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This book gives a
comprehensive and up-to-

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date treatment of the theory of "simple" liquids. The new second edition has been rearranged and considerably expanded to give a balanced account both of basic theory and of the advances of the

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past decade. It presents the main ideas of modern liquid state theory in a way that is both pedagogical and self-contained. The book should be accessible to graduate students and research

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workers, both experimentalists and theorists, who have a good background in elementary mechanics. Compares theoretical deductions with experimental results

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Molecular dynamics Monte Carlo computations Covers ionic, metallic, and molecular liquids

Four-part treatment covers principles of quantum statistical mechanics,

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systems composed of independent molecules or other independent subsystems, and systems of interacting molecules, concluding with a consideration of quantum

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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

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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

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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

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most commonly used ensembles simultaneously with modern computational techniques such as molecular dynamics and Monte Carlo, and important topics including free-energy

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calculations, linear-response theory, harmonic baths and the generalized Langevin equation, critical phenomena, and advanced conformational sampling methods. Burgeoning users

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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

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book to be a useful reference
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describes the use of fast
computers to simulate the
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nonequilibrium properties of gases, liquids, and solids at, and away from equilibrium. The underlying theory is developed from basic principles and illustrated by applying it to the simplest

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possible

examples. Thermodynamics, based on the ideal gas thermometer, is related to Gibb's statistical mechanics through the use of Nose-Hoover heat reservoirs.

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These reservoirs use integral feedback to control temperature. The same approach is carried through to the simulation and analysis of nonequilibrium mass, momentum, and

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energy flows. Such a unified approach makes possible consistent mechanical definitions of temperature, stress, and heat flux which lead to a microscopic demonstration of the Second

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Law of Thermodynamics
directly from mechanics. The
intimate connection linking
Lyapunov-unstable
microscopic motions to
macroscopic"

Lagrangian and Hamiltonian

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The Theory of Polymer
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A Comprehensive Guide

Molecular Thermodynamics

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of Fluid-Phase Equilibria

This book provides a comprehensive account of the modern theory for the dynamical properties of polymer solutions.

The theory has undergone

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dramatic evolution over the last two decades due to the introduction of new methods and concepts that have extended the frontier of theory from dilute solutions in

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which polymers move independently to concentrated solutions where many polymers converge. Among the properties examined are viscoelasticity,

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diffusion, dynamic light scattering, and electric birefringence. Nonlinear viscoelasticity is discussed in detail on the basis of molecular dynamical models. The

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book bridges the gap between classical theory and new developments, creating a consistent picture of polymer solution dynamics over the entire concentration

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range.

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studies on how to answer
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modeling a compositional
gradient subject.

Starting with the basics
on PVT analysis, applied
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derivations of
irreversible

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thermodynamic-based equations, this critical reference explains gravity-modified equations to be applied to reservoirs, enabling engineers to obtain

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fluid composition at any point of the reservoir from measured data to create a stronger model calibration. Once model-parameters are re-estimated, new

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sensibility can be acquired for more accurate modeling of composition, aiding engineers with stronger production curves, reserve estimations, and

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design of future
development strategies.
Multiple examples and
case studies are
included to show the
application of the
theory from very simple

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to more complex systems, such as actual reservoirs influenced by thermal diffusion and gravity simultaneously. Other example include a layer for which

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asphaltene precipitation
takes place in the
reservoir and three
-phase flash algorithms
for liquid-liquid-vapor
equilibrium
calculations, detailing

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the techniques necessary to ensure convergence. The book combines practical studies with the importance in modeling more complex phenomena, filling a gap

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for current and upcoming reservoir engineers to expand on solutions and make sense of their reservoir's output results. Presents a deeper level of detail

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on the heterogeneity
composition and thermo-
physical properties of
petroleum fluids in the
reservoir Includes
tactics on how to
Increase reliability of

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reservoir simulation
initialization, with
practice examples at the
end of each chapter
Helps readers make sense
of compositional
grading, with coverage

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on both theory and application that fulfill a gap in research on reservoir simulation This 2006 textbook discusses the fundamentals and

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applications of
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thermodynamics for
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sciences. Building on

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the prototypical
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and maintaining a step-
by-step development of
the subject, this book
assumes the reader has
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statistics, quantum
mechanics or
spectroscopy. The book
begins with the
essentials of
statistical
thermodynamics, pauses

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to recover needed
knowledge from quantum
mechanics and
spectroscopy, and then
moves on to applications
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highlight of the textbook is its discussion of modern applications, such as laser-based diagnostics. The book concludes with a thorough presentation

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the 'special functions'
of physical science,
cover an extended range
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matter based on physics, particularly on statistical physics. Typical statistical physics courses cover ideal gases (classical and quantum) and interacting units of simple structures. In contrast, even simple biological fluids are solutions of macromolecules, the

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structures of which are very complex. The goal of this book to fill this wide gap by providing appropriate content as well as by explaining the theoretical method that typifies good modeling, namely, the method of coarse-grained descriptions that extract the most

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salient features emerging at mesoscopic scales. The major topics covered in this book include thermodynamics, equilibrium statistical mechanics, soft matter physics of polymers and membranes, non-equilibrium statistical physics covering stochastic processes,

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transport phenomena and hydrodynamics. Generic methods and theories are described with detailed derivations, followed by applications and examples in biology. The book aims to help the readers build, systematically and coherently through

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and statistical mechanics the reader, who will have some previous exposure to thermodynamics, will be guided through each of the two disciplines separately initially to provide an in-

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depth understanding of the area and thereafter the connection between the two is presented and discussed. In addition, mathematical techniques are introduced at appropriate times, highlighting such use as: exact

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and inexact differentials, partial derivatives, Caratheodory's theorem,

Legendre transformation, and combinatorial analysis. *

Emphasis is placed equally on fundamentals and applications *

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Several problems are included
This introductory textbook for
standard undergraduate courses
in thermodynamics has been
completely rewritten to explore a
greater number of topics, more
clearly and concisely. Starting

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with an overview of important quantum behaviours, the book teaches students how to calculate probabilities in order to provide a firm foundation for later chapters. It introduces the ideas of classical

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some unusual topics for a classical mechanics textbook. Most notable examples include the 'classical wavefunction', Koopman-von Neumann theory, classical density functional theories, the 'vakonomic' variational principle for non-

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holonomic constraints, the Gibbs-Appell equations, classical path integrals, Nambu brackets and the full framing of mechanics in the language of differential geometry. This book consists of a number of papers regarding the

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thermodynamics and structure of multicomponent systems that we have published during the last decade. Even though they involve different topics and different systems, they have something in common which can be considered as

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the "signature" of the present book. First, these papers are concerned with "difficult" or very nonideal systems, i. e. systems with very strong interactions (e. g. , hydrogen bonding) between components or systems with large differences in the

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partial molar volumes of the components (e. g. , the aqueous solutions of proteins), or systems that are far from "normal" conditions (e. g. , critical or near-critical mixtures). Second, the conventional thermodynamic methods are not

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sufficient for the accurate treatment of these mixtures. Last but not least, these systems are of interest for the pharmaceutical, biomedical, and related industries. In order to meet the thermodynamic challenges involved in these complex mixtures,

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we employed a variety of traditional methods but also new methods, such as the fluctuation theory of Kirkwood and Buff and ab initio quantum mechanical techniques. The Kirkwood-Buff (KB) theory is a rigorous formalism which is free of

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any of the - proximations usually used in the thermodynamic treatment of multicomponent systems. This theory appears to be very fruitful when applied to the above mentioned "difficult" systems. This revised and expanded edition of

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eclipsing macroscopic thermodynamics, and is integrated into the conceptual framework of physical theory.

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theory. Using the potential distribution theorem (PDT) as the basis, the text provides a discussion of practical theories in conjunction with simulation results. The authors discuss the field in a

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illustrating the text with useful
models of solution
thermodynamics and
numerous exercises. Modern
quasi-chemical theories that
permit statistical

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thermodynamic properties to be studied on the basis of electronic structure calculations are given extended development, as is the testing of those theoretical results with ab initio molecular

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dynamics simulations. The book is intended for students taking up research problems of molecular science in chemistry, chemical engineering, biochemistry, pharmaceutical chemistry,

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and solutions. It is based on the theory of Kirkwood and Buff which was published more than fifty years ago. This theory has been dormant for almost two decades. It has recently become a very

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powerful and general tool to analyze, study and understand any type of mixtures from the molecular, or the microscopic point of view. The traditional approach to mixture has been, for many years, based on the

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study of excess
thermodynamic quantities.
This provides a kind of global
information on the system.
The new approach provides
information on the local
properties of the same system.

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Thus, the new approach supplements and enriches our information on mixtures and solutions.

Physical Chemistry: A

Molecular Approach

Theory of Molecular Fluids

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Statistical Physics

Equilibrium Statistical Physics

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Textbook on modern theoretical chemistry suitable for advanced undergraduate or graduate students. Existing texts on the statistical mechanics of liquids treat only spherical molecules. However, nearly all fluids of practical interest are composed of non-spherical molecules

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that are often dipolar or exhibit other kinds of electrostatic forces. This book describes the statistical mechanical theory of fluids of non-spherical molecules and its application to the calculation of physical properties, and is a sequel to Theory of Molecular Fluids. Volume 1: Fundamentals by

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C.G. Gray and K.E. Gubbins. The emphasis is on the new phenomena that arise due to the non-spherical nature of the intermolecular forces, such as new phase transitions, structural features and dielectric effects. It contains chapters on the thermodynamic properties of pure and

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mixed fluids, surface properties, X-ray and neutron diffraction structure factors, dielectric properties and spectroscopic properties. The book is aimed at beginning graduate students and research workers in chemistry, physics, materials science and engineering.

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"There is a symbiotic relationship between theoretical nonequilibrium statistical mechanics on the one hand and the theory and practice of computer simulation on the other. Sometimes, the initiative for progress has been with the pragmatic requirements of computer simulation

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and at other times, the initiative has been with the fundamental theory of nonequilibrium processes. This book summarises progress in this field up to 1990"--Publisher's description.

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phases of matter and to the phase transitions between them. Throughout, only simple models of both ordinary and soft matter are used but these are studied in full detail. The subject is developed in a pedagogical manner, starting from the basics, going from the simple ideal systems to the

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interacting systems, and ending with the more modern topics. The textbook provides the student with a complete overview, intentionally at an introductory level, of the theory of phase transitions. All equations and deductions are included.

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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

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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

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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

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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

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