WORKSHOP # 10 - Thursday, April 23, 2026

AI Showcase

Organizers: Petra Reinke (University of Virginia), Maya Endoh (Stony Brook University), Gary Harlow (University of Oregon), Anibal Boscoboinik (Brookhaven National Laboratory)

This year we present for the first time a dedicated AI showcase! Scientists working at NSLSII and CFN will present on a diverse range of topics reaching from virtual beamline companions to materials classification, and reaction pathways discovery to robotics for experimentation. AI and machine learning open new ways to experiment and understand complex datasets and will change the way we all work in years to come. We hope the showcase initiates new collaborations and strengthens all our commitments to advance science.

Start Time (ET)	Title	Speaker (Affiliation)
2:00-2:15pm	AI for Science: Virtual Companions at Synchrotrons Beamlines	Shray Mathur
2:15-2:30pm	Quantitative X-ray Imaging Assisted by Machine Learning	Mingyuan Ge
2:30-2:45pm	AI-assisted 2D Material Identification	Houk Jang
2:45-3:15pm	*Break*	
3:15-3:30pm	AI for Tomography Reconstruction	Hanfei Yan
3:30-3:45pm	Machine Learning-Aided Inverse Kinetic Modeling	Qin Wu
3:45-4:00pm	Next Generation MILP for µs Simulation	Xiaohui Qu
4:00-4:30pm	*Break*	
4:30-4:45pm	Frontier Robotics for Experimentation	Aditya Bondada
4:45-5:00pm	AI-Driven Autonomous Nanoparticle Synthesis with In-Situ Synchrotron X-Ray Feedback	Yugang Zhang

ABSTRACTS

AI for Science: Virtual Companions at Synchrotrons Beamlines

Shray Mathur

I will present our work on VISION (Virtual Scientific Companion), a multi-LLM AI assistant designed to enable natural language control of synchrotron X-ray beamlines. VISION allows scientists to perform voice-controlled experimentation, code generation for instrumentation, and data analysis. Its modular architecture is composed of specialized LLM “cogs” dedicated to tasks such as speech transcription, command interpretation, code generation, and data analysis.

Quantitative X-ray Imaging Assisted by Machine Learning

Mingyuan Ge

In this talk, we will present recent advances in machine learning–driven X-ray imaging analysis aimed at enhancing the quantitative interpretation of multimodal datasets. Specifically, we develop data-driven approaches to mitigate reconstruction artifacts arising from incomplete or imperfect data acquisition in X-ray fluorescence tomography (XRF-tomo) and two-dimensional X-ray absorption spectroscopy (2D XANES).

AI-Assisted 2D Material Identification: Universal Optical Identification of 2D Materials by Decoupled Segmentation and Classification

Houk Jang

Automated optical identification of 2D material flakes currently requires either pixel-level classifiers that lack noise robustness or deep-learning models that demand material-specific training data. We decouple segmentation from classification: a visual foundation model segments flakes as coherent objects, and their median color enables statistical layer classification without trained models. Applied to various 2D materials, the framework resolves monolayer through five layers.

AI for Tomographic Reconstruction

Hanfei Yan

Many experimental constraints can result in incomplete, sparse, and noisy datasets that are inadequate for conventional tomographic reconstruction. Here, we demonstrate that by integrating a convolutional neural network—designed to encode perceptual priors—into an iterative reconstruction framework, these otherwise limited datasets can still yield reconstructions that are physically constrained, visually enhanced, and scientifically meaningful.

Machine Learning-Aided Inverse Kinetic Modeling

Qin Wu

Determination of reaction pathways is a critical step in optimizing and controlling chemical systems. We will talk about data-driven approaches that we developed to model reaction pathways by deriving kinetic rate equations from transient kinetic data, featuring physically interpretable parameters that allow for deeper insights into reaction mechanisms. We demonstrate the effectiveness of this approach using experimental data from CO adsorption on a Pd (111) surface and CO oxidation on Pt (111).

Next Generation MILP for μs Simulation

Xiaohui Qu

Machine learning interatomic potentials (MLIPs) accelerate atomistic simulations beyond DFT but often rely on graph neural networks (GNNs) with costly graph construction and message passing. We present a graph- and descriptor-free MLIP using a Deep Sets architecture that builds a continuous structure field from atomic coordinates directly. A voxelized divide-and-consquer sheme ensures efficient atomic environment perception. The model matches GNN accuracy while delivering ~100x speedup.

Frontier Robotics for Experimentation

Aditya Bondada

This talk explores how advanced robotics systems can transform scientific experimentation at synchrotron beamlines. We present work on modular robotic sample handling at NSLS-II, including automated pick-and-place, tool exchange, and integration with the Bluesky experiment framework. We discuss the path toward autonomous beamline operation through extensible robotics architectures and emerging AI-driven control approaches.

AI-Driven Autonomous Nanoparticle Synthesis with In-Situ Synchrotron X-Ray Feedback

Yugang Zhang

We present an autonomous platform integrating a high-throughput droplet-flow microreactor with real-time SAXS/WAXS at NSLS-II for in-situ structural feedback during colloidal nanoparticle synthesis. Applied to gold nanoparticles, the platform achieves precise size control with low polydispersity by sampling only ~150 of ~19,000 possible recipes in under 10 hours. Versatility is further demonstrated through shape-controlled synthesis of other nanomaterials.