

In-situ phase analysis of metal oxide catalysts for selective oxidation

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Heterogeneous catalysts for selective oxidation are commonly metal oxide systems with a high degree of elemental substitution and with additional phases which render their structural chemistry complex. An important property of efficient catalysts is their ability to store or release “lattice oxygen” and so to adapt the oxidation state of the bulk (and surface) to the chemical potential of the gas phase. Consequently, the operation of such a catalyst depends to a great deal on the details of its ideal and real crystal structure.

The structural flexibility of molybdates and molybdo-phosphoric heteropolyacids (HPA) will be discussed using the model reaction of methanol oxidation. Results from in-situ high energy EXAFS, low-energy XAFS, HR-TEM and in-situ XRD will be used to illustrate the structural flexibility and the unexpectedly short time-scale of the accommodation processes of the catalyst systems to various reaction conditions. In-situ UV-VIS-NIR was used to follow the transient behaviour of HPA catalysts under stoichiometric and catalytic reaction conditions.

It will be illustrated that the well-known structures of catalytic systems in their highest oxidation states are a poor representation of the respective working states. Not only the oxidation states of the cations but the whole structural arrangement and the disposition of defects are reversibly altered under reaction conditions. The notion that such transformations can be “frozen in” will be shown to be questionable as well as the notion that fast processes occur on surfaces and slow processes characterise bulk reactions.