

Lectures in Chemical and Biological Engineering

First-Principles approaches to transition metal catalysis: Reaction mechanisms and new catalytic materials



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The detailed *reaction mechanism* and the nature of the *active site* in catalytic chemical transformations have been at the heart of understanding and improving heterogeneous catalysis. Unfortunately, and despite significant advances accomplished so far, determining the nature of the active site for a given reaction under realistic experimental conditions is non-trivial. Similarly, *in-situ* identification of key reactive intermediates is not always possible. In this talk, we will attempt to demonstrate how first-principles electronic structure theory can offer important insights on active sites and reaction mechanisms. These insights, combined with critical information from experiments and *microkinetic modeling*, offer new opportunities for an improved understanding of heterogeneous catalysis and can guide the quest for determining the nature of the active site. In addition, we will show how theory can assist with identifying and designing at the atomic-scale promising, sometimes metastable, catalytic sites with improved catalytic properties. It is then up to modern *inorganic synthesis* to meet the challenge of constructing the predicted catalytic sites.

Examples of catalytic reactions to be discussed include the low temperature Water-Gas-Shift (WGS) reaction and the Preferential Oxidation (PROX) of CO in the presence of H₂, both relevant to H₂ production and purification.



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Thursday November 5th at 4PM in Tech LR4
The Technological Institute
2145 Sheridan Road
Refreshments will be served at 8:45 AM