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

- Predictions of 3D structures of G Protein Coupled Receptors (GPCRs)
- Predictions of selective agonists and antagonists for GPCRs
- Advances in the ReaxFF reactive force; applications to energetic materials, catalysis, bucky tubes
- Shock detonation of energetic materials, with explanation of mechanism underlying sensitivity
- Mechanisms Heterogeneous catalysis: oxidation and ammoniation on multimetal oxides
- The eFF method for electron dynamics; simulation of electron etching semiconductors
- Improved Quantum Monte Carlo and multiscale methods
- New organometallic catalysts for low temperature CH4 to CH3OH
- Properties of dendrimer polymers and environmental applications
- New Organic Frameworks for H2 storage and membranes for high temperature (130C) PEMFC
- Mechanism of dioxgen reduction reaction on Pt alloy and non Pt cathodes
- The plaquette polaron theory of cuprate superconductors
- High ZT thermoelectrics