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Handling Spectrosopic Calculations in Aperiodic Systems[1] ELYSSA ROEDER, Florida State University, JOSHUA KAS, University of Washington — This work is intended to report on a workflow for handling calculations of aperiodic systems with particular focus on calculations of spectroscopy and to demonstrate a sample application of its usage. The workflow is intended to be integrated into the Corvus workflow machinery - a Python-based package designed to automate complex simulations requiring multiple scientific software packages.The workflow has been then applied to the calculation of Ti K-edge X-ray absorption spectra of SrTi1-xSnxO3, in tandem with FEFF9 ab initio code for calculating x-ray and related spectra. Calculated results compare well to experimental results from a recent study, and allow for an interpretation of doping related differences in terms of structure and chemistry. As the workflow and the Corvus machinery are general in nature, the approach can be applied to calculations in a wide variety of systems and phenomena, e.g., glasses, defects, liquids, or vibrational effects.

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