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589 - EVA WASHINGTON

Covers the principles of quantum mechanics and engages those principles in the development of thermodynamics. Coverage includes the properties of gases, the First Law of Thermodynamics, a molecular interpretation of the principal thermodynamic state functions, solutions, non equilibrium thermodynamics, and electrochemistry. Features 10-12 worked examples and some 60 problems for each chapter. A separate Solutions Manual is forthcoming in April 1999. Annotation copyrighted by Book News, Inc., Portland, OR

Learn classical thermodynamics alongside statistical mechanics and how macroscopic and microscopic ideas interweave with this fresh approach to the subjects.

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.

This book offers a comprehensive introduction to polymer rheology with a focus on the viscoelastic characterization of polymeric materials. It contains various numerical algorithms for the processing of viscoelastic data, from basic principles to advanced examples which are hard to find in the existing literature. The book takes a multidisciplinary approach to the study of the viscoelasticity of polymers, and is self-contained, including the essential mathematics, continuum mechanics, polymer science and statistical mechanics needed to understand the theories of polymer viscoelasticity. It covers recent achievements in polymer rheology, such as theoretical and experimental aspects of large amplitude oscillatory shear (LAOS), and numerical methods for linear viscoelasticity, as well as new insights into the interpretation of experimental data. Although the book is balanced between the theoretical and experimental aspects of polymer rheology, the author’s particular interest in the theoretical side will not remain hidden. Aimed at readers familiar with the mathematics and physics of engineering at an undergraduate level, the multidisciplinary approach employed enables researchers with various scientific backgrounds to expand their knowledge of polymer rheology in a systematic way.

Particles and Interfaces: Interaction, Deposition, Structure, Volume 20, Second Edition unifies particle and protein adsorption phenomena by presenting recent developments in this growing field of nanoscience. While experimental data is available in vast quantities, there is a deficit in quality interpretation of that data. This title provides such information, emphasizing the basic physics behind practical problems, thus empowering the reader to estimate relevant effects. The book includes solved problems of particle transport under non-linear conditions and their relevance to predicting protein adsorption, including an entirely new chapter devoted to polyelectrolyte and protein adsorption at solid/liquid and solid/gas interfaces. Unifies information from various fields, such as electrostatics, hydrodynamic, colloid science and biophysics Presents information in a user-friendly manner, including computer aided graphics and schematic drawings Applies a phenomenological approach to the content and provides readily accessible reference data

By uniting basic concepts in equilibrium and time-dependent statistical mechanics with modern computational techniques, the book provides a comprehensive view of how theory proceeds from concepts to model construction to practical algorithms.

The pKa of a compound describes its acidity or basicity and, therefore, is one of its most important properties. Its value determines what form of the compound—positive ion, negative ion, or neutral species—will be present under different circumstances. This is crucial to the action and detection of the compound as a drug, pollutant, or other active chemical agent. In many cases it is desirable to predict pKa values prior to synthesizing a compound, and enough is now known about the salient features that influence a molecule’s acidity to make these predictions. Computational Approaches for the Prediction of pKa Values describes the insights that have been gained on the intrinsic and extrinsic features that influence a molecule’s acidity and discusses the computational methods developed to estimate acidity from a compound’s molecular structure. The authors examine the strengths and weaknesses of the theoretical techniques and show how they have been used to obtain information about the acidities of different classes of chemical compounds. The book presents theoretical methods for both general and more specific applications, covering methods for various acids in aqueous solutions—including oxyacids and related compounds, nitrogen acids, inorganic acids, and excited-state acids—as well as acids in nonaqueous solvents. It also considers temperature effects, isotope effects, and other important factors that influence pKa. This book provides a resource for predicting pKa values and understanding the bases for these determinations, which can be helpful in designing better chemicals for future uses.

This book contains the latest information on all aspects of the most important chemical thermodynamic properties of Gibbs energy and Helmholtz energy, as related to fluids. Both the Gibbs energy and Helmholtz energy are very important in the fields of thermodynamics and material properties as many other properties are obtained from the temperature or pressure dependence. Bringing all the information into one authoritative survey, the book is written by acknowledged world experts in their respective fields. Each of the chapters will cover theory, experimental methods and techniques and results for all types of liquids and vapours. This book is the fourth in the series of Thermodynamic Properties related to liquids, solutions and vapours, edited by Emmerich Wilhelm and Trevor Letcher. The previous books were: Heat Capacities (2010), Volume Properties (2015), and Enthalpy (2017). This book fills the gap in fundamental thermodynamic properties and is the last in the series.

The only text to cover both thermodynamic and statistical mechanics--allowing students to fully master thermodynamics at the macroscopic level. Presents essential ideas on critical phenomena developed over the last decade in simple, qualitative terms. This new edition maintains the simple structure of the first and puts new emphasis on pedagogical considerations. Thermostatistics is incorporated into the text without eclipsing macroscopic thermodynamics, and is integrated into the conceptual framework of physical theory.

This thesis provides a comprehensive description of methods used to compute the vibrational spectra of liquid systems by molecular dynamics simulations. The author systematically introduces theoretical basics and discusses the implications of approximating the atomic nuclei as classical particles. The strengths of the methodology are demonstrated through several different examples. Of particular interest are ionic liquids, since their properties are governed by strong and diverse intermolecular interactions in the liquid state. As a novel contribution to the field, the author presents an alternative route toward infrared and Raman intensities on the basis of a Voronoi tessellation of the electron density. This technique is superior to existing approaches regarding the computational resources needed. Moreover, this book presents an innovative approach to obtaining the magnetic moments and vibrational circular dichroism spectra of liquids, and demonstrates its excellent agreement with experimental reference data.

Gas Bubble Dynamics in the Human Body provides a broad range of professionals, from physicians working in a clinic, hospital or hyperbaric facility, to physical scientists trying to understand and predict the dynamics of gas bubble behavior in the body, with an interdisciplinary perspective on gas-bubble disease. Both iatrogenic and decompression-induced gas bubbles are considered. The basic medical and physiological aspects are described first, in plain language, with numerous illustrations that facilitate an intuitive grasp of the basic underlying medicine and physiology. Current issues in the field, particularly microbubbles and microparticles, and their possible role in gas-bubble disease are included. The physical and mathematical material is given at several levels of sophistication, with the "hard-core" math separated out in sections labelled "For the Math Mavens", so that the basic concepts can be grasped at a descriptive level. The field is large and multi-disciplinary, so that some of the discussion that is at a greater depth is given separately in sections labelled "In Greater Detail". Skipping these sections for whatever reason, shouldn’t materially hamper acquiring an overall appreciation of the field. Demonstrates how physical and mathematical tools help to solve underlying problems across physiology and medicine Helps researchers extend their competence and flexibility to the point that they can personally contribute to the field of hyperbaric medicine and physiology, or to other related biological problems that may interest them Provides clinicians with explicit examples of how mathematical modelling can be integrated into clinical treatment and decision-making

Lectures on elementary statistical mechanics, taught at the University of Illinois and at the University of Pennsylvania.

Quantum physics provides the concepts and their mathematical formalization that lend themselves to describe important properties of biological networks topology, such as vulnerability to external stress and their dynamic response to changing physiological conditions. A theory of networks enhanced with mathematical concepts and tools of quantum physics opens a new area of biological physics, the one of systems biological physics.

This textbook for graduates and advanced undergraduates in physics and physical chemistry covers the major areas of statistical mechanics and concludes with the level of current research. It begins with the fundamental ideas of averages and ensembles, focusing on classical systems described by continuous variables such as position and momentum, and using the ideal gas as an example. It then turns to quantum systems, beginning with diatomic molecules and working up through blackbody radiation and chemical equilibria. The discussion of equilibrium properties of systems of interacting particles includes such techniques as cluster expansions and distribution functions and uses non-ideal gases, liquids, and solutions. Dynamic behavior -- treated here more extensively than in other texts -- is discussed from the point of view of correlation functions. The text concludes with the problem of diffusion in a suspension of interacting hard spheres and what can be learned about such a system from scattered light. Intended for a one-semester course, the text includes several "asides" on topics usually omitted from introductory courses, as well as numerous exercises.

This book presents computer simulations using molecular dynamics techniques in statistical physics, with a focus on macromolecular systems. The numerical methods are introduced in the form of computer algorithms and can be implemented in computers using any desired computer programming language, such as Fortran 90, C/C++, and others. The book also explains how some of these numerical methods and their algorithms can be implemented in the existing computer programming software of macromolecular systems, such as the CHARMM program. In addition, it examines a number of advanced concepts of computer simulation techniques used in statistical physics as well as biological and physical systems. Discussing the molecular dynamics approach in detail to enhance readers understanding of the use of this method in statistical physics problems, it also describes the equations of motion in various statistical ensembles to mimic real-world experimental conditions. Intended for graduate students and research scientists working in the field of theoretical and computational biophysics, physics and chemistry, the book can also be used by postgraduate students of other disciplines, such as applied mathematics, computer sciences, and bioinformatics. Further, offering insights into fundamental theory, it as a valuable resource for expert practitioners and programmers and those new to the field.

Volume 5.

This book provides theoretical concepts and applications of fractals and multifractals to a broad range of audiences from various scientific communities, such as petroleum, chemical, civil and environmental engineering, atmospheric research, and hydrology. In the first chapter, we introduce fractals and multifractals from physics and math viewpoints. We then discuss theory and practical applications in detail. In what follows, in chapter 2, fragmentation process is modeled using fractals. Fragmentation is the breaking of aggregates into smaller pieces or fragments, a typical phenomenon in nature. In chapter 3, the advantages and disadvantages of two- and three-phase fractal models are discussed in detail. These two kinds of approach

have been widely applied in the literature to model different characteristics of natural phenomena. In chapter 4, two- and three-phase fractal techniques are used to develop capillary pressure curve models, which characterize pore-size distribution of porous media. Percolation theory provides a theoretical framework to model flow and transport in disordered networks and systems. Therefore, following chapter 4, in chapter 5 the fractal basis of percolation theory and its applications in surface and subsurface hydrology are discussed. In chapter 6, fracture networks are shown to be modeled using fractal approaches. Chapter 7 provides different applications of fractals and multifractals to petrophysics and relevant area in petroleum engineering. In chapter 8, we introduce the practical advantages of fractals and multifractals in geostatistics at large scales, which have broad applications in stochastic hydrology and hydrogeology. Multifractals have been also widely applied to model atmospheric characteristics, such as precipitation, temperature, and cloud shape. In chapter 9, these kinds of properties are addressed using multifractals. At watershed scales, river networks have been shown to follow fractal behavior. Therefore, the applications of fractals are addressed in chapter 10. Time series analysis has been under investigations for several decades in physics, hydrology, atmospheric research, civil engineering, and water resources. In chapter 11, we therefore, provide fractal, multifractal, multifractal detrended fluctuation analyses, which can be used to study temporal characterization of a phenomenon, such as flow discharge at a specific location of a river. Chapter 12 addresses signals and again time series using a novel fractal Fourier analysis. In chapter 13, we discuss constructal theory, which has a perspective opposite to fractal theories, and is based on optimizationof diffusive exchange. In the case of river drainages, for example, the constructal approach begins at the divide and generates headwater streams first, rather than starting from the fundamental drainage pattern.

Computational Quantum Chemistry: Insights into Polymerization Reactions consolidates extensive research results, couples them with computational quantum chemistry (CQC) methods applicable to polymerization reactions, and presents those results systematically. CQC has advanced polymer reaction engineering considerably for the past two decades. The book puts these advances into perspective. It also allows you to access the most up-to--date research and CQC methods applicable to polymerization reactions in a single volume. The content is rigorous yet accessible to graduate students as well as researchers who need a reference of state-of-the-art CQC methods with polymerization applications. Consolidates more than 10 years of theoretical polymerization reaction research currently scattered across journal articles Accessibly presents CQC methods applicable to polymerization reactions Provides researchers with a one-stop source of the latest theoretical developments in polymer reaction engineering

The advent of laser-based sources of ultrafast infrared pulses has extended the study of very fast molecular dynamics to the observation of processes manifested through their effects on the vibrations of molecules. In addition, non-linear infrared spectroscopic techniques make it possible to examine intra- and intermolecular interactions and how such interactions evolve on very fast time scales, but also in some instances on very slow time scales. Ultrafast Infrared Vibrational Spectroscopy is an advanced overview of the field of ultrafast infrared vibrational spectroscopy based on the scientific research of the leading figures in the field. The book discusses experimental and theoretical topics reflecting the latest accomplishments and understanding of ultrafast infrared vibrational spectroscopy. Each chapter provides background, details of methods, and explication of a topic of current research interest. Experimental and theoretical studies cover topics as diverse as the dynamics of water and the dynamics and structure of biological molecules. Methods covered include vibrational echo chemical exchange spectroscopy, IR-Raman spectroscopy, time resolved sum frequency generation, and 2D IR spectroscopy. Edited by a recognized leader in the field and with contributions from top researchers, including experimentalists and theoreticians, this book presents the latest research methods and results. It will serve as an excellent resource for those new to the field, experts in the field, and individuals who want to gain an understanding of particular methods and research topics.

This book provides a broad and nuanced overview of the achievements and legacy of Professor William (“Bill”) Goddard in the field of computational materials and molecular science. Leading researchers from around the globe discuss Goddard’s work and its lasting impacts, which can be seen in today’s cutting-edge chemistry, materials science, and biology techniques. Each section of the book closes with an outline of the prospects for future developments. In the course of a career spanning more than 50 years, Goddard’s seminal work has led to dramatic advances in a diverse range of science and engineering fields. Presenting scientific essays and reflections by students, postdoctoral associates, collaborators and colleagues, the book describes the contributions of one of the world’s greatest materials and molecular scientists in the context of theory, experimentation, and applications, and examines his legacy in each area, from conceptualization (the first mile) to developments and extensions aimed at applications, and lastly to de novo design (the last mile). Goddard’s passion for science, his insights, and his ability to actively engage with his collaborators in bold initiatives is a model for us all. As he enters his second half-century of scientific research and education, this book inspires future generations of students and researchers to employ and extend these powerful techniques and insights to tackle today’s critical problems in biology, chemistry, and materials. Examples highlighted in the book include new materials for photocatalysts to convert water and CO2 into fuels, novel catalysts for the highly selective and active catalysis of alkanes to valuable organics, simulating the chemistry in film growth to develop two-dimensional functional films, and predicting ligand–protein binding and activation to enable the design of targeted drugs with minimal side effects.

Complex systems that bridge the traditional disciplines of physics, chemistry, biology, and materials science can be studied at an unprecedented level of detail using increasingly sophisticated theoretical methodology and high-speed computers. The aim of this book is to prepare burgeoning users and developers to become active participants in this exciting and rapidly advancing research area by uniting for the first time, in one monograph, the basic concepts of equilibrium and time-dependent statistical mechanics with the modern techniques used to solve the complex problems that arise in real-world applications. The book contains a detailed review of classical and quantum mechanics, in-depth discussions of the most commonly used ensembles simultaneously with modern computational techniques such as molecular dynamics and Monte Carlo, and important topics including free-energy calculations, linear-response theory, harmonic baths and the generalized Langevin equation, critical phenomena, and advanced conformational sampling methods. Burgeoning users and developers are thus provided firm grounding to become active participants in this exciting and rapidly advancing research area, while experienced practitioners will find the book to be a useful reference tool for the field.

The third edition of Van Kampen's standard work has been revised and updated. The main difference with the second edition is that the contrived application of the quantum master equation in section 6 of chapter XVII has been replaced with a satisfactory treatment of quantum fluctuations. Apart from that throughout the text corrections have been made and a number of references to later developments have been included. From the recent textbooks the following are the most relevant. C.W.Gardiner, Quantum Optics (Springer, Berlin 1991) D.T. Gillespie, Markov Processes (Academic Press, San Diego 1992) W.T. Coffey, Yu.P.Kalmykov, and J.T.Waldron, The Langevin Equation (2nd edition, World Scientific, 2004) Comprehensive coverage of fluctuations and stochastic methods for describing them A must for students and researchers in applied mathematics, physics and physical chemistry

Annual Reports in Computational Chemistry provides timely and critical reviews of important topics in computational chemistry as applied to all chemical disciplines. Topics covered include quantum chemistry, molecular mechanics, force fields, chemical education, and applications in academic and industrial settings. Focusing on the most recent literature and advances in the field, each article covers a specific topic of importance to computational chemists. Quantum chemistry Molecular mechanics Force fields Chemical education and applications in academic and industrial settings

Nuclear Structure Physics connects to some of our fundamental questions about the creation of the universe and its basic constituents. At the same time, precise knowledge on the subject has led to the development of many important tools for humankind such as proton therapy and radioactive dating, among others. This book has chapters on some of the crucial and trending research topics in nuclear structure, including the nuclei lying on the extremes of spin, isospin and mass. A better theoretical understanding of these topics is important beyond the confines of the nuclear structure community. Additionally, the book will showcase the applicability and success of the different nuclear effective interaction parameters near the drip line, where hints for level reordering have already been seen, and where one can test the isospin-dependence of the interaction. The book offers comprehensive coverage of the most essential topics, including: • Nuclear Structure of Nuclei at or Near Drip-Lines • Synthesis challenges and properties of Superheavy nuclei • Nuclear Structure and Nuclear models - Ab-initio calculations, cluster models, Shell-model/DSM, RMF, Skyrme • Shell Closure, Magicity and other novel features of nuclei at extremes • Structure of Toroidal, Bubble Nuclei, halo and other exotic nuclei These topics are not only very interesting from a theoretical nuclear physics perspective but are also quite complimentary for ongoing nuclear physics experimental programs worldwide. The book chapters, written by experienced and well-known researchers/experts, will be helpful for master students, graduate students and researchers and serve as a standard and up-to-date research reference book on the topics covered.

A book about statistical mechanics for students.

The book is devoted to the study of the correlation effects in many-particle systems. It presents the advanced methods of quantum statistical mechanics (equilibrium and nonequilibrium), and shows their effectiveness and operational ability in applications to problems of quantum solid-state theory, quantum theory of magnetism and the kinetic theory. The book includes description of the fundamental concepts and techniques of analysis following the approach of N N Bogoliubov's school, including recent developments. It provides an overview that introduces the main notions of quantum many--particle physics with the emphasis on concepts and models. This book combines the features of textbook and research monograph. For many topics the aim is to start from the beginning and to guide the reader to the threshold of advanced researches. Many chapters include also additional information and discuss many complex research areas which are not often discussed in other places. The book is useful for established researchers to organize and present the advanced material disseminated in the literature. The book contains also an extensive bibliography. The book serves undergraduate, graduate and postgraduate students, as well as researchers who have had prior experience with the subject matter at a more elementary level or have used other many-particle techniques.

Molecular processes in nature affect human health, the availability of resources and the Earth’s climate. Molecular modelling is a powerful and versatile toolbox that complements experimental data and provides insights where direct observation is not currently possible. Molecular Modeling of Geochemical Reactions: An Introduction applies computational chemistry to geochemical problems. Chapters focus on geochemical applications in aqueous, petroleum, organic, environmental, bio- and isotope geochemistry, covering the fundamental theory, practical guidance on applying techniques, and extensive literature reviews in numerous geochemical sub-disciplines. Topics covered include: • Theory and Methods of Computational Chemistry • Force Field Application and Development • Computational Spectroscopy • Thermodynamics • Structure Determination • Geochemical Kinetics This book will be of interest to graduate students and researchers looking to understand geochemical processes on a molecular level. Novice practitioners of molecular modelling, experienced computational chemists, and experimentalists seeking to understand this field will all find information and knowledge of use in their research.

"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.

Crystallization is one of the most ancient and interdisciplinary topics of research known to mankind. Crystals can be organic or inorganic and may be produced from melts, liquid solutions, vapors or even in solid state. Notwithstanding its inherently high complexity, the crystallization process is part of our everyday lives, from ice making in our homes to the most state-of-the-art chemical and electronic industry. In this book, our purpose was to present new insights to the reader, as well as crucial and very useful information for researchers working in this field, while simultaneously creating a comprehensive text about crystallization processes which may serve as a starting point for people with different backgrounds.

REVIEWS IN COMPUTATIONAL CHEMISTRY THE LATEST VOLUME IN THE REVIEWS IN COMPUTATIONAL CHEMISTRY SERIES, THE INVALUABLE REFERENCE TO METHODS AND TECHNIQUES IN COMPUTATIONAL CHEMISTRY Reviews in Computational Chemistry reference texts assist researchers in se-

lecting and applying new computational chemistry methods to their own research. Bringing together writings from leading experts in various fields of computational chemistry, Volume 32 covers topics including global structure optimization, time-dependent density functional tight binding calculations, non-equilibrium self-assembly, cluster prediction, and molecular simulations of microphase formers and deep eutectic solvents. In keeping with previous books in the series, Volume 32 uses a non-mathematical style and tutorial-based approach that provides students and researchers with easy access to computational methods outside their area of expertise. The chapters comprising Volume 32 are connected by two themes: methods that can be broadly applied to a variety of systems, and special considerations required when modeling specific system types. Each in-depth chapter contains background and theory, strategies for using the methods correctly, mini-tutorials and best practices, and critical literature reviews highlighting advanced applications. Essential reading for both newcomers and experts in the area of molecular modeling, this state-of-the-art resource: Covers topics such as non-deterministic global optimization (NDGO) approaches and excited-state dynamics calculations Contains a detailed overview of deep eutectic solvents (DESs) and simulation methods Presents methodologies for investigating chemical systems that form microphases with periodic morphologies such as lamellae and cylinders Features step-by-step tutorials on applying techniques to probe and understand the chemical dynamics exhibited in a system Includes detailed subject indices on each volume in the series and up-to-date compendiums of molecular modeling software, services, programs, suppliers, and other useful information Reviews in Computational Chemistry, Volume 32 is a must-have guide for computational chemists, theoretical chemists, pharmaceutical chemists, biological chemists, chemical engineers, researchers in academia and industry, and graduate students involved in molecular modeling.

Reflecting the substantially increased interest in tautomerism, this book demonstrates the transformation of fundamental knowledge into novel concepts and the latest applications. Each chapter introduces the theoretical background, before reviewing and critically discussing the experimental techniques and corresponding applications. Special emphasis is placed on tautomerism under unusual conditions, such as in supramolecular solids and at surfaces, displaying the wide scope between basic research and timely applications.

This textbook covers the basic principles of statistical physics and thermodynamics. The text is pitched at the level equivalent to first-year graduate studies or advanced undergraduate studies. It presents the subject in a straightforward and lively manner. After reviewing the basic probability theory of classical thermodynamics, the author addresses the standard topics of statistical physics. The text demonstrates their relevance in other scientific fields using clear and explicit examples. Later chapters introduce phase transitions, critical phenomena and non-equilibrium phenomena.

Four-part treatment covers principles of quantum statistical mechanics, systems composed of independent molecules or other independent subsystems, and systems of interacting molecules, concluding with a consideration of quantum statistics.

CRC Press is pleased to introduce the new edition of Commonly Asked Questions in Thermodynamics, an indispensable resource for those in modern science and engineering disciplines from molecular science, engineering and biotechnology to astrophysics. Fully updated throughout, this edition features two new chapters focused on energy utilization and biological systems. This edition begins by setting out the fundamentals of thermodynamics, including its basic laws and overarching principles. It provides explanations of those principles in an organized manner, using questions that arise frequently from undergraduates in the classroom as the stimulus. These early chapters explore the language of thermodynamics; the first and second laws; statistical mechanical theory; measurement of thermodynamic quantities and their relationships; phase behavior in single and multicomponent systems; electrochemistry; and chemical and biochemical reaction equilibria. The later chapters explore applications of these fundamentals to a diverse set of subjects including power generation (with and without fossil fuels) for transport, industrial and domestic use; heating; decarbonization technologies; energy storage; refrigeration; environmental pollution; and biotechnology. Data sources for the properties needed to complete thermodynamic evaluations of many processes are included. The text is designed for readers to dip into to find an answer to a specific question where thermodynamics can provide some, if not all, of the answers, whether in the context of an undergraduate course or not. Thus its readership extends beyond conventional technical undergraduates to practicing engineers and also to the interested lay person who seeks to understand the discourse that surrounds the choice of particular technological solutions to current and future energy and material production problems.

Intended for upper-level undergraduate and graduate courses in chemistry, physics, mathematics and engineering, this text is also suitable as a reference for advanced students in the physical sciences. Detailed problems and worked examples are included.

Emphasizes a molecular approach to physical chemistry, discussing principles of quantum mechanics first and then using those ideas in development of thermodynamics and kinetics. Chapters on quantum subjects are interspersed with ten math chapters reviewing mathematical topics used in subsequent chapters. Includes material on current physical chemical research, with chapters on computational quantum chemistry, group theory, NMR spectroscopy, and lasers. Units and symbols used in the text follow IUPAC recommendations. Includes exercises. Annotation copyrighted by Book News, Inc., Portland, OR

Statistical Mechanics discusses the fundamental concepts involved in understanding the physical properties of matter in bulk on the basis of the dynamical behavior of its microscopic constituents. The book emphasizes the equilibrium states of physical systems. The text first details the statistical basis of thermodynamics, and then proceeds to discussing the elements of ensemble theory. The next two chapters cover the canonical and grand canonical ensemble. Chapter 5 deals with the formulation of quantum statistics, while Chapter 6 talks about the theory of simple gases. Chapters 7 and 8 examine the ideal Bose and Fermi systems. In the next three chapters, the book covers the statistical mechanics of interacting systems, which includes the method of cluster expansions, pseudopotentials, and quantized fields. Chapter 12 discusses the theory of phase transitions, while Chapter 13 discusses fluctuations. The book will be of great use to researchers and practitioners from wide array of disciplines, such as physics, chemistry, and engineering.

Statistical mechanics is one of the most exciting areas of physics today, and it also has applications to subjects as diverse as economics, social behavior, algorithmic theory, and evolutionary biology. Statistical Mechanics in a Nutshell offers the most concise, self-contained introduction to this rapidly developing field. Requiring only a background in elementary calculus and elementary mechanics, this book starts with the basics, introduces the most important developments in classical statistical mechanics over the last thirty years, and guides readers to the very threshold of today's cutting-edge research. Statistical Mechanics in a Nutshell zeroes in on the most relevant and promising advances in the field, including the theory of phase transitions, generalized Brownian motion and stochastic dynamics, the methods underlying Monte Carlo simulations, complex systems--and much, much more. The essential resource on the subject, this book is the most up-to-date and accessible introduction available for graduate students and advanced undergraduates seeking a succinct primer on the core ideas of statistical mechanics. Provides the most concise, self-contained introduction to statistical mechanics Focuses on the most promising advances, not complicated calculations Requires only elementary calculus and elementary mechanics Guides readers from the basics to the threshold of modern research Highlights the broad scope of applications of statistical mechanics