

**Telluride Workshop 2019**  
***“Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy”***

Telluride Intermediate School located at 725 W Colorado Ave, Telluride, CO 81435  
 July 16<sup>th</sup> to 20<sup>th</sup>

TSRC Host: Mark Kozak [mark@telluridescience.org](mailto:mark@telluridescience.org) / 970.708.4426

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

Lunches are NOT included in registration.

There is an All-TSRC Meet and Greet event at Oak located at the base of the gondola at 250 W San Juan Avenue (Gus's Way) on Monday, July 15 from 5:00 to 6:30pm. Oak offers walk-up counter service for food and drink.

The scientific program starts at 8:30 am on Tuesday, July 16<sup>th</sup> and ends at 12 pm on Saturday, July 20<sup>th</sup> (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 38 presentations: 10 on Tuesday, 8 on Wednesday and 10 on Thursday and Friday

There is no “town talk” this week

There is a TSRC Picnic/BBQ on Wednesday evening (6 pm – 8 pm under the tent at the Intermediate School). We will have talks leading right up to the picnic.

<b>Monday, July 15th</b>		
5:00-6:30	All TSRC Meet and Greet at the Oak	
<b>Tuesday, July 16th</b>		
8:00	Breakfast	
8:30	Michael Herman	Three Problems in Semiclassical Tunneling
9:10	Sophya Garashchuk	Quantum dynamics employing the quantum trajectory-guided adaptable Gaussian bases
9:50	Craig Martens	Quantum Trajectory Surface Hopping Methodology for Simulating Nonadiabatic Dynamics
10:30	Coffee Break	
10:45	Dima Mozyrsky	Quantum-Classical Approach to Modelling Non-Adiabatic Dynamics
11:25	Eddy Timmermans	Molecular Opacity Challenges for Broad-Band Radiative Transfer
12:05	Lunch (on your own)	

1:30	Xavier Andrade	Non-linear transport from real-time electron dynamics
2:10	Andrew Baczewski	Transport Properties In The Warm Dense Regime Using Time-Dependent Density Functional Theory
2:50	Alexander White	Nonadiabatic Time-Dependent Kohn-Sham & Orbital-Free DFT: Stopping Power in Warm Dense Matter
3:30	Coffee Break	
3:45	Giovanni Vignale	Electron hydrodynamics and thermal transport in graphene-based materials
4:25	Alfredo Correa	First principles non-equilibrium dynamics of electrons and ions, method and applications
Wednesday, July 17th		
8:00	Breakfast	
Open time for Hike / Collaboration		
Lunch (on your own)		
12:00	Galen Craven	Electron transfer in thermally heterogeneous environments
12:40	Yujun Zheng	Non-Markovian decoherence dynamics in nonequilibrium environments
1:20	Pengfei Huo	Using quasi-diabatic propagation scheme to simulate non-adiabatic dynamics
2:00	Coffee Break	
2:15	Luis Rego	Photoinduced Coupled Electronic--Structural Dynamics in Large Molecular Systems
3:55	Hans Lischka	Carbon-based Nanomaterials: from Graphene Sheets to Carbon Nanodots - High-level Theoretical Studies
4:35	Coffee Break	
3:50	Jin Zhao	Ab initio nonadiabatic molecular dynamics investigations on the excited carriers in condensed matter systems
4:30	Thomas Jansen	Exciton dynamics in two-dimensional electronic spectroscopies
5:10	Alexey Akimov	Nonadiabatic dynamics in condensed matter systems: Uncertainty, reliability, (best?) practices.
6:00-8:00	Picnic (under the tent at Telluride Intermediate School)	
Thursday, July 18th		
8:00	Breakfast	
8:30	Roi Baer	Unraveling the nonequilibrium dynamics of an open system of non-interacting electrons
9:10	Maicol Ochoa	Electromechanical molecular detection with graphene nanoresonators in noisy environments
9:50	Xiao Zheng	Fermionic dissipative dynamics: Theories and applications
10:30	Coffee Break	
10:45	Artur Izmaylov	Quantum chemistry on a quantum computer: Recent developments and current challenges
11:25	Mario Barbatti	Dynamics of electronically-excited organic systems: advances, appraisal, applications
12:05	Lunch (on your own)	
1:30	Spiridoula Matsika	Nonadiabatic dynamics in photon and electron driven processes
2:10	Dmitry Shalashilin	Trajectory guided basis sets of Coherent States for nonadiabatic dynamics
2:50	Sergei Tretiak	Multiple cloning and polaritonics in excited state NAMD

3:30	Coffee Break	
3:45	Andre Schleife	Hot-electron mediated ion diffusion and projectile-charge dynamics for radiation damage
4:25	Ivan Infante	A Tale of Perovskite Nanocrystals: How Experiments Inspire Theory and Viceversa
Friday, July 19th		
8:00	Breakfast	
8:30	Zhenfei Liu	Accelerating first-principles GW calculations for molecule-substrate interfaces
9:10	Barry Dunietz	Molecular and dielectric impact on the spectra, energy and charge transfer processes in interfaces of organic semiconducting materials: A predictive comprehensive computational framework
9:50	Xiang Sun	Photo-induced charge transfer dynamics via the linearized semiclassical method
10:30	Coffee Break	
10:45	Eric Bittner	TBD
11:25	Tammie Nelson	Non-Adiabatic Excited-State Molecular Dynamics for Open-Shell Systems
12:05	Lunch (on your own)	
1:30	Maxim Sukharev	Crafting light-matter interactions at plasmonic interfaces: strong coupling and beyond
2:10	Rebecca Giesecking	Semiempirical Modeling of Plasmonic Ag Nanoclusters and Surface-Enhanced Spectroscopy
2:50	Andrei Piryatinski	Theory and simulations of superradiant and lasing regimes in plasmonic cavities
3:30	Coffee Break	
3:45	Run Long	Photoexcitation Dynamics in Perovskite Solar Cells
4:25	Marco Garavelli	Computational Multi-pulse Transient Spectroscopies of Nonadiabatic Photoinduced Events in Biological Systems: Retinal Chromophores, Nucleobases et al.
Saturday, July 20 <sup>th</sup>		
8:00	Breakfast	
8:30	Open time for Collaboration	
12:00	End of Workshop	