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ECXAS: A data aggregation tool for battery study in ROCK beamline

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Present-day material characterization requires insight from multiple techniques if a complete understanding of the material's properties and behaviors is desired. This is often the case with synchrotron-based experiments in which, besides the collected data from a beamline itself, additional data is obtained by simultaneous measurements using other experimental probes and under different in situ environments. This multimodal approach along with the continuously increasing time/space resolution of synchrotron measurements simply translates into higher data dimension and larger data volume, which adds to its complexity during the analysis step. A tool for semi-automated data processing becomes thus decisive during and after each experiment.

Here, we present the case example of ROCK beamline in which time-resolved X-ray absorption spectroscopy (XAS) is coupled to electrochemical cycling (EC) for the study of battery materials. We introduce a tool developed in Python to aggregate data from multiple sources and assemble multi-dimensional maps. The tool allows for a continuous representation of XAS spectra during charge/discharge cycles along with the relevant electrochemical information, thus facilitating the deduction of present phases over the course of the experiment. The initiative is part of the European BIG-MAP (Battery Interface Genome - Materials Acceleration Platform) project.

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