

Tracking the structure of catalysts during birth, work and deactivation/reactivation: Snapshots synchrotron-based in-situ and operando spectroscopy

Institute for Chemical Technology and Polymer Chemistry (ITCP) and Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), grunwaldt@kit.edu

The toolbox for advanced and operando characterization of heterogeneous catalysts has rapidly increased in recent years. This is important because identifying the active site in heterogeneous catalysts and its structure is a demanding task. Catalysts are dynamic entities and depend on the embedding matrix, the surrounding fluid and last but not least the location in the catalytic reactor. Bridging the different time and length scales in heterogeneous catalysis is a challenge at the interface of spectroscopy, model system design, modelling and chemical engineering. This review aims to illustrate this approach with examples from emission reduction for clean air and sustainable production of CO₂-neutral fuels and chemicals.

For example, noble metal catalysts play a key role in the removal of pollutants such as CO, methane, VOCs or residual ammonia. Deactivation and reactivation processes are fundamental, and the dynamics of the noble metal structure can be exploited to increase efficiency and lifetime. However, not only the active site but also the porous network, the shaping and the concentration profiles in the reactor are crucial, making it an excellent showcase for bridging the different scales of complexity in catalysis. This is also part of the Collaborative Research Centre CRC1441 (TrackAct, www.trackact.kit.edu).

Another challenge comes with the development of Power-to-X processes: The simple CO₂-methanation as an exothermic reaction does not appear as simple as often described when looking in a spatially resolved manner. Additionally, Fe-Ni-catalysts are not only bimetallic but also bifunctional improving activity and selectivity as well as stability against H₂ dropouts. Both methanol and Fischer-Tropsch synthesis including the production of higher alcohols require high pressure studies, also when using *operando* spectroscopy. In addition, the use of model catalysts instead of industrial catalysts is needed to answer specific questions like promoter effects – a particular challenge tackled in the projects of the SPP2080 (www.spp2080.org). The examples will show that *operando* spectroscopy has become an indispensable tool in catalysis and that further challenges and exciting work lie ahead.