

MSC 2006 Program

All talks in BI Auditorium unless indicated otherwise

Thursday April 6, 2006

Talk #	Time	Duration	Speaker	Title
Registration	08:00	50	Shirley Wu	BI Patio or NE porch, Coffee
Session A: Biotechnology				
Chairs: Mamadou Diallo				
A0	8:50	10	To be announced	Intro to Caltech
A1	09:00	30	William Goddard	The MSC and Overview of biological applications
A2	09:30	18	Jiyoung Heo	Prediction of the 3D structure for FMRF-amide Peptides Bound to Mouse MrgC11 Receptor with subsequent Experimental Verification
A3	09:48	18	Ravi Abrol	Full Lipid-Solvent Simulations of the Prediction for the BX471/hCCR1 complex and Experimental Verification
A4	10:06	18	Youyong Li	The prediction of human DP receptor structure and bound with endogenous agonist
A5	10:24	18	Jenelle Bray	Structure Prediction and Ligand Binding in Serotonin 2b & 2c Receptors
A6	10:42	18	Leonard Ong	Prediction of Structures and Binding sites for V1BR vasopressin receptor
Break	11:00	20		BI Patio
A7	11:20	18	Changmoon Park	Prediction of Structures and Binding sites for V2R and V1AR vasopressin receptors
A8	11:38	3	Elena Fabrikant	Prediction of the Structure and Binding Properties of a Human Histamine Receptor
A9	11:41	3	Daniel Koslover	The P2Y1 Purinergic Receptor and its Ligand Binding Site
A10	11:44	3	Heather Wiencko	New Structure and Function Predictions for the Beta1 Adrenergic Receptor
A11	11:47	3	Adam Griffith	Structure of D1 dopamine receptor and binding of ligands
A12	11:50	3	Mazyar Kalani	Prediction of Structures and Binding sites for somatostatin receptors
A13	11:53	3	Shebli Mehrazarin	Prediction of Structures and Binding sites for GPR30 Estrogen receptors
A14	11:56	18	Victor Wai Tak Kam	Better binding energies using neutral amino acids and SCREAMED side chain
A15	12:14	18	John A. Wendel	Comparison of old and new docking methods.
A16	12:32	3	Frank Ducheneaux	Benchmarking the APBS and Delphi PBE Solvers for Electrostatic Solvation Energies and the APBS Role within the CMDF Framework
A17	12:35	3	Peter Clark	Cracking the Sulfation Code: Understanding the Interaction Between Glycosaminoglycans and Growth Factors
A18	12:38	3	Ismet Caglar Tanrikulu	In Vivo and In Silico Screening of an E. coli Methionyl-tRNA Synthetase Library for the Incorporation of Azidonorleucine into Proteins
A19	12:41	3	Bjørn H. Lindqvist (Norway)	Virus based self-assembly of protein arrays
Lunch	12:44	76	Poster Preview	BI Patio
Session B: Multi-paradigm Modeling and simulation				
Chairs: Jonas Ongaard, Mario Blanco				
B0	14:00	15	Andres Jaramillo-Botero	Multiscale Modeling and Simulation: The Computational Materials Design Facility (CMDF)
B1	14:15	30	Adri van Duin	Overview of current and developing directions for ReaxFF reactive force fields; applications to catalysis, fuel cells, solar cells, polymers and proteins
B2	14:45	3	Jef Dodson	The Computational Materials Design Facility (CMDF): A Powerful Framework for Multiparadigm Multiscale Simulations
B3	14:48	3	Bill Goddard	Multi-Paradigm Modeling Of Dynamical Crack Propagation in Silicon using the ReaxFF Reactive Force Field
B4	14:51	18	Sergey Zybin	ReaxFF MD of energetic materials: combustion and shock detonation
B5	15:09	3	Sergey Zybin	Atomistic simulation of Richtmyer-Meshkov instability in solids using the IBM Blue Gene Computer
B6	15:12	3	Peng Xu	Integration of simulation ability for metals and alloys into CMDF via ITAP code
B7	15:15	18	Qing Zhang	The Structure and Sliding Friction of Diamond-like Carbon Surfaces from Molecular Dynamics Simulations
B8	15:33	18	Qingsong Zhang	New insights for structural properties of ferroelectrics, predictions of domain wall structures and migration
B9	15:51	3	Qingsong Zhang	Multiscale predictions of domain wall migration in ferroelectrics
B10	15:54	3	Hyungjun Kim	Implicit solvation strategies for coarse grain models of carbohydrates
B11	15:57	18	Tod Pascal	DNA Power: Love Thy Neighbor
Break	16:15	20		BI Patio
B12	16:35	3	Zhitao Xu	Barriers for ATP-ADP hydrolysis from QM and ReaxFF
B13	16:38	3	Youyong Li	General Scaling Rules for Polymers based on the Continuous Self Avoiding Walk
B14	16:41	18	Andreas Bick (Scienomics)	New amorphous builder and applications
B15	16:59	3	Peter Kekenes-Huskey	Free energy from Weighted Histogram Analysis Method (WHAM): Talk MD study of ion flow through silica pores
B16	17:02	3	Prinsa Verma (INDIA)	Nanophosphor Applications
B17	17:05	3	Darryl Willick	Computational Facilities at the MSC
B18	17:08	30	Jamil Tahir-Kheli	Chiral Polaron Theory of Cuprate Superconductors
	17:38	60	Poster Viewing	
Banquet	18:30	90		Avery
Speaker	20:00		Roy A. Periana	Breakthroughs in Activating CH4 and Prospects for the 21st Century

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Friday April 7, 2006

Talk #	Time	Duration	Speaker	Title
Registration	08:00	50	Shirley Wu	BI Patio or NE porch, Coffee
Session C: Catalysis and Fuel Cells				
Chairs: Weiqiao Deng				
	8:50	10		Introduction
C1	09:00	30	Boris Merinov	Overview of Fuel Cell Projects in the MSC (PEMFC, SAFC, SOFC)
C2	09:30	18	Seung Soon Jang	New Molecular Architecture of Water-Soluble Dendrimer-grafted Polymer for PEMFC
C3	09:48	3	Sang Soo Han	Li-Pillared Graphite and Metal Organic Framework as Hydrogen Storage Media
C4	09:51	30	Jonas Oxgaard	Overview of Methane Activation and other Catalysis Research at the MSC
C5	10:21	18	Jason M. Gonzales	Quantum mechanical rapid prototyping of rhenium catalyst for methane activation
C6	10:39	18	John Keith	The Mechanism of the Tsuji-Allylation Reaction
Break	10:57	20		BI Patio
C7	11:17	3	Jason Keith	O ₂ insertion into Palladium Hydride Organometallics
C8	11:20	3	Julius Su	Choosing between reactivity modes of IBX, a hypervalent iodine oxidant
C9	11:23	3	Robert J. Nielsen	Designing Ligands for the Palladium-Catalyzed Oxidative Kinetic Resolution of Chiral Alcohols
C10	11:26	3	John Keith	Inaccessibility of BHE in the Wacker Reaction
C11	11:29	18	William Goddard	Overview of Mechanisms for Selective Oxidation and Ammoxidation
C12	11:47	18	Kimberly Chenoweth	Selective oxidation on mixed- metal oxides using ReaxFF
C13	12:05	3	Sanja Pudar	A DFT Study of Mechanism of Selective Oxidation of Propene on Bismuth Molybdate Catalyst
C14	12:08	3	Mu-Jeng Cheng	QM calculations toward understanding catalysis on Vanadium oxide sites
C15	12:11	3	Chinghang Tong	Secondary Organic Aerosol Formation by Heterogeneous Reactions of Aldehydes and Ketones: A Quantum Mechanical Study
C16	12:14	18	Yongchun Tang (PEER)	Ionic Liquids for Gas to Liquid Conversion
C17	12:32	18	Yongchun Tang (PEER)	Biodesel and Biomass conversion
Lunch	12:50	60	Poster Preview	BI Patio
Session D: Nanotechnology and Quantum Development				
Chairs: Adri van Duin, Boris Merinov				
D1	13:50	30	Wei-Qiao Deng	Design of active nanostructured materials
D2	14:20	3	Wei-Qiao Deng	Rational design of nanostructure for TE materials
D3	14:23	18	Yuki Matsuda	Contact Resistance Properties of Metal-Nanotube Interfaces
D4	14:41	3	Yuki Matsuda	Structural and Electronic Properties of Hydrogen Terminated Silicon Nanowires (QM and Tight-binding studies)
D5	14:44	3	Si-Ping Han	Raman spectra of carbon nanotubes: single and double wall
D6	14:47	3	Gain In Lee (KAIST)	Fullerenes-based multifunctional I-V characteristics using the green functional approach
D7	14:50	18	Santiago Solares	Theoretical Investigation of the Energetics, Structure and Coverage of Alkylated and Methoxylated Silicon (111) Surfaces
D8	15:08	3	Hatem Helal	Low Energy Electron Enhanced Etching: Simulating Processes Involving Highly Excited and Unstable Systems
Break	15:11	20		BI Patio
D9	15:31	18	Mamadou Diallo	Dendrimer Nanotechnology Research at the MSC: Overview of Recent Advances
D10	15:49	3	John Howard (Caltech UG)	Aqua Nanotechnologies: Cleaning the World's Water
D11	15:52	18	Mario Blanco	Quantum Mechanical Solutions to Systems Powering in Space
D12	16:10	18	Abhijit Shevade	Quantum Mechanical Solutions to Environmental Monitoring in Space
D13	16:28	18	Dan Fisher	Investigating pairwise electronic interactions with quantum Monte Carlo
D14	16:46	3	Amos Anderson	Quantum Monte Carlo on Graphics Processing Units
D15	16:49	18	Julius Su	Toward Quantum Monte Carlo Derived Pair Functionals
D16	17:07	3	Min Seong Kim (KAIST)	Grid-based multiscale DFT
	17:10		William Goddard	Wrap-up