Of defects and dynamics - Structural characterization of heterogeneous catalysts in the electron microscope

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Olefins and functionalized hydrocarbons are important building blocks for daily life products. In chemical industry they are usually produced from saturated analogues at the surface of heterogeneous catalysts, e.g. transition metal oxides, or energy intensive routes involving hazardous biproducts. In both cases, they rely on natural gases and crude oil. Thus, there is a strong desire to develop rational design concepts allowing to enhance their ecologic and economic production efficiencies.^[1] However, catalyst's tailoring requires the availability of realistic structure-function correlations. This is not trivial as the most promising oxidic catalysts are structurally complex and known to exhibit a broad defect chemistry and compositional diversity. In addition, catalysts are dynamic and their structures under working conditions depend on the local chemical potential.^[2]

To untangle the structural pluralism and its evolution under reaction conditions of complex oxide catalysts we employ a scale-bridging (*operando*) electron microscopy approach that is complemented by theoretical modelling as well as X-ray diffraction and spectroscopy.^[3]

In this talk, I will show the complexity of Mo- and V- based oxides that are used in the oxidative dehydrogenation of ethane (ODE), the relation between surface structure and real structure of the bulk and their structural changes induced during ODE disclosed by identical location transmission electron microscopy (TEM).^[4] In addition, I will illustrate the evolution of Co_3O_4 catalysts during isopropanol oxidation by combining near ambient pressure X-ray spectroscopy with *operando* TEM and *operando* scanning electron microscopy.^[5]

The data show that working at frustrated phase transitions is key for maintaining the high performance of oxide catalysts under selective oxidation conditions. This gives new momentum in finding strategies for prospective catalyst tailoring.

References:

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