

An introduction to Density Functional Theory and Time-Dependent Density Functional Theory

“Density Functional Theory” (DFT) is undoubtedly one of the most ground breaking theories of modern physics and chemistry. Walter Kohn received the Nobel prize of Chemistry in 1998 for the development of this theory and the seminal papers in this area are among the most cited Physics papers of all times. DFT provides an alternative feasible route to solve the Schrödinger equation of a molecule or a solid by replacing the role of the wavefunction by a computational cheaper quantity which is the electronic spatial density. Although this reformulation is proved to be feasible, the corresponding equations that one needs to solve instead are not explicitly known and need to be approximated.

Nowadays there is a plethora of scientific software available which solves numerically these approximate DFT equations helping to understand from chemical processes that happen in the human body to ones in astrophysical systems. DFT applications involve from drug discovery to developing materials for solar cells.

In this course an introduction to DFT and its Time-Dependent counterpart (TDDFT), which addresses problems of dynamics of matter, will be given. The topics that would be covered is its foundations, actual challenges in the methodological development of it and a short overview of physical applications. A basic hand-on tutorial on how to set up a DFT/TDDFT calculation with a standard electronic structure program will be presented.

Course Prerequisites: Basic Knowledge of Quantum Mechanics

This is a theory course presented in a way that experimentalists could also attend it.

