

ACTC 2011

Schedule of events and sessions

- *All scientific sessions will take place in the Palm Theater.*
- *Scheduled meals will take place under tents on the adjacent field.*

SUNDAY, July 17, 2011

Welcome!	
5:00PM-7:30PM	REGISTRATION
MONDAY AM	
7:30-8:45AM	<i>BREAKFAST served</i>
Session 1 DISC LEADER:	John STRAUB
9:00AM	Opening remarks
9:15	Angel GARCIA
	<i>Simulations of the folding-unfolding equilibrium of proteins under different solvent conditions</i>
10:05	coffee
10:35	Ronald LEVY
	<i>Exploring landscapes for protein binding and folding using replica exchange dynamics, kinetic networks, and Markov state models</i>
11:25	Richard FRIESNER
	<i>Understanding and Predicting Protein-Ligand Binding Affinities: Theory and Practice</i>
	<i>LUNCH on your own</i>

MONDAY PM	
Session 2	
DISC LEADER:	Dmitrii MAKAROV
2:00PM	Steven CORCELLI
	<i>Solvation Dynamics in DNA</i>
2:50	Joan-Emma SHEA
	<i>Simulations of Protein Aggregation in the Cellular Milieu</i>
3:40	Coffee
4:10	Ron ELBER
	<i>Milestoning: Theory and algorithm for long time dynamics from short trajectories</i>
5:00	Dave THIRUMALAI
	<i>Stepping Dynamics of Molecular Motors along Polar Tracks</i>
	<i>Dinner on your own</i>
	FREE TIME
TUESDAY AM	
	FREE/DISCUSSION TIME
	Lunch on your own

TUESDAY PM	
Session 3 DISC LEADER:	Eran RABANI
1:00	Graeme HENKELMAN
	<i>Correlating structure and function for nanoparticle catalysts</i>
1:50	Sergei TRETIAK
	<i>Modeling of photoinduced relaxation pathways in conjugated polymers</i>
2:40	coffee
3::10	Christopher MUNDY
	<i>Ions in solution and at interfaces: What can density functional theory teach us?</i>
4:00	David REICHMAN
	<i>The Role of Thermodynamic Correlations in Vitrification</i>
4:50	Mark RATNER
	<i>Electron and Exciton Motion in Molecular Bridges, Junctions and Patterns: Quantum, Classical and Actual Behaviors</i>
5:45-7:15PM	<i>DINNER served</i>
Session 4	POSTER SESSION 1
7:30-9:30PM	

WEDNESDAY AM	
	FREE/DISCUSSION TIME
	Lunch on your own
WEDNESDAY PM	
Session 5 DISC LEADER:	Lawrence Pratt
1:00	Shekhar GARDE
	<i>Hydration Phenomena at the Interface of Physics and Biology: A New Fluctuations-based Perspective</i>
1:50	Frank BROWN
	<i>Dynamics of lipid bilayer membranes</i>
2:40	coffee
3::10	Gerhard HUMMER
	<i>Theory of single-molecule force spectroscopy</i>
4:00	Richard STRATT
	<i>Who's got the time? The most efficient paths through the potential energy landscapes of liquids.</i>
4:50	Sharon HAMMES-SCHIFFER
	<i>Proton-Coupled Electron Transfer: Electron-Proton Nonadiabaticity and Ultrafast Solvent Dynamics</i>
5:45-7:15PM	<i>DINNER served</i>
Session 6	POSTER SESSION 2
7:30-9:30PM	

THURSDAY AM	
	FREE/DISCUSSION
	TIME
	Lunch on your own
Session 7 DISC LEADER:	Jack SIMONS
1:00PM	Garnet CHAN
	<i>Approaches to electronic structure theory in transition metal clusters and solids</i>
1:50	Jeffrey NEATON
	<i>Excited States at Interfaces: Implications for Charge Transport and Energy Conversion</i>
2:40	coffee
3::10	Joseph SUBOTNIK
	<i>The initial and final states of electron and energy transfer processes: Photochemistry for Quantum Chemists</i>
4:00	David MANOLOPOULOS
	<i>Chemical reaction rates from ring polymer molecular dynamics</i>
5:30-10:00PM	<i>DINNER & PARTY</i>

FRIDAY AM	
7:30-8:45AM	<i>BREAKFAST served</i>
Session 8 DISC LEADER:	Ken JORDAN
9:00AM	Pablo DEBENEDETTI
	<i>Water in Confinement</i>
9:50	Valeria MOLINERO
	<i>Crystallization of water: from bulk to the nanoscale</i>
10:40	James SKINNER
	<i>Three-body interactions and vibrational spectroscopy in water: Ice Ih, liquid, liquid/vapor interface, and clusters</i>
11:30AM	<i>Meeting adjourned</i>