

Investigating Catalysts at Work

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Inhalt Catalyst characterization during their preparation, activation and under reaction conditions is important for a targeted catalyst development. X-ray absorption spectroscopy is a valuable tool for this, since it is element-specific, information both on amorphous and crystalline materials can be gained, and a number of materials can be investigated. To elucidate the active sites in heterogeneous catalysts, it is often not sufficient to uncover the structure of catalysts before and after a catalytic reaction. Structural information is especially required *during* the catalytic reaction or *during* the activation process – in other words, “snapshots” of the catalyst at work are required. Since the use of hard X-rays allows penetrating a number of window materials and reaction media, this opens up the design of *in situ* cells imitating the reaction conditions in real reactors. The strength of this approach will be illustrated for gas-solid and liquid-solid reactions. Even at high pressure, i.e. in supercritical fluids, it is possible to monitor the structure of heterogeneous catalysts and thus to establish structure-activity relationships. Other opportunities of XAS and related techniques are time-resolved studies in the ms-scale, structural identification of low-concentrated constituents of interest (e.g. promoters) using fluorescence detection, resonant inelastic X-ray scattering (RIXS), and spatially resolved X-ray absorption spectroscopy.

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