TOPICS IN FUNDAMENTAL PHYSICS

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Density Functional Theory (DFT)

Introduction: What is a Kohn-Sham calculation?

Functionals: What is a functional? Functional derivatives. Euler-Lagrange equations.

One electron systems: Variational principle, trial wave-functions.

Two electron systems: Antisymmetry, Hartree-Fock and correlation.

Many electron systems: ground state and Hartree-Fock.

Density Functional Theory: Hohenberg-Kohn theorem and Thomas-Fermi.

Kohn-Sham equations: Exchange and correlations.

The Local Density Approximation: uniform electron gas.

Exchange-correlation hole: Density matrices and holes, Hooke's atom and Transferability of a hole.

DFT in practice

Overview of electronic structure codes

Hands on Quantum-espresso: Plane waves; Pseudo-potential calculations: total energy, bands, relaxations; Non-collinear calculations: magnetism and spin-orbit coupling; Density functional perturbation theory: phonons and external fields.