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Quantum Mechanics in Chemistry BoD – Books on Demand

Textbook on modern theoretical chemistry suitable for advanced undergraduate or graduate students.

Prediction and Estimation of Molecular Thermodynamics Courier Corporation

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.

An Advanced Course Cambridge University Press

Solid State Physics is a textbook for students of physics, material science, chemistry, and engineering. It is the state-of-the-art presentation of the theoretical foundations and application of the quantum structure of matter and materials. This second edition provides timely coverage of the most important scientific breakthroughs of the last decade (especially in low-dimensional systems and quantum transport). It helps build readers' understanding of the newest advances in condensed matter physics with rigorous yet clear mathematics. Examples are an integral part of the text, carefully designed to apply the fundamental principles illustrated in the text to currently active topics of research. Basic concepts and recent advances in the field are explained in tutorial style and organized in an intuitive manner. The book is a basic reference work for students, researchers, and lecturers in any area of solid-state physics. Features additional material on nanostructures, giving students and lecturers the most significant features of low-dimensional systems, with focus on carbon allotropes Offers detailed explanation of dissipative and nondissipative transport, and explains the essential aspects in a field, which is commonly overlooked in textbooks Additional material in the classical and quantum Hall effect offers further aspects on magnetotransport, with particular emphasis on the current profiles Gives a broad overview of the band structure of solids, as well as presenting the foundations of the electronic band structure. Also features reported with new and revised material, which leads to the latest research

Molecular Dynamics National Academies Press

Density Functional Theory (DFT) has firmly established itself as the workhorse for atomic-level simulations of condensed phases, pure or composite materials and quantum chemical systems. This work offers a rigorous and detailed introduction to the foundations of this theory, up to and including such advanced topics as orbital-dependent functionals as well as both time-dependent and relativistic DFT. Given the many ramifications of contemporary DFT, the text concentrates on the self-contained presentation of the basics of the most widely used DFT variants: this implies a thorough discussion of the corresponding existence theorems and effective single particle equations, as well as of key approximations utilized in implementations. The formal results are complemented by selected quantitative results, which primarily aim at illustrating the strengths and weaknesses of particular approaches or functionals. The structure and content of this book allow a tutorial and modular self-study approach: the reader will find that all concepts of many-body theory which are indispensable for the discussion of DFT - such as the single-particle Green's function or response functions - are introduced step by step, along with the actual DFT material. The same applies to basic notions of solid state theory, such as the Fermi surface of inhomogeneous, interacting systems. In fact, even the language of second quantization is introduced systematically in an Appendix for readers without formal training in many-body theory.

Advanced Organic Chemistry Wiley-VCH

The book explains the fundamental ideas of density functional theory, and how this theory can be used as a powerful method for explaining and even predicting the properties of materials with stunning accuracy.

The British National Bibliography John Wiley & Sons

Fifty years ago, a new approach to reaction kinetics began to emerge: one based on mathematical models of reaction kinetics, or formal reaction kinetics. Since then, there has been a rapid and accelerated development in both deterministic and stochastic kinetics, primarily because mathematicians studying differential equations and algebraic geometry have taken an interest in the nonlinear differential equations of kinetics, which are relatively simple, yet capable of depicting complex behavior such as oscillation, chaos, and pattern formation. The development of stochastic models was triggered by the fact that novel methods made it possible to measure molecules individually. Now it is high time to make the results of the last half-century

available to a larger audience: students of chemistry, chemical engineering and biochemistry, not to mention applied mathematics. Based on recent papers, this book presents the most important concepts and results, together with a wealth of solved exercises. The book is accompanied by the authors' Mathematica package, ReactionKinetics, which helps both students and scholars in their everyday work, and which can be downloaded from <http://extras.springer.com/> and also from the authors' websites. Further, the large set of unsolved problems provided may serve as a springboard for individual research.

Introduction to Computational Chemistry Cambridge University Press

Mathematical Methods for Physical and Analytical Chemistry presents mathematical and statistical methods to students of chemistry at the intermediate, post-calculus level. The content includes a review of general calculus; a review of numerical techniques often omitted from calculus courses, such as cubic splines and Newton's method; a detailed treatment of statistical methods for experimental data analysis; complex numbers; extrapolation; linear algebra; and differential equations. With numerous example problems and helpful anecdotes, this text gives chemistry students the mathematical knowledge they need to understand the analytical and physical chemistry professional literature.

Materials Modelling Using Density Functional Theory Springer Science & Business Media

The two-part, fifth edition of Advanced Organic Chemistry has been substantially revised and reorganized for greater clarity. The material has been updated to reflect advances in the field since the previous edition, especially in computational chemistry. Part B describes the most general and useful synthetic reactions, organized on the basis of reaction type. It can stand-alone; together, with Part A: Structure and Mechanisms, the two volumes provide a comprehensive foundation for the study in organic chemistry. Companion websites provide digital models for students and exercise solutions for instructors.

Fundamental Aspects of Plasma Chemical Physics Springer Science & Business Media

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.

Symmetry and Spectroscopy Amer Chemical Society

Molecular Symmetry and Spectroscopy deals with the use of group theory in quantum mechanics in relation to problems in molecular spectroscopy. It discusses the use of the molecular symmetry group, whose elements consist of permutations of identical nuclei with or without inversion. After reviewing the permutation groups, inversion operation, point groups, and representation of groups, the book describes the use of representations for labeling molecular energy. The text explains an approximate time independent Schrödinger equation for a molecule, as well as the effect of a nuclear permutation or the inversion of E^* on such equation. The book also examines the expression for the complete molecular Hamiltonian and the several groups of operations commuting with the Hamiltonian. The energy levels of the Hamiltonian can then be symmetrically labeled by the investigator using the irreducible representations of these groups. The text explains the two techniques to change coordinates in a Schrödinger equation, namely, (1) by using a diatomic molecule in the rovibronic Schrödinger equation, and (2) by a rigid nonlinear polyatomic molecule. The book also explains that using true symmetry, basis symmetry, near symmetry, and near quantum numbers, the investigator can label molecular energy levels. The text can benefit students of molecular spectroscopy, academicians, and investigators of molecular chemistry or quantum mechanics.

Molecular Symmetry and Spectroscopy Oxford University Press on Demand

Drug overdose, driven largely by overdose related to the use of opioids, is now the leading cause of unintentional injury death in the United States. The ongoing opioid crisis lies at the intersection of two public health challenges: reducing the burden of suffering from pain and containing the rising toll of the harms that can arise from the use of opioid medications. Chronic pain and opioid use disorder both represent complex human conditions affecting millions of Americans and causing untold disability and loss of function. In the context of the growing opioid problem, the U.S. Food and Drug Administration (FDA) launched an Opioids Action Plan in early 2016. As part of this plan, the FDA asked the National Academies of Sciences, Engineering, and Medicine to convene a committee to update the state of the science on pain research, care, and education and to identify actions the FDA and others can take to respond to the opioid epidemic, with a particular focus on informing FDA's development of a formal method for incorporating individual and societal considerations into its risk-benefit framework for opioid approval and monitoring.

Density Functional Theory John Wiley & Sons

Comprises 20 contributions which grew from the August 1996 symposium. Representative paper topics include estimating phase-change enthalpies and entropies, electrostatic-covalent model parameters for molecular modeling, complete basis-set thermochemistry and kinetics, modeling free energies of solvation and transfer, use of density functional methods to compute heats of reaction, and a density functional study of periodic trends in bond energies. Together the contributions describe all the major methods used for estimating or predicting molecular thermochemistry. Appends information on software and databases for thermochemistry, essential statistical thermodynamics, and worked examples. Annotation copyrighted by Book News, Inc., Portland, OR

Molecular Electronic-Structure Theory John Wiley & Sons

A practical introduction to orbital interaction theory and its applications in modern organic chemistry Orbital interaction theory is a conceptual construct that lies at the very heart of modern organic chemistry. Comprising a comprehensive set of principles for explaining chemical reactivity, orbital interaction theory originates in a rigorous theory of electronic structure that also provides the basis for the powerful computational models and techniques with which chemists seek to describe and exploit the structures and thermodynamic and kinetic stabilities of molecules. Orbital Interaction Theory of Organic Chemistry, Second Edition introduces students to the fascinating world

of organic chemistry at the mechanistic level with a thoroughly self-contained, well-integrated exposition of orbital interaction theory and its applications in modern organic chemistry. Professor Rauk reviews the concepts of symmetry and orbital theory, and explains reactivity in common functional groups and reactive intermediates in terms of orbital interaction theory. Aided by numerous examples and worked problems, he guides readers through basic chemistry concepts, such as acid and base strength, nucleophilicity, electrophilicity, and thermal stability (in terms of orbital interactions), and describes various computational models for describing those interactions. Updated and expanded, this latest edition of Orbital Interaction Theory of Organic Chemistry includes a completely new chapter on organometallics, increased coverage of density functional theory, many new application examples, and worked problems. The text is complemented by an interactive computer program that displays orbitals graphically and is available through a link to a Web site. Orbital Interaction Theory of Organic Chemistry, Second Edition is an excellent text for advanced-level undergraduate and graduate students in organic chemistry. It is also a valuable working resource for professional chemists seeking guidance on interpreting the quantitative data produced by modern computational chemists.

Part B: Reaction and Synthesis Springer Science & Business Media

Computational chemistry has become extremely important in the last decade, being widely used in academic and industrial research. Yet there have been few books designed to teach the subject to nonspecialists. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics is an invaluable tool for teaching and researchers alike. The book provides an overview of the field, explains the basic underlying theory at a meaningful level that is not beyond beginners, and it gives numerous comparisons of different methods with one another and with experiment. The following concepts are illustrated and their possibilities and limitations are given: - potential energy surfaces; - simple and extended Hückel methods; - ab initio, AM1 and related semiempirical methods; - density functional theory (DFT). Topics are placed in a historical context, adding interest to them and removing much of their apparently arbitrary aspect. The large number of references, to all significant topics mentioned, should make this book useful not only to undergraduates but also to graduate students and academic and industrial researchers.

Thermodynamics John Wiley & Sons

Fifty years ago, a new approach to reaction kinetics began to emerge: one based on mathematical models of reaction kinetics, or formal reaction kinetics. Since then, there has been a rapid and accelerated development in both deterministic and stochastic kinetics, primarily because mathematicians studying differential equations and algebraic geometry have taken an interest in the nonlinear differential equations of kinetics, which are relatively simple, yet capable of depicting complex behavior such as oscillation, chaos, and pattern formation. The development of stochastic models was triggered by the fact that novel methods made it possible to measure molecules individually. Now it is high time to make the results of the last half-century available to a larger audience: students of chemistry, chemical engineering and biochemistry, not to mention applied mathematics. Based on recent papers, this book presents the most important concepts and results, together with a wealth of solved exercises. The book is accompanied by the authors' Mathematica package, ReactionKinetics, which helps both students and scholars in their everyday work, and which can be downloaded from <http://extras.springer.com/> and also from the authors' websites. Further, the large set of unsolved problems provided may serve as a springboard for individual research.

Mathematical Methods for Physical and Analytical Chemistry Springer Science & Business Media

Informal, effective undergraduate-level text introduces vibrational and electronic spectroscopy, presenting applications of group theory to the interpretation of UV, visible, and infrared spectra without assuming a high level of background knowledge. 200 problems with solutions. Numerous illustrations. "A uniform and consistent treatment of the subject matter." — Journal of Chemical Education.

Solid State Physics Cambridge University Press

Ab initio quantum chemistry has emerged as an important tool in chemical research and is applied to a wide variety of problems in chemistry and molecular physics. Recent developments of computational methods have enabled previously intractable chemical problems to be solved using rigorous quantum-mechanical methods. This is the first comprehensive, up-to-date and technical work to cover all the important aspects of modern molecular electronic-structure theory. Topics covered in the book include: * Second quantization with spin adaptation * Gaussian basis sets and molecular-integral evaluation * Hartree-Fock theory * Configuration-interaction and multi-configurational self-consistent theory * Coupled-cluster theory for ground and excited states * Perturbation theory for single- and multi-configurational states * Linear-scaling techniques and the fast multipole method * Explicitly correlated wave functions * Basis-set convergence and extrapolation * Calibration and benchmarking of computational methods, with applications to molecular equilibrium structure, atomization energies and reaction enthalpies. Molecular Electronic-Structure Theory makes extensive use of numerical examples, designed to illustrate the strengths and weaknesses of each method treated. In addition, statements about the usefulness and deficiencies of the various methods are supported by actual examples, not just model calculations. Problems and exercises are provided at the end of each chapter, complete with hints and solutions. This book is a must for researchers in the field of quantum chemistry as well as for nonspecialists who wish to acquire a thorough understanding of ab initio molecular electronic-structure theory and its applications to problems in chemistry and physics. It is also highly recommended for the teaching of graduates and advanced undergraduates.

Orbital Interaction Theory of Organic Chemistry Courier Corporation

New edition of the overwhelmingly favorite text for the physical chemistry course.

Computational Thermochemistry Oxford University Press

Molecular Dynamics is a two-volume compendium of the ever-growing applications of molecular dynamics simulations to solve a wider range of scientific and engineering challenges. The contents illustrate the rapid progress on molecular dynamics simulations in many fields of science and technology, such as nanotechnology, energy research, and biology, due to the advances of new dynamics theories and the extraordinary power of today's computers. This first book begins with a general description of underlying theories of molecular dynamics simulations and provides extensive coverage of molecular dynamics simulations in nanotechnology and energy. Coverage of this book includes: Recent advances of molecular dynamics theory Formation and evolution of nanoparticles of up to 106 atoms Diffusion and dissociation of gas and liquid molecules on silicon, metal, or metal organic frameworks Conductivity of ionic species in solid oxides Ion solvation in liquid mixtures Nuclear structures

Introduction to Quantum Mechanics with Applications to Chemistry Oxford University Press

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.