American Conference on Theoretical Chemistry

Agenda

Locations

All Sessions and Registration– Boston University Law Auditorium
The Law School and Auditorium are located behind the School of Theology.
Access the Law School from Marsh Plaza or from the George Sherman Union plaza.

Breaks– Boston University Law School Barrister's Hall

Lunch– George Sherman Union Food Court, 775 Commonwealth Ave. 1st floor

Poster Sessions & Reception– George Sherman Union, 775 Commonwealth Ave. 2nd floor

Monday, July 17

8:00-8:45 am	Registration	
8:45-9:00am	Welcome Opening Remarks	Sharon Hammes-Schiffer Gloria Waters, Vice President & Associate Provost for Research Boston University
	CHAIR: Sharon Hammes-Schiffer	
9:00-9:40am	Alan Aspuru-Guzik	*Can Computers Dream of Electric Molecules?* *Generative Models for Molecular Design*
9:40- 10:20am	Teresa Head-Gordon	*New Methods and Models for Condensed Phase Simulations*
10:20-10:40am	Break	
10:40-11:30am	Victor Batista	*Studies of Natural and Artificial Photosynthesis*
11:20-12:00pm	Rigoberto Hernandez	*Exact Classical TST in Dissipative and Driven Chemical Dynamics*
12:00-1:20pm	Lunch	
	CHAIR: Jack Simons	
1:20-2:00pm	Rommie Amaro	*Multiscale Dynamics: Molecules to Cells*
2:00-2:40pm	Joe Subotnik	*Surface Hopping All Around Us*
2:40-3:20pm	Jim Skinner	*Supercooled Water: Simulations, Theory, and Experiment in No Man's Land and the Liquid-Liquid Critical Point*
3:20-3:40pm	Break	
3:40-4:20pm	Andrew Rappe	*Quantum Mechanical Study of the Bulk Photovoltaic Effect*
4:20-5:00pm	Weitao Yang	*Going Beyond Conventional Density Functional Approximations*
5:00-5:30pm	Preparation for Poster Session	
5:30-7:30pm	Poster Session	

Tuesday, July 18

	CHAIR: John Straub	
9:00-9:40am	David Beratan	*Engineering Nanometer-Scale Electronic Coherence in DNA*
9:40-10:20am	Anastassia Alexandrova	*Statistical Ensemble Nature of Cluster-Decorated Surface Catalysts*
10:20-10:40am	Break	
10:40-11:20am	Filipp Furche	*Chemistry beyond the Born-Oppenheimer Approximation*
11:20-12:00pm	Tom Markland	*Decoding the Spectroscopy and Dynamics of Proton Defects using ab initio Quantum Dynamics Simulations*
12:00-1:20pm	Lunch	
	CHAIR: Heather Kulik	
1:20-2:00pm	Abe Nitzan	*Electron Transfer across Thermal Gradients*
2:00-2:40pm	Monica Olvera de la Cruz	*Polymer Electrolytes Thermodynamics and Microstructures*
2:40-3:20pm	Peter Rossky	*Relating Spectroscopy to Structure for Conjugated Polymers*

Tuesday, July 18 (Continued)

3:20-3:40pm	Break	
3:40-4:20pm	Garnet Chan	*Metalloenzymes from Many-Particle Quantum Mechanics*
4:20-5:00pm	Qiang Cui	*Recent Progress in Understanding Mechanochemical Coupling in Biomolecules*
5:00-5:30pm	Preparation for Poster Session	
5:30-7:30pm	Poster Session	

Wednesday, July 19

	CHAIR: Troy van Voorhis	
9:00-9:40am	Emily Carter	*Quantum Solutions for Sustainable Energy*
9:40-10:20am	Gus Scuseria	*Symmetry Projected Coupled Cluster Theory*
10:20-10:40am	Break	
10:40-11:20am	Laura Gagliardi	*Multireference Methods for Electronically Excited States and Transition-Metal Containing Systems*
11:20-12:00pm	Greg Voth	*Ultra Coarse-Graining: Theory and Applications*
12:00-1:20pm	Lunch	
	CHAIR: David Coker	
1:20-2:00pm	Francesco Paesani	*Chemical Accuracy from the Gas to the Condensed Phase through Many-Body Molecular Dynamics*
2:00-2:40pm	George Schatz	*CO_2 and N_2 Reduction: New Directions*
2:40-3:20pm	Evelyn Goldfield	*NSF's Ten Big Ideas and Their Relevance to Chemistry*
3:20-6:00pm	Free Time	Travel to Seaport World Trade Center Marine Terminal
6:00-7:00pm	Boarding	Spirit of Boston
7:00-9:00pm	Dinner Cruise	Spirit of Boston

Thursday, July 20

	CHAIR: Todd Martinez	
9:00-9:40am	David Coker	*Modeling Excitation Energy Transfer Dynamics and Spectroscopy in Photosynthetic Light Harvesting Systems*
9:40-10:20am	Heather Kulik	*New Computational Tools for Inorganic Molecular Design*
10:20-10:40am	Break	
10:40-11:20am	Francesco Evangelista	*Multireference Electronic Structure Theories Based on the Similarity Renormalization Group*
11:20-12:00pm	Nancy Makri	*Interference, Decoherence, and Quantum-Classical Path Integral Simulations with Thousands of Atoms*
12:00-1:20pm	Lunch	
	CHAIR: Sharon Hammes-Schiffer	
1:20-2:00pm	Ed Valeev	*Reduced Scaling and Controlled Precision: Extending the Reach of Many-Body Electronic Structure*
2:00-2:40pm	Lyudmila Slipchenko	*Polarizable Embedding in Biological Systems: When, Why, and How*
2:40-3:20pm	Ben Levine	*Conical Intersections and Non-Radiative Recombination in Semiconductor Nanocrystals*
3:20-3:40pm	Break	
3:40-4:20pm	David Reichman	*Optical and Excitonic Properties of Emerging Materials*
4:20-5:00pm	Todd Martinez	*Nonadiabatic Excited State Dynamics from First Principles*