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Demonstrates how anyone in math, science, and engineering canmaster DFT calculations Density functional theory (DFT) is one of the most frequentlyused computational tools for studying and predicting the propertiesof isolated molecules, bulk solids, and material interfaces,including surfaces. Although the theoretical underpinnings of DFTare quite complicated, this book demonstrates that the basicconcepts underlying the calculations are simple enough to beunderstood by anyone with a background in chemistry, physics,engineering, or mathematics. The authors show how the widespreadavailability of powerful DFT codes makes it possible for studentsand researchers to apply this important computational technique toa broad range of fundamental and applied problems. Density Functional Theory: A Practical Introductionoffers a concise, easy-to-follow introduction to the key conceptsand practical applications of DFT, focusing on plane-wave DFT. Theauthors have many years of experience introducing DFT to studentsfrom a variety of backgrounds. The book therefore offers severalfeatures that have proven to be helpful in enabling students tomaster the subject, including: Problem sets in each chapter that give readers the opportunityto test their knowledge by performing their own calculations Worked examples that demonstrate how DFT calculations are usedto solve real-world problems Further readings listed in each chapter enabling readers toinvestigate specific topics in greater depth This text is written at a level suitable for individuals from avariety of scientific, mathematical, and engineering backgrounds.No previous experience working with DFT calculations is needed.

Experiential learning is a singularly powerful approach to teaching and learning that is based on the fact that people learn best through experience. In this extensively updated book, the author offers the most complete and up-to-date statement of the theory of experiential learning and its modern applications in education, work, and adult development.

Changes and additions to the new edition of this classic textbook include a new chapter on symmetries, new problems and examples, improved explanations, more numerical problems to be worked on a computer, new applications to solid state physics, and consolidated treatment of time-dependent potentials.

Nanocharacterization Techniques covers the main characterization techniques used in nanomaterials and nanostructures. The chapters focus on the fundamental aspects of characterization techniques and their distinctive approaches. Significant advances that have taken place over recent years in refining techniques are covered, and the mathematical foundations needed to use the techniques are also explained in detail. This book is an important reference for materials scientists and engineers looking for a through analysis of nanocharacterization techniques in order to establish which is best for their needs. Includes a detailed analysis of different nanocharacterization techniques, allowing readers to explore which one is best for their particular needs Provides examples of how each characterization technique has been used, giving readers a greater understanding of how each technique can be profitably used Covers the mathematical background needed to utilize each of these techniques to their best effect, meaning that readers can gain a full understanding of the theoretical principles behind each technique covered Serves as an important, go-to reference for materials scientists and engineers

The Sixth Edition of a classic in organic chemistry continues its tradition of excellence Now in its sixth edition, March's Advanced Organic Chemistry remains the gold standard in organic chemistry. Throughout its six editions, students and chemists from around the world have relied on it as an essential resource for planning and executing synthetic reactions. The Sixth Edition brings the text completely current with the most recent organic reactions. In addition, the references have been updated to enable readers to find the latest primary and review literature with ease. New features include: More than 25,000 references to the literature to facilitate further research Revised mechanisms, where required, that explain concepts in clear modern terms Revisions and updates to each chapter to bring them all fully up to date with the latest reactions and discoveries A revised Appendix B to facilitate correlating chapter sections with synthetic transformations

Introduction to Transfer Phenomena in PEM Fuel Cells presents the fruit of several years of research in the area of fuel cells. The book illustrates the transfer phenomena occurring inside a single cell and describes the technology field of hydrogen, explicitly the production, storage and risk management of hydrogen as an energy carrier. Several applications of hydrogen are also cited, and special interest is dedicated to the PEM Fuel Cell. Mass, charge and heat transfer phenomena are also discussed in this great resource that includes explanations, illustrations and governing equations for each section. Illustrates transfer phenomena occurring within a single cell Describes the technological field of hydrogen (production, storage, and risk and management) Introduces the various applications of hydrogen Presents mass transfer, charge and heat phenomena

For two-semester courses in Organic Chemistry taken primarily by science and pre-health majors. This text, organized with a traditional functional-group approach, applies the most modern teaching and pedagogical techniques to the study of organic chemistry. In a highly accessible fashion, this top-selling text bridges the gap between conceptual understanding and actual application while strongly emphasizing the development of problem-solving skills. Additionally, it provides up-to-date aspects of spectroscopy, relevant photographs, and many applications to polymer chemistry integrated throughout the text.

Designed for students in Nebo School District, this text covers the Utah State Core Curriculum for chemistry with few additional top-

ics.

Molecular models are as vital a tool for the study of chemistry as calculators are for the study of mathematics. Molecular Visions models may be assembled in infinite combinations enabling the user to construct not only familiar configurations but also undiscovered possibilities. Models are intended to inspire the imagination, stimulate thought, and assist the visualization process. They present the user with a solid form of an abstract object that can otherwise only be visualized by the chemist. While chemistry textbooks use letters and graphics to describe molecules, molecular models make them "real". MOLECULAR VISIONS Organic Kit #1 is in a green plastic box, 9"x4"x2"

Those of us who read a daily newspaper or scan a weekly magazine have grown accustomed to being told that the science of genetics influences countless aspects of our existence, from human development, health, and disease to the ecological balance of our planet. We accept this, and yet most of us have only the faintest idea of what a gene really is or how it functions. This book, then, is a primer on modern genetics, and its aim is to teach any interested general reader all he or she needs to know about how genes work - and about how a detailed knowledge of their workings can be applied to some of the most pressing problems of our time. Written by two world-renowned researchers in molecular biology and illustrated with uncommon clarity and precision, Dealing with Genes will satisfy the interest of general readers, including those who have little formal background in biology. It will also serve admirably as an authoritative text for students taking nonmajors courses in biology, genetics, molecular biology, biotechnology, and related disciplines.

Membrane Computing was introduced as a computational paradigm in Natural Computing. The models introduced, called Membrane (or P) Systems, provide a coherent platform to describe and study living cells as computational systems. Membrane Systems have been investigated for their computational aspects and employed to model problems in other fields, like: Computer Science, Linguistics, Biology, Economy, Computer Graphics, Robotics, etc. Their inherent parallelism, heterogeneity and intrinsic versatility allow them to model a broad range of processes and phenomena, being also an efficient means to solve and analyze problems in a novel way. Membrane Computing has been used to model biological systems, becoming with time a thorough modeling paradigm comparable, in its modeling and predicting capabilities, to more established models in this area. This book is the result of the need to collect, in an organic way, different facets of this paradigm. The chapters of this book, together with the web pages accompanying them, present different applications of Membrane Systems to Biology. Deterministic, non-deterministic and stochastic systems paired with different algorithms and methodologies show the full potential of this framework. The book is addressed to researchers interested in applications of discrete biological models and the interplay between Membrane Systems and other approaches to analyze complex systems.

This book provides a myriad of fresh ideas and energetic approaches to the newer aspects of everyday drug modelling. With contributions from some of the best young talents of today, Molecular Modelling and Drug Design encourages a break from old traditions and probes the unexplored avenues of the modelling tool. The contributors' views act as a gauge to future trends in computer-aided drug design-an area that continues to expand and play an ever more significant role in drug discovery.

This book focuses on X-ray spectroscopy for chemical state analysis covering X-ray physics, spectroscopic characteristics used for functional and toxic materials, and the author's ideas related to X-ray experiments. This book also provides novel theoretical interpretations of X-ray spectra along with experimental techniques needed for both synchrotron radiation users and laboratory experimentalists. Presenting not only practical information, this book also covers basic knowledge of commercially available spectrometers and the basic physics of optics and electromagnetism related to X-rays. Furthermore, the author introduces the forgotten history of X-ray physics in the beginning of twentieth century. This book is of use for researchers studying catalysts, charge-transfer materials, surface characterization, and toxic trace elements via X-ray spectroscopy for chemical state analysis as well as quantitative analysis.

This brief guidebook assists you in mastering the difficult concept of pushing electrons that is vital to your success in Organic Chemistry. With an investment of only 12 to 16 hours of self-study you can have a better understanding of how to write resonance structures and will become comfortable with bond-making and bond-breaking steps in organic mechanisms. A paper-on-pencil approach uses active involvement and repetition to teach you to properly push electrons to generate resonance structures and write organic mechanisms with a minimum of memorization. Compatible with any organic chemistry textbook. Important Notice: Media content referenced within the product description or the product text may not be available in the ebook version.

Very broad overview of the field intended for an interdisciplinary audience; Lively discussion of current challenges written in a colloquial style; Author is a rising star in this discipline; Suitably accessible for beginners and suitably rigorous for experts; Features extensive four-color illustrations; Appendices featuring homework assignments and reading lists complement the material in the main text

Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas. The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

Designed for general chemistry courses that consider a lot of organic examples, or for students who plan to continue in organic chemistry. This molecular model set can be used to construct realistic scale models illustrating the molecular structures of many thousands of compounds. With it one can build molecular models of representative compounds.

This kit enables users to build virtually all simple molecules encountered in organic chemistry. Includes space-filling models that simulate the true shape of saturated compounds. Provides open models that form realistic single, double, and triple bonds — even strained rings. Allows smooth rotation of the bonds to make conformational analysis easy. Contains enough components to create several models at once. The components are precision-tooled from quality plastics, are virtually indestructible, and come in a sturdy plastic case for easy storage. Provides a useful Instruction Book — with photos, diagrams, and concise discussions of chemical principles.

In this third edition, core applications have been added along with more recent developments in the theories of chemical reaction kinetics and molecular quantum mechanics, as well as in the experimental study of extremely rapid chemical reactions. * Fully revised concise edition covering recent developments in the field * Supports student learning with step by step explanation of fundamental principles, an appropriate level of math rigor, and pedagogical tools to aid comprehension * Encourages readers to apply theory in practical situations

Up-to-date information on 1,780 colleges and universities.

The two-part, fifth edition of Advanced Organic Chemistry has been substantially revised and reorganized for greater clarity. The material has been updated to reflect advances in the field since the previous edition, especially in computational chemistry. Part A covers fundamental structural topics and basic mechanistic types. It can stand-alone; together, with Part B: Reaction and Synthesis, the two volumes provide a comprehensive foundation for the study in organic chemistry. Companion websites provide digital models for study of structure, reaction and selectivity for students and exercise solutions for instructors.

The growth in the world’s nuclear industry, motivated by peaking world oil supplies, concerns about the greenhouse effect, and domestic needs for energy independence, has resulted in a heightened focus on the need for next-generation nuclear fuel-cycle technologies. Ion Exchange and Solvent Extraction: A Series of Advances, Volume 19 provides a comprehensive look at the state of the science underlying solvent extraction in its role as the most powerful separation technique for the reprocessing of commercial spent nuclear fuel. Capturing the current technology and scientific progress as it exists today and looking ahead to potential developments, the book examines the overall state of solvent extraction in reprocessing, new molecules for increased selectivity and performance, methods for predicting extractant properties, and actinide-lanthanide group separation. The contributors also explore the simultaneous extraction of radionuclides by mixing extractants, the cause and nature of third-phase formation, the effects of radiation on the solvent and its performance, analytical techniques for measuring process concentrations, new centrifugal contactors for more efficient processing, and new chemistry using novel media. The long-term vision of many professionals in the field entails a proliferation-free nuclear energy economy in which little or no waste is stored or released into the environment and all potential energy values in spent nuclear fuel are recycled. This text opens a window on that possibility, offering insight from world leaders on the cutting edge of nuclear research.

Designed to serve as a textbook for postgraduate students of physics and chemistry, this second edition improves the clarity of treatment, extends the range of topics, and includes more worked examples with a view to providing all the material needed for a course in molecular spectroscopy—from first principles to the very useful spectral data that comprise figures, charts and tables. To improve the conceptual appreciation and to help students develop more positive and realistic impressions of spectroscopy, there are two new chapters—one on the spectra of atoms and the other on laser spectroscopy. The chapter on the spectra of atoms is a detailed account of the basic principles involved in molecular spectroscopy. The chapter on laser spectroscopy covers some new experimental techniques for the investigation of the structure of atoms and molecules. Additional sections on interstellar molecules, inversion vibration of ammonia molecule, fibre--coupled Raman spectrometer, Raman microscope, supersonic beams and jet-cooling have also been included. Besides worked-out examples, an abundance of review questions, and end-of-chapter problems with answers are included to aid students in testing their knowledge of the material contained in each chapter. Solutions manual containing the complete worked-out solutions to chapter-end problems is available for instructors.

This text covers new techniques and applications in chemical genomics for researchers, professionals and graduates in biology, biomedicine and chemistry.

"Compatible with standard taper miniscale, 14/10 standard taper microscale, Williamson microscale. Supports guided inquiry"--Cover.

Chemistry 2e is designed to meet the scope and sequence requirements of the two-semester general chemistry course. The textbook provides an important opportunity for students to learn the core concepts of chemistry and understand how those concepts apply to their lives and the world around them. The book also includes a number of innovative features, including interactive exercises and real-world applications, designed to enhance student learning. The second edition has been revised to incorporate clearer, more current, and more dynamic explanations, while maintaining the same organization as the first edition. Substantial improvements have been made in the figures, illustrations, and example exercises that support the text narrative. Changes made in Chemistry 2e are described in the preface to help instructors transition to the second edition.

"The Seventh Edition has been written with students like you in mind who are encountering organic chemistry for the first time. When learning and studying organic chemistry, you first must master fundamental principles of structure and reactivity that will then serve as the foundation on which to lay subsequent information. When we put a puzzle together, as depicted in the cover image of this book, we must work piece by piece until the larger picture comes into view. Similarly, the individual steps to learning organic chemistry are quite simple; each by itself is relatively easy to master. But there are many pieces involved in learning organic chemistry -- far too many to memorize. One would never try to memorize the position of each piece within a 500 piece puzzle! Mastering organic chemistry requires an understanding of fundamental principles and the ability to use those principles to reason, analyze, classify, and predict."--

The sixth edition provides an authoritative and comprehensive vision of molecular biology today. It presents developments in cell birth, lineage and death, expanded coverage of signaling systems and of metabolism and movement of lipids.

This book provides simultaneously a design blueprint, user guide, research agenda, and communication platform for current and future developments in artificial intelligence (AI) approaches to systems biology. It places an emphasis on the molecular dimension of life phenomena and in one chapter on anatomical and functional modeling of the brain. As design blueprint, the book is intended for scientists and other professionals tasked with developing and using AI technologies in the context of life sciences research. As a user guide, this volume addresses the requirements of researchers to gain a basic understanding of key AI methodologies for life sciences research. Its emphasis is not on an intricate mathematical treatment of the presented AI methodologies. Instead, it aims at providing the users with a clear understanding and practical know-how of the methods. As a research agenda, the book is intended for computer and life science students, teachers, researchers, and managers who want to understand the state of the art of the presented methodologies and the areas in which gaps in our knowledge demand further research and development. Our aim was to maintain the readability and accessibility of a textbook throughout the chapters, rather than compiling a mere reference manual. The book is also intended as a communication platform seeking to bride the cultural and technological gap among key systems biology disciplines. To support this function, contributors have adopted a terminology and approach that appeal to audiences from different backgrounds.

The fundamental aim underlying Cellular and Biochemical Sciences is to emphasize diversified topics of current interest to postgraduate students pursuing different courses in the area of biological sciences including Zoology, Botany, Biochemistry and Biotechnology. The text is also relevant to the students of Life Sciences, Biosciences, Cell Biology, Bioengineering and Pharmacology. A total of 58 topics have been incorporated in the book and some of

the topics are rarely found in other books of Biology. New information has been introduced which updates existing knowledge and enables the book to justify its claim as the most comprehensive text in the sphere of cellular and biochemical sciences at the postgraduate and competitive examination levels. Each and every chapter has been designed in lucid and readable manner. There are references, suggested readings, long questions and objective questions at the end of chapters for revision of topics.

For beginners and specialists in other fields: the Nobel Laureate's introduction to atomic spectra and their relationship to atomic structures, stressing basics in a physical, rather than mathematical, treatment. 80 illustrations.

The second edition of MODERN GARDE MANGER: A GLOBAL PERSPECTIVE, was written for both the working chef and the serious student engaged in the practice and study of culinary arts. The first edition was winner of the International Association of Culinary Professionals (IACP) Cookbook Award. Its carefully researched information and fully tested recipes span the international spectrum of the modern garde manger station. Four sections covering twenty chapters focus on the chef's required knowledge and responsibilities. This second edition has been reorganized to provide a clearer transition from subject to subject, and skill set to skill set. Special features include: Chapter Goals; Professional Profiles; Ask the Expert; People, Places, Things; Review Questions; Activities and Applications; and Key Words in Review. The text contains material on molecular cuisine, plus creative equipment used by garde manger chefs. There are more than 800 four--color photographs of which more than 300 are new, including many finished plates, platters, showpieces and step-by-step procedures, plus many additional recipes and expanded content on food show competition, buffet table layouts, ice sculpting techniques and more. . While Modern Garde Manger, 2e still retains its exposure to international recipes and techniques, more traditionally American recipes and techniques have been included in this edition. MODERN GARDE MANGER 2E is the most comprehensive book of its kind available for today's student and professional chef. In addition, a CourseMate website is available to accompany the text. CourseMate includes: an interactive eBook; Engagement Tracker, a first-of-its-kind tool that monitors student engagement in the course; and interactive teaching and learning tools including quizzes, flashcards, crossword puzzles, PowerPoint slides and more. Important Notice: Media content referenced within the product description or the product text may not be available in the ebook version.

Homology modeling is an extremely useful and versatile technique that is gaining more and more space and demand in research in computational and theoretical biology. This book, “Homology Molecular Modeling - Perspectives and Applications”, brings together unpublished chapters on this technique. In this book, 7 chapters are intimately related to the theme of molecular modeling, carefully selected and edited for academic and scientific readers. It is an indispensable read for anyone interested in the areas of bioinformatics and computational biology. Divided into 4 sections, the reader will have a didactic and comprehensive view of the theme, with updated and relevant concepts on the subject. This book was organized from researchers to researchers with the aim of spreading the fascinating area of molecular modeling by homology.

Fully updated and rewritten by a basic scientist who is also a practicing physician, the third edition of this popular textbook remains comprehensive, authoritative and readable. Taking a receptor-based, target-centered approach, it presents the concepts central to the study of drug action in a logical, mechanistic way grounded on molecular and principles. Students of pharmacy, chemistry and pharmacology, as well as researchers interested in a better understanding of drug design, will find this book an invaluable resource. Starting with an overview of basic principles, Medicinal Chemistry examines the properties of drug molecules, the characteristics of drug receptors, and the nature of drug-receptor interactions. Then it systematically examines the various families of receptors involved in human disease and drug design. The first three classes of receptors are related to endogenous molecules: neurotransmitters, hormones and immunomodulators. Next, receptors associated with cellular organelles (mitochondria, cell nucleus), endogenous macromolecules (membrane proteins, cytoplasmic enzymes) and pathogens (viruses, bacteria) are examined. Through this evaluation of receptors, all the main types of human disease and all major categories of drugs are considered. There have been many changes in the third edition, including a new chapter on the immune system. Because of their increasingly prominent role in drug discovery, molecular modeling techniques, high throughput screening, neuropharmacology and genetics/genomics are given much more attention. The chapter on hormonal therapies has been thoroughly updated and re-organized. Emerging enzyme targets in drug design (e.g. kinases, caspases) are discussed, and recent information on voltage-gated and ligand-gated ion channels has been incorporated. The sections on antihypertensive, antiviral, antibacterial, anti-inflammatory, antiarrhythmic, and anticancer drugs, as well as treatments for hyperlipidemia and peptic ulcer, have been substantially expanded. One new feature will enhance the book's appeal to all readers: clinical-molecular interface sections that facilitate understanding of the treatment of human disease at a molecular level.

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