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8 Simulation of Solids Starting from the First Principles ("ab initio" Models)
8.1 Many-Body Problem: Fundamentals; 8.2 Milestones in Solution of the Many-Body Problem; 8.3 More of the Hartree and Hartree-Fock Approximations; 8.4 Density Functional Theory; 8.5 The Kohn-Sham Auxiliary System of Equations; 8.6 Exchange-Correlation Functional; 8.7 Plane Wave Pseudopotential Method; 8.8 Iterative Minimization Technique for Total Energy Calculations; 8.9 Linearized Augmented PlaneWave Method; 9 First-Principle Simulation in Materials Science; 9.1 Strength Characteristics of Solids
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11.3 Applications of the Tight-Binding Method

Sommario/riassunto

The connection between a quantum behavior of the structure elements of a substance and the parameters that determine the macroscopic behavior of materials has a major influence on the properties exhibited by different solids. Although quantum theory and engineering should complement each other, this is not always the case. This book aims to demonstrate how the properties of materials can be derived and predicted proceeding from the features of their structural elements, generally electrons. In a sense, electronic structure forms the glue holding solids as whole, and it is centr
