

Density Functional Theory: Principles, Self-Consistency, and Practical Implementation

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Density Functional Theory (DFT) has become one of the most widely used computational frameworks in materials science, chemistry, and solid-state physics for predicting electronic structure and related physical properties from first principles. In this talk, we will introduce the fundamental concepts underlying DFT, starting from the many-electron Schrödinger equation and the key insight that the ground-state properties of a many-electron system can be uniquely determined by its electron density. Central to DFT is the self-consistent field (SCF) procedure, where the electron density and the effective potential are iteratively refined until convergence is achieved. We will demystify how practical implementations of DFT, such as plane-wave basis sets and pseudopotentials, enable efficient and accurate calculations for real materials. The talk will cover common approximations (e.g., exchange-correlation functionals), the role of convergence thresholds, and how density mixing and other numerical strategies are used to achieve stability. Illustrative examples will demonstrate how DFT is applied using widely adopted software, highlighting both its strengths and limitations. Attendees will leave with a clear conceptual understanding of DFT's core mechanisms.