Implementing the Relaxed Core PAW Method into ABINIT

N. Brouwer[1], V. Recoules[1] and M. Torrent[1]

[1] CEA, DAM, DIF, F91297 Arpajon, France

The projector augmented wave method usually treats core electrons using the frozen core approximation in order to save computational cost in comparison to all-electron codes. However, in certain cases, e. g. under warm dense matter conditions, core wave functions are expected to be altered significantly. Due to the large number of atoms and bands, that might be required under these conditions, the computational cost of all-electron codes can be prohibitive.
As an alternative Marsman and Kresse [1] developed the relaxed core projector augmented wave method (RCPAW), which relaxes the core wave functions with respect to the altered valence band electron density. In this short presentation, we will present our plans for implementing RCPAW into the ABINIT software package.

References

[1] M. Marsman and G. Kressw, J. Chem. Phys. **125**, 104101 (2006).