Electronic Structure Basic Theory And Practical Methods

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TREVINO FRENCH

Density-Functional Theory of Atoms and Molecules Elsevier
DIVThorough, modern study of solid state physics; solid types and symmetry, electron states, electronic properties and cooperative phenomena. /div
Solid State Physics Clarendon Press
While group theory and its application to solid state physics is well established, this textbook raises two completely new aspects. First, it provides a better understanding by focusing on problem solving and making extensive use of Mathematica tools to visualize the concepts. Second, it offers a new tool for the photonics community by transferring the concepts of group theory and its application to photonic crystals. Clearly divided into three parts, the first provides the basics of group theory. Even at this stage, the authors go beyond the widely used standard examples to show the broad field of applications. Part II is devoted to applications in condensed matter physics, i.e. the electronic structure of materials. Combining the application of the computer algebra system Mathematica with pen and paper derivations leads to a better and faster understanding. The exhaustive discussion shows that the basics of group theory can also be applied to a totally different field, as seen in Part III. Here, photonic applications are discussed in parallel to the electronic case, with the focus on photonic crystals in two and three dimensions, as well as being partially expanded to other problems in the field of photonics. The authors have developed Mathematica package GTPack which is available for download from the book's homepage. Analytic considerations, numerical calculations and visualization are carried out using the same software. While the use of the Mathematica tools are demonstrated on elementary examples, they can equally be applied to more complicated tasks resulting from the reader's own research.
Quantum Theory of Materials John Wiley & Sons
This graduate-level text explains the modern in-depth approaches to the calculation of electronic structure and the properties of molecules. Largely self-contained, it features more than 150 exercises. 1989 edition.
Ab Initio Molecular Dynamics World Scientific
The study of the electronic structure of materials is at a momentous stage, with the emergence of new computational methods and theoretical approaches. This volume provides an introduction to the field and describes its conceptual framework, the capabilities of present methods, limitations, and challenges for the future. Many properties of materials can now be determined directly from the fundamental equations of quantum mechanics, bringing new insights into critical problems in physics, chemistry, and materials science.
Handbook of Materials Modeling World Scientific
This book surveys the theory of defects in solids, concentrating on the electronic structure of point defects in insulators and semiconductors. The relations between different approaches are described, and the predictions of the theory compared critically with experiment. The physical assumptions and approximations are emphasized. The book begins with the perfect solid, then reviews the main methods of calculating defect energy levels and wave functions. The calculation and observable defect properties is discussed, and finally, the theory is applied to a range of defects that are very different in nature. This book is intended for research workers and graduate students interested in solid-state physics. From reviews of the hardback: 'It is unique and of great value to all interested in the basic aspects of defects in solids.' Physics Today 'This is a particularly worthy book, one which has long been needed by the theoretician and experimentalist alike.' Nature
Quantum Chemistry Workbook Cambridge University Press
Provides an account of the fundamental principles of the density-functional theory of the electronic structure of matter and its applications to atoms and molecules. This book contains a discussion of the chemical potential and its derivatives. It is intended for physicists, chemists, and advanced students in chemistry.
An Introduction to Electronic Structure Theory Springer Science & Business Media
The first volume of this two part series is concerned with the fundamental aspects of relativistic quantum theory, outlining the enormous progress made in the last twenty years in this field. The aim was to create a book such that researchers who become interested in this exciting new field find it useful as a textbook, and do not have to rely on a rather large number of specialized papers published in this area. · No title is currently available that deals with new developments in relativistic quantum electronic structure theory · Interesting and relevant to graduate students in chemistry and physics as well as to all researchers in the field of quantum chemistry · As treatment of heavy elements becomes more important, there will be a constant demand for this title
Quantum Chemistry Oxford University Press
As well as providing a unified outlook on physics, Information Theory (IT) has numerous applications in chemistry and biology owing to its ability to provide a measure of the entropy/information contained within probability distributions and criteria of their information "distance" (similarity) and independence. Information Theory of Molecular Systems applies standard IT to classical problems in the theory of electronic structure and chemical reactivity. The book starts by introducing the basic concepts of modern electronic structure/reactivity theory based upon the Density Functional Theory (DFT), followed by an outline of the main ideas and techniques of IT, including several illustrative applications to molecular systems. Coverage includes information origins of the chemical bond,

unbiased definition of molecular fragments, adequate entropic measures of their internal (intra-fragment) and external (inter-fragment) bond-orders and valence-numbers, descriptors of their chemical reactivity, and information criteria of their similarity and independence. Information Theory of Molecular Systems is recommended to graduate students and researchers interested in fresh ideas in the theory of electronic structure and chemical reactivity. ·Provides powerful tools for tackling both classical and new problems in the theory of the molecular electronic structure and chemical reactivity ·Introduces basic concepts of the modern electronic structure/reactivity theory based upon the Density Functional Theory (DFT) ·Outlines main ideas and techniques of Information Theory

Physics of Condensed Matter Oxford University Press

The theory of the inhomogeneous electron gas had its origin in the Thomas Fermi statistical theory, which is discussed in the first chapter of this book. This already leads to significant physical results for the binding energies of atomic ions, though because it leaves out shell structure the results of such a theory cannot reflect the richness of the Periodic Table. Therefore, for a long time, the earlier method proposed by Hartree, in which each electron is assigned its own personal wave function and energy, dominated atomic theory. The extension of the Hartree theory by Fock, to include exchange, had its parallel in the density description when Dirac showed how to incorporate exchange in the Thomas-Fermi theory. Considerably later, in 1951, Slater, in an important paper, showed how a result similar to but not identical with that of Dirac followed as a simplification of the Hartree-Fock method. It was Gombas and other workers who recognized that one could also incorporate electron correlation consistently into the Thomas-Fermi-Dirac theory by using uniform electron gas relations locally, and progress had been made along all these avenues by the 1950s.

Electronic Structure of Materials OUP USA

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.

Molecular Electronic-Structure Theory Springer Science & Business Media

Computational chemistry, including electronic structure modeling, is a fast and accurate tool for treating large chemically meaningful systems. Unique among current quantum chemistry texts, Electronic Structure Modeling: Connections Between Theory and Software enables nonspecialists to employ computational methods in their own investigations. The text illustrates theoretical methods with numerical detail and model calculations. It clarifies what these modeling programs can do, their known pathologies, which ones are suited for specific kinds of projects, and how to reproduce them using the accompanying PC-LOBE bundled software. While elucidating gradient-based molecular structure optimization, the text reviews notable successes and unsolved problems or failures in electronic structure modeling. It also describes the theory and computation of circular dichroism and optical rotation, including magnetically induced optical phenomena. Offering an accessible introduction to computational methods, Electronic Structure Modeling permits users to practice modeling with a full understanding of the algorithms that support their calculations.

Basic Theory and Practical Methods John Wiley & Sons

Modern Electronic Structure Theory provides a didactically oriented description of the latest computational techniques in electronic structure theory and their impact in several areas of chemistry. The book is aimed at first year graduate students or college seniors considering graduate study in computational chemistry, or researchers who wish to acquire a wider knowledge of this field.

Ideas of Quantum Chemistry Cambridge University Press

For each of 150 landmark papers in ab initio molecular electronic structure methods, the author provides a lucid commentary that focuses on methodology, rather than particular chemical problems. 1984 edition.

Modern Electronic Structure Theory and Applications in Organic Chemistry OUP Oxford

This volume focuses on the use of quantum theory to understand and explain experiments in organic chemistry. High level ab initio calculations, when properly performed, are useful in making quantitative distinctions between various possible interpretations of structures, reactions and spectra. Chemical reasoning based on simpler quantum models is, however, essential to enumerating the likely possibilities. The simpler models also often suggest the type of wave function likely to be involved in ground and excited states at various points along reaction paths. This preliminary understanding is needed in order to select the appropriate higher level approach since most higher level models are designed to describe improvements to some reasonable zeroth order wave function. Consequently, most of the chapters in this volume begin with experimental facts and model functions and then progress to higher level theory only when quantitative results are required. In the first chapter, Zimmerman discusses a wide variety of thermal and photochemical reactions of organic molecules. Gronert discusses the use of ab initio calculations and experimental facts in deciphering the mechanism of β-elimination reactions in the gas phase. Bettinger et al focus on carbene structures and reactions with comparison of the triplet and singlet states. Next, Hrovat and Borden discuss more general molecules with competitive triplet and singlet contenders for the ground state structure. Cave explains the difficulties and considerations involved with many of the methods and illustrates the difficulties by comparing with the UV spectra of short polyenes. Jordan et al discuss long-range electron transfer using model compounds and model Hamiltonians. Finally, Hiberty discusses the breathing orbital valence bond model as a different approach to introducing the crucial σπ correlation that is known to be important in organic reactions. Contents:Some Theoretical Applications to Organic Chemistry (H E Zimmerman)Ab Initio Studies of Elimination Reaction Mechanisms (S Gronert)Computational Analyses of Prototype Carbene Structures and Reactions (H F Bettinger et al.)Violations of Hund's Rule in Organic Diradicals — Where to Look for Violations and How to Identify Them (D A Hrovat & W T Borden)Ab Initio Methods for the Description of

Electronically Excited States: Survey of Methods and Selected Results (R J Cave)Long-Range Intramolecular Interactions: Implications for Electron Transfer (K D Jordan et al.)The Breathing Orbital Valence Bond Method (P C Hiberty) Readership: Graduate and postgraduate students in organic chemistry. keywords:Electronic Structure;Organic Chemistry;Reaction Mechanisms;Carbene Structures;Diradicals;Excited States;Long-Range Interaction;Valence Bond Theory;Molecular Orbitals

Solid State Theory OUP Oxford

Demonstrates how anyone in math, science, and engineering canmaster DFT calculations Density functional theory (DFT) is one of the most frequentlyused computational tools for studying and predicting the propertiesof isolated molecules, bulk solids, and material interfaces,including surfaces. Although the theoretical underpinnings of DFTare quite complicated, this book demonstrates that the basicconcepts underlying the calculations are simple enough to beunderstood by anyone with a background in chemistry, physics,engineering, or mathematics. The authors show how the widespreadavailability of powerful DFT codes makes it possible for studentsand researchers to apply this important computational technique toa broad range of fundamental and applied problems. Density Functional Theory: A Practical Introductionoffers a concise, easy-to-follow introduction to the key conceptsand practical applications of DFT, focusing on plane-wave DFT. Theauthors have many years of experience introducing DFT to studentsfrom a variety of backgrounds. The book therefore offers severalfeatures that have proven to be helpful in enabling students tomaster the subject, including: Problem sets in each chapter that give readers the opportunityto test their knowledge by performing their own calculations Worked examples that demonstrate how DFT calculations are usedto solve real-world problems Further readings listed in each chapter enabling readers toinvestigate specific topics in greater depth This text is written at a level suitable for individuals from avariety of scientific, mathematical, and engineering backgrounds.No previous experience working with DFT calculations is needed.

Electronic Structure SIAM

With more than 40% new and revised materials, this second edition offers researchers and students in the field a comprehensive understanding of fundamental molecular properties amidst cutting-edge applications. Including ~70 Example-Boxes and summary notes, questions, exercises, problem sets, and illustrations in each chapter, this publication is also suitable for use as a textbook for advanced undergraduate and graduate students. Novel material is introduced in description of multi-orbital chemical bonding, spectroscopic and magnetic properties, methods of electronic structure calculation, and quantum-classical modeling for organometallic and metallobiochemical systems. This is an excellent reference for chemists, researchers and teachers, and advanced undergraduate and graduate students in inorganic, coordination, and organometallic chemistry.

Computational Methods for Large Systems Wiley-Interscience

"In An Introduction to Electronic Structure Theory, Quantum Information Theory is applied to donor-acceptor systems. Reaction stages and charge-transfer phenomena are described, continuities of probability and phase distributions are explored, and resultant information descriptors combining classical and nonclassical contributions are summarized. The authors describe the most efficient method for studying the electronic structure of solids, the magnetic dilution method, or the study of the magnetic susceptibility of diluted solid solutions of paramagnetic oxides in diamagnetic isomorphous matrices. A review of the mathematical modeling and investigation of the electronic structure of some nanomaterials, composite materials, and graphene is presented using the Parameterized Model number 3 (PM3) semi-empirical method. A basic introduction of electronic structure theory with commonly used notation is provided, as well as its applications for studying the physical properties of materials. Lastly, based on a concept of "different prescription for different correlation", a multireference Brillouin-Wigner perturbation scheme with improved virtual orbitals is presented as an accurate and affordable computational protocol for treating electronic states plagued by quasidegeneracy"--

Theory and Computational Methods Cambridge University Press

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.

Basic Theory and Practical Methods John Wiley & Sons

Over the past twenty-five years, mathematical concepts associated with geometric phases have come to occupy a central place in our modern understanding of the physics of electrons in solids. These 'Berry phases' describe the global phase acquired by a quantum state as the Hamiltonian is changed. Beginning at an elementary level, this book provides a pedagogical introduction to the important role of Berry phases and curvatures, and outlines their great influence upon many key properties of electrons in solids, including electric polarization, anomalous Hall conductivity, and the nature of the topological insulating state. It focuses on drawing connections between physical concepts and provides a solid framework for their integration, enabling researchers and students to explore and develop links to related fields. Computational examples and exercises throughout provide an added dimension to the book, giving readers the opportunity to explore the central concepts in a practical and engaging way.

Materials Modelling Using Density Functional Theory Cambridge University Press

Publisher Description