Sample Environment, Data Acquisition and Data Processing Pipeline for High Throughput X-ray Absorption Spectroscopy Measurements at the Inner Shell Spectroscopy Beamline at NSLS-II

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Inner shell spectroscopy (ISS) beamline which entered user operations in early 2017, operates at very high flux (10^{14} ph/s) and allows for fast energy scanning (1000 eV/s). This performance enables the ability to perform high-throughput X-ray spectroscopy measurements. In this contribution, I will present the asynchronous data acquisition system developed at ISS. The high throughput operando sample environments which allow electro- and heterogeneous catalysis, and battery experiments with multiple cell/reactors will be discussed. Leveraging these developments, a novel material characterization pipeline is being created that yields atomistic-level snapshot of the active site in action. The high-throughput X-ray spectroscopic data streams into a spectral database. Operando spectral series will be deconvoluted into pure response spectra, which will be compared on-line with available body of experimental data as well as low-level calculations, derived from, e.g., Materials Project. Once preliminary matches are established, the computational engine will perform high-level DFT calculations, as well as multi-parameter correlation search (aka machine learning) to refine the model. This scheme will provide immediate feedback to the experimenter, allowing to select most promising areas of the parameter space and optimize experimental conditions. With this approach, self-guiding operando experiments will become possible.