

Physical Chemistry Seminar



Professor Alexis T. Bell

Dept. of Chemical Engineering &
Biomolecular Engineering
University of California, Berkeley

In Pursuit of a Molecular-Scale Understanding of Catalyzed Reactions - Lessons Learned from Experiments and Theory

A continuing goal of research in the field of catalysis is the development of a fundamental, atomic-scale understanding of the influence of catalyst composition and structure on catalyst activity and selectivity. The effects of catalyst composition and structure on catalyst performance has largely been revealed through experimental studies, but recent advances in theoretical methods and computer speed have opened the door for understanding and exploring the influence of catalyst composition and structure through the application of theory. This talk will illustrate how experimental and theoretical methods can be used to develop an understanding of the factors controlling catalyst performance. It will be shown that in the case of active centers contained in a zeolite, catalyst activity and selectivity depend on both the electronic properties and confinement of the active site. In the case of reactions occurring on the surface of metal nanoparticles, it will be shown that particle size and composition strongly influence the activity, selectivity, and stability of the catalyst, whereas for metal oxides non-bonding interactions can play a critical role.

Monday, April 22, 2013

4:00 P.M.

2033 Young Hall