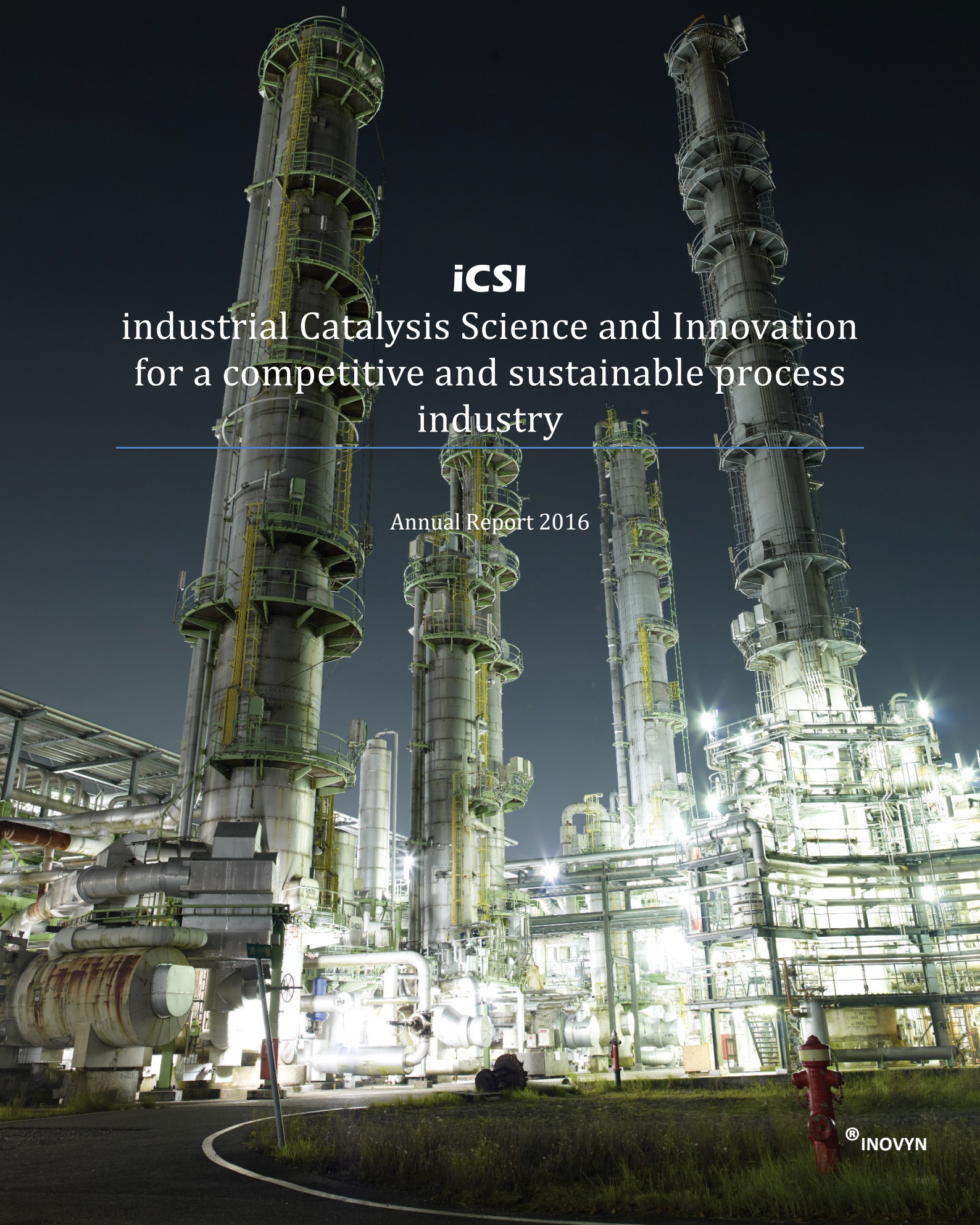
sfi Centre for Research-based Innovation

The Research Council of Norway

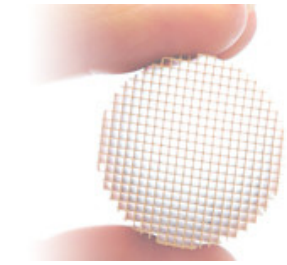


iCSI

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

Annual Report 2016

INOVYN



iCSI

Centre for Research-based Innovation

NTNU – Trondheim
Norwegian University of Science and Technology

The **iCSI** main objective is to boost industrial innovation and competitiveness and promote world class energy and raw material efficiency , through:

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

6 PhD candidates

3 Postdoctoral fellows

11 Professors

3 Scientific Advisors

14 Research Scientists from SINTEF

16 Scientists from industry

...and more to come!

UiO : Universitetet i Oslo

SINTEF

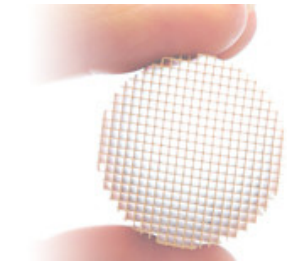
YARA

dynea

inovyn

K.A.Rasmussen Norway

HALDOR TOPSØE



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NTNU – Trondheim Norwegian University of Science and Technology

iCSI 2016 Summary

2016 was the ***first full running year*** of iCSI, during which all contracts, plans and budgets have come into place. The recruitment of PhD candidates and postdoctoral fellows for the first 4-year period is close to complete and the Centre is proud to present its motivated and competent personell. All research activities (Industrial Innovation Areas - IIA1-6) are fully up and running and a taste of achievements so far are given in the following pages. A large number of NTNU and UiO students also chose to work within iCSI for their Master and Specialization projects (p. 34-35)

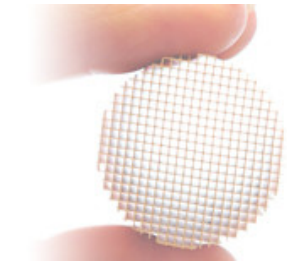
The iCSI Centre is pleased to announce the establishment of its ***Scientific Advisory Committee*** (SAC). Professor Alessandra Beretta (Politecnico di Milano), Professor Enrique Iglesia (UC Berkeley) and Professor Graham Hutchings (Cardiff University) are scientists from prominent institutions who have excelled within iCSI relevant areas of heterogeneous catalysis and represent the international research forefront. They have accepted to advise and be critical, but most importantly to serve as an inspiration to the young iCSI scientists.

The ***iCSI Kick-off meeting*** was held in November 23-24 in Trondheim. 50 participants attended the meeting, with all the industry partners represented and all the PhD and Postdocs recently hired present. Prof. Alessandra Beretta (SAC) gave an inspiring and highly relevant lecture on her efforts to combine kinetic analysis and characterization in investigating catalytic partial oxidation of hydrocarbons. Both the scientific and the social program was a success, providing inspiration and ideas across the IIAs and work packages, potential new collaborations within the Centre, as well as new friends.

The ***first iCSI paper*** in a peer reviewed journal has been published. "**Highly Active and Stable CeO_2-Promoted $CuCl_2/Al_2O_3$ Oxychlorination Catalysts Developed by Rational Design Using a Rate Diagram of the Catalytic Cycle**", by K. R. Rout, E. Fenes, M. F. Baidoo, R. Abdollahi, T. Fuglerud, D. Chen, appeared in *ACS Catalysis* thanks to the collaboration between NTNU, SINTEF and the industry partner INOVYN within the Industrial Innovation Area 4. See the publication list on p. 37-43 for a full overview over iCSI researchers' dissemination, including co-publications with many of the institutions mentioned as international partners (p. 32).

International collaboration and visibility are important success parameters for iCSI. iCSI researchers have given ***41 presentations*** at national and international conferences. Among these are plenary, invited and keynote lectures at NGCS11 (Tromsø), 6th EuChemS Chemistry Congress (Sevilla), and 11th International Congress of Catalysis (Beijing) by Prof. Unni Olsbye (UiO) and Prof. De Chen (NTNU). Some of our PhDs and post docs have attended international courses within state-of-the-art catalysis research, and iCSI researchers also taught at the "Molecules@Surfaces" International Winter School in Bardonnecchia (Italy). See the list of presentations (p. 37-43).

The iCSI partners also hosted the ***NGCS11 - 11th Natural Gas Conversion Symposium*** in Tromsø, Norway in June 2016 (p. 32).



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Centre for Research-based Innovation

NTNU – Trondheim Norwegian University of Science and Technology

iCSI Looking ahead

So far so good! The iCSI organization is in place, the research activities are up and running, and the first results have emerged. The challenge now is to reach our goals with respect to quality and relevance, with good visibility of our achievements. The following elements are identified as key in this respect, and they are also linked to each other.

The first is collaboration between the industry and the research partner personnel. The core in this is frequent interaction within the Industrial Innovation Areas and the specific Work Packages, through research activities, discussion of results, joint publications and planning of further work. But, we have also recognized the importance of a broader iCSI arena, where all the personnel exchange results and get inspired by each other. This was strikingly apparent at the first iCSI seminar, and will be further strengthened.

Next is internationalization. This is essential for cutting edge research and for looking into the future. As shown here, the iCSI research partners have many international collaborations, whereas the industrial partners have international operations to an extent that goes beyond description here. Some of the industrial partners also have highly successful collaborations with research partners world-wide on other topics, which can serve as inspiration also for iCSI. At the core of the internationalization is dissemination; through joint conference presentations and publications. From 2017, a scheme for international exchange to other research groups is being implemented. A future challenge will be additional activities within European research and other international programs.

The final element is recruitment and education. We have hired skilled postdoctoral fellows who will be trained at the interface between academic research and industrial innovation. The new PhD candidates are a good mix between competencies and nationalities, but have in common a high quality MSc education and almost unprecedented enthusiasm for their projects and the Centre. And not the least - a considerable number of aspiring chemical engineers and chemists choose to complete their Master theses under iCSI. All these young men and women represent the future of the Norwegian chemical process industry, and several will likely also have international impact. They clearly state their motivation as interaction with industry and knowing the relevance of their work, as well as “knowledge for a better world” and “technology for a better society”.

Odd-Arne Lorentsen

iCSI Board Chair

Professor Hilde Venvik

iCSI Centre Director

UiO : Universitetet i Oslo

SINTEF

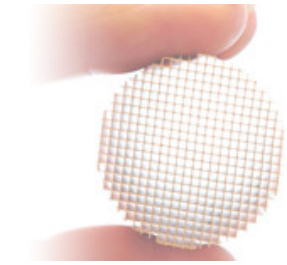
YARA

dynea

inovyn

K.A.Rasmussen Norway

HALDOR TOPSØE



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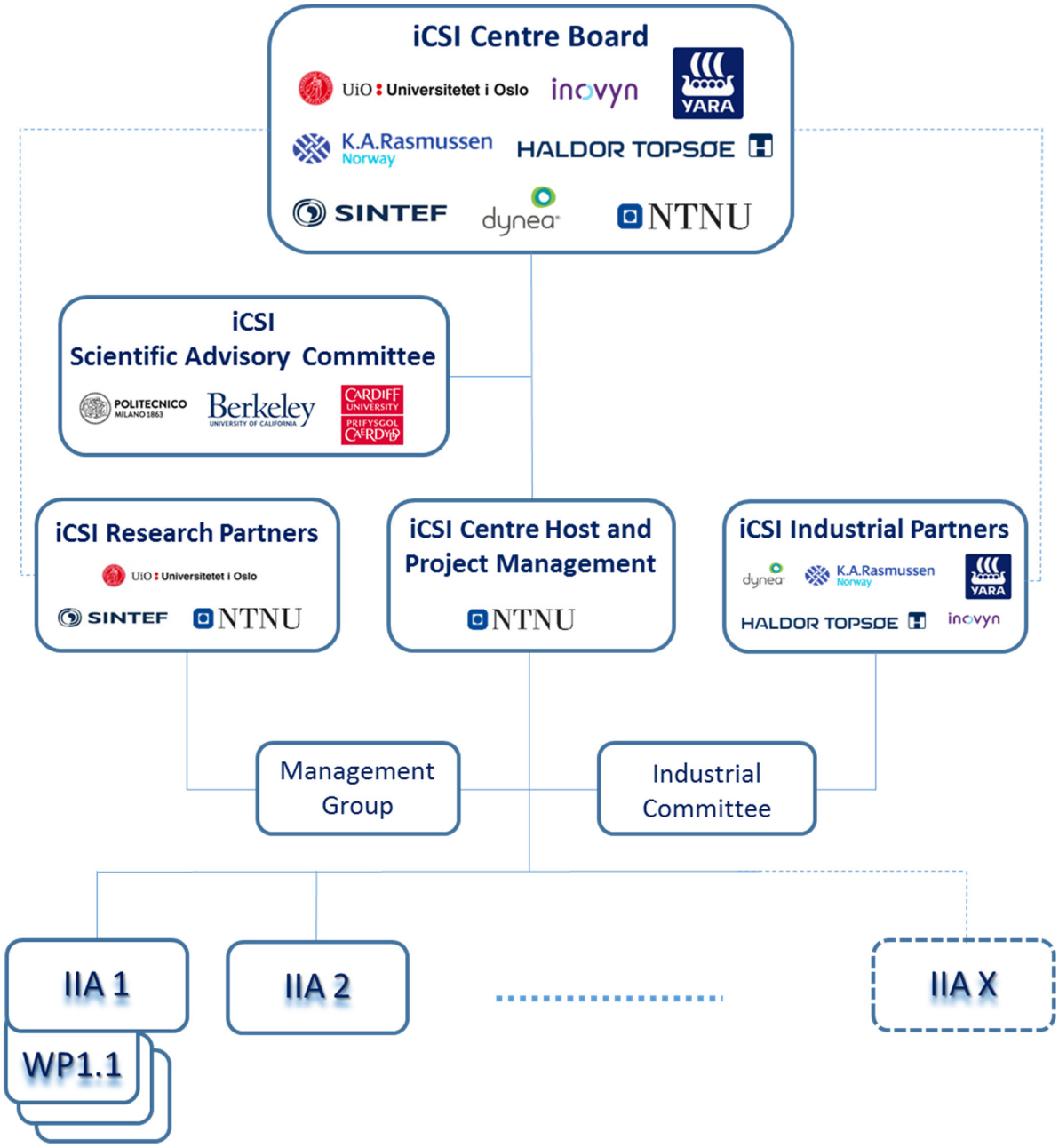
sfi Centre for Research-based Innovation

NTNU – Trondheim Norwegian University of Science and Technology

Contents

Organization

The Norwegian University of Science and Technology (NTNU) is Centre Host and Manager of iCSI. The iCSI research partners, NTNU, SINTEF Materials and Chemistry 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 represent significant R&D activity. The collaboration enables optimized use of complementary competence and a shared, highly advanced, instrumental infrastructure that will be further utilized, expanded and developed within iCSI.



The Centre Board and Management

Odd-Arne Lorentsen, Yara (Chair)
Pablo Beato, HALDOR TOPSØE (Vice-Chair)
Lars Axelsen, DYNEA
Duncan Akporiaye, SINTEF
Vebjørn Bakken, UiO
Tor Grande, NTNU
Steinar Kvisle, INOVYN
Terje Pedersen, KA RASMUSSEN
Aase Marie Hundere, Research Council (Observer)
Hilde J. Venvik (Secretary)
Estelle Vanhaecke (Vice-secretary)

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.*" Innovation transfer will be ensured throughout the lifetime of iCSI through follow-up by the Board with majority and Chairperson among the industrial partners. Each partner is represented (permanent + deputy) and has one vote, and the Research Council of Norway is represented by an observer.

The ICSI Management and Administration consist of:

- Professor Hilde J. Venvik, Director
- Dr. Estelle Vanhaecke, Coordinator and vice-director
- Torgrim Mathisen, economy advisor

The Scientific Advisory Committee


Prof. Alessandra Beretta

POLITECNICO MILANO 1863

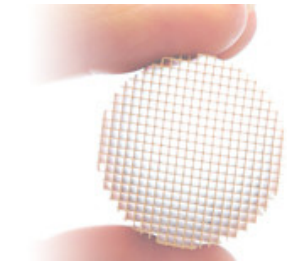

Prof. Enrique Iglesia

Berkeley UNIVERSITY OF CALIFORNIA


Prof. Graham Hutchings

CARDIFF UNIVERSITY
PRIFYSGOL CAERDYDD

The iCSI SAC appointment was finalized in 2016. 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. The Board and whole iCSI team look forward to hearing their presentations at our annual seminar and receiving their – sometimes critical – advice. Most important is, however, that the SAC appointment allows our young researchers to interact and draw inspiration from the very forefront of research in catalysis.



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The Industrial Partners

An overall ambition 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.

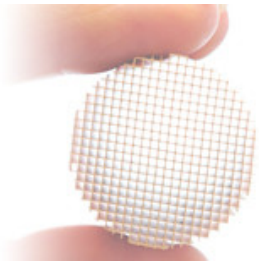
Yara International ASA is a Norwegian-based chemical company with fertilizer as its largest business area, but with industrial gases, catalyst production and NOx abatement solutions for industrial plants, vehicles and vessels also in its product portfolio. In addition to being present in more than 51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

KA RASMUSSEN AS is a refiner of precious metals, supplier of catalysts, products based on precious metals as dental products 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. By entering the iCSI Centre, KA Rasmussen wants to expand its catalyst market base, contribute to meeting emissions targets, as well as minimizing the consumption of noble and scarce metals in their product range.

DYNEA AS is a Norwegian-owned company for wood adhesives production, with productions sites in Norway, Denmark and Hungary. DYNEA holds now several unique technologies for licensing and its further technology R&D is based in Norway. By joining the iCSI Centre, 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 petrochemical company with 20 production sites worldwide. The company was established in 2015 as a result of INEOS and SOLVAY combining their respective European chlorvinyls activities in a 50-50 joint Venture. By entering the iCSI Centre, INOVYN targets further improvements in VCM technology, with world class energy and raw material efficiency.

HALDOR TOPSØE AS is a catalyst producer and process plants technology developer based in Denmark. HTAS is known for its emphasis on research and scientific excellence as a basis for its business. By joining the iCSI Centre, HTAS 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.



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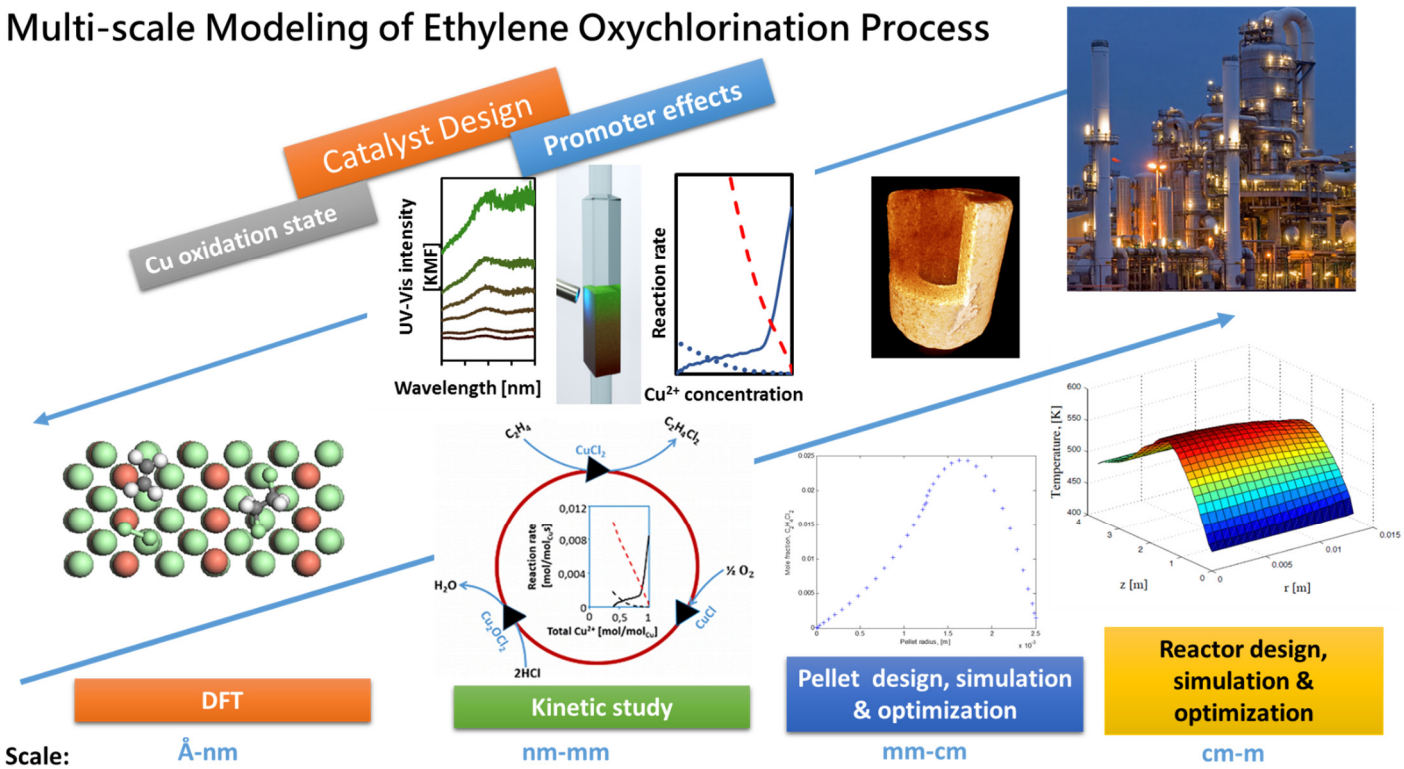
iCSI Highlight 2016

PVC Value Chain Project: a NTNU-SINTEF-INOVYN Collaboration

In 2016 the first iCSI publication was released in ACS Catalysis: "***Highly Active and Stable CeO_2-Promoted $CuCl_2/Al_2O_3$ Oxychlorination Catalysts Developed by Rational Design Using a Rate Diagram of the Catalytic Cycle***" by Kumar R. Rout (SINTEF, Trondheim), Endre Fenes, Martina Baidoo, Reza Abdollahi, De Chen (NTNU) and Terje Fuglerud (INOVYN). Reference: *ACS Catal.*, **2016**, 6 (10), pages 7030–7039

In this study, the team has developed a method to predict the steady-state rate and Cu oxidation state during ethylene oxychlorination from a reaction rate diagram of the individual steps involved in the catalytic oxychlorination cycle. The steady state of the redox cycle is represented by a cross point of the reaction rates of the reduction and oxidation steps as a function of the Cu^{2+} in the rate diagram. Transient kinetics of elementary reactions and steady-state kinetics of the overall catalytic cycle were investigated in an operando study using combined mass and UV–vis-NIR spectrophotometry.

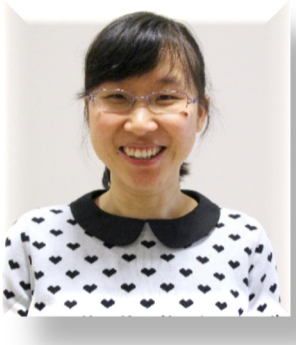
A multiscale approach is applied to the ethylene oxychlorination process to integrate density functional theory (DFT), microkinetic modeling, pellet- and reactor modeling. This is to provide better understanding of the surface reactions in the catalytic cycle, and thereby enable rational design of oxychlorination catalyst and the industrial reactor optimization.

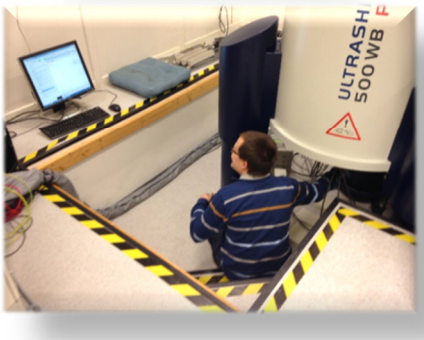


Recruitment

By 2016, seven young professionals from six different countries have joined iCSI to form our young task force of PhD candidates and postdoctoral fellows. Five of those entering in 2016 were asked about themselves and their motivations.





Have a look at the next pages and get to know Asbjørn, Oleksii, Stine, Yanying and Samuel!

Asbjørn - The Cyclist!

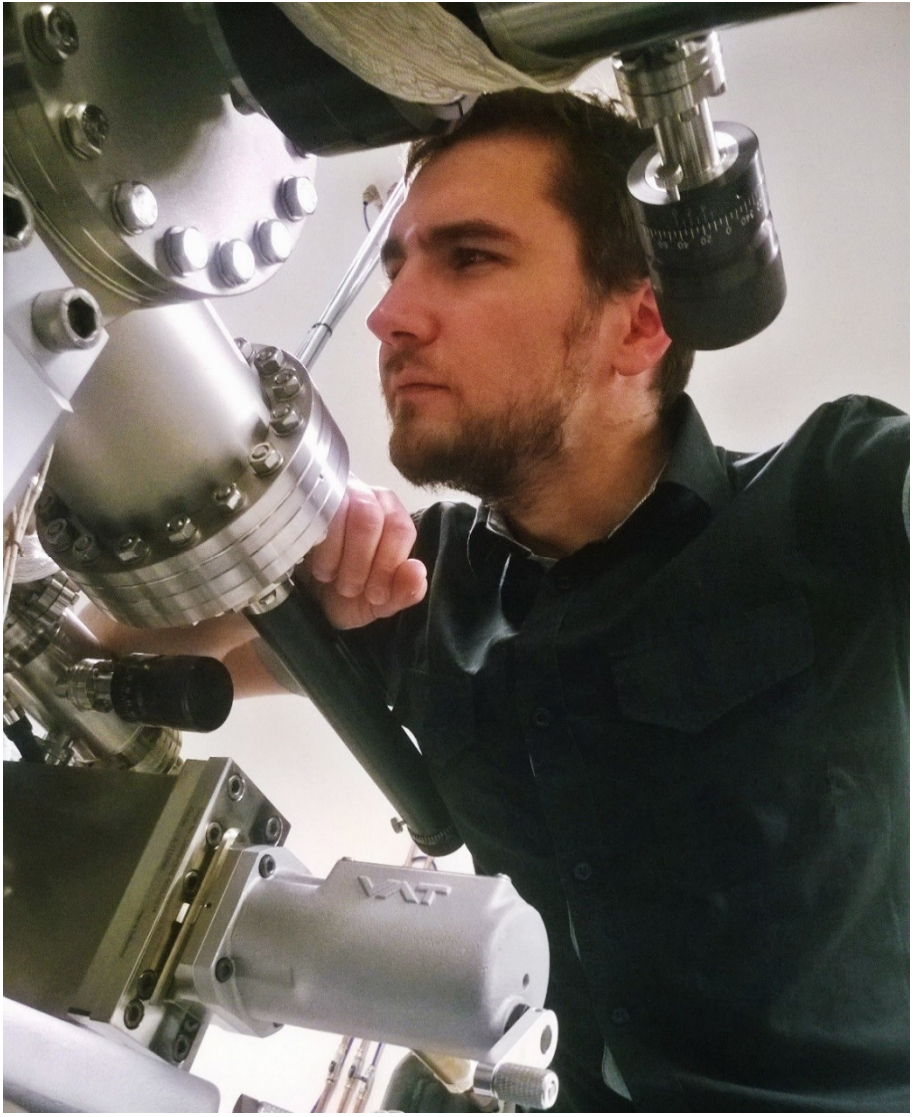
Asbjørn Slagtern Fjellvåg is born and raised in Oslo, Norway, to a family of scientists and did his MSc at UiO. He started his PhD last August on new solid state catchment systems (see page 18) and he is enjoying a lot his daily schedule in the lab. “I expect to improve my efficiency at work, and to know more about science. “

All about cycling….and research too

When you ask Asbjørn about his motivation for doing a PhD, he will first explain his need to satisfy his curiosity: “I decided to take a PhD because I learned very much during my masters, and I felt like there was so much more I could still learn. If I had left the university to work elsewhere, I probably wouldn't have had the chance to continue with research in the same manner.”

“I'm also cycling for the team called OSI Selmer, but the most important part is that I really enjoy being outside using my body to move forward. It's a great feeling, and it relieves me of all stress. It's also nice to have a flexible workday. It means that I can train in the morning if I need to, which makes it easier for me to keep motivated and to get the work done.”

Aikido and Yoga help me to connect better with myself and surrounding nature, increasing also my concentration and open-mindedness in the lab



Oleksii Ivashenko comes from Ukraine and graduated with a Master degree in Applied Physics from National Taras Shevchenko University of Kyiv in 2009.

First a PhD in the Netherlands…

"I was always fascinated with natural sciences and doing a PhD was a logical step after my Master degree. It was a tryout of the academic world. I had several European Universities in mind and chose the University of Groningen in the Netherlands (Zernike Institute for Advanced Materials) due to its high scientific level...and the Dutch cycling culture. It was an unforgettable experience, but after the PhD there is a choice; research in company or a postdoc. Although the Netherlands is booming with industry and startups, I was not ready to settle down in a company. There was still a whole world of unknown science in front of me! "

…then Canada

"So, at some point during the last year I understood that my adventure should continue outside of Europe. Doing a postdoc in Canada (National Institute for Nanotechnology, University of Alberta) was my next challenge!" After 2.5 years there, the next question was why a postdoc after a postdoc, and where? This time it was harder. Canada, with its warm summers and cold winters, reminded me of home. Moreover, polite, English-speaking people, incredible nature and really high quality science...What can beat that?

NORWAY!

I had been to Norway several times before that and found Bergen and Oslo magical, mysterious cities. Hard to cycle those hills, hard to speak the language, everything overtaxed, so, finally, a challenging scientific project on Reactor STM at UiO was an obvious choice! Besides that, funding for important science in Norway focused on climate change, renewable energy, and emissions abatement is good...it was LOVE FROM THE FIRST HIKE

Stine Lervold was born at Røros and has been living in Trondheim since. She took her master degree in the Chemical Engineering Department at NTNU with Prof. Hilde Venvik. Since August 2016, she works on her PhD on "Reaction mechanisms and surface Ag species in catalytic oxidation of methanol to formaldehyde" in cooperation with DYNEA and K.A. Rasmussen.

From media and communication to natural science and engineering

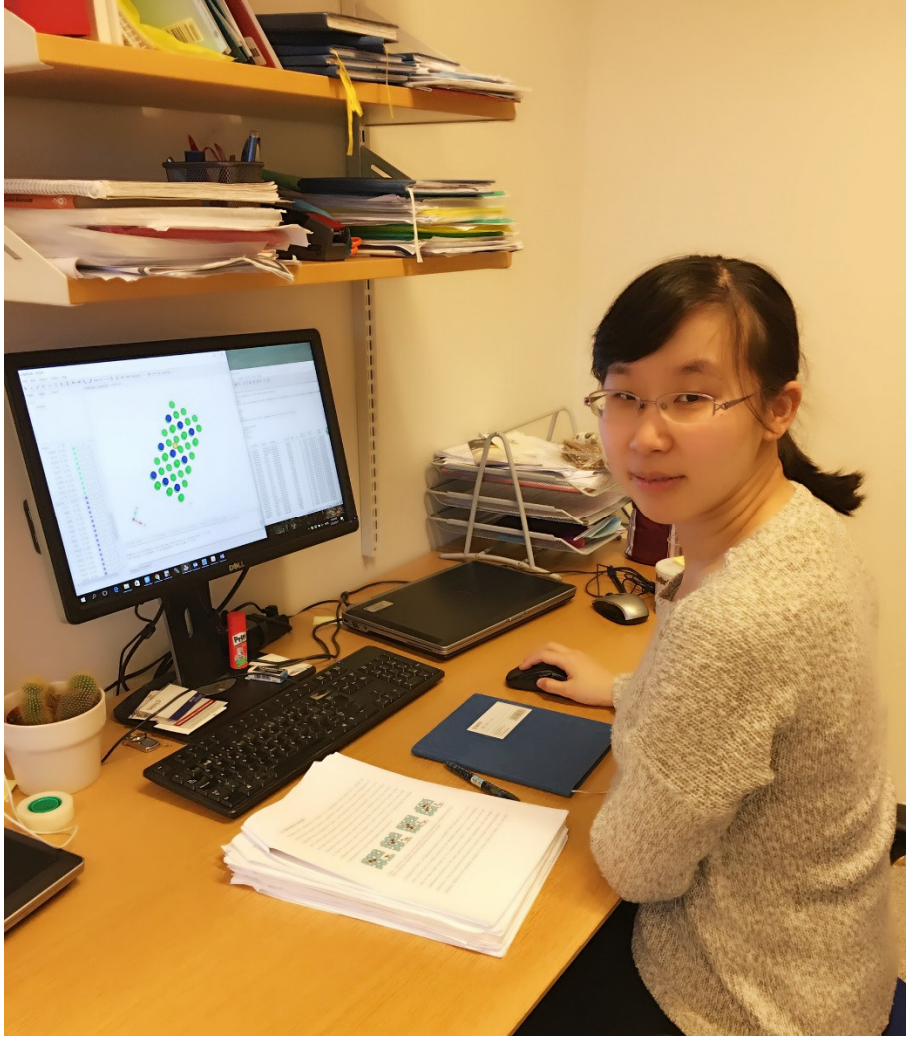
Stine specialized in Media and communication in upper secondary school and then moved on to do one year of Psychology at NTNU. She learned a lot about herself, found the topics pretty challenging but was missing the classroom learning environment. And maybe she was also thinking back to one of her high school teachers, who was sure that Stine would eventually take the natural science path. So, she proceeded to obtain a bachelor in Chemical Technology at the University College, and finally decided for a Master degree in Chemical Engineering at NTNU because of its relevance to environmental questions and future solutions!

A perfect working place

It may be Stine's somewhat curly path into science and technology that makes her appear with high motivation and clear priorities. And if you ask Stine about her working environment, you may not know where it will end. First she starts with the daily lunch/coffee she is sharing with her PhD colleagues on the second floor of the K5 building. An excellent way of having break and socializing! Then she will also speak about her main supervisor, Hilde Venvik, whom she finds a lot of motivation from. And also her inspiring and easy going contact with supervisors at DYNEA and KA Rasmussen remind her that someone is actually awaiting her results.

Jointly with the IIA3 team, she won for her first poster ever the Poster Prize at the iCSI Kick-off seminar in November 2016 - still finding it hard to believe.

The knowledge is like a sea and I want to explore it deeply.



Yanying Qi comes from Cangzhou, Hebei province – a town with over 7 million inhabitants, and she graduated with a degree in 2012 from the University of Tianjin. In fact, the Master degree programs last one year longer in China than in Europe. The first year is only classes and exams, followed by a two-year research project where you should publish some scientific articles. Yanying worked on DFT calculations during her master thesis.

The love of challenge: from a stable job in China to a PhD in Norway!

Yanying likes challenges and experiencing other cultures and meeting new people. "When I graduated, I got a very stable job as a Chemical Engineer and could almost image my whole future life. However, I thought I was still young and needed to see the world. I wanted to experience more before settling down." Many fellow master students were going KTH in Sweden on a scholarship, but Yanying decided to try her chances in Norway. After only one month working in a refinery, she quit her job and left China to settle down in Trondheim and work with Prof. De Chen. And apparently she was not the only one at her student house: among four girls living together, two are currently in the US and one in Norway! She loves Norway and the beautiful nature.

Second step: The Postdoc

"Curiosity and enterprise drive me to continue my research career. Although I completed my PhD thesis, I am far from an expert and there are lots of things that I need to learn. Research is very interesting and motivating. There are always new theories, new methods and new results coming out. Moreover, the topics of DFT and microkinetic calculations fit my background from the Master and PhD research very well."

The next step? Possibly exploring research even further. Difficult to know exactly where and what because it will depend also on external factors such as opportunity and…family!

Photo: Per Henning, NTNU

Samuel K. Regli comes from Luzern, Switzerland. In addition to German, English and French that he speaks fluently, Samuel is learning Norwegian and there is no doubt he will succeed.

From ETH to NTNU

He finished his Master of Science in Process Engineering from the prestigious university ETH Zürich in 2016 and decided to come to Norway to take a PhD. Why Norway? For many reasons: family, the beautiful country, going abroad and also for the prestige of NTNU! Samuel started his PhD in June 2016 and is enjoying a lot the working environment at Department of Chemical Engineering, NTNU – "people with different backgrounds and nationalities, and especially the Scandinavian culture. During my time here in Trondheim, I have already met many great people at NTNU, SINTEF and in iCSI."

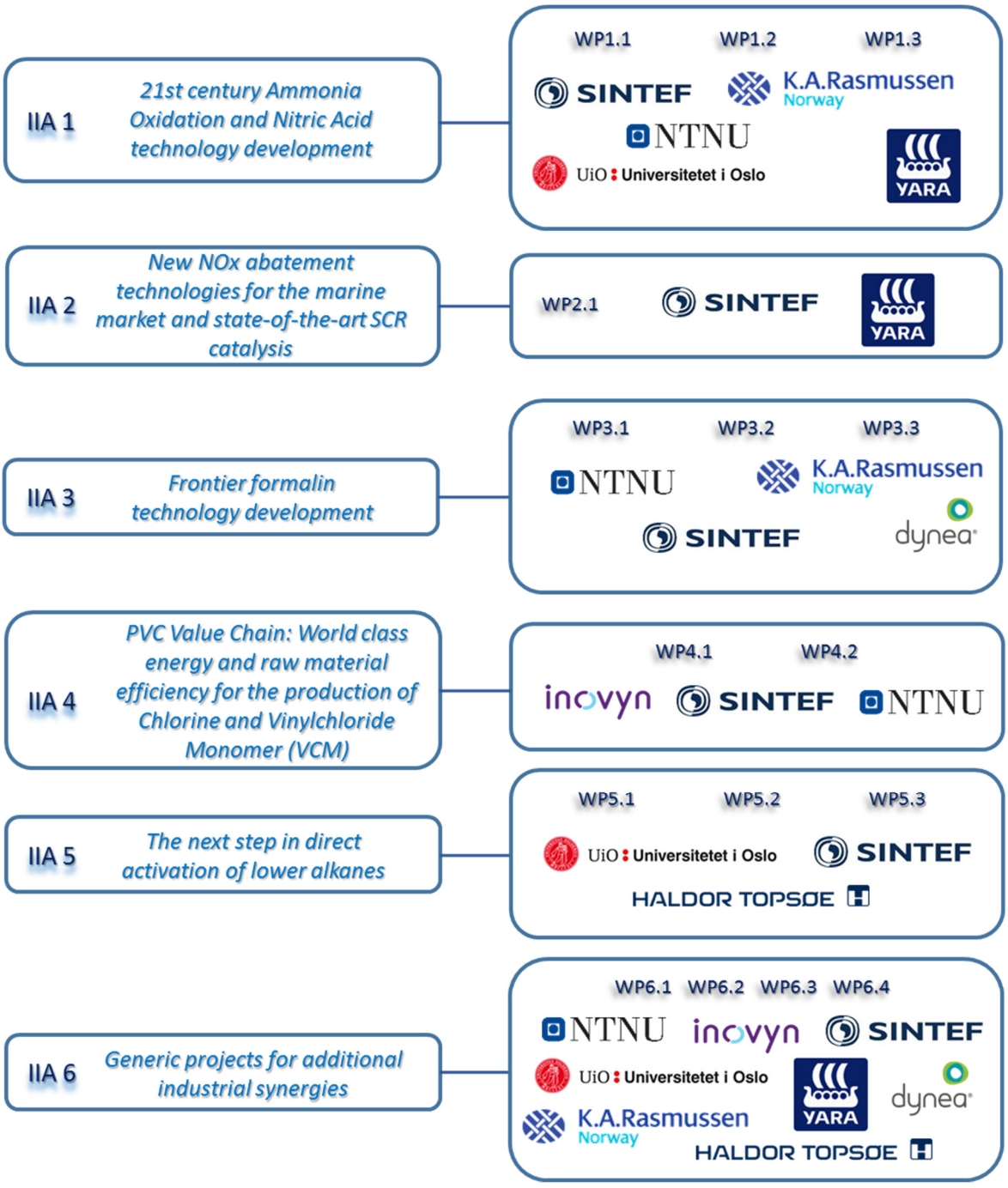
"The opportunity to specialize in and contribute to current research in catalysis appeals to me. Furthermore, I enjoy the academic environment with its intellectual stimulation and mixture of practical and theoretical work. I enjoy working together with the young and young at heart in contributing ideas and effort towards a common goal. I expect to build a strong network with colleagues working in the same field and to improve on doing research in a good way. I work on developing my skills and deepen my knowledge on different characterization methods."

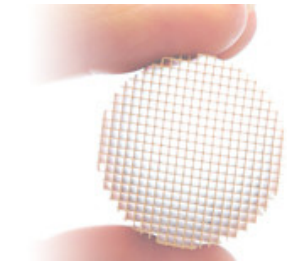
What's next?

"I see myself staying in science and research. I am feeling more and more drawn towards academia and dissemination, so I might pursue this direction. In the long run somewhere in Europe, probably Norway or Switzerland. Although a position abroad, Asia or America, for one or two years would be very interesting."

Scientific activities

iCSI main Industrial Innovation Areas (IIA) and Work Packages (WP) for 2016:





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

The Team in 2016

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)
Oleksii Ivashenko	UiO	Postdoctoral fellow (WP 1.1)
Maximilian Warner	Yara	Industry researcher (WP1.1-1.2)
Johan Skjelstad	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)
Roman Tschenscher	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)
Mohan Menon	Yara	Industry researcher (WP1.3)
Bjørn Christian Enger	SINTEF	Researcher (WP1.3)

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 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.

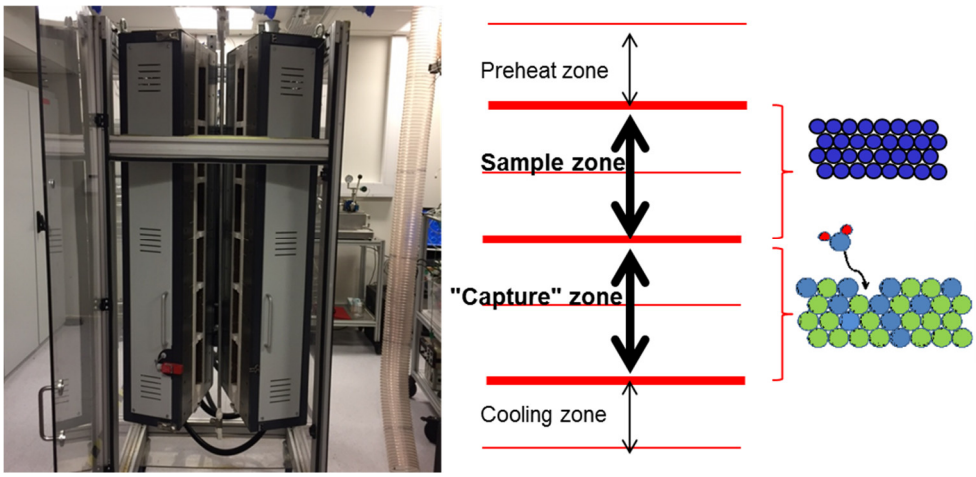
A major technological challenge is loss of Pt and Rh in the highly exothermic first step. The noble metals are brought into the gas phase in elemental form or as oxide and either re-deposited on the catalyst in the form of “cauliflower” structures or transported away from the reaction zone. To avoid permanent loss or costly recovery of Pt or Rh, 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 help to reduce the capital investment and increase the energy recovery by replacing the bulky homogeneous oxidation by a compact, heterogeneously catalyzed process.

Pt-group metal oxides in catchment processes - PhD project

A new, 5-zone furnace system for investigating noble metal oxide transport and the subsequent catchment mechanism is under implementation. Introductory TGA experiments of platinum and rhodium oxides are conducted to investigate their decomposition as well as their volatility. Preliminary results point in direction of Pt_3O_4 as prime candidate for catchment investigations in the 5-zone furnace system. Furthermore, from XRD it is understood that PtO_2 is a heavily distorted material and total scattering analysis will be adopted to provide a satisfactory description of the atomic arrangement. Double perovskites described by the formula RE2MM'O6 (RE = Y, La, Nd; M = Co, Ni, Fe; M' = PGM) are identified as potential alternative catchment materials. Several new compositions are successfully synthesized and established as phase pure. Samples are in the pipeline for more detailed characterization of structural arrangement, electronic properties as well as their catchment capacities.

Experimental investigations of Pt/PtRh volatilization and catchment - Researchers SINTEF

The design and construction of a dedicated reactor system for generating volatile Pt species and subsequent catchment on pure Pd and a range of Pd/Pt alloy materials has been performed. A six-zone oven system is used to achieve temperature gradients in the range 800-1200 °C, representative of those between the location for Pt volatilization and the catchment material. Flow regime and feed composition will furthermore be adjusted to provide realistic conditions and appropriate vapor phase concentrations of the Pt species. Scaling test conditions for practical campaign durations will be determined, taking into account also Pd loss from the catchment material.

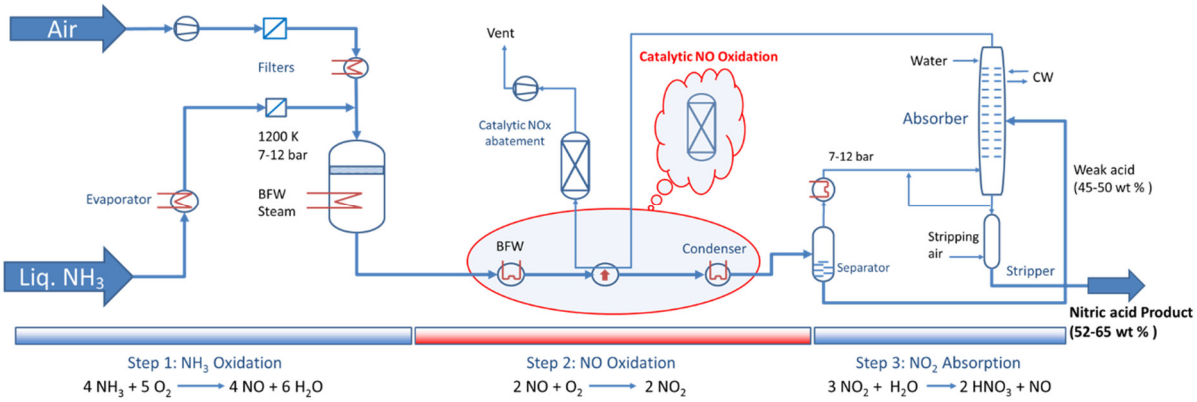


Dedicated reactor designed and constructed for generating volatile Pt species and the subsequent catchment on model Pd and a range of Pd/Pt alloy materials.

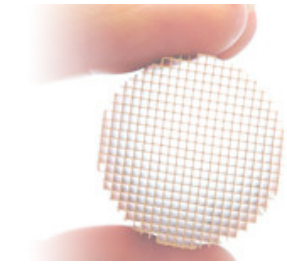
Key analytical methods (SIMS, SEM etc.) have been evaluated and put into operation using model, polycrystalline Pt/Pd alloy samples. Target for the evaluation has been to identify an analysis "toolbox" for determination of diffusion gradients generated in the model samples after treatment in the reactor system described above. Data derived this way will in the following be used as input in model development.

Catalysts for attaining NO/NO_2 equilibrium - PhD project

An experimental setup capable of testing catalysts for NO oxidation under industrial conditions was designed and built. NO oxidation was investigated both with and without the catalyst. Pt/Al_2O_3, prepared by incipient wetness impregnation, was chosen as a reference catalyst and characterized by H_2 and CO Chemisorption, XRF, TPR and BET. The catalyst activity and stability was investigated under different NO concentrations, ranging from dilute diesel oxidation conditions to concentrated nitric acid plant compositions, for varying residence time and temperature. The Pt/Al_2O_3 catalyst showed promising activity towards oxidation of NO under industrial conditions.



Process flow diagram of a single pressure nitric acid plant indicating substitution of gas phase NO oxidation with a catalytic converter. Figure modified based on Moulijn, J.A., M. Makkee, and A.E. Van Diepen, *Chemical process technology*, 2013: Ed, John Wiley & Sons.



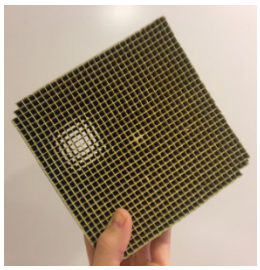
IIA 2 New NO_x abatement technologies for the marine market and state-of-the-art SCR catalysis

The Team in 2016

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 Tschenscher	SINTEF	Researcher (WP2.1)
Arne Karlsson	SINTEF	Researcher (WP2.1)
Spyros Diplas	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)

Motivation

Selective Catalytic Reduction (SCR) is a core technology in the treatment of exhaust gases (NOx) 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, instead, may involve the addition of an active phase to recover the original activity. It would be highly beneficial if the catalyst activity could be recovered in a simpler way, and this is targeted in WP2.1 through first gaining a deeper understanding of the mechanisms causing the catalyst deactivation through thorough characterization of the catalyst at different stages of the its lifetime, and then translating this knowledge into new measures.

Research project

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 activity of the catalyst is among other things connected to the type and amount of active sites. Figure 1 compares the acidity of the fresh and the spent catalyst, which is important for ammonia adsorption. The first sample of the spent catalyst (red curve) represents the average catalyst composition, while the second sample (orange curve) consists only of monolith walls (the corners were cut out). The idea behind having different samples of spent catalyst is to investigate if certain parts of the monolith are more prone to deactivation and poisoning. The difference between the two spent catalyst samples is minor, while the comparison with fresh catalyst reveals a loss of both density and strength of the acid sites. It is expected that this will have major impact on the activity of the SCR catalyst.

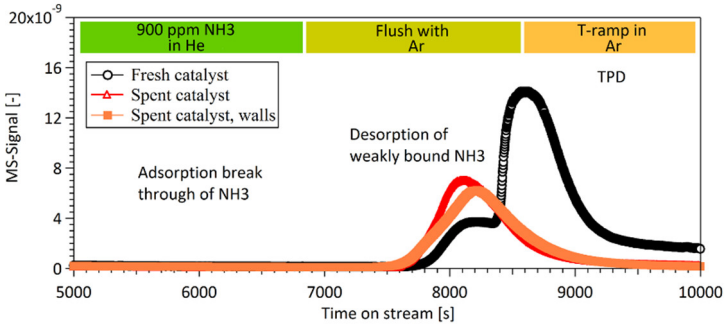


Figure 1: Probing of acid sites with NH_3 temperature programmed reaction.

The SEM-EDS analysis of the fresh and spent catalysts did not reveal significant changes in the catalyst morphology nor distribution of elements. However, the analysis indicated slight enrichment of sulphur on the surface of the spent catalyst (Figure 2). Mapping of other elements showed strong correlation of sulphur and calcium maps, suggesting sulphur to be present as $CaSO_4$. The sulphur compounds can be responsible for the blocking of acid sites and reduction in acidity discussed above.

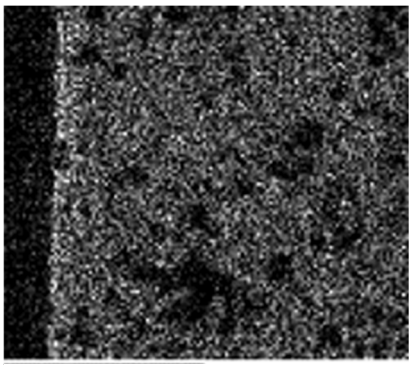


Figure 2: SEM-EDS analysis of spent SCR monolith cross-section; sulphur mapping.

Changes in the vanadium concentration and distribution were also investigated by both SEM-EDS and TEM analysis. Due to overlap, however, differentiation between Ti and V requires very precise peak convolution. Further investigations of vanadium species will therefore be performed with spectroscopic techniques such as Raman and XPS.

IIA 3 Frontier formalin technology development

The Team in 2016

Jasmina Hafizovic Cavka	SINTEF	IIA leader
Kristin Bingen	DYNEA	Industrial senior, industry researcher (WP3.1-3.2-3.3), WP responsible (3.2-3.3)
Terje Pedersen	KA Rasmussen	Industrial senior, industry researcher (WP3.1)
Hilde Venvik	NTNU	PhD supervisor, WP responsible (WP3.1), advisor (WP3.3)
Jia Yang	NTNU	PhD supervisor (WP3.1), advisor (WP3.3)
Stine Lervold	NTNU	PhD student (WP3.1)
Rune Lødeng	SINTEF	PhD supervisor (WP3.1), researcher (WP3.2-3.3)
Alma Engelbrecht	DYNEA	Industry researcher (WP3.2-3.3)
Mohammad Washi Uddin	DYNEA	Industry researcher (WP3.2)
Roman Tschenscher	SINTEF	Researcher (WP3.2-3.3)

Motivation

Formalin is a base chemical that is widely used for adhesives and resins applied in the wood industry. Production proceeds by catalytic oxidation of methanol to formaldehyde, in excess air over a mixed base 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%.

Improving selectivity is the main target, and because of the fast and exothermic nature of the reactions involved, it requires understanding of the heat and mass transfer phenomena as well as the surface chemistry proceeding on the silver. Gas phase chemistry may also play a role at the typical processing temperatures 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 taking better control of the reaction conditions and tuning of the silver particle/bed morphology, thus controlling both selectivity and stability.

The three work packages are partly integrated through addressing the 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).

Main Findings and Conclusions

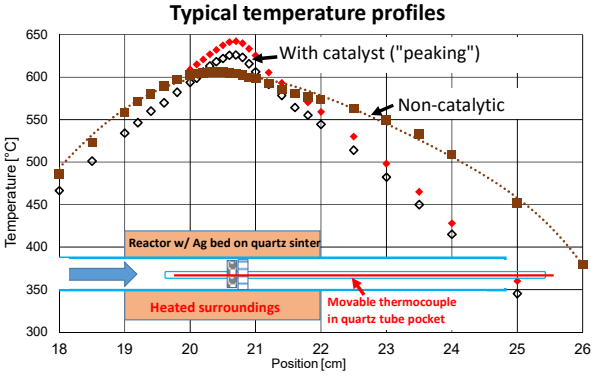
One of the main project goals is further increasing an already high yield of formaldehyde. An increment improvement would have a significant impact on the economics of the overall process. A precision of ±2% is thus necessary in the investigations of this chemical reaction system; which is challenging due to several factors (packing of catalyst bed, temperature measurement and control, accuracy of feed system and analytics, product stability). Two complementary experimental set-ups have been designed for establishing high precision data. One is optimized for kinetic studies at laboratory scale (Reactor 1) and targeting close control of the temperature conditions, and the other for screening of parameters at industrial conditions (Reactor 2).

Examples of high precision, reproducible results obtained in Reactor 1 are illustrated below. Initially, it had to be confirmed that the conversion in the empty reactor is at a satisfactorily low level; established as below 2.5% CH_3OH conversion with a non-detrimental selectivity. In the figure, the range of conditions investigated is given alongside a graph illustrating the temperature inside the tubular quartz reactor with and without catalyst present. The tubular reactor sketch is showing the case of an Ag granular bed supported on a quartz sinter. The bottom plot shows the methanol conversion and corresponding product selectivity distribution for a catalytic case. These initial results illustrate well the catalyst properties and the set-up performance. The low level of CO formation indicates that the reactor design prevents gas phase decomposition of the formaldehyde product. The data corresponds to formaldehyde yields close to 90%, which is a good starting point for exploring further improvements. Finally, the conditioning period during the initial period on-stream, as observed by the gradually increasing CH_3OH conversion, should be noted as it is indicative of beneficial structural changes in the surface of the silver granules due to the temperature and the ongoing surface chemistry.

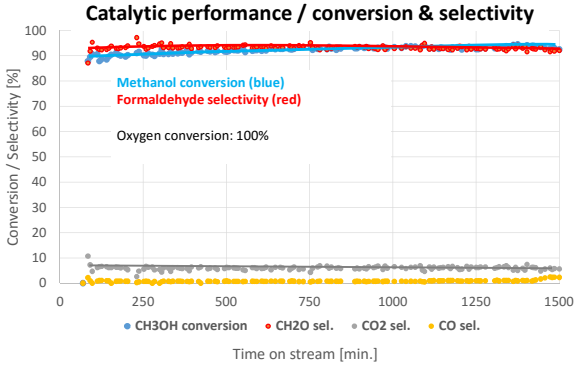
Typical conditions

Quartz reactor	; i.d. 11 mm
Catalyst granules	; 100 – 500 mg (0.25 – 0.5 mm)
Temperatures	; < 700 °C
Total flow	; 250 – 750 ml/min
Feed composition (vol.%)	
Methanol	; 8
Water	; 9.44
Oxygen	; 3.46
Nitrogen	; 79.1

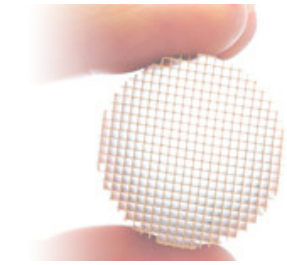
Typical temperature profiles



Catalytic performance / conversion & selectivity



Typical conditions (top left), sketch of reactor with typical temperature profiles (top right), and catalytic performance of 450 mg Ag (left) at ~600 °C and 500 Nml/min reactant gas flow (bottom).




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

The Team in 2016

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)
Kumar R. Rout	SINTEF	Researcher (WP4.1-4.2-4.3)
Torbjørn Gjervan	SINTEF	Researcher (WP4.2)

Published paper: **Highly Active and Stable CeO_2-Promoted $CuCl_2/Al_2O_3$ Oxychlorination Catalysts Developed by Rational Design Using a Rate Diagram of the Catalytic Cycle,** K. R. Rout, E. Fenes, M. F. Baidoo, R. Abdollahi, T. Fuglerud, D. Chen, *ACS Catalysis* 2016, 6 (10), 7030-7039.

Oral contribution: **Quantitatively defining promotor influence on catalytic activity and stability in ethylene oxychlorination**, E. Fenes, K. Rout, M.F. Baidoo, T. Fuglerud, D. Chen, Oral presentation, 11th Natural Gas conversion symposium, June 2016, Tromsø, Norway

Motivation

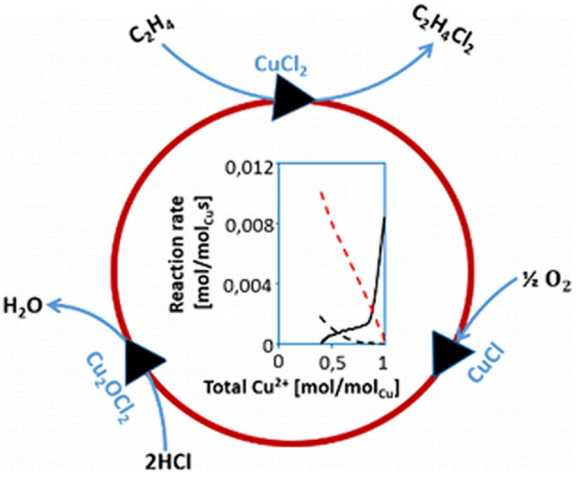
Polyvinylchloride (PVC) produced by polymerization of the monomer vinyl chloride (VCM, C_2H_3Cl), is the third-most widely produced plastic and finds application in flooring, piping, profiles, cables, etc. VCM production based on ethylene was introduced in the 1950's and is a mature process where high plant reliability and continuous improvement of energy and raw material efficiency is still required to remain competitive. VCM is produced from ethylene and chlorine in a process involving several chemical conversion steps, one being the oxychlorination of ethylene to EDC, i.e. 1,2 dichloroethane ($(CH_2)_2Cl_2$), in a fixed or fluidized bed reactor.

The $CuCl_2/\gamma$-Al_2O_3 system is the commonly used catalyst in this process and it is generally agreed that the oxychlorination reaction involves a redox process in which copper cycles between $Cu^{(I)}$- 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. An operando fixed bed reactor set-up combined with UV/Vis- and mass spectroscopy has been established at NTNU to measure spatial-time quantitative kinetics of the reaction while characterizing the active catalyst component involved. A strategy of combined transient- and steady-state kinetic investigations then enables prediction of the reaction rate and the copper oxidation state at steady-state conditions.

Another main challenge of this process is that the $Cu^{(I)}$ forms on the surface of the catalyst during the reaction thereby causing the aggregation and loss of active Cu. Compounds of alkali and/or rare earth

metals are often used as promoters to increase the activity, selectivity and stability. KCl is the most common promoter used for Cu based fixed bed catalysts. In the project, the promoter effect of on reduction, oxidation and steady state reactions is studied. The aim is to provide more detailed scientific insights to the effect of such promoters, and eventually to identify descriptors for the promoter effects that enable rational catalyst design principles.

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



We developed here a new kinetic diagram to approximately predict the steady-state reaction rate and Cu oxidation state based on the kinetic evolution of the single steps in the catalytic cycle. At steady-state, the reduction- and oxidation reaction rates should be identical, represented as the intersection point of the two curves. In this respect, the rate and the Cu oxidation state corresponding to the intersection point represent the steady-state rate and Cu oxidation state at the given reaction conditions. An analysis of the unpromoted catalyst, rate diagram in the Figure points out that significantly increasing the oxidation rate, represented in the Figure as a theoretical oxidation rate (red dashed line) of an ideal catalyst, could remarkably increase the steady-state reaction rate and Cu^{2+} concentration, hence improving catalytic stability. By using the catalyst design tool, highly active and stable catalysts could be obtained. The rate diagram is a useful tool that allows understanding the mechanism of the catalytic cycle at an unprecedented level, but also facilitating catalyst design of the redox reaction cycle, achieving high activity, selectivity and stability. The method is expected to have a significant implication for the rational design of highly active and stable heterogeneous catalysts in general.

Two papers coming soon

Understanding of Potassium Promoter Effects on Oxychlorination of Ethylene by Operando Spatial-time Resolved UV-Vis-NIR Spectrometry, K. R. Rout, M. F. Baidoo, E. Fenes, J. Zhu, T. Fuglerud, and D. Chen, J. Catal. 2017; **Accepted**

On the Effects of K and La Co-promotion on $CuCl_2/\gamma$-Al_2O_3 Catalysts for the Oxychlorination of Ethylene, Martina F. Baidoo, Endre Fenes, Kumar Ranjan Rout, Terje Fuglerud, De Chen, Catalysis Today, 2017, **Submitted**

IIA 5 The next step in direct activation of lower alkanes

The Team in 2016

Stian Svelle	UiO	IIA Leader, PhD supervisor, WP responsible (WP5.1-5.2-5.3)
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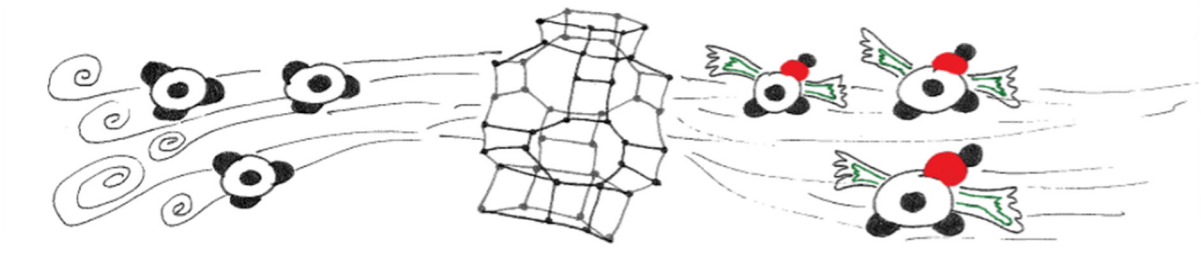
Dimitrios Pappas	UiO	PhD student (WP5.1-5.2)
Michael Dyballa	UiO	Postdoctoral fellow (WP5.1-5.2-5.3)
Lars Fahl Lundegaard	HTAS	Industry researcher (WP5.1)
Ton Janssens	HTAS	Industry researcher (WP5.2-5.3)
Bjørnar Arstad	SINTEF	Researcher (WP5.3)

Motivation

Researchers at UiO and Haldor Topsøe AS are working on developing new nanostructured catalyst materials, with potential for breakthrough discoveries within direct conversion of lower alkanes to chemicals or liquid fuels.

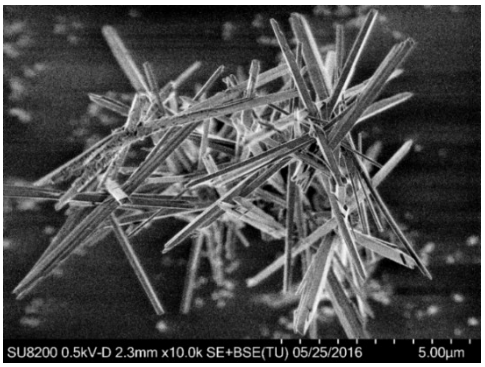
Current industrial routes for exploitation of natural gas (methane) for chemicals production rely on synthesis gas (CO + H_2) as an intermediate. Therefore, a low temperature activation and transformation of methane as well as other lower alkanes directly into valuable chemicals, such as methanol, is commonly considered "a dream reaction" due to its enormous industrial potential. While Haldor Topsøe AS supplies essential technology to most existing routes, new pathways are considered an essential extension of current portfolio and competence within synthesis, functionalization and application of zeotype materials.

Recent discoveries indicate that certain zeotype materials hold remarkable potential as catalysts for direct conversion of methane. Remaining key challenges are easily identified, however, that translates into a need for rational design of zeolite materials with tailored properties, advanced operando characterization of the active site, and process engineering. The iCSI consortium members possess all the competences required to successfully tackle these challenges and progress towards a viable process. (Illustration by Karoline Kvande, Master student, UiO)



Synthesis of new zeolite catalysts – Postdoctoral fellowship

The main goal of 2016 was synthesizing a library of potential catalysts, developing new synthesis methods and implementing standard characterization procedures. This resulted in the development of a basic protocol for further research, and also a substantial amount of highly interesting materials of which one is illustrated in the figure below. In addition to that, completely new characterization methods have been developed, involving also the collaboration partners at SINTEF. This means a good starting point for thorough research in 2017 in a wider collaboration. We intend to develop the new characterization methods further in 2017 and bring all the results from different approaches together. This includes especially own characterization, XAS results from external cooperation partners and MAS NMR (Magic Angle Spinning –Nuclear Magnetic Resonance Spectroscopy) results obtained at SINTEF.

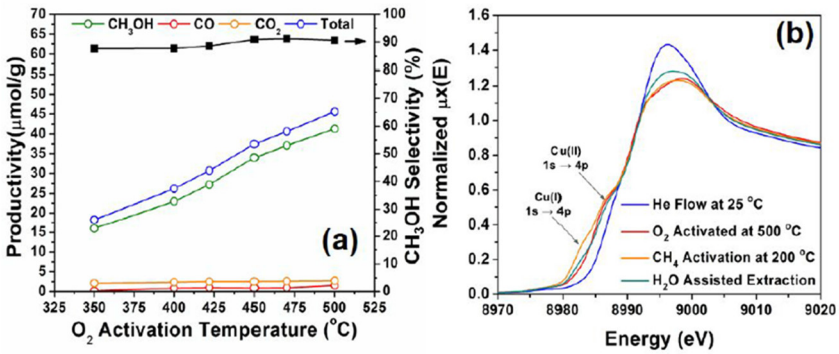


New zeolite catalyst

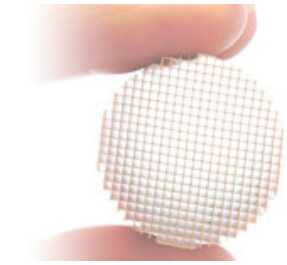
Catalytic performance – PhD project

A new catalytic performance evaluation setup has been built in order to test materials for the direct conversion of methane to methanol. Different catalysts for the reaction have been explored, in particular Cu-exchanged zeolites supplied by Haldor Topsøe AS or as well as synthesized at UiO.

Different studies were conducted to get insights into the reaction and be able to optimize the testing in terms of conditions and catalysts. In addition to that, operando X-Ray Absorption Spectroscopy (XAS) and Emission Spectroscopy (XES) using Synchrotron X-Rays were performed at ESRF (European Synchrotron Radiation Facility) in Grenoble, France. The location, coordination and oxidation state of Cu during the different steps of a partial oxidation reaction cycle were studied for different Cu-exchanged zeolites, with one example presented in the figure below.



Performance and characteristics of the material Cu-SSz-13 (Si/Al = 12, Cu/Al = 0.5) in the stepwise, stoichiometric partial methane oxidation to methanol. (a) Productivity (left axis) and selectivity (right axis) plotted as a function of O_2 activation temperature. (b), Cu K-Edge X-Ray Absorption Near Edge Structure (XANES) spectra of Cu-SSZ-13 (Si/Al=12, Cu/Al=0.5) collected after each step of a reaction cycle. (Submitted to the 25th North American Meeting (NAM) of the Catalysis Society, June 4-9, 2017, Denver, USA).




IIA 6 Generic projects for additional industrial synergies

The Team in 2016

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)
Hilde Venvik	NTNU	PhD supervisor (WP6.1)
John Walmsley	SINTEF	Researcher (WP6.1-6.4)
Oleksii Ivashenko	UiO	Postdoctoral fellow (WP 6.2)
David Waller	Yara	Industrial senior, industry researcher (WP6.2)
Helmer Fjellvåg	UiO	Researcher (WP6.2)
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Terje Fuglerud	INOVYN	Industry researcher (WP6.3)
Kumar R. Rout	SINTEF	Researcher (WP6.3)
Rune Lødeng	SINTEF	Researcher (WP6.4)
Patricia Almeida Carvalho	SINTEF	Researcher (WP6.4)
Martin F. Sunding	SINTEF	Researcher (WP6.4)

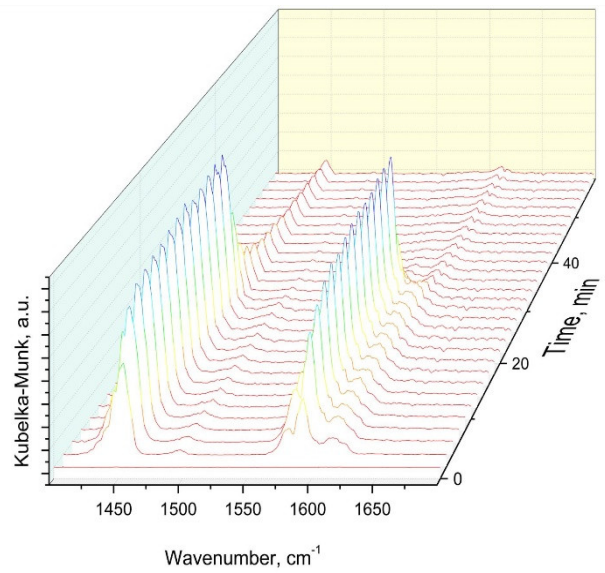
Motivation

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 IIA1-5 in the future. In particular, advanced spectroscopic and microscopic investigations under conditions highly relevant to industrial operation is targeted. The second pillar in this effort is to advance atomistic and kinetic modeling of metals and oxides, as well as reactor modeling, to eventually enable an integrated, multiscale approach.

In situ characterization methodology for catalytic active sites determination – PhD project

For heterogeneous catalytic systems, an experimental mode combining both the acquisition of kinetic and structural information in the same setup, called in situ or operando, is highly desirable as well as challenging. Such an approach could bring more mechanistic insights to the 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.



Waterfall plot of diffuse reflectance infrared Fourier transform spectroscopy of *in situ* pyridine adsorption (1-30 minutes) and desorption (31-60 minutes) at 423 K and atmosphere pressure.

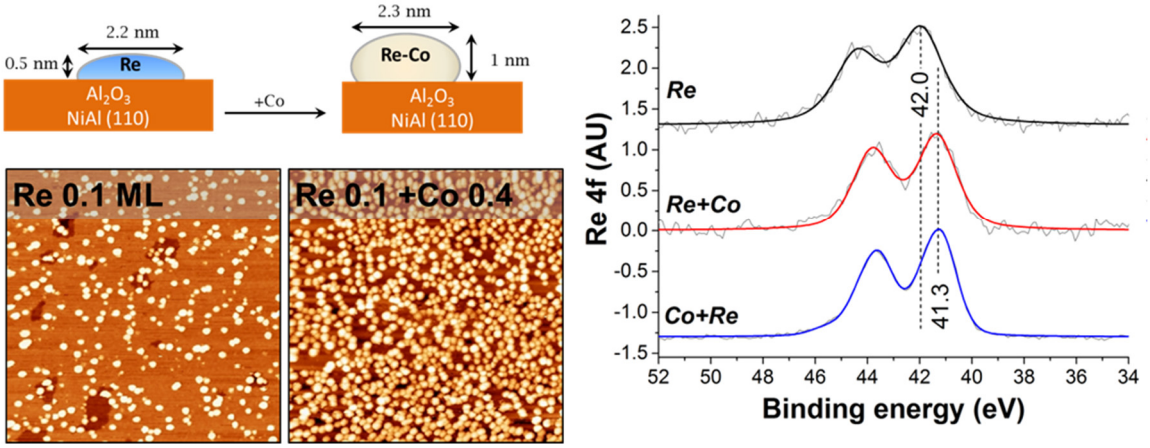
The first catalyst investigated is commercial y-Al_2O_3 modified with W and Pt, relevant to nitric acid technology. The spectroscopic data (see Figure) show distinct vibrational modes of pyridine on strong and medium strong Lewis acid sites of the catalyst even after desorption, thus suggesting a strong interaction between acid site and probe molecule. Comparing and quantifying the acidity of different materials is the key for tuning the acidity for specific processes and applications.

Advanced synthesis and characterization – novel thin film preparation and reactor STM – Postdoctoral fellowship

A new Reactor-STM (Scanning Tunneling Microscope) has been in operation at UiO since June 2016. The system, which is the 5th of its type worldwide, is capable of scanning surfaces in the temperature interval from 20 to 300^{o}C and pressures from ultra-high vacuum (UHV) conditions to 6 bar in presence of reactive gasses such as NH_3, NO, H_2 and CO. The first stages of surface preparation and characterization of a PtRh/Pt(111) model catalyst under UHV have so far been accomplished, and further results will be relevant to understanding the performance of ammonia oxidation catalysts (see IIA1, page 19). In addition, initial experiments on a TiO_2 (110) single crystal have been performed, and this is a relevant model system for NO_x removal catalysts (see IIA2, p. 20-21)

Part of the training on the Reactor-STM system was performed in Leiden, a leading environment for this type of investigations. This took place both at LPM (Leiden Probe Microscope), the company that produces the Reactor-STM and at the University of Leiden. During this training, the preparation and characterization (STM+XPS) of a Cobalt (Co) catalyst promoted with rhenium (Re) and supported on Al_2O_3/NiAl(110) crystal was performed. The elucidation of the role of Re associated with Co is

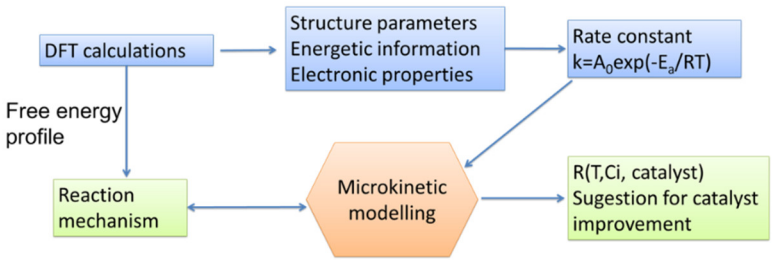
important to the Fischer-Tropsch process, utilized in the conversion of natural gas or biomass to liquid fuels.



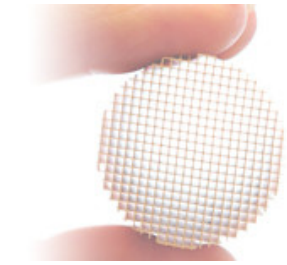
Scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) of Re nanoparticles on Al_2O_3/NiAl(110) before and after sequential deposition of Co nanoparticles, realized at the University of Leiden, the Netherlands.

Reaction mechanism investigation by combined DFT calculations and microkinetic modelling – Postdoctoral fellowship

Density functional theory (DFT) calculations is based on the fundamental equations governing 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 to be able to tailor catalysts atom by atom. 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. A schematic figure of DFT based microkinetic modelling is shown in the figure below. By developing this methodology, the project has enabled to bridge the gap from the atomic level to kinetic analysis at macro-scale. This is currently being employed to reaction systems of vinyl chloride monomer synthesis and formaldehyde synthesis. In the former case, understanding the details of the alkali and/or rare earth promoter mechanism is targeted (see IIA4, p. 24-25). For the latter, the details of the interaction between the Ag catalyst and O_2/H_2O is investigated; understanding which is key to tuning the selectivity of the process (see IIA3, p. 22-23).



Schematic figure of DFT-based microkinetic modelling



iCSI

sfi Centre for Research-based Innovation

NTNU – Trondheim Norwegian University of Science and Technology

The **iCSI** Kick-off seminar

The ***Annual iCSI seminar*** takes place to share and discuss the results obtained in IIAs and the work packages, to ensure good interaction between the industrial and the research partners, and to provide a training arena for the PhD candidates and postdoctoral fellows.

The iCSI Kick-off seminar was held in Trondheim in Nov 22 to 23 2016 at NTNU. In total 50 participants were present including the first SAC member appointed, Professor Alessandra Beretta from Politecnico di Milano. She presented her lecture "***CPO of hydrocarbon fuels on Rh: kinetic analysis and Raman characterization in annular reactor***".

The Seminar program included presentations from the IIA leaders and the Industrial Committee as well social activities. The Board also was officially presented to all the participants and the PhD candidates and Postdocs presented their work and further plans.

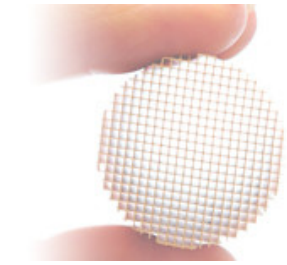
iCSI Kick off Seminar November 23-24 2016

Wednesday 23/11/2016 ***Rådssalen, Main Building, NTNU***

11.30 - 12.00	**Registration**
12.00 - 12.30	**Welcome opening** Professor Johan E. Hustad, Pro-rector Innovations, NTNU Dr. Odd-Arne Lorentsen, iCSI Board Chairman, YARA International Professor Hilde Venvik, iCSI Director, NTNU
12.30 - 13.30	**Lunch**
13.30 - 14.30	**IIAs Presentations by IIA leaders and Industrial Seniors** IIA 1 *21st century Ammonia Oxidation and Nitric Acid technology development.* Prof. Anja Sjålstad, NAFUMA, UiO. IIA 2 *New NOx abatement technologies for the marine market and state-of-the-art SCR catalysis.* Dr. Karl-Isak Skau, YARA International. IIA 3 *Frontier formalin technology development.* Dr. Jasmina Hafizovic Cavka, SINTEF Materials and Chemistry. IIA 4 *PVC Value Chain: World class energy and raw material efficiency for the production of Chlorine and Vinylchloride Monomer (VCM).* Dr. Terje Fuglerud, INOVYN. IIA 5 *The next step in direct activation of lower alkanes.* Prof. Stian Svelle, UiO and Dr. Pablo Beato, HTAS.
14.30 - 15.00	**Coffee Break**
15.00 - 15.45	**The iCSI Scientific Advisory Committee presents** ***CPO of hydrocarbon fuels on Rh: kinetic analysis and Raman characterization in annular reactor*** Professor Alessandra Beretta, Politecnico di Milano
16.30 - 19.30	**Team building activity**
20.00 - 22.00	**iCSI Dinner** (*Banksalen Restaurant, Kongens Gate 4, 7010 Trondheim)*

Thursday 24/11/2016, ***Konferansesenteret i SpareBank 1 SMN, Trondheim***

9.00 - 10.30	**Research presentations – 20 min + questions** **9.00** *IIA 5, Partial Methane Oxidation to Methanol Over Copper Exchanged Zeolites*. Dimitrios Pappas and Dr. Michael Dyballa, UiO/Haldor Topsøe **9.30** *IIA 4, Oxychlorination of Ethylene: Catalysts, Kinetics and Process Optimization* . Dr. Kumar Ranjan Rout, SINTEF/NTNU **10.00** *IIA 1, Reducing platinum losses during ammonia combustion.* Dr. David Waller, Dr Børge Holme and Asbjørn Slagtern Fjellvåg, YARA/SINTEF/UiO/K.A. Rasmussen
10.30 - 11.45	**Posters Session –** Snacks / Coffee will be served
11.45 - 12.30	**Panel discussion Industrial Committee / SAC**
12:30 - 13.00	**Closing session** - iCSI Industrial Poster prize - iCSI SAC poster prize - Closing remarks
13.00 - 14.00	**Lunch**



iCSI Internationalization 2016

Sabbatical leave

Professor Magnus Rønning (NTNU), Stanford University (US), from July 2016 to June 2017.

Overview of international collaborations

- 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 Helsinski, 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

European research projects:

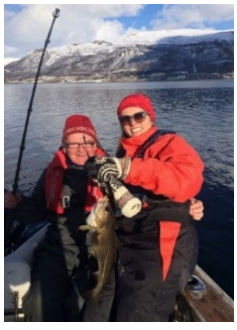
- ***ZeoMorph***, FP7-ITN-EID, 5 PhD projects, iCSI Partners involved: UiO/HTAS
- ***FASTCARD***, FP7-NMP-2017-LARGE-7, iCSI Partners involved: SINTEF/NTNU
- ***Horizon 2020 Projects: PrintCr3dit*** and ***ProDIA,*** iCSI Partner involved in both: SINTEF

Research Council of Norway projects with international collaborations:

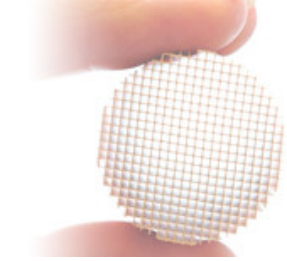
- ***EmX 2025***, TRANSPORT 2025, iCSI Partners involved: NTNU/ SINTEF
- ***Development of Catalysts and Materials for Compact Steam Reformer***, GASSMAKS, iCSI Partners involved: NTNU/ SINTEF
- ***GAFT-Fischer Tropsch synthesis of biofuels***, EnergiX, iCSI Partner involved: SINTEF
- ***FutureFeed***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

NGCS 11 Tromsø 2016
The 11th Natural Gas Conversion Symposium

The iCSI partners hosted the ***NGCS11 - 11th Natural Gas Conversion Symposium*** in Tromsø, Norway in June 2016. 300 participants from 30 countries of all continents attended the conference, which is a triannual event under the auspices of the Natural Gas Conversion Board. The local organizing committee was composed of Hilde Venvik (NTNU, Chair), Anders Holmen (NTNU, Chair), Unni Olsbye (UiO), Erling Rytter (NTNU, Statoil), De Chen (NTNU), Duncan Akporiaye (SINTEF) and Steinar Kvisle (INOVYN).



Co-chairs: Professors Anders Holmen and Hilde Venvik



Communication and dissemination

Invited lectures

Professor De Chen was invited to the 11th International Congress of Catalysis (ICC 11) held in July 3-8 in Beijing, China to give a lecture entitled "**A New Insight into Reaction Mechanism of Fischer-Tropsch synthesis on Cobalt catalysts: A Combined Study of DFT and SSITKA**".

Prof. Unni Olsbye gave a plenary lecture "**MTH revisited, status and prospects from fundamental studies**" during the NGCS 11, Tromsø, Norway.
She was also invited speaker at the 6th EuChemS Chemistry Congress in Sevilla in September 2016 about "**Catalysis in confined space - ethene oligomerisation in Ni-containing zeolites and MOFs**".

Keynotes lectures

Professor Unni Olsbye gave a keynote lecture "**MTH revisited - Status and prospects from fundamental studies**" at the Post-Symposium on Catalysis for Syngas and Methanol Conversion of ICC-2016, July 9-11, Beijing, China.

Professor De Chen gave several keynote lectures in 2016:

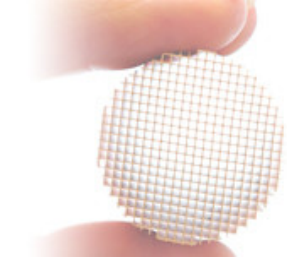
- **Ni Based Steam Reforming Catalysts: From Molecular Understanding to Catalyst Design**, at NGCS 11, June 3-9, Tromsø, Norway.
- **Synthesis and applications of carbon based multifunctional catalysts for biomass conversion** at the Symposium on Carbon for Catalysis (CarboCat), June 12-15, Strasbourg, France.
- **Methane steam reforming on Ni based bimetallic catalysts** at the Symposium on Nano and Interfacial Catalysis, July 9-13, Dalian, China.

Popular dissemination

Hilde Johnsen Venvik and Rune Lødeng, **Feil om katalysatorer**, *Dagens næringsliv,* September 16 2016

Special Publications

Elsevier has appointed iCSI Partners as **Guest Editors** for a Special Issue of Catalysis Today for NGCS 11 Tromsø. The Guest editors are professors Hilde Venvik, Anders Holmen and De Chen (NTNU), Erling Rytter (NTNU, Statoil) and Duncan Akporiaye (SINTEF). Catalysis Today will publish a special issue in 2017 based on selected papers from NGCS 11.



Education within iCSI

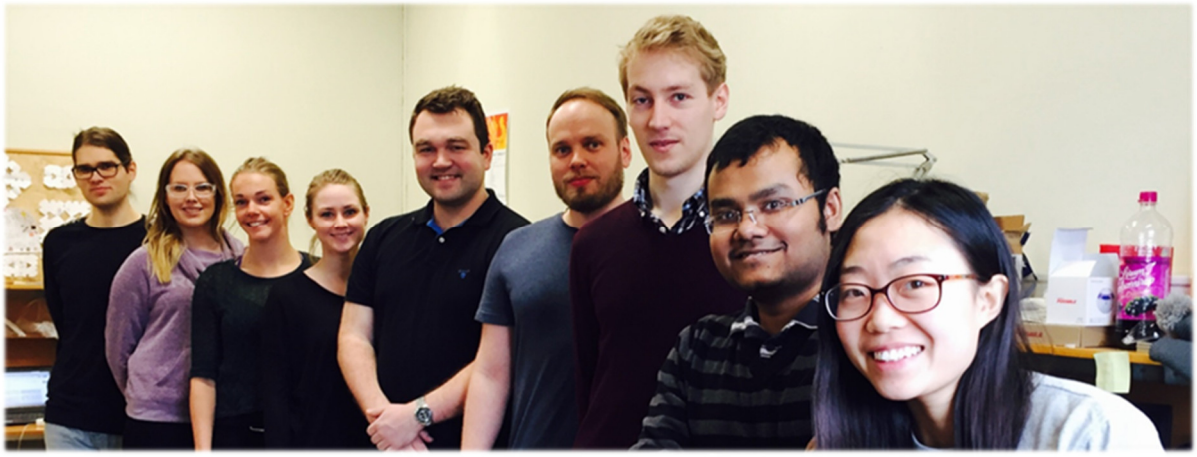
Master Theses

Master Thesis projects in the Department of Chemical Engineering (NTNU) and the Department of Chemistry (UiO) associated or affiliated with iCSI:

Name		Topic
2016: Master thesis projects		
Ellinor Sofie Smith Wiker	NTNU	Reactor model for oxychlorination of ethylene in multi-tubular fixed bed reactors
Annemari Løberg Larsen	NTNU	Reduction of Cu-ZnO water-gas shift catalysts in presence of water
Mads Alexander Lid	NTNU	Efficient catalysts for achieving NO /NO_2 equilibrium
Ole H. Bjørkedal	NTNU	Efficient catalysts for achieving NO /NO_2 equilibrium
Stine Lervold	NTNU	Characterization of Ag catalysts for formalin production
Vegard Andreas Naustdal	NTNU	Characterization of Ag catalysts for formalin production
Hanna Marie Storvik	NTNU	Catalysis for control of methane slip in marine machinery
Helene Sandvik	NTNU	Catalysis for control of methane slip in marine machinery
Tor Erik Sørensen	NTNU	Catalytic conversion of kerogen in enhanced oil production from shales
Debashish Chowdhury	NTNU	Synthesis and characterization of tungsten carbide
Wei Ge	NTNU	Multifunctional proppants for enhanced oil production from shales
Marthe Meyer	NTNU	Catalytic conversion of kerogen in enhanced oil production from shales
Shawn Christopher Apan	NTNU	Photocatalytic H_2-production through photo-reforming of hydrocarbons
Benedicte Hovd	NTNU	Direct conversion of methane to C2 hydrocarbons, aromatics and hydrogen
Mustafa Kømurcu	UiO	Ethene oligomerization on Ni containing beta zeolite catalysts
Daniel Wolseop Lee	UiO	Formulation of metal organic framework compounds
Maria Mykland	UiO	Synthesis and characterization of AFI zeotype materials
2016: Specialization projects		
Rakel Johanne Ekholt	NTNU	Oxidation of Methanol to Formaldehyde over Ag – Kinetic Modelling using Comsol **(WP3.1)**
Ragnhild Brokstad Lund-Johansen	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
Sebastian Langfjæran	NTNU	Synthesis and characterization of Tungsten Carbide

Exchange Students in 2016

Exchange Bachelor students 2016 at NTNU		
Ruiyu Zhang	China	Metal anticorrosion applications of electrochemical exfoliated graphene
Yaki Qin	China	Application of biomass derived carbon materials in waste oil recycling
Exchange Master students 2016 at NTNU		
David Kovacic	Slovakia	Cellulose conversion by hybrid catalysts
Marc Greuel	Germany	Catalytic conversion of biomass in biphasic system
Thomas Naumayer	Germany	Fischer-Tropsch synthesis catalysts for CO_2-rich syngas
Exchange Master students 2016 at UiO		
Koen Bossers	Netherlands	CO_2 reduction over functionalized MOFs
Stefano Palliggiano	Italy	Characterization of porous solid materials for industrial application
Exchange PhD students 2016 at NTNU		
Ting Cui	China	One pot synthesis of chemicals from biomass
Niu Juntian	China	Steam reforming of methane on bimetallic catalysts



2015-2016 Master students at NTNU (from left to right): exchange student David Kovacic (Slovakia), Stine Lervold, Marthe Meyer, Ellinor Sofie Smith Wiker, Ole Bjørkedal, Vegard Andreas Naustdal, Mads Alexander Lid, Debashish Chowdhury, exchange PhD student Ting Cui (China). Photo: Estelle Vanhaecke, NTNU

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

Accounts 2016

Table 1 summarizes the costs in 2016 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

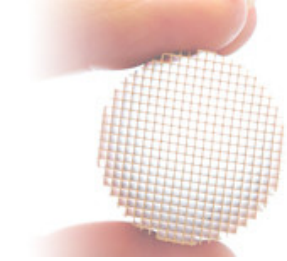
Cost code	Costs 2016	2015-2023 Total budget
Payroll and indirect expenses	5382	62692
Procurement of R&D services	9985	92038
Equipment	596	6650
Other operating expenses	4364	30755
Totals	**20328**	**192135**

Table 2 presents the cost and financing per partner. The Industrial Partners are Yara ASA, DYNEA AS, INOVYN AS, K.A. RASMUSSEN AS and HALDOR TOPSØE AS.

Cost and Financing per partner	2016 Accounts		2015-2023 Total budget	
Partner	Costs	Financing	Costs	Financing
NTNU	6560	2760	76098	27914
University of Oslo	4627	1272	48538	12363
SINTEF	5359	998	43500	7858
Industrial partners	3782	6782	24000	48000
Research Council of Norway	-	8516	-	96000
Totals	**20328**	**20327**	**192136**	**192135**

Table 3 presents the costs per Industry Innovation Area (IIA). The iCSI Management and administration include the overall administration of the Centre (Director, Coordinator and economy Advisor, meetings, seminars, SAC members compensation, international exchange funding).

Industrial Innovation Area (IIA)	Costs 2016	2015-2023 Total budget
IIA1 21st century Nitric Acid technology development	4343	41149
IIA2 New NOx abatement technologies	899	7322
IIA3 Frontier formalin technology development	3092	21027
IIA4 PVC Value Chain	2395	31339
IIA5 The next step in direct activation of methane	3920	34708
IIA6 Generic projects	3989	39701
iCSI Management and administration	1690	16889
Totals	**20328**	**192135**



iCSI

Centre for Research-based Innovation

NTNU – Trondheim Norwegian University of Science and Technology

Publications 2016

The first publication by iCSI was accepted in 2016. The other publications listed are all associated with projects funded from other sources but all affiliated to the iCSI research partners.

Publication by iCSI

Rout, Kumar Ranjan; Fenes, Endre; Baidoo, Martina Francisca; Abdollahi, Reza; Fuglerud, Terje; Chen, De, **Highly Active and Stable CeO_2-Promoted $CuCl_2/Al_2O_3$ Oxychlorination Catalysts Developed by Rational Design Using a Rate Diagram of the Catalytic Cycle**, *ACS Catalysis* 2016, 6, 7030-7039

iCSI associated journal publications

Arstad, Bjørnar; Lind, Anna Maria; Cavka, Jasmina Hafizovic; Thorshaug, Knut; Akporiaye, Duncan; Wragg, David; Fjellvåg, Helmer; Grønvold, Arne; Fuglerud, Terje, **Structural changes in SAPO-34 due to hydrothermal treatment. A NMR, XRD, and DRIFTS study**, *Microporous and Mesoporous Materials*, 2016, 225, 421-431

Bokach, D.; Ten H., Sander; Muthuswamy, N.; Buan, M. E. M.; Rønning, M., **Nitrogen-doped carbon nanofiber catalyst for ORR in PEM fuel cell stack: Performance, durability and market application aspects**, *International Journal of Hydrogen Energy*, 2016, 41, 17616-17630

Borfecchia, Elisa; Øien-Ødegaard, Sigurd; Svelle, Stian; Mino, Lorenzo; Braglia, Luca; Agostini, Giovanni; Gallo, Erik; Lomachenko, Kirill A.; Bordiga, Silvia; Guda, Alexander A.; Soldatov, Mikhail A.; Soldatov, Alexander V.; Olsbye, Unni; Lillerud, Karl Petter; Lamberti, Carlo, **A XAFS study of the local environment and reactivity of Pt- sites in functionalized UiO-67 MOFs**, *Journal of Physics, Conference Series 712*, 2016, 012125, 1-4

Bremmer, Marien G.; 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*, 2016,

Brogaard, Rasmus Yding; Olsbye, Unni, **Ethene Oligomerization in Ni-Containing Zeolites: Theoretical, Discrimination of Reaction Mechanisms**, *ACS Catalysis*, 2016, 6, 1205-1214

Buan, M. E. M.; Muthuswamy, N.; Walmsley, J.; Chen, D.; Rønning, M., **Nitrogen-doped carbon nanofibers on expanded graphite as oxygen reduction electrocatalysts**, *Carbon*, 2016, 101, 191-202

Dadgar, F.; Myrstad, R.; Pfeifer, P.; Holmen, A.; Venvik, Hilde J., **Direct dimethyl ether synthesis from synthesis gas: The influence of methanol dehydration on methanol synthesis reaction**, *Catalysis Today* 2016, 270, 76-84

Del Campo, Pablo; Slawinski, Wojciech Andrzej; Henry, Reynald Philippe; Westgård Erichsen, Marius; Svelle, Stian; Beato, Pablo; Wragg, David; Olsbye, Unni, **Time- and space-resolved high energy operando X-ray diffraction for monitoring the methanol to hydrocarbons reaction over H-ZSM-22 zeolite catalyst in different conditions**, *Surface Science*, 2016, 648, 141-149

Del Campo, Pablo; Slawinski, Wojciech Andrzej; Henry, Reynald Philippe; Westgård Erichsen, Marius; Svelle, Stian; Beato, Pablo; Wragg, David; Olsbye, Unni**, Time- and space-resolved high energy operando X-ray diffraction for monitoring the methanol to hydrocarbons reaction over H-**

ZSM-22 zeolite catalyst in different conditions, *Surface Science*, 2016, 648, 141-149

den Otter, J. H.; Yoshida, H.; Ledesma, C.; Chen, D.; de Jong, K. P., **On the Superior Activity and Selectivity of Ptco/Nb_2O_5 Fischer Tropsch Catalysts,** *Journal of Catalysis,* 2016, *340*, 270-275.

Duan, X. Z.; Ji, J.; Yan, X. D.; Qian, G.; Chen, D.; Zhou, X. G., **Understanding Co-Mo Catalyzed Ammonia Decomposition: Influence of Calcination Atmosphere and Identification of Active Phase**, *ChemCatChem*, 2016, 8, 938-945

Duan, X. Z.; Wang, D.; Qian, G.; Walmsley, J. C.; Holmen, A.; Chen, D.; Zhou, X. G., **Fabrication of K-Promoted Iron/Carbon Nanotubes Composite Catalysts for the Fischer-Tropsch Synthesis of Lower Olefins,** *Journal of Energy Chemistry*, 2016, 25, 311-317

Esteban-Díez, G.; Gil, M. V.; Pevida, C.; Chen, D.; Rubiera, F., E**ffect of Operating Conditions on the Sorption Enhanced Steam Reforming of Blends of Acetic Acid and Acetone as Bio-Oil Model Compounds,** *Applied Energy*, 2016, 177, 579-590

Feng, X.; Chen, D.; Zhou, X. G., **Thermal Stability of TPA Template and Size-Dependent Selectivity of Uncalcined Ts-1 Supported Au Catalyst for Propene Epoxidation with H_2 and O_2**, *RSC Advances*, 2016, 6, 44050-44056

Feng, X.; Liu, Y.; Li, Y.; Yang, C.; Zhang, Z.; Duan, X.; Zhou, X.; Chen, D., **Au/Ts-1 Catalyst for Propene Epoxidation with H_2/O_2: A Novel Strategy to Enhance Stability by Tuning Charging Sequence**, *AIChE Journal*, 2016

Fernandes, V. R. P.; Van der Bossche, M.; Knudsen, J.; Farstad, M. H.; Gustafson, J.; Venvik, H. J.; Grönbeck, H.; Borg, A., **Reversed Hysteresis during CO Oxidation over $Pd_{75}Ag_{25}$(100)**, *ACS Catalysis,* 2016, 6, 4154-4161

Gil, M. V.; Fermoso, J.; Pevida, C.; Chen, D.; Rubiera, F., **Production of Fuel-Cell Grade H-2 by Sorption Enhanced Steam Reforming of Acetic Acid as a Model Compound of Biomass-Derived Bio-Oil**, *Applied Catalysis B: environmental*, 2016, 184, 64-76

Huang, X.; Li, H.; Xiao, W. D.; Chen, D., **Insight into the Side Reactions in Methanol-to-Olefin Process over HZSM-5: A Kinetic Study**, *Chemical Engineering Journal*, 2016, 299, 263-275

Ledesma Rodriguez, C.; Yang, J.; Blekkan, E. A.; Holmen, A.; Chen, D., **Carbon number dependence of reaction mechanism and kinetics in CO hydrogenation on a Co-based catalyst**, *ACS Catalysis* 2016, 6, 6674-6686

Lei, J. Q.; Dong, H.; Duan, X. Z.; Chen, W. Y.; Qian, G.; Chen, D.; Zhou, X. G., **Insights into Activated Carbon-Supported Platinum Catalysts for Base-Free Oxidation of Glycerol**, *Industrial & Engineering Chemistry Research*, 2016, 55, 420-427

Lou, Fengliu; Buan, Marthe Emelie Melandsø; Muthuswamy, Navaneethan; Walmsley, John; Rønning, Magnus; Chen, De, **One-step electrochemical synthesis of tunable nitrogen-doped graphene**, *Journal of Materials Chemistry A*, 2016, 4, 1233-1243

Mahmoodinia, M.; Astrand, P. O.; Chen, D., **Influence of Carbon Support on Electronic Structure and Catalytic Activity of Pt Catalysts: Binding to the Co Molecule**, *Journal of Physical Chemistry C*, 2016, 120, 12452-12462

Mudu, Federica; Olsbye, Unni; Arstad, Bjørnar; Diplas, Spyros; Li, Yanjun; Fjellvåg, Helmer, **Aluminium substituted lanthanum based perovskite type oxides, non- stoichiometry and performance in methane partial oxidation by framework oxygen**, *Applied Catalysis A : General,* 2016, 523, 171-181

Øien-Ødegaard, Sigurd; Bouchevreau, Boris; Hylland, Knut Tormodssønn; Wu, Lianpao; Blom, Richard; Grande, Carlos Adolfo; Olsbye, Unni; Tilset, Mats; Lillerud, Karl Petter, **UiO-67-type Metal-Organic Frameworks with Enhanced Water Stability and Methane Adsorption Capacity**, *Inorganic Chemistry*, 2016, 55, 1986- 1991

Olsbye, Unni, **Single-Pass Catalytic Conversion of Syngas into Olefins via Methanol**, *Angewandte Chemie International Edition*, 2016, 55, 7294-7295

Phan, X. K.; Walmsley, J. C.; Bakhtiary Davijany, H.; Myrstad, R.; Pfeifer, P.; Venvik, H. J.; Holmen, A.**, Pd/CeO_2 catalysts as powder in a fixed-bed reactor and as coating in a stacked foil microreactor for the methanol synthesis**, *Catalysis Today* 2016, 273, 25-33

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*, 2016

Romar, H.; Lillebø A. H.; Tynjälä P.; Hu T.; Holmen A.; Blekkan E. A.; Lassi U., **H_2-TPR, XPS and TEM Study of the Reduction of Ru and Re promoted Co/γ-Al_2O_3, Co/TiO_2 and Co/SiC Catalysts**, *Journal of Materials Science Research*, 2016, 5, 39-49

Rytter, E.; Souskova, K.; Lundgren, M. K.; Ge, W.; Nannestad, Å. D.; Venvik, H. J.; Hillestad, M., **Process concepts to produce syngas for Fischer-Tropsch fuels by solar thermochemical splitting of water and/or CO_2**, *Fuel processing technology* 2016, 145, 1-8

Shearer, Greig Charles; Chavan, Sachin Maruti; Bordiga, Silvia; Svelle, Stian; Olsbye, Unni; Lillerud, Karl Petter, **Defect Engineering: Tuning the Porosity and Composition of the Metal-Organic Framework UiO-66 via Modulated Synthesis**, *Chemistry of Materials*, 2016 , 28, 3749-3761

Shearer, Greig Charles; Vitillo, Jenny G.; Bordiga, Silvia; Svelle, Stian; Olsbye, Unni; Lillerud, Karl Petter, **Functionalizing the Defects: Post Synthetic Ligand Exchange in the Metal Organic Framework UiO-66**, *Chemistry of Materials,* 2016, 28, 7190-7193

Tsakoumis, N.; Johnsen, R. E.; van Beek, W.; Rønning, M.; Rytter, E.; Holmen, A., **Capturing metal-support interactions in situ during the reduction of a Re promoted Co/γ-Al_2O_3 catalyst**, *Chemical Communications*, 2016, 52, 3239-3242

Van Belleghem, J.; Ledesma Rodriguez, C.; Yang, J.; Toch, K.; Chen, D.; Thybaut, J. W.; Marin, G. B., **A Single-Event MicroKinetic model for the cobalt catalyzed Fischer-Tropsch Synthesis**, *Applied Catalysis A : General*, 2016, 524, 149-162

Wang, D.; Ji, J.; Chen, B.; Chen, W.; Qian, G.; Duan, X.; Zhou, X.; Holmen, A.; Chen, D.; Walmsley, J. C., **Novel Fe/Mnk-Cnts Nanocomposites as Catalysts for Direct Production of Lower Olefins from Syngas**, *AIChE Journal*,2016

Wang, X.; Zhou, H.; Lou, F.; Li, Y.; Buan, M. E. M.; Duan, X.; Walmsley, J. C.; Sheridan, E.; Chen, D., **Boosted Supercapacitive Energy with High Rate Capability of aCarbon Framework with Hierarchical Pore Structure in an Ionic Liquid**, *ChemSusChem*, 2016, 9, 3093-3101.

Wang, X.; Zhou, H.; Sheridan, E.; Walmsley, J. C.; Ren, D.; Chen, D., **Geometrically Confined Favourable Ion Packing for High Gravimetric Capacitance in Carbon-Ionic Liquid Supercapacitors**, *Energy & Environmental Science*, 2016, 9, 232-239.

Xie, J.; Yang, J.; Dugulan, A. I.; Holmen, A.; Chen, D.; de Jong, K. P.; Louwerse, M. J., **Size and Promoter Effects in Supported Iron Fischer-Tropsch Catalysts: Insights from Experiment and Theory**, *ACS Catalysis*, 2016, 6, 3147-3157.

Xie, J.; Yang, J.; Dugulan, A.I.; Holmen, A.; Chen, D.; de Jong, K. P.; Louwerse, M. J., **Size and Promoter Effects in Supported Iron Fischer-Tropsch Catalysts: Insights from Experiment and Theory**, *ACS Catalysis* 2016, 6, 3147-3157

Yang, J.; Eiras, S.B.; Myrstad, Rune; Venvik, H.J.; Pfeifer, P.; Holmen, A., **Fischer-Tropsch Synthesis on Co-Based Catalysts in a Microchannel Reactor: Effect of Temperature and Pressure on Selectivity and Stability**, I: *Fischer-Tropsch Synthesis, Catalysts, and Catalysis: Advances and Applications*, CRC Press 2016 ISBN 978-1-4665-5529-7, 223-241

Yang, J.; Frøseth, V.; Chen, D.; Holmen, A., **Particle size effect for cobalt Fischer-Tropsch catalysts based on in situ CO chemisorption**, *Surface Science* 2016, 648, 67-73

Zacharaki, Eirini; Kalyva, Maria Evangelou; Fjellvåg, Helmer; Sjåstad, Anja Olafsen, **Burst nucleation by hot injection for size controlled synthesis of ε-cobalt nanoparticles**, *Chemistry Central Journal 2016*, 10:10

Zhang, J.; Sui, Z. J.; Zhu, Y. A.; Chen, D.; Zhou, X. G.; Yuan, W. K., **Composition of the Green Oil in Hydrogenation of Acetylene over a Commercial Pd-Ag/Al_2O_3 Catalyst**, *Chemical Engineering & Technology*, 2016, 39, 865-873

Zhou, H.; Wang, X.; Sheridan, E.; Gao, H.; Du, J.; Yang, J.; Chen, D., **Boosting the Energy Density of 3D Dual-Manganese Oxides-Based Li-Ion Supercabattery by Controlled Mass Ratio and Charge Injection,** *Journal of The Electrochemical Society*, 2016, 163, A2618-A2622

Popular Science Article

Venvik, Hilde Johnsen; Lødeng, Rune, **Feil om katalysatorer**, *Dagens Næringsliv*, September 16, 2016

iCSI Presentations

Martinez-Espin, Juan Salvador; Joensen, Finn; Beato, Pablo; Olsbye, Unni, **Syngas to clean-burn fuel via Oxygenates: effect of effluent recycling, Molecules @ surfaces,** International Winter School, January 31-Feb 5, Bardonnecchia, Italy

Braglia, Luca; Borfecchia, Elisa; Agostini, Giovanni; Lomachenko, Kirill A.; Bleken, Bjørn Tore Lønstad; Øien-Ødegaard, Sigurd; Bordiga, Silvia; Lillerud, Karl Petter; Olsbye, Unni; Lamberti, Carlo, **XAS for studying the duality of UiO-67 Pt functionalized MOFs depending on the content of H2 in the gas feeding**, 24th SILS Conference, Feb 21-23, Bari, Italy

Nielsen, Malte; Brogaard, Rasmus Yding; Falsig, Hanne; Swang, Ole; Svelle, Stian, **Modeling Catalysis in Zeolites**, Topsøe PhD Workshop, Februar 25, Copenhagen, Denmark

M. Rønning, **Fischer-Tropsch synthesis catalysts: Strategies to enhance the sensitivity of in situ characterization techniques**, Invited lecture: 251st ACS National Meeting, March 13-17, San Diego, USA

Olsbye, Unni; Mudu, Federica; Palcheva, Radostina Dimitrova; Arstad, Bjørnar; Diplas, Spyros; Li, Yanjun; Palcut, Marion; Rauwel, Protima; Fjellvåg, Helmer, **On the performance of aluminium or gallium substituted lanthanum based perovskite type oxides in methane partial oxidation by framework oxygen,** 251st ACS National Meeting, March 13-17, San Diego, USA

M. Rønning, **Nitrogen-doped carbon nanofibres as alternative catalysts for the oxygen reduction reaction in PEM fuel cells**, Invited lecture: SUNCAT seminar, March 21, Stanford University, USA

Mahmoodinia, Mehdi; Åstrand, Per-Olof; Chen, De, **CO Activation on Edge Functionalized Graphene-based Pt Clusters: Electronic and Catalytic Properties**, Girona Seminar 2016: "Predictive Catalysis: Transition-Metal Reactivity by Design", April 17-20, Girona, Spain

Arstad, Bjørnar; Lind, Anna Maria; Thorshaug, Knut; Cavka, Jasmina Hafizovic; Akporiaye, Duncan; Kalantzopoulos, Georgios N.; Lundvall, Fredrik; Wragg, David; Fjellvåg, Helmer; Grønvold, Arne Gidløv; Fuglerud, Terje, **Structural changes in the methanol-to-olefin (MTO) catalyst SAPO-34 after/during hydrothermal treatment**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Chen, Qingjun; Svenum, Ingeborg-Helene; Qi, Yanying; Gavrilovic, Ljubisa; Chen, De; Holmen, Anders; Blekkan, Edd Anders, **Potassium adsorption behaviors on hcp cobalt: A density functional theory calculation**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Dam, Anh Hoang; Wang, Hongmin; Liland, Shirley Elisabeth; Holmen, Anders; Chen, De, **The methane adsorption activation energy dependency on**

different three-hollow sites, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Fenes, Endre; Rout, Kumar Ranjan; Baidoo, Martina Francisca; Fuglerud, Terje; Chen, De, **Quantitatively defining promotor influence on catalytic activity and stability in ethylene oxychlorination**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Gavrilovic, Ljubisa; Blekkan, Edd Anders; Venvik, Hilde Johnsen; Holmen, Anders; Brandin, Jan, **Influence of potassium species on Co based Fischer-Tropsch catalyst,** NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Guo, Xiaoyang; Panditha Vidana, Daham S G; Vanhaecke, Estelle Marie M.; Hwang, Jihye; Walmsley, John Charles; Chen, De; Venvik, Hilde Johnsen, **Material degradation by metal dusting corrosion on instrumentation used in natural gas conversion technologies**, NGCS 11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Ledesma C., Yang J., Blekkan E. A., A. Holmen, D. Chen: **The Use of Multicomponent SSITKA as a Tool to Study the Reaction Mechanism in CO Hydrogenation over Cobalt Catalysts.** Oral presentation, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway.

Patanou, Eleni; Tsakoumis, Nikolaos; Myrstad, Rune; Blekkan, Edd Anders, **The effect of CO pre-treatment on a Co/Re /γ-Al2O3 catalyst for Fischer-Tropsch synthesis**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Qi, Yanying; Yang, Jia; Aaserud, Christian; Holmen, Anders; Chen, De, **Mechanistic insights into olefin selectivity on cobalt-catalyzed Fischer-Tropsch synthesis**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Redekop, Evgeniy; Fushimi, Rebecca; Yablonsky, Gregory; Gleaves, John; Olsbye, Unni, **Temporal Analysis of Products (TAP): advanced kinetic characterization of microporous materials**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Wang, Yalan; Qi, Yanying; Zhu, Yi-An; Chen, De, Mechanism research of light olefin formation in **Fischer-Tropsch synthesis over cobalt catalyst by combination of DFT calculations and microkinetic analysis**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Yang, Jia; Eiras, Sara Boullosa; Myrstad, Rune; Pfeifer, Peter; Venvik, Hilde Johnsen; Holmen, Anders**, Fischer-Tropsch Synthesis on Co-Based Catalysts in a Microchannel Reactor: Effect of Temperature and Pressure on Selectivity and Stability**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd Anders, **Co-Mn catalysts for Fischer-Tropsch production of light olefins**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Zhu, Yi-An; Chen, De, **Descriptor-based microkinetic analysis of propane dehydrogenation**, 24th International Symposium on Chemical Reaction Engineering, June 12-15, Minneapolis Minnesota, U.S.A

Bleken, Bjørn Tore Lønstad; Braglia, Luca; Øien-Ødegaard, Sigurd; Lomachenko, Kirill A.; Lamberti, Carlo; Olsbye, Unni, **Pt-incorporated UiO-67 material for CO2 hydrogenation**, 17th Nordic Symposium on Catalysis, June 14-16, Lund, Sweden

Strømsheim, Marie Døvre; Knudsen, Jan; Guo, Xiaoyang; Sørvik, Linn Cecilie; Fernandes, Vasco Rafael; Venvik, Hilde Johnsen; Borg, Anne. **Near ambient pressure XPS investigation of CO oxidation over Pd3Au (100).** 17th Nordic Symposium on Catalysis (NSC17), June 14-16, Lund, Sweden

Svelle, Stian; Martinez-Espin, Juan Salvador; Westgård Erichsen, Marius; De Wispelaere, Kristof; Van Speybroeck, Véronique; Beato, Pablo; Olsbye,

Unni, **Distinct reactivity of methanol and dimethyl ether toward benzene within MTH context**, 17th Nordic Symposium on Catalysis, June 14-16, Lund, Sweden

Arstad, Bjørnar; Lind, Anna Maria; Cavka, Jasmina Hafizovic; Akporiaye, Duncan; Kalantzopoulos, Georgios N.; Lundvall, Fredrik; Wragg, David; Fjellvåg, Helmer; Grønvold, Arne; Fuglerud, Terje, **Characterization of catalytic sites in microporous materials using solid-state NMR. An ex-situ and in-situ high temperature flow study**, 14th National MR meeting, June 16-17, Bergen, Norway

Martinez-Espin, Juan Salvador; Westgård Erichsen, Marius; De Wispelaere, Kristof; Beato, Pablo; Van Speybroeck, Veronique; Svelle, Stian; Olsbye, Unni, **Distinct reactivity of methanol and dimethyl ether toward benzene within MTH context**, 18th International Zeolite Conference, June 19-24, Rio de Janeiro, Brazil

Nielsen, Malte; Brogaard, Rasmus Yding; Falsig, Hanne; Swang, Ole; Svelle, Stian, **Kinetics of Zeolite Dealumination: Insights from H-SSZ-13**, 18th International Zeolite Conference, June 19-24, Rio de Janeiro, Brazil

Chen, Qingjun; Svenum, Ingeborg-Helene; Qi, Yanying; Gavrilovic, Ljubisa; Chen, De; Holmen, Anders; Blekkan, Edd Anders, **Potassium adsorption behavior and its influence on the CO adsorption and activation on hcp cobalt in Fischer-Tropsch synthesis**, 16th ICC, July 3-8, Beijing, China

Liland, Shirley Elisabeth; Yousaf, Bilal; Rout, Kumar Ranjan; Wang, Yalan; Chen, De, **Unprecedented Active and Stable Ni-Co Bimetallic Catalyst for Steam Methane Reforming**, 16th ICC, July 3-8, Beijing, China

Olsbye, Unni; Lillerud, Karl Petter, Nanoporous catalysts - from zeolites and zeotypes to metal-organic frameworks, 16th ICC, July 3-8, 2016, Beijing, China

Qi, Yanying; Yang, Jia; Aaserud, Christian; Holmen, Anders; Chen, De, **New insights to the effect of water on selectivity in cobalt catalyzed Fischer-Tropsch synthesis**, 16th ICC, July 3-8, Beijing, China

Wang, Yalan; Qi, Yanying; Zhu, Yi-An; Chen, De, **Mechanistic research of light olefin formation in Fischer-Tropsch synthesis over cobalt catalyst by combination of DFT calculations and UBI-QEP method**, 16th ICC, July 3-8, Beijing, China

Yang, Jia; Lødeng, Rune; Venvik, Hilde Johnsen, **Co and Ni spinel catalysts for low temperature methane total oxidation**, 9th International Conference on Environmental Catalysis - ICEC 9, July 10-13, Newcastle, Australia

Lomachenko, Kirill A.; Borfecchia, Elisa; Agostini, Giovanni; Øien-Ødegaard, Sigurd; Bleken, Bjørn Tore Lønstad; Braglia, Luca; Olsbye, Unni; Lillerud, Karl Petter; Soldatov, Alexander V.; Bordiga, Silvia; Lamberti, Carlo, **Local environment and electronic structure of Pt centers in UiO-67-Pt MOFs**, Nano 2016, XIII International Conference on Nanostructured Materials; August 7-12, Québec City, Canada

Farstad, Mari Helene; Strømsheim, Marie Døvre; Knudsen, Jan; Guo, Xiaoyang; Gavrilovic, Ljubisa; Fernandes, Vasco Rafael P; Borg, Anne; Venvik, Hilde Johnsen, **CO oxidation over Pd-based alloys**, CMD26, September 4-9, Groningen, The Netherlands

Farstad, Mari Helene; Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Borg, Anne; Venvik, Hilde Johnsen, **The effect of K impurities on Co(11-20) with respect to Fisher-Tropsh catalysis**, CMD26, September 4-9, Groningen, The Netherlands

Redekop, Evgeniy; Fushimi, Rebecca; Martinez-Espin, Juan Salvador; Mortén, Magnus; Bleken, Bjørn Tore Lønstad; Mykland, Maria; Gleaves, John; Olsbye, Unni, **Kinetic characterization of zeolitic MTO/MTH catalysts with Temporal Analysis of Products (TAP-3),** CHEMREACTOR-22, September 19-23, London, UK

Zhu, Yi-An; Chen, De, **Rational Catalyst Design for Propane Dehydrogenation**, 8th International Conference on Molecular Simulations and

Informatics Technology Application. September 24-26, Dalian, China

M. E. M. Buan, N. Muthuswamy, A. Cognigni, J. C. Walmsley, D. Chen, and M. Rønning, **Nitrogen-Doped Carbon Nanofibers for the Oxygen Reduction: The Role of Iron As Growth Catalyst**, ECS PRiME 2016, October 2-7, Honolulu, USA

Mahmoodinia, Mehdi; Chen, De; Åstrand, Per-Olof, **Platinum clusters with a carbon support material as catalysts: ReaxFF simulations and DFT calculations**, Magical Mystery Tour of Electron Correlation, October 24-26, Oslo, Norway

Henry, Reynald; Redekop, Evgeniy; Olsbye, Unni, **Study of CO2 reduction by non-stoichiometric cerium oxide with transient response experiments**, International Conference on Carbon Dioxide Utilisation, November 11-15, Sheffield, UK

Lectures at International Winter School "Molecules@Surfaces", January 31-Feb 5, Bardonnecchia, Italy

"Molecules@Surfaces" Winter Schools offered to PhD students and Post-Docs updated "tools" for acting as relevant scientific players in surface-related materials science and technology. Prof. Stian Svelle, UiO was part of the Scientific Committee. Pablo Beato (HTAS) and Karl Petter Lillerud (UiO) presented two lectures.

Pablo Beato, **Molecules@Industrial Surfaces, Molecular Dynamics in Catalysis for Sulfur Chemistry**

Karl Petter Lillerud, **Surfaces In nanoporous materials: Zeolites and MOFs**

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