The role of early transition metal oxides in heterogeneous selective oxidation catalysis

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The activation and oxidative functionalisation of small aliphatic hydrocarbon molecules using molecular oxygen are prime targets of heterogeneous catalysis research. The needs of chemical industry and the scientific challenge drive the development that is largely dominated by empirical search strategies. Catalytic systems are complex oxide mixtures containing several phases and a variety of cations. Heuristic principles of site isolation, phase cooperation and lattice oxygen participation dominate the conceptual discussion.

Functional concepts based on rigorous experiments are scarce due to the lack of in-situ experimentation and the incompatibility of reactions and catalysts with surface science techniques that were so successful in understanding other classes of catalytic processes.

The selective oxidation of butane to maleic anhydride will be used as example to show how in-situ experimentation on real-world systems and the design of experimental and theoretical model systems start to cooperate in an effort to understand the reaction steps governing the chemically so “simple” processes.

To exploit such in-depth understanding requires the ability to taylor the solid-state synthesis of catalytic materials to functional requirements. As these are largely determined by defect structures, the real structure of a material decides over its catalytic function. Very little is known on the synthetic side of “simple” inorganic systems. The missing toolboxes that work so well in molecular chemistry present a major bottleneck in the development of heterogeneous catalytic processes suitable for large-scale applications.