Telluride Workshop

"Machine Learning and Informatics for Chemistry and Materials"

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 each day.

Lunches are NOT included in registration

The scientific program starts at 8:10 am on Monday, October 14th and ends at 12:00 pm on Friday, October 18th. Wednesday morning, October 16th is reserved for group activity. Friday, October 18th is reserved for code sharing, tutorials, demos, group discussions, collaborations, etc.

Each talk is scheduled for 25 minutes + 15 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. Gift cards to Oak will be provided for each participant.

Cash-bar Meet & Greet at Alibi – 157 S. Fir Street on Sunday, October 13, from 5:00pm to 6:30pm. This is a good chance to meet up with fellow participants before your meeting. A staff member will be on hand to welcome you, distribute badges, and answer questions.

All times shown are Mountain Time (MT).

Monday, October 14

Morning

7:30 am	*Breakfast*
8:20 am	*Pinhead Institute*
8:30 am	*Introductory remarks*
8:40 am	Scott Reed, University of Colorado Denver *"Optimizing GPTs for research in molecular sciences while minimizing hallucinations"*
9:20 am	Yasemin Basdogan, University of Rochester *"Machine Learning-Guided Discovery of Polymer Membranes for Gas Separation with Genetic Algorithm"*
10:00 am	*Coffee Break*
10:30 am	Aikaterini Vriza, Argonne National Laboratory "AI-guided inverse design of functional polymers"
11:10 am	Justin Smith, NVIDIA ""
11:50 pm	*Lunch (on your own)*

Afternoon

1:40 pm	Michelle Kelley, Rensselaer Polytechnic Institute *"A Universal Machine-Learning Approach for Approximating Nonlocal Functionals in Electronic and Classical DFT"*
2:20 pm	Matthew R. Carbone, Brookhaven National Laboratory ""
3:00 pm	*Coffee Break*
3:30 pm	Mike Tynes, University of Chicago ""
4:10 pm	Robert Paton, Colorado State University ""

Tuesday, October 15

Morning

7:30 am	*Breakfast*
8:20 am	Rebecca Lindsey, University of Michigan “”
9:00 am	Brian DeCost, NIST “”
9:40 am	*Coffee Break*
10:10 am	Wissam Saidi, National Energy Technology Lab *“Modeling Extreme Environments with Machine Learning Atomistic Potentials”*
10:50 am	Yulia Pimonova, Los Alamos National Laboratory *“Substructural Meta Learning for Interpretable Cheminformatics”*
11:30 pm	*Lunch (on your own)*

Afternoon

1:20 pm	Maksim Kulichenko, Los Alamos National Laboratory “”
2:00 pm	Steven Torrisi, Toyota Research Institute *“Towards Closing the ML / Experiment Gap in Synthesis & Characterization”*
2:40 pm	James Goff, Sandia National Laboratories “”

Wednesday, October 16

Morning

7:30 am *Breakfast*

8:30 am Group Activity
TBD

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

Afternoon

1:50 pm Aditi Krishnapriyan, University of California, Berkeley
“”

2:30 pm Massimiliano Lupo-Pasini, Oak Ridge National Laboratory
“”

3:10 pm *Coffee Break*

3:40 pm Harry Moore, University of Cambridge
“Biomolecular Free Energy Calculations at Ab Initio Accuracy with Machine Learned Potentials”

4:20 pm Benjamin Kurt Miller, University of Amsterdam
“FlowMM and more: Generative Models for proposing material candidates”

Thursday, October 17

Morning

7:30 am *Breakfast*

8:20 am Dmitry Zubarev, IBM
“”

9:00 am Teerachote Pakornchote, University of South Carolina
“”

9:40 am *Coffee Break*

10:10 am Wenhao Gao, Massachusetts Institute of Technology
“”

10:50 am Adil Kabylda, University of Luxembourg
“Molecular Simulations with a Pretrained Neural Network and Universal Pairwise Force Fields”

11:30 pm *Lunch (on your own)*

Afternoon

1:20 pm Christopher Sutton, University of South Carolina
“”

2:00 pm Nick Lubbers, Los Alamos National Laboratory
“”

Friday, October 18

Morning

7:30 am	*Breakfast*
8:20 am	Code sharing/tutorials
12:00 pm	Closure / Informal Discussions, Collaborations