MolSSI/SETCA 2019 Schedule

Wednesday, May 15, 2019

11:00am-1:00pm	MolSSI/SETCA Check-in/Nametag Pickup and On-site Registration	Strong Hall B1
12:00-1:00pm	Lunch for MolSSI Participants	Strong Hall B1
12:30-1:00pm	Computer Setup Help Available for MolSSI Participants	Strong Hall B1
1:00-5:00pm	MolSSI Workshop Session 1	Strong Hall B1

Thursday, May 16, 2019

9:00am-12:00pm	MolSSI Workshop Session 2	Strong Hall B1
12:00-1:00pm	Lunch for MolSSI Participants	Strong Hall B1
1:00-4:00pm	MolSSI Workshop Session 3	Strong Hall B1
3:00-5:00pm	SETCA Check-in/Nametag Pickup and On-site Registration	Strong Hall Atrium

SETCA BEGINS

5:00-7:00pm	Pizza and Thursday (R) Poster Session	Strong Hall Atrium

Friday, May 17, 2019

7:00-8:00am	Breakfast	Strong Hal Atrium
7:30-10:30am	SETCA Check-in/Nametag Pickup and On-site Registration	Strong Hall Atrium
8:00-8:10am	Opening Remarks	Strong Hall 101
8:10-10:00am	Session A	Strong Hall 101
	Chair: R. J. Hinde, The University of Tennessee, Knoxville	

8:10am	IL1	Nicholas Mayhall, Virginia Tech	Picking the right gates at the right time: an adaptive quantum algorithm for simulating molecular systems on quantum computers
8:40am	IL2	Devin Matthews, Southern Methodist University	Practical Experiences with Tensor Hypercontraction
9:10am	CT1	Filip Pawlowski, Auburn University	Cluster perturbation theory for energies and molecular properties
9:30am	IL3	Dmytro Bykov, Oak Ridge National Laboratory	Quantum Chemistry on Supercomputers

10:00-10:20am	Coffee Break – Refreshments Provided	Strong Hall Atrium
10:20-11:30am	Session B	Strong Hall 101
	Chair: Francesco Evangelista, Emory University	

10:20am	IL4	Jefferson Bates, Appalachian State University	Asymmetric Hubbard Dimer: Exact adiabatic-connection analysis of beyond-RPA correlation
10:50am	CT2	Shuming Bai, Duke University	Practical Proxies of Couplings and Quantum Interferences among Pathways for Dexter Energy Transfer
11:10am	CT3	Run R. Li, Florida State University	The role of orbital angular momentum constraints in the variational optimization of the two-electron reduced-density matrix

11:30am-1:20pm	Lunch	On Your Own
1:20-2:20pm	Session C	Strong Hall 101
	Chair: Sharani Roy, The University of Tennessee, Knoxville	

1:20pm	IL5	Lee Thompson, University of Louisville	Single reference wavefunctions as first-order approximations for efficient variational and orthogonal description of multistate reaction pathways
1:50pm	IL6	Tao Yu, Tennessee Tech	Essential Diabatic Orbital Method to Calculate Electronic Couplings and Simulate Charge Transfer in Organic Semiconducting Polymers

Friday, May 17, 2019 (continued)

2:20-2:40p		Coffee Break – Refreshments Provided	Strong Hall Atrium
2:40-4:00pm		Session D Chair: Evangelos Miliordos, Auburn University	Strong Hall 101
2:40pm	IL7	Sophya Garashchuk, University of South Carolina	Molecular Dynamics with Nuclear Quantum Effects; the H/D substitution effect in materials
3:10pm	IL8	Samer Gozem, Georgia State University	Spectral Tuning Maps and Average Protein Configurations: Strategies to Aid in Studying Flavoproteins
3:40pm	CT4	James H. Thorpe, The University of Florida, Gainesville	Dangers of the SCF-level DBOC: NO and NO_2 as examples
4:00-6:00pm		Friday (F) Poster Session	Strong Hall Atrium
6:20-9:00pm		Dinner & Banquet	UTK Student Union Ballroom
		Weitao Yang, Duke University	Symmetry, Degeneracy, Fractionals and Excitations

Saturday, May 18, 2019

7:30-8:30am		Breakfast	Strong Hal Atrium
8:30-10:10am		Session E Chair: Ashley McDonald, Cal Poly	Strong Hall 101
8:30am	IL9	Rachel Getman, Clemson University	A Multiscale Sampling Model for Calculating Energies, Free Energies, Activation Energies, and Rate Constants of Heterogeneously Catalyzed Reactions under Liquid Phase
9:00am	IL10	Akbar Salam, Wake Forest College	Discriminatory Effects in Resonance Energy Transfer
9:30am	CT5	Danil Kaliakin, Purdue University	Elucidation of Potent Methane Clathrate Stabilizing Agents by Means of Molecular Dynamics, Effective Fragment Potential Method and Density Functional Theory
9:50am	CT6	David Lingerfelt, Oak Ridge National Laboratory	A TD-DFT Method for the Prediction of Electronic Response to Electron Beam Irradiation
10:10-10:30am		Coffee Break – Refreshments Provided	Strong Hall Atrium
10:30am-12:10pm		Session F Chair: Konstantinos Vogiatzis, The University of Tennessee, Knoxville	Strong Hall 101
10:30am	IL11	Konrad Patkowski, Auburn University	Precious metal standards of intermolecular interaction energy calculations
11:00am	CT7	Doug Barlow, Abraham Baldwin Agricultural College	On the Unification of Three Theories for the Kinetics of Crystal Nucleation
11:20am	CT8	Dominic A. Sirianni, Georgia Tech	Improving Efficiency in Symmetry-Adapted Perturbation Theory via Empirical Dispersion
11:40am	IL12	Jesse McDaniel, Georgia Tech	First Principles Modeling of Electrochemical Interfaces
12:10-12:30pm		Business Meeting	Strong Hall 101
12:30pm		Meeting Adjourns	

Conference Locations:

Strong Hall: 1621 Cumberland Avenue, Knoxville, TN 37916
UTK Student Union: 1502 Cumberland Avenue, Knoxville, TN 37916