1. Record Nr. UNISA996466722403316 Autore **Eyert Volker** Titolo The Augmented Spherical Wave Method [[electronic resource]]: A Comprehensive Treatment / / by Volker Eyert Pubbl/distr/stampa Berlin, Heidelberg:,: Springer Berlin Heidelberg:,: Imprint: Springer, , 2013 **ISBN** 3-642-25864-6 Edizione [2nd ed. 2013.] Descrizione fisica 1 online resource (XV, 379 p.) Collana Lecture Notes in Physics, , 0075-8450;; 849 Disciplina 530.4/11 Soggetti Condensed matter **Physics** Chemistry, Physical and theoretical Materials science **Condensed Matter Physics** Numerical and Computational Physics, Simulation Theoretical and Computational Chemistry Materials Science, general Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Bibliographic Level Mode of Issuance: Monograph Nota di bibliografia Includes bibliographical references and index. Introduction -- The Standard ASW Method -- Envelope Functions and Nota di contenuto Structure Constants -- The Plane-Wave Based Full-Potential ASW Method -- The Sperical-Wave Based Full-Potential ASW Method --Details of the Standard ASW Method -- Details of the Envelope Functions -- Details of the Full-Potential ASW Methods -- Brillouin-Zone Integration -- Further Reading -- Index. Sommario/riassunto 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.