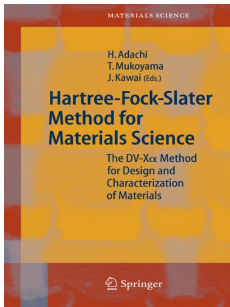


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Molecular-orbital calculations for materials design such as alloys, ceramics, and coordination compounds are now possible for experimentalists. Molecular-orbital calculations for the interpretation of chemical effect of spectra are also possible for experimentalists. The most suitable molecular-orbital calculation method for these purpose is the DV-Xa method, which is robust in such a way that the calculation converges to a result even if the structure of the molecule or solid is impossibleu0026#xa0;in the pressure and temperature ranges on earth. This book specially addresses the methods to design novel materials and to predict the spectralline shape of unknown materials using the DV-Xa molecular-orbital method, but is also useful for those who want to calculate electronic structures of materials using any kind of method.

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