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ISBN	9783031068782 9783031068775
Edizione	[1st ed. 2023.]
Descrizione fisica	1 online resource (686 pages)
Disciplina	546.7112
Soggetti	Electronic structure Hydrides
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.
Nota di contenuto	Introduction (theory and computational details) -- Alkali metal mono-hydrides -- Alkaline earth metal mono-hydrides -- 3d Transition-metal mono-hydrides -- 4d Transition-metal mono-hydrides -- 5d Transition-metal mono-hydrides -- Free-electron-like metal mono-hydrides -- C-Si-Ge-Sn mono-hydrides -- Pnictogen mono-hydrides -- Chalcogen mono-hydrides -- Halogen mono-hydrides -- Noble gas mono-hydrides -- Lanthanide mono-hydrides -- Actinide mono-hydrides.
Sommario/riassunto	This book compiles detailed results of electronic structure calculations for most possible cubic monohydrides, dihydrides and selected trihydrides related to superconductivity, comprising elements with atomic numbers up to 103. Beginning with an introduction to the theory and details of the computational methods implemented, this handbook presents a collection of chapters containing results for different classes of cubic hydrides, featuring tables of three-centre and two-centre tight-binding parameterizations, diagrams of energy bands, and densities of states with angular momentum decomposition. Equilibrium lattice parameters and bulk moduli are also included, along with the electron-ion matrix element (Hopfield-McMillan parameter), Stoner criterion for ferromagnetism and values of Fermi velocities and plasmon energies. Each chapter features a brief text explaining the

results presented with comparison to experimental values when available. A selection of the implemented computer codes is reproduced for the reader's own use. This handbook is an ideal complement to any standard electronic structure text for students and researchers in materials science, condensed matter physics, and quantum chemistry.
