Handbook of the Band Structure of Elemental Solids: From Z = 1 To Z = 112

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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.

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