

1. Record Nr.	UNINA9910140179403321
Autore	Levitin Valim
Titolo	Interatomic bonding in solids : fundamentals, simulation, applications / / Valim Levitin
Pubbl/distr/stampa	Weinheim an der Bergstrasse, Germany : , : Wiley-VCH, , 2014 ©2014
ISBN	3-527-67155-2 3-527-67158-7 3-527-67157-9
Descrizione fisica	1 online resource (322 p.)
Disciplina	541.224
Soggetti	Chemical bonds Density functionals - Computer simulation Materials science - Computer simulation Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Cover; Title Page; Contents; Preface; 1 Introduction; 2 From Classical Bodies to Microscopic Particles; 2.1 Concepts of Quantum Physics; 2.2 Wave Motion; 2.3 Wave Function; 2.4 The Schrodinger Wave Equation; 2.5 An Electron in a Square Well: One-Dimensional Case; 2.6 Electron in a Potential Rectangular Box: k-Space; 3 Electrons in Atoms; 3.1 Atomic Units; 3.2 One-Electron Atom: Quantum Numbers; 3.3 Multi-Electron Atoms; 3.4 The Hartree Theory; 3.5 Results of the Hartree Theory; 3.6 The Hartree-Fock Approximation; 3.7 Multi-Electron Atoms in the Mendeleev Periodic Table; 3.8 Diatomic Molecules 4 The Crystal Lattice 4.1 Close-Packed Structures; 4.2 Some Examples of Crystal Structures; 4.3 The Wigner-Seitz Cell; 4.4 Reciprocal Lattice; 4.5 The Brillouin Zone; 5 Homogeneous Electron Gas and Simple Metals; 5.1 Gas of Free Electrons; 5.2 Parameters of the Free-Electron Gas; 5.3 Notions Related to the Electron Gas; 5.4 Bulk Modulus; 5.5 Energy of Electrons; 5.6 Exchange Energy and Correlation Energy; 5.7 Low-Density Electron Gas: Wigner Lattice; 5.8 Near-Free Electron Approximation: Pseudopotentials; 5.9 Cohesive Energy of Simple Metals

6 Electrons in Crystals and the Bloch Waves in Crystals
6.1 The Bloch Waves; 6.2 The One-Dimensional Kronig-Penney Model; 6.3 Band Theory; 6.4 General Band Structure: Energy Gaps; 6.5 Conductors, Semiconductors, and Insulators; 6.6 Classes of Solids; 7 Criteria of Strength of Interatomic Bonding; 7.1 Elastic Constants; 7.2 Volume and Pressure as Fundamental Variables: Bulk Modulus; 7.3 Amplitude of Lattice Vibration; 7.4 The Debye Temperature; 7.5 Melting Temperature; 7.6 Cohesive Energy; 7.7 Energy of Vacancy Formation and Surface Energy; 7.8 The Stress-Strain Properties in Engineering
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 Plane Wave Method; 9 First-Principle Simulation in Materials Science; 9.1 Strength Characteristics of Solids
9.2 Energy of Vacancy Formation
9.3 Density of States; 9.4 Properties of Intermetallic Compounds; 9.5 Structure, Electron Bands, and Superconductivity of MgB₂; 9.6 Embrittlement of Metals by Trace Impurities; 10 Ab initio Simulation of the Ni₃Al-based Solid Solutions; 10.1 Phases in Superalloys; 10.2 Mean-Square Amplitudes of Atomic Vibrations in γ -based Phases; 10.3 Simulation of the Intermetallic Phases; 10.4 Electron Density; 11 The Tight-Binding Model and Embedded-Atom Potentials; 11.1 The Tight-Binding Approximation; 11.2 The Procedure of Calculations
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
