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Volker Eyert

# The Augmented Spherical Wave Method

A Comprehensive Treatment

 Springer

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*To my children, Florian and Carolin*

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## Preface

The origin of this book dates back to the beginning of the year 1987, when I started to work on my PhD in the group of Prof. J. Kübler at the Technical University of Darmstadt. The discussions in those days were much influenced by the discovery of the high- $T_c$  superconductors and, hence, it became clear quite early that a full-potential augmented spherical wave (ASW) code capable of calculating elastic properties and phonon frequencies via the frozen-phonon approach was desirable. The development and implementation of such a code became the subject of my thesis.

Yet, learning the basic notions of the ASW method was hampered by the fact that review articles were not available and the original work by Williams, Kübler, and Gelatt, while being very concise, did not answer the simple questions a beginner would ask. Benefiting from the diploma theses of D. Hackenbracht and M. Methfessel, I started to write down a first detailed description of both the standard and the full-potential ASW method, which eventually formed the backbone of my PhD thesis. It laid ground for the present notes, which by now cover many aspects of the ASW method.

This book addresses all those readers who want to learn the basic functionality of methods for electronic structure calculations in general and of the ASW method in particular. In addition, being quite detailed, it tries to capture many of the above-mentioned beginners' and non-specialists' questions. Moreover, it provides a guiding hand to the many practioners who started using the ASW method and want to learn more about the details. Of course, the large amount of background material should also content the experts in the field. Finally, since the ASW method shares much of the basic formalism with other spherical-wave-based schemes as the Korringa–Kohn–Rostoker (KKR) and the linear muffin-tin orbital (LMTO) method, the book may also be valuable for researchers familiar with these.

In writing this book and setting up a completely new implementation of the ASW program package, I have much benefited from various support and numerous discussions. My memory is with my friend and colleague Dr. Jürgen Sticht, who deceased much too early one month ago. Jürgen introduced me into the mysteries of the ASW method and with him I share a very fruitful time of code

optimization and vectorization. My thanks include many other people, who in one way or the other had a strong impact on my work. Without being complete, I am particularly grateful to Prof. O. K. Andersen, Prof. R. Claessen, Prof. U. Eckern, Prof. R. Frésard, PD Dr. K.-H. Höck, Prof. S. Horn, Prof. T. Kopp, Prof. J. Kübler, Prof. J. Mannhart, Prof. S. F. Matar, Dr. T. Maurer, Dr. A. Mavromaras, Dr. M. S. Methfessel, Prof. W. Nolting, Prof. W. Scherer, Prof. P. C. Schmidt, Prof. K. Schwarz, Dr. M. Stephan, Prof. D. Vollhardt, and Dr. E. Wimmer. Last but not least, it is a great pleasure to thank Dr. C. Caron, Mrs. G. Hakuba, and Mrs. J. Lenz of the Springer-Verlag for their professional help during the final phase of this book. This project has been partially supported by the Deutsche Forschungsgemeinschaft through Sonderforschungsbereich 252 and 484.

Potsdam, January 2007

*Volker Eyert*

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