Telluride Workshop

"*Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy*"

Location: Telluride Elementary School, 447 West Columbia Ave, Telluride
The Elementary School is at a separate location from the Telluride Intermediate School. There will be a sign on Main Street helping to direct participants to the Elementary School.

TSRC Host: Mark Kozak mark@telluridescience.org / 970.708.4426

Breakfast will be served daily before the talks at the workshop location.

Lunches are NOT included in registration.

The scientific program starts at 9:00 am on Monday, July 20 and ends at 1 pm on Friday, July 24 (the last half-day is reserved for group discussions, collaborations, etc.). The first half day of Wednesday, July 22 is reserved for group discussions, collaborations, group hike, etc.

Each talk is scheduled for 35 minutes + 5 minutes for discussion. Interruptions and questions during talks are encouraged.

We have 35 presentations: 10 on Monday Tuesday and Thursday, and 5 on Wednesday.

There is a "town talk" on Tuesday evening and a TSRC Picnic/BBQ on Wednesday evening (6 pm – 9 pm under the tent at the Elementary School).

Monday, July 20

Morning

8:30 am *Breakfast*

9:00 am Artur Izmaylov, U. Toronto
"Geometric Phase Effects in Quantum-Classical Dynamics through Conical Intersections"

9:40 am Joseph Subotnik, UPenn
"Surface Hopping, Time-Reversibility, Detailed Balance, and Transition State Theory: How Well Do they Match up?"

10:20 am Elena Jakubikova, NCSU
"Exploring intersystem crossing in Fe(II)-polypyridine complexes"

11:00 am *Coffee Break*

11:15 am Carlos Silva, U Montreal
"Ultrafast carrier generation in polymer solar cells"

11:55 pm Andriy Zhugayevych, Skolkovo
"First-principle effective Hamiltonian modeling of charge and energy transport in molecular systems"

12:35 pm *Lunch (on your own)*

Afternoon

2:00 pm John Parkhill, U Notre Dame
"Non-equilibrium Self-Consistent Field Theory at Second Order (OSCF2)"

2:40 pm Vitaly Rassolov, U South Carolina
"Electron Correlation Operator approach for description of Excited States"

3:20 pm John Herbert, Ohio State
"Analytic Derivative Couplings for Time-Dependent DFT"

4:00 pm *Coffee Break*

4:15 pm Koji Ando, U. Kyoto
"A wave packet modeling of chemical bond and dynamics"

4:55 pm Arindam Chakraborty, Syracuse U
"Development of multicomponent coupled-cluster theory"

Tuesday, July 21

Morning

8:30 am *Breakfast*

9:00 am Jun Jiang, USTC
"Modeling of Electron Kinetics in Complex Systems"

9:40 am Ignacio Franco, U Rochester
"New frontier in electronic structure: Establishing the fundamental connection between electronic correlation and decoherence"

10:20 am Rudolph Magyar, Sandia Labs
"Non-Adiabatic Dynamics of Electrons and Ions in Warm Dense Matter"

11:00 am *Coffee Break*

11:15 am Alex White, Los Alamos Lab
"Accelerated Semiclassical Monte Carlo: Efficient Nonadiabatic Dynamics from First Principles"

11:55 pm Craig Martens, UCI
"Fully Coherent Quantum State Hopping"

12:35 pm *Lunch (on your own)*

Afternoon

2:00 pm Eric Bittner, U houston
"Role of quantum tunneling, delocalization, and spin statistics in organic photovoltaics"

2:40 pm Tammie Nelson, Los Alamos
"NA-ESMD modeling of energy transfer in linked chromophores as insight for molecular design"

3:20 pm *Coffee Break*

3:35 pm Tonu Pullerits, Lund U
"Electronic dynamics in colloidal quantum dots probed by coherent multidimensional spectroscopies"

4:15 pm Dhara Trivedi, USC
"Non-adiabatic Excited State Dynamics in Semiconductor Quantum Dots"

4:55 pm Guanhua Chen, HKU
"Predicting long time dynamics of open quantum system"

6:00 pm *Town Talk,* Telluride Conference Center in Mountain Village

Wednesday, July 22

Morning

8:30 am *Breakfast*

9:00 am – 12:30 pm Informal Discussions, Collaborations, Group hike

12:35 pm *Lunch (on your own)*

Afternoon

2:00 pm Suggy Jang, CUNY
"Molecular level design principle behind optimal sizes of LH2 complex of purple bacteria"

2:40 pm Vladimir Mandelshtam, UCI
"Dynamics and equilibrium properties of quantum Lennard-Jones liquids and clusters"

3:20 pm Sougata Pal, USC
"Non adiabatic molecular dynamics for thousand atoms systems: A tight binding approach towards PYXAID"

4:00 pm *Coffee Break*

4:15 pm Ben Nebgen, USC
"The Fragment Molecular Orbital Method and PYXAID: A New Way to do Surface Hopping Calculations"

4:55 pm Sophya Garashchuk, U South Carolina
"Identification of the low-energy eigenstates and collective modes from quantum dynamics"

6:00 pm *Picnic*, under the tent at the Elementary School

Thursday, July 23

Morning

8:30 am *Breakfast*

9:00 am Barry Dunietz, Kent U
"Photoinduced electron transfer through molecular-resolved interfaces: Insight by ab-initio modeling"

9:40 am William Barford, Oxford U
"Excitons in pi-conjugated polymers: Localization, spectroscopy and dynamics"

10:20 am James Lewis, UCI
"High-throughput computational design of azo-functional materials"

11:00 am *Coffee Break*

11:15 am Jacky Even, Rennes U
"Electronic and structural properties of hybrid perovskites"

11:55 pm Heather Jaeger, Lehigh U
"Ab initio modeling of electronic processes in hybrid coordination polymers"

12:35 pm *Lunch (on your own)*

Afternoon

2:00 pm Andrei Piryatinski, Los Alamos
"Influence of Exciton Diffusion and Exciton-Exciton Annihilation on Photon Emission Properties of Carbon Nanotubes"

2:40 pm Sergei Tretiak, Los Alamos
"Chemical functionalization and optical properties of carbon nanotube materials"

3:20 pm Laurent Pedesseau,
"Static and dynamic properties of sodium-borosilicate liquids and glasses: Ab initio simulations"

4:00 pm *Coffee Break*

4:15 pm Hyeon-Deuk Kim, Kyoto U
"Photoexcited Nonadiabatic Dynamics in Nanomaterials Based on Exciton Bases"

4:55 pm Alexander Schubert, Würzburg U
"Atomistic simulation of dissipative processes and direct decoherence observation via non-linear spectroscopy"

Friday, July 24

8:30 am	*Breakfast*
9:00 am – 1:00 pm	Informal Discussions, Collaborations
1:00 pm	Closure