Machine Learning and Informatics for Chemistry and Materials

September 30th through October 4th, 2019

Telluride Science Research Center

Located in the Telluride Firehouse at 131 W Columbia Ave Telluride, CO 81435.

Workshop Details

Meet and Greet
TSRC will host a Meet and Greet event at the Phoenix Bean (221 W Colorado Ave.) on Sunday, September 29th from 5:00 to 6:30pm. The Phoenix Bean offers walk-up counter service for food and drink and is an easy place to get together prior to your workshop.

Workshop Location
The workshop will be held in the meeting room at the Telluride Firehouse located at 131 W Columbia Ave Telluride, CO 81435.

Information
Conference committee:

- Justin S. Smith (Just@lanl.gov; 205-335-3278)
- Benjamin Nebgen
- James Lewis
- Adrian E. Roitberg
- Sergei Tretiak

TSRC Contact Info:
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Schedule

Monday, September 30th

Breakfast	7:30am-8:30am
Thomas Hammerschmidt, ICAMS, Ruhr University Bochum *Electronic-structure based descriptors of local atomic environments*	8:30am-9:20am
Kipton Barros, Los Alamos National Lab *Towards fully automated machine learning of molecular dynamics potentials*	9:20am-10:10am
Break	10:10am-10:25am
David Yaron, Carnegie Mellon University *Deep Learning of Electronic Hamiltonians*	10:25am-11:15am
Ben Nebgen, Los Alamos National Lab *Resurrecting Huckel Theory with Machine Learning*	11:15am-12:05pm
Lunch (on your own)	12:05pm-1:30pm
Open time for Hike/Collaboration	1:30pm-5:00pm

Tuesday, October 1st

Breakfast	7:30am-9:00am
Open time for Hike/Collaboration	9:00am-11:45am
Lunch (on your own)	11:45am-1:00pm
Jenna A. Pope, Pacific Northwest National Lab *Better Learning Through Chemistry*	1:00pm-1:50pm
Jason Goodpaster, University of Minnesota Twin Cities *Transfer Learning for Electron Correlation*	1:50pm-2:40pm
Seonah Kim, National Renewable Energy Laboratory *Prediction of chemical properties from molecular structure*	2:40pm-3:30pm
Break	3:30pm-3:45pm
Arthur Mar, University of Alberta *Machine-Learning Predictions of Half-Heusler Structures*	3:45pm-4:35pm
Robert Paton, Colorado State University *Chemical Reaction Prediction - Combining Quantum Chemistry with Graph Neural Networks*	4:35pm-5:25pm

Wednesday, October 2nd

Breakfast	7:30am-8:30am
Jon Paul Janet, Massachusetts Institute of Technology *Machine-learning assisted workflows for inorganic molecular discovery*	8:30am-9:20am
Olexandr Isayev, University of North Carolina at Chapel Hill *Chemistry-Informed ML and Interpretable AI*	9:20am-10:10am
Break	10:10am-10:25am
Nicholas Lubbers, Los Alamos National Lab *Considerations of Architectures for Deep Learning of Atomistic Information*	10:25am-11:15am
Alexandre Tkatchenko, University of Luxembourg *Bringing Physics and Machine Learning Together*	11:15am-12:05pm
Lunch (on your own)	12:05pm-1:30pm
Open time for Hike/Collaboration	1:30am-5:00pm

Thursday, October 3rd

Breakfast 7:30am-9:00am

Open time for Hike/Collaboration 9:00am-11:45am

Lunch (on your own) 11:45am-1:00pm

Michael Willatt, EPFL - IMX - COSMO 1:00pm-1:50pm
Accurate and Informative Machine-Learning Models from Density-Based Representations

Yu-Hang Tang, Lawrence Berkeley National Lab 1:50pm-2:40pm
Kernel-based learning methods for molecular dynamics

Roman Zubatyuk, University of North Carolina at Chapel Hill 2:40pm-3:30pm
Atoms-in-molecules multitask neural network potential

Break 3:30pm-3:45pm

Andrew Sifain, Army Research Lab 3:45pm-4:35pm
Machine Learning Transition Temperatures from 2D Structure

Sameer Varma, University of South Florida 4:35pm-5:25pm
Identifying time-resolved protein signaling pathways using machine learning

Friday, October 4nd

Breakfast 7:30am-8:30am

Arindam Chakraborty, Syracuse University 8:30am-9:20am
Combining deep neural nets with quantum Monte Carlo: Achieving linear-scaling calculation of electron ionization and excitation energies by learning from semi-simple high-dimensional kernels

Alberto Gobbi, Genentech 9:20am-10:10am
Computing Ligand Strain Energy with Neural Net Potentials

Break 10:10am-10:25am

James P. Lewis, West Virginia University 10:25am-11:15am
TBA

Joshua Schrier, Fordham University 11:15am-12:05am
Discovering reactions and uncovering mechanisms of perovskite formation (with robots)

Closing Remarks 12:05pm-12:10pm

End of Workshop