Computational Methods In Condensed Matter Electronic Structure

This series of books covers all areas of computational physics, collecting together reviews where a newcomer can learn about the state of the art regarding methods and results. Articles are submitted by e-mail before deadlines which are kept by the editor.Biologically motivated simulations, glasses, world-record molecular dynamics, deposition on surfaces, and hydrodynamics are discussed in this volume which ends with an explanation of elementary particle physics (QCD) and their phase transitions.

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, addresses the computational implications and issues in the implementation, as well as present representative examples. A link to the most common computational codes, commercial or open source is listed in each chapter. The strengths and deficiencies of the variety of techniques discussed in this book are presented in detail and visualization tools commonly used to make the simulation data more comprehensive are also discussed. In the end, specific techniques are used as bridges across different disciplines. To this end, examples of different systems tackled with the same methods are presented. The appendices include elements of physical theory which are prerequisites in understanding the simulation methods.

Over the past several decades, computational approaches to studying strongly-interacting systems have become increasingly varied and sophisticated. This book provides a comprehensive introduction to state-of-the-art quantum Monte Carlo techniques relevant for applications in correlated systems. Providing a clear overview of variational wave functions, and featuring a detailed presentation of stochastic samplings including Markov chains and Langevin dynamics, which are developed into a discussion of Monte Carlo methods. The variational technique is described, from foundations to a detailed description of its algorithms. Further topics discussed include optimisation techniques, real-time dynamics and projection methods, including Green's function, reptation and auxiliary-field Monte Carlo, from basic definitions to advanced algorithms for efficient codes, and the book concludes with recent developments on the continuum space. Quantum Monte Carlo Approaches for Correlated Systems provides an extensive reference for students and researchers working in condensed matter theory or those interested in advanced numerical methods for electronic simulation.

Computational Methods in Condensed Matter: Electronic StructureSpringer Science & Business Media

Since the first attempts to model proteins on a computer began almost thirty years ago, our understanding of protein structure and dynamics has dramatically increased. Spectroscopic measurement techniques continue to improve in resolution and sensitivity, allowing a wealth of information to be obtained with regard to the kinetics of protein folding and unfolding, and complementing the detailed structural picture of the folded state. Concurrently, algorithms, software, and computational hardware have progressed to the point where both structural and kinetic problems may be studied with a fair degree of realism. Despite these advances, many major challenges remain in understanding protein folding at both the conceptual and practical levels. Computational Methods for Protein Folding seeks to illuminate recent advances in computational modeling of protein folding in a way that will be useful to physicists, chemists, and chemical physicists. Covering a broad spectrum of computational methods and practices culled from a variety of research fields, the editors present a full range of models that, together, provide a thorough and current description of all aspects of protein folding. A valuable resource for both students and professionals in the field, the book will be of value both as a cutting-edge overview of existing information and as a catalyst for inspiring new studies. Computational Methods for Protein Folding is the 120th volume in the acclaimed series Advances in Chemical Physics, a compilation of scholarly works dedicated to the dissemination of contemporary advances in chemical physics, edited by Nobel Prize-winner Ilya Prigogine.

"Blurb & Contents" This current and comprehensive treatment of the physics of small- amplitude waves in hot magnetized plasmas provides a thorough update of the author's classic Theory of Plasma Waves. New topics include quasi-linear theory, inhomogeneous plasmas, collisions, absolute and convective instability, and mode conversion. Valuable for graduates and advanced undergraduates and an indispensable reference work for researchers in plasmas, controlled fusion, and space science.

Interacting many-body systems are the main subjects of research in theoretical condensed matter physics, and they are the source of both the interest and the difficulty in this field. In order to understand the macroscopic properties of matter in terms of macroscopic knowledge, many analytic and approximate methods have been introduced. The contributions to this proceedings volume focus on the most recent developments of computational approaches in condensed matter physics. Monte Carlo methods and molecular dynamics simulations applied to strongly correlated classical and quantum systems such as electron systems, quantum spin systems, spin glassss, coupled map systems, polymers and other random and comlex systems are reviewed. Comprising easy to follow introductions to each field covered and also more specialized contributions,this proceedings volume explains why computational approaches are necessary and how different fields are related to each other.

This comprehensive collection of lectures by leading experts in the field introduces and reviews all relevant computer simulation methods and their applications in condensed matter systems. Volume 1 is an in-depth introduction to a vast spectrum of computational techniques for statistical mechanical systems of condensed matter. Volume 2 is a collection of state-of-the-art surveys on numerical experiments carried out for a great number of systems.

Prominent multinational contributors present articles on condensed matter physics, quantum biology and quantum chemistry. Among the topics covered: reactive molecular collisions, density-functional theory, atomic and molecular phenomena in astrophysics, non-Born-Oppenheimer methods, thin films and surfaces.

This volume presents computer simulation methods and mathematical modelling of physical processes used in surface science research. It offers in-depth analysis of advanced theoretical approaches to behaviours of fluids in contact with porous, semiporous and nonporous solid surfaces. The book also explores interfacial systems for a wide variety of p

Electronic structure problems are studied in condensed matter physics and theoretical chemistry to provide important insights into the properties of matter. This 2006 graduate textbook describes the main theoretical approaches and computational techniques, from the simplest approximations to the most sophisticated methods. It starts with a detailed description of the various theoretical approaches to calculating the electronic structure of solids and molecules, including density-functional theory and chemical methods based on Hartree-Fock theory. The basic approximations are thoroughly discussed, and an in-depth overview of recent advances and alternative approaches in DFT is given. The second part discusses the different practical methods used to solve the electronic structure problem computationally, for both DFT and Hartree-Fock approaches. Adopting a unique and open approach, this textbook is aimed at graduate students in physics and chemistry, and is intended to improve communication between these communities. It also serves as a reference for researchers entering the field.

This textbook introduces modern techniques based on computer simulation to study materials science. It starts from first principles calculations enabling to calculate the physical and chemical properties by solving a many-body Schroedinger equation with Coulomb forces. For the exchange-correlation term, the local density approximation is usually applied. After the introduction of the first principles treatment, tight-binding and classical potential methods are briefly introduced to indicate how one can increase the number of atoms in the system. In the second half of the book, Monte Carlo simulation is discussed in detail. Problems and solutions are provided to facilitate understanding. Readers will gain sufficient knowledge to begin theoretical studies in modern materials research. This second edition includes a lot of recent theoretical techniques in materials research. With the computers power now available, it is possible to use these numerical techniques to study various physical and chemical properties of complex materials from first principles. The new edition also covers empirical methods, such as tight-binding and molecular dynamics.

This volume presents, for the very first time, an exhaustive collection of those modern numerical methods specifically tailored for the analysis of Strongly Correlated Systems. Many novel materials, with functional properties emerging from macroscopic quantum behaviors at the frontier of modern research in physics, chemistry and material science, belong to this class of systems. Any technique is presented in great detail by its own inventor or by one of the world-wide recognized main contributors. The exposition has a clear pedagogical cut and fully reports on the most relevant case study where the specific technique showed to be very successful in describing and enlightening the puzzling physics of a particular strongly correlated system. The book is intended for advanced graduate students and post-docs in the field as textbook and/or main reference, but also for other researchers in the field who appreciate consulting a single, but comprehensive, source or wishes to get acquainted, in a as painless as possible way, with the working details of a specific technique.

Computer Simulation Studies in Condensed-Matter Physics VI provides a broad overview of recent developments in this field. Based on the last workshop, it presents invited and contributed papers which describe new physical results, simulational techniques and ways of interpreting simulational data. Both classical and quantum systems are discussed.

This volume contains the lectures given at the Third Gordon Godfrey International Workshop on Computational Approaches to Novel Condensed Matter Systems which was held at The University of New South Wales July 12-17, 1993. Lecturers from Asia, Australia, Europe and North America gave a total of twenty-nine lectures which were spread over the five days. Unfortunately we were not able to include in this volume the lectures of S. Das Sarma from the University of Maryland on "Non-Equilibrium Growth as a Self-Organised Phenomenon" due to constraints of time. The workshops have been held annually since 1991 in Sydney, each covering a novel research area in condensed matter physics that is of topical interest. Australia has a strong tradition of research in condensed matter physics. The workshops are jointly organised by the School of Physics at the University of New South Wales (Sydney) and the Department of Theoretical Physics, Research School of Physical Sciences and Engineering at the Australian National University (Canberra). The late Gordon God frey was an Associate Professor of Physics at the University of New South Wales. He bequeathed his estate for the promotion and teaching of theoretical physics within the university. The primary purpose of each workshop is to expose post-graduate students in physics to both informal interaction and formal lectures from recognised international leaders in topical research areas. Past experience has demonstrated again and again that to be informed about a new field there is no substitute for personal contact and interaction.

Readership: Undergraduates, graduate students, and research scientists in computational physics, engineering, physical science, applied physics, and fractals.

Unlike existing texts, this book blends for the first time three topics in physics - symmetry, condensed matter physics and computational methods - into one pedagogical textbook. It includes new concepts in mathematical crystallography; experimental methods capitalizing on symmetry aspects; non-conventional applications such as Fourier crystallography, color groups, quasicrystals and incommensurate systems; as well as concepts and techniques behind the Landau theory of phase transitions. Adopting a computational approach to the application of group theoretical techniques to solving symmetry related problems, it dramatically alleviates the need for intensive calculations usually found in the presentation of symmetry. Writing computer programs helps the student achieve a firm understanding of the underlying concepts, and sample programs, based on Mathematica, are presented throughout the book. Containing over 150 exercises, this textbook is ideal for graduate students in condensed matter physics, materials science, and chemistry. Solutions and computer programs are available online at www.cambridge.org/9780521828451.

At the interface of quantum information and condensed matter physics, the study of entanglement in quantum many-body systems requires a new toolset which combines concepts from each. This thesis introduces a set of computational methods to study phases and phase transitions in lattice models of quantum systems, using the Renyi

entropies as a means of quantifying entanglement. The scaling of entanglement entropy can give valuable insight into the phase of a condensed matter system. It can be used to detect exotic types of phases, to pinpoint transitions between phases, and can give us universal information about a system. The first approach in this thesis is a technique to measure entanglement in finite size lattice systems using zero-temperature quantum Monte Carlo simulations. The algorithm is developed, implemented, and used to explore anomalous entanglement scaling terms in the spin-1/2 Heisenberg antiferromagnet. In the second part of this thesis, a new and complementary numerical technique is introduced to study entanglement not just in finite size systems, but as we approach the thermodynamic limit. This “numerical linked-cluster expansion” is used to study two different systems at their quantum critical points - continuous phase transitions occurring at zero temperature, at which these systems exhibit universal properties. Remarkably, these universal properties can be reflected in the scaling of entanglement. Entanglement offers a new perspective on condensed matter systems, one which takes us closer to genuinely understanding what goes on in these materials at the quantum mechanical level. This thesis demonstrates the first steps in developing an extensive list of computational tools that can be used to study entanglement over a wide range of interacting quantum many-body systems. With the ever increasing computational power available, it may be only a matter of time before these tools are used to create a comprehensive framework for the characterization of condensed matter phases and phase transitions.

This book is part of a two volume set which presents the analysis of nonlinear phenomena as a long-standing challenge for research in basic and applied science as well as engineering. It discusses nonlinear differential and differential equations, bifurcation theory for periodic orbits and global connections. The integrability and reversibility of planar vector fields and theoretical analysis of classic physical models are sketched. This first volume concentrates on the mathematical theory and computational techniques that are essential for the study of nonlinear science, a second volume deals with real-world nonlinear phenomena in condensed matter, biology and optics.

Computional physics involves the use of computer calculations and simulations to solve physical problems. This book describes computational methods used in theoretical physics with emphasis on condensed matter applications. Coverage begins with an overview of the wide variety of topics and algorithmic approaches studied in this book. The next chapters concentrate on electronic structure calculations, presenting the Hartree-Fock and Density Functional formalisms, and band structure methods. Later chapters discuss molecular dynamics simulations and Monte Carlo methods in classical and quantum physics, with applications to condensed matter and particle field theories. Each chapter details the necessary fundamentals, describes the formation of a sample program, and includes problems that address related analytical and numerical issues. Useful appendices on numerical methods and random number generators are also included. This volume bridges the gap between undergraduate physics and computational research. It is an ideal textbook for graduate students as well as a valuable reference for researchers.

Volume 71 of Reviews in Mineralogy and Geochemistry represents an extensive review of the material presented by the invited speakers at a short course on Theoretical and Computational Methods in Mineral Physics held prior (December 10-12, 2009) to the Annual fall meeting of the American Geophysical Union in San Francisco, California. The meeting was held at the Doubletree Hotel & Executive Meeting Center in Berkeley, California. Contents: Density functional theory of electronic structure: a short course for mineralogists and geophysicists The Minnesota density functionals and their applications to problems in mineralogy and geochemistry Density-functional perturbation theory for quasi-harmonic calculations Thermodynamic properties and phase relations in mantle minerals investigated by first principles quasiharmonic theory First principles quasiharmonic thermoelasticity of mantle minerals An overview of quantum Monte Carlo methods Quantum Monte Carlo studies of transition metal oxides Accurate and efficient calculations on strongly correlated minerals with the LDA+U method: review and perspectives Spin-state crossover of iron in lower-mantle minerals: results of DFT+U investigations Simulating diffusion Modeling dislocations and plasticity of deep earth materials Theoretical methods for calculating the lattice thermal conductivity of minerals Evolutionary crystal structure prediction as a method for the discovery of minerals and materials Multi-Mbar phase transitions in minerals Computer simulations on phase transitions in ice Iron at Earth’s core conditions from first principles calculations First-principles molecular dynamics simulations of silicate melts: structural and dynamical properties Lattice dynamics from force-fields as a technique for mineral physics An efficient cluster expansion method for binary solid solutions: application to the halite-silvite, NaCl-KCl, system Large scale simulations Thermodynamics of the Earth’s mantle

The study of the electronic structure of materials is at a momentous stage, with the emergence of computational methods and theoretical approaches. Many properties of materials can now be determined directly from the fundamental equations for the electrons, providing insights into critical problems in physics, chemistry, and materials science. This book provides a unified exposition of the basic theory and methods of electronic structure, together with instructive examples of practical computational methods and real-world applications. Appropriate for both graduate students and practising scientists, this book describes the approach most widely used today, density functional theory, with emphasis upon understanding the ideas, practical methods and limitations. Many references are provided to original papers, pertinent reviews, and widely available books. Included in each chapter is a short list of the most relevant references and a set of exercises that reveal salient points and challenge the reader.

Unlike existing texts, this book blends for the first time three topics in physics - symmetry, condensed matter physics and computational methods - into one pedagogical textbook. It includes new concepts in mathematical crystallography, experimental methods capitalizing on symmetry aspects, non-conventional applications such as Fourier crystallography, color groups, quasicrystals and incommensurate systems, as well as concepts and techniques behind the Landau theory of phase transitions. Ideal for graduate students in condensed matter physics,

materials science, and chemistry.
On June 1St 2004 the Faculty of Electrical Engineering and Information Technology of the Technische Universitat Miinchen bestowed the degree of the doctor honoris causa to Leopold B. Felsen, for extraordinary achievements in the theory of electromag netic fields. On this occasion on June 1St and 2nd 2004 at the Technische Universitat Miinchen a symposium on "Fields, Networks, Computational Methods, and Systems: A Modern View of Engineering Electrodynamics" in honor of Leopold B. Felsen was organized. The symposium topic focused on an important area of Leopold Felsen research interests and, as the title emphasizes, on a modern view of applied Electro dynamics. While the fundamental physical laws of electrodynamics are well known, research in this field is experiencing a steady continuous growth. The problem -solving approaches of, say, twenty years ago may seem now fairly obsolete since considerable progress has been made in the meantime. In this monograph we collect samples of present day state of the art in dealing with electromagnetic fields, their network theory representation, their computation and, finally, on system applications. The network formulation of field problems can improve the problem formulation and also contribute to the solution methodology. Network theory systematic approaches for circuit analysis are based on the separation of the circuit into the connection circuit and the circuit elements. Many applications in science and technology rely on computations of the electromagnetic field in either man-made or natural complex structures.
This textbook for graduate students in physics and chemistry describes the theoretical approaches and computational techniques for studying the behavior of electrons. The first part covers the theoretical methods, including both density-functional theory and Hartree-Fock theory and the latter part discusses the different computational methods.
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.
This book provides a relatively complete introduction to the methods used in computational condensed matter. A wide range of electronic structure theories are introduced, including traditional quantum chemistry methods, density functional theory, many-body perturbation theory, and more. Molecular dynamics simulations are also discussed, with extensions to enhanced sampling and free-energy calculation techniques including umbrella sampling, meta-dynamics, integrated tempering sampling, etc. As a further extension beyond the standard Born-Oppenheimer molecular dynamics, some simulation techniques for the description of quantum nuclear effects are also covered, based on Feynman's path-integral representation of quantum mechanics. The book aims to help beginning graduate students to set up a framework of the concepts they should know before tackling the physical/chemical problems they will face in their research. Contents: Introduction to Computer Simulations of Molecules and Condensed MatterQuantum Chemistry Methods and Density-Functional TheoryPseudopotentials, Full Potential, and Basis SetsMany-Body Green's Function Theory and the GW ApproximationMolecular DynamicsExtension of Molecular Dynamics, Enhanced Sampling and the Free-Energy CalculationsQuantum Nuclear EffectsAppendices: Useful Mathematical RelationsExpansion of a Non-Local FunctionThe Brillouin-Zone IntegrationThe Frequency IntegrationReferencesAcknowledgements Readership: Researchers in computational condensed matter physics. Keywords: Electronic Structures;First-Principle;Molecular Dynamics;Path-IntegralReview: Key Features: Elaboration on a framework of concepts based on the authors' research experiencesIllustrations of methods ranging from electronic structures to molecular dynamicsDetailed explanation of the path-integral method
Looking for the real state of play in computational many-particle physics? Look no further. This book presents an overview of state-of-the-art numerical methods for studying interacting classical and quantum many-particle systems. A broad range of techniques and algorithms are covered, and emphasis is placed on their implementation on modern high-performance computers. This excellent book comes complete with online files and updates allowing readers to stay right up to date.
Soft condensed matter physics relies on a fundamental understanding at the interface between physics, chemistry, biology, and engineering for a host of materials and circumstances that are related to, but outside, the traditional definition of condensed matter physics. Featuring contributions from leading researchers in the field, this book uniquely discusses both the contemporary experimental and computational manifestations of soft condensed matter systems. From particle tracking and image analysis, novel materials and computational methods, to confocal microscopy and bacterial assays, this book will equip the reader for collaborative and interdisciplinary research efforts relating to a range of modern problems in nonlinear and non-equilibrium systems. It will enable both graduate students and experienced researchers to supplement a more traditional understanding of thermodynamics and statistical systems with knowledge of the techniques used in contemporary investigations. Color versions of a selection of the figures are available at www.cambridge.org/9780521115902.
Computational Approaches in Condensed-Matter Physics presents the most recent theoretical investigations using Monte Carlo methods and molecular dynamics simulations. Instructive introductory reviews and specialized contributions cover up-to-date results on strongly correlated classical and quantum systems, quantum spin systems, spin glasses, coupled map systems, polymers and other complex systems.
This book describes computational methods used in theoretical physics with emphasis on condensed matter applications.
There is an increasing need for undergraduate students in physics to have a core set of computational tools. Most problems in physics benefit from numerical methods, and many of them resist analytical solution altogether. This textbook presents numerical techniques for solving familiar physical problems where a complete solution is inaccessible using traditional mathematical methods. The numerical techniques for solving the problems are clearly laid out, with a focus on the logic and applicability of the method. The same problems are revisited multiple times using different numerical techniques, so readers can easily compare the methods. The book features over 250 end-of-chapter exercises. A website hosted by the author features a complete set of programs used to generate the examples and figures, which can be used as a starting point for further investigation. A link to this can be found at www.cambridge.org/9781107034303.