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Nota di contenuto	Chapter 1. Review of approximations for the exchange-correlation energy in density-functional theory -- Chapter 2. On connecting density functional approximations to theory -- Chapter 3. Universal functionals in density functional theory -- Chapter 4. The strong-interaction limit of density functional theory -- Chapter 5. Moreau–Yosida regularization in DFT -- Chapter 6. Thermodynamic limits of electronic systems -- Chapter 7. Numerical methods for Kohn–Sham

models: discretization, algorithms, and error analysis -- Chapter 8. Recent progress in evaluating the Kohn–Sham map -- Chapter 9. Augmented plane wave methods for full-potential calculations -- Chapter 10. Finite Element Methods for Density Functional Theory -- Chapter 11. Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations -- Chapter 12. Accurate approximations of density functional theory for large systems with applications to defects in crystalline solids -- Glossary -- Notation.

Sommario/riassunto

Density functional theory (DFT) provides the most widely used models for simulating molecules and materials based on the fundamental laws of quantum mechanics. It plays a central role in a huge spectrum of applications in chemistry, physics, and materials science. Quantum mechanics describes a system of N interacting particles in the physical 3-dimensional space by a partial differential equation in $3N$ spatial variables. The standard numerical methods thus incur an exponential increase of computational effort with N, a phenomenon known as the curse of dimensionality; in practice these methods already fail beyond $N=2$. DFT overcomes this problem by 1) reformulating the N-body problem involving functions of $3N$ variables in terms of the density, a function of 3 variables, 2) approximating it by a pioneering hybrid approach which keeps important ab initio contributions and re-models the remainder in a data-driven way. This book intends to be an accessible, yet state-of-art text on DFT for graduate students and researchers in applied and computational mathematics, physics, chemistry, and materials science. It introduces and reviews the main models of DFT, covering their derivation and mathematical properties, numerical treatment, and applications. .