Telluride Workshop

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

Location: Ah Haa School for the Arts, 155 W Pacific Ave, Telluride, CO 81435
Launchpad room, top floor.

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

Breakfast: Gift cards to Baked, across from Ah Haa School for the Arts.

Lunches are NOT included in registration.

The scientific program starts at 9:00 am on Monday, September 27th and ends at noon on Friday, October 1st. Wednesday Morning, September 29th is reserved for group activity. Friday, October 1st is reserved for 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 meet and greet, Sunday, September 26 5:00 to 6:30 pm at the Phoenix Bean.

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

All times shown are Mountain Time (MT).

Zoom link: https://zoom.us/j/91844081005?pwd=VlpVb0xJdk1OZUk5Q2FGenB6enB6UT09

Monday, September 27

Morning

8:30 am *Breakfast*

9:00 am Pavlo Dral, Xiamen University
"Quantum Chemistry Assisted by Machine Learning"

9:40 am Andrea Grisafi, École Polytechnique Fédérale de Lausanne
"Symmetry-adapted and long-range representations in atomic-scale machine learning"

10:20 am *Coffee Break*

10:40 am David Pfau, DeepMind
"Deep Neural Networks for Ab Initio Quantum Chemistry"

11:20 am Matthew Foulkes, Imperial College London
"Approximating Many-Electron Wave Functions using Deep Neural Networks"

12:00 pm *Lunch (on your own)*

Afternoon

2:00 pm Anton Oliynyk, Manhattan College
"Inorganic Crystal Structure Prediction Problems: Data, Descriptors, and Discovery Acceleration"

2:40 pm Sameer Varma, University of South Florida
"Toward machine learning molecular dynamics."

3:20 pm *Coffee Break*

3:40 pm Luis Briceno-Mena, Louisiana State University
"Machine Learning and Model Thin Films for High-Temperature Polymer Electrolyte Membrane (HT-PEM) Fuel Cells"

4:20 pm Kipton Barros, Los Alamos National Laboratory
"Exploring approaches to charge equilibration in ML potentials"

Tuesday, September 28

Morning

8:30 am *Breakfast*

9:00 am Cecilia Clementi, Freie Universität Berlin
"Learning molecular models by machine learning and experimental data"

9:40 am Gábor Czakó, University of Szeged
"Automated potential energy surface developments for chemical reaction dynamics simulations"

10:20 am C*offee Break*

10:40 am Tomas Kubar, Karlsruhe Institute of Technology
"Machine learning potentials for molecular dynamics simulation of condensed phase reactions"

11:20 pm Tim Mueller, Johns Hopkins University
"Machine-learned interatomic potential models for practical applications"

12:00 pm *Lunch (on your own)*

Afternoon

2:00 pm Johannes Hachmann, University at Buffalo, SUNY
"Tailoring Machine Learning for the Chemistry Domain"

2:40 am Matthew Welborn, Entos, Inc.
"Towards a Foundation Model for Quantum Chemistry"

3:20 pm *Coffee Break*

3:40 pm Guoqing Zhou, Los Alamos National Laboratory
"Machine Learning with Domain Knowledge in Quantum Chemistry"

4:20 pm Jason Goodpaster, University of Minnesota Twin Cities
"Neural Network Potentials for Reactive Chemical Simulations"

Wednesday, September 29

Morning

8:30 am *Breakfast*

9:00 am Group Activity
TBD

12:00 pm *Lunch (on your own)*

Afternoon

2:00 pm Matthias Ihme, Stanford University
TBD

2:40 pm Steve Whitelam, Lawrence Berkeley National Laboratory
"Learning to Grow: Control of Materials Self-Assembly Using Evolutionary Reinforcement Learning"

3:20 pm *Coffee Break*

3:40 pm Taylor Sparks, University of Utah
"Discovery of Novel Inorganic Crystal Structures via GANs"

4:20 pm Alejandro Lopez-Bezanilla, Los Alamos National Laboratory
"Data-Driven Solution of PDEs with a Machine Learning-Based Algorithm."

5:00 pm Olexander Isayev, Carnegie Mellon University
"TBD"

Thursday, September 30

Morning

8:30 am	*Breakfast*
9:00 am	Jörg Behler, University of Göttingen "Four Generations of Neural Network Potentials"
9:40 am	Bjork Hammer, Aarhus University "Global optimization with image recognition and reinforcement learning"
10:20 am	C*offee Break*
10:40 am	Kim Jelfs, Imperial College London "Remembering the lab in computational molecular material discovery"
11:20 am	Keith Butler, Rutherford Appleton Laboratory "Matrices, Graphs and Natural Language—Ways to Represent Materials for Machine Learning."
12:00 pm	*Lunch (on your own)*
2:00 pm	Francesca Tavazza, National Institute of Standards and Technology "Uncertainty prediction for regression models of crystalline material properties"
2:40 am	Ian Robinson, Brookhaven National Laboratory "Machine Learning Improvements to Coherent Imaging of Nanocrystals"
3:20 pm	*Coffee Break*
3:40 pm	Ben Nebgen, Los Alamos National Laboratory "Automated discovery of metallic interatomic potentials."
4:20 pm	Anjana Talapatra, Los Alamos National Laboratory "A hierarchical machine learning based screening strategy for discovery of novel scintillator chemistries"

Friday, October 1

8:30 am	*Breakfast*
9:00 am	Informal Discussions, Collaborations, Demos
1:00 pm	Closure