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Nota di contenuto	DENSITY FUNCTIONAL THEORY; CONTENTS; Preface; 1 What Is Density Functional Theory?; 1.1 How to Approach This Book; 1.2 Examples of DFT in Action; 1.2.1 Ammonia Synthesis by Heterogeneous Catalysis; 1.2.2 Embrittlement of Metals by Trace Impurities; 1.2.3 Materials Properties for Modeling Planetary Formation; 1.3 The Schrodinger Equation; 1.4 Density Functional Theory-From Wave Functions to Electron Density; 1.5 Exchange-Correlation Functional; 1.6 The Quantum Chemistry Tourist; 1.6.1 Localized and Spatially Extended Functions; 1.6.2 Wave-Function-Based Methods; 1.6.3 Hartree-Fock Method 1.6.4 Beyond Hartree-Fock1.7 What Can DFT Not Do?; 1.8 Density Functional Theory in Other Fields; 1.9 How to Approach This Book (Revisited); References; Further Reading; 2 DFT Calculations for Simple Solids; 2.1 Periodic Structures, Supercells, and Lattice Parameters; 2.2 Face-Centered Cubic Materials; 2.3 Hexagonal Close-Packed Materials; 2.4 Crystal Structure Prediction; 2.5 Phase Transformations; Exercises;

Further Reading; Appendix Calculation Details; 3 Nuts and Bolts of DFT Calculations; 3.1 Reciprocal Space and k Points; 3.1.1 Plane Waves and the Brillouin Zone
3.1.2 Integrals in k Space3.1.3 Choosing k Points in the Brillouin Zone; 3.1.4 Metals-Special Cases in k Space; 3.1.5 Summary of k Space; 3.2 Energy Cutoffs; 3.2.1 Pseudopotentials; 3.3 Numerical Optimization; 3.3.1 Optimization in One Dimension; 3.3.2 Optimization in More than One Dimension; 3.3.3 What Do I Really Need to Know about Optimization?; 3.4 DFT Total Energies-An Iterative Optimization Problem; 3.5 Geometry Optimization; 3.5.1 Internal Degrees of Freedom; 3.5.2 Geometry Optimization with Constrained Atoms; 3.5.3 Optimizing Supercell Volume and Shape; Exercises; References Further ReadingAppendix Calculation Details; 4 DFT Calculations for Surfaces of Solids; 4.1 Importance of Surfaces; 4.2 Periodic Boundary Conditions and Slab Models; 4.3 Choosing k Points for Surface Calculations; 4.4 Classification of Surfaces by Miller Indices; 4.5 Surface Relaxation; 4.6 Calculation of Surface Energies; 4.7 Symmetric and Asymmetric Slab Models; 4.8 Surface Reconstruction; 4.9 Adsorbates on Surfaces; 4.9.1 Accuracy of Adsorption Energies; 4.10 Effects of Surface Coverage; Exercises; References; Further Reading; Appendix Calculation Details
5 DFT Calculations of Vibrational Frequencies5.1 Isolated Molecules; 5.2 Vibrations of a Collection of Atoms; 5.3 Molecules on Surfaces; 5.4 Zero-Point Energies; 5.5 Phonons and Delocalized Modes; Exercises; Reference; Further Reading; Appendix Calculation Details; 6 Calculating Rates of Chemical Processes Using Transition State Theory; 6.1 One-Dimensional Example; 6.2 Multidimensional Transition State Theory; 6.3 Finding Transition States; 6.3.1 Elastic Band Method; 6.3.2 Nudged Elastic Band Method; 6.3.3 Initializing NEB Calculations; 6.4 Finding the Right Transition States
6.5 Connecting Individual Rates to Overall Dynamics

Sommario/riassunto

Demonstrates how anyone in math, science, and engineering can master DFT calculations Density functional theory (DFT) is one of the most frequently used computational tools for studying and predicting the properties of isolated molecules, bulk solids, and material interfaces, including surfaces. Although the theoretical underpinnings of DFT are quite complicated, this book demonstrates that the basic concepts underlying the calculations are simple enough to be understood by anyone with a background in chemistry, physics, engineering, or mathematics. The authors show how the widespread