Telluride Workshop

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

Location: Telluride Fire House, 131 West Columbia Ave. Telluride, CO 81435

TSRC Host: Mark Kozak mark@telluridescience.org / 970.708.4426
TSRC Managing Director: Cindy Fusting cindy@telluridescience.org / 970.708.5069

Breakfast will be served daily before the talks at the workshop location.

Lunches are NOT included in registration.

The scientific program starts at 9:00 am on Monday, October 1st and ends in the afternoon on Friday, October 5th (the last day is reserved for small group discussions, collaborations, etc.). Wednesday, October 3rd is reserved for group discussions, collaborations, etc.

Each talk is scheduled for 35 minutes + 5 minutes for discussion. Interruptions and questions during talks are encouraged.

There will be a group dinner at Village Table (located in Mountain Village) on Wednesday night, 6pm.

Monday, October 1

Morning

8:30 am	*Breakfast*
9:00 am	Arthur Mar, University of Alberta "Accelerating the discovery of solid state materials: From traditional to machine-learning approaches"
9:40 am	David Yaron, Carnegie Mellon University "A Density functional tight binding theory layer for deep learning of electronic properties"
10:20 am	C*offee Break*
10:40 am	Olexander Isayev, University of North Carolina, Chapel Hill "AI driven design of molecules and materials"
11:20 am	Arindam Chakraborty, Syracuse University "Solving the stochastic Kohn-Sham equation: Unraveling structure in random matrices using deep artificial neural networks"
12:00 pm	*Lunch (on your own)*

Afternoon

2:00 pm	Sorelle Friedler, Haverford College "Interpretable machine learning for scientific discovery"
2:40 pm	Ghanshyam Pilania, Los Alamos National Laboratory "Machine learning for high throughput screening of potential scintillator chemistries"
3:20 pm	*Coffee Break*
3:40 pm	Nicholas Lubbers, Los Alamos National Laboratory "Hierarchically Interacting Particle Neural Networks"
4:20 pm	Yu-Hang Tang, Lawrence Berkeley National Laboratory "Predicting molecular energy using graph kernels and active learning"

Tuesday, October 2

Morning

8:30 am	*Breakfast*
9:00 am	David Koes, University of Pittsburg "Deep learning for structure-based drug design"
9:40 am	Jason Goodpaster, University of Minnisota, Twin Cities "Machine learning of electron correlation for full configuration interaction"
10:20 am	C*offee Break*
10:40 am	Ying Wai Li, Oak Ridge National Laboratory "Model Hamiltonian construction from materials properties"
11:20 am	Matthew Welborn, Caltech "Transferable learning of correlation energy from molecular orbital features"
12:00 pm	*Lunch (on your own)*

Afternoon

2:00 pm	Xian-Guo Li, University of San Diego "Quantum-accurate force fields from machine learning of large materials data"
2:40 pm	Justin Smith, Los Alamos National Laboratory "Accurately predicting experimental observations with neural network potentials"
3:20 pm	*Coffee Break*
3:40 pm	Heather Kulik "Accelerating inorganic discovery with machine learning and automation"
4:20 pm	Yousung Jung, Korea Advanced Institute of Science and Technology "Machine learning approaches for materials discovery: Predictive and generative models"

Wednesday, October 3

Morning

8:30 am	*Breakfast*
9:00 am – 12:30 pm	Informal Discussions, Collaborations on ML for materials
12:00 pm	*Lunch (on your own)*

Afternoon

2:00 pm – 4:00 pm	Informal Discussions, collaborations on ML for methods
6:30 pm – 8:00 pm	Group dinner, 6pm, Village Table (located in Mountain Village)

Thursday, October 4

Morning

8:30 am	*Breakfast*
9:00 am	James Lewis, West Virginia University "Machine learning approach for designing catalysts and evaluating reaction mechanisms"
9:40 am	Sameer Varma, University of South Florida "ML approaches for evaluating correlations and causalities in allosteric signaling"
10:20 am	C*offee Break*
10:40 am	Alejandro Lopez-Bezanilla, Los Alamos National Laboratory "Modeling quantum physics with machine learning: Transmission coefficients and density of states"
11:20 am	Koji Tsuda, University of Tokyo "Designing complex materials with machine learning: organic compounds, metamaterials and proteins"
12:00 pm	*Lunch (on your own)*
2:00 pm	Kipton Barros, Los Alamos National Laboratory "Challenges and opportunities in ML for strongly correlated electron materials"
2:40 pm	Marina Meila, Washington State University "Understanding configuration spaces of molecules with manifold learning"
3:20 pm	Sergei Tretiak, Los Alamos National Laboratory "Machine learning for molecular properties"
4:20 pm	Concluding remarks, path forward

Friday, October 5

8:30 am	*Breakfast*
9:00 am – 1:00 pm	Informal Discussions, collaborations, small group meetings
1:00 pm	Closure