Density Functional Theory
(KDIT33)

topics

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1. Brief introduction to functionals: Mathematical background; functional derivative; role of functionals in physics.
2. Schrodinger equation for atoms and molecules: Reduction of the number of variables. Stationary case, adiabatic and Born-Oppenheimer approximation, independent particle model.
3. Theoretical background of the Hartree-Fock method, the terms of the Fock operator.
4. Derivation of the Hohenberg–Kohn theorems for non-degenerate, ground state N-electron systems.
5. The early stage of Density Functional Theory: Derivation of the Thomas–Fermi kinetic functional.
6. The Kohn–Sham picture. Derivation of the Kohn–Sham equations.
7. Exchange functionals in DFT: The local density approximation. Derivation of the Xα energy functional.
8. Beyond the local density approximation: Functionals with gradient corrections. Hybrid functionals.
9. Correlation in DFT.: Local Density Approximation and Gradient corrections.
10. Investigation of excited state systems: ensemble DFT; The fundamentals of linear response theory.
11. Outlook on some current research directions: Density matrix functional theory. Strongly Interacting Electron systems and its Kohn–Sham picture.