Fundamental Catalysis: From Reaction Mechanisms to New Catalytic Materials

Manos Mavrikakis[1]*
[1]*Department of Chemical & Biological Engineering, University of Wisconsin-Madison, Madison, Wisconsin 53718 (USA)*
*manos@engr.wisc.edu

Abstract

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 H_2, both relevant to H_2 production and purification. Furthermore, opportunities for improved bimetallic and ternary alloy electrocatalysts for the oxygen reduction reaction (ORR), which is critical for low temperature fuel cells, will be highlighted.