

APS Scientific Computation Seminar Series

- Speaker:** In-Hui Hwang, Postdoctoral Researcher, X-ray Science Division, Argonne
- Title:** Argonne X-ray Emission Analysis Packages: A Comprehensive Solution for Processing and Analyzing X-ray Emission Spectroscopy (XES) Data
- Date:** October 2, 2023
- Time:** 1:00 p.m. (Central Time)
- Location:** Join ZoomGov Meeting
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- Hosts:** Mathew Cherukara and Nicholas Schwarz
- Abstract:** The Argonne X-ray Emission Analysis Package (AXEAP) comprises two distinct versions designed for the calibration, processing, and analysis of X-ray emission spectroscopy (XES) data obtained using a two-dimensional position-sensitive detector. AXEAP1 utilizes unsupervised machine learning to swiftly convert raw data into XES spectra, enabling immediate comparisons during data acquisition [1]. In addition, the software includes a variety of features that allow correcting any issues that might arise, as well as experiment steering to make sure that the data collected is useful. AXEAP2 is designed to offer insights into electron spin states, 3d-3p electron exchange forces, and emission core-hole lifetimes with minimal user intervention [2]. In addressing the challenges of XES data analysis, a methodology includes three aspects. The first is the XES calculation that is based on the CTM4XAS program. The second is the convolution after XES calculation. The last part is the parameter optimization driven by a genetic algorithm (GA) that efficiently finds optimized values in multiple parameter spaces and is widely used to generate high-quality solutions for optimization problems. Since the program achieves optimization through extensive simulation, scientists can interpret the analysis results through various models generated during optimization. Both AXEAP1 and AXEAP2 are implemented in MATLAB and compatible with the Windows OS.