Introduction to Density Functional Theory (DFT)

Marie-Liesse DOUBLET

Institut Charles Gerhardt – CNRS et Université de Montpellier - France

Abstract: First-principles approaches to condensed matter consist in starting from what we know about a material, i.e. its chemical composition, and to calculate its energy and properties. In the Born-Oppenheimer approximation, the electrons are the particles setting the many-body problem. Amongst the theoretical methods available to solve this many-body problem, Density Functional Theory (DFT) [1] is the most widely used formalism in condensed matter as it combines numerical efficiency with acceptable accuracy and reliability. It is regarded as the main computational tool to perform electronic structure calculations for periodic systems with a realistic complexity. Within the framework of Kohn–Sham DFT (KS DFT) [2] the intractable many-body problem of interacting electrons moving in a static external potential is reduced to a tractable problem of non-interacting electrons moving in an effective potential $v_{\mathrm{eff}}(\vec{r})$. This formalism will be briefly introduced together with the main classes of energy functionals developed so far to reach an accurate description of $v_{\mathrm{eff}}(\vec{r})$. [3] The strength and weakness of each class of functional will then be discussed in regard to specific material properties.

References:

[1] P. Hohenberg and W. Kohn., Phys. Rev., 136, B864 (1964).
[2] W. Kohn and L. J. Sham, Phys. Rev., 140, A1133 (1965).
[3] A review of the different classes of energy functionals can be found in any textbook dedicated to DFT. Specific references will be given during the school.