



BERKELEY CATALYSIS CENTER

Seminar

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The McCollum Room

775-A Tan Hall

2:00 PM

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First-Principles Modeling of Chemical Reactions on Heterogeneous Catalysts

ABSTRACT:

First-principles, quantum-based simulations of elementary chemical processes are emerging as a powerful tool for the analysis and design of heterogeneous, transition metal catalysts. These simulations can provide detailed, molecular-level information about the energies, geometries, and electronic structures of chemical species on metal surfaces. This information, which is often inaccessible through experiment alone, in turn permits the determination of catalytically-relevant quantities such as adsorption energies, adsorbate entropies, and activation barriers of elementary reaction steps.

In this talk, I will present two illustrations of the use of first-principles calculations to analyze chemical reactions on heterogeneous catalysts. The first example, of relevance to the design of direct methanol fuel cells, focuses on the elucidation of the detailed reaction mechanism for the decomposition of methanol on Pt(111). The second example involves the determination of trends in the binding and dissociation of H₂ on a variety of binary, transition metal alloys. Analysis of these trends may contribute to the design of improved catalysts for hydrogenation reactions.