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Conjuring the Universe Springer Science & Business Media

Portrays the structures of the substances that make up our everyday world.

Density Functional Theory Royal Society of Chemistry

Contains the author's detailed solutions of almost every one of the 267 problems contained in the second edition of this textbook.

Quantum Mechanics in Chemistry W. H. Freeman

Most people remember chemistry from their schooldays as largely incomprehensible, a subject that was fact-rich but understanding-poor, smelly, and so far removed from the real world of events and pleasures that there seemed little point, except for the most introverted, in coming to terms with its grubby concepts, spells, recipes, and rules. Peter Atkins wants to change all that. In this Very Short Introduction to Chemistry, he encourages us to look at chemistry anew, through a chemist's eyes, in order to understand its central concepts and to see how it contributes not only towards our material comfort, but also to human culture. Atkins shows how chemistry provides the infrastructure of our world, through the chemical industry, the fuels of heating, power generation, and transport, as well as the fabrics of our clothing and furnishings. By considering the remarkable achievements that chemistry has made, and examining its place between both physics and biology, Atkins presents a fascinating, clear, and rigorous exploration of the world of chemistry - its structure, core concepts, and exciting contributions to new cutting-edge technologies. ABOUT THE SERIES: The Very Short Introductions series from Oxford University Press contains hundreds of titles in almost every subject area. These pocket-sized books are the perfect way to get ahead in a new subject quickly. Our expert authors combine facts, analysis, perspective, new ideas, and enthusiasm to make interesting and challenging topics highly readable.

A Modern Approach to Quantum Mechanics Elsevier

Classic undergraduate text explores wave functions for the hydrogen atom, perturbation theory, the Pauli exclusion principle, and the structure of simple and complex molecules. Numerous tables and figures.

An Introduction to Theoretical Chemistry Macmillan

The aim of this book is to give a simple, short, and elementary introduction to the second quantized formalism as applied to a many-electron system. It is intended for those, mainly chemists, who are familiar with traditional quantum chemistry but have not yet become acquainted with second quantization. The treatment is, in part, based on a series of seminars held by the author on the subject. It has been realized that many quantum chemists either interested in theory or in applications, being educated as chemists and not as physicists, have never devoted themselves to taking a course on the second quantized approach. Most available textbooks on this topic are not very easy to follow for those who are not trained in theory, or they are not detailed enough to offer a comprehensive treatment. At the same time there are several papers in quantum chemical literature which take advantage of using second quantization, and it would be worthwhile if those papers were accessible for a wider reading public. For this reason, it is intended in this survey to review the basic formalism of second quantization, and to treat some selected chapters of quantum chemistry in this language. Most derivations will be carried out in a detailed manner, so the reader need not accept gaps to understand the result.

Solutions Manual for Quanta, Matter and Change Oxford University Press, USA

At a level accessible to advanced undergraduates, this textbook explains the fundamental role of quantum mechanics in determining the structure, dynamics, and other properties of molecules. Readers will come to understand the quantum-mechanical basis for harmonic oscillators, angular momenta and scattering processes. Exercises are provided to help readers deepen their grasp of the essential phenomena.

Second Quantized Approach to Quantum Chemistry Springer

Peter Atkins and Julio de Paula offer a fully integrated approach to the study of physical chemistry and biology.

Chemical Principles Oxford University Press, USA

This revision of the introductory textbook of physical chemistry has been designed to broaden its appeal, particularly to students with an interest in biological applications.

Elements of Physical Chemistry Elsevier

Methods of Molecular Quantum Mechanics This advanced text introduces to the advanced undergraduate and graduate student the mathematical foundations of the methods needed to carry out practical applications in electronic molecular quantum mechanics, a necessary preliminary step before using commercial programmes to carry out quantum chemistry calculations. Major features of the book include: Consistent use of the system of atomic units, essential for simplifying all mathematical formulae Introductory use of density matrix techniques for interpreting properties of many-body systems An introduction to valence bond methods with an explanation of the origin of the chemical bond A unified presentation of basic elements of atomic and molecular interactions The book is intended for advanced undergraduate and first-year graduate students in chemical physics, theoretical and quantum chemistry. In addition, it is relevant to students from physics and from engineering sub-disciplines such as chemical engineering and materials sciences.

Quantum Chemistry CRC Press

"The Sixth Edition of this widely used textbook presents quantum chemistry for beginning graduate students and advanced undergraduates. The subject is carefully explained step-by-step, allowing students to

easily follow the presentation. Necessary mathematics is reviewed in detail. Worked examples aid learning. A solutions manual for the problems is available. Extensive discussions of modern abinitio, density functional, semiempirical, and molecular mechanics methods are included."--BOOK JACKET.

Four Laws That Drive the Universe Cambridge University Press

Previous ed published: 1989 Periodic table and text on lining papers Includes index and appendices.

Molecules Macmillan

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

Physical Chemistry for the Life Sciences Macmillan

Any literate person should be familiar with the central ideas of modern science. In his sparkling new book, Peter Atkins introduces his choice of the ten great ideas of science. With wit, charm, patience, and astonishing insights, he leads the reader through the emergence of the concepts, and then presents them in a strikingly effective manner. At the same time, he works into his engaging narrative an illustration of the scientific method and shows how simple ideas can have enormous consequences. His choice of the ten great ideas are: * Evolution occurs by natural selection, in which the early attempts at explaining the origin of species is followed by an account of the modern approach and some of its unsolved problems. * Inheritance is encoded in DNA, in which the story of the emergence of an understanding of inheritance is followed through to the mapping of the human genome. * Energy is conserved, in which we see how the central concept of energy gradually dawned on scientists as they mastered the motion of particles and the concept of heat. * All change is the consequence of the purposeless collapse of energy and matter into disorder, in which the extraordinarily simple concept of entropy is used to account for events in the world. * Matter is atomic, in which we see how the concept of atoms emerged and how the different personalities of the elements arise from the structures of their atoms. * Symmetry limits, guides, and drives, in which we see how concepts related to beauty can be extended to understand the nature of fundamental particles and the forces that act between them. * Waves behave like particles and particles behave like waves, in which we see how old familiar ideas gave way to the extraordinary insights of quantum theory and transformed our perception of matter. * The universe is expanding, in which we see how a combination of astronomy and a knowledge of elementary particles accounts for the origin of the universe and its long term future. * Spacetime is curved by matter, in which we see the emergence of the theories of special and general relativity and come to understand the nature of space and time. * If arithmetic is consistent, then it is incomplete, in which we learn the origin of numbers and arithmetic, see how the philosophy of mathematics lets us understand the nature of this most cerebral of subjects, and are brought to the limits of its power. C. P. Snow once said 'not knowing the second law of thermodynamics is like never having read a work by Shakespeare'. This is an extraordinary, exciting book that not only will make you literate in science but give you deep enjoyment on the way.

Physical Chemistry Volume 1: Thermodynamics and Kinetics OUP Oxford

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.

Atkins' Physical Chemistry 11e John Wiley & Sons

Demonstrates how anyone in math, science, and engineering can master DFT calculations Density functional theory (DFT) is one of the most frequently used computational tools for studying and predicting the properties of isolated molecules, bulk solids, and material interfaces, including surfaces. Although the theoretical underpinnings of DFT are quite complicated, this book demonstrates that the basic concepts underlying the

calculations are simple enough to be understood by anyone with a background in chemistry, physics, engineering, or mathematics. The authors show how the widespread availability of powerful DFT codes makes it possible for students and researchers to apply this important computational technique to a broad range of fundamental and applied problems. Density Functional Theory: A Practical Introduction offers a concise, easy-to-follow introduction to the key concepts and practical applications of DFT, focusing on plane-wave DFT. The authors have many years of experience introducing DFT to students from a variety of backgrounds. The book therefore offers several features that have proven to be helpful in enabling students to master the subject, including: Problem sets in each chapter that give readers the opportunity to test their knowledge by performing their own calculations Worked examples that demonstrate how DFT calculations are used to solve real-world problems Further readings listed in each chapter enabling readers to investigate specific topics in greater depth This text is written at a level suitable for individuals from a variety of scientific, mathematical, and engineering backgrounds. No previous experience working with DFT calculations is needed.

Quantum Mechanics of Molecular Structures W.H. Freeman

This text is designed for a rigorous course in introductory chemistry. Its central theme is to challenge students to think and question while providing a sound foundation in the principles of chemistry.

Molecular Physics and Elements of Quantum Chemistry Oxford University Press
Advanced graduate-level text looks at symmetry, rotations, and angular momentum addition; occupation number representations; and scattering theory. Uses concepts to develop basic theories of chemical reaction rates. Problems and answers.

Quantum Chemistry John Wiley & Sons

Chemistry is widely considered to be the central science: it encompasses concepts on which all other branches of science are developed. Yet, for many students entering university, gaining a firm grounding in chemistry is a real challenge. Chemistry3 responds to this challenge, providing students with a full understanding of the fundamental principles of chemistry on which to build later studies. Uniquely amongst the introductory chemistry texts currently available, Chemistry3's author team brings together experts in each of organic, inorganic, and physical chemistry with specialists in chemistry education to provide balanced coverage of the fundamentals of chemistry in a way that students both enjoy and understand. The result is a text that builds on what students know already from school and tackles their misunderstandings and misconceptions, thereby providing a seamless transition from school to undergraduate study. Written with unrivalled clarity, students are encouraged to engage with the text and appreciate the central role that chemistry plays in our lives through the unique use of real-world context and photographs. Chemistry3 tackles head-on two issues pervading chemistry education: students' mathematical skills, and their ability to see the subject as a single, unified discipline. Instead of avoiding the maths, Chemistry3 provides structured support, in the form of careful explanations, reminders of key mathematical concepts, step-by-step calculations in worked examples, and a Maths Toolkit, to help students get to grips with the essential mathematical element of chemistry. Frequent cross-references highlight the connections between each strand of chemistry and explain the relationship between the topics, so students can develop an understanding of the subject as a whole. Digital formats and resources Chemistry3 is available for students and institutions to purchase in a variety of formats, and is supported by online resources. The e-book offers a mobile experience and convenient access along with functionality tools, navigation features, and links that offer extra learning support: www.oxfordtextbooks.co.uk/ebooks The e-book also features interactive animations of molecular structures, screencasts in which authors talk step-by-step through selected examples and key reaction mechanisms, and self-assessment activities for each chapter. The accompanying online resources will also include, for students: DT Chapter 1 as an open-access PDF; DT Chapter summaries and key equations to download, to support revision; DT Worked solutions to the questions in the book. The following online resources are also provided for lecturers: DT Test bank of ready-made assessments for each chapter with which to test your students; DT Problem-solving workshop activities for each chapter for you to use in class; DT Case-studies showing how instructors are successfully using Chemistry3 in digital learning environments and to support innovative teaching practices; DT Figures and tables from the book

Elements of Physical Chemistry Springer Science & Business Media

Thoroughly rewritten from start to finish, the second edition of this text provides a complete, highly accessible introduction to quantum chemistry.

Quantum Mechanics for Chemists Courier Corporation

Uses illustrations to discuss the various chemical reactions, both simple and complex, between atoms and molecules.