Second-Principles Density Functional Theory: A systematically improvable multi-scale method including electrons and lattice degrees of freedom

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During the last two decades first-principles methods, particularly Density Functional Theory (DFT), have become an indispensable tool in the study of solid-state systems. However, interpreting or predicting the results of experiments requires, in many cases, to go beyond the length and/or time scales allowed by current computational power. Based on the idea that not all electrons play a relevant role in the determination of the physical magnitudes under scrutiny, we present a non-empirical, systematically improvable approximation to DFT based on a rigorous separation of these active electrons and holes from those of a reference electron density [1]. Using a similar expansion to that found in Tight-binding DFT methods we obtain a large term containing the energy of the reference system, and a second, much smaller one, associated to the active part of the electron density. By employing a well-tested model Hamiltonian to reproduce the energy surface associated to the reference system and representing the active electrons with a small but accurate Wannier function basis-set we obtain an efficient simulation method that can be used to calculate systems with tens of thousands of atoms with approximations that are systematically improvable towards DFT-quality. This method has been implemented in the SCALE-UP code (http://secondprinciples.unican.es; twitter @2nd_Principles). We provide several examples of its application in complex oxides including magnetism, metallic states and ferroelectricity [2,3].

References

[1] P. García-Fernández et al. Phys. Rev. B 93 (2016)195137.
[2] A. R. Damodaran et al. Nature Materials 16 (2017) 1003
[3] P. Shafer et al. Proceedings of the National Academy of Sciences (2018) Early edition

Figures

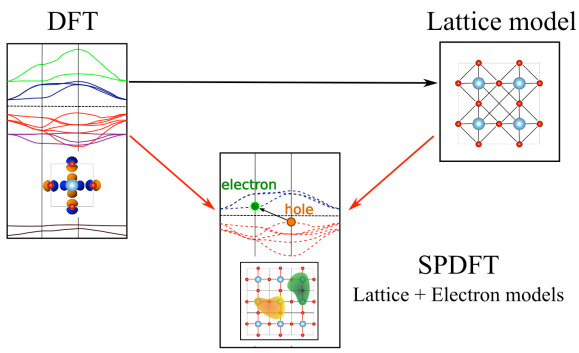

Figure 1: Illustration of second-principles density functional theory with respect to other related simulation methods