

Chemical Engineering Thermodynamics By Gopinath Halder

This comprehensive volume brings together an extensive collection of systematic computer-aided tools and methods developed in recent years for CO2 capture applications, and presents a structured and organized account of works from internationally acknowledged scientists and engineers, through: Modeling of materials and processes based on chemical and physical principles Design of materials and processes based on systematic optimization methods Utilization of advanced control and integration methods in process and plant-wide operations The tools and methods described are illustrated through case studies on materials such as solvents, adsorbents, and membranes, and on processes such as absorption / desorption, pressure and vacuum swing adsorption, membranes, oxycombustion, solid looping, etc. Process Systems and Materials for CO2 Capture: Modelling, Design, Control and Integration should become the essential introductory resource for researchers and industrial practitioners in the field of CO2 capture technology who wish to explore developments in computer-aided tools and methods. In addition, it aims to introduce CO2 capture technologies to process systems engineers working in the development of general computational tools and methods by highlighting opportunities for new developments to address the needs and challenges in CO2 capture technologies.

Organic and nanoscale materials and organic molecules are building blocks of nanodevices, whether they are designed to perform molecular level computing, sense the environment or improve the catalytic properties of a material. The key to creation of these hybrid nanostructures lies in understanding the chemistry at a fundamental level. This book serves as a reference book for researchers by providing fundamental understanding of many nanoscopic materials.

Nano-biotechnology crosses the boundaries between physics, biochemistry and bioengineering, and has profound implications for the biomedical engineering industry. This book describes the quantum chemical simulation of a wide variety of molecular systems, with detailed analysis of their quantum chemical properties, individual molecular configurations, and cutting-edge biomedical applications. Topics covered include the basic properties of quantum chemistry and its conceptual foundations, the nanoelectronics and thermodynamics of DNA, the optoelectronic properties of the five DNA/RNA nucleobase anhydrous crystals, and key examples of molecular diode prototypes. A wide range of important applications are described, including protein binding of drugs such as cholesterol-lowering, anti-Parkinson and anti-migraine drugs, and recent developments in cancer biology are also discussed. This modern and comprehensive text is essential reading for graduate students and researchers in multidisciplinary areas of biological physics, chemical physics, chemical engineering, biochemistry and bioengineering.

This textbook is designed for undergraduate courses in chemical engineering and related disciplines such as biotechnology, polymer technology, petrochemical engineering, electrochemical engineering, environmental engineering, safety engineering and industrial chemistry. The chief objective of this text is to prepare students to make analysis of chemical processes through calculations and also to develop in them systematic problem-solving skills. The students are introduced not only to the application of law of combining proportions to chemical reactions (as the word 'stoichiometry' implies) but also to formulating and solving material and energy balances in processes with and without chemical reactions. The book presents the fundamentals of chemical engineering operations and processes in an accessible style to help the students gain a thorough understanding of chemical process calculations. It also covers in detail the background materials such as units and conversions, dimensional analysis and dimensionless groups, property estimation, P-V-T behaviour of fluids, vapour pressure and phase equilibrium relationships, humidity and saturation. With the help of examples, the book explains the construction and use of reference-substance plots, equilibrium diagrams, psychrometric charts, steam tables and enthalpy composition diagrams. It also elaborates on thermophysics and thermochemistry to acquaint the students with the thermodynamic principles of energy balance calculations. Key Features : • SI units are used throughout the book. • Presents a thorough introduction to basic chemical engineering principles. • Provides many worked-out examples and exercise problems with answers. • Objective type questions included at the end of the book serve as useful review material and also assist the students in preparing for competitive examinations such as GATE.

Engineering Thermodynamics, Heat Transfer and Fluid Flow in Natural and Industrial Processes

Synthesis, Characteristics and Applications

Fundamental and Advanced Topics

From Molecule to Enterprise

New Technologies, Challenges and Opportunities

A TEXTBOOK OF CHEMICAL ENGINEERING THERMODYNAMICS

This second volume of the Metabolic Pathway Engineering Handbook delves into evolutionary tools and gene expression tools for metabolic pathway engineering. It covers applications of emerging technologies including recent research genome-wide technologies, DNA and phenotypic microarrays, and proteomics tools for experimentally determining flux through pathways. This volume also looks at emerging applications for producing fine chemicals, drugs, and alternative fuels. Christine Smolke, who recently developed a novel way to churn out large quantities of drugs from genetically modified brewer's yeast, is regarded as one of the most brilliant new minds in biomedical engineering. In this handbook, she brings together pioneering scientists from dozens of disciplines to provide a complete record of accomplishment in metabolic pathway engineering. With a wealth of cutting edge research and analysis, this work also serves as an invaluable resource for those seeking to add their own contributions. Organized by topic, this 3000 page reference is available as two volumes that can be purchased individually or as a set.

During last couple of years there has been an increasing recognition that problems arising in biology or related to medicine really need a multidisciplinary approach. For this reason some special branches of both applied theoretical physics and mathematics have recently emerged such as biomechanics, mechanobiology, mathematical biology, biothermodynamics. This first section of the book, General notes on biomechanics and mechanobiology, comprises from theoretical contributions to Biomechanics often providing hypothesis or rationale for a given phenomenon that experiment or clinical study cannot provide. It deals with mechanical properties of living cells and tissues, mechanobiology of fracture healing or evolution of locomotor trends in extinct terrestrial giants. The second section, Biomechanical modelling, is devoted to the rapidly growing field of biomechanical models and modelling approaches to improve our understanding about processes in human body. The last section called locomotion and joint biomechanics is a collection of works on description and analysis of human locomotion, joint stability and acting forces.

Advances in Feedstock Conversion Technologies for Alternative Fuels and Bioproducts: New Technologies, Challenges and Opportunities highlights the novel applications of, and new methodologies for, the advancement of biological, biochemical, thermochemical and chemical conversion systems that are required for biofuels production. The book addresses the environmental impact of value added bio-products and agricultural modernization, along with the risk assessment of industrial scaling. The book also stresses the urgency in finding creative, efficient and sustainable solutions for environmentally conscious biofuels, while underlining pertinent technical, environmental, economic, regulatory and social issues. Users will find a basis for technology assessments, current research capability, progress, and advances, as well as the challenges associated with biofuels at an industrial scale, with insights towards forthcoming developments in the industry. Presents a thorough overview of new discoveries in biofuels research and the inherent challenges associated with scale-up highlights the novel applications and advancements for biological, biochemical, thermochemical and chemical conversion systems that are required for biofuels production Evaluates risk management concerns, addressing the environmental impact of value added bio-products and agricultural modernization, and the risk assessment of industrial scaling

Introduction to CHEMICAL ENGINEERING THERMODYNAMICSPH Learning Pvt. Ltd.

The Basics, With Examples

Basic Theory with Engineering Applications

The Soft-Hard Tissue Junction

The Metabolic Pathway Engineering Handbook

Fluid Mechanics and Convective Transport Processes

Volume 6: Molecular Systems Engineering

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.

This textbook comprehensively covers the fundamentals and advanced concepts of thermodynamics in a single volume. It provides a detailed discussion of advanced concepts that include energy efficiency, energy sustainability, energy security, organic Rankine cycle, combined cycle power plants, combined cycle power plant integrated with organic Rankine cycle and absorption refrigeration system, integrated coal gasification combined cycle power plants, energy conservation in domestic refrigerators, and next-generation low-global warming potential refrigerants. Pedagogical features include solved problems and unsolved exercises interspersed throughout the text for better understanding. This textbook is primarily written for senior undergraduate students in the fields of mechanical, automobile, chemical, civil, and aerospace engineering for courses on engineering thermodynamics/thermodynamics and for graduate students in thermal engineering and energy engineering for courses on advanced thermodynamics. It is accompanied by teaching resources, including a solutions manual for instructors. FEATURES Provides design and experimental problems for better understanding Comprehensively discusses power cycles and refrigeration cycles and their advancements Explores the design of energy-efficient buildings to reduce energy consumption Property tables, charts, and multiple-choice questions comprise appendices of the book and are available at https://www.routledge.com/9780367646288.

Inspired by the leading authority in the field, the Centre for Process Systems Engineering at Imperial College London, this book includes theoretical developments, algorithms, methodologies and tools in process systems engineering and applications from the chemical, energy, molecular, biomedical and other areas. It spans a whole range of length scales seen in manufacturing industries,

from molecular and nanoscale phenomena to enterprise-wide optimization and control. As such, this will appeal to a broad readership, since the topic applies not only to all technical processes but also due to the interdisciplinary expertise required to solve the challenge. The ultimate reference for years to come.

An internationally acclaimed reference work recognized as one of the most authoritative and comprehensive sources of information on excipients used in pharmaceutical formulation with this new edition providing 340 excipient monographs. Incorporates information on the uses, and chemical and physical properties of excipients systematically collated from a variety of international sources including: pharmacopaeias, patents, primary and secondary literature, websites, and manufacturers' data; extensive data provided on the applications, licensing, and safety of excipients; comprehensively cross-referenced and indexed, with many additional excipients described as related substances and an international supplier's directory and detailed information on trade names and specific grades or types of excipients commercially available.

STOICHIOMETRY AND PROCESS CALCULATIONS

Structure, Mechanics and Function

Unit Operations of Chemical Engineering

Process Planning and Cost Estimation

Nanoscale Materials

Product-driven process design - from molecule to enterprise provides process engineers and process engineering students with access to a modern and stimulating methodology to process and product design. Throughout the book the links between product design and process design become evident while the reader is guided step-by-step through the different stages of the intertwining product and process design activities. Both molecular and enterprise-wide considerations in design are introduced and addressed in detail. Several examples and case studies in emerging areas such as bio- and food-systems, pharmaceuticals and energy are discussed and presented. This book is an excellent guide and companion for undergraduate, graduate students as well as professional practitioners.

The fundamental aspects of classical thermodynamics are presented in a simple compact way. The equations derived are illustrated by numerous (111) examples, often direct application of the relations just obtained. The (four) laws of thermodynamics are presented and illustrated. The need to define thermodynamic temperature, the meaning of auxiliary thermodynamic functions, the origin, usefulness and use of partial molar quantities are all examined. Gaseous systems, phase equilibria and chemical reactions are quantitatively treated. It is shown how chemical reactions can provide work. Ideal and non ideal solutions are presented with the various standard states and activity coefficients. This book will be of use to a wide audience of students and professionals in the fields of Chemistry, Chemical Engineering, Materials Science and Bio related Sciences. REVIEW Dr. Infelta has prepared a compact Introductory Thermodynamics book which will serve well for mature students who need a command of the important field. Undergraduate students will find the presentation logical, the examples thoughtful, and the coverage thorough. Students and professionals for whom memory or mastery of previous thermodynamics courses have dimmed, will find, in addition to the above virtues, careful derivation of the properties of non-ideal systems and emphasis on when to use these results instead of ideal system results. treatment of multireaction equilibria, and (a personal favorite) a succinct elucidation of that odd proposition of thermodynamics, Le Châtelier's Principle. These students will value this small volume packed with the power of classical thermodynamics. Lynn Melton, Professor of Chemistry, University of Texas, Dallas.

Air and water pollution occurs when toxic pollutants of varying kinds (organic, inorganic, radioactive and so on) are directly or indirectly discharged into the environment without adequate treatment to remove these potential pollutants. There are a total of 13 book chapters in three sections contributed by significant number of expert authors around the world, aiming to provide scientific knowledge and up-to-date development of various solid wastes based cost-effective adsorbent materials and its sustainable application in the removal of contaminants/pollutants from air, gas and water. This book is useful for the professions, practicing engineers, scientists, researchers, academics and undergraduate and post-graduate students' interest on this specific area. ? Key Features: [] Exclusive compilation of information on use of industrial and agricultural waste based adsorbents for air and water pollution abatement. [] Explores utilization of industrial solid wastes in adsorptive purification and agricultural and agricultural by-products in separation and purification. [] Discusses cost-effective solid wastes based emerging adsorbents. [] Alternative adsorbents in the removal of a wide range of contaminants and pollutants from water is proposed. [] Includes performance of unit operations in waste effluents treatment.

New York Times Bestseller Discover the critical link between your brain and the food you eat and change the way your brain ages. In this cutting-edge, practical guide to eliminating brain fog, optimizing brain health, and achieving peak mental performance from media personality and leading voice in health Max Lugavere. After his mother was diagnosed with a mysterious form of dementia, Max Lugavere put his successful media career on hold to learn everything he could about brain health and performance. For the better half of a decade, he consumed the most up-to-date scientific research, talked to dozens of leading scientists and clinicians around the world, and visited the country's best neurology departments—all in the hopes of understanding his mother's condition. Now, in Genius Foods, Lugavere presents a comprehensive guide to brain optimization. He uncovers the stunning link between our dietary and lifestyle choices and our brain functions, revealing how the foods you eat directly affect your ability to focus, learn, remember, create, analyze new ideas, and maintain a balanced mood. Weaving together pioneering research on dementia prevention, cognitive optimization, and nutritional psychiatry, Lugavere distills groundbreaking science into actionable lifestyle changes. He shares invaluable insights into how to improve your brain power, including the nutrients that can boost your memory and improve mental clarity (and where to find them); the foods and tactics that can energize and rejuvenate your brain, no matter your age; a brain-boosting fat-loss method so powerful it has been called "biochemical liposuction"; and the foods that can improve your happiness, both now and for the long term. With Genius Foods, Lugavere offers a cutting-edge yet practical road map to eliminating brain fog and optimizing the brain's health and performance today—and decades into the future.

Classical and Quantum Dynamics in Condensed Phase Simulations

Indian National Bibliography

Theoretical Biomechanics

Theory and Practice

PRINCIPLES OF MASS TRANSFER AND SEPERATION PROCESSES

Computer Aided Molecular Design

A succinct introduction to the field of biomaterials engineering, packed with practical insights.

Biosensors have been employed for numerous applications from medical diagnosis, environmental monitoring, pharmaceutical engineering, and security purposes. Their development encompasses chemistry, physics, materials science, nanotechnology, and engineering. Being at the intersection of these multiple disciplines, this book is suitable for academic, clinical, and commercial researchers, as well as graduate students. This book reviews the latest studies and developments in the use of a range of biosensor platforms for the analysis of viral infections. This Book Presents A Systematic Account Of The Concepts And Principles Of Engineering Thermodynamics And The Concepts And Practices Of Thermal Engineering. The Book Covers Basic Course Of Engineering Thermodynamics And Also Deals With The Advanced Course Of Thermal Engineering. This Book Will Meet The Requirements Of The Undergraduate Students Of Engineering And Technology Undertaking The Compulsory Course Of Engineering Thermodynamics. The Subject Matter Of Book Is Sufficient For The Students Of Mechanical Engineering/Industrial-Production Engineering/Thermodynamic Engineering/Heat Engineering/Applied Thermodynamics Etc. Presentation Of The Subject Matter Has Been Made In Very Simple And Understandable Language. The Book Is Written In SI System Of Units And Each Chapter Has Been Provided With Sufficient Number Of Typical Numerical Problems Of Solved And Unsolved Questions With Answers.

This textbook is targeted to undergraduate students in chemical engineering, chemical technology, and biochemical engineering for courses in mass transfer, separation processes, transport processes, and unit operations. The principles of mass transfer, both diffusional and convective have been comprehensively discussed. The application of these principles to separation processes is explained. The more common separation processes used in the chemical industries are individually described in separate chapters. The book also provides a good understanding of the construction, the operating principles, and the selection criteria of separation equipment. Recent developments in equipment have been included as far as possible. The procedure of equipment design and sizing has been illustrated by simple examples. An overview of different applications and aspects of membrane separation has also been provided. "Humidification and water cooling", necessary in every process industry, is also described. Finally, elementary principles of 'unsteady state diffusion' and mass transfer accompanied by a chemical reaction are covered. SALIENT FEATURES : • A balanced coverage of theoretical principles and applications. • Important recent developments in mass transfer equipment and practice are included. • A large number of solved problems of varying levels of complexities showing the applications of the theory are included. • Many end-chapter exercises. • Chapter-wise multiple choice questions. • An Instructors manual for the teachers.

Modelling, Design, Control and Integration

Process Systems Engineering

Become Smarter, Happier, and More Productive While Protecting Your Brain for Life

Tools and Applications

Statistical Physics and Thermodynamics of Nonlinear Nonequilibrium Systems

Advances in Feedstock Conversion Technologies for Alternative Fuels and Bioproducts

The fourth edition of Ludwig's Applied Process Design for Chemical and Petrochemical Plants, Volume Three is a core reference for chemical, plant, and process engineers and provides an unrivalled reference on methods, process fundamentals, and supporting design data. New to this edition are expanded chapters on heat transfer plus additional chapters focused on the design of shell and tube heat exchangers, double pipe heat exchangers and air coolers. Heat tracer requirements for pipelines and heat loss from insulated pipelines are covered in this new edition, along with batch heating and cooling of process fluids, process integration, and industrial reactors. The book also looks at the troubleshooting of process equipment and corrosion and metallurgy. Assists engineers in rapidly analyzing problems and finding effective design methods and mechanical specifications Definitive guide to the selection and design of various equipment types, including heat exchanger sizing and compressor sizing, with established design codes Batch heating and cooling of process fluids supported by Excel programs

Discover how the detailed structures of musculoskeletal tissue junctions relate to their mechanical function. This pioneering book, richly illustrated with tissue images, offers a rigorous, biomechanical approach to understanding the soft-hard tissue interface across multiple scales of resolution.

Modern Engineering and Physics very often deal with the need for the design of natural or induced phenomena and processes and this is especially true in the problems involving heat transfer or fluid flows, often on the basis of a Thermodynamic viewpoint or of the Constructal Law. These broad areas of research are presented in this special issue of the journal "Defect and Diffusion Forum".

This book provides an in-depth discussion of the principles of thermodynamics. It focuses on engineering applications of theory and sound techniques for solving thermodynamic problems. The book presents the fundamental concepts of thermodynamics and describes the theory of work and heat. The text covers in detail the first law and the second law of thermodynamics with their applications. It also explains the concepts of entropy and availability and irreversibility. In addition, the book presents thermodynamic properties of pure substances, ideal gases and mixtures of ideal gases, as well as real gases. This book is designed for undergraduate students of mechanical engineering, industrial and production engineering, automobile engineering and aeronautical engineering for their courses in thermodynamics.

Introduction to CHEMICAL ENGINEERING THERMODYNAMICS

Process Calculations

Advanced Transport Phenomena

Ludwig's Applied Process Design for Chemical and Petrochemical Plants

Engineering Thermodynamics

Handbook of Pharmaceutical Excipients

Polystyrene represents one of the oldest and the most widespread polymers in the world. Its starts as far back as 1839 when a German apothecary Edmon Simon distilled an oily liquid named styrol from the resin of Turkish sweet gum trees. In several days, the sterol converted into a jelly product that he thought resulted from the oxidation process. For that reason, the jelly product received the name styroloxide. This book discusses the synthesis of polystyrene, as well as the characteristics and applications of this polymer.

This book offers a full account of thermodynamic systems in chemical engineering. It provides a solid understanding of the basic concepts of the laws of thermodynamics as well as their applications with a thorough discussion of phase and chemical reaction equilibria. At the outset the text explains the various key terms of thermodynamics with suitable examples and then thoroughly deals with the virial and cubic equations of state by showing the P-V-T (pressure, molar volume and temperature) relation of fluids. It elaborates on the first and second laws of thermodynamics and their applications with the help of numerous engineering examples. The text further discusses the concepts of exergy, standard property changes of chemical reactions, thermodynamic property relations and fugacity. The book also includes detailed discussions on residual and excess properties of mixtures, various activity coefficient models, and group contribution methods. In addition, the text focuses on vapour-liquid and other phase equilibrium calculations, and analyzes chemical reaction equilibria and adiabatic reaction temperature for systems with complete and incomplete conversion of reactants. Key Features ? Includes a large number of fully worked-out examples to help students master the concepts discussed. ? Provides well-graded problems with answers at the end of each chapter to test and foster students' conceptual understanding of the subject. The total number of solved examples and end-chapter exercises in the book are over 600. ? Contains chapter summaries that review the major concepts covered. The book is primarily designed for the undergraduate students of chemical engineering and its related disciplines such as petroleum engineering and polymer engineering. It can also be useful to professionals. The Solution Manual containing the complete worked-out solutions to chapter-end exercises and problems is available for instructors.

Designed as an undergraduate-level textbook in Chemical Engineering, this student-friendly, thoroughly class-room tested book, now in its second edition, continues to provide an in-depth analysis of chemical engineering thermodynamics. The book has been so organized that it gives comprehensive coverage of basic concepts and applications of the laws of thermodynamics in the initial chapters, while the later chapters focus at length on important areas of study falling under the realm of chemical thermodynamics. The reader is thus introduced to a thorough analysis of the fundamental laws of thermodynamics as well as their applications to practical situations. This is followed by a detailed discussion on relationships among thermodynamic properties and an exhaustive treatment on the thermodynamic properties of solutions. The role of phase equilibrium thermodynamics in design, analysis, and operation of chemical separation methods is also deftly dealt with. Finally, the chemical reaction equilibria are skillfully explained. Besides numerous illustrations, the book contains over 200 worked examples, over 400 exercise problems (all with answers) and several objective-type questions, which enable students to gain an in-depth understanding of the concepts and theory discussed. The book will also be a useful text for students pursuing courses in chemical engineering-related branches such as polymer engineering, petroleum engineering, and safety and environmental engineering. New to This Edition • More Example Problems and Exercise Questions in each chapter • Updated section on Vapour-Liquid Equilibrium in Chapter 8 to highlight the significance of equations of state approach • GATE Questions up to 2012 with answers

This book, now in its second edition, continues to provide a comprehensive introduction to the principles of chemical engineering thermodynamics and also introduces the student to the application of principles to various practical areas. The book emphasizes the role of the fundamental principles of thermodynamics in the derivation of significant relationships between the various thermodynamic properties. The initial chapter provides an overview of the basic concepts and processes, and discusses the important units and dimensions involved. The ensuing chapters, in a logical presentation, thoroughly cover the first and second laws of thermodynamics, the heat effects, the thermodynamic properties and their relations, refrigeration and liquefaction processes, and the equilibria between phases and in chemical reactions. The book is suitably illustrated with a large number of visuals. In the second edition, new sections on Quasi-Static Process and Entropy Change in Reversible and Irreversible Processes are included. Besides, new Solved Model Question Paper and several new Multiple Choice Questions are also added that help develop the students' ability and confidence in the application of the underlying concepts. Primarily intended for the undergraduate students of chemical engineering and other related engineering disciplines such as polymer, petroleum and pharmaceutical engineering, the book will also be useful for the postgraduate students of the subject as well as professionals in the relevant fields.

Thermodynamic Models

Genius Foods

Statistical Physics

Applied Thermodynamics

Product-Driven Process Design

Introduction to Biomaterials

In these proceedings, it is shown that thermodynamical concepts are not 'old fashioned' but still are most useful at the frontiers of modern science. Among the contributors are well-known experts such as Andresen (Copenhagen), Eu (Montreal), Großmann (Marburg), Kawasaki (Fuhuoha), Maugin (Paris), Nicolis (Bruxelles) and Szépfalusy (Budapest). The subject covers a wide field including: recent developments in phenomenological thermodynamics, statistical foundation of thermodynamical concepts, thermodynamical concepts in nonlinear dynamics, applications to nonlinear (neural) networks, stochastic theory and transition processes. Contents: Random Stresses in Potts Models of Disordered Plastic Crystals (A Gützel et al.)Sensitivity to Initial Conditions in Complex Systems (G Nicolis et al.)Nonlinear Dynamics in Low-Dimensional Lattices: A Chemical Reaction Model (A Provata & J W Turner)Resonant Pair Nucleation in an Overdamped Sine-Gordon Chain (F Marchesoni)Finite-Time Optimization of Chemical Reactions and Connections to Thermodynamic Speed (J Ch Schön & B Andresen)A Variation Principle for Differential Transport Coefficients (M Ichiyanaqi)Higher-Order Fluxes and Effective Relaxation Times in Extended Thermodynamics (D Jou)Projection Operators in Statistical Formulation of Nonlinear and Extended Thermodynamics (R R Nettleton)Thermodynamics of Light and Sound (I Müller)Entropy, Predictability and Historicity of Nonlinear Processes (W Ebeling)Symmetry and Coherent Approximations in Non-Equilibrium Systems (M Suzuki)and other papers Readership: Statistical and thermodynamical working physicists.

This textbook offers original and new approaches to the teaching of electrochemical concepts, principles and applications. Throughout the text the authors provide a balanced coverage of the thermodynamic and kinetic processes at the heart of electrochemical systems. The first half of the book outlines fundamental concepts appropriate to undergraduate students and the second half gives an in-depth account of electrochemical systems suitable for experienced scientists and course lecturers. Concepts are clearly explained and mathematical treatments are kept to a minimum or reported in appendices. This book features: - Questions and answers for self-assessment - Basic and advanced level numerical descriptions - Illustrated electrochemistry applications This book is accessible to both novice and experienced electrochemists and supports a deep understanding of the fundamental principles and laws of electrochemistry.

The school held at Villa Marigola, Lerici, Italy, in July 1997 was very much an educational experiment aimed not just at teaching a new generation of students the latest developments in computer simulation methods and theory, but also at bringing together researchers from the condensed matter computer simulation community, the biophysical chemistry community and the quantum dynamics community to confront the shared problem: the development of methods to treat the dynamics of quantum condensed phase systems. This volume collects the lectures delivered there. Due to the focus of the school, the contributions divide along natural lines into two broad groups: (1) the most sophisticated forms of the art of computer simulation, including biased phase space sampling schemes, methods which address the multiplicity of time scales in condensed phase problems, and static equilibrium methods for treating quantum systems; (2) the contributions on quantum dynamics, including methods for mixing quantum and classical dynamics in condensed phase simulations and methods capable of treating all degrees of freedom quantum-mechanically. Contents:Barrier Crossing; Classical Theory of Rare but Important Events (D Chandler)Monte Carlo Simulations (D Frenko)Molecular Dynamics Methods for the Enhanced Sampling of Phase Space (B J Berne)Constrained and Nonequilibrium Molecular Dynamics (G Cicciotti & M Ferrario)From Erving to Kramers: Computation of Diffusive Barrier Crossing Rates (M J Ruiz-Montero)Monte Carlo Methods for Sampling of Rare Event States (W Janke)Proton Transfer in Ice (D Marx)Judged Elastic Band Method for Finding Minimum Energy Paths of Transitions (H Jönsson et al.)RAW Quantum Transition State Theory (G Mills et al.)Dynamics of Peptide Folding (R Elber et al.)Theoretical Studies of Activated Processes in Biological Ion Channels (B Roux & S Crouzy)The Semiclassical Initial Value Representation for Including Quantum Effects in Molecular Dynamics Simulations (W H Miller)Tunneling in the Condensed Phase: Barrier Crossing and Dynamical Control (N Makri)Feynman Path Centroid Methods for Condensed Phase Quantum Dynamics (G A Voth)Quantum Molecular Dynamics Using Wigner Representation (V S Filinov et al.)Nonadiabatic Molecular Dynamics Methods for Diffusion (D Laria et al.)and other papers Readership: Computational and statistical physicists. Keywords:Quantum,Molecular Dynamics,DynamicsReviews: "... this volume is a useful introduction to currently popular, and widely-used techniques in chemical and statistical physics. The authors are well-respected researchers in the field and the level is appropriate to graduate students and researchers." Journal of Statistical Physics

CAMD or Computer Aided Molecular Design refers to the design of molecules with desirable properties. That is, through CAMD, one determines molecules that match a specified set of (target) properties. CAMD as a technique has a very large potential as in principle, all kinds of chemical, bio-chemical and material products can be designed through this technique. This book mainly deals with macroscopic properties and therefore does not cover molecular design of large, complex chemicals such as drugs. While books have been written on computer aided molecular design relating to drugs and large complex chemicals, a book on systematic formulation of CAMD problems and solutions, with emphasis on theory and practice, which helps one to learn, understand and apply the technique is currently unavailable. This title brings together the theoretical aspects related to Computer Aided Molecular Design, the different techniques that have been developed and the different applications that have been reported. · Contributing authors are among the leading researchers and users of CAMD · First book available giving a systematic formulation of CAMD problems and solutions

Chemical Engineering Thermodynamics

Basic Thermodynamics

Mass Transfer-II

Biosensors for Virus Detection

Process Systems and Materials for CO2 Capture

Introductory Thermodynamics

Advanced Transport Phenomena is ideal as a graduate textbook. It contains a detailed discussion of modern analytic methods for the solution of fluid mechanics and heat and mass transfer problems, focusing on approximations based on scaling and asymptotic methods, beginning with the derivation of basic equations and boundary conditions and concluding with linear stability theory. Also covered are unidirectional flows, lubrication and thin-film theory, creeping flows, boundary layer theory, and convective heat and mass transport at high and low Reynolds numbers. The emphasis is on basic physics, scaling and nondimensionalization, and approximations that can be used to obtain solutions that are due either to geometric simplifications, or large or small values of dimensionless parameters. The author emphasizes setting up problems and extracting as much information as possible short of obtaining detailed solutions of differential equations. The book also focuses on the solutions of representative problems. This reflects the book's goal of teaching readers to think about the solution of transport problems.

Polystyrene

Quantum Chemistry Simulation of Biological Molecules

