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Frontiers in Catalysis Science and Engineering
Seminar Series

Structure-Activity Relations in Heterogeneous Catalysis - A View from Computational Chemistry

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University of California, Los Angeles

Wednesday, February 22, 2017
9:00am
EMSL Auditorium

The understanding of the catalytic properties of nanoparticle catalysts and the design of optimal composition and structures demands fast methods for the calculation of adsorption energies. By exploring the adsorption of O and OR (R=OH, OOH, OCH_3) adsorbates on a large range of surface sites with 9 transition metals, we propose new structure sensitive scaling relations between the adsorption energy of two adsorbates that are valid for all metals and for all surface sites. This opens the way for a new class of activity volcano plots where the descriptor is not an energy but a structure-related descriptor. In addition, to better grasp finite size effects in the nanoparticles, a generalized coordination number is proposed as a leading descriptor for the adsorption strength. Simple descriptors as generalized coordination show a strong predictive potential exemplified in the design of optimal oxygen reduction reaction catalysts, with strong impact on efficient storage of energy. In a second part, smaller clusters (Pt_{13}) will be considered, supported on a g-alumina surface. We will show how the structure of the cluster is modified upon interaction with the support. The system will then be submitted to a pressure of H_2. The cluster is covered by a high coverage of H atoms (up to 3H per surface Pt) and its structure is modified, with strong implications on its reactivity. Finally I will show how the ordering of the surface of an alloy between Ag and Pd is modified between vacuum and a gas phase of acetylene. The molecule hence create the active site on the alloy surface for its own reactivity.

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