# Improving Optical and X-Ray Spectroscopy in ABINIT

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The prediction and analysis of optical and X-Ray spectra of materials under warm dense matter conditions is of great scientific interest. The ABINIT implementation of the PAW formalism is well suited to treat this highly excited state of matter. One important aspect when treating optical and X-Ray spectroscopy, especially for heavier elements, is the spin-orbit coupling.

In this talk, we will present our improvments of the prtnabla option and the conducti post-processing tool, which take advantage of ABINIT's PAW spinor implementation in the calculation of optical and X-Ray spectra. Spinors are now treated correctly and an option to take spin-orbit coupling into account in the dipole matrix element as well has been added for optical spectroscopy. Furthermore, it is now possible to import spinor core wave functions provided by the new version of atompaw, which allows to predict the spin-orbit splitting and the ratio of the X-ray absorption edges correctly. In addition, we have added NetCDF and MPI support for the conducti post-processing tool. Finally, we will present our plans for the implementation of the relaxed core approximation in ABINIT.