Workshop Agenda: Artificial Intelligence for Materials Science (AIMS)
NIST, Gaithersburg, MD, Red Auditorium, August 1-2, 2019

	August 1, 2019
7:30-8:30 AM	Registration/Badging
8:30-8:40 AM	Welcome, F. Tavazza, NIST
8:40-8:55 AM	J. Warren, NIST, Director MGI, "MGI and AI"
8:55-9:30 AM	M. Scheffler, FHI-Berlin, "When The New Science Is In The Outliers"
9:30-10:05 AM	S. R. Kalidindi, Georgia Tech, "A Machine Learning Framework for Materials Knowledge Systems"
10:05-10:15 AM	Break
10:15-10:50 AM	M. Aykol, Toyota Research Institute, "Artificial intelligence for accelerating the discovery of materials for emission-free technologies"
10:50-11:25 AM	S. P. Ong, UCSD, "Materials Graphs, Environments and Machine Learning"
11:25 AM-12:00 PM	K. Choudhary, NIST, "Smart Metrics for High-Performance Material-Design"
12:00-12:35 PM	S. Curtarolo, Duke Univ., "From meta-data to meta-properties with only a bit of meta-physics"
12:30-2:05 PM	Lunch on your own
2:05- 2:40 PM	G. Pilania, LANL, "Materials that Glow: discovering and designing new scintillators with machine learning"
2:40-3:15 PM	S. V. Kalinin, ORNL, "Deep Dive into the Scanning Transmission Electron Microscopy of Quantum Materials: From Learning Physics to Atomic Manipulation"
3:15-3:50 PM	Deyu Lu, Brookhaven Nat. Lab., "Predicting local atomic structures from X-ray absorption spectroscopy using theory and machine learning"
3:50-4:25 PM	C. Niu, QuesTek, "A Framework and Infrastructure for Uncertainty Quantification and Management in Materials Design"
4:25-4:30 PM	Group-photo
4:30- 6:00 PM	Poster-session (30 registered posters, poster size recommended: 46 inch x 46 inch)
	August 2, 2019
8:30-9:05 AM	Nicola Marzari, EPFL
9:05-9:40 AM	T. Mueller, JHU, "Fast and accurate interatomic potentials by genetic programming"
9:40-10:15 AM	Gus Hart, Brigham Young University, "Machine-learned Interatomic Potentials"
10:15-10:30 AM	Break
10:30-11:05 AM	Zachary Ulissi, Carnegie Mellon University, "Challenges in Data Science Methods for Catalyst Design and Discovery"
11:05-11:40 AM	Olexandr Isayev, U. North Carolina, "Predicting properties of inorganic materials with machine learning"
11:40AM-12:30PM	Panel discussion
12:30 -2:00 PM	Lunch on your own
2:00 -5:00 PM	D. Wheeler, B. DeCost, K. Garrity, J. Hickman, L. Hale, K. Choudhary, Hands-on session, (Using Google-Colab notebook, JARVIS-ML dataset, Basic regression and

	classification examples, Uncertainty quantification in ML), Participants should bring their laptops

Posters:

1. Jeffery Aguiar, Idaho National Laboratory, **Realizing Real Time Crystallographic and Materials Based Analysis Using Deep Learning**

2. Lewis Geer, NIST, **Using generalized chemical artificial intelligence to calculate molecular properties, including GC retention indices**

3. Yuling An, Schrodinger, Inc, **Data-Centric Informatics Platform for Next-Generation of Discovery and Innovation in Materials Science**

4. Alba Avila, Universidad de los Andes, **AI applied to nancomposites for evaluation EMI´s materials performance.**

5. Adarsh Dave, Carnegie Mellon University, **Automated Electrolyte Design with Robotic Experiment and Machine-learning**

6. Anthony DiGiovanni, Army Research Laboratory, **Comparing Quantified Microstructural Features Obtained from Segmentation Algorithms to those Derived from a Modified U-Net CNN in Biphasic Ceramic Systems using SEM Image Mapping**

7. Zeeshan Ahmad, Carnegie Mellon University, **Machine Learning Enabled Computational Screening of Inorganic Solid Electrolytes for Suppression of Dendrite Formation in Lithium Metal Anodes**

8. Meenakshi Dutt, Rutgers, The State University of New Jersey, **Computational Design of Peptide-Based Materials**

9. Hassna EL-BOUSIYDY, Laboratoire de Réactivité et Chimie des Solides (LRCS), **Batteries Lifetime Prediction by Artificial Intelligence**

10. Uday Gajera, The Max-Planck-Institut für Eisenforschung GmbH, **Solution enthalpies of hydrogen using data-mining**

11. Kamalika Ghatak, New Jersey Institute of Technology, **Contribution of various stacked bilayer TMDs With different degree of rotation of the top layer towards the growth mechanism.**

12. Luis Felipe Giraldo Trujillo, University of los Andes, **Nanocomposites descriptors for correlation of properties and synthesis**

13. Olle Heinonen, Argonne National Laboratory, **Phase Segmentation in Atom-Probe Tomography Using Deep Learning-Based Edge Detection**

14. Shweta Jindal, Indian Institute of Technology Indore, **Machine learning advances in nanochemistry**

15. Naghma Khan, Csir- National Physical laboratory India, **Alpha quartz a powder diffraction standard**

16. Soo Kim, Lawrence Livermore National Laboroatory, **Optimizing 3D structure of H2O molecule using DDPG**

17. Ravinder Kumar, Csir- National Physical laboratory, **Alpha alumina powder x-ray diffraction standard**

18. Vipin Kumar, U. Ulsan, **Themoelctrc propeties of the group -III**

19. Wei Li, University of Delaware, **Machine learning models for accurate predictions of crystal**

20. Vubangsi Mercel, HIBUMS Polytechnic University, Bafoussam, Cameroon, **Simulation of laser based processing of polycrystalline composites combining analytical and machine learning models**

21. Rohan Mishra, Washington University in St. Louis, **Designing stable perovskites for energy applications one atom at a time**

22. Jungho Shin, Korea Research Institute of Chemical Technology, **Database for thermometric material's properties: electronic structure calculations, experiments and machine learning**

23. Blair Tuttle, Penn State Behrend, **Band Gaps in nano-porous SiC using Machine Learning**

24. Selam Waktola, Lodz University of Technology, **Stagnant zone segmentation with U-net**

25. Qimin Yan, Temple University, **Machine learning the periodic table from compound formula**

26. Fei Zhou, Lawrence Livermore National Laboratory, **Unsupervised learning and prediction of microstructure evolution with recurrent neural networks**

27. Li Zhu, Carnegie Institution for Science, **Carbon-boron clathrates as a new class of sp3-bonded framework materials**

28. Sanjeev K. Nayak, University of Connecticut, **Polarization rotation in Bi4Ti3O12 by selective sublattice doping**

29. Sanjubala Sahoo**,** University of Connecticut, **Single-site heterogeneous catalysts for hydrocarbon conversion**

30. Haleem Ud Din, Hazara University, **Van der waals heterostructures of SIC TMDCs**