

## Arvoisa Katalyysiseuran jäsen! Dear member of Catalysis Society!

Summer starts to be behind in Finland and the most significant catalyst conferences of this year have already been held. 17<sup>th</sup> Nordic Symposium on Catalysis (NSC17) was held in June in Lund and 16<sup>th</sup> International Congress on Catalysis (ICC 16) in July in Beijing. At NSC17, there was a big delegation from Finland with many oral and poster presentations. Unfortunately, arrangements for the symposium cannot be said to be fully on a high level if comparing e.g. to NSC in Mariehamn in 2012. There was also a delegation from Finland at ICC16, however, relatively small one. A keynote talk was given by prof. Dmitry Murzin and an oral presentation by Dr. Karoliina Honkala.

The main event of this year for our society was 1<sup>st</sup> Young Scientist Forum on Catalysis which was held 8<sup>th</sup> April in Tampere. The event was a success with over 40 participants and ~20 presentations by young scientists. Furthermore, fourth Doctoral Thesis award of the Finnish Catalysis Society was awarded to Marko Melander and Prof. Riitta Keiski and Prof. Outi Krause were invited to honorary members of our society.

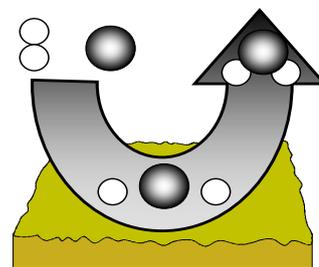
Our target is to organize this event annually to promote the interaction and networking of Finnish catalysis researchers and in order to provide an opportunity for young researchers to present their research. We have also gone through the feedback from the first event being mainly positive. However, the program was considered to be too tight with too many presentations in a row. Based on this, we consider next time to have a looser program

with possibly two parallel sessions. Furthermore, we may group the presentations based on themes. Next Young Scientist Forum will be held in Jyväskylä in late March or early April in 2017.

Another ongoing activity of the board of Catalysis Society is updating of presentation material for Finnish high schools. The aim of the material is to promote knowledge on significance of catalysis. Generally spoken, there is also a worry about number of high level chemistry and chemical engineering students in Finland. This material may also promote a more positive picture of chemistry among high school students.

I warmly welcome all new members of our society! Our target is really to make our society attractive for all catalyst researchers in Finland. I wish you all the best for the challenges of starting fall season!

*Chair Prof. Juha Lehtonen*



## The 1<sup>st</sup> Finnish Young Scientist Forum on Catalysis on 8<sup>th</sup> of April, 2016

Finnish Catalysis Society organized the first Finnish Young Scientist Forum on Catalysis on 8<sup>th</sup> of April, 2016, at the Finnish Labour Museum Werstas, Tampere, in connection with the annual meeting of the Finnish Catalysis Society.

The catalysis related event gathered totally 43 participants, both from academia but also from industry. The program consisted of welcoming address, a keynote lecture given by Dr. Mats Kåldström (Neste), prize winner's lecture and presentations of PhD theses. Totally 22 PhD theses were presented during the day, covering widely the field of catalysis. The day ended with the annual meeting of the Finnish Catalysis Society or a museum tour.

Thank you all for the nice day!



Dr. Mats Kåldström



## The fourth Doctoral thesis award of the Finnish Catalysis Society to Dr. Marko Melander

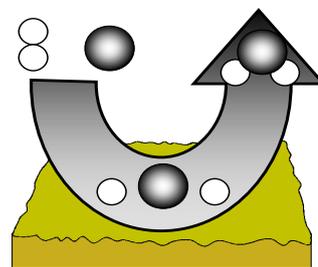
**Dr. Marko Melander** was selected as the award winner of the fourth Doctoral Thesis award of the Finnish Catalysis Society. He defended his thesis in Aalto University in August, 2015. His thesis is entitled "Reactivity of Iron Nanostructures from Density Functional Theory".

The selection was made by an external expert, Prof. Daniel Duprez (University of Poitiers). The reasoning for the selection is presented below:

*"Iron catalysts are widely used in Industry, for instance in the Fischer-Tropsch process, in ammonia synthesis, in ethylbenzene dehydrogenation to styrene and in many other processes. Carbon monoxide can play a crucial role, either as reactant (FT synthesis) or contaminant (NH<sub>3</sub> synthesis, ...). CO dissociation, a key-step in the above processes, has been studied by computational chemistry methods on a variety of Fe nanostructures. Among all the discoveries of Marko Melander, the impact of magnetic*

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*moment in catalysis by Fe clusters should be highlighted. This important result paves the way for the development of Catalysis under magnetic field control. Even if several attempts have been made in the past to take advantage of this catalyst property, the work of Marko Melander could clarify the horizon of this new strategy.*

*Finally, I hope that this Award will be an encouragement for the School of theoretical chemistry of Finland, in the framework of an extremely competitive domain of Research.”*

The award is worth 2000 €. The Catalysis Society warmly congratulates Dr. Marko Melander!



Dr. Marko Melander

## Two honorary members of Finnish Catalysis Society: Outi Krause and Riitta Keiski

As the Finnish Catalysis Society decided to introduce honorary membership, two names appeared spontaneously to discussion: professor Riitta Keiski from University of Oulu and Professor Outi Krause from Aalto

University. Both Outi and Riitta have made tremendous contributions to the academic world and society, in Finland and abroad. Their work is very well recognized. Outi has obtained the Innovation Prize of Finnish Chemical Industry and Riitta has been appointed by Professor's Union the Professor of the Year. Finnish Catalysis Society wanted to give the honorary membership to Outi and Riitta for their excellent scientific merits in heterogeneous catalysis, their effort in the teaching of the subject and their activities in the global catalysis community.



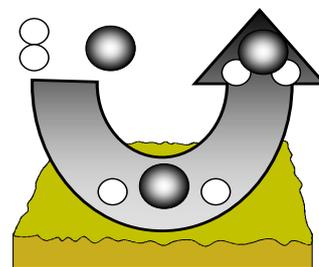
Prof. Outi Krause



Prof. Riitta Keiski

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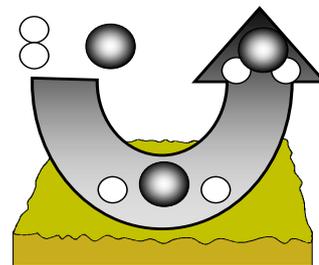
Very much thanks to Outi and Riitta, the Finnish research in catalysis is today on a high international level and globally visible. Two German words come here in my mind: Weltklasse and Weltbühne. Outi is an internationally known researcher particularly in the field of catalysis related to fuels. In young years, she presented a top-class doctoral dissertation at TU Eindhoven. The topic of the work was the Fischer-Tropsch process. During the career at the Finnish oil company Neste, she lifted the research and development to a completely new level: the research centre in Porvoo became one of the leading ones in Europe. After returning to the Alma Mater, Helsinki University of Technology, she put a strong focus on the research and development of etherification processes, which lead to several doctoral theses and numerous international publications, which still are very frequently cited. Outi understood very early the strongly interdisciplinary character of heterogeneous catalysis emphasizing the coupling between catalyst preparation, characterization and kinetic studies. The early HETEKA project was a good example of this.

During the recent 25 years, Riitta has created a strong Oulu school in catalysis. The Oulu group combines catalysis and separation technologies in a unique manner in our country. Today the research work done in Oulu is very well recognized on the international arena. The doctoral thesis of Riitta was devoted to water-gas shift reaction in a non-isothermal fixed bed reactor. Publications based on this early work are still very well cited. Riitta spent a post-doc year in Berkeley, in the world-famous group of Professor Gabor Somorjai, a brilliant scientist of Hungarian origin and a warm friend of Finland. This period gave Riitta the final

maturity to become a university professor. The strong focus in Riitta's research is on environmental issues, from automotive exhaust catalysis to destruction of volatile organic components. The Oulu group is on the Weltbühne of environmental technology. Riitta is the real catalyst of the Oulu group; she encourages young scientists in a tireless manner, and new generation of docents and professors has been educated.

Outi and Riitta have modernized the education in the field of catalysis at their universities. This is an extensive effort and often not that much recognized by the academic community. Catalysis has to be included in chemical and chemical engineering education. Heterogeneous catalysis is one of the key technologies in current chemical and process industry, but even more: catalysis is the key technology in the tedious transfer to sustainable development of the mankind. By education we push this message to young students. With a born charisma, Outi and Riitta have done a great job in university education, on the undergraduate level and in postgraduate education, being very active in the national Graduate School in Chemical Engineering (GSCE).

Many excellent researchers remain in the golden cage of science, but Outi and Riitta have been very active in industrial collaboration and in international catalysis organisations. They have been board members in the Nordic Federation of Catalysis Societies and organizers of Nordic Catalysis Symposia on Finnish soil. They participated actively in the organization of the largest European event in catalysis, Europacat in Finland (2007). Outi and Riitta have been members of the EFCATS council, Outi being



one of the founding members of this organization and board member of EFCATS. This work has been extremely important for a small country not being in the core of Europe. Outi and Riitta have demonstrated that we exist and we exist on a high level.

How to serve the own university, is always a question - by research and education; that is what most professors do, but Outi and Riitta have done much more. Who is active, gets more and more tasks, which results in a heavy workload. Outi and Riitta have always been loyal to their Alma Maters and accepted many duties and positions: membership of numerous committees, positions as dean and vice rector. Without complaining, they have given their energy and intelligence to the disposal of the university.

The decision about the honorary members of Finnish Catalysis Society was unanimous. It was the right decision. On behalf of the Finnish Society and personally, I convey cordial congratulations to the grand ladies of Finnish catalysis. I wish you good health and sustainable energy in life and catalysis.

Kuressaare/Arensburg, August 2016

Tapio Salmi  
Professor in chemical reaction engineering  
Board member of Finnish Catalysis Society

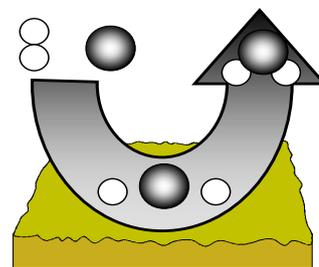
## ICC greetings

The 16th International Congress on Catalysis held from July 3 to 8, 2016 in Beijing, China with the theme of Catalysis for the Sustainable Development of the World, has attracted researchers working in the field of catalysis science and technology. The

presentations during the conferences covered important methodological aspects as well as applications in energy production, utilization of fossil and renewable resources for fuels and chemicals and in environmental protection. The congress served its a purpose as a venue to exchange new ideas and discuss the advances in all areas of catalysis. The organizers were able to attract amazing plenary speakers setting the tone for the whole congress and clearly showing how design of new catalysts and development of practically important processes can be inspired and guided by theory.

In fact a distinct feature of the congress was that in addition to outstanding keynote lectures there were several dozens of invited lectures given by the well-recognized leaders in respective subdisciplines. In this respect ICC-16 was clearly different from the previous international congresses. The congress gathered a substantial amount of local Chinese scientists, thus the total number of attendees was approaching three thousand. This presented some challenges from the organizational viewpoint regarding poster sessions, lunches, excursions, which were successfully solved. Finally it should be noted that even if the number of participants from Finland was limited, our contribution to the overall success of the congress was clearly visible.

*Written by Prof. Dmitry Murzin, Åbo  
Akademi*



## Travel reports

### Travel report of the 16<sup>th</sup> international congress on catalysis (16th ICC)

The 16<sup>th</sup> ICC was arranged at July 3-8, 2016 at Beijing China by International Association of Catalysis Science (IACS) and Catalysis Society of China (CSC). The main theme of this conference was Catalysis for the Sustainable Development of the World and the scope was especially on the catalysis role in the clean and efficient production/utilization of traditional fossil resources, development of renewable energies and abating environmental pollutants to achieve low carbon economy.

The ICC is held only every 4<sup>th</sup> year and it is the largest conference in the field of catalysis. This time more than 2500 people from over 50 countries were participated in that congress. The 16<sup>th</sup> ICC included around 1700 posters and more than 300 oral presentations which were arranged in 6 parallel sessions including catalysis for energy, catalytic materials, catalytic mechanisms, environmental catalysis, industrial catalysis, photocatalysis, catalysis for biomass conversion etc. The conference venue CNCC was a really huge building! (Fig. 1)



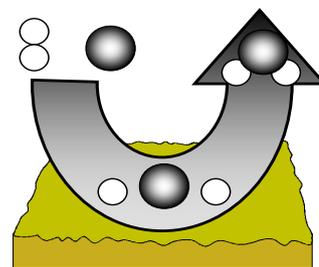
Fig. 1. China national convention center (CNCC).

The conference was started at Sunday 3<sup>rd</sup> of July in the afternoon with oral presentation of the 2016 international catalysis lecture Prof. Davide Farrusseng from IRCELYON, CNRS, France (Fig. 2.). The topic of his presentation was “Catalysis inside a box” dealing the impregnation of active metals to zeolites by novel technique. Typically, the loading of active metal to the zeolites have been performed by ion-exchange or wetness impregnation but unfortunately the sintering of the active metal may occur. Farrusseng and his group has been studied the encapsulation of the metal particles in to the microporous of zeolites which is presented as a solution towards sintering. Due to the encapsulation of bimetallic nanoparticles in hollow zeolites the most important properties of the catalyst i.e. activity, stability and selectivity were significantly improved compared to traditional preparation method. I found this presentation very interesting and perhaps I will apply these preparation techniques in my own research☺.



Fig. 2. Prof. David Farrusseng received the 2016 international catalysis award.

Prof. Paolo Fornasiero from University of Trieste, Italy was awarded by Heinz Heinemann prize (Fig. 3.) The topic of his



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presentation was “Hybrid nanocatalysts for energy related applications”. In this research several carbon nanostructures (CNs) such as single-wall carbon nanohorns (SWCNHs), multiwalled carbon nanotubes (MWCNTs) and carbon nanocones (CNCs) were modified e.g. by oxidation to achieve functionalization of the materials. The hybrid catalysts were prepared via sol-gel method by addition of Pd@TiO<sub>2</sub> to the functionalized CNs and the produced materials were studied in the photo and electro-chemical production of hydrogen or electro-reduction of CO<sub>2</sub>.



Fig. 3. Prof. Paolo Fornasiero received the Heinz Heinemann prize.

Totally five plenary lectures were presented in the conference. The topic of Prof. Bruce C. Gates (University of California, USA) presentation was “Molecular and single-site metal catalysts on surface” in which he presented for example different characterization techniques for site-isolated supported metal catalysts. Prof. Charles T. Campbell (University of Washington, USA) was concentrated in his presentation in the thermodynamics and kinetics of elementary reaction steps on transition metal catalysts. The recent advances in the application of zeolites in the production of fuels and petrochemicals was the topic of Dr. José G.

Santiesteban (ExxonMobil Research and Engineering Company, USA). In my opinion the most interesting plenary lectures were presented by Prof. Krijn P. de Jong (Utrecht University, Netherlands) and Prof. Matthias Beller (University of Rostock, Germany). Prof. de Jong was talking about nanoscale effects in heterogeneous catalysis and especially particle size in supported catalysts and spatial distribution of nanoparticles in mono and bi-functional catalysts. In his talk he was concentrated on the Fischer Tropsch and Fischer Tropsch to Olefins i.e. Cu, Fe, Ni and Co catalysts. Prof. Beller was talking about the differences and similarities between homogeneous and heterogeneous catalysis. His group was open-minded studied how homogeneous and heterogeneous catalysts can benefit from each other for example in hydrogenation and dehydrogenation processes. I was impressed with the enthusiasm which Prof. Beller still has in the catalysis research! I think we all should keep our mind open and studied sometimes also the most strangest ideas. Only that way we can invent something new.

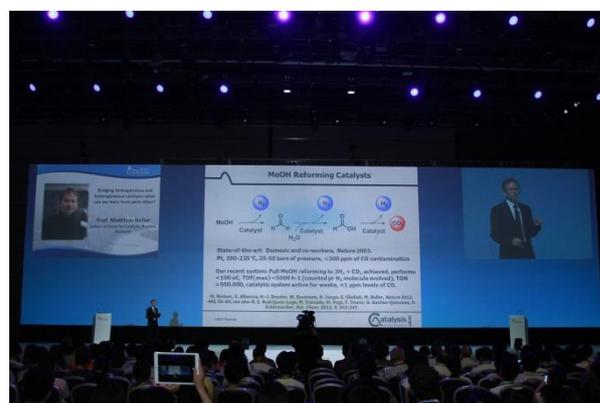
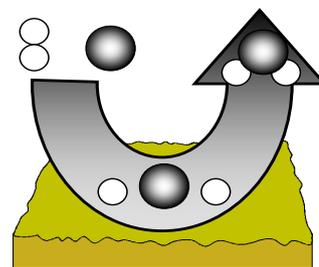


Fig. 4. Prof. Matthias Beller gave an interesting plenary presentation.

The poster sessions were at Tuesday and Thursday afternoons. I had my poster



presentation at Tuesday from the topic “Industrial by-product as a source of novel catalytic materials” (Fig. 5). In this poster I was presented two catalytic materials prepared from waste materials: carbon residue (CR) from wood gasification process and lignin waste from Kraft lignin process. These materials were modified as catalyst supports for catalytic wet peroxide oxidation and Fischer Tropsch processes.

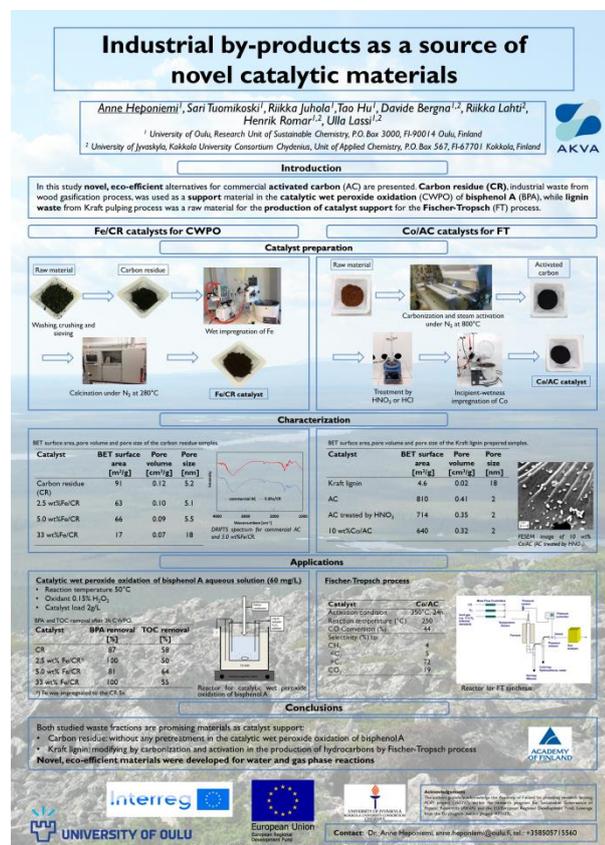


Fig. 5. The poster of Anne Heponiemi at 16<sup>th</sup> ICC.

Probably due to the occasion of conference (the typical holiday time in Finland) only few participants from Finland were present at the conference. Prof. Dimitry Murzin (Åbo Akademi) had a key note presentation from

the topic “Catalytic transformation of lipids to fuels and chemicals” (Fig. 6.)



Fig. 6. Prof. Murzin was a keynote speaker.

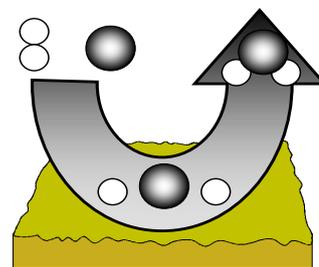
and Dr. Karoliina Honkala (University of Jyväskylä) presentation was concerning the acrolein hydrogenation from first principles calculations (Fig. 7.).



Fig. 7. Dr. Karoliina Honkala had an oral presentation at 16<sup>th</sup> ICC on Thursday.

In addition, posters from University of Jyväskylä and Aalto University were presented.

At Wednesday half day excursion was arranged by conference organizers. There were several options of travel routes such as Forbidden city, Temple of Heaven, Tian’anmen Square etc. but I was chosen the



travel trip to the Great Wall at Badaling (Fig. 8.).



Fig. 8. The excursion to Great Wall at Badaling.

This place is located at around 50 km from the city center of Beijing. It was a very hot day (around 35 °C) but unfortunately the bus had an air conditioning! The Great Wall was truly impressive attraction and you can't understand the size of that construction without seeing it (Fig. 9.).



Fig. 9. The Great Wall is truly impressive construction.

Finally, the 16th ICC was the biggest conference in which I have visited. I listened several interesting presentations and met new and old colleagues from different countries. The next ICC will be held at San Diego in 2020. I want to acknowledge the Finnish

Catalysis Society to given me the travel grant to this conference!

*Dr. Anne Heponiemi, University of Oulu,  
Research unit of Sustainable Chemistry*

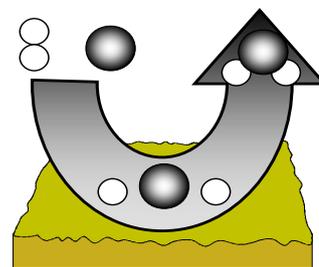
## 17<sup>th</sup> Nordic Symposium on Catalysis

*June 14-16, 2016*

*Lund, Sweden*

The 17th Nordic Symposium on Catalysis was organized on the university campus in Lund, Sweden and was held on June 14-16<sup>th</sup> 2016. This year the topics of the biannual conference NSC17 were chosen to emphasize surface science and catalysis for sustainable development as well as the use of large scale facilities for catalysis research. These fields were covered by 5 invited presentation, 57 contributed oral presentations and 86 poster presentations.

The winner of the 2016 Berzelius Price was Anders Riisager from Technical University of Denmark. His Berzelius lecture was entitled "Supported Ionic Liquid Phase (SILP) catalysis - A new era for homogeneous catalysis?". Other plenary speakers were Martin Skov-Skjöth Rasmussen from Haldor Topsoe and lecture "Going green with chemicals and fuels. Sustainable at a premium or not?", Jesper Andersen from MAX IV Laboratory and presentation of "Future possibilities for studying heterogeneous catalysis at the MAX IV Laboratory", Jeroen van Bokhoven from ETH Zürich and lecture "From porosity to active sites in heterogeneous catalysis" and Karoliina Honkala Winner of the 2014 Berzelius Price from University of Jyväskylä and lecture "Heterogeneous catalysts from first principles and beyond".



Other interesting topics of the oral presentation included structured materials and reactions, surface science and modelling, syngas and syngas, alternative feedstocks and oxidation fundamentals.



Figure 1 - Lecture about VOC abatement from Adj. Prof. in University of Oulu - Satu Ojala



Figure 2 - Lecture about catalytic active sites from Prof. Dr. ETH Zurich - Jeroen van Bokhoven

The conference also included a study visit to the MAX IV laboratory in Lund, facility that hosts the most brilliant X-Ray source for scientists and industry to perform research in different fields. The facilities enable scientists to develop innovative materials and products

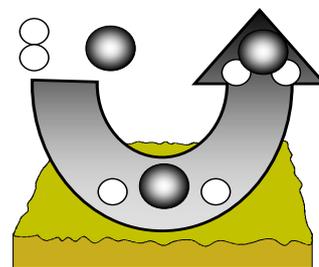
that could improve our life and our environment. MAX IV consists of an electron gun that generates electrons injecting them through a linear accelerator where they are loaded with energy to close the speed of light. The thin and focused electron beam generated is one of the unique features of MAX IV laboratory. The facility also operates with two rings (small and big rings) that enables generation of hard and soft X-Rays and a total of 28 beamlines for research. The short pulse facility provides pulses that allows the study of how chemical bonds are formed or broken or how atoms move. Projects in different areas such as biology, physics, chemistry, environmental science, geology, engineering, pharmacology and cultural heritage can benefit from this facility. It was extremely fascinating to visit this research facility and being able to understand how technology is developing and enabling more and more advanced tools to support scientists achieving a better understanding of science.



Figure 3 MAX IV laboratory in Lund - Sweden

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The Finnish Catalysis Society granted five master and PhD students from Finnish universities, namely Felipe Lopes (University of Oulu), Riikka Lahti (Kokkola University Consortium), Tiia Viinikainen (Aalto University), Yaseen Khan (Aalto University) and Ricardo Pezoa-Conte (Åbo Akademi University) to give poster and oral presentations in different interesting topics within the catalysis field. The presenters covered topics where catalyst can be applied into different applications such as treatment of wastewaters, hydrolysis of marine carbohydrates among other interesting uses. As a result, the presenters gave an overview of the activities that young researchers are carrying out in Finland on the field of catalysis, demonstrating the big contribution the country provides to the Nordic countries and the world scientific society on this field.



Figure 4 - Poster presentation about Felipe's Master thesis results

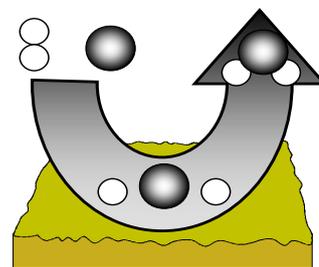


Figure 5 – Oral presentation about Ricardo's PhD thesis results

Overall the experience of being able to attend the conference and watch all the wonderful presentations was a very enriching experience. Not only the presentations, but also the interaction and networking of meeting researchers and students from different parts of the world and exchange information about research and other fields of work was extremely valuable, a great chance to interact with interesting people working on the field and to develop plans and future projects with new collaborations.

Regards

Felipe Lopes, Riikka Lahti, Tiia Viinikainen,  
Yaseen Khan and Ricardo Pezoa-Conte



## Membership fees in 2016

Members are requested to transfer the membership fee directly to the following bank account:

Nordea FI08 1107 3000 6085 17

### Payment due September 30, 2016.

The amount of the membership fee for year 2016 is 10 euros. The fee for industry members is 250 €. The members can also pay a LIFE-TIME MEMBERSHIP FEE (called 'ainaisjäsenmaksu'). The amount of life-time membership fee is 100 euros. Life-time members do not need to pay annual membership fees. When paying the membership fees, please indicate your name in the 'Lisätietoja' section of the invoice.

## Catalysis related dissertations in spring and autumn 2016

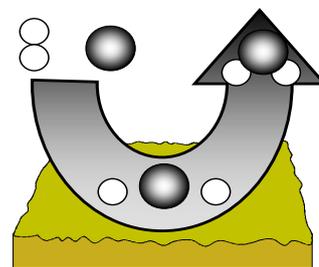
**M.Sc.(Chem.) Anne-Riikka Rautio** from the Faculty of Information Technology and Electrical Engineering, University of Oulu, defended her thesis on 18<sup>th</sup> of March, 2016. Her thesis entitled "*On the stability of carbon nanotube and titania nanowire based catalyst materials: from synthesis to applications*".

Opponent: Prof. Saikat Talapatra, Southern Illinois University, USA and Doctor Toni Kinnunen

Custodian: Prof. Krisztian Kordas, University of Oulu

### Abstract

Degradation of the support and sintering of catalyst nanoparticles inherently leads to a loss of functionality of catalyst materials in converters and sensors. Malfunction in such devices may lead to serious economic and environmental damage. The quest for novel and sustainable catalyst materials with better durability is thus ongoing. In this thesis, one-dimensional nanomaterials such as carbon nanotubes and titanium dioxide nanowires are studied and compared to their conventional zero-dimensional counterparts in regard to their structural and functional stability. With the combination of several catalyst nanomaterials and supporting surfaces, aging properties of more than 70 different materials are assessed by the means of X-ray diffraction, transmission electron microscopy and energy-dispersive X-ray analyses. Although CNTs were shown to be thermally the most stable carbonaceous supports for metal nanoparticles, they are, similar to other carbon supports, more sensitive to high temperatures than metal oxide supports and can suffer deactivation by catalytic oxidation and gasification even at moderate temperatures. In addition, the irradiation of the samples with e-beams caused the most dramatic changes in CNT based materials, where nanosized deformities (voids, channels) were formed when either nanoparticles or defects were present. The prepared nanocompositions have been utilized successfully in three different applications including (i) synthesis of hydrogen from ethanol via a steam reforming reaction, (ii) hydrogenation of citral to form value added chemicals and (iii) the application of advanced electrode materials in electric double-layer capacitors. Both CNT and TiO<sub>2</sub> nanowire based nanomaterials were shown to outperform their conventional nano-



and microparticle based counterparts in the studied catalytic reactions, i.e. in citral hydrogenation and steam reforming of ethanol, respectively. Furthermore, nanostructured CNTs obtained by catalytic partial oxidation of the material showed an increased specific surface area, which could be exploited in supercapacitor electrodes with enhanced specific capacitance.

**M.Sc. Cesar Augusto de Araujo Filho** from the Laboratory of Industrial Chemistry and Reaction Engineering, Johan Gadolin Process Chemistry Centre, Faculty of Science and Engineering/Chemical Engineering, Åbo Akademi, defended his thesis on 20<sup>th</sup> of May, 2016. His thesis entitled “*A reaction engineering approach to homogeneously catalysed glycerol hydrochlorination*”.

Opponent: Professor Juan Garcia Serna, University of Valladolid, Spain

Custodian: Professor Tapio Salmi, Åbo Akademi

## Abstract

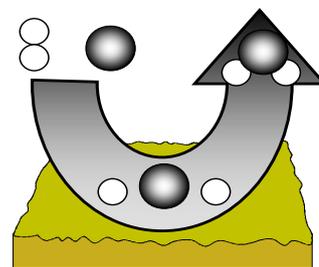
The production of biodiesel through transesterification of fatty acid esters has created a surplus of glycerol on the international market. In few years, glycerol has become an inexpensive and abundant raw material, subject to numerous plausible valorisation strategies. Glycerol hydrochlorination stands out as an economically attractive alternative to the production of bio-based epichlorohydrin, an important raw material for the manufacturing of epoxy resins and plasticizers.

Glycerol hydrochlorination using gaseous hydrogen chloride (HCl) was studied from a reaction engineering viewpoint. Firstly, a

more general and rigorous kinetic model was derived based on a consistent reaction mechanism proposed in the literature. The model was validated with experimental data reported in the literature as well as with new data of our own.

Semi-batch experiments were conducted in which the influence of the stirring speed, HCl partial pressure, catalyst concentration and temperature were thoroughly analysed and discussed. Acetic acid was used as a homogeneous catalyst for the experiments. For the first time, it was demonstrated that the liquid-phase volume undergoes a significant increase due to the accumulation of HCl in the liquid phase. Novel and relevant features concerning hydrochlorination kinetics, HCl solubility and mass transfer were investigated. An extended reaction mechanism was proposed and a new kinetic model was derived. The model was tested with the experimental data by means of nonlinear regression analysis, in which kinetic and mass transfer parameters were successfully estimated. A dimensionless number, called Catalyst Modulus, was proposed as a tool for corroborating the kinetic model.

Reactive flash distillation experiments were conducted to check the commonly accepted hypothesis that removal of water should enhance the glycerol hydrochlorination kinetics. The performances of the reactive flash distillation experiments were compared to the semi-batch data previously obtained. An unforeseen effect was observed once water was let to strip out from the liquid phase, exposing a strong correlation between the HCl liquid uptake and the presence of water in the system. Water has revealed to play an important role also in the HCl



dissociation: as water was removed, the dissociation of HCl was diminished, which had a retarding effect on the reaction kinetics. In order to get a further insight on the influence of water on the hydrochlorination process, additional semi-batch experiments were conducted in which various initial amounts of water and the desired product were added. This study revealed the possibility to use the desired product  $\alpha$ -dichlorohydrin as an ideal “solvent” for the glycerol hydrochlorination process.

A co-current bubble column was used to investigate the glycerol hydrochlorination process under continuous operation. The influence of liquid flow rate, gas flow rate, temperature and catalyst concentration on the glycerol conversion and the product distribution was studied. The fluid dynamics of the system showed a remarkable behaviour, which was carefully investigated and described. High-speed camera images and residence time distribution experiments were conducted to collect relevant information about the flow conditions inside the column reactor. A model based on the axial dispersion concept was developed and confronted with the experimental data. The kinetic and solubility parameters estimated from the semi-batch experiments were successfully used for describing the mass transfer and the fluid dynamics of the bubble column reactor.

On the light of the results brought by the present work, the glycerol hydrochlorination reaction mechanism has been finally clarified. It has been demonstrated that the reactive distillation technology might impair the glycerol hydrochlorination rate under certain conditions. Furthermore, the continuous reactor technology showed a high selectivity

towards monochlorohydrins, whilst semi-batch technology was demonstrated to be more efficient towards the production of dichlorohydrins. Based on the novel and revealing discoveries brought by the present work, many insightful suggestions were made towards the improvement of the  $\alpha$ -dichlorohydrin production in industrial scale.

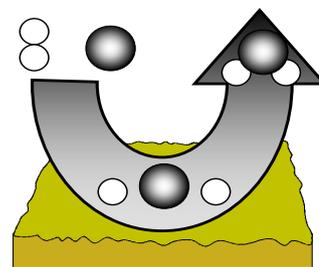
**M.Sc. (Chem.) Lakhya Jyoti Konwar** from the Laboratory of Industrial Chemistry and Reaction Engineering, Johan Gadolin Process Chemistry Centre, Faculty of Science and Engineering, Åbo Akademi University, defended his thesis on 17<sup>th</sup> of June, 2016. His thesis entitled “*New biomass derived carbon catalysts for biomass valorization*”.

Opponent: Docent Ahmad Kalantar Neyestanaki, Shell Global Solutions, Amsterdam

Custodian: Professor Jyri-Pekka Mikkola

### *Abstract*

Due to diminishing petroleum reserves, unsteady market situation and the environmental concerns associated with utilization of fossil resources, the utilization of renewables for production of energy and chemicals (biorefining) has gained considerable attention. Biomass is the only sustainable source of organic compounds that has been proposed as petroleum equivalent for the production of fuels, chemicals and materials. In fact, it would not be wrong to say that the only viable answer to sustainably convene our future energy and material requirements remain with a *bio-based economy* with biomass based industries and products. This has prompted biomass valorization (biorefining) to become an



important area of industrial research. While many disciplines of science are involved in the realization of this effort, catalysis and knowledge of chemical technology are considered to be particularly important to eventually render this dream to come true.

Traditionally, the catalyst research for biomass conversion has been focused primarily on commercially available catalysts like zeolites, silica and various metals (Pt, Pd, Au, Ni) supported on zeolites, silica etc. Nevertheless, the main drawbacks of these catalysts are coupled with high material cost, low activity, limited reusability etc. – all facts that render them less attractive in industrial scale applications (poor activity for the price). Thus, there is a particular need to develop active, robust and cost efficient catalytic systems capable of converting complex biomass molecules.

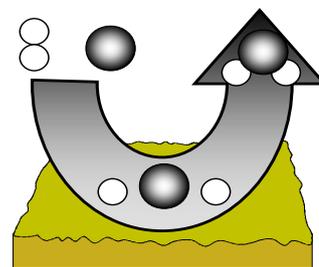
Saccharification, esterification, transesterification and acetylation are important chemical processes in the valorization chain of biomasses (and several biomass components) for production of platform chemicals, transportation fuels, food additives and materials. In the current work, various novel acidic carbons were synthesized from wastes generated from biodiesel and allied industries, and employed as catalysts in the aforementioned reactions. The structure and surface properties of the novel materials were investigated by XRD, XPS, elemental analysis, SEM, TEM, TPD and N<sub>2</sub>-physisorption techniques.

The agro-industrial waste derived sulfonic acid functionalized novel carbons exhibit excellent catalytic activity in the aforementioned reactions and easily outperformed liquid H<sub>2</sub>SO<sub>4</sub> and conventional solid acids (zeolites, ion-exchange resins etc). The experimental results indicated strong influence of catalyst pore-structure (pore size,

pore-volume), concentration of –SO<sub>3</sub>H groups and surface properties in terms of the activity and selectivity of these catalysts. Here, a large pore catalyst with high –SO<sub>3</sub>H density exhibited the highest esterification and transesterification activity, and was successfully employed in biodiesel production from fatty acids and low grade acidic oils. Also, a catalyst decay model was proposed upon biodiesel production and could explain that the catalyst loses its activity mainly due to active site blocking by adsorption of impurities and by-products.

The large pore sulfonated catalyst also exhibited good catalytic performance in the selective synthesis of triacetin via acetylation of glycerol with acetic anhydride and outperformed the best zeolite H-Y with respect to reusability. It also demonstrated equally good activity in acetylation of cellulose to soluble cellulose acetates, with the possibility to control cellulose acetate yield and quality (degree of substitution, DS) by a simple adjustment of reaction time and acetic anhydride concentration.

In contrast, the small pore and highly functionalized catalysts obtained by hydrothermal method and from protein rich waste (Jatropha de-oiled waste cake, DOWC), were active and selective in esterification of glycerol with fatty acids to monoglycerides and saccharification of cellulosic materials, respectively. The operational stability and reusability of the catalyst was found to depend on the stability of –SO<sub>3</sub>H function (leaching) as well as active site blocking due to adsorption of impurities during the reaction. Thus, our results corroborate the potential of DOWC derived sulfated mesoporous active carbons as efficient integrated solid acid catalysts for valorization of biomass to platform



chemicals, biofuel, bio-additive, surfactants and cellulose-esters.

**M.Sc. Terhi Suoranta** from Faculty of Natural Sciences (Chemistry), University of Oulu, defended her thesis on 12<sup>th</sup> of August, 2016. Her thesis entitled “*Advanced analytical methods for platinum group elements. Applications in the research of catalyst materials, recycling and environmental issues*”.

Opponent: Professor Sebastian Rauch, Chalmers University of Technology

Custodian: Docent Paavo Perämäki, University of Oulu

### Abstract

Platinum group elements (PGEs) have a high commercial value and variety of applications in different fields of industry. One of the well-known applications is the use of palladium, platinum and rhodium in the catalytic converters of automobiles to reduce the amount of harmful gases emitted to the environment. Advanced analytical methods are needed to deal with issues related to development of new catalyst materials, recycling of PGEs from spent materials and for monitoring PGE emissions to the environment.

In the first part of this study the emphasis was on the catalyst materials. Especially, reliable determination of ruthenium content in catalyst materials required further studies. Consequently, acid digestions in closed vessels using a microwave oven or high pressure asher were compared with a previously reported fusion method. Furthermore, the recovery of PGEs from

spent materials is important due to many factors, for example, the high value of these metals, environmental aspects related to their production and possible availability issues in the future. Thus, utilization of microwave-assisted leaching and cloud point extraction (CPE) for the recovery of palladium, platinum, rhodium and ruthenium from catalyst materials was investigated.

The second part of this study concentrated on the PGEs in environmental samples and the analytical challenges related to PGE determinations with inductively coupled plasma mass spectrometry (ICP-MS). Due to the use of PGEs in catalytic converters of automobiles, they are emitted to the roadside environment. The use of *Pleurozium schreberi*, a terrestrial moss, for active biomonitoring of these emissions was evaluated. Advanced analytical methods were needed to perform interference-free determinations of palladium, platinum and rhodium in these samples. Two alternative approaches for interference elimination were studied. Firstly, the interfering elements were removed using CPE as a chemical separation method. Secondly, interferences were eliminated using ammonia as a reaction gas with the novel ICP-MS/MS (inductively coupled plasma tandem mass spectrometry) technique.

### Conferences and symposia

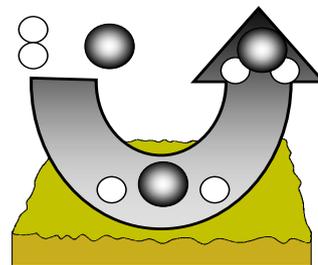
See also e.g.

[www.conference-service.com](http://www.conference-service.com)

[www.iacs-icc.org/Events/events.html](http://www.iacs-icc.org/Events/events.html)

# Katse

Suomen katalyysiseura  
Finska katalyssällskapet  
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## Web pages

<http://www.katalyysiseura.org>

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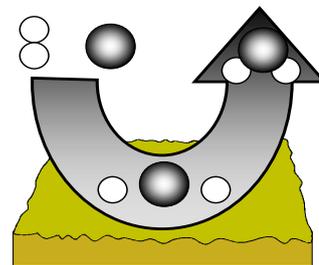
<http://www.efcats.org>

<http://www.elsevier.com>

Katalyysiseuran hallitus toivoo, että saisimme jäsenkunnaltamme palautetta Katse-lehdestämme ja uutisia julkaistavaksi (esim. väitökset, kansalliset ja kansainväliset tapahtumat, palkinnot, kurssit yms.)! Palautteet ja uutiset voi toimittaa hallituksen jäsenille.

# Katse

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