The DFT-1/2 method for gap correction

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Abstract

For the past 40 years density functional theory (DFT) has been the dominant method for the quantum mechanical simulation of periodic systems, predicting the ground state properties of metals, semiconductors, and insulators with great success. This success not only encompasses standard bulk materials but also complex materials such as proteins, polymers, solids, nanostructures and DNA. Practical applications of DFT are based on approximations for the so-called exchange-correlation potential. Common approximations are the so-called Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA), which produce semiconductor band gaps significantly smaller than experiment. This fact raises the issue of how to obtain reliable excited-state properties. We addressed this question by proposing the DFT-1/2 method in 2008 and provide general form to calculate one-particle excitations in solids [1,2]. The method consists of calculating the self-energy as the quantum mechanical average of a “self-energy potential”, which is added to the local part of the pseudopotential or to the -2Z/r part of the all-electron potential. We obtained band gaps of several semiconductors that compare very well with experiment, with the precision of the GW method, but at negligible computational cost. This great advantage of the method allows approximate quasiparticle correction for more complex systems as alloys, interfaces, perovskites etc. The method was also applied to 34 different 2D materials showing results in their majority superior to the HSE06. Moreover, based on the knowledge of the method and chemical information of the material, we can predict the small number of cases in which the method is not so effective and provide the best recipe for an optimized DFT-1/2 method based on the electronegativity difference of the bonding atoms. The method is nowadays used in several codes by several groups around the world.

In this tutorial we will provide a basic theoretical overview and perform a few hands-on practices.

References

1. L. G. Ferreira, M. Marques and L. K. Teles, Phys. Rev. B 78, 125116 (2008).
2. L. G. Fereira, M. Marques and L. K. Teles, AIP Adv. 1032119 (2011).