



MSC 2008 Research Conference

Materials and Process Simulation Center (MSC)

Caltech, Pasadena California



Thursday and Friday, April 3-4, 2008

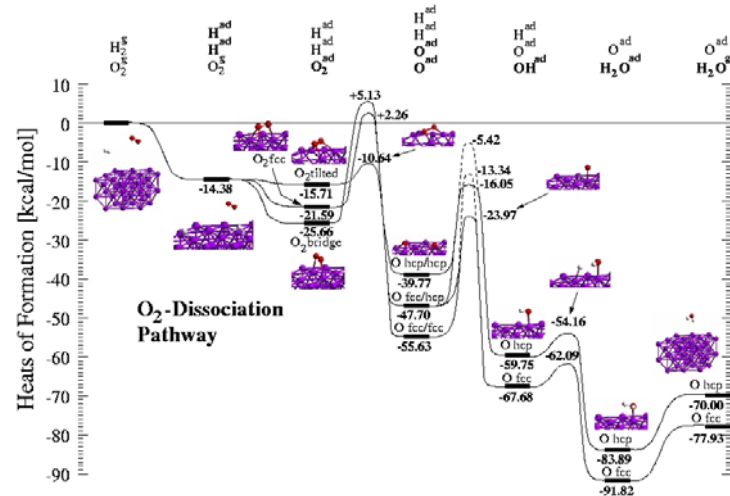
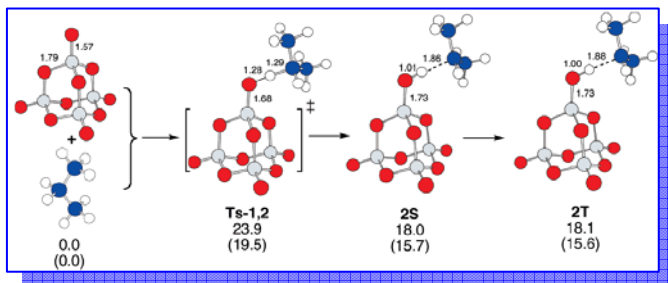
Co-sponsored by Caltech Corporate Affiliates Program

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

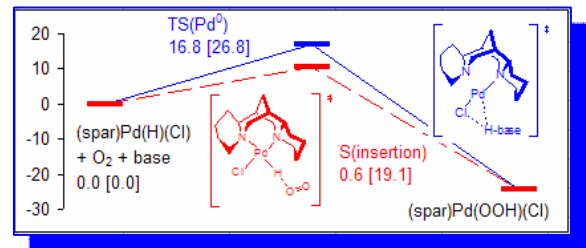
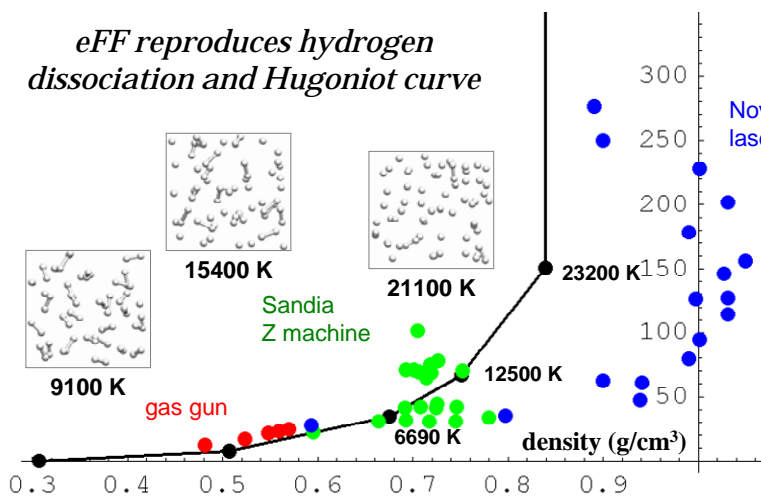
The mission of the MSC is to develop first-principles methods for describing the structures and properties of chemical, biological, and materials systems and to apply them to *de novo* design of industrial catalysts, drugs, nanoscale materials, and processes using a multiscale hierarchy based on quantum,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

Highlights of MSC2008 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
9. Thermoelectrics: figure merit nanowires.
10. Multiparadigm Computational Materials Design Facility (CMDF)



eFF reproduces hydrogen dissociation and Hugoniot curve



MSC 2008 Research Conference Tentative Schedule

Thursday April 3, 2008

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 Methods Quantum Mechanics
4. Electron Dynamics and warm dense matter
5. Entropy, Free Energy, Phase diagrams from MD
6. Atomistic based Mesoscale Force Fields

Friday, April 4, 2008

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 CH₄ to CH₃OH
6. Catalysts Oxidation and Ammoxidation

Afternoon: Application to nanotechnology

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

Registration Fee: \$185, Meals-breaks Fee: \$90

<http://www.wag.caltech.edu/msc/2008/registration.html>

Program for MSC2007: <http://www.wag.caltech.edu/msc/2007/>

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, Pfizer**

Pharma, Boehringer-Ingelheim, Allozyne

MSC Industrial Associates, **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,

Sun Microsystems.

Contact: Professor William A. Goddard, III, Director, Materials and Process Simulation Center (139-74),

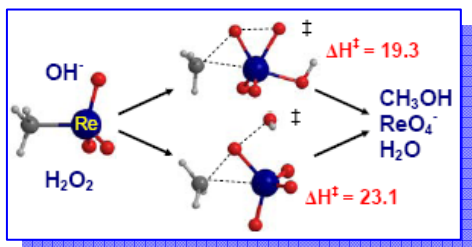
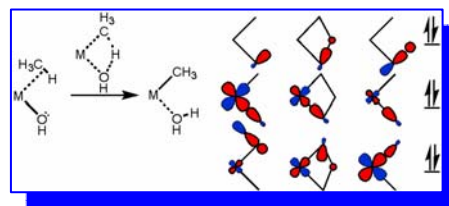
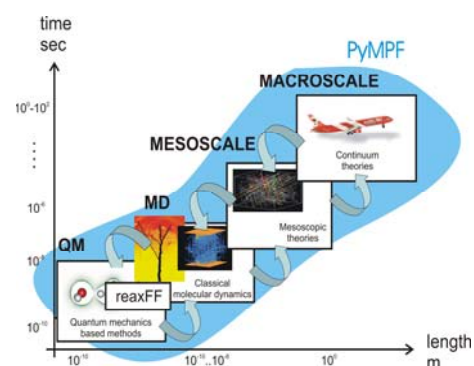
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Predicted Human DP
receptor structure binds
PGD2 selectively

