

Challenges for the Design of Catalytic Material from First Principles

Alexis T. Bell
Department of Chemical Engineering
University of California, Berkeley

One of the long standing challenges in the field of catalysis is to design catalytic material from first principles. Advances in theory, computational algorithms, and computer speed have come to a point where considerable insights into the factors governing the performance of catalysts at many length scales can be addressed by the application of a hierarchy of theoretical methods. This talk examine what can be done to describe the kinetics of a catalyzed reaction occurring at the Brønsted acid centers of a zeolite and how the kinetics are related to multicomponent adsorption and diffusion in the zeolite. Finally, it will be shown that it is possible to develop a theoretical link between the microkinetics, intraparticle mass transfer dynamics, and overall reactor performance. Additional illustrations will be presented to show what can be learned from a theoretical analysis of the factors involved in stabilizing transition states and how an analysis of the effects of ligand composition contributes to an understanding of what ligand properties are needed to achieve high activity and selectivity for homogeneous catalysts. This presentation will end with some comments about the need for faster algorithms to perform quantum chemical calculations with high accuracy on very large cluster representation of the catalyst.