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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;

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