Overview of the Materials and Process Simulation Center
Methods for First Principles Design of Materials
Applications to Catalysis, Nanoelectronics, Fuel Cells, and Pharma

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Advances in theoretical and computational chemistry are making it practical to consider fully first principles (de novo) predictions of important systems and processes in the Chemical, Biological, and Materials Sciences. To apply first principles to such systems the approach at the MSC is to build hierarchies of models each based on the results of more fundamental methods but coarsened to make practical the consideration of much larger length and time scales. Connecting this hierarchy back to quantum mechanics enables the application of first principles to the coarse levels essential for practical simulations of complex systems.

We will highlight some recent advances in methodology and will illustrate them with recent applications to materials problems involving Catalysis, Nanoelectronics, Fuel Cells and pharma including Organometallic reactions (Wacker process, IBX, Tsuji Allylation)

- Mechanisms Heterogeneous catalysis: oxidation and ammoxidation on multimetal oxides
- Predictions of 3D structures of G Protein Coupled Receptors (GPCRs)
- Predictions of selective agonists and antagonists for GPCRs
- Conductance properties of Nanoelectronic switches and carbon nanotube interconnects
- De novo Force Fields (from QM) to describe reactions and phase transitions (ReaxFF)
- New membranes for high temperature (130°C) PEMFC
- Mechanism of dioxygen reduction reaction on Pt alloy and non Pt cathodes
- Simulations of Solid Oxide and Solid Acid membranes for Fuel Cells
- simulation of electron stimulated desorption and plasma etching the eFF electron force field
- The plaquette polaron theory of cuprate superconductors
- Predictions of thermoelectric power, electrical and thermal conductivity for nanowires