

MSC 2006 Research Conference

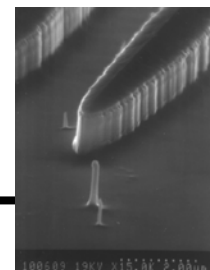
Materials and Process Simulation Center (MSC)

Caltech, Pasadena California



Thursday and Friday, April 6-7, 2006

Co-sponsored by Caltech Corporate Affiliates Program

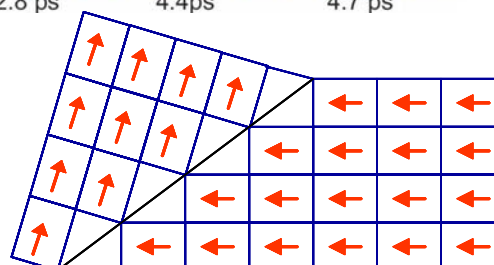
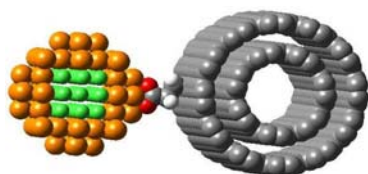
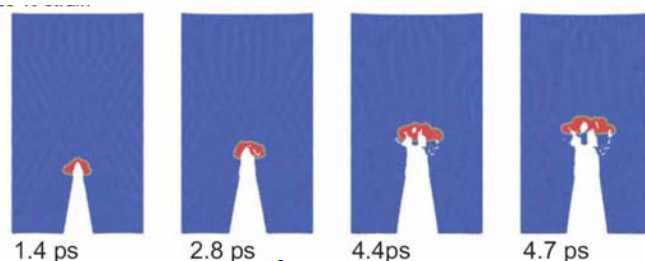
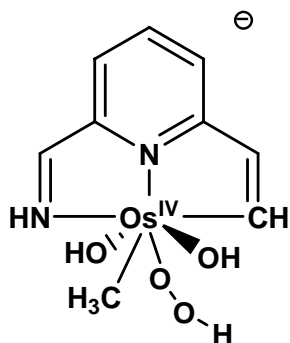
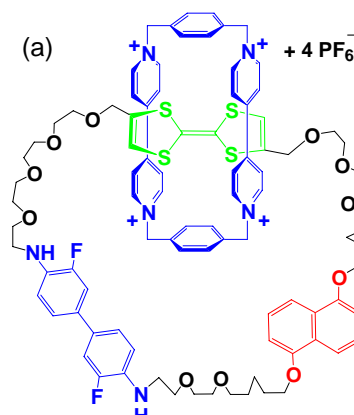
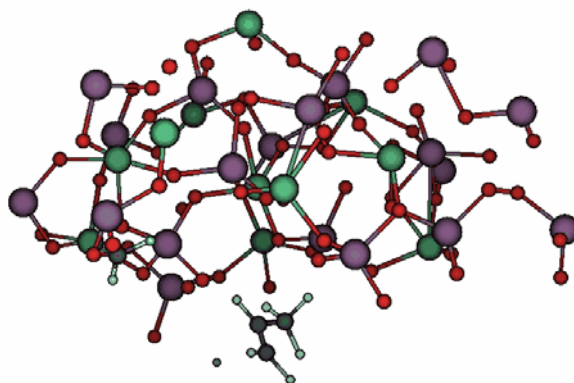
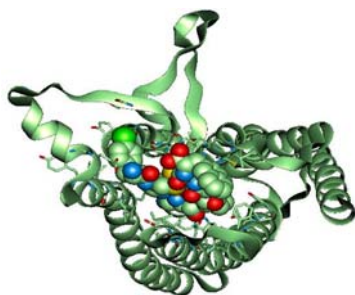
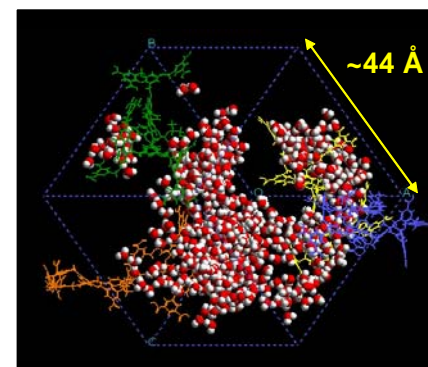


The MSC research conference is held annually to inform the industrial and government sponsors about the progress made at the MSC each year.

The mission of the MSC is to develop first-principles methods for describing the structures and properties of chemical, biological, and materials systems and to apply them to *de novo* design of industrial catalysts, drugs, nanoscale materials, and processes using a multiscale hierarchy based on quantum, atomistic, mesoscale, and continuum simulations.

Highlights of MSC2006 will include:

1. 3D structure and function of many GPCR's (include lipids, peptides)
2. Fuel Cells: H₂ Storage, water free membranes PEM and SOFC
3. Catalysts for methane activation, oxidation, fuel cells
4. Reactive Force Fields for metal oxide catalysts, combustion, proteolysis
5. Mesoscale simulations: lipids, polysaccharides
6. New Density Functionals and Quantum Monte Carlo methods
7. Nanotechnology: carbon nanotubes, DNA devices, nanoelectronics
8. Molecular Electronics: hole mobilities, contact resistance
9. Thermoelectrics, Ferroelectrics, Nonlinear optical Materials
10. Multiparadigm Computational Materials Design Facility (CMDF)



MSC 2006 Research Conference Tentative Schedule

Thursday April 6

Morning: Application to Biological Systems

1. Predict 3D Structures of GPCRs
2. Predict binding sites to GPCR's
3. New methods biological systems

Afternoon: Multiparadigm Simulation Materials

1. CMDF Coupling hierarchies of simulation paradigms
2. Reactive forcefields for organics and inorganics
3. New DFT Functionals
4. Quantum Monte Carlo
5. Entropy, Free Energy, Phase diagrams from MD
6. Atomistic based Mesoscale Force Fields

Friday, 7, 2006

Morning: Application to Fuel Cells and Catalysis

1. Membranes for fuel cells (PEM and SOFC)
2. Reaction mechanisms in Cathode Electrocatalysis
3. Mechanisms for organic oxidations at fuel cell anodes
4. H₂ generation and storage
5. Soluble catalysts for CH activation
6. Heterogeneous Multi-metal Oxidation Catalysts

Afternoon: Application to nanotechnology

1. Nanoelectronics, Molecular electronics
2. Organic and nanotube Nanotechnology
3. carbon-like diamond, tribology
4. DNA based Nanotechnology
5. Etching nm sizes with low energy electrons

Registration Fee: \$175, Meals-breaks Fee: \$80

<http://www.wag.caltech.edu/msc/2006/msc2006registration.html>

Program for MSC2005:

<http://www.wag.caltech.edu/anmeeting/2005/msc2005-program/>

Registration is free for MSC Participants and Associates, MSC Government Sponsors, PEER Associates, Caltech Corporate Associates. Caltech faculty and students

MSC Industrial Participants: **Sanofi-Aventis Pharma, Berlex Pharma Chevron, Dow Corning, Intel, Nissan Corp, Pfizer Pharma**

MSC Industrial Associates **Allozyme, Beckman Institute. Software Partners: Schrödinger**

Hardware Partners: **Dell**

MSC Federal Funding: **ONR, DARPA, DOE, NIH, NSF, ARO.**

PEER Associates: **Exxon, Shell, Chevron, Aramco, Total, ENI**

Caltech Corporate Associates members

3M Company, Aerospace Corp., Amgen Inc, AstraZeneca Pharma, Beckman Coulter, Berlex, Bristol-Myers Squibb,

California Technology Ventures, Cisco Systems, Dell, General Motors,

Hitachi America, IBM, Intel, Johnson & Johnson, Merck, Microsoft, Northrop Grumman, Novartis Pharma, Pfizer,

QUALCOMM, Raytheon, Sanofi-Aventis, SAFRAN, SeeBeyond Technology Corporation,

Sumitomo Chemical America, Sun Microsystems.

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