

Computational Methods in Solid State Physics

V.V. Nemoshkalenko and V.N. Antonov

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Computational Methods in Solid State Physics V V Nemoshkalenko, N.V. Antonov, 1999-02-19 The combination of theoretical physics methods numerical mathematics and computers has given rise to a new field of physics known as computational physics The purpose of this monograph is to present the various methods of computational physics in particular the methods of band theory The first chapter of the book provides an introduction to the field and presents the theoretical foundations of band theory In the second and third chapters the authors describe both traditional and more modern methods of band theory and include practical recommendations for their use Methods which are discussed include APW augmented plane wave Green s function method LMTO linear method of MT orbitals LKKR linear Korringor Kohn and Rostocker method LAPW linear augmented plane wave ASW augmented spherical waves and LASO linear method of augmented Slater orbitals Great attention is paid to the practical aspects of these theories and the book is structured in such a way as to enable the reader to use any method in practice without reference to other sources [Quantum Chemistry, Solid-state Physics, and Computational Methods](#) Per-Olov Lowdin, 1990 [Computational Methods for Large Molecules and Localized States in Solids](#) F. Herman, 2012-12-06 During the past few years there has been dramatic progress in theoretical and computational studies of large molecules and localized states in solids Various semi empirical and first principles methods well known in quantum chemistry have been applied with considerable success to ever larger and more complex molecules including some of biological importance as well as to selected solid state problems involving localized electronic states In creasingly solid state physicists are adopting a molecular point of view in attempting to understand the nature of electronic states associated with a isolated structural and chemical defects in solids b surfaces and interfaces and c bulk disordered solids most notably amorphous semiconductors Moreover many concepts and methods already widely used in solid state physics are being adapted to molecular problems These adaptations include pseudopotentials statistical exchange approxi mations muffin tin model potentials and multiple scattering and cellular methods In addition many new approaches are being de vised to deal with progressively more complex molecular and local ized electronic state problems *Quantum Chemistry, Solid-state Physics, and Computational Methods* N. Yngve Ohrn, John R Sabin, Michael C Zerner, 1991

Computational Solid State Physics F. Herman, 1972-03-01 During the past 20 years solid state physics has become one of the major branches of physics 1 2 Today over one third of all scientific articles published in physics deal with solid state 3 topics During the last two decades there has also been ra id growth of scientific computation in a wide variety of fields 5 The combination of solid state physics and comp tation may be termed computational solid state physics This emerging field is distin guished from theoretical solid state physics only to the extent that electronic computers rather than slide rules or backs of envelopes are used to solve numerical or logical problems test scientific hypotheses and discover the essential physical content of formal mathematical theories Papers in computational solid state physics are widely scatter ed

in the literature They can be found in the traditional physics journals and review series such as The Physical Review and Solid State Physics in more specialized publications such as Journal of Computational Physics Computer Physics Communications and Methods in Computational Physics and in the proceedings of a number of recent conferences and seminar courses Plans for holding an International Symposium on Computational Solid State Physics in early October 1971 were formulated by Dr **Computational Methods for Nanoscale Applications** Igor Tsukerman,2020-08-21 Positioning itself at the common boundaries of several disciplines this work provides new perspectives on modern nanoscale problems where fundamental science meets technology and computer modeling In addition to well known computational techniques such as finite difference schemes and Ewald summation the book presents a new finite difference calculus of Flexible Local Approximation Methods FLAME that qualitatively improves the numerical accuracy in a variety of problems

Computational Methods in Band Theory Paul M. Marcus,2013-03-13 This volume contains the papers presented at the Conference on Computational Methods in Band Theory sponsored jointly by IBM and the American Physical Society and held at the IBM Thomas J Watson Research Center Yorktown Heights New York on May 14 15 1970 The purpose of the conference was a sharing of information on the computational problems involved in relating models for the electron electron and electron ion interactions to experimentally measurable quantities The papers comprising this volume therefore present up to date methodology for the calculation of single particle energies and wave functions for periodic and near periodic systems the integration over these states required to describe experiment and computationally practicable procedures for the introduction of exchange and correlation and the achievement of self consistency The proceedings is actually an expansion of the conference in that unlike the oral presentations the papers were not limited as to length Furthermore time was allowed after the conference to permit the papers to be written with the conference in retrospect and five prepared discussion papers written by attendees of the conference but not on the original program are included The latter are indicated in the table of contents by asterisks The explicit emphasis of the conference on comparison of technique generated much lively argument which is surely an indication of the current interest in the subject and the vigor of those working in it It is our hope that the proceedings will make these comparisons available to the widest possible audience **Introductory Solid State Physics with MATLAB Applications** Javier E. Hasbun,Trinanjana Datta,2019-10-08 Solid state physics the study and prediction of the fundamental physical properties of materials forms the backbone of modern materials science and has many technological applications The unique feature of this text is the MATLAB based computational approach with several numerical techniques and simulation methods included This is highly effective in addressing the need for visualization and a direct hands on approach in learning the theoretical concepts of solid state physics The code is freely available to all textbook users Additional Features Uses the pedagogical tools of computational physics that have become important in enhancing physics teaching of advanced subjects such as solid state physics Adds visualization and simulation to the subject in a way that

enables students to participate actively in a hand on approach Covers the basic concepts of solid state physics and provides students with a deeper understanding of the subject matter Provides unique example exercises throughout the text Obtains mathematical analytical solutions Carries out illustrations of important formulae results using programming scripts that students can run on their own and reproduce graphs and or simulations Helps students visualize solid state processes and apply certain numerical techniques using MATLAB making the process of learning solid state physics much more effective Reinforces the examples discussed within the chapters through the use of end of chapter exercises Includes simple analytical and numerical examples to more challenging ones as well as computational problems with the opportunity to run codes create new ones or modify existing ones to solve problems or reproduce certain results

Computational Methods for Large Systems Jeffrey R. Reimers, 2011-08-24 While its results normally complement the information obtained by chemical experiments computer computations can in some cases predict unobserved chemical phenomena Electronic Structure Computational Methods for Large Systems gives readers a simple description of modern electronic structure techniques It shows what techniques are pertinent for particular problems in biotechnology and nanotechnology and provides a balanced treatment of topics that teach strengths and weaknesses appropriate and inappropriate methods It s a book that will enhance the your calculating confidence and improve your ability to predict new effects and solve new problems

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Computational Approaches in Physics Maria Fyta, 2016-11-01 Computational Approaches in Physics reviews computational schemes which are used in the simulations of physical systems These range from very accurate ab initio techniques up to coarse grained and mesoscopic schemes The choice of the method is based on the desired accuracy and computational efficiency A bottom up approach is used to present the various simulation methods used in Physics starting from the lower level and the most accurate methods up to particle based ones The book outlines the basic theory underlying each technique and its complexity

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