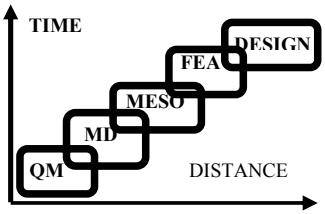
"De Novo Multiscale Simulations Of Materials"

William A. Goddard, III
Charles and Mary Ferkel Professor of
Chemistry, Materials Science, and Applied Physics
Director, Materials and Process Simulation Center (MSC)
California Institute of Technology (139-74)
Pasadena, CA 91125



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. Quantitative models based on theory and computation are starting to become the basis for design and operations in industry, but strategies for linking the time scales from electrons to macroscale are required for the most important applications.

We will highlight some recent advances in methodology with applications to nanotechnology, materials science, protein folding, drug design, and catalysis on topics such as:

- nanoelectronic switches, prediction of current/voltage and switching performance
- Plasticity and failure in crystalline and amorphous metal alloys
- Mesoscale Dynamics: Diffusion of water in complex polysaccharides and polymers
- De novo Force Fields (from QM) to describe reactions and phase transitions (ReaxFF)
- Mechanisms of Catalysts and Nafion membrane for PEM fuel cells
- First principles predicted 3D structures of G Protein Coupled Receptors (GPCRs)
- Predictions on drugs for GPCRs (receptors for dopamine, serotonin, histamine, lipids)