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First-Principles Elucidation and Design of Catalytic Sites and their Environments

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Heterogeneous catalysis is at the heart of over 90% of all chemical transformations of molecules into useful products. Catalytic processes are responsible for the production of the energy necessary to power our homes and cars, the purification of the air that we breathe; the fabrication of the materials we use each day, the manufacturing of the foods that we eat, and the synthesis of pharmaceutical intermediates. Knowledge of the atomic structure at and near the active sites of the catalyst and how it influences reactivity could revolutionize our ability to design more active and selective catalysts. Significant advances in both theory and simulation have occurred over the past decade thus making theoretical chemistry an invaluable partner to experiment in this endeavor. Theory and simulation can be used to begin to predict properties of different catalytic surfaces. The nature and strength of the adsorbate-surface bonds that form are important in dictating its surface chemistry. The influence of the local molecular environment within the vicinity of the active site, however, can be just as important. We can model the atomic structure along with the effects of the local molecular topography about the active site. More importantly, we can begin to probe ways to exploit them in the design of active metal particles.

In this talk, we describe the use of ab initio methods along with ab initio-based dynamic and kinetic methods to simulate the catalytic performance over supported metal particles. We show that it is now possible to track the nature of the active surface site along with the local “molecular” environment about the active surface ensemble. We specifically probe the influence of surface coverage, bimetallic alloys, and the molecular networks that form at a liquid/metal interface on catalytic activity. This talk will focus on the application of these tools to simulating the synthesis of oxygenates and the electrocatalytic oxidation of methanol and CO.