

Telluride Workshop 2021
“Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy”

Telluride Intermediate School located at 725 W Colorado Ave, Telluride, CO 81435
 July 19th to 23rd

Room 1209

Sunday, July 18 th		
5:00-6:30	All-TSRC Meet and Greet Phoenix Bean located at 221 W. Colorado Ave <i>*The Phoenix Bean offers walk-up counter service for food and drink and is an easy place to get together prior to your workshop. Telluride Science staff will be there to welcome participants and distribute workshop badges.</i>	
Monday, July 19 th		
Breakfast (Grab and Go)		
8:30	Ben Levine	Nonadiabatic Dynamics on Many Electronic States
9:15	Craig Martens	Zombie Cats on the Quantum-Classical Frontier
10:00	Coffee Break	
10:15	Sophya Garaschuk	Quantum molecular dynamics with time-dependent Gaussian bases
11:00	Lin-Wang Wang	Natural orbital branching: a new algorithm for wave function collapsing in nonadiabatic MD simulations
11:45	Lunch (on your own)	
1:15	Sergei Tretiak	From NAMM method comparisons to modeling of coherent photoexcited dynamics
2:00	Tammie Nelson	Multiconfigurational Ehrenfest with ab initio multiple cloning (MCE-AIMC)
2:45	Coffee Break	
3:00	Mark Tuckerman	Machine learning the theorems of density functional theory
Tuesday, July 20 th		
Breakfast (Grab and Go)		
8:30	Jianshu Cao	Coherent dynamics induced by strong light-matter interactions
9:15	Pengfei Huo	Theoretical Investigations of Polariton Chemistry and Molecular Cavity Quantum Electrodynamics
10:00	Coffee Break	
10:15	Andre Piryatinski	Nonlinear response of plasmonic cavity and quantum emitters in the strong coupling regime
11:00	Eric Bittner	Multiexciton dynamics in organic and hybrid semiconductors: biexcitons and dark background processes
11:45	Lunch (on your own)	

1:15	Jacek Jakowski	Modeling electronic structure, dynamics and properties of conducting polymers for optoelectronic applications
2:00	Amanda Neukirch	Nonadiabatic Dynamics Shines Light on How to Best Harness Perovskite Properties for Use in Optoelectronic Devices
2:45	Coffee Break	
3:00	Barry Dunietz	Predictive description of photo or bias-induced electron transfer or transport processes through molecular-resolved interfaces using an environment polarization consistent framework
6:30-7:30	Town Talk: Sergei Tretiak "Telluride Transfer Warehouse" - 201 S Fir Street, Telluride	
Wednesday, July 21 st		
Breakfast (Grab and Go)		
8:30	Federica Agostini	Excited-state molecular dynamics with the exact factorization.
9:15	Neepa Maitra	A tale of two studies: (i) Exact-factorization-derived decoherence corrections, and (ii) Minimizing TDDFT errors in Ehrenfest dynamics
10:00	Coffee Break	
10:15	Spiridoula Matsika	Exploring nonadiabatic dynamics by modeling experimental observables
11:00	Michele Pavanello	Excited states of large systems with subsystem and orbital-free DFT
11:45	In-person group activity / collaboration time	
5:30	Telluride Science Group Picnic Outside at Telluride Intermediate School (Family & Friends welcome)	
Thursday, July 22 nd		
Breakfast (Grab and Go)		
8:30	Guanhua Chen	Revealing generation, migration and dissociation of electron-hole pairs and current emergence in an organic photovoltaic device
9:15	Michael Galperin	Nonadiabatic Dynamics and Spectroscopy in Single Molecule Junctions: A Green's Function Perspective
10:00	Coffee Break	
10:15	Maicol Ochoa	Electronic structure and transport in silicon nanostructures for quantum simulations and quantum computing
11:00	Ignacio Franco	Theory of dissipation pathways in open quantum systems
11:45	Lunch (on your own)	
1:15	Andre Schleife	Electron and ion dynamics in materials due to particle radiation and optical excitation
2:00	Xavier Andrade	INQ: a state-of-the-art implementation of TDDFT
2:45	Coffee Break	
3:00	Alfredo Correa	TBD
Friday, July 23 rd		
Breakfast (Grab and Go)		
8:30	Filipp Furche	Decoherence and multi-state nonadiabatic dynamics using TDDFT

9:15	Alexey Akimov	Including many-body effects in nonadiabatic dynamics of nanoscale systems.
10:00	Coffee Break	
10:15	Nancy Makri	Nonadiabatic dynamics of excitation energy transfer
11:00	Vitaly Rassolov	Energy flow in quantum systems