An Introduction to Density Functional Theory and Application

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Abstract: Density-functional theory (DFT) is a theoretical and computational quantum mechanical method used in physics, chemistry, biology and materials science to investigate the electronic of many-body systems, in particular atoms, molecules, crystal structures, and the condensed phases. DFT has been very popular for calculations in solid-state physics since the 1970s. Unlike the wavefunction, which is not a physical reality but a mathematical construct, electron density is a physical characteristic of all molecules. A functional is defined as a function of a function, and the energy of the molecule is a functional of the electron density. The electron density is a function with three variables – x-, y-, and z-position of the electrons. Unlike the wavefunction, which becomes significantly more complicated as the number of electrons increases, the determination of the electron density is independent of the number of electrons. Using this theory, the properties of a many-electron system can be determined by using functionals, i.e. functions of another function. In the case of DFT, these are functionals of the spatially dependent electron density. DFT is among the most popular and versatile methods available in condensed-matter physics, computational physics, computational materials physics, and materials chemistry. We will describe the DFT method in short and we will show how the DFT methods can apply to solve various problems in condensed matter nanoscience and materials science in detail.

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