Institutsseminar

Mass Spectrometry and Theoretical Chemistry in Service of Catalysis Research: A Menage-a-Trois at Its Best

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The ultimate goal in heterogeneous catalysis is to make use of each and every atom of supported (metal) catalysts, i.e. in the extreme to perform single-atom catalysis (SAC). While this arduous task constitutes a non-trivial, if not daunting challenge in 'real-life' chemistry, in the gas phase SAC can be achieved in a rather straightforward manner by conducting experiments with mass-selected species under (near) single-collision conditions. These mass spectrometry-based studies on isolated reactants, when complemented by state-of-the-art computational and spectroscopic work, provide an ideal arena for probing the energetics and kinetics of a chemical process in an unperturbed environment at a strictly molecular level without being obscured by ill-defined side effects. Thus, the concept of SAC can be explored or, more generally, the mechanisms of reactions and the active parts of single-site catalysts, the so-called 'aristocratic' atoms, can be identified. Examples discussed include:

(i) The room-temperature, cluster-oxide mediated redox reactions of the CO/N2O couple which, arguably constitute one of the most prominent oxidation processes, and
(ii) novel metal-mediated C-H bond activation and C-C coupling of methane, which are regarded as one of the holy grails in chemistry.

References

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