

# **Recent Progress in Autonomous X-ray Scattering\***

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## **Abstract**

Autonomous control of complex scientific instruments holds enormous promise for accelerating experiments and materials discovery. This talk will present recent progress in the deployment of autonomous experimentation (AE) methods on synchrotron x-ray scattering beamlines at NSLS-II. Deep learning is used to classify x-ray detector images, with performance improving when domain-specific data transformations are applied. To close the autonomous loop, we deploy a general-purpose algorithm based on gaussian processes. The underlying modeling can exploit system-specific information, while the objective function can be tailored to a particular experiment, balancing knowledge gain, cost, and search targets. We have identified three classes of scattering experiments that benefit from AE: real space mapping, combinatorial exploration, and real-time processing. Examples from recent autonomous experiments will be presented, including measuring nanoparticle ordering, 3D-printed materials, multi-dimensional combinatorial libraries, and real-time photo-thermal processing.

\* Title and Abstract of an Invited Presentation at the Workshop: AI/ML for Particle Accelerator, X-Ray Beamlines and Electron Microscopy at Argonne National Laboratory, November 1-3, 2021.