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. The 2010 program has not been planned but it will have a coverage similarly to 2009, listed here.

Thursday AM, March 26

Chairs Smith and Sergey

A. Biotechnology
A00 J Barton Welcome to Caltech
A01 W Goddard Overview of the MSC in 2009
A02 R Abrol Overview of progress in GPCR Structure Prediction and Rational Drug Design
A03 J Bray SuperBriHelix: Predictions of the 3D structures GPCRs
A04 C Tanrikulu DarwinDock-Rapid Complete Sampling and Selection of Optimal Ligand Structures
A05 A Griffith DarwinDock- Validation from dopamine receptors
A06 H Wiencko Predicted Adrenergic GPCR Structures
A07 Y Li Validation of GPCR Struccre and Ligand Predictions: Adenosine Receptors
A08 SK Kim Ligand inding site and Activation of Histamine and Serotonin receptors
A09 B Trzaskowski Predicted 3D Structure and Binding Sites for CCR5 Chemokine Receptor
A10 A Kirkpatrick Predicted Structure and Binding Site for CXCR4 Chemokine Receptor
A11 C Scott Determining the structure for the CB1 Cannabanoid Receptor
A12 H Levenson Muscarinic Acetylcholine Receptors: NMS/Xanolamine/M1
A13 Pascal, Sowers Progress in understanding DNA repair enzymes
A14 Pascal, Nemani Progress toward vaccines for neo-natal meningitis

Thursday PM, March 26

B. Frontiers QM

B01 Goddard XYG3: Rigorous inclusion London Forces into Density Functional Theory
B02 E Tkatchouk Validation of M06 DFT for catalysis and mechanically interlocked structures
B03 S.Bryantsev DFT for Predicting Binding Energies of Neutral, Protonated, Deprotonated H2O Clusters
B04 Y Liu Can DFT describe the weak interaction? Empirical dispersion correction for DFT"
B05 Pascal New generation force field based on accurate QM
B06 Anderson Advances in Quantum Monte Carlo for High Accuracy ab initio Calculations
B07 Fisher Quantum Monte Carlo studies
B08 Goddard the eFF method for electron dynamics of highly excited electronic systems
B09 H Kim Application of eFF to Lithium at high pressure
B10 Q An Application of eFF to warm dense matter

C. Multiscale Technology

C1 Jaramillo-Botero Multiparadigm, Multiscale Methodologies, application to network polymers
C2 G McGuinness Hydrogels for Vascular Tissue Engineering
C3 Goddard ReaxFFreactive force field developments and applications to mixed metal oxide catalysts
C4 Tahir-Kheli Chiral Plaquette Polarones Theory of Cuprate Superconductors
C5 MJ Cheng Density Functional Study of the Spin Coupling in VPO
C6 MJ Cheng (FeAs)(LaO) superconductors
C7 Pascal Interfacial Free Energies from MD

Thursday Night March 26 Banquet at Goddards

D Rachid Yazami Lithium Batteries, the next generation
Friday AM  
Session Chairs: Andres and Mario

E. Catalysis
E0  E Abbott Introduction to Caltech Corporate Associates
E1  Nielsen Progress in organometallic catalysts for functionalization of CH4
E2  Ahlquist Strategies for oxidation and functionalization in CH activation catalysts
E3  Ess Charge-transfer Polarization in CH Bond Activation and Functionalization Reactions
E4  Tkatchouk Methane Activation with Ru Complexes: countercation and pH dependance
E5  Theofanis CH Activation by Intramolecular Coordinated Bases
E6  Benitez Selectivity on Ruthenium Catalyzed Olefin Metathesis
E7  WG Liu new Au catalyst for converting methane to methanol
E8  MJ Cheng Mechanism Study of the Oxidation of the Alkyl Ligand in Rhenium(V) Oxo compounds
E9  Mueller Hydrocarbon Adsorption and Dissociation on Nickel (talk)
E10 Ahlquist ReaxFF Description of CH3OH Fuel Cell Anode Catalysis
E11 Blanco Chemical Catalysis Networks in Gas/Surface Reactions
E12 Q Wang Biomass conversion
E13 T Baker ab initio MD to understand oxidation of the Au(111) surface

F. Environmental
F1  Diallo Cellular Uptake and Toxicity of Dendrimers not 12:30 to 2:30
F2  Shah Perchlorate Recovery by Dendrimer Enhanced Crossflow Filtration
F3  Y Liu (Giri) Drug delivery using pH induced dense-core to dense-shell transition in PAMAM dendrimer
F4  Fang-Wang Highly Sensitive Micro-Biosensors for in-situ Monitoring of Mercury (II) Contaminants
F5  Bryantsev complexation and hydrolysis of copper(II) in aqueous solution
F6  Tang The Power, Energy, Environmental Research (PEER) Institute
F7  S. Wu Sensors for bio-process and carbon sequestration monitoring

Friday PM  
Session Chairs: Soo-Kyung and Ravi

G. Fuel cells and Batteries
G1  B Merinov Progress in Fuel Cell Research in the MSC
G2  Y Sha Non-Pt Metal Catalysts for Oxygen Reduction Reaction
G3  T Yu segregation in Pt, Pd, and Rh based alloys as cathode catalysts for fuel cells.
G4  M Blanco New Perspective in Battery Technology
G5  T Yu Structures and F migration in CFx for cathode in batteries.
G6  Mendoza-Cortés Hydrogen and Methane Storage in Omar Yaghi Framework Structures

H Nanotechnology
H1  SP Han DNA Origami Nanoscaffold Directed Self-Assembly of Carbon Nanotube Devices
H2  D Benitez Molecular Based Memory Devices
H3  H Kim Negative Differential Resistance of OPE SAM On Au (111) Surface

I Energetic Materials
I1  S Zybin Overview of energetic materials research at MSC
I2  P Xu Computational protocol to predict sensitivity; validation for PETN
I3  WG Liu Explanation of the colossal detonation sensitivity of Si-PETN
I4  Q An Shear Sensitivity simulation of RDX Energetic Materials
I5  S. Dasgupta Hypergolic Propellants

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

MSC Industrial Participants: Chevron, GPC-Rx, Dow Corning, Intel, Toshiba, Pfizer, Boehringer-Ingelheim
MSC Federal Funding: ARO, DARPA, DOE, NIH, NSF, ONR.

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

Caltech Corporate Associates: 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.

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