Artificial Intelligence and Machine Learning for Ceramics and Glasses

March 26 and 27, 2024



March 26: Day 1

11:00 am – 11:05 am—Workshop Introduction and Welcome

11:05 am – 12:05 pm—Session I: How to Get Started with Materials and Machine Learning

11:05 am - 11:35 am—A Diversity of AI Opportunities Revealed by High Throughput Experimentation

Speaker: John Gregoire, California Institute of Technology

11:35 am – 12:05 pm—Innovating at the Interface: Opinionated Tips for Materials Scientists Exploring Machine Learning
Speaker: Daniel R. Cassar, Ilum School of Science

12:05 pm – 2:20 pm—Session II: Machine Learning and Materials Synthesis

12:05 pm - 12:35 pm—Nuclear Waste Glass Formulation Using Machine Learning Property Models with Prediction Uncertainty

Speaker: Xiaonan Lu, Pacific Northwest National Laboratory

12:35 pm - 1:05 pm—Combinatorial Printing for High-Throughput Materials Discovery

Speaker: Yanliang Zhang, University of Notre Dame

1:05 pm - 1:20 pm— Break

1:20 pm – 1:50 pm—*Collaborative Intelligence in Laboratory Materials Research*

Speaker: Shijing Sun, University of Washington-Seattle

1:50 pm – 2:20 pm—Accelerating Inorganic Materials Synthesis and Characterization in Autonomous Laboratories

Speaker: Yan Zeng, Florida State University

2:20 pm—Closing Remarks

March 27: Day 2

11:00 am – 11:05 am—Workshop Welcome

11:05 am – 12:05 pm—Session III: Machine Learning and Materials Modeling

11:05 am - 11:35 am—Application of Statistical Approaches to Proton-Conducting Phosphate Glasses: Study of the Effect of Oxide Components on Proton Mobility and Thermal Stability

Speaker: <u>Takahisa Omata</u>, Tohoku University

11:35 am – 12:05 pm—*Materials Design from Atomistic Simulations and Electron Microscopy Guided by Explainable Scientific Machine Learning* Speaker: Ayana Ghosh, Oak Ridge National Laboratory

12:05 pm – 2:20 pm—Session IV: Machine Learning and Materials Characterization

12:05 pm — 12:35 pm—*Theory-informed AI/ML for Materials Characterization* Speaker: Maria Chan, Argonne National Laboratory

12:35 pm - 1:05 pm—Deep Learning Defect Detection in Electron Microscopy of Radiation Damage

Speaker: Dane Morgan, University of Wisconsin-Madison

1:05 pm - 1:20 pm—Break

1:20 pm – 1:50 pm—Machine Learning for High-Throughput Characterization of Nanoelectronics

Speaker: Matthew Hauwiller, Seagate Technology

1:50 pm – 2:20 pm—Boosting Prediction of NMR Properties in Disordered Solids with Machine Learning

Speaker: Thibault Charpentier, Université Paris-Saclay

2:20 pm—Closing Remarks