**Telluride Workshop**

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

Location: Telluride Intermediate School  
721 W. Colorado Ave Telluride, CO 81435

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

Breakfast: served at the Telluride Intermediate School at 7:30am each day.

Lunches are NOT included in registration

The scientific program starts at 8:10 am on Sunday, June 25th and ends at 12:00 pm on Thursday, June 29th. Tuesday morning, June 27th is reserved for group activity. Thursday, June 29th 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 the All-Telluride Science Picnic on Wednesday. Free BBQ, Beer, Wine and Non-Alcoholic Beverages. Friends and Family are invited free of charge.

All times shown are Mountain Time (MT).

**Sunday, June 25**

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| **Morning** |  |
| *7:30 am* | *Breakfast* |
| 8:10 am | Albert Musaelian  *“Scaling up equivariant potentials”* |
| 8:50 am | Daniel Schwalbe Koda, Lawrence Livermore National Laboratory  *“Data efficiency and extrapolation trends in neural network interatomic potentials”* |
| *9:30 am* | *Coffee Break* |
| 9:50 am | Aditya Nandy, MIT  *“Data-driven exploration of transition metal complexes and metal-organic frameworks by leveraging computational and experimental data”* |
| 10:30 am | Arun Mannodi Kanakkithodi, Purdue University  *“Discovering Novel Halide Perovskites using Multi-Fidelity Machine Learning and Graph Neural Networks”* |
| *11:10 pm* | *Lunch (on your own)* |
| **Afternoon** |  |
| 1:10 pm | Mingjie Liu, University of Florida  *“Data-driven computational platform for carbon-based materials in energy applications”* |
| 1:50 pm | Dylan Anstine, Carnegie Mellon University  *“Neural Networks for Diverse Species and Chemical Reactions”* |
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**Monday, June 26**

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| **Morning** |  |
| *7:30 am* | *Breakfast* |
| 8:10 am | Michael Chen, Stanford University  *“Transfer learning for the data-efficient modeling of ab initio ground and excited state potential energy surfaces for condensed phase systems”* |
| 8:50 am | Alice Allen, Los Alamos National Laboratory  *“Learning Together: Training interatomic potentials to multiple datasets”* |
| *9:30 am* | *Coffee Break* |
| 9:50 am | Aparna Subramanyam, Los Alamos National Laboratory  *“Training data generation for machine learning-based interatomic potentials”* |
| 10:30 am | Sameer Varma, University of South Florida  *“Machine learning of molecular dynamics”* |
| *11:10 pm* | *Lunch (on your own)* |
| **Afternoon** |  |
| 1:10 pm | Steven Torrisi, Toyota Research Institute  *“The Role of Materials Representations in Machine Learning”* |
| 1:50 pm | Ganesh Sivaraman, Argonne National Laboratory  *“Accelerating the Modeling of Materials with Machine Learning and High Energy X-ray Diffraction”* |
| 2:30 pm | Muratahan Aykol, Google Brain  *“Accelerating materials discovery and synthesis by combining physics with machine learning”* |

**Tuesday, June 27**

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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 | Todd Martinez, Stanford University  *“Delta Machine Learning for Basis Set Incompleteness and Neural Nets for Molecular Image Captioning* |
| 2:40 pm | David Balcells, University of Oslo  *“Machine Learning for Metal-Organic Chemistry”* |
| *3:20 pm* | *Coffee Break* |
| 3:40 pm | Maksim Kulichenko, Los Alamos national Laboratory *“Advancing Semiempirical Quantum Chemistry with Extended Lagrangian and Machine Learning”* |
| 4:20 pm | Seonah Kim, Colorado State University *“Computational Design Principles for Sustainable Chemistry: from Biomass to Renewable Biofuel and Biomaterials”* |

**Wednesday, June 28**

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| **Morning** |  |
| *7:30 am* | *Breakfast* |
| 8:10 am | Aidan Thompson, Sandia National Laboratories  *“The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources”* |
| 8:50 am | Grant M. Rotskoff, Stanford University |
| *9:30 am* | *Coffee Break* |
| 9:50 am | Fang Liu, Emory University  *“Machine learning aided quantum chemistry discovery in the solution phase”* |
| 10:30 am | Christopher Sutton, University of South Carolina *“Training reliable machine learned potentials for simulating the behavior of liquids under an external potential”* |
| *11:10 pm* | *Lunch (on your own)* |
| **Afternoon** |  |
| 1:10 pm | Rebecca K. Lindsey, University of Michigan  *“The ChIMES ML Interatomic Model: Recent Developments Toward Enhanced Robustness and Transferability”* |
| 1:50 | Nick Lubbers, Los Alamos National Laboratory |
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**Thursday, June 29**

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| **Morning** |  |  |
| *7:30 am* | *Breakfast* |  |
| 8:10 am | Code sharing/tutorials |  |
| *12:00 pm* | Closure / Informal Discussions, Collaborations |  |