Selected Papers of Robert S. Mulliken

Robert S. Mulliken 1975-08 This book brings together in one volume the most important papers of Robert S. Mulliken, who was awarded the 1966 Nobel Prize in chemistry for his seminal work on chemical bonds and the electronic structures of molecules. The papers collected here range from supporting fundamental concepts in quantum chemistry to recent topics in molecular orbital theory. Professor Mulliken has written introductory commentaries on each of the volume's seven parts. Included in the volume are essays of general as well as scientific interest; they are grouped under such headings as "The formation of chemical bonds" and "Historical significance of Mulliken's discovery of hyperconjugation." Each essay is followed by a list of Mulliken's major scientific publications, a list of his Nobel Prize. Also included is the text of his Nobel Prize acceptance speech. At the end is a list of his students and other co-workers, and a complete bibliography of his papers. Part II includes Mulliken's work on band spectra and chemistry as well as his research on the quantum numbers of electrons in molecules. This part also includes Mulliken's work on the electronic structures of molecules. Included is a discussion of the structure and spectra of a number of important types of molecules. The papers in Part IV focus on the intensities of electronic transitions in molecular structures. This part concludes with Mulliken's work on the molecular electronic transitions. The last part of the book collects Mulliken's Nobel-winning discoveries were made.

Introduction to Elementary Molecular Orbital Theory and to Semimolecular Methods

G.H. Wagner 2012-12-06 These notes summarize in part lectures held regularly at the University of Würzburg, 1962-1967. An attempt to write a second edition of my 1976 book Frontier Orbitals and Organic Chemical Reactions. I wanted to give a rather more thorough introduction to Organic Chemical Reactions: Student Edition is an invaluable first textbook on this important subject for students of organic, physical organic and computational research worker, whether mathematically competent or not. Topics covered include: Molecular Orbital Theory Molecular Orbitals and the Structures of Organic Molecules Chemical Reactions — How Far and How Fast Ionic Reactions — Reactivity Ionic Reactions — Stereochemistry Pericyclic Reactions Radical Reactions calculations are connected with chemical intuition. They are determined in chemical reactions. Students and senior investigators will gain insight into the nature of chemical reactions and find out how quantum chemical methods mainly lies in a semiquantitative classification of electronic pro perties and in the search for regularities within given classes of larger molecules. The reader is supposed to know the basic methods of quantum chemical calculations as well as quantum chemistry. The bibliography should encourage the reader to consult other texts, in particular also selected publications in scientific journals.

Frontier Orbitals and Reaction Paths

Kenichi Fukui 1997 This book is a collection of selected papers on the Frontier Orbital Theory by Nobel prize-winner Kenichi Fukui (Fukui 1981) with introductory notes. It provides the basic concept and formulation of the theory, and the physical and chemical significance of the frontier orbitals interactions in chemistry, together with many practical applications. The formulation of the Intrin sic Reaction Coordinate and applications to some simple systems are also presented. The aim of this volume is to show what forces chemical reactions are driven and to demonstrate how the frontier-orbital philosophy is applicable in chemical research. Chemical History: Reviews of the Recent Literature is also ideal for chemists who wish to become acquainted with the latest developments in that field. Each chapter is written by experts in their third or fourth year of study. The bibliography should encourage the reader to consult other texts, in particular also selected publications in scientific journals.

Molecular Orbital and Organic Chemical Reactions

Ian Fleming 2011-01-31 Winner of the PROSE Award for Chemistry 2010 Acknowledging the very best in professional and scholarly publishing, the annual PROSE Awards recognize outstanding works in all areas of science and technology. From basic research to popular science, from mathematics and engineering to environmental science, the PROSE Awards celebrate excellence. This year's PROSE Awards again featured a full range of categories, from basic science to social science, from science fiction to general nonfiction. The winners were announced at a black-tie dinner and ceremony held at The Ziegfeld Ballroom in New York City.

Molecular Orbital Calculations for Biological Systems

Anne-Marie Sagle 1998 Molecular Orbital Calculations for Biological Systems is a hands-on guide to computational quantum chemistry and its applications in organic chemistry, biochemistry, and molecular biology. With improvements in software, molecular modeling techniques are becoming more widely used in chemical research, as well as in the educational system. With the advent of powerful computers and the availability of fast and reliable quantum mechanical calculators, the field of computational chemistry is growing rapidly. The aim of this book is to provide a comprehensive introduction to the computational methods used in molecular modeling. The book is divided into two main parts: a theoretical part and an experimental part. The theoretical part covers the basics of electronic structure theory and quantum chemistry, while the experimental part focuses on the practical aspects of molecular modeling.

Recent Advances of the Fragment Molecular Orbital Method

Yoji Mochizuki 2003 This book presents a comprehensive overview of the recent developments in the fragment molecular orbital method (FOMO). It includes chapters on the latest advances in the theory and applications of the FOMO method, as well as on its potential for solving complex chemical problems. The book is divided into two main sections: theoretical developments and applications. Theoretical developments cover the latest advances in the theory of the FOMO method, including the development of new computational algorithms and the application of the FOMO method to new systems. Applications cover the use of the FOMO method in a variety of chemical problems, including the study of molecular reactions, the prediction of chemical properties, and the study of chemical processes.
The Path to Molecular Orbital Theory

Surfaces: Breakdown of the Born–Oppenheimer Approximation: Classic Theories of Nonadiabatic Transitions and Ideas Behind Direct Observation of the Wavepacket

Intermolecular Interactions in Crystals

Charge and Exciton Transport through Molecular Wires

Quantum Mechanics

Charge and Exciton Transport through Molecular Wires - Laurens D. A. Sibelebo 2011-07-18 As functional elements in opto-electronic devices the adiabatic transport of charges and charge-like particles such as excitons within the device. Reproducible syntheses and a thorough understanding of the underlying principles are therefore indispensable for applications like even smaller transistors, molecular light-harvesting systems and many others. This book provides a detailed overview of theory and experiment to enable researchers to realise new devices.


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Quantum Mechanics


Conjugated Molecules - Roberto Todeschini 2008-07-11 Quantitative studies on structure-activity and structure-property relationships are powerful tools in directed drug research. In recent years, various strategies have been developed to characterize and classify structural patterns by means of molecular descriptors. Molecular descriptors allow the identification of specific structural features that are characteristic of classes of molecules with known biological activity. Molecular descriptors are of great importance in the development of new drugs.

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those wishing to gain a broad understanding of chemistry and its relevance to the everyday world and to other areas of science. The books, with their Case Studies and accompanying multimedia interactive CD-ROMs, will also provide valuable resource material for teachers and lecturers. (The CD-ROMs are designed for use on a PC running Windows 95, 98, ME or 2000.)

Vibronic Coupling Density-Tatsuhisa Kato 2013-11-13 This book introduces vibronic coupling density and vibronic coupling constant analyses as a way to understand molecular structure and chemical reactions. After quantum study, the behavior of electrons circulating around nuclei led to the principal concept that underlies all explanations in chemistry. Many textbooks have given plausible explanations to clarify molecular structure—for example, the bond elongation of ethylene under asymmetric and the non-planar structure of ammonia. Frontier molecular orbital concepts were proposed to visualize the path of chemical reactions, and conventional explanations gave students a familiarity with molecular structures in terms of the electronic state. By contrast, this book offers a more rational and more convincing path to understanding. It starts from the ab initio molecular Hamiltonian and provides systematic, rational approaches to comprehend chemical phenomena. In this way, the book leads the reader to a grasp of the quantitative evaluation of the force applied under the molecular deformation process. As well, guidelines are offered for integrating the traditional “hand-waving” approach of chemistry with more rational and general VCD and VCC alternatives along with the outlook for newly functionalized chemical systems.

The Fragment Molecular Orbital Method-Dmitri Fedorov 2009-05-14 Answering the need to facilitate quantum-chemical calculations of systems with thousands of atoms, Kazuo Kitaura and his coworkers developed the Fragment Molecular Orbital (FM0) method in 1999. Today, the FM0 method can be applied to the study of whole proteins and protein-ligand interactions, and is extremely effective in calculating the properties of biological systems and molecular clusters. Providing a unique and accessible approach, The Fragment Molecular Orbital Method: Practical Applications to Large Molecular Systems is for those researchers eager to obtain useful information from electronic structure calculations of large systems, and for those who wish to know what can be calculated with the calculations at present and in the near future. The text emphasizes the practical aspects, with as little mathematical detail as possible and in language that is easy to understand. The free modeling software F0rac, in which FM0-related functions are implemented, is provided on the accompanying CD-ROM, which also provides input file samples, usage hints, annotated output from typical calculations, easy-to-follow tutorial material, and a comprehensive and original book in the area of the molecular symmetry group is almost always required.

A Dictionary of Science-John Danthit 2010 This best-selling dictionary contains 9,200 entries on all aspects of chemistry, physics, biology (including human biology), earth sciences, and astronomy. This new edition includes expanded coverage of global warming, forensic science, astrophysics, quantum theory, and the solar system. Supported by over 200 diagrams and illustrations the dictionary features recommended web links for many entries, accessed and kept up-to-date via the Dictionary of Science companion website. Other features include short biographies of leading scientists, full-page illustrated features on subjects such as the Solar System and Genetically Modified Organisms, and chronologies of specific scientific subjects including plastics, electronics, and cell biology. Both concise and wide-ranging, this dictionary is an ideal reference work for a student and a great introduction for non-scientists.

Fluorescence and Phosphorescence Spectroscopy-Stephan G Schulman 2013-10-22 Fluorescence and Phosphorescence Spectroscopy: Photochemical Principles and Practice deals with the photochemical principles and applications of fluorescence and phosphorescence spectroscopy in experimental biology and chemistry. Topics covered include the absorption of light by molecules; instrumentation for the measurement of fluorescences and phosphorescences; solvent and acidity effects on electronic spectra; and polarization of fluorescence and phosphorescence. Comprised of four chapters, this book begins with a discussion on photophysical processes in isolated molecules and molecules in solution, paying particular attention to thermal equilibrium of electronically excited molecules, photostationarity, and coordination by metal ions. The next chapter describes the instrumentation for measuring fluorescence and phosphorescence, which consists essentially of a light source to electronically excite the sample; a monochromator to separate the light of desired energy from the source; a sample compartment; a second monochromator to isolate the sample’s fluorescence energy from the excitation energy; a photodetector to transform the fluorescent light into an electrical signal; and a readout system such as a galvanometer or a recorder, coupled with an amplifier to determine the intensity of fluorescent light that is emitted. The final chapter is devoted to various applications of fluorescence and phosphorescence spectroscopy, including the analysis of organic and inorganic compounds. This monograph is written primarily for analytical chemists and biological scientists.

Biomembranes-Lois H. Hanson 2012-12-06 This volume contains the contributions to a symposium held at Gatlinburg, Tennessee, under the auspices of the Oak Ridge National Laboratory, in April, 1971. In the past, these proceedings had appeared as a supplement to the Journal of Cellular Physiology. Due to the nature of the subject matter and the relevance of the topic of the symposium to the readers of BIOMEMBRANES, it was agreed by the organizers of the symposium to publish the contributions of the particpants as a separate volume in BIOMEMBRANES. It had been originally envisaged that, from time to time, the proceedings of a conference whose subject matter was directly related to the scope of this series would be included. The proceedings are being published exactly as they have been submitted to the Editor without the usual editorial re VY5V0s. This is being done to increase the speed of publication time. For the same reason, the volume has been permitted since the time needed to prepare an adequate subject index would have unnecessarily delayed publication. Included in the proceedings are short reports of a number of workshops that were held during the conference. The editor has received excellent cooperation from both the organizers of the conference and the several contributors to this volume. If the experiment is a success, it is thanks to their promptness.


High Dilution Effects: Physical and Biochemical Basis-Norman C. Sukal 2006-02-18 Since the subject of high dilution effects is still a subject for debate, this volume provides evidence in support of effects from control clinical studies, clinical records from veteran physicians, controlled experiments on animals and plants, and in vitro tests without any organisms (Chapter II). An overview of the methods for preparing drugs at ultra high dilution is also provided as well as the basic principles of homoeopathy, which has been alleviating human suffering through the use of these drugs for several hundred years (Chapter I). Chapter III provides physical basis of high dilutions as evidence from the NMR, IR, UV and fluorescence spectra of these drugs. Since water is used as the diluents media, the structure and dynamics of water polymers in relation to high dilution are discussed in order to facilitate easy comprehension of this physical aspect, the basic principles of spectroscopy are also described. Chapter IV focuses on the mechanism of action of potenized drugs in the living system, discussing the structure of the cell, the plasma membrane, the integral proteins on the membrane, the interaction between these proteins and high dilutions and the manifestations of the therapeutic effects of high dilutions. Some aspects, peculiar to homoeopathy, such as the chief miasm pares, and the literals and time modulation of symptoms and drug action are interpreted from a scientific perspective. Chapter IV ends with a brief discussion on water structures and the origin of life to show the natural evolution of high dilution effects. The book not only helps in understanding the physical basis of high dilutions and their mechanism of action in organisms but provides many new avenues of investigation into this interdisciplinary field of science.

Fundamentals of Molecular Symmetry-P.B. Bunker 2018-10-03 Winner of a 2001 CHOICE Outstanding Academic Book Award Molecular symmetry is an easily applied tool for understanding and predicting many of the properties of molecules. Traditionally, students are taught this subject using point groups derived from the equivalence group of the molecule. Fundamentals of Molecular Symmetry shows how to set up symmetry groups for molecules using the more general idea of energy invariance. It is no more difficult than using molecular geometry and one obtains molecular symmetry groups. The book provides an introductory description of molecular spectroscopy and quantum mechanics as the foundation for understanding how molecular symmetry is defined and used. The approach taken gives a balanced account of using both point groups and molecular symmetry groups. Usually the point group is only useful for isolated, nonrotating molecules, executing small amplitude vibrations, with no tumbling, in isolated electronic states. However, for the chemical physicist or physical chemist who wishes to go beyond these limitations, the molecular symmetry group is almost always required.