MSC 2003

All talks presented in Beckman Institute Auditorium (134 BI) – Posters in Beckman Institute Courtyard

Thursday, March 20, 2003

Time		Speaker	Title
8:00 AM		**Registration**	**BI Courtyard**
8:45		Gray, Harry	Advances at the BI-LRC over the last decade recent activities
8:55	B1	Goddard, William	Overview of MSC and recent activities
Computational Biology Session: Rick Muller, Chair			
9:25	B2	Vaidehi, Nagarajan	Overview of Progress in Computational Biochemistry
9:55	B3	Freddolino, Peter	Structure and Function of Adrenergic Receptors
10:05	B4	Kalani, Yashar	Structure and Function of Dopamine, Histamine, and Traceamine GPCRs
10:30	B5	Hall, Spencer	Structure and Function of Olfactory Receptors
10:50		**Break**	**BI Courtyard**
11:10	B6	Trabanino, Rene	Structure and Function of Opsins
11:25	B7	Heo, Jiyoung	Predicted binding site in MrgC11 pain receptor and experimental validation
		Choi, Eun Jung	Structure and Function of S1P4 and LPA2 GPCRs
11:40	B8	Shen, Huazhang	Structure and Function of Serotonin Receptors
11:43	B9	Floriano, Wely	Overview of Function Prediction Projects (Cassandra)
12:13	B10	Huskey, Pete	Design of amino acyl -tRNA synthetases for non-natural amino acids
12:38	B11	Tanrikulu, Caglar	Design of Isoleucyl-tRNA Synthetase (IleRS) Mutants for the Incorporation of Hexafluorovaline into Proteins *In Vivo*
12:41	B12	Wendel, John	Predicting Geometries of Protein-Ligand Complexes with MPSim-Dock
12:44	B13	Kam, Victor	Accurate Placement of Amino-acid Sidechains: The Program SCREAM
12:47	B14	Datta, Deepshikha	ReaxFF reactive force fields for proteins: Applications to enzymes
12:50	B15	Heo, Jiyoung	Molecular dynamics simulation of DNA containing 5-formyl-uridine
12:53	B16	Zhang, David	Simulate the Electrostatic Interactions in the Ribosome and RNA-Virus Using APBS
12:56		**Lunch+Posters**	**BI Courtyard**
Catalysis + Fuel Cell Session: Vaidehi, Chair			
13:55	FC1	Merinov, Boris	Overview of Fuel Cell Projects
14:15	FC2	Jacob, Timo	DFT Studies on the Catalytic Cathode Reactions in PEM-Fuel Cells
14:35	FC3	Jang, YunHee	Water dissociation on Ru(001)
14:38	FC4	Molinero, Valeria	Nanostructure and water transport in Nafion membranes
14:58	FC5	Blanco, Mario	Quantum Hopping Molecular Dynamics (*QHMD*)
15:18	FC6	Dorso, Claudio	Towards a Microscopic description of proton conduction in perovskites
15:21	C1	Muller, Rick	Toward Computational Materials Design
15:41	C2	Oxgaard, Jonas	Oxidative Hydrogen Migration: Ir-Catalyzed Arylation of Olefins through a Novel Mechanism
16:01		**Break**	**BI Courtyard**
16:21	C3	Nielsen, Smith	Enantioselective Oxidation of Secondary Alcohols by Pd(II) Complexes
16:36	C4	Su, Julius	Tandem Wolff-Cope Rearrangement: Substrate Scope and Reactivity Control
16:51	C5	Keith, John	Studies of the Wacker Process
16:54	C7	Deng, Weiqiao	Mechanism of Metallic Catalyzed Growth of Single-Wall Carbon Nanotubes
16:57	C8	van Duin, Adri	Application of the ReaxFF reactive force fields to catalysis
17:27		Dismiss	
6:00 PM		**Dinner**	**Avery Dining Hall**
7:30 PM		Derek Debe, CEO Eidogen	The Post-Proteomics Era: View from Eidogen (Caltech Spin-off)

Friday, March 21, 2003

Time		Speaker	Title
7:00 AM		**MSC Board of Directors**	**Athenaeum (Invitation Only)**
8:00 AM		**Registration**	**BI courtyard**
8:45		Kevin Doody (CorpRel)	Corporate Relations at Caltech
Materials and Nanotechnology Session: Mario Blanco, Chair			
8:55	M1	Meulbroek, Peter	The Computational Materials Design Facility (CMDF).
9:15	M2	Su, Haibin	Studies on Ferroelectric Polymers via Multiscale Approches
9:25	M3	Zhang, Luzheng	Energetic Materials Simulation for Computational Materials Design Facilities
9:35	M4	Lee, Hyon Jee	AlTiNI Bulk metallic glasses
9:55	M5	Xu, Peng	Viscosities of liquid metals and alloys and dependence on pressure
10:15	M6	Zhang, Qing	Wear in Al/Al2O3 systems
10:35	M7	Zhang, Qingsong	Polarizable ReaxFF for BaTiO3/PbTiO3 ferroelectrics
10:45	M8	Miyata, Masayasu	Structure at semiconductor-oxide Interface
10:48	M9	Hiefets, Eugene	Structures at perovskite surfaces
10:51		**Break**	**BI Courtyard**
11:11	M10	Tahir-Kheli, Jamil	NMR, Neutron Scaling, and Resistivity from Dynamic Polarons in Cuprate Superconductors
11:31	N1	Cagin, Tahir	Nanomechanics: elasticity and beyond
11:51	N2	Deng, Weiqiao	Computational simulation at molecular electronics and molecular devices
12:11	N3	JangYH, JangSS	QM and FF simulations for SAMs of Stoddart-Heath devices
12:36	N5	Kim, Yong-Hoon	Electron transport through SAMs of Stoddart-Heath devices
12:56		**Lunch+Posters**	**BI Courtyard**
13:55	N6	Chen, Quanhua	Field emission from carbon nanotubes
14:15	N7	Han, Si-Ping	Simulation of Hongjai Dai nanogloves for bucky tubes and improvements
14:25	N8	Solares, Santiago	Design of Nanotech devices
14:28	N10	Pascal, Tod	Building crossover structures of DNA systems
14:48	N9	Maiti, Prabal	DNA based nanotechnology
14:51	N11	Diallo, Mamadou	Dendritic Nanocale Chelating Agents
Polymers and Theory Session: Tahir Cagin, Chair			
14:54	P1	Jang, SS	Effect of Cyclic Chain Architecture on Dilute Solutions Properties…
15:09	P2	Li, Youyong	CCBTX MC, Structure of Percec polymer
15:29	P3	Taiko, Hiroshi	Forming Dendrimer Templates using Grubbs Metathesis
15:32	P4	Lin/JangSS	Zimmerman Dendrimer
15:35	P5	Maiti, Prabal	Structure and dynamics of PAMAM dendrimers
15:38	P13	Su, Julius	Acidity amplification via Rapidly Interchanging Proximate Functionality
15:41	P6	Li, Youyong	Structure and Properties of N6/AMCC Nylon
15:44		**Break**	**BI Courtyard**
16:04	P7	Diallo, Mamadou	Structure/Properties of Humic Acid
16:24	P8	Lin, Shiang-Tai	Atomistic Predictions Solvation and Vapor Pressure
16:44	P9	Niemer, Rachel	First Principle Predictions of VLE Phase Diagrams
16:47	P10	Tong, Chinghang	Predicting Thermodynamic Properties for Atmospherically Relevant Compounds
16:50	P11	Sisk/Lin/ Shevadi/Blanco	Predicting Properties for Electronic Noses
16:53	Pet5	Meulbroek, Peter	The HCToolkit for Performing Continuum Phase Equilibria Calculations
16:56	Pet1	Tang, Yongchun	Molecular Modeling and experiments on Hydrocarbon Chemistry at PEER
17:16	Pet2	Ma, Qisheng	Mechanism of Alkylation of phenol by Sulfonic Resin
17:26	Pet3	Ma/Cheung	Ionic Liquids: DFT and ReaxFF Studies
17:36	Pet4	Shular, Pat	Surfactants for low Interfacial Surface Tension: Experiments and calculation
		Zhao, Yang	Electronic and Mechanic Properties of Carbon Nanotubes
		Mhin, Byung Jin	DFT Calculation on the Electron Affinity of Polychlorinated Dibenzo-p-dioxins
17:39	T1	Accelrys	New methods from Accelrys
17:59	T2	Feldmann/FisherDan	Advances in Quantum Monte Carlo
18:02	T3	Goddard, William	Closure
18:12			**The end, informal dinner for guests**