**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