state under steady state conditions.

Another aim is to develop one- and two-dimensional non-isothermal models in order 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, and pressure drop, will be evaluated.

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

The work package focuses on additive effects, i.e. the impact of alkali, alkali earth and lanthanide elements on turnover frequency, catalytic activity, selectivity and stability of the $CuCl_2/\gamma\text{-}Al_2O_3$ based catalyst. The analysis capability of our in-house developed operando setup, combining mass- and UV-Vis-NIR spectrometry, has significantly increased during the last year. A corrosion resistant gas chromatograph has been added alongside increased capacity for temperature programmed reduction. Application of additional characterization techniques such as infrared-, Raman- and x-ray photoelectron spectroscopy was also implemented in an effort to investigate the nature of oxygen in the catalyst.

Mapping the Cu^{II}/Cu^{I} ratio of the oxychlorination catalyst by X-ray absorption spectroscopy (XAS) will be performed during beam time at ESRF. An operando study using XAS techniques (XANES and EXAFS) will be done in order to further validate our novel approach of kinetic rate diagram used for rational catalyst design of $CuCl_2$ oxychlorination catalysts. Both transient and steady-state reaction experiments will be performed to improve the understanding of the distribution of Cu valence states during the reaction, and promoter (K, La, Cs and La) effects on the Cu oxidation states using XRD and XAS. Efforts will be made to investigate the oxidation state of the promoters during reaction, of which little is known this far.



Reactor Modelling (WP4.2):

A master student is currently working in collaboration with SINTEF on kinetic- and multi-scale reactor modelling based on laboratory kinetic data. The aim is to reproduce temperature profiles provided by INOVYN from an industrial reactor. 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.

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

In this research activity we will establish a method for in situ investigations of Cu migration and carbon formation on the $CuCl_2$ based catalysts. Through coupling the characterization data with the kinetics of Cu migration and coke formation, a detailed understanding of the deactivation mechanism can be established. Furthermore, the effects of promoters such as K, Li, Ce, Mg and La on the Cu migration and carbon and byproduct formation will be studied. Eventually, the aim is to perform kinetic modeling of the Cu migration that incorporates the relationship of Cu^{2+}/Cu^{+1}.

This part of the project was initiated during the last part 2017. Since the work will pay special attention to copper mobility and fixation on the support, we are designing a new setup with larger catalyst capacity. This will be better suited for mapping spatial copper oxidation state variations within both fixed bed reactors and individual catalyst pellets, using one or more *in situ* UV-Vis spectrometers. Since water is formed during the reaction, a H_2O feed will be added to investigate possible effects on the reaction kinetics. We have been preliminary limited to HCl-free experiments due to the extremely corrosive nature of humid hydrochloric acid. Additionally, recognizing that our existing methodology for quantitative UV-Vis analysis and prediction of catalyst steady-state performance might have application to several catalytic systems with cyclic redox processes, we have opted to extend the number of connections in the new setup to accommodate both iCSI- and external research cooperation on related systems. We expect the setup to be fully functioning during 2018.

Manuscripts in preparation

1. Fenes, Endre; Baidoo, Martina M.; Ma, Hongfei; Rout, Kumar R.; Fuglerud, Terje; Chen, De, **New approach of kinetic modelling and analysis of catalytic cycle: evolution of production and catalyst composition in ethylene oxychlorination on $CuCl_2/\gamma$ -Al_2O_3**

2. Rout, Kumar R.; Fenes, Endre; Ma, Hongfei; Fuglerud, Terje; Chen, De, **Modelling and Simulation of oxychlorination Fixed bed reactor: Effect of process parameters**

IIA 5 The next step in direct activation of lower alkanes

The Team in 2017

Stian Svelle	UiO	IIA Leader, PhD supervisor, WP responsible (WP5.1-3)
Pablo Beato	HTAS	Industrial senior, Industry researcher (WP5.1-3), PhD supervisor (WP5.1)
Unni Olsbye	UiO	PhD supervisor (WP5.1-2)
Dimitrios Pappas	UiO	PhD student (WP5.1-2)
Michael Dyballa	UiO	Postdoctoral fellow (WP5.1-3)
Karoline Kvande	UiO	Master student (WP5.1-2)
Lars Fahl Lundegaard	HTAS	Industry researcher (WP5.1)
Ton Janssens	HTAS	Industry researcher (WP5.2-3)
Bjørnar Arstad	SINTEF	Researcher (WP5.3)

Published papers

1) Pappas, Dimitrios; Borfecchia, Elisa; Dyballa, Michael Martin; Pankin, Ilia A.; Lomachenko, Kirill A.; Martini, Andrea; Signorile, Matteo; Teketel, Shewangizaw; Arstad, Bjørnar; Berlier, Gloria; Lamberti, Carlo; Bordiga, Silvia; Olsbye, Unni; Lillerud, Karl Petter; Svelle, Stian; Beato, Pablo, **Methane to methanol: structure-activity relationships for Cu-CHA**, *Journal of the American Chemical Society*, 2017, 139, 42, 14961-14975

2) Pappas, Dimitrios; Borfecchia, Elisa; Dyballa, Michael Martin; Pankin, Ilia A.; Lomachenko, Kirill A.; Martini, Andrea; Signorile, Matteo; Teketel, Shewangizaw; Arstad, Bjørnar; Berlier, Gloria; Lamberti, Carlo; Bordiga, Silvia; Olsbye, Unni; Lillerud, Karl Petter; Svelle, Stian; Beato, Pablo, **XAS reveals structure-activity relationships for the Methane-to-Methanol conversion over Cu-zeolites,** *ESRF Highlights 2017,* 49-51

Oral contributions

1) Pappas, Dimitrios; Borfecchia, Elisa; Dyballa, Michael Martin; Pankin, Ilia; Lomachenko, Kirill A.; Berlier, Gloria; Arstad, Bjørnar; Lamberti, Carlo; Bordiga, Silvia; Beato, Pablo; Olsbye, Unni; Svelle, Stian, **Key Reaction Steps in the Partial Oxidation of Methane to Methanol over Cu-SSZ-13**, NAM25 | North American Catalysis Society Meeting, 2017, June 4-9, Denver, USA
2) Berlier, Gloria; Borfecchia, Elisa; Negri, C; Bordiga, Silvia; Beato, Pablo; Lomachenko, Kirill A.; Pankin, Ilia; Lamberti, Carlo; Pappas, Dimitrios; Dyballa, Michael Martin; Olsbye, Unni; Svelle, Stian, **Comparing small and large pore Cu-zeolites for the partial oxidation of methane to methanol: operando spectroscopic study**, Congress on Oxidation Catalysis; September 3-8, Krakow, Poland
3) Pappas, Dimitrios; Borfecchia, Elisa; Dyballa, Michael Martin; Lomachenko, Kirill A.; Signorile, Matteo; Berlier, Gloria; Lamberti, Carlo; Bordiga, Silvia; Olsbye, Unni; Lillerud, Karl Petter; Svelle, Stian; Beato, Pablo, **Searching for the Active Sites Responsible for the CH_4 to CH_3OH Conversion over Cu-Chabazite Materials**, Norwegian Catalysis Symposium 2017; November 6-7, Hurdalsjøen, Norway

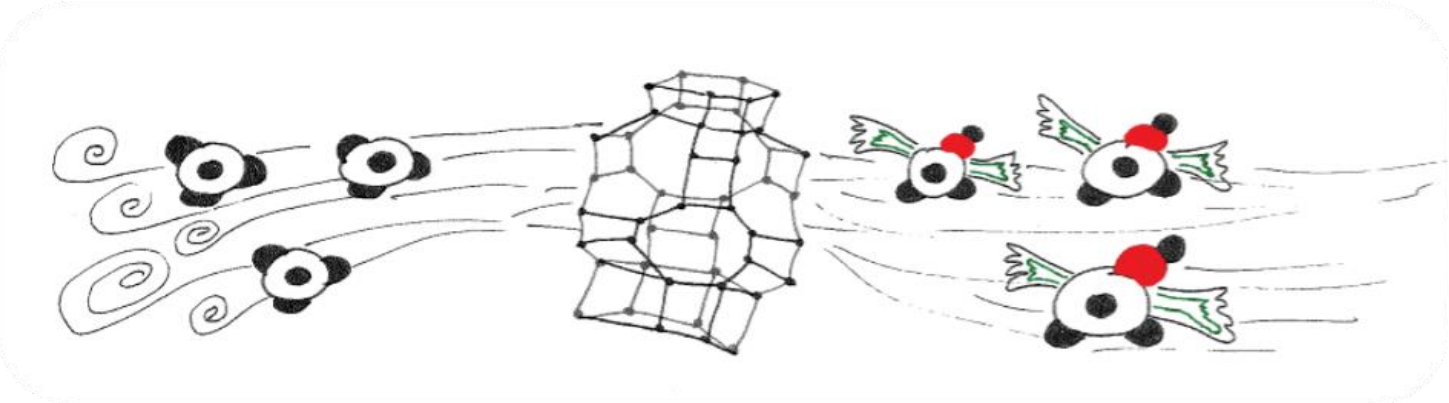
Poster contributions

1) Dyballa, M.M.; Arstad, B.; Pappas, D.; Svelle, S.; Olsbye, U.; Beato, P.; Bordiga, S.; Borfecchia, E., **On the preparation of Cu-containing Zeolites - How to avoid comparing Apples to Oranges,** NAM25 | North American Catalysis Society Meeting, 2017, June 4-9, Denver, USA.
2) Kvande, K., **Direct conversion of methane to methanol**, Norwegian Catalysis Symposium 2017; November 6-7, Hurdalsjøen, Norway
3) Pappas, D.; Borfecchia, E.; Dyballa, M. M.; Lomachenko, K. A.; Signorile, M.; Berlier, G.; Lamberti, C.; Bordiga, S.; Olsbye, U.; Lillerud, K. P.; Svelle, S.; Beato P., **Searching for the Active Sites Responsible for the CH_4 to CH_3OH Conversion over Cu-Chabazite Materials,** Norwegian Catalysis Symposium 2017; November 6-7, Hurdalsjøen, Norway

Motivation

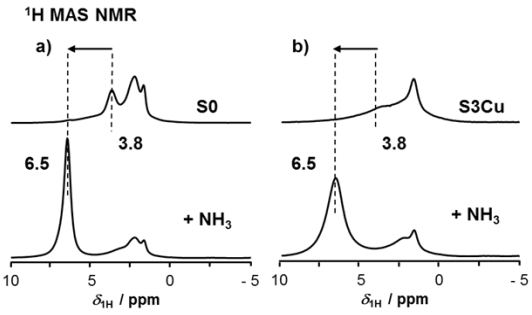
Researchers at UiO and Haldor Topsøe AS join forces for developing new nanostructured catalyst materials. Therefore, they try to reveal the mechanism of the direct conversion of lower alkanes to chemicals or liquid fuels over copper-doped zeolite catalysts.

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



"Giving Methane Wings", drawing by Master student Karoline Kvande (UiO)

Synthesis of new zeolite catalysts – Postdoctoral fellowship



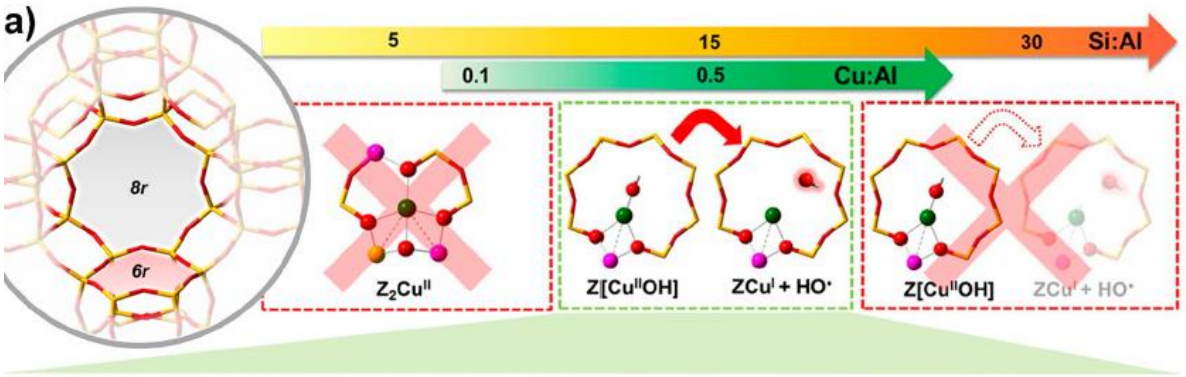
^{1}H MAS NMR spectroscopy performed at SINTEF, Oslo, NO. Use of a new-installed setup for probe-loading zeolite catalysts useful for example for the quantification of acidity. Here ammonia loaded on copper-exchanged SUZ-4 catalysts.

As a follow-up to 2016 we thoroughly investigated the developed catalyst library in terms of physicochemical properties and catalytic performance. This included use of *operando* XAS measurements during multiple stays at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, with our external cooperation partners from Torino, Italy and from Haldor Topsøe, Denmark. The collaboration with SINTEF in terms of MAS NMR (Magic Angle Spinning – Nuclear Magnetic Resonance Spectroscopy) spectroscopy was further extended and the tool used for the characterization of acid properties of catalysts as well as the zeolite framework stability. SUZ-4 catalysts were investigated in terms of their reactivity in the methane oxidation reaction. The low activity of the topology could be assigned to partial pore blocking and an unfortunate strong copper binding in paired aluminum sites in the 6-membered rings of the SZR topology. For 2018, additional studies on the reaction mechanism of the methane conversion reaction are planned. These measurements will include *in situ* Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) available through the cooperation partner SINTEF in Oslo, Norway.

Catalytic performance – PhD project

Our newly synthesized catalysts were successfully tested and found active in the conversion of methane to methanol. First results on Cu-exchanged SSZ-13 zeolites that were supplied by Haldor Topsøe AS or synthesized at UiO were successfully summarized and published in 2017. Also the catalytic performance of Mordenite-based copper catalysts was evaluated. The results are currently evaluated with respect to the catalyst properties and will be finalized in 2018.

During 2018, the focus of further investigations will be on copper exchanged Ferrierite-based catalysts as well as SAPO-34 catalysts (CHA topology) synthesized by varying approaches.



Rationalization of the effect of composition (Cu/Al and Si/Al ratios) on the productivity for the methane-to-methanol conversion over Cu-SSZ-13 as part of combined catalytic and *operando* XAS measurements.

Paper coming soon

Dyballa, Michael; Pappas, Dimitrios K.; Borfecchia, Elisa; Beato, Pablo; Olsbye, Unni; Lillerud, Karl Petter; Arstad, Bjørnar; Svelle, Stian, **Tuning the material and catalytic properties of SUZ-4 zeolites for the conversion of methanol or methane**, Microporous and Mesoporous Materials, **submitted.**

IIA 6 Generic projects for additional industrial synergies.

The Team in 2017

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)

Oral contribution

Ivashenko, Oleksii; Zheng, Jian; Fjellvåg, Helmer; Sjåstad, Anja Olafsen, **Operando Investigations of Surfaces for NO_x Abatement Catalysis**, International Conference on Advances in Functional Materials, 2017, January 6-8, Chennai, India

Motivation

Some iCSI work packages have been allocated to research unspecific to a particular technology, with the intention of moving the research forefront and providing a methodological basis for the industrial innovation areas IIA1 to 5. In particular, advanced spectroscopic and microscopic investigations under conditions highly relevant to industrial operation are targeted. The second pillar in this effort is to advance 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)

The aim of this research is to study heterogeneous catalytic systems, combining both the acquisition of kinetic and structural information in the same setup at the same time. Such an approach, although challenging, could bring more mechanistic insights to kinetic modelling and subsequently make more accurate predictions of the relevant kinetic steps. The key characterization techniques in this project – X-ray absorption spectroscopy and X-ray diffraction with synchrotron radiation, Fourier-transform infrared spectroscopy and Raman spectroscopy – can be combined 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.

In 2017, three visits to the Swiss-Norwegian Beamlines (SNBL) at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, with a total of 54 shifts, allowed collection of data on a number of heterogeneous catalysts for NO oxidation as well as the selective catalytic reduction (SCR) of NO and NO_2.

Two master students are affiliated with the research. They are working on challenges with operando DRIFTS studies of ammonia SCR over mesoporous alumina based catalysts, and with in situ Raman spectroscopy of perovskites for NO oxidation.

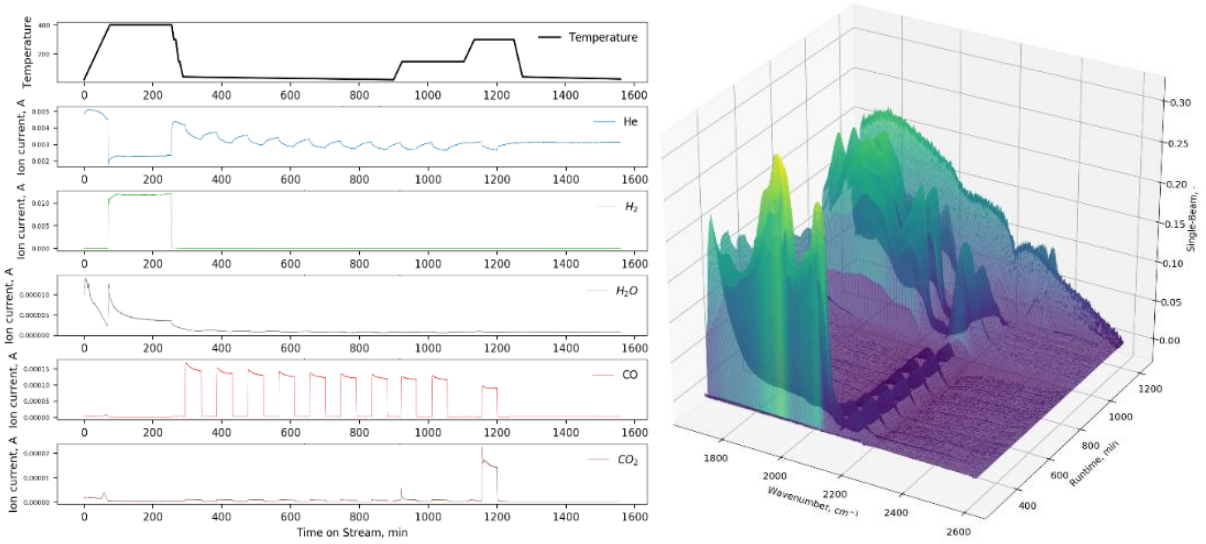


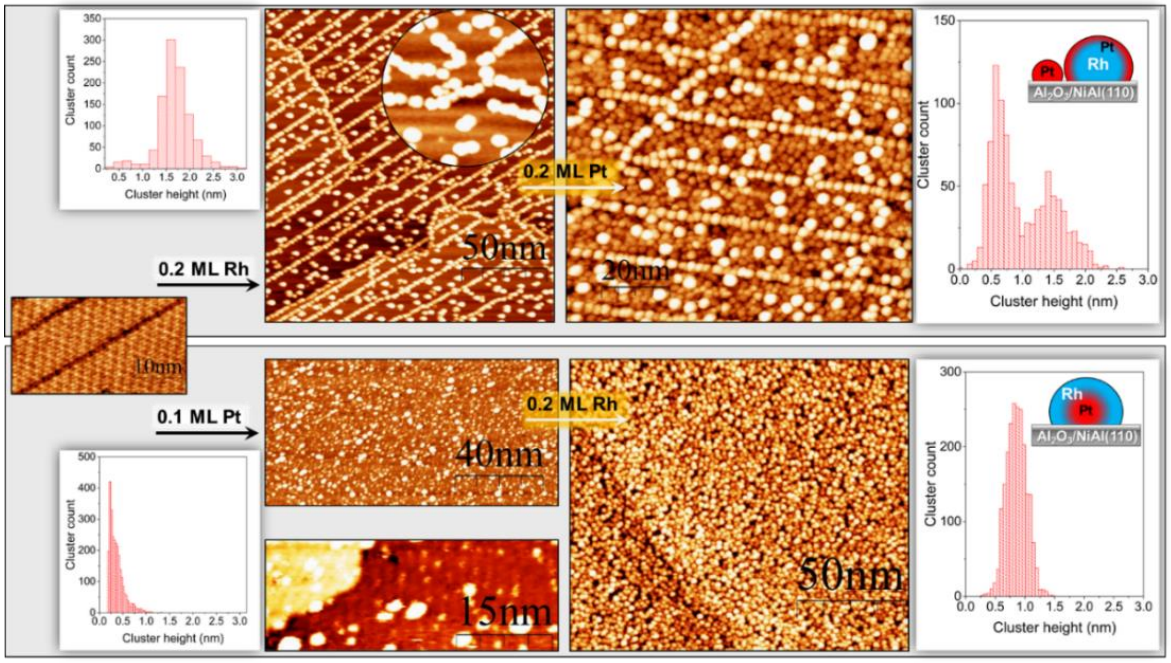
Figure 1. Example of DRIFTS study (right panel) of time resolved in situ adsorption and desorption of carbon monoxide in helium on Ni on a hydrotalcite derived support at different temperatures over time with monitoring of downstream gas composition using mass spectrometry (left panel).

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 subsequently utilized in surface sensitive operando studies by means of Reactor-STM (Scanning Tunneling Microscopy) and (near) ambient-pressure photoelectron spectroscopy (APPES).

Currently we have recipes at hand that provide well-defined bimetallic Co-Re[1] and Pt-Rh nanoparticles supported on Al_2O_3/NiAl(110). The surfaces are suited as model catalysts for Fischer-Tropsch synthesis and ammonia oxidation, respectively. Some recent results obtained for Pt-Rh/Al_2O_3/NiAl(110) are presented in the figure below. Another effort has been towards the preparation of PtRh/Pt(111) surfaces for exploring the role of Rh in the PtRh alloy for intermediate temperature ammonia oxidation[2]. This includes STM imaging at UHV and elevated oxygen pressure (~2 bar). Obtained model surfaces were also studied using APPES at the Advanced Light Source at Berkeley, in collaboration with international partners at Lund University/MAXIV and Leiden University.

An important decision in 2017 is to host an international meeting on ***Operando Surface Catalysis Methods*** in Oslo at the beginning of 2019. Funding has been obtained from the Research Council of Norway NANO2021 program, and an international scientific committee has been appointed.



Sequential deposition of Pt and Rh on Al_2O_3/NiAl(110) can yield two distinct morphologies observed using Reactor STM. Top: Rh followed by Pt gives two types of particles pure Pt (smaller, 0.6 nm) and Rh mixed with Pt (larger, 1.5 nm). Bottom: Pt followed by Rh results in a uniform morphology containing mainly 0.8-1 nm clusters.

Papers coming soon

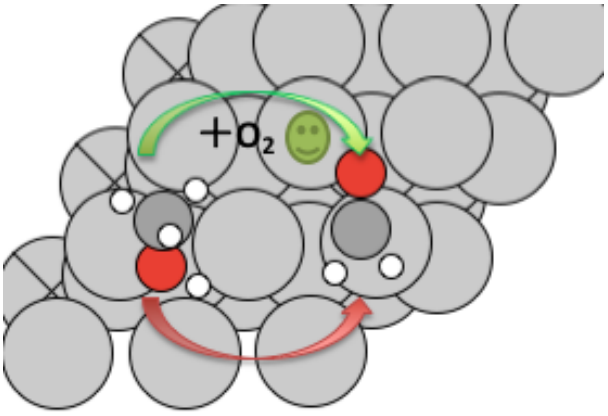
[1]Mom, R.; Ivashenko, O.; Frenken W.M.J.; Groot, I.M.N.; Sjåstad, A.O., **The Nucleation, Alloying, and Stability of Co-Re Bimetallic Nanoparticles on Al_2O_3/NiAl(110**), Journal of Physical Chemistry C, **Accepted**

[2]Zheng, J.; Ivashenko, O.; Fjellvåg, F.; Groot, I.M.N.; Sjåstad, A.O., **Well-Defined RhPt/Pt(111) Model Surfaces for Ammonia Oxidation, in preparation**

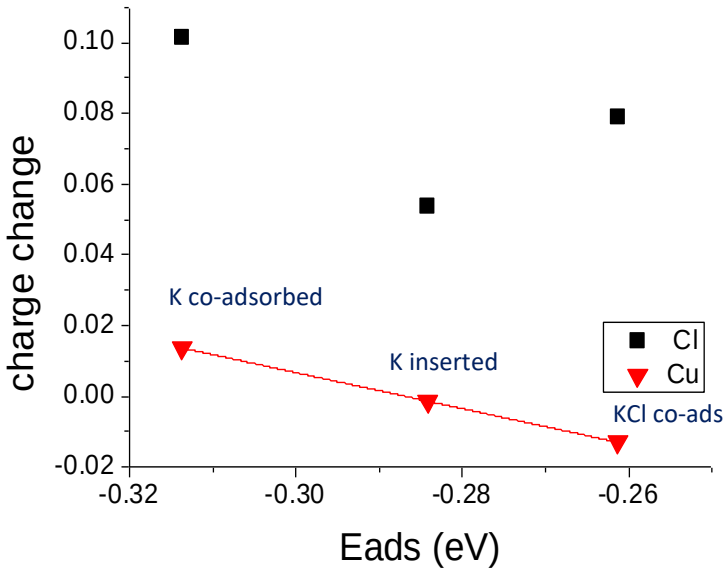
Reaction mechanism investigation by combined by density functional theory (DFT) calculations and microkinetic modelling – Postdoctoral fellowship (WP6.3)

Density functional theory (DFT) calculations are based on the fundamental mathematical description of how atoms interact; the Schrödinger equation. Assumptions and approximations are required to be able to model complex systems, but thanks to modern computer technology, this has reached an advanced stage. DFT can be used to describe surface reactions and provide so-called descriptors of catalytic activity and selectivity. Microkinetic modelling is utilized to investigate the reaction mechanism and predict information about surface coverages and relative rates of various elementary steps under reaction conditions. By the two methodologies, the project aims to bridge the gap from the atomic level to macro-scale kinetic analysis to be able to tailor catalysts atom by atom. This is currently being employed to understand the details of the alkali and/or rare earth promoter mechanism in the oxychlorination reaction (see IIA4, p. 30). With respect to formaldehyde formation (see IIA3, p. 27), the interaction between the Ag surface and oxygen surface species is being modelled to find a key to further tuning of the selectivity of the process.

The adsorption energies of the main species in the reaction of methanol and oxygen to formaldehyde over on Ag (211) and Ag (111) were obtained from DFT, and it was generally found that the adsorption on Ag (211) is stronger. Moreover, microkinetic modelling was performed to investigate the reaction mechanism and predict the relevant surface coverages and relative rates of different elementary steps under reaction conditions. It is found that adsorbed oxygen facilitates both the reaction rate and the selectivity towards the desired product, compared to direct dissociation of methanol (schematic figure, right). The effect of water on the selectivity to formaldehyde will be studied next.



Regarding oxychlorination of ethylene, the $CuCl_2$ catalyst promoter (i.e. potassium (K) and sodium (Na)) effect on ethylene adsorption has been investigated. From Bader charge analysis and analysis of charge density difference during K or Na adsorption on a $CuCl_2$ (100) surface surface it is found that adsorbed K or Na change the electronic distribution of the $CuCl_2$ surface and slightly enhances ethylene adsorption. The adsorption energy of ethylene with co-adsorbed K/KCl correlates to the charge change of surface Cu rather than Cl (figure, left). The K/Na promoter effect on oxychlorination of ethylene will be investigated further. Moreover, the interaction between the support (i.e. γ-Al_2O_3) and $CuCl_2$ will also be studied.



SINTEF Fundamental Catalysis Investigations

The SINTEF activity in the iCSI-associated EmX project (RCN Transport 2025 program, contract no. 246862) is focusing on CH_4 slip. The low-temperature catalytic combustion kinetics of CH_4 has been addressed for abatement of slip from LNG fueled machinery, though the challenge has wider perspectives.

Materials synthesized include co-precipitated mixed Ni-Co oxides of different metal ratios, with and NiO and Co_2O_4 as limits (NiO, Ni_2CoO_4, $NiCoO_4$, $NiCo_2O_4$, $Ni_{0.75}Co_{2.25}O_4$, $Ni_{0.5}Co_{2.5}O_4$, Co_3O_4). Noble metal based catalysts, i.e. 0.2 and 2wt.% of Pd and Pt on γ-Al_2O_3 were included as reference materials. Also subsequent impregnation 0.5wt.% Pd on $NiCo_2O_4$ spinel has been studied. The complete oxidation reaction was studied in a fixed-bed quartz reactor performing temperature heating and cooling cycles in the range 100 – 550 °C, covering the relevant temperature range, at GHSVs of 24000 ml/g.h. and 58800 ml/g.h. Feed compositions representative of methane containing exhaust, also relevant for marine LNG engines, were used. The CH_4 concentration was in the range 1000 – 20000 ppm, with 10% O_2, 10 – 15% H_2O, and N_2 as balance. In a pursuit of in-depth understanding of the origin of the catalytic activity, the morphology, structure and composition of the catalysts have been characterized by a range of techniques, including N_2-physisoption, X-ray diffraction (XRD), Raman spectroscopy, H_2 and CO chemisorption, X-ray fluorescence (XRF), temperature programmed reduction (TPR), and scanning/transmission electron microscopy (SEM-, TEM-EDS).

The observed order of performance was 2wt.% Pd/Al_2O_3 > 0.5%$Pd/NiCO_2O_4$ > mixed Co-Ni oxides ≈ Co_3O_4 > NiO > 2wt.% Pt/Al_2O_3. Activation energies (Ea = 80 ± 4 kJ/mol, for oxides and 0.5%$Pd/NiCO_2O_4$) were estimated. Dependencies of E_a upon the CH_4 and H_2O concentrations have been found. H_2O in the feed caused significant reduction in the activity (**Figure** below). This was, however, a reversible effect and could be explained by competitive adsorption. Kinetic parameters (A_{freq}, E_a) were estimated by fitting a simple power rate law with first order dependence in CH_4 and second order in O_2 to experimental data. Promising catalyst stability was shown in a test with duration over one month.

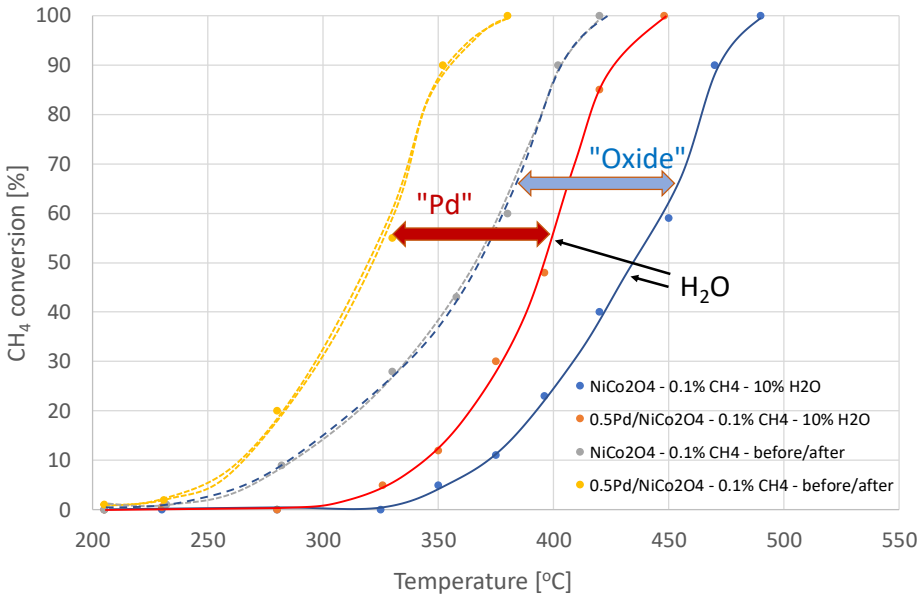


Figure: A comparison of catalytic combustion behavior at dry condition and with 10% H_2O in the feed for the $NiCo_2O_4$ and 0.5wt.%$Pd/NiCo_2O_4$ catalysts.

Internationalization 2017

Sabbatical leave

Professor Magnus Rønning (NTNU), Stanford University (US) *from July 2016 to June 2017.*
Professor De Chen (NTNU), Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai, China *from July 2017 to 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:

- ***ZeoMorph***, FP7-ITN-EID, 5 PhD projects, iCSI Partners involved: UiO/HTAS
- ***FASTCARD***, FP7-NMP-2017-LARGE-7, iCSI Partners involved: SINTEF/NTNU
- ***Horizon 2020 Projects: PrintCr3dit*** and ***ProDIA,*** iCSI Partner involved in both: SINTEF

Research Council of Norway projects with international collaborations:

- ***EmX 2025***, TRANSPORT 2025, iCSI Partners involved: NTNU/ SINTEF
- ***Development of Catalysts and Materials for Compact Steam Reformer***, GASSMAKS, iCSI Partners involved: NTNU/ SINTEF
- ***GAFT-Fischer Tropsch synthesis of biofuels***, EnergiX, iCSI Partner involved: SINTEF
- ***FutureFeed*** Nano 2021, iCSI Partners involved: SINTEF/ UiO
- ***Bio4Fuels,*** Centre for Environment-friendly Energy Research (FME), iCSI Partners involved: SINTEF/ NTNU

Communication and dissemination

iCSI Keynote lectures

Chen, De, **New Approach of Kinetic Modeling of Redox Catalytic Cycles: Study of Ethylene Oxy-chlorination Process**, the 8th Asian-Pacific Chemical Reaction Engineering Symposia (APCRE 2017), 2017, November 12-15, China

Chen, De, **Kinetics and design of catalytic redox cycles on MX (X=O, Cl),** National conference on catalysis, 2017, October 16-21, Tianjin, China

Olsbye, Unni, **Structure - composition - activity correlations for zeolites and zeotypes as alkene and arene methylation catalysts**, keynote lecture, EuCheMS Inorganic Chemistry Conference (EICC-4), 2017, July 2-5, Copenhagen, Denmark

iCSI associated invited lectures

Rønning, Magnus, **In situ characterisation of catalysts without compromising process conditions,** ESRF User Meeting, 2017, February 6-8, Grenoble, France

Holmen, Anders; Rytter, Erling, **Fischer-Tropsch Synthesis on Cobalt Catalysts – On the Effect of Water**, 253rd American Chemical Society National Meeting, April 2-6, San Francisco, California, USA

Chen, De, **Perspectives of low carbon technologies**, Zhanjiang conference on low carbon Technologies, 2017, August 1, Zhanjiang, China

Sjåstad, Anja Olafsen; Zacharaki, Eirini; Bundli, Silje; Jensen, Martin; Kalyva, Maria Evangelou; Dhak, Prasanta; Kooyman, Patricia J.; Bremmer, Marien G.; Slawiniski, Wojciech Andrzej; Fjellvåg, Helmer, **Nanoparticles for heterogeneous catalysis of industrial relevant processes**, International Conference on Advances in Functional Materials, 2017, January 6-8, Chennai, India

Periyasamy, Manimuthu; Fjellvåg, Helmer; Sjåstad, Anja Olafsen, **Role of defects on the functional properties of mixed transition metal oxides**, International Conference on Advances in Functional Materials, 2017, January 6-8, Chennai, India

Olsbye, Unni, **Elucidating the Influence of Process and Material Parameters on Methylation versus Hydrogen Transfer Rates in Zeotype Materials**, Gordon Research Conference on Nanoporous Materials and their Applications, 2017, August 6-11, Andover, USA

Olsbye, Unni, **Catalysis with zeolites**, SUNCAT Summer Institute 2017, August 14-18, Stanford University, California, USA

Chen, De, **Green Metal free catalysts for oxygen reduction reaction and applications in metal –air batteries**, Jiangsu University of science and technology, 2017, November 1, Zhanjiang, China

Yang, Jia, **The Use of Multicomponent SSITKA as a Tool to Study the Reaction Mechanism in CO Hydrogenation over Cobalt Catalysts**, the 8th Asian-Pacific Chemical Reaction Engineering Symposia (APCRE 2017), 2017, November 12-15, China

Chen, De, **Nanocatalysis beyond activity, a kinetic perspective**, Dalian institute of physical chemistry, 2017, November 23, Dalian, China

Chen, De, **Kinetic analysis and design of catalytic redox cycles**, Dalian university of science and Technology, 2017, November 24, Dalian, China

Chen, De, **Nanocatalysis beyond activity**, International workshop on nanocatalysis, 2017, October 23, Shanghai normal university, China

Chen, De, **Nanostructured carbon based 3D electrodes for energy storage: principles of rational design**, Sino-Norway conference on light metals and new energy technologies, 2017, December 4, Shanghai, China

Popular Dissemination

Rønning, Magnus, **A catalyst for discussion**, ESRF News, 2017, March 15

Education

Master Theses

2016-2017 and 2017-2018 Specialization and Master Thesis projects in Chemical Engineering at NTNU associated or affiliated with iCSI:

2017: Master thesis projects		
Martin Jensen (2015-17)	**IIA 1&6** UiO-Nafuma	Synthesis and Characterization of $Pt_{1-x}Pd_x$ Nanoparticles and their Suitability for NH_3 Oxidation Catalysis
Galina Tenkova Yavasheva (2017-19)	**IIA 1&6** UiO-Nafuma	Synthesis and characterization of bimetallic nanoparticles for selective catalytic conversion of ammonia
Rakel Johanne Ekholt	**IIA 3** NTNU	Oxidation of Methanol to Formaldehyde over Ag – Kinetic Modelling using Comsol
Karoline Kvande (2017-19)	**IIA 5** UiO-Catalysis	Selective oxidation of methane to methanol over Cu loaded SAPO-34 catalysts
Ragnhild Brokstad Lund-Johansen	**IIA 6** NTNU	Catalysis for control of methane slip in marine machinery over a nickel cobalt spinel.
Stine Hansen	NTNU	Catalytic conversion of biomass derived oxygenates to aviation fuel
Jianyu Ma	NTNU	Metal Dusting
Björn Frederik Baumgarten	NTNU	One-pot conversion of biomass to chemicals on Ni-Cu-Zn alloy catalysts
Moses Mawanga	NTNU	CO_2 Capture using CaO-based (doped and synthetic) sorbents.
Daniel Skodvin	NTNU	Synthesis and applications of carbon spheres
Petter Kaalstad	NTNU	One-pot conversion of cellulose to 5-hydroxymethylfurfural
Joakim Tafjord	NTNU	Introduction of rhenium into porous supports
Sebastian Langfjæran	NTNU	Synthesis and characterization of Tungsten Carbide
Maria Mykland	UiO-Catalysis	Synthesis and characterization of AFI zeotype materials

2016-2017 Master students at NTNU (from left to right): Moses Mawanga, Jianyu Ma, Leyman Maleki Bakali-Hemou (exchange Master student, France), Ragnhild Lund-Johansen, Sebastian Langfjæran, Stine Hansen, Daniel Skodvin, Signe Marit Hyrve, Björn Frederik Baumgarten, Petter Kaalstad. Photo: Estelle Vanhaecke, NTNU

Pictures p.3

Top left to right: Kamilla Arnesen, Stine Lervold; Samuel K. Regli My Nhung Thi Tran (NTNU),
Middle top left to right: IIA 5 team: Terje Fuglerud (INOVYN), Endre Fenes, Kumar Ranjan Rout (SINTEF), Erling Olav Sollund (Master student NTNU), Hongfei Ma; NTNU iCSI PhD students: Hongfei Ma, Endre Fenes, Stine Lervold, Samuel K. Regli, Ata ul Rauf Salman;
Middle down left to right: Oleksii Ivashenko, Asbjørn Slagtern Fjellvåg (UiO); Jane Eiane Aarsland, Samuel K. Regli (NTNU);
Bottom from left to right: UiO Master students: Karoline Kvande; Martin Jensen, Galina Tenkova Yavasheva;
NTNU Master students: Henrik Jenssen Gremmetsen, Beate Meisland Østrådt, Signe Marit Hyrve with Ata ul Rauf Salman

2017: Specialization Projects NTNU		
Henrik Jenssen	**IIA 1**	Efficient catalysts for achieving NO/NO_2 equilibrium
Beate Meisland Østrådt	**IIA 1**	Efficient catalysts for achieving NO/NO_2 equilibrium
Signe Marit Hyrve	**IIA 1**	Tuning of perovskite composition for NO oxidation
Kamilla Arnesen	**IIA 3**	Oxidation of Methanol to formaldehyde over Ag catalysts
Erling Olav Sollund	**IIA 4**	Kinetic study and reactor modeling of ethylene oxychlorination
My Nhung Thi Tran	**IIA 6**	In situ characterization of industrial catalysts
Jane Eiane Aarsland	**IIA 6**	In situ characterization of industrial catalysts
Helene Marie Eng Granlund	**IIA 6**	Catalytic methane abatement for natural gas engines
Amalie Tysseland		Carbon formation and catalysis in the conversion of methylchloride and silicon into dimethyldichlorosilane
Ane Sofie Lilleng		Synthesis of solid sorbents and kinetic study for CO_2 capture
Dani Espevik		Artifical photosynthesis Visible-light photocatalysts for water splitting
Eline Nesdal Sundli		Catalytic conversion of biomass derived oxygenates to fuel and chemicals
Gaute Osaland Hådem		Nanoscale investigations and modifications of catalysts and catalytic model systems
Ion Cotorobai		Direct conversion of methane
John Helms		Initial stages of metal dusting corrosion
Jonas Save		The effect of alkali on cobalt-based Fischer-Tropsch catalysts
Karoline Aasen Nilsen		New catalysts for low-temperature selective catalytic reduction (SCR)
Kin Hui		New catalysts for low-temperature selective catalytic reduction (SCR)
Maria Oslvik		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		Catalytic combustion of natural gas
Siri Stavnes		Sorbents for sulfur removal from biomass-derived syngas

2017-2018 Master students at NTNU (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.. Photo: Estelle Vanhaecke, NTNU

Exchange students in 2017

Exchange Master students 2017 (from January to June) at NTNU		
Nicolas Beck	Karlsruhe Institute of Technology (KIT), Germany	Oxidation of methanol to formaldehyde over Ag catalysts (**IIA 3**)
Maleki Bakali-Henou	Sorbonne University, France	Catalytic combustion of methane on nickel cobalt based catalysts derived from hydrotalcite precursors
Matus Bodnar	Slovak University of Technology in Bratislava, Slovakia	Direct Non-Oxidative Conversion of Methane to C_2 Hydrocarbons, Aromatics and Hydrogen
Exchange PhD students 2017 at NTNU		
Niu Juntian	Chongqing University, China	Dry (CO_2) reforming of methane on Ni and Ni-Pt surface alloy catalysts studied by experiment and DFT.
Fan Guifang	Tsinghua University, China	Biomass conversion; Cellulose hydrolytic hydrogenation to vicinal diols
Chen Wenyao	East China University of Science and Technology, China	CO oxidation

PhD students in 2017

Hongfei Ma was recruited to IIA4 in 2017. He holds his Master of Science in Physical Chemistry (July 2017) from Dalian Institute of Chemical Physics under the supervision of Professor Xinhe Bao.

Endre Fenes	NTNU	Norway	2015-18
Ata ul Rauf Salman	NTNU	Pakistan	2015-18
Dimitrios Pappas	UiO - Catalysis	Greece	2016-19
Samuel K. Regli	NTNU	Switzerland	2016-19
Stine Lervold	NTNU	Norway	2016-20
Asbjørn Slagtern Fjellvåg	UiO - Nafuma	Norway	2016-20
Hongfei Ma	NTNU	China	2017-20

Postdocs in 2017

Michael Dyballa	UiO - Catalysis	Germany	2016-18
Yanying Qi	NTNU	China	2016-18
Oleksii Ivashenko	UiO – Nafuma	Ukraine	2016-18

Accounts 2017

Table 1 summarizes the costs in 2017 and the total budget for the period of the Centre. 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 2017	2015-2023 Total budget
Payroll and indirect expenses	6383	59004
Procurement of R&D services	11231	92039
Equipment	1075	7094
Other operating expenses	4488	33997
Totals	**23176**	**192135**

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 AS.

Cost and Financing per partner	2017 Accounts		2015-2023 Total budget	
Partner	Costs	Financing	Costs	Financing
NTNU	8363	4465	76095	27914
University of Oslo	5824	1987	48539	12363
SINTEF	5407	1006	43501	7858
Industrial partners	3582	6581	24000	48000
Research Council of Norway	-	9136	-	96000
Totals	**23176**	**23176**	**192135**	**192135**

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 2017	2015-2023 Total budget
IIA1 21st century Nitric Acid technology development	5542	41176
IIA2 New NOx abatement technologies	1004	7331
IIA3 Frontier formalin technology development	3359	20502
IIA4 PVC Value Chain	3073	30237
IIA5 The next step in direct activation of methane	3900	33780
IIA6 Generic projects	4609	32254
IIA7 2020 Catalysis	-	7402
iCSI Management and administration	1689	19453
Totals	**23176**	**192135**

Publications

iCSI Publications

Baidoo, Martina Francisca; Fenes, Endre; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De, **On the effects of K and La co-promotion on $CuCl_2/\gamma$-Al_2O_3 catalysts for the oxychlorination of ethylene**, *Catalysis Today*, 2017, 299, 164-171

Rout, Kumar Ranjan; Baidoo, Martina Francisca; Fenes, Endre; Zhu, Jun; Fuglerud, Terje; Chen, De, **Understanding of potassium promoter effects on oxychlorination of ethylene by operando spatial-time resolved UV–vis–NIR spectrometry**, *Journal of Catalysis*, 2017, 352, 218-228

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Pappas, Dimitrios; Borfecchia, Elisa; Dyballa, Michael Martin; Pankin, Ilia A.; Lomachenko, Kirill A.; Martini, Andrea; Signorile, Matteo; Teketel, Shewangizaw; Arstad, Bjørnar; Berlier, Gloria; Lamberti, Carlo; Bordiga, Silvia; Olsbye, Unni; Lillerud, Karl Petter; Svelle, Stian; Beato, Pablo, **XAS reveals structure-activity relationships for the Methane-to-Methanol conversion over Cu-zeolites,** *ESRF Highlights 2017,* 49-51

Qi, Yanying; Ledesma Rodriguez, Cristian; Yang, Jia; Duan, Xuezhi; Zhu, Yi-An; Holmen, Anders; Chen, De, **Adsorption energy-driven carbon number-dependent olefin to paraffin ratio in cobalt-catalyzed Fischer-Tropsch synthesis**, *Journal of Catalysis*, 2017, 349, 110-117

Venvik, Hilde Johnsen; Yang, Jia, **Catalysis in microstructured reactors - Short review on smallscale syngas production and further conversion into methanol, DME and Fischer-Tropsch products**, *Catalysis Today*, 2017, 285, 135-146

iCSI Presentations

Ivashenko, Oleksii; Zheng, Jian; Fjellvåg, Helmer; Sjåstad, Anja Olafsen, **Operando Investigations of Surfaces for NO_x Abatement Catalysis**, International Conference on Advances in Functional Materials, 2017, January 6-8, Chennai, India

Fenes, Endre; Baidoo, Martina Francisca; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De, **Rational Design of $CuCl_2/Al_2O_3$ based Oxychlorination Catalysts**, NAM25 | North American Catalysis Society Meeting, 2017, June 4-9, Denver, USA

Pappas, Dimitrios; Borfecchia, Elisa; Dyballa, Michael Martin; Pankin, Ilia; Lomachenko, Kirill A.; Berlier, Gloria; Arstad, Bjørnar; Lamberti, Carlo; Bordiga, Silvia; Beato, Pablo; Olsbye, Unni; Svelle, Stian, **Key Reaction Steps in the Partial Oxidation of Methane to Methanol over Cu-SSZ-13**, NAM25 | North American Catalysis Society Meeting, 2017, June 4-9, Denver, USA

Dyballa, Michael Martin; Arstad, Bjørnar; Pappas, Dimitrios; Svelle, Stian; Olsbye, Unni; Beato, Pablo; Bordiga, Silvia; Borfecchia, Elisa, **On the preparation of Cu-containing Zeolites - How to avoid comparing Apples to Oranges,** NAM25 | North American Catalysis Society Meeting, 2017, June 4-9, Denver, USA

Fenes, Endre; Baidoo, Martina F.; Rout, Kumar R.; Fuglerud, Terje; Chen, De, **First Ionization Energy as a Descriptor of Alkali Metals promoted Oxychlorination Cu-based Catalyst,** 13th Europacat 2017, August 27-31, Florence, Italy

Pappas, Dimitrios; Borfecchia, Elisa; Dyballa, Michael Martin; Lomachenko, Kirill A.; Signorile, Matteo; Berlier, Gloria; Lamberti, Carlo; Bordiga, Silvia; Olsbye, Unni; Lillerud, Karl Petter; Svelle, Stian; Beato, Pablo, **Searching for the Active Sites Responsible for the CH_4 to CH_3OH Conversion over Cu-Chabazite Materials**, Norwegian catalysis symposium, 2017, November 6-7, Hurdal, Norway

iCSI associated journal publications

Ahoba-Sam, Christian; Olsbye, Unni; Jens, Klaus-Joachim, **Low temperature methanol synthesis catalyzed by copper nanoparticles**, *Catalysis Today*, 2017, 299, 112-119

Ahoba-Sam, Christian; Olsbye, Unni; Jens, Klaus-Joachim, **The Role of Solvent Polarity on Low-Temperature Methanol Synthesis Catalyzed by Cu Nanoparticles**, *Frontiers in Energy Research*, 2017, 5, 15

Bergem, Håkon; Xu, Run; Brown, Robert C.; Huber, George W., **Low temperature aqueous phase hydrogenation of the light oxygenate fraction of bio-oil over supported ruthenium catalysts**, *Green Chemistry*, 2017, 19, 14, 3252-3262

Braglia, Luca; Borfecchia, Elisa; Lomachenko, Kirill A.; Bugaev, Alexander L.; Guda, Alexander A.; Soldatov, Alexander V.; Bleken, Bjørn Tore Lønstad; Øien-Ødegaard, Sigurd; Olsbye, Unni; Lillerud, Karl Petter; Bordiga, Silvia; Agostini, Giovanni; Manzoli, Maela; Lamberti, Carlo, **Tuning Pt and Cu sites population inside functionalized UiO-67 MOF by controlling activation conditions**, *Faraday discussions*, 2017, 201, 277-298

Bremmer, G Marien; Zacharaki, Eirini; Sjåstad, Anja Olafsen; Navarro, Violeta; Frenken, Joost W. M.; Kooyman, Patricia J., **In situ TEM observation of the Boudouard reaction: Multi-layered graphene formation from CO on cobalt nanoparticles at atmospheric pressure**, *Faraday discussions*, 2017, 197, 337- 351

Buan, Marthe Emelie Melandsø; Muthuswamy, Navaneethan; Walmsley, John; Chen, De; Rønning, Magnus, **Nitrogen-doped Carbon Nanofibers for the Oxygen Reduction Reaction: Importance of the Iron Growth Catalyst Phase**, *ChemCatChem*, 2017, 9, 1663-1674

Cao, Yueqiang; Sui, Zhijun; Zhu, Yian; Zhou, Xinggui; Chen, De, **Selective Hydrogenation of Acetylene over Pd-In/Al2O3 Catalyst: Promotional Effect of Indium and Composition-Dependent Performance**, *ACS Catalysis*, 2017, 7, 7835-7846

Chen, Qingjun; Svenum, Ingeborg-Helene; Qi, Yanying; Gavrilovic, Ljubisa; Chen, De; Holmen, Anders; Blekkan, Edd Anders, **Potassium adsorption behavior on hcp cobalt as model systems for the Fischer–Tropsch synthesis: a density functional theory study**, *Physical Chemistry, Chemical Physics – PCCP*, 2017, 19, 12246-12254

Chen, Wenyao; Li, Dali; Peng, Chong; Qian, Gang; Duan, Xuezhi; Chen, De; Zhou, Xinggui, **Mechanistic and kinetic insights into the Pt-Ru synergy during hydrogen generation from ammonia borane over PtRu/CNT nanocatalysts**, *Journal of Catalysis*, 2017, 356, 186-196

Chen, Wenyao; Li, Dali; Wang, Zijun; Qian, Gang; Sui, Zhijun; Duan, Xuezhi; Zhou, Xinggui; Yeboah, Isaac; Chen, De, **Reaction mechanism and kinetics for hydrolytic dehydrogenation of ammonia borane on a Pt/CNT catalyst**, *AIChE Journal*, 2017, 63, 60-65

Chytil, Svatopluk; Kure, Milly; Lødeng, Rune; Blekkan, Edd Anders, **Performance of Mn-based H_2S sorbents in dry, reducing atmosphere – Manganese oxide support effects**, *Fuel*, 2017, 196, 124-133

Dadgar, Farbod; Myrstad, Rune; Pfeifer, Peter; Holmen, Anders; Venvik, Hilde Johnsen, **Catalyst Deactivation During One-Step Dimethyl Ether Synthesis from Synthesis Gas**, *Catalysis Letters*, 2017, 147, 865-879

Feng, Xiang; Sheng, Nan; Liu, Yibin; Chen, Xiaobo; Chen, De; Yang, Chaohe; Zhou, Xinggui, **Simultaneously Enhanced Stability and Selectivity for Propene Epoxidation with H_2 and O_2 on Au Catalysts Supported on Nano-Crystalline Mesoporous TS-1**, *ACS Catalysis*, 2017, 7, 2668-2675

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Guo, Xiaoyang; Gunawardana, Daham; Chen, De; Vanhaecke, Estelle Marie M.; Venvik, Hilde Johnsen; Walmsley, John, **Investigation of metal dusting corrosion process over UNS N08800 alloy**,

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Kalyva, Maria Evangelou; Wragg, David; Fjellvåg, Helmer; Sjåstad, Anja Olafsen, **Engineering Functions into Platinum and Platinum-Rhodium Nanoparticles in a One-Step Microwave Irradiation Synthesis**, *ChemistryOpen*, 6, 2, 273-281

Lillebø, Andreas Helland; Rytter, Erling; Blekkan, Edd Anders; Holmen, Anders, **Fischer–Tropsch Synthesis at High Conversions on Al_2O_3-Supported Co Catalysts with Different H_2/CO Levels**, *Industrial & Engineering Chemistry Research*, 2017, 56, 13281-13286

Lødeng, Rune; Bergem, Håkon, **Stabilization of pyrolysis oils. I: Direct thermochemical liquefaction for energy applications**, Woodhead Publishing Limited, 2017, ISBN 978-0-08-101029-7, 193-247

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Lundvall, Fredrik; Kalantzopoulos, Georgios N.; Wragg, David; Arstad, Bjørnar; Blom, Richard; Sjåstad, Anja Olafsen; Fjellvåg, Helmer, **Thermogravimetric Analysis – A Viable Method for Screening Novel Materials for the Sorbent Enhanced Water-gas Shift Process**, *Energy Procedia*, 2017, 114, 2294- 2303

Mahmoodinia, Mehdi; Åstrand, Per-Olof; Chen, De, **Tuning the Electronic Properties of Single-Atom Pt Catalysts by Functionalization of the Carbon Support Material**, *Journal of Physical Chemistry C*, 2017, 121, 20802-20812

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Martinez-Espin, Juan Salvador; De Wispelaere, Kristof; Westgård Erichsen, Marius; Svelle, Stian; Janssens, Ton V.W.; Van Speybroeck, Veronique; Beato, Pablo; Olsbye, Unni, **Benzene co-reaction with methanol and dimethyl ether over zeolite and zeotype catalysts: Evidence of parallel reaction paths to toluene and diphenylmethane**, *Journal of Catalysis*, 2017, 349, 136-148

Martinez-Espin, Juan Salvador; Mortén, Magnus; Janssens, Ton V.W.; Svelle, Stian; Beato, Pablo; Olsbye, Unni, **New insights in catalyst deactivation and product distribution of zeolites in the Methanol-To-Hydrocarbons (MTH) reaction with methanol and dimethyl ether feeds**, *Catalysis science & technology*, 2017, 7,2700-2716

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Pinilla-Herrero, Irene; Olsbye, Unni; Marquez-Alvarez, Carlos; Sastre, Enrique, **Effect of framework topology of SAPO catalysts on selectivity and deactivation profile in the methanol-to-olefins reaction**, *Journal of Catalysis*, 2017, 352, 191-207

Rojo-Gama, Daniel; Etemadi, Samaneh; Kirby, Eliot; Lillerud, Karl Petter; Beato, Pablo; Svelle, Stian; Olsbye, Unni, **Time- and space-resolved study of the Methanol to Hydrocarbons (MTH) reaction - influence of zeolite topology on deactivation patterns**, *Faraday discussions*, 2017, 197, 421-446

Rojo-Gama, Daniel; Nielsen, Malte; Wragg, David; Dyballa, Michael Martin; Holzinger, Julian; Falsig, Hanne; Lundegaard, Lars Fahl; Beato, Pablo; Brogaard, Rasmus Yding; Lillerud, Karl Petter; Olsbye, Unni; Svelle, Stian, **A Straightforward Descriptor for the Deactivation of Zeolite Catalyst H-ZSM-5**, *ACS Catalysis*, 2017, 7, 8235-8246

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Rytter, Erling; Holmen, Anders, **Perspectives on the Effect of Water in Cobalt Fischer-Tropsch Synthesis**, *ACS Catalysis,* 2017, 7, 5321-5328

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