O.24 Calculating X-ray absorption spectra in ABINIT including spin-orbit effects

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X-ray spectroscopy is sensitive to core levels and valence band electronic structure and can be used to study materials ranging from bio-molecules to warm dense matter. With the advent of X-ray free electron lasers, it is possible to employ X-ray spectroscopy in experiments on new timescales with increased intensity and resolution. However, to interpret the results of these experiments, they have to be accompanied by improved calculations, that need to take into account as many relevant effects as possible.

In this talk, we will focus on the effect of spin-orbit coupling and how we implemented it into X-ray spectroscopy in ABINIT. To this end we will describe how to obtain relativistic core wave functions from ATOMPAW and how we use them to calculate transition matrix elements in ABINIT. These matrix elements are then evaluated with the CONDUCTI post-processing tool within the Kubo-Greenwood formalism to calculate X-ray absorption near edge spectra (XANES). We will show example results for gold and warm dense copper.