**Telluride Workshop**

**“*Machine Learning and Informatics for Chemistry and Materials***

Location: The Depot  
300 S. Townsend St. Telluride, CO 81435

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

Breakfast: served at the Depot starting at 7:30am each day.

Lunches are NOT included in registration

The scientific program starts at 8:10 am on Monday, October 3rd and ends at 1:00 pm on Friday, October 7th. Wednesday Morning, October 5th is reserved for group activity. Friday, October 7th is reserved for code sharing, tutorials, demos, group discussions, collaborations, etc.

Each talk is scheduled for 30 minutes + 10 minutes for discussion. Interruptions and questions during talks are encouraged.

There will be a group dinner at Oak, date will be decided on the first day of the workshop.

Participants will be provided $25/person gift cards to Oak on Monday morning.

All times shown are Mountain Time (MT).

Zoom link:

**Monday, October 3**

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| **Morning** |  |  |
| *7:30 am* | *Breakfast* |  |
| 8:10 am | Joel Bowman, Emory University “*Machine Learning and* D*-Machine Learning for Potentials and “Exact” Rate Constants: Contrasts in Data Availability*” | (online) |
| 8:50 am | Aditi Krishnapriyan  “*Physics-based machine learning with differentiable solvers*” | (in person) |
| *9:30 am* | *Coffee Break* |  |
| 9:50 am | Wissam Saidi, University of Pittsburgh “*Accelerating Simulations-Assisted Materials Design Using Machine Learning*” | (in person) |
| 10:30 am | Connor Coley, MIT “*AI for Chemical Space Navigation*” | (online) |
| *11:10 pm* | *Lunch (on your own)* |  |
| **Afternoon** |  |  |
| 1:10 pm | Y Z, University of Michigan “*Interpretation of Autoencoder Generated Collective Variables Using Morse-Smale Complex* | (in person) |
| 1:50 pm | Andrew White, University of Rochester “*Large language models understand chemistry, but can we understand them*” | (in person) |
| *2:30 pm* | *Coffee Break* |  |
| 2:50 pm | Michael Taylor, Los Alamos National Laboratory "*Architector: towards learning across the mononuclear periodic table*” | (in person) |
| 3:30 pm | Olexander Isayev, Carnegie Mellon University “*Neural Networks Learning Chemical Reactivity*” | (online) |

**Tuesday, October 4**

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| **Morning** |  |  |
| *7:30 am* | *Breakfast* |  |
| 8:10 am | Michele Ceriotti, EPFL, Switzerland “*Blurring the lines between quantum chemistry and machine learning*” | (online) |
| 8:50 am | Moritz Thürlemann, ETH Zürich “*Regularized by Physics: Graph Neural Network Parametrized Force Fields*” | (in person) |
| *9:30 am* | *Coffee Break* |  |
| 9:50 am | Christopher Sutton, University of South Carolina “*Machine learning of experimental datasets to enable materials discovery*” | (in person) |
| 10:30 am | Nikita Fedik, Los Alamos National Laboratory “*Machine learnable chemical properties along the atomistic scale*” | (in person) |
| *11:10 pm* | *Lunch (on your own)* |  |
| **Afternoon** |  |  |
| 1:10 pm | Oleg Prezhdo, University of Southern California,  “*Accelerating and Analyzing Nonadiabatic Molecular Dynamics with Machine Learning*” | (online) |
| 1:50 pm | Artur Meller, Washington University in St. Louis  “*Predicting the locations of cryptic pockets from single structures using graph neural networks*” | (in person) |
| *2:30 pm* | *Coffee Break* |  |
| 2:50 pm | Matthew Carbone, Brookhaven National Laboratory *“Forward and inverse modeling of molecules and materials”* | (in person) |
| 3:30 pm | Nick Lubbers, Los Alamos National Laboratory “*Lightweight and Effective Tensor Sensitivity for Atomistic Neural Networks*” | (in person) |

**Wednesday, October 5**

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| **Morning** |  |  |
| *7:30 am* | *Breakfast* |  |
| 8:30 am | Group Activity TBD |  |
| *12:00 pm* | *Lunch (on your own)* |  |
| **Afternoon** |  |  |
| 2:00 pm | Gabe Gomes, Carnegie Mellon University “*Stereoelectronics-Aware Molecular Representation Learning*” | (in person) |
| 2:40 pm | Teresa Head-Gordon, UC Berkeley “*Physics-Inspired Machine Learning Methods: A Status Report on Predictive Chemistry*” | (online) |
| *3:20 pm* | *Coffee Break* |  |
| 3:40 pm | Maksim Kulichenko, Los Alamos national Laboratory “*Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials*” | (in person) |
| 4:20 pm | Robert Paton, Colorado State University “*Predictions of organic reactivity & selectivity with QM and ML*” | (in person) |

**Thursday, October 6**

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| **Morning** |  |  |
| *7:30 am* | *Breakfast* |  |
| 8:10 am | Markus Reiher, ETH Zurich “*Quantum chemical roots of machine-learning molecular similarity descriptors*” | (online) |
| 8:50 am | Heather Kulik, MIT “*Overcoming challenges of data scarcity and data quality for machine learning*” | (online) |
| *9:30 am* | *Coffee Break* |  |
| 9:50 am | Reinhard Maurer, University of Warwick “*Machine learning of electronic structure for quantum dynamics and molecular design”* | (online) |
| 10:30 am | Adela Habib, Los Alamos national Laboratory “*Atomistic simulation of plasmonic hot carriers in silver nanoparticles using machine learning*” | (in person) |
| *11:10 pm* | *Lunch (on your own)* |  |
| **Afternoon** |  |  |
| 1:10 pm | Daniel Schwalbe-Koda, Lawrence Livermore National Laboratory “*Exploring materials synthesis landscapes with high-throughput simulations, machine learning, and adversarial attacks*” | (in person) |
| 1:50 pm | Peter St John, National Renewable Energy Laboratory  “*Reinforcement learning for battery material design*” | (in person) |
| *2:30 pm* | *Coffee Break* |  |
| 2:50 pm | Ben Nebgen, Los Alamos national Laboratory “*Interfacing Metallic Machine Learned Interatomic Potentials with Experiment*” | (in person) |

**Friday, October 7**

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| **Morning** |  |  |
| *7:30 am* | *Breakfast* |  |
| 8:10 am | Code sharing/tutorials |  |
| *1:00 pm* | Closure / Informal Discussions, Collaborations |  |