

The ABINIT software project

Xavier GONZE

Unite PCPM, U. Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium

Douglas C. ALLAN

Corning Inc., Fundamental Res., SP FR 5, Corning, NY 14831

and the ABINIT group

The computation of electronic structure, total energy, forces and many related properties of condensed matter, thanks to density-functional theory (DFT), is a field in constant progress. A DFT software project that wants to stay at the frontier of knowledge cannot be the work of a single individual, neither of a small group. Also, up-to-date software engineering concepts can considerably ease the harmonious development of such software.

The ABINIT project relies upon these ideas : reliability, portability, readability and freedom of sources are emphasized, in the course of developping a sophisticated plane-wave pseudopotential code. More than 200 automated tests secure existing capabilities (concept of self-testing), despite heavy development efforts and the associated bug generation; thanks to MAKE and PERL scripts, and CPP directives, the unique set of Fortran90 source files (about 100000 lines) can generate sequential (or parallel) object code for many platforms, under Unix/Linux, DOS/Windows and MacOS; strict coding rules have been followed to make the source readable; the documentation is extensive, including online help files, tutorials, HTML-formatted sources. Moreover, the whole package is distributed under the GNU General Public Licence, often nicknamed 'copyleft'. For more information, see <http://www.pcpm.ucl.ac.be/ABINIT>.