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The Augmented Spherical Wave Method

A Comprehensive Treatment

Second Edition

Springer

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To Kerstin
and to my children, Florian and Carolin

Preface

Only four years after the first edition was published, new developments of the augmented spherical wave (ASW) methodology made an update of this book necessary. In particular, the successful implementation and widespread application of the spherical-wave based full-potential ASW method was reflected by many requests for a comprehensive description of the new approach. This is accounted for by the present edition, which complements the variety of ASW methods dealt with in this book by a detailed outline of the spherical-wave based full-potential ASW method in Chap. 5.

It is probably not exaggerated to say that the spherical-wave based full-potential ASW method, the development and implementation of which has kept me busy over many years, marks the present highlight of the spherical wave methods. Indeed, it combines the simplicity and very high computational efficiency of Andersen's atomic sphere approximation (ASA) with the high accuracy of modern full-potential methods. This is even more remarkable, as the spherical wave methods, while being conceptionally simple and allowing for an intuitive interpretation of results in terms of atomic-like orbitals, suffered for a long time from severe approximations, which prevented highly accurate total energy calculations. So far, the latter could be achieved only by considerable loss in computational efficiency, an obstacle, which has been overcome with the present spherical-wave based full-potential ASW method.

The recent developments and the implementation of the corresponding code have been accompanied and supported by many friends and colleagues. Without being complete, I would like to thank particularly Prof. U. Eckern, Prof. R. Frésard, PD Dr. K.-H. Höck, Prof. T. Kopp, Prof. J. Mannhart, Prof. S. F. Matar, Dr. A. Mavromaras, Prof. W. Scherer, Prof. P. C. Schmidt, Dr. M. Stephan, Prof. D. Vollhardt, and Dr. E. Wimmer. Again, I want to express my gratitude to Dr. C. Caron, Mrs. G. Hakuba, and Mrs. A. Schulze-Thomin from Springer Verlag for their expertise in guiding me through the final phase of this book. Last but not least, many thanks go to all the readers of the first edition as well as the users of the ASW program package worldwide, for their interest, feedback, suggestions, and the numerous fruitful discussion on the method and its applications. I both enjoyed and

benefited a lot from these collaborations. This project has been partially supported by the Deutsche Forschungsgemeinschaft through SFB 252, SFB 484, and TRR 80.

Potsdam, July 2011 Volker Eyert

Preface to the First Edition

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 practitioners 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.

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