

Introduction

Density functional theory (DFT) is a quantum many-body theory used in physics and chemistry to investigate the electronic structural (principally the ground state) of many body system, in particular atoms, molecules, and the condense phase. According to this theory, the properties of the system are mathematical functions of the electron density which is itself a function of the position. In other words, the properties of the system are determined as a functional (functional of other function), the electron density, hence the name density functional theory. The DFT has been extensively used in solid state physics and quantum chemistry. In most cases, compare to other theoretical method of solving many-body Schrodinger equation (such as Hatree-Fork Method), the calculation results from DFT under the Local Density Approximation (LDA) match the experimental results extreme well! However, although the DFT is the leading theory method for electronic calculation in all kinds of area, it encountered some difficulties in describing the interaction between molecules, especially “Vandwas force”. It is also difficult to be used in of semiconductor research.

Inspired by the Thomas-Fermi model, DFT was put on a firm theoretical footing by the Hohenberg—Kohn theorems (H-K) in 1964. H-K is the origination of the DFT. The basic ideas of the H-K theorems are listed as follow:

First, the ground state properties of the system are uniquely defined by the spatial dependent electron density; Second, it defines a functional of electron density for the system, and proved that the correct ground state electron density minimized this energy functional.

After the great idea had been created, the next step is how to realize it. In 1965, Kohn and Sham showed that the Hamiltonian equation derived from this variational approach took a very simple form. The so-called **Kohn-Sham equation** is similar in form to the time-independent Schrodinger equation, except that the potential experienced by the electrons

is formally expressed as a functional of the electron density. Again it is effectively a single-particle equation. In addition to the contribution from the electron-ion interaction, the electron-electron interaction potential is split for convenience into two parts: the Hartree potential, which we have met before, and an **exchange-correlation potential**, whose form is, in general, unknown.