Presenting Abinit

Abstract

The following abstract can be useful when asked to present Abinit to other scientific communities.

ABINIT is an open-source suite of programs for materials science, distributed under the GNU General Public License. ABINIT implements density function theory by solving the Kohn-Sham equations describing the electrons in a material, expanded in a plane wave basis set. Computational efficiency is achieved through the use of fast Fourier transforms, and pseudopotentials or projector-augmented waves to describe core electrons. Materials that can be treated by ABINIT include insulators, metals, and magnetically ordered systems including Mott-Hubbard insulators. In addition to computing the electronic ground state of materials, ABINIT implements density functional perturbation theory to compute response functions including phonons, dielectric response, Born effective charges and IR oscillator strength tensor, response to strain and elastic properties, and nonlinear responses, including piezoelectric response, Raman cross sections, and electro-optic response. ABINIT can also compute excited-state properties via time-dependent density functional theory, as well as through many-body perturbation theory using the GW approximation and Bethe-Salpeter equation.