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The ABINIT software project

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The ABINIT software project aims at providing the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) thanks to a first-principle approach. The ground state properties are calculated in the framework of the Density-Functional Theory (DFT). The excited states properties are computed within the Many-Body Perturbation Theory (MBPT). Finally, the response properties are obtained from Density-Functional Perturbation Theory (DFPT).
The ABINIT software project was started in 1997 as an open software project, without a definite goal, developed using several software engineering techniques to allow international collaboration of many different groups. The first publicly available version of ABINIT was released in December 2000 under the GNU GPL. The software has already been described in various articles [1-4]. The last stable version of the package (7.10.4) has now a 70 MBytes size, consisting in nearly 1400 files written in F90 (830000 lines) and including documentation, tutorials and more than one thousand tests. The code is developed by an always opened community (around fifty people) and it is used by more than a thousand individuals worldwide.

References

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