**Charge and Energy Transfer in Photoreactions and Photodynamics**  
Telluride Science Research Center Workshop  
**07/04/2016 - 07/08/2016**  
Telluride Elementary School

**TSRC Hosts:** Mark Kozak, 970-708-4426  
**Organizers:** Dmitri Kilin, Sebastian Fernandez-Alberti, and Kirill Velizhanin  
**Meeting Venue:** Telluride Elementary School 447 W. Columbia Ave Telluride CO 81435  
Each talk is 40 minutes + 5 minutes for questions  
Website: [https://www.telluridescience.org/meetings/workshop-details?wid=522](https://www.telluridescience.org/meetings/workshop-details?wid=522)

**Monday, 7/4**

8:30am  Breakfast at Telluride Elementary School  
8:55am  Introductory word

**Half-day Session on Semi-classics and Path Integrals,**  
**chair: Haobin Wang**

9:00am  Miller, William H., University of California Berkeley,  
*Classical Molecular Dynamics Simulation of Electronically Non-Adiabatic Processes in Complex Molecular Systems*

9:45am  Herman, Michael, Tulane University,  
*Approximate Semiclassical Method that Uses Real Valued Trajectories for Time Dependent (and other) Tunneling Calculations*

10:30am  **Coffee Break**

10:45am  Makhov, Dmitry, University of Leeds,  
*Towards Fully quantum modeling of Ultrafast Photodynamics*

11:30am  Huo, Pengfei, University of Rochester,  
*Semi-classical Path-Integral Dynamics for understanding energy transfer and charge separation*

12:15am  White, Alexander, LANL,  
*Coupled Wavepackets for non-adiabatic molecular dynamics*

1:00pm  **Lunch on your own, free time,**  
2:30pm  *group hike along Bear Creek trail,*  
*watching 4th of July fireworks from Smugglers*
Tuesday, 7/5

8:30am Breakfast at Telluride Elementary School

8:45am Free time, an opportunity to attend session honoring 60th birthday of V. Chernyak

1:00pm Lunch on your own

**Half-day session on nonadiabatic dynamics and Bond breaking, chair: Sebastian Fernandez-Alberti**

2:00pm Muuronen, Mikko, University of California Irvine, *First Electron-Proton Transfer of Water Oxidation on small TiO₂ nanoparticles*

2:45pm Fernandez Alberti, Sebastian, Universidad Nacional de Quilmes, *Electronic and vibrational energy relaxation and redistribution in chlorophylls*

3:30pm Coffee Break

3:45pm Nelson, Tammie, LANL, *Improved Efficiency for Nonadiabatic Molecular Dynamics in Extended Systems*

4:30pm Chen, Lipeng, Nanyang Technological University, *GPU-assisted simulation of energy and charge transfer dynamics in light harvesting systems*

5:15pm Gondola ride to Mountain Village

5:30pm Cash bar for Town Talk

6:00pm **Telluride Town Talk** at Conference Center in Mountain Village
Paul O’Shea, The University of Nottingham, “*Science & Healthcare: This Time It’s Personal!*”
Wednesday, 7/6

8:30am  Breakfast at Telluride Elementary School

**Half-day session on electron transport dynamics.**
**Chair: Kirill Velizhanin**

9:00am  Wang, Haobin, University of Colorado Denver,
_Quantum Dynamics Simulation of Ultrafast Photoinduced Electron Transfer Processes_

9:45am  Yam, Chi Yung, Beijing Comp. Science Research Center,
_Quantum Mechanical Simulations of Open Electronic Systems: From Molecular Electronics to Optoelectronics_

10:30am  **Coffee Break**

10:45am  Zwolak, Michael, Natl. Instit. of Standards & Technology,
_The simulation of real-time charge transport: Landauer formula with finite-time relaxation_

11:30am  Jaeger, Heather, Lehigh University,
_A quantum chemist’s view of electronic conductivity in molecular materials_

12:15pm  Lunch on your own

**Half-day Session on**
**Optoelectronic properties of organic-inorganic perovskite materials:**
**Chair: Andrei Kryjevski**

2:00pm  Tretiak, Sergei, LANL,
_On the way toward efficient perovskite photovoltaics and beyond_

2:45pm  Jankowska, Joanna, University of Southern California,
_Understanding the role of organic-inorganic layer coupling in perovskite materials from photovoltaics_

3:30pm  **Coffee Break**

3:45pm  Kilin, Dmitri, NDSU,
_Dynamics of Electronic Excitations at Interfaces_

6:00pm  **TSRC Picnic** at Telluride Elementary School, under the tent
Thursday, 7/7

8:30am  Breakfast at Telluride Elementary School

Half-day Session on Excitations in Carbon Materials,
Chair: Svetlana Kilina

9:00am  Piryatinski, Andrei, LANL,
Exciton dynamics in semiconductor carbon nanotubes and photon emission properties

9:45am  Kryjevski, Andrei, North Dakota State University,
Multiple Exciton Generation in Chiral Single-Wall Carbon Nanotubes: DFT-based study

10:30am  Coffee Break

10:45am  Velizhanin, Kirill A., LANL,
Exciton Fate in Functionalized Carbon Nanotubes: Thermodynamics and Relaxation Dynamics

11:30am  Marom, Noa, Carnegie Mellon University,
Effect of crystal packing on Electronic properties of molecular crystals

12:15am  Sahar, Sharifzadeh, Boston University,
Understanding Optical Excitations in Ordered Organic Molecular Assemblies from First-Principles Theory

1:00pm  Lunch on your own
an opportunity to attend session honoring 60th birthday of V. Chernyak
**Friday, 7/8**

8:30am  Breakfast at Telluride Elementary School

**Half day Session on Excited State Processes, Chair: Dmitri Kilin**

9:00am  Chakraborty, Arindam, Syracuse University,  
*Describing electronic excitations in atoms, molecules, clusters and quantum dots using electron-home multicomponent coupled cluster theory*

9:45am  Kilina, Svetlana, North Dakota State University,  
*Dephasing, dynamics, energy relaxation and surface chemistry of semiconductor nanostructures*

**10:30am  Coffee Break**

10:45am  Krylov, Anna, USC,  
*On density matrices, non-adiabatic couplings, and singlet fission*

11:30am  Kocherzhenko, Aleksey, UC Merced,  
*Model Hamiltonians for Studies of Charge Separation and Spectroscopy in Organic Optoelectronic Materials*

12:15 am  Concluding remarks

12:20pm  Adjourn