Record Nr. UNINA9910300434403321 Autore Papaconstantopoulos Dimitris A **Titolo** Handbook of the Band Structure of Elemental Solids: From Z = 1 To Z = 112 / / by Dimitris A. Papaconstantopoulos New York, NY:,: Springer US:,: Imprint: Springer,, 2015 Pubbl/distr/stampa 1-4419-8264-7 **ISBN** Edizione [2nd ed. 2015.] 1 online resource (663 p.) Descrizione fisica 530 Disciplina 530.1 530.41 548 Soggetti Solid state physics Spectrum analysis Microscopy Materials science Condensed matter Crystallography Mathematical physics Solid State Physics Spectroscopy and Microscopy Materials Science, general **Condensed Matter Physics** Crystallography and Scattering Methods Theoretical, Mathematical and Computational Physics Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Includes index. Introduction -- Hydrogen and The Alkali Metals -- The Alkali Earth Nota di contenuto Metals -- The 3d Transition Metals -- The 4d Transition Metals -- The 5d Transition Metals -- Free-Electron-Like Metals of Groups III and IV

-- The Diamond Structure -- Group 15 Elements: Pnictogens -- Group 16 Elements: Chalcogens -- Group 17 Elements: Halogens -- The Noble Gases -- Lanthanides -- Actinides -- Transactinides -- Al: Spin-

Sommario/riassunto

Orbit Coupling -- AII: Modifications and Extensions to Harrison's Theory -- AIII: Alternative Structures -- AIV: Computer Programs.

This handbook presents electronic structure data and tabulations of Slater-Koster parameters for the whole periodic table. This second edition presents data sets for all elements up to Z = 112, Copernicium, whereas the first edition contained only 53 elements. In this new edition, results are given for the equation of state of the elements together with the parameters of a Birch fit, so that the reader can regenerate the results and derive additional information, such as Pressure-Volume relations and variation of Bulk Modulus with Pressure. For each element, in addition to the equation of state, the energy bands, densities of states, and a set of tight-binding parameters is provided. For a majority of elements, the tight-binding parameters are presented for both a two- and three-center approximation. For the hcp structure, new three-center tight-binding results are given. Other new material in this edition include: energy bands and densities of states of all rare-earth metals, a discussion of the McMillan-Gaspari-Gyorffy theories, and a tabulation of the electron-ion interaction matrix elements. The evaluation of the Stoner criterion for ferromagnetism is examined and results are tabulated. This edition also contains two new appendices discussing the effects of spin-orbit interaction and a modified version of Harrison's tight-binding theory for metals which puts the theory on a quantitative basis.