Scale-Up: An implementation of Second-Principles DFT

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Second-Principles Density Functional Density (SPDFT) [1] is a first-principles-based method designed to have an accuracy similar to DFT, at a much smaller computational cost. The resulting method, that allows for a systematical improbable approximation of DFT and that is related to self-consistent tight-binding DFT, can be used to perform simulations in large systems (typically tens of thousands of atoms) and is able to deal with metals and magnetic systems. In SPDFT a material is divided into two subsystems; the lattice, corresponding with a reference, electronic state (usually the ground state) whose energy is calculated using a force-field [2] and the electrons, that are activated to correct the results when the state of the system deviates from the reference. Here, we will focus on giving an overview of current capabilities and limitations of the method.
Scale-Up is our implementation of SPDFT and it allows obtaining many of the magnitudes that a DFT code typically provides, from the total energy or the forces to the charge or spin distribution over the atoms. This package can be used as a library by other Second Principles codes like Multibinit in order to complement these codes with extra functionality. Finally, we will devote some time to discuss how to generate electron models from first-principles simulations and the interface between Scale-Up and Siesta.

References

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