

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

Location: Telluride Intermediate School, 725 West Colorado Ave, Telluride

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 17 and ends at 1 pm on Friday, July 21 (the last half-day is reserved for group discussions, collaborations, etc.). The first half day of Wednesday, July 19 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 9 presentations on Monday and Tuesday, and 4 on Wednesday. On Thursday we will have a special joint session with two other workshops “*Regulating the Interfacial Physicochemical Processes of Organic Semiconductors by Design*” (Chad Risko and Natalie Stingelin) and “*Spontaneous Coherence and Collective Dynamics*” (Eric Bittner, Carlos Silva)

There is WELCOME RECEPTION on Sunday at the Phoenix Bean (Cash Bar). The Phoenix bean is located at 221 W. Colorado Ave Main Street. They are opening their coffee shop/ bar to scientists on Sunday nights with drink specials from 6:00-9:00pm. A representative from TSRC will be there 6-8pm to hand out badges

There is a Town Talk at the Conference Center in Mountain Village on Tuesday night from 6-7 pm. (Cash bar starts at 5:30 pm on Tuesday evening) and a TSRC Picnic/BBQ on Wednesday evening (6 pm – 9 pm under the tent at the Intermediate School).

Monday, July 17

Morning

8:30 am

Breakfast

9:00 am

Craig Martens, UC, Irvine

“Rigorous Trajectory-Based Methods for Simulating Nonadiabatic Dynamics”

9:40 am

Hans Lishka, U of Vienna

“Excitonic Coupling and Charge Transfer in Organic Semiconductor Polymers: Ab Initio and Density Functional Calculations”

10:20 am

Ignacio Franco, U of R

“Atomistic modeling of electromechanical spectroscopies in molecular junctions”

11:00 am

Coffee Break

11:15 am

Luis Rego, U de Santa Catarina

“Environmental effects on charge and energy quantum dynamics”

11:55 pm

Tammie Nelson, Los Alamos National Lab

“Electronic Delocalization, Vibrational Dynamics and Energy Transfer in Organic Chromophores”

12:35 pm

Lunch (on your own)

Afternoon

2:00 pm

Piryatinski Andrei, Los Alamos National Lab

“Fano resonances in Raman response of carbon nanotube bundles as signature of interacting intra- and inter-tube excitons”

2:40 pm

Sergei Shenogin, U of Dayton Research Institute

“Multiscale modeling of electron and thermal transport in CNT composites”

3:20 pm

Coffee Break

3:35 pm

Svetlana Kilina, North Dakota State U

“Comparing Contribution of Organic and Inorganic Surface Shells into Light-Driven Processes in Nanostructures”

4:15 pm

Vladimir Chernyak, Wayne State U

“TBA”

Tuesday, July 18

Morning

8:30 am

Breakfast

9:00 am

Ryoji Asahi, Toyota R&D Lab
“Theoretical study of semiconductor surface modifications for photocatalytic reactions”

9:40 am

Jorge Morales, Texas Tech U
“The Electron Nuclear Dynamics (END) Method and Its Applications to Cancer Proton Therapy Reactions and Other High-Energy Reactions”

10:20 am

Benjamin Nebgen, Los Alamos National Lab
“Ab-initio Based Methods for Simulating Molecular Properties on the Fly”

11:00 am

Coffee Break

11:15 am

Dmytro Kosenkov, Monmouth U
“Exciton Energy Transfer in Pigment-Protein Complexes”

11:55 pm

Ravithree Senanayake, Kansas State U
“Theoretical investigation of electron and nuclear dynamics in the [Au₂₅(SR)₁₈]-1 (R = CH₃, C₂H₅, MPA)”

12:35 pm

Lunch (on your own)

Afternoon

2:00 pm

Barros Kipton, Los Alamos National Lab
“Introduction to machine learning for quantum chemistry”

2:40 pm

James Lewis, West Virginia U
“Machine Learning to Evaluate Reaction Pathways from Nonadiabatic Molecular Dynamics Simulations”

3:20 pm

Coffee Break

3:35 pm

Artur Izmaylov, U of Toronto Scarborough
“Fully Quantum Nonadiabatic On-the-Fly Dynamics Accounting for Geometric Phases”

4:15 pm

Arindam Chakraborty, Syracuse U
“Development of effective stochastic potential method using random matrix theory for describing electronic excitation in noisy quantum systems”

6:00 pm

Town Talk, Telluride Conference Center in Mountain Village

Wednesday, July 19

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

Eric Bittner, U of Houston

“Kinetics and Dynamics of Charge and Energy Transfer at Organic Photovoltaic Interfaces”

2:40 pm

Dmitri Kilin, North Dakota State U

“Role of spin for excited state dynamics in nano-structures”

3:20 pm

Coffee Break

3:35 pm

Thomas Frauenheim, U of Bremen

“DFTB+ - An approximate DFT method: Applications to excited state simulations of nanomaterials”

4:15 pm

Sergei Tretiak, Los Alamos National Lab

“Advances and Promises of Layered Halide Hybrid Perovskites Semiconductors”

6:00 pm

Picnic, under the tent at the Intermediate School

Thursday, July 20

Joint session of workshops “*Regulating the Interfacial Physicochemical Processes of Organic Semiconductors by Design*” (Chad Risko and Natalie Stingelin), “*Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy*” (Alexey Akimov, Vladimir Chernyak, Sergei Tretiak) and “*Spontaneous Coherence and Collective Dynamics*” (Eric Bittner, Carlos Silva)

Morning

8:30 am *Breakfast*

9:00 am Oliver Kuhn, U of Rostock
“Exciton-Vibrational Dynamics in Natural and Artificial Light-Harvesting”

9:45 am Carlos Silva, Georgia Institute of Technology
“TBA”

10:30 am *Coffee Break*

10:45 am Andriy Zhugayevych, SkolTech, Moscow
“Modeling of conjugated polymers: non-oligomer approach”

11:30 am Natalie Banerji, University of Fribourg
“Excited- state properties and charge mobility in a doped conjugated polyelectrolyte”

12:15 pm *Lunch (on your own)*

Afternoon

2:00 pm Guglielmo Lanzani, Istituto Italiano di Tecnologia (IIT) at Politecnico di Milano
“Vibrational coherence in carbon conjugated materials”

2:45 pm Barry Dunitz, Kent U
“Predictive descriptions of voltage-biased or photo-induced processes through interfaces of molecular semi-conducting systems”

3:30 pm *Coffee Break*

3:45 pm Garry Rumbles, NREL
“Generating Long-lived Charges in Doped Conjugated Polymers: Controlling Carrier Delocalization”

4:30 pm Frank Pengfei, U of R
“Singlet fission and charge transfer quantum dynamics in organic photovoltaic”

Friday, July 21

8:30 am *Breakfast*

9:00 am – 1:00 pm Informal Discussions, Collaborations

1:00 pm Closure