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Quantum Chemistry New Age International

This is the physical chemistry textbook for students with an affinity for computers! It offers basic and advanced knowledge for students in the second year of chemistry masters studies and beyond. In seven chapters, the book presents thermodynamics, chemical kinetics, quantum mechanics and molecular structure (including an introduction to quantum chemical calculations), molecular symmetry and crystals. The application of physical-chemical knowledge and problem solving is demonstrated in a chapter on water, treating both the water molecule as well as water in condensed phases. Instead of a traditional textbook top-down approach, this book presents the subjects on the basis of examples, exploring and running computer programs (Mathematica®), discussing the results of molecular orbital calculations (performed using Gaussian) on small molecules and turning to suitable reference works to obtain thermodynamic data. Selected Mathematica® codes are explained at the end of each chapter and cross-referenced with the text, enabling students to plot functions, solve equations, fit data, normalize probability functions, manipulate matrices and test physical models. In addition, the book presents clear and step-by-step explanations and provides detailed and complete answers to all exercises. In this way, it creates an active learning environment that can prepare students for pursuing their own research projects further down the road. Students who are not yet familiar with Mathematica® or Gaussian will find a valuable introduction to computer-based problem solving in the molecular sciences. Other computer applications can alternatively be used. For every chapter learning goals are clearly listed in the beginning, so that readers can easily spot the highlights, and a glossary in the end of the chapter offers a quick look-up of important terms.

Essentials of Computational Chemistry Univ Science Books

Physical Chemistry: A Molecular Approach Sterling Publishing Company

Solutions Manual to Accompany Quantum Chemistry Univ Science Books

Completely revised and updated, Chemical Analysis: Second Edition is an essential introduction to a wide range of analytical techniques and instruments. Assuming little in the way of prior knowledge, this text carefully guides the reader through the more widely used and important techniques, whilst avoiding excessive technical detail. Provides a thorough introduction to a wide range of the most important and widely used instrumental techniques. Maintains a careful balance between depth and breadth of coverage. Includes examples, problems and their solutions. Includes coverage of latest developments including supercritical fluid chromatography and capillary electrophoresis.

Physical Chemistry, 4th Edition Royal Society of Chemistry

Following in the wake of Chang's two other best-selling physical chemistry textbooks (Physical Chemistry for the Chemical and Biological Sciences and Physical Chemistry for the Biosciences), this new title introduces laser spectroscopist Jay Thoman (Williams College) as co-author. This comprehensive new text has been extensively revised both in level and scope. Targeted to a mainstream physical chemistry course, this text features extensively revised chapters on quantum mechanics and spectroscopy, many new chapter-ending problems, and updated references, while biological topics have been largely relegated to the previous two textbooks. Other topics added include the law of corresponding states, the Joule-Thomson effect, the meaning of entropy, multiple equilibria and coupled reactions, and chemiluminescence and bioluminescence. One way to gauge the level of this new text is that students who have used it will be well prepared for their GRE exams in the subject. Careful pedagogy and clear writing throughout combine to make this an excellent choice for your physical chemistry course.

Problems and Solutions to Accompany McQuarrie and Simon, Physical Chemistry: a Molecular Approach W. H. Freeman

"Atoms First seems to be the flavor of the year in chemistry textbooks, but many of them seem to be little more than rearrangement of the chapters. It takes a master like McQuarrie to go back to the drawing board and create a logical development from smallest to largest that makes sense to students."---Hal Harris, University of Missouri-St. Louis "McQuarrie's book is extremely well written, the order of topics is logical, and it does a great job with both introductory material and more advanced concepts. Students of all skill levels will be able to learn from this book."---Mark Kearley, Florida State University This new fourth edition of General Chemistry takes an atoms-first approach from beginning to end. In the tradition of McQuarrie's many previous works, it promises to be another ground-breaking text. This superb new book combines the clear writing and wonderful problems that have made McQuarrie famous among chemistry professors and students worldwide. Presented in an elegant design with all-new illustrations, it is available in a soft-cover edition to offer professors a fresh choice at an outstanding value. Student supplements include an online series of descriptive chemistry Interchapters, a Student Solutions Manual, and an optional state-of-the-art Online Homework program. For adopting professors, an Instructor's Manual and a CD of the art are also available.

Quantum Chemistry Sterling Publishing Company

Part A.: Overviews of biological inorganic chemistry : 1. Bioinorganic chemistry and the biogeochemical cycles -- 2. Metal ions and proteins: binding, stability, and folding -- 3. Special cofactors and metal clusters -- 4. Transport and storage of metal ions in biology -- 5. Biominerals and biomineralization -- 6. Metals in medicine. --

Part B.: Metal ion containing biological systems : 1. Metal ion transport and storage -- 2. Hydrolytic chemistry -- 3. Electron transfer, respiration, and photosynthesis -- 4. Oxygen metabolism -- 5. Hydrogen, carbon, and sulfur metabolism -- 6. Metalloenzymes with radical intermediates -- 7. Metal ion receptors and signaling. -- Cell

biology, biochemistry, and evolution: Tutorial I. -- Fundamentals of coordination chemistry: Tutorial II.

Essentials of Nuclear Chemistry Allyn & Bacon

The Students Solutions Manual to Accompany Physical Chemistry: Quanta, Matter, and Change 2e provides full worked solutions to the 'a' exercises, and the odd-numbered discussion questions and problems presented in the parent book. The manual is intended for students and instructors alike, and provides helpful comments and friendly advice to aid understanding.

Quantum Mechanics for Chemists Macmillan

This text provides students with concise reviews of mathematical topics that are used throughout physical chemistry. By reading these reviews before the mathematics is applied to physical chemical problems, a student will be able to spend less time worrying about the math and more time learning the physical chemistry.

Problems and Solutions in Quantum Chemistry and Physics Elsevier

Physical Chemistry for the Biosciences has been optimized for a one-semester introductory course in physical chemistry for students of biosciences.

Introduction to Computational Physical Chemistry Sterling Publishing Company

"Intended for upper-level undergraduate and graduate courses in chemistry, physics, math and engineering, this book will also become a must-have for the personal library of all advanced students in the physical sciences. Comprised of more than 2000 problems and 700 worked examples that detail every single step, this text is exceptionally well adapted for self study as well as for course use."--From publisher description.

Physical Chemistry Wiley Global Education

Written by Ira Levine, the Student Solutions Manual contains the worked-out solutions to all of the problems in the text. The purpose of the manual is help the student learn physical chemistry and as an incentive to work problems, not as a way to avoid working problems.

Solutions Manual for Quanta, Matter and Change Springer Science & Business Media

A leading book for 80 years, Silbey's Physical Chemistry features exceptionally clear explanations of the concepts and methods of physical chemistry for students who have had a year of calculus and a year of physics. The basic theory of chemistry is presented from the viewpoint of academic physical chemists, but the many practical applications of physical chemistry are integrated throughout the text. The problems in the text also reflect a skillful blend of theory and practical applications. This text is ideally suited for a standard undergraduate physical chemistry course taken by chemistry, chemical engineering, and biochemistry majors in their junior or senior year.

Mathematics for Physical Chemistry Elsevier

This book is a physical chemistry textbook that presents the essentials of physical chemistry as a logical sequence from its most modest beginning to contemporary research topics. Many books currently on the market focus on the problem sets with a cursory treatment of the conceptual background and theoretical material, whereas this book is concerned only with the conceptual development of the subject. Comprised of 19 chapters, the book will address ideal gas laws, real gases, the thermodynamics of simple systems, thermochemistry, entropy and the second law, the Gibbs free energy, equilibrium, statistical approaches to thermodynamics, the phase rule, chemical kinetics, liquids and solids, solution chemistry, conductivity, electrochemical cells, atomic theory, wave mechanics of simple systems, molecular orbital theory, experimental determination of molecular structure, and photochemistry and the theory of chemical kinetics.

Computer-Aided Analysis of Rigid and Flexible Mechanical Systems John Wiley & Sons

This book will revolutionize the way physical chemistry is taught by bridging the gap between the traditional "solve a bunch of equations for a very simple model" approach and the computational methods that are used to solve research problems. While some recent textbooks include exercises using pre-packaged Hartree-Fock/DFT calculations, this is largely limited to giving students a proverbial black box. The DIY (do-it-yourself) approach taken in this book helps student gain understanding by building their own simulations from scratch. The reader of this book should come away with the ability to apply and adapt these techniques in computational chemistry to his or her own research problems, and have an enhanced ability to critically evaluate other computational results. This book is mainly intended to be used in conjunction with an existing physical chemistry text, but it is also well suited as a stand-alone text for upper level undergraduate or intro graduate computational chemistry courses.

Quantum Chemistry 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.

Molecular Thermodynamics University Science Books

"Topics are organized into three parts: algebra, calculus, differential equations, and expansions in series; vectors, determinants and matrices; and numerical analysis and statistics. The extensive use of examples illustrates every important concept and method in the text, and are used to demonstrate applications of the mathematics in chemistry and several basic concepts in physics. The exercises at the end of each chapter, are an essential element of the development of the subject, and have been designed to give students a working understanding of the material in the text."--BOOK JACKET.

Concise Physical Chemistry Oxford University Press

With its modern emphasis on the molecular view of physical chemistry, its wealth of contemporary applications, vivid full-color presentation, and dynamic new media tools, the thoroughly revised new edition is again the most modern, most effective full-length textbook

available for the physical chemistry classroom. Volume 1 of Physical Chemistry, Ninth Edition, contains the new edition's new Fundamentals chapters (Chapter 0), plus coverage of thermodynamics (Chapters 1-6) and kinetics (Chapters 20-23)

General Chemistry World Scientific

Integrating many new computer-oriented examples and problems throughout, this modern introduction to quantum chemistry covers quantum mechanics, atomic structure, and molecular electronics, and clearly demonstrates the usefulness and limitations of current quantum-mechanical methods for the calculation of molecular properties. Covers such areas as the Schrödinger Equation, harmonic oscillator, angular momentum, hydrogen atom, theorems of quantum mechanics, electron spin and the Pauli Principle, the Virial Theorem and the Hellmann-Feynman Theorem, and more. Contains solid presentations of the mathematics needed for quantum chemistry, clearly explaining difficult or subtle points in detail. Offers full, step-by-step examinations of derivations that are easy to follow and understand. Offers comprehensive coverage of recent, revolutionary advances in modern quantum-chemistry methods for calculating molecular electronic structure, including the ab initio and semiempirical methods for molecular calculations. Now integrates over 500 problems throughout, with a substantial increase in the amount of computer applications, and fully updated discussions of molecular electronic structure calculations. For professionals in all branches of chemistry.

Univ Science Books

Fifty years ago solution chemistry occupied a major fraction of physical chemistry textbooks, and dealt mainly with classical thermodynamics, phase equilibria, and non-equilibrium phenomena, especially those related to electrochemistry. Much has happened in the intervening period, with tremendous advances in theory and the development of important new experimental techniques. This book brings the reader through the developments from classical macroscopic descriptions to more modern microscopic details.

Mathematics for Physical Chemistry: Opening Doors University Science Books

Martin's Physical Pharmacy and Pharmaceutical Sciences is considered the most comprehensive text available on the application of the physical, chemical and biological principles in the pharmaceutical sciences. It helps students, teachers, researchers, and industrial pharmaceutical scientists use elements of biology, physics, and chemistry in their work and study. Since the first edition was published in 1960, the text has been and continues to be a required text for the core courses of Pharmaceutics, Drug Delivery, and Physical Pharmacy. The Sixth Edition features expanded content on drug delivery, solid oral dosage forms, pharmaceutical polymers and pharmaceutical biotechnology, and updated sections to cover advances in nanotechnology.