

# Strategies towards an efficient development of heterogeneous catalysts: Selective oxidation as case study

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The traditional way of developing catalytic materials is through trial and error methods which are combined with an increasing amount of intuitive experience. All our present catalysts were found and optimised by this method. Besides the modern approach of „combinatorial catalysis“ there is now the alternative to direct the research efforts towards an in-depth atomistic understanding of catalysis and its exploitation as a directed material development with a rational working hypothesis.

A central challenge for heterogeneous catalysis is oxidative functionalisation of small molecules. Selective oxidation of alkanes and alcohols, alkane-to-olefine conversion and methane activation are relevant topics. One major problem in all these reactions is the control of the activity of the oxidant which is derived from activated molecular oxygen. The main strategy for this control is the diffusion/segregation of surface oxygen atoms through the bulk of the catalyst. The ratio of the kinetic constants of these two processes and the details of the surface chemical bonding of oxygen atoms will control the oxidising potential of the oxygen.

Elemental silver is used as a case study to illustrate the moderation of oxygen for either selective oxidation of methanol or oxidative coupling of methane. Multi-element oxides are used as efficient catalyst in selective oxidation. Using molybdo-heteropoly-acids (HPA) the concept of bulk-oxygen activation is illustrated which resides on a combination of redox. And polymerisation steps within the crystal of molecular oxo-anionic species.

The application of a suite of in-situ analytical techniques allows to study fundamental catalytic processes in quasi-realistic conditions and to derive the understanding necessary for the rational approach to heterogeneous catalysis with much less extrapolation problems as it does the surface-science approach using idealised materials and reaction conditions with very little surface coverage (UHV).

The contribution will illustrate how such understanding has been derived so far and what perspectives can be expected for the implementation of the rational approach towards heterogeneous catalysis.