Preface

This is a book describing electronic structure theory and application within the framework of a methodology implemented in the computer code RSPt. In 1986, when the code that was to become RSPt was developed enough to be useful, it was one of the first full-potential, all-electron, relativistic implementations of DFT (density functional theory). While RSPt was documented parasitically in many publications describing the results of its application, it was many years before a publication explicitly describing aspects of the method appeared. In the meantime, several excellent all-electron, full-potential methods had been developed, published, and become available. So why a book about RSPt now?

The code that became RSPt was initially developed as a personal research tool, rather than a collaborative effort or as a product. As such it required some knowledge of its inner workings to use, and as it was meant to be maximally flexible, the code required experience to be used effectively. These attributes inhibited, but did not prevent, the spread of RSPt as a research tool. While applicable across the periodic table, the method is particularly useful in describing a wide range of materials, including heavier elements and compounds, and its flexibility provides targeted accuracy and a convenient and accurate framework for implementing and assessing the effect of new models. A fair number of informal developers arose in the course of doctoral, postdoctoral, and professional research, principally at Uppsala University and at many other institutions as well. As a consequence, a number of innovative extensions to the code were developed, many of which were never integrated in the "official" version of RSPt and were consequently lost or shelved, often to be re-invented at a later date.

This situation started to change in 2006 when a group of researchers with a stake in the methodology met to establish a protocol for continuous development of a single RSPt thread. We established a code repository with developing branches merged periodically and a web site to facilitate communication, disseminate stable versions of the code, and provide a forum for user support and discussion. This group meets yearly to evolve the organization and suggest

ongoing and future efforts. The results of this organization have been gratifying. Computationally, data structures and memory allocation have been substantially reworked, eliminating non-standard and annoying remnants of Fortran 77 and enhancing modularity. RSPt is now k-point-, band-, and FFT-parallel. In methodology, physics modules such as DMFT and SIC are now present in the stable version, and forces are finally available without restriction.

No one is explicitly paid to do this development. At best, code and method development support particular research directions. The development continues, however, largely because the developers believe that expanding the capability and efficiency of RSPt will benefit their research, and that making RSPt more accessible will enhance the research of others. This book, encompassing electronic structure theory, technical detail, and representative application, is another step in this process.

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Full-Potential Electronic Structure Method
Energy and Force Calculations with Density Functional and Dynamical Mean Field Theory

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