ABINIT: first-principles approach to material and nanosystem properties

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ABINIT [http://www.abinit.org] allows one to study, frorn first-principles, systems made of electrons and nuclei (e.g. periodic solids, molecules. nanostructures, etc.), on the basis of Density-Functional Theory (DFT) and Many-Body Perturbation Theory. Beyond the computation of the total energy, charge density and electronic structure of such systems, ABINIT also implements many dynamical, dielectric, thermodynamical, mechanical. or electronic properties, at different levels of approximation. The present paper provides an exhaustive account of the capabilities of ABINIT. It should be helpful to scientists that are not familiarized with ABINIT, as well as to already regular users. First, we give a broad overview of ABINIT, including the list of the capabilities and how to access them. Then, we present in more details the recent, advanced, developments of ABINIT, with adequate references to the underlying theory, as well as the relevant input variables, tests and, if available, ABINIT tutorials. Program summary Program title: ABINIT Catalogue identifier: AEEU-v1-0 Distribution fop-mat: tar.gz Joumal reference: Comput. Phys. Comm. Programming language: Fortran95, PERL scripts, Python scripts Computer: All systems with a Fortran95 compiler Operating system: All systems with a Fortran95 compiler Has the code been vectorized or parallelized?: Sequential, or parallel with proven speed-up up to one thousand processors. RAM: Ranges from a few Mbytes to several hundred Gbytes, depending on the input file. Classification: 7.3. 7.8 External routines: (all optional) BigDFT [1], ETSF 10 [2], libxc [3]. NetCDF [4], MPI [5], Wannier90 [6] Nature of problem: This package has the purpose of computing accurately material and nanostructure properties: electronic structure, bond lengths, bond angles, primitive cell size, cohesive energy, dielectric properties, vibrational properties, elastic properties, optical properties, magnetic properties, non-linear couplings, electronic and vibrational lifetimes, etc. Solution method: Software application based on Density-Functional Theory and Many-Body Perturbation Theory, pseudopotentials, with planewaves, Projector-Augmented Waves (PAW) or wavelets as basis functions. Running time: From less than one second for the simplest tests, to several weeks. The vast majority of the >600 provided tests run in less than 30 seconds. References: [1] http://inac.cea.fr/LSim/BigDFr. [2] http://etsLeu/index.php?page=standardization. [3] http://www.tddft.org/programs/octopus/wiki/index.php/Libxc. [4] http://www.uniciata.ucar.edti/software/iietcdL [5] http://en.wikipedia.org/wiki/MessagePassinginterface. [6] http://www.wannier.org.

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