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in Solids

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