2021 "Computational Materials Chemistry" Telluride Workshop
In-person (IP) venue: Telluride Intermediate School, 725 W Colorado Ave, Telluride, CO 81435
Virtual (V): Zoom link will be distributed a week before the workshop starts
Sunday morning, 27 June 2021 to Thursday noon, 1 July 2021; Breakfast starts 7:30am at School for in-person
(all times are local or Mountain Time; 8am Telluride = 3pm London = 4pm Berlin = 11pm Tokyo)

Sunday, 27 June 2021
8:00am-8:10am opening remarks
Session I: Accelerated discovery; Chairs: De-en Jiang (IP)/Eva Zurek (V)
8:10am-9:00am Ryoji Asahi (V), U. of Nagoya; Design and Discovery of Ionic Conductors Based on High-Throughput Computation and Experiment
9:00am-9:50am Brett Savoie (V), Purdue U.; Transfer Learning for Materials Discovery and Simulation
9:50am-10:20am Coffee Break
10:20am-11:10am Joshua Schrier (IP), Fordham Univ.; Does machine learning accelerate experimental discovery of new materials? Case studies in halide perovskite synthesis
11:10am-12:00pm Alan Asparu-Guzik (V), U. of Toronto; Closed loop discovery of organic materials

Monday, 28 June 2021
Session II: Structure prediction; Chairs: Graeme Henkelman (IP)/Jason Goodpaster (IP)
8:10am-9:00am Richard Hennig (IP), U. Florida; Structure prediction with the UF3 ML framework
9:00am-9:50am Eva Zurek (V), SUNY Buffalo; Theoretical Predictions of Superhard Materials
9:50am-10:20am Coffee Break
10:20am-11:10am De-en Jiang (IP), UC Riverside; Locating hydrides in metal nanoclusters via CNNs
11:10am-12:00pm Taylor Sparks (V), U. Utah; Discovery of Novel Inorganic Crystal Structures via GANs

Tuesday, 29 June 2021
Session III: NN potentials and test of DFT; Chairs: Richard Hennig (IP)/Hongliang Xin (V)
8:10am-9:00am Gabor Csanyi (V), Cambridge U.; Machine learned force fields and potential energy surfaces
9:00am-9:50am Matthias Rupp (V), U. of Konstanz; ML Potentials: Splines, Kernels, Neural Networks
9:50am-10:20am Coffee Break
10:20am-11:10am Aleksey Kolmogorov (V), SUNY Binghamton; Structure prediction with ML potentials
11:10am-12:00pm Heather Kulik (IP), MIT; Putting DFT to the test in ML-accelerated discovery

Wednesday, 30 June 2021
Session IV: Spectroscopy and properties; Chairs: Heather Kulik (IP)/Zack Ulissi (IP)
8:10am-9:00am Greg Beran (IP), UC Riverside; Machine-learning NMR chemical shifts with DFT accuracy
9:00am-9:50am Maria Chan (V), Argonne National Lab; Modeling and ML for Spectroscopy and Microscopy
9:50am-10:20am Coffee Break
10:20am-11:10am Giulia Galli (V), U. of Chicago; ML Dielectric Screening for the Simulation of Excited States
11:10am-12:00pm Diego Gómez-Gualdrón (IP), Colorado School of Mines; Alchemical data as tool to develop recyclable, multitask deep learning models to predict adsorption in nanoporous materials

Thursday, 1 July 2021
Session V: Catalysis, surface, reactivity, and electronic structure; Chair: Greg Beran (IP)/Matthias Rupp (V)
8:00am-8:45am Ichigaku Takigawa (V), RIKEN, JAPAN; A ML view on heterogeneous catalyst design and discovery
8:45am-9:30am Jason Goodpaster (IP), U. Minnesota; DFT and ML methodologies for electrocatalytic systems.
9:30am-9:45am Coffee Break
9:45am-10:30am Zack Ulissi (IP), Carnegie Mellon; Exploring the limits and generalizability of graph models on large surface science datasets
10:30m-11:15am Hongliang Xin (V), Virginia Tech; Theory-infused NNs for Interpretable Reactivity Prediction
11:15am-12:00pm Victor Fung (V), ORNL; Exploring electronic structure-property relationships with ML.