KEMIJSKI INŠTITUT

Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium

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Velika predavalnica Kemijskega inštituta /
Great Lecture Hall
National Institute of Chemistry
Hajdrihova 19, Ljubljana, Slovenia

Surface catalysis beyond the binding site

The chemical properties of bound intermediates and transition states and of binding sites act in concert to select reaction channels in surface catalysis, with theory and experiments now able to uncover site requirements and mechanism with unprecedented precision. The deprotonation energy of a solid and the proton affinity of organic moieties determine reactivity and selectivity for elementary steps mediated by proton transfer and ion-pair transition states on solid acids. Oxidation turnovers on redox-active oxides involve C-H activation and the reduction of metal centers, with transition states involving electron transfer and di-radical pairs, rendering the energy of formation of O-H at surfaces and of C-H bonds in reactants as the relevant reactivity descriptors. The outer sphere environments around binding sites complement their chemical properties through solvation effects that stabilize specific bound intermediates and transition states through weak concerted van der Waals or H-bonding interactions. Such stabilization is particularly evident when sites reside within inorganic voids of molecular dimensions, but also when such sites reside are in contact with dense phases, whether present as liquids or crowded adlayers. These inner and outer sphere consequences for reactivity and selectivity, together with the use of well-defined catalyst architectures suitable for theoretical treatments, are bringing us another step closer to purposeful design in surface catalysis.

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Vljudno vabljeni / Kindly invited