MSC2011 at Caltech (William A. Goddard III)

Thursday March 24 and Friday March 25, 2011

topics will be similar to those for MSC2010, see below

Thursday AM March 24

A Biotechnology

08:50	10	A00	E Abbott	Introduction to Caltech Corporate Associates
09:00	15	A01	W Goddard	Overview of the MSC in 2010 - 15
	25	A02	R Abrol	Overview of Computational Biology at the MSC 25
	20	A03	R Abrol	Gensemble: Predictions of the 3D structures GPCRs - 20
	20	A04	C Tanrikulu	DarwinDock: Predictions of Optimal Ligand-protein Structures 20
	20	A05	SK Kim	Applications: 4 Adenosine Receptors and Ligands - 20
	15	A06	B Trzaskowski	Applications: CCR5 Receptor and Ligands against HIV - 15
10:55	20	115	break	
11:15	15	A07	A Griffith	Applications: 5 Dopamine Receptors and Ligands - 15
	15	A08	C Scott	Applications: CB1 Cannabanoid Receptor and Ligands - 15
	15	A09	SK Kim	Applications: 4 Histamine Receptors and Ligands - 15
	10	A10	SK Kim	Applications: 2b and 2c Serotonin Receptors and Ligands 10
	10	A11	SK Kim	Applications: CXCR3 Chemokine Receptor and Ligands 10
	5	A12	SK Kim	Applications: Urotensin II Receptor and Ligands 5
	15	A13	A Kirkpatrick	Applications: CXCR4 Chemokine Receptor and Ligands 15
	3	A14	H Levenson	Applications: M1 Muscarinic Acetylcholine Receptor and Ligands POSTER
	3	A15	J. Tan	Applications: TAS2R38 Taster Receptor and Ligands - POSTER
	0	A16	V Cvicek	Applications: GPR81 (Lactate) Receptor and Ligands Cancelled
12:46	54	91	lunch	

13:40 Thursday PM March 24

15	A17	T Pascal	neo-natal meningitis: New ligands to block OmpA-HBMEC(Ec-gp96) binding 15
10	A18	C Scott	Inhibition of bacterial invasion: small ligand docking to human Ecgp protein 10
10	A19	R Abrol	Apoptosis Pathways - Design of Bclxl inhibitors -10
15	A20	T Pascal	The 2PT MD method for entropies - toward accurate FREE energies of binding
15	A21	SP Han	new strategies for therapeutics based on sequence activated RNA interference
15	A22	Y Liu	Drug delivery using pH induced dense-core to shell transition in PAMAM dendrimer

B. Frontiers QM

10	B01	Goddard	XYG3: Rigorous inclusion London Forces into Density Functional Theory
10	B03	Y Liu	Practical inclusion of London interaction into first principles based DFT
15:40	100	break	
15	B04	Anderson	Advances in Quantum Monte Carlo for High Accuracy ab initio Calculations
15	B05	Pascal	New generation force fields based on accurate QM
20	B06	J. Su	the eFF method for electron dynamics of highly excited electronic systems
20	B07	Jaramillo-Boter	Large-scale, long-term MD with pEFF-LAMMPS
10	B08	H Kim	Application of eFF to Lithium at high pressure
10	B09	Q An	Application of eFF to Carbon phases under extreme conditions
10	B10	P Theofanis	Effective Core approximaitons in eFF
20	B11	J Tahir-Kheli	Universal properties of cuprate superconductors explained by Plaquette pairing
20	B02	Y Jung	Fast, accurate doubly hybrid density functional method toward chemical accuracy

18:00 Thursday night March 24 Banquet at Goddards

18:30	D	Yousung Jung	Energy Environment water Sustainability at KAIST, Daejeon Korea

Friday AM March 25

E. Catalysis

09:00	25	E1	Nielsen	Progress in organometallic catalysts for functionalization of CH4
	15	E2	MJ Cheng	CH4 C-H Activation, Functionalization by Os(II) and Ru(II) Bipyridine complexes
	15	E3	WG Liu	new Au catalyst for converting methane to methanol
	10	E4	Theofanis	CH Activation by Intramolecular Coordinated Bases
	15	E5	MJ Cheng	Magnetic Structure of Vanadyl Pyrophosphate butane to maleic anhdride catalyst
	15	E6	J. Mueller	ReaxFF Reactive Dynamics: Early Stages CNT Growth on Ni468
	15	E7	J. Mueller	catalysts
10:50	20	110	break	

G. Fuel cells, Batteries, solar

	20	G1	B Merinov	Progress in Fuel Cell Research in the MSC
	20	G2	Y Sha	Mechanism of the Oxygen Reduction Reaction on Pt and alloys
	15	G3	T Yu	new alloys for fuel cell cathode catalysts
	20	G4	R Yazami	New strategies for Li-ion Battery Technology
	15	G5	HW Cho	Calculation of the intercalation free energy potential of LiC6 using 2PT method
	15	G6	H Xiao	Electronic structure+defects in Copper-Indium-Gallium-Selenide (CIGS) solar cells
12:55	45	125	lunch	

Friday PM March 25

13:40	15	G7	Mendoza-Corté	Storage of CH4 and H2 in Yaghi MOFs & COFs)
	15	G8	Mendoza-Corté	Trapping CO2 in Omar Yaghi's Zeolitic Imidazolate Frameworks (ZIFs)
	15	G9	P Pascal	New advanced material 4% reversible H2 storage at 300K, cheap as water

F. Environmental

	10	F1	M Diallo	Global Research Laboratory: Advanced Materials for Water Sustainability
	0	F2	H Mishra	Synthesis of hyperbranched PEI polymers for water disinfection'
	15	F3	Ma	Integrated Carbon Capture and Storage (CCS) Program at PEER.
	10	F4	S. Wu	Sensors for bio-process and carbon sequestration monitoring
	10	F5	T. Pascal	How much does nature hate vacuums?

H Multiscale/Nanotechnology

	15	C1	Jaramillo-Boter	Multiparadigm, Multiscale Methodologies, application to network polymers
15:25	20	105	break	
15:45	15	C3	J. Su	Multiscale Methodologies for protien-protein interactions
	10	C4	T Pascal	novel nucleation mechanisms in water graphene systems
	15	C5	H Kim	Dynamics of Localized Electrons in graphene: a metamaterial for electrons
	10	C6	W Ford	QM optimized charge equilibration using genetic algorithms
	15	C7	SP Han	Self assembly of DNA-CNT ladders on charged surfaces
	10	C8	R Barish	Using Nucleic Acids to Imprint Knot Topologies on Organic, Inorganic Substrates

I Energetic Materials

	20	I1	S Zybin	Overview of energetic materials research at MSC
	15	I2	WG Liu	First principles study of the ignition mechanism of hypergolic propellants
	15	I3	Y Liu	Reactive dynamics study of hypergolic propellants
	15	I4	Q An	HTPB based PBX study during shock loading using ReaxFF ?
	10	I5	Q An	Shear Sensitivity simulation of RDX Energetic Materials

Registration Fee: $195, Meals&breaks Fee: $95 To register, go to:
http://citrix1.wag.caltech.edu/EXEC/0/0xnfr5v0oz6wr0160glry0q3tkda
Registration is free for corporate and government sponsors of the MSC also for Caltech Corporate Associates. Caltech faculty and students