

PAW Atomic Data Generation for ABINIT

M. Torrent and F. Jollet

*Commissariat à l'Energie Atomique, Centre d'Etudes de
Bruyères-le-Chatel, BP 12, F-91680 Bruyères-le-Chatel*

Two PAW atomic data generators have been developed for ABINIT. The first one comes from the code ATOMPAW, written by N. Holzwarth and co-workers, that has been adapted for ABINIT. The second one comes from the ultrasoft generator from D. Vanderbilt. The presentation will include the following topics:

- Which data do we need?
- How are they generated?
- What is available on the web site?
- How to generate a new set of atomic data?
- How do the two generators compare?