

MSC2004 Program
 All talks in BI Auditorium unless indicated otherwise
Thursday April 1, 2004

			Duration	Time	Speaker	Title
Registration, coffee				08:00	Wu, Shirley	BI Patio
Session A					<i>Chair: Jonas Oxgaard</i>	<i>Facilitator: Frank Ducheaneaux</i>
A1	Gen	Talk	10	08:40	Wold, Barbara	Overview of BI
A2	Gen	Talk	20	08:50	Goddard, Bill	overview of progress at MSC
A3	Bio	Talk	25	09:10	Vaidehi	overview of progress in computational biochemistry
A4	Bio	Talk	15	09:35	Kalani, Yashar	Structure and Function of Dopamine receptors including blind test
A5	Bio	Talk	15	09:50	Freddolino, Peter	Predictions for histaminergic and beta-adrenergic receptors
A6	Bio	Talk	15	10:05	Trabanino, Rene	Distinguishing colors with Human Opsins
A7	Bio	Talk	20	10:20	Floriano, Wely	Structure and Function predictions for taste receptors
Break			20	10:40		
Session B					<i>Chair: Vaidehi</i>	<i>Facilitator: Dan Fisher</i>
B1	Bio	Talk	10	11:00	Spencer Hall	Structure and Function predictions for Olfactory receptors (OR)
B2	Bio	Talk	12	11:10	Heo, Jiyoung	Structure and Function predictions for pain receptors including blind tests
B3	Bio	Talk	12	11:22	Kalani, Yashar	Predictions for lipid G2A receptors including blind tests
B4	Bio	Talk	10	11:34	Shen, Huazhang	Structure and Function predictions for 5HT2A serotonin receptor
B5	Bio	Talk	10	11:44	Hummel, Patrick	Predicting the difference between human and mouse 912-93 OR
B6	Bio	Talk	10	11:54	Tanrikulu, Caglar	Design of phenylalanyl tRNA synthetases
B7	Bio	Talk	12	12:04	Pete Huskey	New MC Methods and Analog design for Phenylalanyl tRNA synthetase
B8	Bio	Poster	3	12:16	Kalani, Maziyar	Calculations of GPCR's
B9	Bio	Poster	3	12:19	Nierner, Rachel	Structure and Function of LPA receptors
B10	Bio	Poster	3	12:22	Peng, Joyce	Structure and Function of 2 muscarinic acetylcholine receptors
B11	Bio	Poster	3	12:25	Yoyong, Ducheaneaux	Structure and function of adenosine receptors
B12	Bio	Poster	3	12:28	Kam, Victor	Development of accurate side chain optimization techniques
B13	Bio	Poster	3	12:31	Wendel, John	Accurate free energy of binding calculations for trypsin inhibitors
B14	Bio	Poster	3	12:34	Floriano, Wely	MSC biodefense applications
B15	Bio	Poster	3	12:37	Oelschlaeger, Peter	Catalytic Mechanism and Specificities of Metallo-beta-lactamases from MD
Lunch, Posters			60	12:40		BI Patio
Session C					<i>Chair: Peter Meulbroek</i>	<i>Facilitator: Amos Anderson</i>
C1	Cat	Talk	20	01:40	Oxgaard, Jonas	Mechanistic Analysis of Hydroarylation Catalysts
C2	Cat	Poster	0	02:00	Oxgaard, Jonas	The Oxidative Hydrogen Migration mechanism in CH activation
C3	Cat	Talk	10	02:00	Su, Julius	Rational Design of Substrates for the Tandem Wolff/Cope Reaction
C4	Cat	Talk	10	02:10	Nielsen, Robert	Enantioselective Oxidation of Alcohols by PdII-Sparteine Complexes
C5	Cat	Talk	10	02:20	Keith, Jason	Pd-mediated activation of molecular oxygen
C6	Cat	Talk	10	02:30	Keith, John	Mechanism of the Wacker reaction in aqueous solution
C7	Cat	Talk	10	02:40	Jacob, Timo	Hydrocarbon rearrangements on Pt surface
C8	QM	Talk	15	02:50	Su, Julius	Accurate Energies, Structures for Large Water Clusters Using X3LYP QM
C9	Cat	Poster	3	03:05	Nielsen, Robert	gold(III) catalyzed methane to methanol conversion
C10	Cat	Poster	3	03:08	Mhin, Bynn Jin	The Interstitial Electron Model: Tests for Ni clusters
C11	Cat	Poster	3	03:11	DiStasio, Robert	CH activation by Re homogeneous catalysts
C12	QM	Poster	3	03:14	Fisher, Dan	Quantum Monte Carlo methods
C13	FC	Talk	20	03:17	Jacob, Timo	The reaction mechanism at a fuel cell cathode
Break, Posters			18	03:37		BI Patio
Session D					<i>Chair: Tahir Cagin</i>	<i>Facilitator: Rob DiStasio</i>
D1	FC	Talk	20	03:55	Blanco, Mario	Water free proton exchange materials for fuel cells
D2	FC	Talk	10	04:15	Jang, Yun Hee	QM studies of Pt-Ru-RuOxOH _y system
D3	FC	Talk	15	04:25	Merinov, Boris	Solid Oxide Fuel Cells: Zr _{1-x} Y _x O ₂
D4	FC	Talk	15	04:40	Jang, Seung Soon	New molecular architecture for PEMFC: Dendrimer-PTFE copolymer
D5	FC	Talk	15	04:55	Molinero, Vale	Water Dynamics in Nafion
D6	FC	Talk	15	05:10	Deng, Weiqiao	Practical Reversible Hydrogen Storage for Transportation
D7	FC	Talk	10	05:25	Cheung, Sam	Simulations of H ₂ storage in Mg
D8	EE	Talk	15	05:35	Tahir-Kheli, Jamil	Origin of Dielectric breakdown in semiconductor oxides
D9	EE	Talk	10	05:50	Deng, Weiqiao	Hole Mobilities in Oligoacene Organic Semiconductors from QM
End Session D				06:00		
Dinner				06:30		Athenaeum
Speaker			60	08:00	Prof. Sossina Haile	Fuel Cells: Novel Promising Technologies for Practical systems

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Friday April 2, 2004

			Duration	Time	Speaker	Title
Breakfast				07:00	Executive Committee	Athenaeum (by invitation)
Registration, coffee				08:00	Wu, Shirley	BI Patio
Session E					Chair: Boris Merinov	Facilitator: Yuki Matsuda
E1	Gen	Talk	10	08:50	Gorchow-Stuart, Sheryl	Corporate Relations
E2	FF	Talk	30	09:00	van Duin, Adri	Reactive force fields applied to catalysis and materials
E3	FF	Talk	10	09:30	Datta, Dee	ReaxFF Molecular dynamics of Serine protease
E4	FF	Poster	3	09:40	Persson, Petter	reactive force fields for TiOx and VOx systems.
E5	FF	Poster	3	09:43	Chenoweth, Kim	reactive force fields for BiOx and MoOx systems.
E6	FF	Poster	3	09:46	Han, Si-Ping	Extraction of reaction mechanisms from Reaction Chemistry
E7	FF	Poster	3	09:49	Dodson	bucky Balls and tubes having fun
E8	FF	Poster	3	09:52	Su, Julius	Automated sampling of key solvation configurations
E9	FF	Talk	15	09:55	Zhang, Qingsong	Application of Polarizable Charge Equilibration Force Field to Ferroelectrics
E10	FF	Poster	3	10:10	McClendon, Chris	Charge Consistent Force fields for proteins
E11	Met	Talk	10	10:13	Xu, Peng	Adam-Gibbs and energy landscape thermodynamics of Liquid Metals
E12	Met	Talk	10	10:23	Zhang, Qing	Friction at Al/Al and Al2O3/Al2O3 surface.
E13	Met	Talk	10	10:33	Cagin, Tahir	Maximum superheating and undercooling in metals and ceramics
E14	Met	Poster	3	10:43	Zhang, Guoyun	Force Fields for metal alloys
E15	Met	Poster	3	10:46	Zhang, Qing	Force field and MD simulation of reentry melting in NiTiZr system
Break, Posters			20	10:49		
Session F					Chair: Adri van Duin	Facilitator: Guoyun Zhang
F1	Nan	Talk	15	11:09	Jang, Yun Hee	Electronic structure and tunneling of Rotaxane SAMs on Au.
F2	Nan	Talk	15	11:24	Jang, Seung Soon	Self-Assembled Monolayer of the Rotaxanes from FF
F3	Nan	Talk	10	11:39	Solares, Santiago	Atomistic simulations of atomic force microscope images
F4	Nan	Poster	3	11:49	Jacob, Timo	Designing a better alligator clip for molecular electronics
F5	Nan	Poster	3	11:52	Han, Si-Ping	Molecule Assemblies on nanotubes
F6	Nan	Poster	3	11:55	Matsuda, Yuki	Mesoscale modeling of nanodevices
F7	Nan	Talk	10	11:58	Pascal, Tod	Effect of Mg(+2) ions on the stability of JX DNA crossover motifs
F8	Nan	Talk	10	12:08	Pascal, Tod	the Seeman DNA Paranemic Crossover in Salt Solution
F9	Mes	Talk	15	12:18	Moliner, Vale	The M3B coarse model for the MD of malto oligosaccharides
F10	Mes	Talk	10	12:32	Moliner, Vale	non-exponential relaxation in supercooled glucose solutions
F11	Mes	Talk	10	12:42	Spjiker, Peter	Mesoscale FF for lipid bilayers
Lunch, Posters			60	12:52		
Session G					Chair: Mamadou Diallo	Facilitator: Candi Tong
G1	Tc	Talk	15	01:52	Tahir-Kheli, Jamil	New insights on high Tc superconductors
G2	Pol	Talk	15	02:07	Cagin, Tahir	The Effect of solvent and pH on the structure of PAMAM dendrimers
G3	Pol	Talk	15	02:22	Lin, Shiang-Tai	Free energies and entropies of Water in PAMAM Dendrimers
G4	Pol	Talk	10	02:37	Li, Youyong	Thermodynamics and structures of Percec Dendrimer liquid crystals
G5	Pol	Talk	10	02:47	Taiko, Hiroshi	Molecular Imprinting using Dendrimers
G6	pol	Talk	10	02:57	Kavarnos, George	Electroactive Polymers ?
G7	Pol	Poster	3	03:07	Li, Youyong	Thermodynamic Functions and Critical Exponents for Polymer Chains
G8	Pol	Poster	3	03:10	Taiko, Hiroshi	Modeling Partially crystalline polymers (PET)
G9	MS	Talk	20	03:13	Meulbroek, Peter	The Computational Materials Design Facility
G10	MS	Talk	15	03:33	Su, Haibin	energetics and kinetics of electro-active polymers: PVDF and P(VDF-TrFE)
G11	MS	Talk	15	03:48	Zhang, Luzheng	Reaction Kinetics from Molecular Dynamics (ReaxFF)
Break, Posters			20	04:03		
Session H					Chair: Mario Blanco	Facilitator: Adam Griffith
H1	Env	Talk	20	04:23	Diallo, Mamadou	Molecular Environmental Technology (Humic Acid, Cu-PAMAM)
H2	Env	Talk	10	04:43	Lin, Shiang-Tai	Prediction of Vapor Pressures and Enthalpies of Vaporization
H3	Env	Poster	3	04:53	Tong, Candy	Cloud condensation nucleation by multioxygenates
H4	PER	Talk	20	04:56	Tang, Yongchun	Overview of Power, Energy, Environmental Research Center
H5	PER	Talk	10	05:16	Shuler, Pat	Experiments toward improved surfactants for enhanced oil recovery
H6	PER	Talk	10	05:26	Jang, Seung Soon	MD low interfacial tension in enhanced oil recovery surfactants
H7	PER	Talk	10	05:36	Ma, Qisheng	Naphthenic acids
H8	PER	Poster	3	05:46	Ma, Qisheng	Ionic Liquids
H9	PER	Poster	3	05:49	Wu, Sheng	New On-line Instrumentation to Detect and Measure Particulates
H10	Gen	Talk	8	05:52	Goddard, Bill	Wrap-up
Finish				06:00		Informal Dinner for out-of-town guests at Goddard house. RSVP