Machine Learning and Informatics for Chemistry and Materials

Telluride Workshop

Dates: September 7–11, 2025

Location: Telluride Science & Innovation Center 300 S. Townsend St. Telluride, CO 81435
TSRC Host: Mark Kozak mark@telluridescience.org / 970.708.4426
Breakfast: served at Telluride Science & Innovation Center at 7:30am everyday.
Lunches and dinners are NOT included in registration.

The scientific program starts at 8:15 am on Sunday, September 7th and ends at 12:00 pm on Thursday, September 11th. Tuesday morning, September 9th is reserved for group activity (hike). Thursday, September 11th is reserved for code sharing, tutorials, demos, group discussions, collaborations, etc. Each talk is scheduled for 25 minutes + 10 minutes for discussion. Interruptions and questions during talks are encouraged.

Meet & Greet: Informal gathering before the workshop; badges will be available for pickup. This is a good chance to meet up with fellow participants before your meeting. The venue hosts live music later in the evening - this time window is planned for a quieter meet-up.
When: Saturday, September 6, 2025, 5:00–6:30 pm
Where: Cash-bar The Alibi, 121 S Fir St, Telluride, CO 81435

All times are Mountain Time (MT).

Sunday, September 7, 2025

7:30–8:15	Breakfast
8:15–8:30	Introductory Remarks

Morning Session

8:30–9:05	**Nima Karimitari**, University of South Carolina *"A Generalized Machine-learned Interatomic Potential for Chemical Reaction Pathways and Transition States"*
9:05–9:40	**Michael Kilgour**, New York University *"Geometric Deep Learning for the Molecular Solid State"*
9:40–10:00	Coffee Break
10:00–10:35	**Mary Alice Cusentino**, Sandia National Laboratory *"Atomistic Modeling of Materials for Fusion Energy using Machine Learned Interatomic Potentials"*
10:35–11:10	**Gia-Wei Chern**, University of Virginia *"TBD"*
11:10–1:00	Lunch (on your own)

Afternoon Session

1:00–1:35	**Rodrigo Freitas**, Massachusetts Institute of Technology *"Machine Learning for Chemistry–Microstructure Interactions"*
1:35–2:10	**Massimiliano Lupo-Pasini**, Oak Ridge National Laboratory *"Multi-Task Parallelism for Robust Pre-Training of Graph Foundation Models on Multi-Source, Multi-Fidelity Atomistic Modeling Data"*
2:10–2:30	Coffee Break
2:30–3:05	**Yulia Pimonova**, Los Alamos National Laboratory *"Adaptive Linear Models via Meta-Learning for Molecular Property Prediction"*
3:05–3:40	**Jith Subramanian**, Toyota Research Institute *"Structure Agnostic Multimodal Learning for Materials Science"*

Monday, September 8, 2025

7:30–8:30	Breakfast

Morning Session

8:30–9:05	**Olexandr Isayev**, Carnegie Mellon University *"TBD"*
9:05–9:40	**Megan J. McCarthy**, Sandia National Laboratory *"Keeping It Simple (or Not): Tackling Complexity in the Training of Machine Learning Models"*
9:40–10:00	Coffee Break
10:00–10:35	**Arun Mannodi Kanakkithodi**, Purdue University *"ML-Augmented First Principles Simulations for Understanding Point Defects and Designing Next-Generation Semiconductors"*
10:35–11:10	**Ganesh Sivaraman**, University at Buffalo *"TBD"*
11:10–1:00	Lunch (on your own)

Afternoon Session

1:00–1:35	**Oleg Prezhdo**, University of New Mexico *"Nonadiabatic Molecular Dynamics with Machine Learning"*
1:35–2:10	**Maksim Kulichenko**, Los Alamos National Laboratory *"Leveraging AI Hardware and Graph Theory for Large Scale Quantum Simulations"*
2:10–2:30	Coffee Break
2:30–4:00	Group Activity — AI in Science Group Discussion

Tuesday, September 9, 2025

7:30–8:30	Breakfast
8:30–12:00	Group Activity — Hike
12:00–1:30	Lunch (on your own)

Afternoon Session

1:30–2:05	**Aurora Clark**, University of Utah *"Opportunities and Challenges in Feature Selection for Solution Phase"*
2:05–2:40	**Nicholas Lubbers**, Los Alamos National Laboratory *"Knowledge Distillation for Augmenting Atomistic Datasets"*
2:40–3:00	Coffee Break
3:00–3:35	**Robert Paton**, Colorado State University *"TBD"*
3:35–4:10	**Alexei Kananenka**, University of Delaware *"Accelerating Quantum Dynamics Simulations with Machine Learning"*

Wednesday, September 10, 2025

7:30–8:30	Breakfast
Morning Session	
8:30–9:05	**Avanish Mishra**, Los Alamos National Laboratory *"Accelerating Materials Discovery via Generative AI"*
9:05–9:40	**Igor Poltavskyi**, University of Luxembourg *"Crash Testing Machine Learning Force Fields for Molecules, Materials, and Interfaces"*
9:40–10:00	Coffee Break
10:00–10:35	**Christopher Sutton**, University of Toronto *"TBD"*
11:10–1:00	Lunch (on your own)
5:30–7:00	Group Picnic at Telluride Science & Innovation Center

Thursday, September 11, 2025

7:30–8:30	Breakfast
Morning Session	
8:30–11:30	Code sharing, tutorials, informal chats
11:30–12:00	Closing remarks