Telluride Workshop 2023

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

Ah Haa School for the Arts
Silver Bell Building
Transformation Room
155 W Pacific Ave., Telluride, CO 81435
October 2nd-6th, 2023

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

$50 gift card to Baked in Telluride (127 S Fir St, Telluride, CO 81435) **provided.**

Lunches are NOT included in registration.

There is a Meet and Greet at Oak, The New Fat Alley BBQ located at the base of the gondola at 250 W San Juan Avenue on Sunday, October 1st from 5:00 to 6:30pm. Oak offers walk-up counter service for food and drink. Badges can be picked up.

The scientific program starts at 8:50 am on Monday, Oct 2nd and ends at 12 pm on Friday, Oct 6th (the last half-day is reserved for group discussions, collaborations, etc.). The workshop closes at 5 pm on Friday, Oct 6th. The first half day of Wednesday, Oct 4th is reserved for group discussions, collaborations, group hike, etc.

Each talk is scheduled for 40 minutes + 10 minutes for discussion. Interruptions and questions during talks are encouraged.

We have 28 presentations: 7 on Monday/Tuesday, 4 on Wednesday, 7 on Thursday and 3 on Friday.

There is no "town talk" this week.

Fall meetings **do not** include a Picnic/BBQ. Instead, each registrant we will receive a $25 gift card to Oak, The New Fat Alley BBQ. We intend to meet as a group at Oak on Wednesday following the scientific talks.

Sunday, Oct 1st		
5:00-6:30 PM	All TSRC Meet and Greet at the Oak (Badge Pickup)	
Monday, Oct 2nd		
8:50	Opening Remarks	
9:00	Sergei Tretiak	Chemical bonding in photophysics and photochemistry of organic chromophores
9:50	Coffee Break (10 minutes)	
10:00	Xiang Sun	Modeling Photoinduced Charge Transfer Dynamics in Complex Condensed Phase
10:50	Vidushi Sharma	Exploring Photon-mediated Water Splitting On Perovskite Surfaces With Accelerated Density Functional Theory Methods.
11:40	Lunch (on your own, 1 hour 50 minutes)	
1:30	Alina Kononov	Electron dynamics in nonequilibrium warm dense matter
2:20	Alexander White	Nonadiabatic TD-DFT for warm dense matter
3:10	Coffee Break (10 minutes)	
3:20	Michele Pavanello	Beyond Equilibrium: Electronic Structure Methods for Mesoscale System
4:10	Reserved	Reserved
Tuesday, Oct 3rd		
9:00	Dmitry Shalashilin	A brief review of Coherent State based methods of quantum dynamics and their applications in chemistry and physics
9:50	Coffee Break (10 minutes)	
10:00	Ben Levine	Ab Initio Molecular Dynamics on Many Electronic States
10:50	Arthur Izmaylov	Quantum Chemistry on a Quantum Computer
11:40	Lunch (on your own, 1 hour 50 minutes)	
1:30	Leeor Kronik	Three generations of optimally-tuned density functionals for quantitative spectroscopy
2:20	Barry Dunietz	Dielectric Screened Range Separated Hybrid Functionals - A Polarization Consistent Framework for Describing Photoinduced Electron Transfer and Transport Processes
3:10	Coffee Break (10 minutes)	
3:20	Seung Kyu Min	Correlated Electron-Nuclear Dynamics Toward Extended Systems Based on Exact Factorization
4:10	Reserved	Reserved
Wednesday, Oct 4th		
Open time for Hike / Collaboration		
	Lunch (on your own)	
12:00		
1:30	Jerome Daligault	Nature of Non-Adiabatic Electron−Ion Forces in Liquid Metals and Warm Dense Matter
2:20	Dmitry Mozyrsky	Fermi Golden Rule in degenerate coupled plasmas
3:10	Coffee Break (10 minutes)	
3:20	Michael Galperin	Quantum thermodynamics of nanoscale molecular systems
4:10	Jianshu Cao	Quantum Diffusion in Organic Materials: Disorder, Phonons, and Photons
5:30	Meet at Oak ($25 gift card included w/ registration)	

Thursday, Oct 5th		
9:00	Eric Bittner	Non-equilibrium Stochastic exciton scattering dynamics
9:50	Coffee Break (10 minutes)	
10:00	Andrei Piryatinski	Nonequilibrium exciton-plasmon-polariton dynamics in nonlinear plasmonic nanostructures under a strong coupling regime with quantum emitters
10:50	Andre Schleife	Secondary electron emission from cold and hot graphene layers
11:40	Lunch (on your own, 1 hour 50 minutes)	
1:30	Lucien Dupuy	Developments in Exact Factorization-based mixed quantum-classical methods
2:20	Vitaly Rassolov	Factorized Electron-Nuclear Dynamics with an Effective Complex Potential
3:10	Coffee Break (10 minutes)	
3:20	Craig Martens	Surface Hopping Demystified
4:10	Austin Green	TBD
Friday, Oct 6th		
9:00	Vladimir Mandelstam	Magic numbers versus quantum delocalization and disordering in neutral and anionic hydrogen clusters
9:50	Coffee Break (10 minutes)	
10:00	Eleftherios Lambros	Proton Quantization as a Gateway to the Non-Adiabatic Regime
10:50	Basile Curchod	Driving new developments in excited-state molecular dynamics through challenging photochemical applications
11:40	Closing Remarks	
12:00	Lunch (on your own) / Collaboration Time	
5:00	End of Workshop	