Machine Learning-Assisted Approaches for Materials Design & Characterization

Organizers: Xiaohui Qu (CFN), Deyu Lu (CFN), Gregory Doerk (CFN), Yugang Zhang (CFN), Hanfei Yan (BNL/NSLS-II)

Description - Discovery of new materials with superb targeted properties is a key driver of innovation in a wide range of technology sectors, such as photovoltaics, energy storage, catalysis, to name a few. With the recent advances in shortening the life cycle of materials discovery, the paradigm has transformed from the Edisonian approach to a data-driven approach that embraces big data and machine learning to navigate the high-dimensional materials design space with unprecedented efficiency and accuracy. Notably, materials design is accompanied by materials characterization. Interpreting complex characterization (e.g., in microscopy, spectroscopy, and diffraction) in real-time and at scale has become an essential element in autonomous experimentation, which is an emerging technical challenge. In light of this, this workshop will highlight recent progress in materials research and demonstrate the impact of big data and machine learning. The workshop will bring together scientists in the fields of energy, catalysis, electron microscopy, chemistry, polymer science, condensed matter physics, and data science. By focusing on exemplary machine learning-assisted approaches in materials design, synthesis and characterization, the workshop will inspire potential developments in hardware and data distillation as well as new research opportunities, at BNL user facilities at CFN and NSLS-II. The workshop will include new developments in several topics: Microscopy, small-angle scattering, core-level spectroscopy, computational modeling, and autonomous experiments.

Start Time (ET)	Title	Speaker (Affiliation)
09:58	Opening Remarks (2 minutes)	Xiaohui Qu (BNL)
10:00	Physical Theory Session	Deyu Lu (BNL, Chair)
10:00	AI-assisted Materials Discovery (Keynote)	Rajeev Surendran Assary (ANL)
10:45	Elucidating Structural Heterogeneity of Complex Materials with Spectroscopy, Machine Learning, and Atomistic Simulations	Tuan Anh Pham (LLNL)
11:15	BigSMILES and Other Informatics Tools to Make Data More Open in Materials Chemistry	Bradley Olsen (MIT)
11:45	Group Photo	All
12:00	Break (Lunch, 1 hour)	
1:00	Materials Dynamics Session	Yugang Zhang (BNL, Chair)
1:00	Unveiling Supported Catalyst Evolution: Harnessing Machine Learning for Environmental Transmission Electron Microscopy Image Analysis	Dmitri Zakharov (BNL)
1:30	Machine Learning Enabled High Performance Coherent X-ray Diffraction Imaging	Longlong Wu (BNL)
2:00	Machine Learning for Accelerated Understanding of Dynamic Catalysts	Prahlad Routh (BNL)
2:30	Break	
2:45	Autonomous Experiment Session	Gregory Doerk (BNL, Chair)
2:45	Autonomous Experimentation for Acceleration of Materials Research & Development (Keynote)	Benji Maruyama (Air Force)

3:30	Complex decision-making for problem-fluent closed-loop campaigns	Kristofer Reyes (U Buffalo)
4:00	AI-guided precision synthesis of Gold nanoparticles: leveraging automated fluidics and in-situ SAXS	Hyeong Jin Kim (BNL)
4:30	Break	
4:45	Experimental Data Interpretation Session	Hanfei Yan (BNL, Chair)
4:45	Data-driven computational approaches for interpreting high-throughput structural characterization of soft materials	Arthi Jayaraman (U Delaware)
5:15	Highly sensitive full field X-ray absorption spectroscopy via self-supervised Machine Learning	Mingyuan Ge (BNL)
5:45	Closing Remarks (2 minutes)	Xiaohui Qu (BNL)