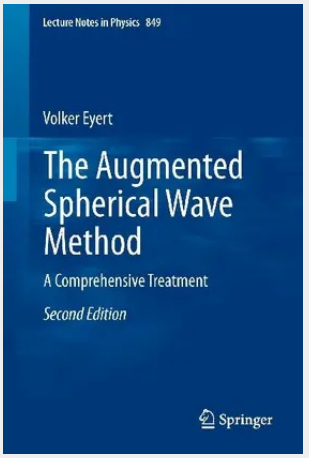
Eyert

The Augmented Spherical Wave Method

A Comprehensive Treatment



The Augmented Spherical Wave (ASW) method is one of the most powerful approaches to handle the requirements of finite basis sets in DFT calculations. It is particularly suited for the calculation of the electronic, magnetic, and optical properties of solid-state materials. Recent developments allow application, in addition, to the elastic properties and phonon spectra. Due to the localized nature of the ASW basis set these properties can be easily interpreted in terms of atomic-like orbitals.

The book addresses all those who want to learn about methods for electronic structure calculations and the ASW method in particular.

This new edition has been thoroughly revised and extended. In particular, a chapter on the new, both very efficient and accurate spherical-wave based full potential ASW method has been added.

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