TSIC Workshop

Reactive chemistry modeling in the age of AI

Dates
Tuesday, 16th – Saturday 20th of September 2025

Venue
Telluride Science & Innovation Center
300 South Townsend St., Telluride, CO

TSIC Host
Mark Kozak mark@telluridescience.org / 970.708.4426

Workshop organizer's contact phone:
Alejandro Lopez 865.360.9616

Breakfast
Breakfast will be served in the common area outside of the workshop classrooms.

Lunches
NOT included in registration.

Notes

Meet & Greet at Alibi – 121 S Fir St, Telluride, on Tuesday, Sept. 16th from 5:00 pm to 6:30 pm.

The scientific program starts at 9:00 am on Wednesday, Sept.17th, ends at noon on Saturday, Sept 20th.

Saturday 20th morning is reserved for group discussions, collaborations, etc.

Breakfast will be served at the Center each day at 8:30 am.

Snacks, coffee, and other drinks will be available throughout the day.

Thursday evening group dinner: TSIC will provide a gift card to each participant to Oak, a casual and an easy place to gather, a couple of blocks away from the Conference Center.

Each presenter is scheduled for a total of 35 minutes with about 5-10 minutes for Q&A.

Interruptions and questions during talks are encouraged.

All times are in Mountain Time Zone.

Wednesday, 17th of September

Morning

8:30 am	Breakfast
9:00 am	Opening remarks/Welcome (Organizers & Mark Kozak)
9:05 am	**Anders Niklasson** (**Los Alamos National Laboratory**) *Workshop presentation*
9:15 am	**David Yaron** (***Carnegie Mellon University***) *Learning Semiempirical Quantum Chemical Models from Data*
10:00 am	**Nir Goldman** (**Lawrence Livermore National Laboratory**) *ML-driven simulations of reactive materials: Energetic Materials, Astrobiology, and Actinide Corrosion*
10:45 am	Break
11:15 am	**Michael Wall** (**Los Alamos National Laboratory**) *Fast Graph-Based Quantum-Mechanical Molecular Dynamics Simulations on AI Supercomputers*
12:00 am	Lunch (on your own)

Afternoon

1:30 pm	**Susan Atlas** (**University of New Mexico**) *Latent space design of reactive charge-transfer force fields*
2:15 pm	**Cheng-Han Li** (**Los Alamos National Laboratory**) *Shadow Molecular Dynamics with Machine-Learned Flexible Charges: Combining Speed, Stability, and Accuracy*
3:00 pm	Break
3:30 pm	**Rae Corrigan Grove** (**Los Alamos National Laboratory**) *Shadow Molecular Dynamics with Flexible Multipoles: Towards Accurate and Stable Electrostatics for Machine Learned Interatomic Potentials*
4:15 pm	
5:00 pm	**Adjourn**

Thursday, 18th of September

Morning

8:30 am	Breakfast
	Free morning
12:30 pm	**Anna Delin** (**Royal Institute of Technology, Sweden**) *Harnessing AI-Inspired Techniques to Explore Topological Spin Structures*
1:15 pm	**Yihan Shao** (**University of Oklahoma**) *Enzyme Reaction Modeling with Machine Learning*
2:00 pm	Break
2:30 pm	**Jacek Jakowski** (**Oak Ridge National Laboratory**) *Modeling Reactive Dynamics: Real-Time Electronic Structure and Beyond*
3:15 pm	**Anders Niklasson** (**Los Alamos National Laboratory**) *Quantum-Mechanical Molecular Dynamics using Deep-NN solvers and AI-Hardware*
4:00 pm	Panel session & discussions *Teaching Machines: Flexible Charges, Polarization, and Spin for Complex Systems; AI hardware acceleration for general scientific calculations; On-the-fly AI-guided analysis of atomistic simulations; Future directions, …*
5:00 pm	**Adjourn**

Friday, 19th of September

Morning

8:30 am	Breakfast
9:00 am	**Romain Perriot** (**Los Alamos National Laboratory**) *Atomistic simulations of energetic materials I*
9:45 am	**William Bricker** (**University of New Mexico**) *Machine-learned electronic structure for biomolecules: Theory and applications*
10:30 am	Break
11:00 am	**Seaton Ullberg** (**Los Alamos National Laboratory**) *High-throughput computations of energetic materials*
11:45 am	Lunch (on your own)

Afternoon

1:30 pm	**Ming Chen** (**University of Purdue**) *Beyond Foundation Model: Guided Sampling of Protein Conformations*
2:15 pm	**Christian Negre** (**Los Alamos National Laboratory**) *SEDACS: Scalable Ecosystems, Driver and Analyzer for Complex Chemistry Simulations*
3:00 pm	**Anders Niklasson** (**LANL**) *Closing remarks on the future of atomistic modeling in the age of AI*
4:30 pm	***Adjourn***

Saturday, 20th of September

Morning

8:30 am	*Breakfast*
9:00 am	*Informal Discussions, Collaborations, ...*