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 MSC2007 will include:
1. 3D structure and function of several GPCR’s (include lipids, peptides)
2. Fuel Cells: Alloy Cathode catalysts, H₂ Storage, high temperature PEM membranes
3. Catalysts for methane activation, oxidation
4. Reactive Force Fields for metal oxide catalysts, combustion, hydrolysis ATP
5. Mesoscale simulations: DNA
6. Electron FF for describing electron etching
7. Nanotechnology: carbon nanotubes, DNA devices, nanoelectronics
8. Molecular Electronics: contact resistance
10. Multiparadigm Computational Materials Design Facility (CMDF)
MSC 2007 Research Conference Tentative Schedule

Thursday April 5, 2007
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, April 6, 2007
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

Program for MSC2006:
http://www.wag.caltech.edu/anmeeting/2006/msc2006-program/

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

MSC Industrial Participants: Chevron, Dow Corning, Intel, Nissan
Corp, Pfizer Pharma, Boehringer-Ingelheim,
MSC Industrial Associates Allozyne, 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,
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Predicted Human DP receptor structure binds PGD2 selectively