

## Conference report

### **44. Jahrestreffen Deutscher Katalytiker mit Jahrestreffen Reaktionstechnik**

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The 44<sup>th</sup> Jahrestreffen Deutscher Katalytiker was organized by the DECHEMA at the conference center in Weimar in March 2011 together with the 4<sup>th</sup> Jahrestreffen Reaktionstechnik. The intention of this joint conference was to intensify the communication between the scientific communities of homogeneous/heterogeneous catalysis and reaction engineering, which are mutually connected in many areas. The conference attracted 680 participants from academia and industry with a broad range of interest in the fields of homogeneous and heterogeneous catalysis as well as reaction engineering. As a consequence of the large number of contributions, the oral and poster presentations were organized in two sessions focusing on catalysis and reaction engineering. The joint community presented 34 oral and seven plenary lectures in the fields of homogeneous/heterogeneous catalysis and reaction engineering. Moreover two presentations were held by the awardees of the “Jochen Block Preis 2010” and “Hanns Hofmann Preis 2011” showing the recent research activities in the fields of chemical usage of biomass and in-situ methods for high temperature catalytic reactions. Further highlights of the conference were the two poster workshops on “Transformation of Renewable Feedstocks” and “Electro- and Photocatalysis”. A group of poster authors presented the summary of their work in order to stimulate an intensive discussion among the participants in these emerging fields of research and application.

In the field of heterogeneous catalysis the broad interest in renewable feedstocks was evident. Already in the first plenary lecture Prof. Ib Chockendorf was discussing the potential and limitations of the photocatalytic production of hydrogen from water splitting. The recent developments in the usage of bio renewable compounds such as cellulose and lignin as building blocks for organic synthesis were presented by the “Jochen Block Preis 2010” laureate Regina Palkovits. The current applicability and the future lines of development in the field of electromobility were presented in a very illustrative contribution by Prof. Hubert

Gasteiger, discussing not only the wide expectations, but also the limitations related to the future (CO<sub>2</sub> neutral) mobility.

From reaction engineering point of view the dominating topics were exhaust gas treatment, as well as the use of modelling and simulation as a tool in reaction engineering and industrial processes. These topics are strongly interconnected to heterogeneous catalysis and of great interest to both the scientific communities. The exhaust gas treatment session compiled contributions dealing with catalyst aging during operation and controlling of automotive three way catalysts. Starting with a presentation from industry Martin Votsmeier discussed that neither the control of automotive convertors under dynamic operation nor the deactivation mechanisms of the applied catalytic materials are completely understood. Additionally, the requirements in the catalysts in terms of air pollution control increase in the future. The close link between the interests of both communities became evident by the broad variety of the presentations in this section ranging from kinetic simulations to an example of the application of Fe-zeolites as catalysts for the NH<sub>3</sub>-SCR reaction in diesel engines. Modelling and simulation was applied in several contributions including model predictive control and flow fields in fixed-bed reactors. An interesting presentation by Kristian Voelskow applied modelling tools to describe the production of carbon nanotubes in a technical fluidized bed reactor. In this challenging application it could be shown, how modelling and simulation can contribute to the comprehension of complex multi-scale processes. Large scale industrial processes discussed included the oxidation of o-xylene to phthalic anhydride and industrial carbohydrate chemistry, where the improvement in selectivity for bulk chemicals plays an important role in industrial research and development. This is underlined by the efforts in understanding the reaction network and the search for novel classes of catalysts for the partial oxidation of o-xylene presented by Robert Marx and Stephan Schunk, respectively. Further emerging topics are in-situ methods for investigation flow and concentration fields in chemical reactors and electricity storage for use in individual transportation. It would be desirable to address these topics at the next conference.

This year the homogenous catalysis was embossed by sustainability and renewable resources. From new techniques for process optimization and the exchange of the catalyst metal to water splitting the range was quite broad. In this respect, Thomas Müller from the RWTH Aachen presented his recent results in the usage of CO<sub>2</sub> as a renewable C<sub>1</sub> building block. His group was able to convert CO<sub>2</sub> with epoxides to cyclic carbonates, aliphatic polycarbonates, as well as polyether carbonates and could show that the product formation is selectively steered by the choice of homogenous catalyst. This contribution was a nice example for the application

of greenhouse gas CO<sub>2</sub> as a renewable building block. The photocatalytic water splitting represents another way to avoid greenhouse gases and a potentially sustainable hydrogen source. In this regard, Nicolas Marquet from the Leibniz-Institut für Katalyse e.V. demonstrated new homogenous iridium-based water oxidizing catalysts, which efficiently oxidize water in significant amounts. Notably, in the majority of existing systems ruthenium is used for this purpose. For the well-known cross-coupling reactions, Axel Jacobi von Wangelin from University of Cologne presented how iron catalysts are able to form various C-C bonds under rather simple reaction conditions with a unifying concept. His group opened up new possibilities to avoid expensive and also toxic nickel and palladium complexes, by the use of naturally preferred iron. Inspired by nature, Prof. Feringa from the University of Groningen showed his challenging developments for sustainable organic synthesis by integration of biocatalysis and homogeneous catalysis. The highlight was the usage of DNA in asymmetric catalysis, as highly chiral biomolecule. Following the main intention, Katja Seifert from the TU Berlin illustrated an interesting process concept, which allows the combination of a palladium-catalyzed Suzuki-coupling with a rhodium-catalyzed transfer hydrogenation. In the process the advantages of microemulsion were used to affect the phase properties, thus the catalyst could be easily separated and reused. This example shows how catalytic reactions could be intensified by the combination of reaction engineering and catalysis. Apart from that, the poster of Sebastian Bähn about the homogenous ruthenium catalyzed synthesis of primary amines was awarded with the poster price. The contribution disclosed how ruthenium catalysts enable primary amines generation from secondary amines as well as from secondary alcohols. Noteworthy, both reactions employed ammonia a nitrogen source.

In summary the intention of intensified interactions was successfully realized on the joint conference on catalysis and reaction engineering, which was impressively underlined by the final plenary lecture of Götz Vesper, who covered the whole range from heterogeneous catalysis to classical reaction engineering. The contributions were carefully chosen to be as interdisciplinary as possible. In addition the scientific exchange was also enhanced among young scientists/chemists by the well accepted poster workshops.