Workshop: Artificial Intelligence for Materials Science (AIMS)

(Virtual) NIST, Gaithersburg, MD, July 12-14, 2022

(Eastern Standard Time/Washington DC Time)

	Day: 1, July 12, 2022, Tuesday
10:00-10:15 AM	Welcome Note, James Warren, Director MGI, NIST
	INVITED TALKS (SESSION CHAIR: Francesca Tavazza)
10:15-10:45 AM	Kamal Choudhary, NIST, Deep-learning Frameworks for Materials Data
10:45-11:15 AM	Shyue Ping Ong, UC San Diego, Exploring the Matterverse with Machine Learning
11:15-11:45 AM	Tim Mueller, Johns Hopkins, Acceleration of materials research using machine-learned interatomic potentials
11:45-12:15 PM	Jorg Behler, University of Goettingen, Simulations of Complex Systems with High-Dimensional Neural Network Potentials
12:15-12:30 PM	Break
12:30-1:00 PM	Jacqueline Cole, Cambridge University, Data-driven Materials Discovery
1:00 -1:30 PM	Boris Kozinsky, Harvard University
1:30-2:00 PM	Keith Butler, UKRI, Interpretable Machine Learning for Materials' Design and Characterization
2:00-2:15 PM	Break
	LIGHTNING TALKS (SESSION CHAIR: Daniel Wines)
2:15-2:30 PM	Jan Janssen, Los Alamos National Laboratory, Predicting melting temperatures from bulk properties with pyiron
2:30-2:45 PM	Ramya Gurunathan, NIST, Rapid Prediction of Phonon Structure and Properties using the Atomistic Line Graph Neural Network
2:45-3:00 PM	Jianjun Hu, University of South Carolina, Physics Guided Generative Adversarial Networks for Generations of Crystal Materials with High Symmetry Constraints

3:00-3:15 PM	Ming Hu, University of South Carolina, Million-Scale Atomic Data Integrated Deep Neural Network for Predicting Phonon Properties of Crystals Spanning the Periodic Table
3:15-3:30 PM	Fei Zhou, Lawrence Livermore National Lab, Accelerated microstructure simulations with graph neural networks
3:30-3:45 PM	Kwang-Ryeol Lee, Korea Institute of Science and Technology, Materials R&D Data Structure in Korea based on Materials System
3:45-4:00 PM	Break
	E-POSTER SESSION (SESSION CHAIR: Daniel Wines)
4:00-4:10 PM	Vahe Gharakhanyan, Columbia University, Predicting Melting Temperatures of Solids with Combined Clustering and Regression
4:10-4:20 PM	Vahe Gharakhanyan, Columbia University, Thermodynamics of Redox Reactions at High Temperatures with Combined Machine Learning and Density Functional Theory
4:20- 4:30 PM	Henry Sprueill, Pacific Northwest National Laboratory, Active Sampling for Atomistic Potentials: A Neural Network Potential for Dynamic Shear Simulations of Binary Metal Systems
4:30-4:40 PM	Chenru Duan, MIT, Transforming Automated Quantum Chemistry Calculation Workflows via Machine Learning: Towards Accelerated Chemical Discovery with Higher Fidelity
4:40-4:50 PM	Diana L. Ortiz-Montalvo, NIST, AI for Climate Change: Guiding Discovery of Sorbent Materials for Direct Air Capture of CO_2
	Day: 2, July 13, 2022, Wednesday
	INVITED TALKS (SESSION CHAIR: Brian DeCost)
10:00-10:30 AM	Rama Vasudevan, ORNL, Machine learning and automated experiment for manipulation and characterization of nanoscale materials
10:30-11:00 AM	Tian Xie, Microsoft, Forward and inverse design of solid materials with graph neural networks
11:00-11:30 AM	Heather Kulik, MIT, Revealing molecular design blueprints for open shell transition metal materials and catalysts with machine learning
11:30-12:00 noon	Chris Rackauckas, MIT, Accurate and Efficient Physics-Informed Learning Through Differentiable Simulation

12:00-12:30 PM	Break
12:30-1:00 PM	Geoffrey Hautier, Dartmouth college, Beyond the bulk, zero-Kelvin computations: growing complexity in high-throughput computational databases
1:00-1:30 PM	Raymundo Arroyave, TAMU, Bayesian Materials Discovery
1:30-2:00 PM	Maria Chan, ANL, Theory-guided AI/ML for Microscopy and Spectroscopy
2:00-2:30 PM	Break
	LIGHTNING TALKS (SESSION CHAIR: Kevin Garrity)
2:30 -2:45 PM	Niloy Ganguly, Leibniz university of Hannover, CrysXPP: An explainable property predictor for crystalline materials
2:45 -3:00 PM	Arghya Bhowmik, Technical University of Denmark, Equivariant graph neural networks for fast electron density estimation of molecules, liquids, and solids
3:00 -3:15 PM	Mahesh R. Neupane, DEVCOM US Army Research Laboratory, Engineering structural, chemical and electronic properties of doped MoO_3 (010) surface via Neural Network (NN) Approach
3:15-3:30 PM	Break
	E-POSTER SESSION
3:30 -3:40 PM	Mustapha Ait Boukideur, University Ibn Zohr, Agadir, Morocco., The combination of the DFT method and the CALPHAD approach for the thermodynamic optimization of the Er-As system.
3:40-3:50 PM	Akram Ibrahim, University of Maryland Baltimore County, A machine-learned molecular dynamics modeling of the self-assembly of one-dimensional nanostructures from MoS2 monolayers using defect engineering
3:50-4:00 PM	Scott Muller, Pacific Northwest National Laboratory, Introducing a database of bulk ternary transition metal dichalcogenides
4:00-5:00 PM	Hands-on session (SESSION CHAIR: Ramya Gurunathan, Brian DeCost)
	Day: 3, July 14, 2022, Thursday

	INVITED TALKS (SESSION CHAIR: Kamal Choudhary)
10:00-10:30 AM	Ekin Dogus Cubuk, Google
10:30-11:00 AM	Kedar Hippalgaonkar, NTU/A*STAR, Data-driven Design of Functional Inorganic Materials
11:00-11:30 AM	Zachary Ulsisi, Carnegie Mellon University
11:30-12:00 PM	Wei Chen, Mixed Variable Latent Variable Gaussian Process for Materials Design, Northwestern University
12:00-12:30 PM	Trevor David Rhone, RPI, Artificial intelligence guided studies of van der Waals magnets
12:30-1:00 PM	Break
	LIGHTNING TALKS (SESSION CHAIR: Ramya Gurunathan)
1:00-1:15 PM	J. I. Gomez-Peralta, CINVESTAV Mérida, Bandgap assessment using X-ray powder diffraction and Artificial Intelligence
1:15-1:30 PM	Fadwa El Mellouhi, Hamad Bin Khalifa University, Machine Learning from Large and Sparse Data for Novel materials discovery
	E-POSTER SESSION (SESSION CHAIR: Ramya Gurunathan)
1:30-1:40 PM	Wei Li, Los Alamos National Laboratory, Transition path sampling framework for active learning of robust machine learning potentials
1:40-1:50 PM	Gracie Chaney, University of Maryland, Baltimore County, Development of a universal machine learning descriptor from density functional theory data of ion adsorption properties on Sulfur-functionalized MXenes for battery applications
1:50-2:00 PM	Ruijie Zhu, Northwestern University, Accelerated Discovery of i-MAX phases using high-throughput computation and machine learning
2:00-2:10 PM	Sukhbir Singh, Panjab University, Modeling Electronic and Transport Properties of Armchair Silicene Nanoribbon for PIN-FET Design
2:10-2:20 PM	Fadla Mohamed Abdelilah, Laghouat university, Algeria, Machine Learning for point defect in halide perovskite from Elemental Properties
2:20-2:30 PM	Thank You Note & Survey