MoISSI/SETCA 2019 Schedule

Wednesday, May 15, 2019

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

Thursday, May 16, 2019

9:00am-12:00pm  MolISSI Workshop Session 2  Strong Hall B1
12:00-1:00pm  Lunch for MolISSI Participants  Strong Hall B1
1:00-4:00pm  MolISSI 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 Hall 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
8:10am-10:00am  Session A  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
10:20-11:30am  Session B  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  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
Chair: Evangelos Miliordos, Auburn University

2:40-4:00pm Session D
Strong Hall 101
Chair: Evangelos Miliordos, Auburn University

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 NO₂ 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 Hall Atrium

8:30-10:10am Session E
Strong Hall 101
Chair: Ashley McDonald, Cal Poly

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
Chair: Konstantinos Vogiatzis, The University of Tennessee, Knoxville

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