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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

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. Volume 5. Lectures on elementary statistical mechanics, taught at

the University of Illinois and at the University of Pennsylvania. *Molecular Driving Forces, Second Edition E-book* is an introductory statistical thermodynamics text that describes the principles and forces that drive chemical and biological processes. It demonstrates how the complex behaviors of molecules can result from a few simple physical processes, and how simple models provide surprisingly accurate insights into the workings of the molecular world. Widely adopted in its First Edition, *Molecular Driving Forces* is regarded by teachers and students as an accessible textbook that illuminates underlying principles and concepts. The Second Edition includes two brand new chapters: (1) "Microscopic Dynamics" introduces single molecule experiments; and (2) "Molecular Machines" considers how nanoscale machines and engines work. "The Logic of Thermodynamics" has been expanded to its own chapter and now covers heat, work, processes, pathways, and cycles. New practical applications, examples, and end-of-chapter questions are integrated throughout the revised and updated text, exploring topics in biology, environmental and energy science, and nanotechnology. Written in a

clear and reader-friendly style, the book provides an excellent introduction to the subject for novices while remaining a valuable resource for experts. - Gives unified presentation of many of the major principles in nanotechnology: molecular-based study of condensed matter in small systems. - Authored by an expert in the molecular-based study of matter - Accessible to students, yet of interest to experts - Emphasizes the intrinsic beauty of methods of bottom-up nanotechnology - Includes many full-color figures Classic text combines thermodynamics, statistical mechanics, and kinetic theory in one unified presentation. Topics include equilibrium statistics of special systems, kinetic theory, transport coefficients, and fluctuations. Problems with solutions. 1966 edition. "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 groundbreaking 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. Con esta obra se pretenden unificar los fundamentos, métodos y técnicas de la química teórica y computacional. Además, cabe comentar que la presente edición no sólo va dirigida a estudiantes de doctorado (a fin de proporcionarles un nivel

adecuado para sus estudios), sino que la materia se trata de manera suficientemente detallada para que lectores no tan expertos puedan acceder a ella sin ninguna dificultad. 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. 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 a renowned and accessible introduction to the subject, containing a large number of chapter-ending problems for students. 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 This is a textbook for the standard undergraduate-level course in thermal physics. The book explores applications to engineering, chemistry, biology, geology, atmospheric science, astrophysics, cosmology, and everyday life. The first reference of its kind in the rapidly emerging field of computational approaches to materials research, this is a compendium of perspective-providing and topical articles written to inform students and non-specialists of the current status and capabilities of modelling and simulation. From the standpoint of methodology, the development follows a multiscale approach with emphasis on electronic-structure, atomistic, and mesoscale methods, as well as mathematical analysis and rate processes. Basic models are treated across traditional disciplines, not only in the discussion of methods but also in chapters on crystal defects, microstructure, fluids, polymers and soft matter. Written by authors who are actively participating in the current development, this collection of 150 articles has the breadth and depth to be a major contributor toward defining the field of computational materials. In addition, there are 40

commentaries by highly respected researchers, presenting various views that should interest the future generations of the community. Subject Editors: Martin Bazant, MIT; Bruce Boghosian, Tufts University; Richard Catlow, Royal Institution; Long-Qing Chen, Pennsylvania State University; William Curtin, Brown University; Tomas Diaz de la Rubia, Lawrence Livermore National Laboratory; Nicolas Hadjiconstantinou, MIT; Mark F. Horstemeyer, Mississippi State University; Efthimios Kaxiras, Harvard University; L. Mahadevan, Harvard University; Dimitrios Maroudas, University of Massachusetts; Nicola Marzari, MIT; Horia Metiu, University of California Santa Barbara; Gregory C. Rutledge, MIT; David J. Srolovitz, Princeton University; Bernhardt L. Trout, MIT; Dieter Wolf, Argonne National Laboratory. Statistical physics has its origins in attempts to describe the thermal properties of matter in terms of its constituent particles, and has played a fundamental role in the development of quantum mechanics. Based on lectures taught by Professor Kardar at MIT, this textbook introduces the central concepts and tools of statistical physics. It contains a chapter on probability and related issues

such as the central limit theorem and information theory, and covers interacting particles, with an extensive description of the van der Waals equation and its derivation by mean field approximation. It also contains an integrated set of problems, with solutions to selected problems at the end of the book and a complete set of solutions is available to lecturers on a password protected website at www.cambridge.org/9780521873420. A companion volume, *Statistical Physics of Fields*, discusses non-mean field aspects of scaling and critical phenomena, through the perspective of renormalization group. Thermodynamics is one of the most exciting branches of physical chemistry which has greatly contributed to the modern science. Being concentrated on a wide range of applications of thermodynamics, this book gathers a series of contributions by the finest scientists in the world, gathered in an orderly manner. It can be used in post-graduate courses for students and as a reference book, as it is written in a language pleasing to the reader. It can also serve as a reference material for researchers to whom the thermodynamics is one of the area of interest. 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. This self-contained primer covers statistical thermodynamics in a rigorous yet approachable manner, making it the perfect text for undergraduates. This book is the distilled essence of the author teaching

statistical mechanics to juniors, seniors and graduate students for over 50 years in various course settings. It uses a unique approach that leads naturally into the development of all possible ensembles. Much of the later chapters on polymers has previously been available only in the literature. Throughout the book, the assumption is made that the reader is still relatively raw, and mathematical detail is provided that other books leave to the abilities of the reader. While this produces a plethora of equations that mature scientists would regard as unnecessary, it is intended to help those just coming into the field and who want to get the idea without suffering hours of agony wondering, "where did that come from?". Request Inspection Copy This text aims to help students understand energy, its different forms and transformations, and the key role of entropy, as applied to chemical systems. "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. This textbook is for graduate students and young scientists, who are looking for an introduction to the physics and physical chemistry of crystal growth and nucleation phenomena. 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 is a presentation of the main ideas and methods of modern nonequilibrium statistical mechanics. It is the perfect introduction for anyone in chemistry or physics who needs an update or background in this time-dependent field. Topics covered include fluctuation-dissipation theorem; linear response theory; time correlation functions, and projection

operators. Theoretical models are illustrated by real-world examples and numerous applications such as chemical reaction rates and spectral line shapes are covered. The mathematical treatments are detailed and easily understandable and the appendices include useful mathematical methods like the Laplace transforms, Gaussian random variables and phenomenological transport equations. This widely acclaimed text, now in its sixth edition and translated into many languages, continues to present a clear, simple and concise introduction to chemical thermodynamics. An examination of equilibrium in the everyday world of mechanical objects provides a starting point for an accessible account of the factors that determine equilibrium in chemical systems. This straightforward approach leads students to a thorough understanding of the basic principles of thermodynamics, which are then applied to a wide range of physical chemical systems. The book also discusses the problems of non-ideal solutions and the concept of activity, and provides an introduction to the molecular basis of thermodynamics. Over six editions, the views of teachers of the subject and their

students have been incorporated. Reference to the phase rule has been included in this edition and the notation has been revised to conform to current IUPAC recommendations. Students taking courses in thermodynamics will continue to find this popular book an excellent introductory text. 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. For many processes and applications in science and technology a basic knowledge of liquids and solutions is a must. Gaining a better understanding of the behavior and properties of pure liquids and solutions will help to improve many processes and to advance research in many different areas. This book provides a comprehensive, self-contained and integrated survey of this topic and is a must-have for many chemists, chemical engineers and material scientists, ranging from newcomers in the field to more experienced researchers. The author offers a clear, well-structured didactic approach and provides an overview of the most important types of liquids and solutions. Special topics

include chemical reactions, surfaces and phase transitions. Suitable both for introductory as well as intermediate level as more advanced parts are clearly marked. Includes also problems and solutions.

Publisher Description This textbook concerns thermal properties of bulk matter and is aimed at advanced undergraduate or first-year graduate students in a range of programs in science or engineering. It provides an intermediate level presentation of statistical thermodynamics for students in the physical sciences (chemistry, nanosciences, physics) or related areas of applied science/engineering (chemical engineering, materials science, nanotechnology engineering), as they are areas in which statistical mechanical concepts play important roles. The book enables students to utilize microscopic concepts to achieve a better understanding of macroscopic phenomena and to be able to apply these concepts to the types of sub-macroscopic systems encountered in areas of nanoscience and nanotechnology. In this clear and concise introduction to thermodynamics and statistical mechanics the reader, who will have some previous exposure to thermodynamics, will be guided through

each of the twodisciplines separately initially to provide an in-depthunderstanding of the area and thereafter the connection between thetwo is presented and discussed. In addition, mathematical techniques are introduced at appropriatetimes, highlighting such use as: exact and inexact differentials, partial derivatives, Caratheodory's theorem, Legendretransformation, and combinatory analysis. * Emphasis is placed equally on fundamentals and applications * Several problems are included

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