WORKSHOP # 3 – Tuesday, April 21, 2026

Physics-Informed Autonomous Experimentation from Synthesis to Understanding

Organizers: Yugang Zhang, Xiaohui Qu, Gregory Doerk, Jason kahn, Fang Lu, Oleg Gang (CFN, BNL);
Sanjit Ghose, Ruipeng Li, Eliot Gann, Xiaogang Yang (NSLS-II, BNL);
Susan Minkoff, Kristofer Reyes (Computational Science, BNL)

High-throughput experimentation and AI-driven optimization are transforming materials discovery. However, many existing autonomous experimental systems function largely as black boxes, identifying correlations without delivering mechanistic insight. This workshop aims to bridge three critical communities: researchers developing high-throughput synthesis and manufacturing platforms, experts in advanced in situ characterization techniques, and computational scientists working on physics-informed machine learning methods. The workshop will highlight state-of-the-art capabilities and examine strategies for integrating them into closed-loop autonomous systems. Emphasis will be placed on approaches in which prior knowledge from literature, kinetic and thermodynamics models, and physical constraints guide both experimental design and interpretation. Key topics include establishment of practical experimental realizations of autonomous synthesis and measurement workflows across diverse material classes; physics-informed Bayesian optimization, multi-fidelity modeling combining simulation and experiment, symbolic regression for discovering governing equations, and addressing reproducibility through metadata standards. Case studies will span nanocolloidal synthesis, thin film growth, and self-assembly, integrating multimodal characterization emphasizing both in situ real-time monitoring, and comprehensive ex situ structural characterization. Through invited talks and interactive breakout sessions, we will identify infrastructure, software tools, and data standards needed to move beyond black-box optimization toward systems that truly understand materials synthesis and assembly. This workshop addresses a timely need as NSLS-II and CFN users increasingly adopt autonomous workflows while seeking deeper mechanistic insights from their high-throughput data.

Start Time (ET)	Title	Speaker (Affiliation)
09:00 – 09:05	Opening Remarks	Yugang Zhang (CFN, BNL)
09:05 – 09:30	The Future of AI-Empowered Physical Science	Kevin Yager (CFN, BNL)
09:30 – 09:55	Accelerated Discovery of High-Entropy Materials via Integrated High-Throughput Computation and Synthesis	Wei Chen (University at Buffalo)
09:55 – 10:15	*Morning Coffee Break*	
10:15 – 10:40	Data-Rich Autonomous Labs for Accelerated Materials Discovery	Milad Abolhasani (NC State)

10:40 – 11:00	Toward Self-Driving Labs: High Throughput, Automation and AI for the Next Era of Materials Innovation	Mahshid Ahmadi (U. Tennessee)
11:00 – 11:25	Leveraging Specialized Databases, Data Mining, and Machine Learning for Self-Driving Laboratories	Bin Ouyang (Florida State University)
11:25 – 11:50	Physics-informed active learning for functional polymer design and assembly	Michael Webb (Princeton University)
11:50 – 01:50	*Lunch Break (travel to/from SUSC to Berkner Hall)*	
02:00 – 02:25	Extracting knowledge from polymeric data with AI	Debbie Audus (NIST)
02:25 – 02:50	The Weak Link in Autonomous Experimentation: If You Want to Understand Function, Study Spectra	Anatoly I. Frenkel (Stony Brook)
02:50 – 03:15	From Optimization to Understanding: Scientist-in-the-Loop Autonomous Experimentation	Klaus Mueller (Stony Brook)
03:15– 03:35	*Break*	
03:35 – 04:00	Model-Guided User Facility Experimentation and Control	Nathan Urban (CDS, BNL)
04:00 – 04:25	TBD	Henry Chan (ANL)
04:25 – 05:30	Panel Discussion: Bridging the Gap from Synthesis to Understanding	Moderators: Yugang Zhang, et al.
05:30 – 06:00	Closing Remarks & Future Outlook	Organizing Committee