The SIESTA Code: Basis Set Construction Strategy. Comparing Solid State DFT Codes

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Abstract

SIESTA is both a method and its computer program implementation, to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.[1] In the SIESTA code, finite-support atomic orbitals are used as basis set.[2] In this work we have designed a basis set construction strategy to generate efficient basis set. The optimization target has been the minimization of the average energy of a set of Ndi symmetric dimers at different bond distances (di).

The reproducibility of results is one of the underlying principles of science. In spite of the absence of one absolute reference code, the reproducibility of DFT results can be established by a broad and comprehensive test for precision; Δ-DFT test. [3] As a second stage of this project, the original Δ-DFT protocol will be applied to the SIESTA method firstly to test the quality of the newly generated basis, and secondly to demonstrate SIESTA competitiveness against other codes. Applying the Δ-DFT test, the precision is assessed by means of a pairwise comparison of a wide range of codes and methods respect to their predictions of the equations of state of the elemental crystals. This test has already been performed for more than ten atomic-scale simulation codes with characteristics similar to SIESTA code (WIEN2k, GPAW, VASP, ABINIT, etc.).

After the Δ-DFT test is successfully completed, the basis set database generated in this project will be incorporated into the software SIESTA PRO. SIESTA PRO, computer program currently developed by SIMUNE (www.simune.eu), has the aim to automatize and increase the efficiency of the use of the SIESTA code.

References

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