Catalysis Today 155 (2010) 155–156

Contents lists available at ScienceDirect

Catalysis Today

journal homepage: www.elsevier.com/locate/cattod

Preface

Catalysis is a key technology for chemical production processes, more than 80% of which include at least one catalytic step. Knowledge-based and hence time-effective catalyst design, which goes beyond the scope of the empirical methodology being currently still dominating, requires a scientific understanding of the relationship between synthesis parameters and structure of catalysts on the one hand and their mode of action on the other hand. Both pieces of information must be obtained under at least approximately real reaction conditions. This is only possible by methods of "operando spectroscopy", a label which has been introduced for spectroscopic studies, in which the analytical cell operates as a catalytic reactor which is coupled to on-line product analysis. Such techniques experienced a lively development in recent years which has been impressively reflected by the 3rd International Congress on Operando Spectroscopy held in Rostock (Germany) in April 2009. Initiated by two conferences in 2003 in Lunteren (The Netherlands) and 2006 in Toledo (Spain) this conference series has become an important opportunity for many researchers to share their latest results and future ideas on direct insights in catalyst synthesis and operation for knowledge-driven catalyst design.

Thanks to many high-quality contributions in both heterogeneous and homogeneous catalysis as well as in catalyst synthesis, 24 of which are contained as full papers in this special issue, the 3rd International Congress on Operando Spectroscopy became a true success and provided an exciting discussion forum for about 125 participants from Europe, Asia, North America and South Africa. Five plenary and five keynote lectures introduced current hot topics of in situ and operando spectroscopy, such as increasing time and space resolution, realizing operation conditions as close as possible to those of technical processes, design of new reactor cells and coupling techniques, development of advanced data processing and chemometric tools, and the combination of operando spectroscopy and molecular theory.

Lynn Gladden (University of Cambridge) highlightened in her plenary lecture the potential of Magnetic Resonance Imaging for catalytic studies. Heiko Oosterbeek (Shell Technology Center, Amsterdam) tackled the challenges of operando spectroscopy from an industrial point of view, with special emphasis on Fischer–Tropsch and polymerization reactions. The plenary lecture of Marc Garland (Institute of Chemical and Engineering Science, Singapore) illustrated benefits that derive for spectra interpretation from a combination of experimental design and advanced chemometric procedures. Zbigniew Sojka (Jagiellonian University, Krakow) underlined the deeper insight in reaction mechanisms that can be gained by combining spectroscopy and molecular modeling and Bert M. Weckhuysen provided spatially resolved views on reactions proceeding in catalysts by combining spectroscopy and microscopy.

Keynote presentations were dedicated to the application of time-resolved vibrational techniques for the study of DeNO$_x$ processes (Atsushi Urakawa), the use of X-ray scattering and spectroscopy for analyzing the synthesis of nanoclusters (Stefan Vajda), the analysis of Pd catalysts in liquid-phase reactions by a variety of techniques (Davide Ferri), the combination of DRIFT spectroscopy with quantitative kinetic analysis (Frederic C. Meunier) and the space and time-resolved analysis of zeolites during hydrocarbon transformations by optical and fluorescence micro-spectroscopy (Marianne H. F. Kox).

The majority of papers presented in this special issue comprise the application of vibrational spectroscopies such as Raman and infrared spectroscopy in transmission, diffuse reflectance (DRIFTS), attenuated total reflectance (ATR) and polarization-modulated reflection–absorption mode (PM-IRRAS) for the study of heterogeneous and homogeneous catalytic reactions as well as for the analysis of surface adsorption and catalyst synthesis processes. Moreover, there are several studies which used X-ray diffraction and absorption methods to shed some light on structural changes proceeding during heterogeneous catalytic gas-phase reactions such as Fischer–Tropsch synthesis and oxidation reactions. Besides these techniques which became well-known for in situ-studies during recent years, there are also few papers on less frequently applied methods such as in situ-measurements of electrical conductivity and the use of neutron scattering after quenching active catalysts.

Thanks to many intriguing results presented by the participants of the 3rd International Congress on Operando Spectroscopy, we remember this event with pleasure and look forward to the 4th International Congress on Operando Spectroscopy, which will take place on April 29–May 3, 2012 at Brookhaven National Laboratory, Upton, NY, USA.

Last but not least I would like to take the advantage of these lines to thank our Major Sponsor EVONIC Industries and our sponsors Avantes, Kaiser Optical Systems, HORIBA Jobin–Yvon, Ocean Optics, Thermo Fisher Scientific Inc. and Parr Instruments for their very important support. Moreover, we appreciate the support by the Royal Society of Chemistry, Elsevier (Catal. Today), Westphal Mess- und Regeltechnik, STOE, BASF, UOP and GDCH. Special thanks go to the Program Committee and the Local Organizing Committee as well as to the DFG Research Training Group 1213, who all did a great job to make the congress a success.

I hope that you enjoy this special issue of Catalysis Today and I am looking forward to seeing you again at Operando IV, 2012 at Brookhaven National Laboratory.

0920-5861/$ – see front matter
doi:10.1016/j.cattod.2010.06.024

Angelika Brückner*
Leibniz-Institut für Katalyse e. V., an der Universität Rostock, Albert-Einstein-Str. 29a, D-18059 Rostock, Germany

*Tel.: +49 381 1281 244; fax: +49 381 1281 51244.
*E-mail address:*angelika.brueckner@catalysis.de

Available online 17 July 2010