Weimar – The place to be for Catalysis in Germany

Conference Report

45. Jahrestreffen Deutscher Katalytiker

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Catalysis in Weimar has a long standing tradition, dating back to the time of Johann Wolfgang von Goethe (1749-1832). He was one of the first owners of a "Döbereiner's lamp", which is an early example of applied and successfully commercialized catalysis. Nearly two centuries later the 45th annual meeting of the German Catalysis Society (GeCatS) took place in Weimar on March 14th-16th, 2012. The conference was organized by DECHEMA and attracted 524 participants from academia and industry. Beside homogeneous and heterogeneous catalysis also more specialized nonetheless highly important topics such as photocatalysis, electrocatalysis, biomass valorization as well as novel catalyst materials and *in situ* characterization techniques were represented. The great importance of catalysis for today's but even more for tomorrow's society is emphasized by the large number of contributions. Six plenary talks, 29 oral presentations organized in two parallel sessions and a presentation of recent research activities of the awardee of the "Jochen-Block-Preis 2011" delivered insights to the state of the art in catalysis research. During the poster sessions 247 posters were presented. Additionally, the posters could be accessed as electronic posters on two poster-sized screens during the whole conference initiating intense scientific discussions and exchange. A further highlight was the poster workshop on "Electrochemistry in Catalysis: Experiment and Theory". Therein, chosen posters were presented in short and intensively discussed among the participants. On the edge of the conference, a meeting of young

scientists from academia and industry took place for the first time to discuss the future of catalysis and build up a platform for intense networking. “YounGeCatS” (www.gecats.de/youngecats) will organize future meetings and events for the discussion of scientific as well as career-related issues.

The topics in heterogeneous catalysis were focused on the characterization and understanding of the interactions between surfaces and molecular species. In the first plenary lecture Prof. Michel Che from the University Pierre and Marie Curie (Paris, France) presented the “Elaboration of supported catalysts: between water and fire”. He discussed the formation of different oxide-supported catalytic active species and the influence of complex formation on their reactivity. Prof. Hans-Peter Steinrück from the University Erlangen-Nürnberg (Germany) showed impressive results on the behavior of metalloporphyrins on metal surfaces characterized by scanning tunneling microscopy. The “Jochen-Block-Preis” awardee Dr. Swetlana Schauermann from the Fritz Haber Institute of the Max Planck Society (Berlin, Germany) provided valuable insights in the interactions of gas phase molecules with nanostructured supported model catalysts by applying molecular beam techniques. The characterization of such model systems leads to a better understanding of the diffusion processes of hydrogen on as well as under the surface of catalysts particles. Beside these highlights, various oral presentations proved the usefulness of novel *in situ* and *operando* characterization methods for a deeper understanding of catalytic processes. The presented methods ranged from classical spectroscopic methods such as IR and UV/Vis to more exotic techniques such as microwave cavity perturbation, *in situ* XAS and XRD, TOF-SIMS and *operando* SSITKA/DRIFTS/MS.

Next to characterization techniques also theoretical approaches played an important role as shown by the plenary lecture of Prof. Olaf Deutschmann from the Karlsruhe Institute of Technology (Germany) on multi-scale modeling in heterogeneous catalysis. He nicely demonstrated how different theoretical approaches can lead to valuable insights on scales of several orders of magnitude. It started with DFT modeling on the molecular scale went on to the application of Monte Carlo and Molecular Dynamic Simulations to describe diffusion processes and ended with modeling approaches in the field of reaction engineering. In further oral presentations the usefulness of computational methods in combination with experimental results in biomass upgrading as well as in concerted CO_2 utilization has been emphasized.

The valorization of renewable resources such as biomass in general proved to be of great interest within the catalysis community. E.g. model compounds have been used for the investigation of lignin depolymerization and novel porous polymers were applied as solid acid catalysts in the dehydration of fructose to hydroxymethylfurfural. Also hydrogen as an energy carrier was of interest. Results showing the production of hydrogen from biomass as well as

by electrochemical and photocatalytic watersplitting using novel catalyst materials were presented. The general challenges associated with hydrocarbon conversion were emphasized by Dr. Marcello Rigutto from Shell Global Solutions (Amsterdam, Netherlands) giving a plenary lecture from the industrial perspective on catalysis research. Further oral presentations dealt with the catalytic oxidation of methanol as well as with the oxidative coupling of methane using MgO as a model catalyst. But also exhaust gas catalysis with a high environmental impact such as a SO_2 oxidation catalyst screening by high throughput methods or the investigation of catalyst species in automotive three-way catalytic converters was presented.

Along with presentations on heterogeneous catalysis new insights on homogeneous catalysis were reported. In this regard, the development of sustainable, efficient and selective procedures to access organic compounds with higher values is still one of the fundamental research goals in modern chemistry. Especially the requirements for “Green Chemistry” have become one of the major issues for organic synthesis and were the subject of discussion in previous “Jahrestreffen Deutscher Katalytiker”. This year Prof. David Milstein from the Weizmann Institute of Science (Israel) provided an overview of his recent achievements in this field, e.g., the sustainable synthesis of esters or amides starting from alcohols. Noteworthy, these reactions are highly atom economical and generate molecular hydrogen as the only by-product. A milestone for achieving remarkable catalytic activity was the application of Ruthenium complexes modified by “cooperating” pincer ligands, which are nowadays a prominent ligand class in homogeneous catalysis. Furthermore, the understanding of the underlying processes, e.g., the interplay between aromatization and dearomatization of the coordinated ligand, creates a huge number of possibilities for organic transformations. Apart from metal-based catalysis, Prof. Gerhard Erker from the University of Münster (Germany) reported on investigations in the research field of transition metal-free catalytic systems for the activation of dihydrogen, which can be applied for the reduction of organic molecules. Clearly, most of the applied transition metals for hydrogenation chemistry displayed difficulties by their high price or toxicity. In this regard, the application of a combination of sterically encumbered *Lewis* acid and *Lewis* base, which are highly “frustrated”, because they cannot form a “classical” *Lewis* acid/*Lewis* base adduct, can be an interesting alternative.

In summary, this year´s “Jahrestreffen Deutscher Katalytiker” added benefits to all researchers in the field of catalysis with the well-balanced program and the creation of a platform for bridging the gap between the different disciplines in catalysis. Also in 2013 the “Jahrestreffen Deutscher Katalytiker” in Weimar should be the place to be for the catalysis community in Germany.