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| Nota di contenuto | Computational Chemistry of Solid State Materials; Contents; Foreword Materials: the Bridge Between Chemistry and Physics; Preface; 1 Classical Approaches; 1.1 Ionic Radii and Related Concepts; 1.2 Electrostatics; 1.3 Pauling's Rules; 1.4 Volume Increments; 1.5 The Bond-valence Method; 1.6 Symmetry Principles; 2 Quantum-chemical Approaches; 2.1 Schrodinger's Equation; 2.2 Basis Sets for Molecules; 2.3 Three Myths of Chemical Bonding; 2.4 Bloch's Theorem; 2.5 Reciprocal Space and the k Quantum Number; 2.6 Band Structures; 2.6.1 One-dimensional Systems; 2.6.2 Structural Distortions 2.6.3 Higher Dimensions2.7 Density-of-states and Basic Electron Partitioning; 2.8 Energy-resolved Electron and Energy Partitioning; 2.9 Exchange and Correlation; 2.10 Electron Localization; 2.11 How to Deal with Exchange and Correlation; 2.11.1 Ignoring it or Pretending to do so; 2.11.2 The Hartree Approximation; 2.11.3 The Hartree-Fock Approximation; 2.12 Density-functional Theory; 2.12.1 Exchange-Correlation Functionals; 2.13 Beyond Density-functional Theory; 2.14 Absolute Electronegativity and Hardness; 2.15 Potentials and Basis Sets |

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2.15.1 Empirical Tight-binding and Nonempirical Relatives2.15.2 Pseudopotentials; 2.15.3 Cellular (Augmentation) Methods; 2.15.4 Linear Methods; 2.15.5 Modern Developments; 2.16 Structure Optimization; 2.17 Molecular Dynamics; 2.18 Practical Aspects; 2.18.1 Structural Models; 2.18.2 Energy, Enthalpy, Entropy and Gibbs Energy; 2.19 Computer Implementations; 3 The Theoretical Machinery at Work; 3.1 Structure and Energetics: Calcium Oxide; 3.2 Structural Alternatives: Transition-metal Nitrides; 3.3 Structure and Physical Properties: Cerium Pnictides

3.4 Structures by Peierls Distortions: Tellurium3.5 Itinerant Magnetism: The Transition Metals; 3.6 Itinerant Magnetism: Transition-metal Compounds; 3.7 Atomic Dynamics in Fe:AlN Nanocomposites; 3.8 Structural versus Electronic Distortions: MnAl; 3.9 Challenging Theory: Mercury Carbodiimide and Cyanamide; 3.10 Quasi-binary Oxynitrides: TaON and CoO(1-x)N(x); 3.11 Into the Void: The Sn/Zn System; 3.12 Predicting Oxynitrides: High-pressure Phases and VON; 3.13 Predicting Magnetic Cyanamides and Carbodiimides; 3.14 Predicting Ternary Magnetic Nitrides; 4 Epilogue; Bibliography; Index Acknowledgments

Sommario/riassunto

This is the first book to present both classical and quantum-chemical approaches to computational methods, incorporating the many new developments in this field from the last few years. Written especially for ""non""-theoretical readers in a readily comprehensible and implemental style, it includes numerous practical examples of varying degrees of difficulty. Similarly, the use of mathematical equations is reduced to a minimum, focusing only on those important for experimentalists. Backed by many extensive tables containing detailed data for direct use in the calculations, this is the ideal co