**ACTC2014**

Schedule of talks, breaks, meals, and poster sessions

Sunday July 20

 6:00pm-9:00pm Welcome, registration. At Arroyo, 220 E Colorado Ave.

Monday July 21

 7:30 Breakfast

 8:45 TSRC Intro

 8:55 ACTC Intro (Jim Skinner)

 9:00 Giulia Galli (U. Chicago)

 *Computational spectroscopy of heterogeneous interfaces*

 9:40 Joan-Emma Shea (UC Santa Barbara)

 *Surface-mediated protein folding and aggregation*

 10:20 Break

 10:40 Joel Bowman (Emory U.)

 *Dynamics on ab initio potential energy surfaces: from roaming to the IR spectra of ice and hydrated ions*

 11:20 Chris Jarzynski (U. of Maryland)

 *Introduction to nonequilibrium thermodynamics of small systems*

 12:00 Lunch

 1:00 Martin Head-Gordon (UC Berkeley)

 *Some new developments in the description of electron correlation*

 1:40 Alexei Stuchebrukhov (UC Davis)

 *Electron tunneling and Redox-driven proton pumps*

 2:20 Anna Krylov (USC)

 *A fresh look at resonances: an equation-of-motion coupled-cluster based approach*

 3:00 Break

 3:30 Jeff Saven (U. Pennsylvania)

 *Statistical thermodynamic approach to protein design and redesign*

 4:10 Will Noid (Penn State U.)

 *Advances in coarse-graining structure*

 4:50 Evelyn Goldfield (NSF)

 *Funding opportunities at NSF for theoretical and computational chemists*

Tuesday July 22

 11:00 Hang posters for Session A

 1:00 Bill Miller (UC Berkeley)

 *Classical molecular dynamics approach to electronically non-adiabatic processes*

 1:40 So Hirata (U. Illinois)

 *Ab initio solid-state chemistry*

 2:20 Sal Torquato (Princeton U.)

 *Disordered hyperuniform materials: new states of matter*

 3:00 Break

 3:30 Cecilia Clementi (Rice U.)

 *Multiscale characterization of the photocycle of photoactive yellow protein*

 4:10 Sotiris Xantheas (PNNL)

 *New scalable forms of potential energy functions describing intermolecular interactions: from the very weak to the very strong*

 4:50 Sherwin Singer (Ohio State U.)

 *The water-amorphous silica interface: analysis of the Stern layer and surface conduction*

 5:30 Cash bar

 6:00 Dinner

 7:00 Poster Session A

Wednesday July 23

 11:00 Hang posters for Session B

 1:00 Hans Andersen (Stanford U.)

 *Dynamic force matching - construction of models for coarse grained dynamics*

 1:40 Marina Guenza (U. of Oregon)

 *Modeling across multiple length scales while preserving thermodynamics and structure*

 2:20 Zhen-Gang Wang (CalTech)

 *Self-energy effects of salt ions on phase behavior and interfacial properties*

 3:00 Break

 3:30 Patrick Charbonneau (Duke U.)

 *A soft-matter perspective on protein crystallization*

 4:10 Yu-Shan Lin (Tufts U.)

 *Computational studies of peptides*

 4:50 Ilan Benjamin (UC Santa Cruz)

 *Electron transfer at liquid/liquid interfaces: recent advances and open questions*

 5:30 Cash bar

 6:00 Dinner

 7:00 Poster Session B

Thursday July 24

 7:30 Breakfast

 9:00 John Weeks (U. of Maryland)

 *Solvation and structure for systems with strong Coulomb interactions*

 9:40 Nandini Ananth (Cornell U.)

 *Path integrals for photochemistry*

 10:20 Break

 10:40 Garyk Papoian (U. of Maryland)

 *Mechano-chemical modeling of the eukaryotic cytoskeleton*

 11:20 J. R. Schmidt (U. of Wisconsin-Madison)

 *First-principles force fields from symmetry-adapted perturbation theory*

 12:00 Lunch

 1:00 Todd Martinez (Stanford U.)

 *Leveraging stream processors and machine learning for molecular simulation*

 1:40 Troy Van Voorhis (MIT)

 *Excited states that look like ground states: diabatic pictures of electronic reactions*

 2:20 Tom Miller (CalTech)

 *Quantum dynamics from classical trajectories: new approaches to simulating biological and molecular catalysts*

 3:00 Break

 3:30 Joe Francisco (Purdue U.)

 *Carboxylic acid catalyzed hydration of formic acid*

 4:10 Sharon Hammes-Schiffer (U. of Illinois)

 *Theoretical perspectives on proton-coupled electron transfer and applications to catalysis*

 5:00 Open bar

 5:30 Closing Dinner/Party