

Special Issue on Density Functional Theory

Call for Papers

Density functional theory (DFT) is a quantum mechanical modelling method used in physics and chemistry to investigate the electronic structure (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases. With this theory, the properties of a many-electron system can be determined by using functionals, i.e. functions of another function, which in this case is the spatially dependent electron density. Hence the name density functional theory comes from the use of functionals of the electron density. DFT is among the most popular and versatile methods available in condensed-matter physics, computational physics, and computational chemistry.

DFT has been very popular for calculations in solid-state physics since the 1970s. However, DFT was not considered accurate enough for calculations in quantum chemistry until the 1990s, when the approximations used in the theory were greatly refined to better model the exchange and correlation interactions. In many cases the results of DFT calculations for solid-state systems agree quite satisfactorily with experimental data. Computational costs are relatively low when compared to traditional methods, such as Hartree–Fock theory and its descendants based on the complex many-electron wavefunction.

In this special issue, we intend to invite front-line researchers and authors to submit original research and review articles on exploring **Density Functional Theory**.

Authors should read over the journal's [Author's Guidelines](#) carefully before submission, Prospective authors should submit an electronic copy of their complete manuscript through the journal [Paper Submission System](#).

Please kindly notice that the “**Special Issue**” under your manuscript title is supposed to be specified and the research field “**Special Issue-Density functional theory**” should be chosen during your submission.

According to the following timetable:

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