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Time-resolved XAS in Heterogeneous Catalysis – Evolution of Catalyst Structure under Reaction Conditions

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Structure-activity relationships constitute important subjects in heterogeneous catalysis research. In addition to reactions of the catalyst bulk during preparation and activation, the active phase and its surface can be influenced or even determined by the "real" structure (i.e. under reaction conditions) of the catalyst bulk. Time-resolved X-ray absorption spectroscopy (TR-XAS) possesses excellent capabilities to reveal quantitative phase composition and average valence together with the evolution of the local structure of a system under dynamic reaction conditions. From a combination of TR-XAS and, for instance, mass spectrometry, reliable relationships between the "real" structure of a catalyst and its function can be obtained. Here, time-resolved in situ XAS investigations will be presented aiming, first, at understanding the evolution of the structure of the catalyst under dynamic conditions and, second, at revealing properties of the system studied not available from investigations under stationary conditions (e.g. reaction intermediates or the solid-state kinetics of the reaction). The structural evolution of various molybdenum oxide based catalysts under partial oxidation reaction conditions will be discussed emphasizing the potentials and the limitations of TR-XAS.