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

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 TiO_2 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