

WORKSHOP #13
Thursday, May 26th, 2022

Data-Driven Analysis, Characterization and Modeling in Battery Development and Manufacturing

Feng Wang (IS), Deyu Lu (CFN), Sooyeon Hwang (CFN), Matthew R. Carbone (CSI), Shinjae Yoo (CSI), and Mingyuan Ge (NSLS-II)

Lithium-ion battery technology provides critical energy-storage needs for society, ranging from everyday electronics to electrified transportation and power grids. The demand for lighter, more powerful devices continues to fuel the need for energy-dense batteries. This, in turn, requires designing new battery materials, understanding how they function and, ultimately, developing scalable processes to manufacture them. As witnessed by the development of the 1st generation Li-ion batteries, it took decades to move from early discovery to commercial deployment due to the lifetime, safety, cost, and environmental impact requirements. With the advances in data-driven and artificial intelligence and machine learning (AI/ML) techniques, in silico tools and workflows for automated characterization and data analysis are emerging and show great promise in high-throughput automated and autonomous experimentation pipelines and computational modeling. Data-driven analysis, characterization and modeling play an increasingly important role in accelerating the otherwise ultra-long process from battery materials discovery to manufacturing and commercial deployment.

This workshop highlights the emerging opportunities for developing next-generation battery materials and manufacturing processes using the synchrotron x-ray, electron microscopy, and computational facilities/infrastructures at NSLS-II, CFN and CSI. Through this workshop, we intend to advocate the existing and up-to-coming capabilities/resources at the user facilities and learn from the battery community about their research needs. It will provide a platform for developing collaboration among AI/ML developers, data scientists, theorists, facility leads, and battery researchers broadly from industry, academia and national laboratories.

Start Time (ET)	Title	Speaker (Affiliation)
Session 1		
8:20 – 8:30 a.m.	Opening Remarks	Organizers (Brookhaven National Laboratory; BNL)
8:30 – 9:00	Keynote: Advancing Battery Manufacturing with Data Origami Approach	Changwon Suh (Advanced Manufacturing Office, Department of Energy)
9:00 – 9:30	Physics-based Machine Learning for Enhanced Life Prediction and Cell Design	Eric Dufek (Idaho National Laboratory)
9:30 – 10:00	Smart Giga Machine: A Long-Term Friendship between Molecules, Machines and the Data	Shailesh Upreti (C4V, LLC; iM3NY)
10:00 – 10:30	Understanding Oxygen Redox in Cathode Materials from Modeling and Characterization	Maria Chan (Argonne National Laboratory; ANL)
10:30 – 10:45	Break	N/A
10:45-11:45	Capabilities/resources at BNL for “Data-Driven Analysis, Characterization and Modeling in Battery Development and Manufacturing”	
10:45 – 11:00	NLSII Capabilities	Yong Chu (BNL)
11:00 – 11:15	CFN Capabilities and Data/ML research	Kevin Yager (BNL)
11:15 – 11:30	Energy Storage/IS	Amy Marschilok (BNL)
11:30 – 11:45	CSI Capabilities	Kerstin Kleese van Dam (BNL)
11:45 – 12:30 p.m.	Panel Discussion	Speakers from Session 1
12:30 – 1:30	Lunch	N/A
Session 2		
1:30 – 2:00	Electrode Performance and Degradation: Coupling Continuum Modeling, Experiment, and Machine Learning	Alan West (Columbia University)
2:00 – 2:30	Application of AI in X-ray Emission Spectroscopy	Chengjun Sun (ANL)
2:30 – 3:00	Using Time-resolved Electron Microscopy and Data Analytics to Quantify the Evolution of Supported Metal Nanoparticles	Eric Stach (University of Pennsylvania)
3:00 – 3:10	Vendor	N/A
3:10 – 3:20	Break	N/A
Session 3		
3:10 – 3:40	Accelerating the Prediction of Microstructure Evolution with Machine Learning Models	Ming Tang (Rice University)
3:40 – 4:10	Machine Learning Models for Simulating Complex Battery Materials with Non-Crystalline Structures	Nongnuch Artrith (Utrecht University)
4:10 – 5:00	Panel Discussion	Chris Brown (Schrödinger) Don DeRosa (Eonix) Nongnuch Artrith (Utrecht University) Chengjun Sun (ANL) Ming Tang (Rice University)