In-situ Methods for Catalyst Characterisation

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A rational approach for catalyst development requires the solid understanding of the solid state and surface chemistry of the material intended to be used as a catalyst. Surface science can provide a very detailed understanding of elementary surface reactions which are useful for practical catalysis when the reaction conditions and the material properties of the model systems allow a scientifically based extrapolation to practical conditions.

Structural in situ characterisation of reacting solids can be performed with modified laboratory X-ray diffraction methods or with synchrotron based EXAFS or diffraction experiments. A report will be given on the performance of simpler experiments which occur always under in-situ control of the catalytic performance. The partial oxidation of methanol to formaldehyde over copper and the phase inventory of reacting heteropoly acid catalysts will be used as examples.

These examples will further be used to illustrate the range of methods to investigate surface electronic properties by in-situ low energy NEXAFS at oxygen K edge and by in-situ UV-VIS spectroscopy.

Fundamental studies in catalysis as well as practical development efforts rely on efficient and versatile detector systems to monitor catalytic performances. A novel mass spectrometric technique based on ion molecule reaction (IMR) ionisation will be presented. The technique offers low fragmentation, chemical selectivity and quantification of reactor responses with a time resolution of below 1 s. In combination with TG-DTA valuable data on solid state transformations can be obtained. In combination with catalytic reactors it will be illustrated how multiple reaction pathways in selective oxidation reactions can be identified very quickly. The time resolution capabilitis will be shown by the analysis of kinetic oscillations of the methanol oxidation reaction over copper catalysts.