Excited States and Time-dependent Electronic Structure Theory

July 14-18, 2014

- Location: Telluride Intermediate School, 725 W. Colorado Ave, Telluride CO 81435
- Invited talks will be 30 minutes plus 10 minutes for questions and discussion
- Graduate student talks will be 20 minutes plus 5 minutes for questions and discussion
- A twenty minute coffee break is scheduled for both morning and afternoon sessions

- Any questions about the schedule should be directed to workshop organizers: Christine Isborn (cisborn@ucmerced.edu), Svetlana Kilina (Svetlana.Kilina@ndsu.edu), and Xiaosong Li (xsli@uw.edu)
- Any questions about logistics should be directed to TSRC hosts: Nana Naisbitt (nana@telluridescience.org), 970-708-0004 and Rory Sullivan (rory@telluridescience.org), 970-708-4542

- **Picnic on Monday, July 14,** 6-9 pm, Ah Haa School for the Arts, 300 S. Townsend (family and guests welcome free of charge)

- **TSRC Town Talk on Tuesday, July 15**, 6-7:15 pm, Conference Center in Mountain Village

- Breakfast Monday-Friday is included in the registration cost and will be provided at TSRC from 8:00 – 9:00 am

- Lunch Monday-Thursday is included in the registration cost and will be provided at TSRC from 12:40 – 1:30 pm

	8:00 – 9:00 AM	MORNING 9:00 AM – 12:40 PM	12:40 –1:30 PM	AFTERNOON 2:00 PM – 5:00 PM	EVENING
Mon July 14th	Breakfast at TSRC	***I(A) Electronic Dynamics*** Isborn Maitra **Break** Wong Lopata Govind	Lunch at TSRC	***II(A) Wavefxn methods*** Valeev Caricato **Break** Ding Goings **End at 4:45**	TSRC Picnic, **6:00 – 9:00 PM** (Ah Haa School for the Arts, 300 S. Townsend)
Tues July 15th	Breakfast at TSRC	***III(A) Electronic Structure and Dynamics*** Varganov DePrince **Break** Autschbach W. Yang Liu	Lunch at TSRC	***III(B) Electronic Structure and Dynamics*** Shiozaki Scuseria **Break** Li Q. Zhang **End at 4:45**	Town Talk, **6:00-7:15 PM** (Conference Center in Mountain Village)
Wed July 16th	Breakfast at TSRC	***I(B) Electronic Dynamics*** Tretiak Furche **Break** Lu Izmaylov Levine	Lunch at TSRC	Hiking / Free time	Free time / 6:00 PM social gathering in Smugglers Brewpub
Thurs July 17th	Breakfast at TSRC	***III(C) Electronic Structure and Dynamics*** Chakraborty Kilina **Break** Jaeger Chen Fuks	Lunch at TSRC	***IV. Charge and Energy Transfer*** Kilin Jakubikova **Break** Nelson You **End at 5:00**	Free
Fri July 18th	Breakfast at TSRC	***II(B) Wavefxn methods*** Hoffman Bravaya **Break** Y. Yang D. Zhang **Discussion & Wrap up**	End by 12:00 PM	Free	Free

Full Agenda

July 14

Monday Morning

8:00-8:50	**Breakfast at TSRC** (for participants)
8:50-9:00	Organizational Remarks
9:00 am -12:40 pm	**SECTION I(A): ELECTRONIC DYNAMICS**
	Chair: Xiaosong Li
9:00-9:40	Christine Isborn, University of California, Merced, CA *Oddities of Real-time TDDFT Electron Dynamics: Peak-shifting and Two-electron Rabi Oscillations*
9:40-10:20	Neepa Maitra, Hunter College, New York, NY *Electron Dynamics in Strong and Weak Fields: Studies of the Exact Correlation Potentials*
10:20-10:40	**Coffee Break**
10:40-11:20	Bryan Wong, University of California, Riverside CA *Charge-Transfer Dynamics with Explicit Solvent: Insights from RT-TDDFTB*
11:20-12:00	Ken Lopata, Lousiana State University, Baton Rouge, LA *Optical and X-Ray Absorption of Insulators Using Non-Hermitian Real-Time TDDFT*
12:00-12:40	Niri Govind, Pacific Northwest National Lab, Richland, WA *Recent TDDFT Developments in NWChem for Valence and Core Spectroscopies*
12:40-1:30	**Lunch at TSRC**
2:00 pm - 4:30 pm	**SECTION II(A): Wave function methods**
	Chair: Elena Jakubikova
2:00-2:40	Ed Valeev, Virginia Tech, Blacksburg, VA *Chasing Strong Scaling Concurrency for Electronic Structure and Dynamics*
2:40-3:20	Marco Caricato, University of Kansas, Lawrence, KS *Exploring Excited States in Solution With Coupled Cluster and Polarizable Solvation Methods*
3:20-3:40	**Coffee Break**
3:40- 4:20	Feizhi Ding, University of Washington, Seattle, WA *An Efficient Algorithm for Determinant-Based Configuration Interaction*
4:20- 4:45	Joshua Goings, University of Washington, Seattle, WA *Low-Scaling Approximations to the Equation of Motion Coupled-Cluster Singles and Doubles Equations*
6:00-dark	**TSRC Picnic** at the Ah Haa Art School at 300 S. Townsend

July 15

Tuesday Morning

8:00-9:00 **Breakfast at TSRC** (for participants)

9:00 am -12:40 pm **SECTION III (A): ELECTRONIC STRUCTURE & DYNAMICS**

Chair: Christine Isborn

9:00-9:40 Sergey Varganov, University of Nevada, Reno, NV
Non-adiabatic Spin-Forbidden Reactions: From Biology to Astrochemistry

9:40-10:20 Eugene DePrince, Florida State University, Tallahassee, FL
Time-Dependent Variational Two-Electron Reduced-Density-Matrix Method

10:20-10:40 **Coffee Break**

10:40-11:20 Jochen Autschbach, University at Buffalo, The State University of New York, Buffalo, NY
Kohn-Sham Calculations of Response Properties and the Impact of the Delocalization Error

11:20-12:00 Weitao Yang, Duke University, Durham, NC
Electronic Excitations from Pairing Matrix Fluctuation and Particle-Particle Random Phase Approximation

12:00-12:40 Wenjian Liu, Peking University, Beijing, China
Recent Advances in TD-DFT

12:40-1:30 **Lunch at TSRC**

Tuesday Afternoon

2:00 pm - 4:45 pm **SECTION III(B): ELECTRONIC STRUCTURE & DYNAMICS**

Chair: Ksenia Bravaya

2:00-2:40 Toru Shiozaki, Northwestern University, Chicago, IL
Product Wave Functions for Diabatic Model Hamiltonians of Exciton Dynamics

2:40-3:20 Gustavo Scuseria, Rice University, Houston, TX
Accurate Excited States via Multi-Component Projected Hartree-Fock Theory

3:20-3:40 **Coffee Break**

3:40- 4:20 Xiaosong Li, University of Washington, Seattle, WA
Ab initio Time-Dependent Two-Component Spinor

4:20- 4:45 Qing Zhang, University of Hong Kong, Hong Kong
Time-domain First Principle Quantum Transport Theory with Nuclei Dynamics

6:00-7:15 **Town Talk** at Conference Center in Mountain Village

July 16

Wednesday Morning

8:00-9:00	**Breakfast at TSRC** (for participants)
9:00 am -12:40 pm	**SECTION I(B): ELECTRONIC & NON-ADIABATIC DYNAMICS**
	Chair: Dmitri Kilin
9:00-9:40	Filipp Furche, University of California, Irvine, CA *Improving the Efficiency of Linear Response Calculations for Non-Adiabatic Molecular Dynamics*
9:40-10:20	Sergei Tretiak, Los Alamos National Lab, Los Alamos, NM *Efficient Non-Adiabatic Excited State Dynamics Simulations in Extended Molecular Systems*
10:20-10:40	**Coffee Break**
10:40-11:20	Gang Lu, California State University Northridge, Los Angeles, CA *First-Principles Study of Exciton Dynamics in Organic and Hybrid Photovoltaics: Practical Implementations and Theoretical Challenges*
11:20-12:00	Artur Izmaylov, University of Toronto Scarborough, Toronto, Canada *Topological Effects In Non-Adiabatic Dynamics near Conical Intersections*
12:00-12:40	Benjamin G. Levine, Michigan State University, East Lansing, MI *Conical Intersections and Non-Radiative Recombination at Semiconductor Defects*
12:40-1:30	**Lunch at TSRC**

Wednesday Afternoon

2:00 pm - 6:00 pm	**Hiking & Free Time**
6:00-9:00	**Social gathering in Smugglers Brewpub**

July 17

Thursday Morning

8:00-9:00 **Breakfast at TSRC** (for participants)

9:00 am -12:40 pm **SECTION III(C): ELECTRONIC STRUCTURE & DYNAMICS**

Chair: Marco Caricato

9:00-9:40 Arindam Chakraborty, Syracuse University, New York, NY
Investigation of Electron-Hole Interaction in Nano Particles Using Explicitly Correlated Wavefunction Based Methods

9:40-10:20 Svetlana Kilina, North Dakota State University, Fargo, ND
First-Principles Simulations of Dissipation and Time-Resolved Emission in Nanocrystals

10:20-10:40 **Coffee Break**

10:40-11:20 Heather Jaeger, Lehigh University, Bethlehem, PA
Excited States of Metal-Organic Frameworks.

11:20-12:00 Guanhua Chen, University of Hong Kong, Hong Kong
Time-Dependent Density-Functional Theory for Open System

12:00-12:40 Johanna Fuks Hunter College, New York, NY
Non-Perturbative Charge-Transfer within TDDFT: Simulations in Exactly-Solvable Model Systems

12:40-1:30 **Lunch at TSRC**

Thursday Afternoon

2:00 pm - 5:30 pm **SECTION IV: SIMULATIONS OF CHARGE & ENERGY TRANSFER**

Chair: Sergei Tretiak

2:00-2:40 Dmitri Kilin, University of South Dakota, Vermillion, SD
Quantum Dynamics at Liquid-Solid Interfaces: Limitations to Redfield Theory

2:40-3:20 Elena Jakubikova, North Carolina State University, Raleigh, NC
Computational Design of Fe-Based Sensitizers for Dye-Sensitized Solar Cells

3:20-3:40 **Coffee Break**

3:40- 4:20 Tammie Nelson, Los Alamos National Lab, Los Alamos, NM
Delocalization Dynamics and Energy Transfer in Conjugated Chromophores

4:20- 5:00 Zhi-Qiang You, Ohio State University, Columbus, OH
Quantum Chemistry Study of Electronic Excited States and Excitation Energy Transfer for an Organic Semiconductor Nanotube

July 18

Friday Morning

8:00-9:00	**Breakfast at TSRC** (for participants)
9:00 am -12:00 pm	**SECTION II(B): Wave function methods**
	Chair: Ben Levine
9:00-9:40	Mark Hoffmann, University of North Dakota, Grand Forks, ND *GVVPT2 Multireference Perturbation Theory Studies of Transition Metals*
9:40-10:20	Ksenia Bravaya, Boston University, Boston, MA *Energies and Lifetimes of Autoionizing Electronic States: EOM-CCSD Suite of Methods*
10:20-10:40	**Coffee Break**
10:40-11:05	Yang Yang, Duke University, Durham, NC *Excitation Energies from Particle-Particle Random Phase Approximation: Davidson Algorithm and Benchmark Studies*
11:05-11:30	Du Zhang, Duke University, Durham, NC *Analytic gradient, geometry optimization and excited state potential energy surfaces from pairing matrix fluctuations and the particle-particle random phase approximation*
11:30 – 12:00	Discussion and closing remarks by Svetlana Kilina
12:00	**Lunch on your own**