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Experimental studies on the Structure of Active Sites in Heterogeneous Catalysis

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The efforts in understanding heterogeneous catalysts in their working state have a long tradition. They are motivated by the view that only the knowledge of the structure of the active catalysts allows to understand the function of the catalyst at an atomic level. This understanding is, however, prerequisite to any efforts to improve or to redesign more efficient catalysts. Surface Science has provided us with an enormous amount of insight into the course of heterogeneous reactions forming elementary processes in practical catalysis. Hence, these facts are difficult to apply to practical cases leading to the identification of gaps in catalysis science.

The origin of this discrepancy between surface science and catalysis is not the “black magic” character of catalysis but merely the fact that the models used in fundamental studies do not match the reality. Thus the structural analysis of working catalysts in the bulk as well at their surfaces is of paramount importance in order to device the correct model substrates for fundamental studies.

The selective oxidation of methanol over silver and copper metal will be used to illustrate the complexity of structures arising from the application of these simple catalysts under atmospheric conditions. They form metastable structures and can no longer be modeled by single crystal surfaces. The use of heteropoly acid derivatives as selective oxidation catalysts was partly triggered by apparent simplicity of a well-defined single properties to optimize catalytic performance. The paper will show that the structural anticipations are incorrect and well-defined molecular oxide is only a precursor structure to an oligomeric oxide which is, however, distinctly different in its properties of the final decomposition product MoO_3.

Active sites occur as atomic ensembles preferably in metastable derivatives of the parent catalyst materials which exist only under catalytic reaction conditions including the correct partial pressure of all reactants. It is thus absolutely essential to retro-synthesize these metastable structures under conditions enabling the application of rigorous surface science techniques in order to unravel the function of active sites. First attempts to accept this synthetic challenge will be presented for iron oxide and zirconia.

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