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Synchrotron Radiation and Neutrons for Catalysis, Materials Research and Development

The participants of the INFOday "Synchrotron Radiation and Neutrons for Catalysis, Materials Research and Development" at DECHEMA. © DECHEMA.

With the present and future synchrotron radiation (SR) and neutron facilities in Germany and in Europe, new and attractive possibilities for the analysis, understanding, and development of materials and catalysts have arisen. The large-scale facilities PETRA III, ESRF, BESSY, ILL, ISIS, and smaller synchrotron radiation sources, such as those in Karlsruhe (KIT-Synchrotron, formerly ANKA) or Dortmund (DELTA), are now up and running, and some of them will be upgraded in the near future. New sources like FLASH, XFEL, ESS, and MAX IV have recently or will soon go into operation. This exciting situation, both for academic and industrial users, was the trigger for the GeCatS Infoday "Synchrotron Radiation and Neutrons for Catalysis, Materials Research and Development" at the DECHEMA in Frankfurt/Germany. The Infoday was organized by Peter Albers (Evonik), Dana Demtröder (DECHEMA), and Jan-Dierk Grunwaldt (KIT) on October 23, 2017, and was supported by the German Catalysis Society (GeCatS), the Committee for Synchrotron Research (KFS), and the Committee for Neutron Research (KFN). The workshop started with a welcome address by the BMBF (Oda Keppler) and the workshop organizers (Jan-Dierk Grunwaldt). The German government strongly supports not only the facilities, but also the infrastructure, and therefore its interest at this Infoday was highly appreciated, especially by German participants.

More than 80 participants from academia, facilities, and industry discussed questions such as: How do catalysts, fuel cells, batteries, or sensors work on an atomic, mesoscopic, or macroscopic scale? What kind of changes occur under working conditions upon gas exposure, temperature, as a function of time, or at elevated pressure? Some direction was given in the welcome address by Jan-Dierk Grunwaldt, highlighting the prominent role of a sensitive microstructure and structural dynamics in catalysts and batteries. Their understanding is paramount for solving current and future challenges within the "Energiewende" or environmental catalysis. In the morning talks, Robert Schlögl (MPI Mülheim, FHI Berlin) and Tobias Unruh (FAU Erlangen) demonstrated the need and the potential of synchrotron X-rays and neutrons to probe catalysts and related materials in situ and

even operando. Robert Schlögl, for example, showed that the structure of Cu- or Ru-catalysts during methanol oxidation or Bi-Mo-O catalysts during propane dehydrogenation strongly depends on the reaction atmosphere. Near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) has been developed at BESSY to ensure that the structure of these catalysts could be ascertained in time, while the catalyst is working. In fact, the joint laboratory for electrochemical interfaces with special infrastructures was recently founded in Berlin; e.g., for focusing on photo-electrochemistry. Likewise, Tobias Unruh demonstrated the indispensible need for neutrons and synchrotron radiation for understanding the formation of colloidal ZnO particles, including the outer shell. Neutrons are also excellent for providing insight into battery materials, as shown on a poster by Gilles and co-workers.

Peter Albers (Evonik) demonstrated the strength of both synchrotron radiation and neutrons for industrial research in his talk. The advantages of SR (high brilliance and penetration power) and neutrons (high penetration power and detection of light elements) were illustrated by excellent examples, such as fuel-cell catalysts (studied by SR), Lindlar catalysts (β-Pd-hydride probed by neutrons), or the coking of catalysts (examined by neutron scattering). According to Albers, both "work-horse" beamlines and high-end spectrometers/beamlines are needed for the understanding of catalytic processes and to ensure the steady improvement of materials. The use of high-end stations additionally needs long-term collaboration, including not only large-scale facilities, but also expert groups from universities. For daily industrial R&D high-intensity beamlines, professional support and rapid access are essential, as Volodomyr Boyko (BASF) outlined in his talk. Rapid access is required for standard experiments (e.g., diffraction, scattering), and expert knowledge for more demanding techniques such as PDF analysis or nanotomography. In other cases, such as those shown by Peter Albers and Kirill Lomachenko (ESRF), long-term research studies, in collaboration with expert university groups, and novel infrastructure at synchrotron radiation sources are demanded. Hence, the industrial interest—whether a "work-horse beamline" or a "Ferrari" with all possible techniques is needed—depends on the target question.

This requires a strong synergy between large-scale facility and university research, as excellently demonstrated by Stewart Parker (ISIS) and Anatoly Frenkel (Stony Brook University/Brookhaven National Laboratory). In the U.K., a Catalysis hub was founded in 2013 with five team leaders in various fields of catalysis (design, energy, environmental, chemical transformation, and biotransformations). Neutrons, for example, allowed a mechanistic insight into methanol-to-hydrocarbon processes, whereas the structure of a Au-Pd alloy could be uniquely studied by a combination of XAS, XRD, and DRIFTS. The catalysis consortium in the U.S. was founded in 2005, and facilitates bridging SR-related work and applied research, not only by providing infrastructure at the synchrotrons, including a combination of techniques, but also through education by offering annual short courses and training at large-scale facilities. Examples are the identification of the role of Cr in water gas shift catalysts using combined XAFS, XRD, and Raman spectroscopy and correlative studies at the nanoscale by XAS, STEM, and IR during the ethylene hydrogenation process over Pt and Pd catalysts in an operando microreactor.

This joint effort, as found in the U.K. and the U.S., is extremely important; nevertheless, the keys are and remain the facilities themselves, as highlighted in a session chaired by Ronald Frahm (Univ. Wuppertal). Andreas Stierle (DESY, Hamburg), Marco Favaro (BESSY II), Andreas Schreyer (ESS), and Kirill Lomachenko (ESRF) demonstrated, in convincing talks, the possibilities at today's large-scale facilities and provided further excellent exemplary studies. This was extended by a poster session, where facilities presented their research and special infrastructures, such as those at ILL, DESY, BESSY, and the KIT Synchrotron, among others. In addition, spe-

A lively panel discussion on the question "How to achieve synergies between large-scale facilities, academic research, and industry?" at the end of the workshop. © DECHEMA.

cial techniques for in-situ studies of Li-ion batteries (neutrons as a probe, Gilles, TU Munich), catalysts (dedicated catalysis beamline, Zimina, KIT), tomography (Sheppard, KIT), or gas sensors (Degler, Tübingen) were presented and discussed.

The talks and posters earlier during the Infoday provided an excellent basis for the panel discussion on the question "How to achieve synergies between large-scale facilities, academic research, and industry?" The panel was well-represented by scientists from academia (Behrens, Duisburg-Essen), industry (Albers), synchrotron and neutron sources (Stierle, Frenkel, Parker), and the BMBF (Meyer-Klaucke, PT-DESY). For the panelists, it was very obvious that, in Germany, much progress has already been achieved in solving problems in catalysis and materials science. Not only in Germany, but also in the U.K., the U.S., and other countries, government agencies have invested hundreds of millions of euros in building large user facilities. What remains to be improved are the research infrastructures in Germany and worldwide, with help from the user communities and with the help of funding agencies to maximize the scientific output. This requires a joint effort from both universities and large-scale facilities on the one hand, and industry on the other. Significant manpower is needed to provide appropriate support for industrial users and to run the research infrastructures. It is particularly important that governmental funding agencies play leading roles in bringing all parties together and, as in the case of the U.S. Synchrotron Catalysis Consortium, providing the funding for supporting the user organizations that do research at the synchrotrons.

The Infoday's talks and discussions demonstrated that new consortia have recently emerged (such as those in the U.K. and U.S.), but their experience should be actively disseminated to establish continuous fruitful transfer between large-scale facilities, university groups, and industry across the globe. The Infoday's participants concluded the day by looking forward to the opportunity for further discussions at conferences like the international X-ray absorption spectroscopy conference XAFS17 in July 2018 in Poland, and the synchrotron, neutron, ion conference (SNI2018) in September 2018 in Munich. ■

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