Workshop: Artificial Intelligence for Materials Science (AIMS), NIST, Gaithersburg, Red auditorium, August 7-8, 2018

AGENDA:

	August 7, 2018
8:00-8:30 AM	Registration/badging
8:30-8:40 AM	Welcome note, Francesca Tavazza
8:40-9:00 AM	James Warren, NIST, "MGI and AI"
9:00-9:30 AM	Krishna Rajan, University at Buffalo, "AI for Discovering Materials Design Pathways"
9:30-10:00 AM	Caleb Phillips, NREL, "Applications of Machine Learning for Materials Discovery using the NREL High Throughput Experimental Materials Database"
10:00-10:15 AM	Break
	Density functional theory data and AI
10:15-10:45 AM	Anubhav Jain, LBNL, "Data Mining to Discovery for Inorganic Solids: Software Tools and Applications"
10:45-11:15 AM	Ankit Agrawal, Northwestern university, "Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science"
11:15-11:45 AM	Logan Ward, University of Chicago, "Accelerating Materials Discovery and Design with Machine Learning"
11:45 AM-12:15 PM	Kamal Choudhary, NIST, "JARVIS-ML: fast screening and mapping energy landscape of materials"
12:15-12:30 PM	Discussion
12:30-2:00 PM	Lunch
2:00- 2:30 PM	Richard Hennig, University of Florida, "Pathways Towards a Hierarchical Discovery of Materials"
2:30-3:00 PM	Evan Reed, Stanford university, "Statistical learning for small data materials challenges: Solid lithium-ion conductors for batteries"
3:00-3:30 PM	Rampi Ramprasad, Georgia Tech., "Polymer Genome: An Informatics Platform for Rational Polymer Dielectrics Design and Beyond"
3:30-4:00 PM	Noa Marom, Carnegie Mellon university
4:00-4:30 PM	Yuri Mishin, George Mason university, "Classical force fields as physics-based neural networks"
4:30- 6:00 PM	Poster-session
	August 8, 2018
	Experimental data and AI
8:30-9:00 AM	Ichiro Takeuchi, University of Maryland, "Combinatorial Experimentation and Machine Learning for Materials Discovery"
9:00-9:30 AM	Aaron Gilad Kusne, NIST, "Unsupervised Machine Learning for materials"
9:30-10:00 AM	Turab Lookman, LANL

10:00-10:15 AM	Discussion
10:15-10:30 AM	Break
10:30-11:00 AM	J. C. Zhao, Ohio state university
11:00-11:30 AM	Apurva Mehta, Stanford university, "Coupling of Artificial Intelligence with High-throughput Experimentation for Orders of Magnitude Acceleration in Discovery of Amorphous Alloys"
11:30 AM-12:00 PM	Jason-Hattrick Simpers, NIST, "High-throughput experimental synthesis and characterization"
12:00-12:30 PM	Max Hutchinson, Citrine Informatics, "One does not simply apply off the shelf machine learning tools to materials discovery"
12:30-1:30 PM	Lunch
	Development of classical potentials and natural language processing
1:30-2:00 PM	Aidan Thompson, Sandia National lab, "Automated Generation of High-accuracy Interatomic Potentials Using Quantum Data"
2:00-2:30 PM	Elsa Olivetti, MIT, "Progress in Natural Language Processing of Materials Science Text"
2:30-3:00 PM	Olga Kononova, UC Berkeley, "Making steps toward predictive synthesis of new materials by using data mining and machine learning approaches"
3:00-3:30 PM	Haoyan Huo, UC Berkeley, "Machine Learning Approach for Identifying Reported Materials Synthesis Experiments in Scientific Articles"
3:30-4:00 PM	Discussion
4:00 PM	Adjourn

Some poster titles:

1) **Bayesian Inference enabled experimental determination of materials and transport descriptors in thermoelectrics**, D V Maheswar Repaka , A Suwardi , R Zekun , T Buonassisi and K Hippalgaonkar
2) **Accelerate Searching for Singlet Fission Materials: Feature Selection and Model Construction for GW+BSE Method with SISSO**, Xingyu Liu, Xiaopeng Wang, Maituo Yu, Rithwik Tom, Noa Marom
3) **Size and Temperature Transferability of Direct and Local Deep Neural Networks for Atomic Forces**, Nataly Kuritz
4) **Machine Learning Models with a Mix of Sparse and Dense Data for Predicting Metallic Glasses**, Brenna Gibbons, Cooper Elsworth, Jason Hattrick-Simpers, Logan Ward, and Apurva Mehta
5) **Fostering machine learning through coordination descriptors, site fingerprints, and structure similarity measures**, Nils Zimmermann
6) **Machine learning prediction of the electronic properties in double perovskites**, Jino Im, Seongwon Lee, Tae-Wook Ko, Hyun Woo Kim, YunKyong Hyon,and Hyunju Chang