Elementary Molecular Quantum Mechanics

Ideas of Quantum Chemistry shows how quantum mechanics is applied to chemistry to give it a theoretical foundation. The structure of the book (a TREE-form) emphasizes the logical relationships between various topics, facts and methods. It shows the reader which parts of the text are needed for understanding specific aspects of the subject matter. Interspersed throughout the text are short biographies of key scientists and their contributions to the development of the field. Ideas of Quantum Chemistry has both textbook and reference work aspects. Like a textbook, the material is organized into digestable sections with each chapter following the same structure. It answers frequently asked questions and highlights the most important conclusions and the essential mathematical formulae in the text. In its reference aspects, it has a broader range than traditional quantum chemistry books and reviews virtually all of the pertinent literature. It is useful both for beginners as well as specialists in advanced topics of quantum chemistry. The book is supplemented by an appendix on the Internet. * Presents the widest range of quantum chemical problems covered in one book * Unique structure allows material to be tailored to the specific needs of the reader * Informal language facilitates the understanding of difficult topics

Single-volume account of methods used in dealing with the many-body problem and the resulting physics. Single-particle approximations, second quantization, many-body perturbation theory, Fermi fluids, superconductivity, many-boson systems, more. Each chapter contains well-chosen problems. Only prerequisite is basic understanding of elementary quantum mechanics. 1967 edition.

As quantum theory enters its second century, it is fitting to examine just how far it has come as a tool for the chemist. Beginning with Max Planck’s agonizing conclusion in 1900 that linked energy emission in discreet bundles to the resultant black-body radiation curve, a body of knowledge has developed with profound consequences in our ability to understand nature. In the early years, quantum theory was the providence of physicists and certain breeds of physical chemists. While physicists honed and refined the theory and studied atoms and their component systems, physical chemists began the foray into the study of larger, molecular systems. Quantum theory predictions of these systems were first verified through experimental spectroscopic studies in the electromagnetic spectrum (microwave, infrared and ultraviolet/visible), and, later, by nuclear magnetic resonance (NMR) spectroscopy. Over two generations these studies were hampered by two major drawbacks: lack of resolution of spectroscopic data, and the complexity of calculations. This powerful theory that promised understanding of the fundamental nature of molecules faced formidable challenges. The following example may put things in perspective for today’s chemistry faculty, college seniors or graduate students: As little as 40 years ago, force field calculations on a molecule as simple as ketene was a four to five year dissertation project.

Elementary Molecular Quantum MechanicsMathematical Methods and ApplicationsElsevier

Two Nobel Laureates present a systematic, comprehensive account of the theory, techniques, experimental data, and interpretation involved in the study of microwave spectroscopy. Ideal as reference or text. 1955 edition.

This book provides non-specialists with a basic understanding ofthe underlying concepts of quantum chemistry. It is both a text for second or third-year undergraduates and a reference for researchers who need a quick introduction or refresher. All chemists and many biochemists, materials scientists, engineers, and physicists routinely user spectroscopic measurements and electronic structure computations in their work. The emphasis of Quantum Chemistry on explaining ideas rather than enumerating facts or presenting procedural details makes this an excellent foundation text/reference. The keystone is laid in the first two chapters which deal with molecular symmetry and the postulates of quantum mechanics, respectively. Symmetry is woven through the narrative of the next three chapters dealing with simple models of translational, rotational, and vibrational motion that underlie molecular spectroscopy and statistical thermodynamics. The next two chapters deal with the electronic structure of the hydrogen atom and hydrogen molecule ion, respectively. Having been armed with a basic knowledge of these prototypical systems, the reader is ready to learn, in the next chapter, the fundamental ideas used to deal with the complexities of many-electron atoms and molecules. These somewhat abstract ideas are illustrated with the venerable Huckel model of planar hydrocarbons in the penultimate chapter. The book concludes with an explanation of the bare minimum of technical choices that must be made to do meaningful electronic structure computations using quantum chemistry software packages.

Quantum Mechanics, Second Edition discusses the fundamental concepts and governing principles of quantum mechanics. The title details the physical ideas and the mathematical formalism of the quantum theory of the non-relativistic and quasi-relativistic motion of a single particle in an external field. The text first covers the basic concepts, and then proceeds to tackling the change of quantum states in time. Next, the selection examines the connection between quantum mechanics and classical mechanics. The book also discusses the simplest applications of quantum mechanics, along with the elementary representation theory. The book will be most useful to students of physics who are studying quantum mechanics. The text will also serve expert quantum physicists as a reference.

An introductory journey through the periodic table explains how every tangible object is comprised of the various elements, while chronicling the history of element discovery and explaining how elemental knowledge can be applied

Quantum mechanics is a general theory of the motions, structures, properties, and behaviors of particles of atomic and subatomic dimensions. While quantum mechanics was created in the first third of the twentieth century by a handful of theoretical physicists working on a limited number of problems, it has further developed and is now applied by a great number of people working on a vast range of problems in wide areas of science and technology. Basic Molecular Quantum Mechanics introduces quantum mechanics by covering the fundamentals of quantum mechanics and some of its most important chemical applications: vibrational and rotational spectroscopy and electronic structure of atoms and molecules. Thoughtfully organized, the author builds up quantum mechanics systematically with each chapter preparing the student for the more advanced chapters and complex applications. Additional features include the following: This book presents rigorous and precise explanations of quantum

mechanics and mathematical proofs. It contains qualitative discussions of key concepts with mathematics presented in the appendices. It provides problems and solutions at the end of each chapter to encourage understanding and application. This book is carefully written to emphasize its applications to chemistry and is a valuable resource for advanced undergraduates and beginning graduate students specializing in chemistry, in related fields such as chemical engineering and materials science, and in some areas of biology.
This book deals with a central topic at the interface of chemistry and physics - the understanding of how the transformation of matter takes place at the atomic level. Building on the laws of physics, the book focuses on the theoretical framework for predicting the outcome of chemical reactions. The style is highly systematic with attention to basic concepts and clarity of presentation. Molecular reaction dynamics is about the detailed atomic-level description of chemical reactions. Based on quantum mechanics and statistical mechanics or, as an approximation, classical mechanics, the dynamics of uni- and bi-molecular elementary reactions are described. The book features a detailed presentation of transition-state theory which plays an important role in practice, and a comprehensive discussion of basic theories of reaction dynamics in condensed phases. Examples and end-of-chapter problems are included in order to illustrate the theory and its connection to chemical problems.
Useful introductory course and reference covers origins of quantum theory, Schrödinger wave equation, quantum mechanics of simple systems, electron spin, quantum states of atoms, Hartree-Fock self-consistent field method, more. 1990 edition.
"The standard work in the fundamental principles of quantum mechanics, indispensable both to the advanced student and to the mature research worker, who will always find it a fresh source of knowledge and stimulation." --Nature "This is the classic text on quantum mechanics. No graduate student of quantum theory should leave it unread"--W.C Schieve, University of Texas
This textbook introduces the molecular and quantum chemistry needed to understand the physical properties of molecules and their chemical bonds. It follows the authors' earlier textbook "The Physics of Atoms and Quanta" and presents both experimental and theoretical fundamentals for students in physics and physical and theoretical chemistry. The new edition treats new developments in areas such as high-resolution two-photon spectroscopy, ultrashort pulse spectroscopy, photoelectron spectroscopy, optical investigation of single molecules in condensed phase, electroluminescence, and light-emitting diodes.
The last twenty years have seen remarkable advances in molecular quantum mechanics. The traditional methods expounded in the first successful edition of this book have been implemented on a grand scale. In the Second Edition, McWeeny has completely revised the text and has added a wealth of new material and example problems. Key Features * Self-contained development of modern quantum theory of molecular electronic structure and properties *

Assumes only an elementary quantum mechanics background * Mathematical methods (vector spaces, representations, group theory, etc.) built up as required * Latest advances (use of second quantization, unitary group, propagators all developed assuming no previous knowledge)

As a consequence of new experimental techniques in optical and collision physics, such as multiphoton excitation and VUV radiation generation, quantum defect theory (QDT) has become more widely used as a theoretical tool for experimentalists. Drawing together a historical body of work that contains key research and review papers, Molecular Applica

Quantum Mechanics for Organic Chemists is based on the author's first-year graduate course on quantum mechanics for Organic Chemistry majors. The book not only makes a gradual transition from elementary to advanced, but also tries an approach that allows students to have a more intuitive learning. The book covers concepts in quantum physics and topics such as the LCAO-MO Huckel Approach; group theory; and extensions, modifications, and applications of the Huckel approach. Also included in the book are the areas of three-dimensional treatments; polyelectron wave functions; the Slater determinant; and Pople's SCF equations. The text is recommended for graduate students of organic chemistry who would like to know more about the applications of quantum mechanics in their field. Quantum physicists who are interested in the field of organic chemistry would also find the book appealing.

This book introduces readers in material chemistry/engineering to elementary quantum mechanics of atoms, molecules and solids and then goes on to make them acquainted with methods of statistical mechanics (classical as well as quantum) along with elementary principles of classical MD simulation.

Theories of Chemistry reviews the theories that underpin chemistry, but yet are not traditionally recognized as such, being normally considered as part of physics. Based on the argument that the needs of chemistry are distinctive, a mathematical structure of topics such as quantum mechanics, relativity theory, thermodynamics and statistical mechanics, suiting the needs of chemistry, is outlined. The subject matter is arranged in a sequence that reveals the foundations of chemistry. Starting from the mathematical basis, the sequence runs through the general concepts (mechanics and wave formalism) and the elementary building blocks, to molecules and macrosystems. The book is the product of the author's reading of original literature rather than of standard texts. It differs from what is conventionally emphasized because of the different approach that it argues for the recognition of chemistry as an emergent discipline, ultimately based on the properties and structure of space and time. Hence the emphasis on otherwise unexpected topics such as quaternions, lie groups, polarized light, compressed atoms, rydberg atoms, solitons, molecular hydrogen, and phase transitions, amongst others. The topic is the understanding of chemistry from first principles. The book is self-contained and can be used without reference to other sources. - All chemisty theories are covered in this one

volume. - The book is self-contained and can be used without reference to other sources. - Many topics, routinely referred to in advanced chemistry texts, without making them accessible to the non-specialist, are brought together.
Quantum mechanics is one of the most fascinating, and at the same time most controversial, branches of contemporary science. Disputes have accompanied this science since its birth and have not ceased to this day. Uncommon Paths in Quantum Physics allows the reader to contemplate deeply some ideas and methods that are seldom met in the contemporary literature. Instead of widespread recipes of mathematical physics, based on the solutions of integro-differential equations, the book follows logical and partly intuitional derivations of non-commutative algebra. Readers can directly penetrate the abstract world of quantum mechanics. First book in the market that treats this newly developed area of theoretical physics; the book will thus provide a fascinating overview of the prospective applications of this area, strongly founded on the theories and methods that it describes. Provides a solid foundation for the application of quantum theory to current physical problems arising in the interpretation of molecular spectra and important effects in quantum field theory. New insight into the physics of anharmonic vibrations, more feasible calculations with improved precision.
Computational chemistry has become extremely important in the last decade, being widely used in academic and industrial research. Yet there have been few books designed to teach the subject to nonspecialists. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics is an invaluable tool for teaching and researchers alike. The book provides an overview of the field, explains the basic underlying theory at a meaningful level that is not beyond beginners, and it gives numerous comparisons of different methods with one another and with experiment. The following concepts are illustrated and their possibilities and limitations are given: - potential energy surfaces; - simple and extended Hückel methods; - ab initio, AM1 and related semiempirical methods; - density functional theory (DFT). Topics are placed in a historical context, adding interest to them and removing much of their apparently arbitrary aspect. The large number of references, to all significant topics mentioned, should make this book useful not only to undergraduates but also to graduate students and academic and industrial researchers.
Volume 1 of the 5-volume Quantum Nanochemistry set presents an overall perspective of nuclear, atomic, molecular, and solids structures, and the observability and quantum properties as based on the quantum principles in their various levels of applications, from Planck, Bohr, Einstein, Schrödinger, Hartree-Fock, up to Feynman Path Integral approaches. The volume presents in a balanced manner the fundamental and advanced concepts, principles, and models as well as their first and novel combinations and applications in modeling complex natural or designed phenomena.

The Center for Computational Quantum Chemistry (CCQC) at the University of Georgia in Athens, Georgia, offers the full text of the August 1997 paper entitled "A Brief Review of Elementary Quantum Chemistry," written by C. David Sherrill. The paper highlights quantum mechanics, the Schrodinger equation, postulates of quantum mechanics, and molecular quantum mechanics, as well as some analytically soluble problems.

The new experiments underway at the Large Hadron Collider at CERN in Switzerland may significantly change our understanding of elementary particle physics and, indeed, the universe. Suitable for first-year graduate students and advanced undergraduates, this textbook provides an introduction to the field Fundamentals of Quantum Mechanics, Third Edition is a clear and detailed introduction to quantum mechanics and its applications in chemistry and physics. All required math is clearly explained, including intermediate steps in derivations, and concise review of the math is included in the text at appropriate points. Most of the elementary quantum mechanical models—including particles in boxes, rigid rotor, harmonic oscillator, barrier penetration, hydrogen atom—are clearly and completely presented. Applications of these models to selected “real world topics are also included. This new edition includes many new topics such as band theory and heat capacity of solids, spectroscopy of molecules and complexes (including applications to ligand field theory), and small molecules of astrophysical interest. Accessible style and colorful illustrations make the content appropriate for professional researchers and students alike Presents results of quantum mechanical calculations that can be performed with readily available software Provides exceptionally clear discussions of spin-orbit coupling and group theory, and comprehensive coverage of barrier penetration (quantum mechanical tunneling) that touches upon hot topics, such as superconductivity and scanning tunneling microscopy Problems given at the end of each chapter help students to master concepts

Presenting a concise, basic introduction to modelling and computational chemistry this text includes relevant introductory material to ensure greater accessibility to the subject. Provides a comprehensive introduction to this evolving and developing field Focuses on MM, MC, and MD with an entire chapter devoted to QSAR and Discovery Chemistry. Includes many real chemical applications combined with worked problems and solutions provided in each chapter Ensures that up-to-date treatment of a variety of chemical modeling techniques are introduced.

Introduction to Molecular Energy Transfer intends to provide an elementary introduction to the subject of molecular energy transfer and relaxation. The book covers the foundation of molecular energy transfer such as quantum mechanics; the vibrational state of molecules; and vibrational energy transfer and the experimental methods for its study. Coverage also includes the different kinds of energy transfer in gases; vibrational relaxation in condensed phases; electronic states and interactions; electronic energy as a result of intermolecular interaction;

radiationless electronic transition; and rotational energy transfer. The text is recommended for students, graduates, and researchers in the fields of physics and chemistry, especially those who would like to know more about molecular energy transfer.

Graduate-level text develops group theory relevant to physics and chemistry and illustrates their applications to quantum mechanics, with systematic treatment of quantum theory of atoms, molecules, solids. 1964 edition.

The second edition of Elementary Molecular Quantum Mechanics shows the methods of molecular quantum mechanics for graduate University students of Chemistry and Physics. This readable book teaches in detail the mathematical methods needed to do working applications in molecular quantum mechanics, as a preliminary step before using commercial programmes doing quantum chemistry calculations. This book aims to bridge the gap between the classic Coulson's Valence, where application of wave mechanical principles to valence theory is presented in a fully non-mathematical way, and McWeeny's Methods of Molecular Quantum Mechanics, where recent advances in the application of quantum mechanical methods to molecular problems are presented at a research level in a full mathematical way. Many examples and mathematical points are given as problems at the end of each chapter, with a hint for their solution. Solutions are then worked out in detail in the last section of each Chapter. Uses clear and simplified examples to demonstrate the methods of molecular quantum mechanics Simplifies all mathematical formulae for the reader Provides educational training in basic methodology

Quantum mechanics and the Schrodinger equation are the basis for the de scription of the properties of atoms, molecules, and nuclei. The development of reliable, meaningful solutions for the energy eigenfunctions of these many is a formidable problem. The usual approach for obtaining particle systems the eigenfunctions is based on their variational extremum property of the expectation values of the energy. However the complexity of these variational solutions does not allow a transparent, compact description of the physical structure. There are some properties of the wave functions in some specific, spatial domains, which depend on the general structure of the Schrodinger equation and the electromagnetic potential. These properties provide very useful guidelines in developing simple and accurate solutions for the wave functions of these systems, and provide significant insight into their physical structure. This point, though of considerable importance, has not received adequate attention. Here we present a description of the local properties of the wave functions of a collection of particles, in particular the asymptotic properties when one of the particles is far away from the others. The asymptotic behaviour of this wave function depends primarily on the separation energy of the outmost particle. The universal significance of the asymptotic behaviour of the wave functions should be appreciated at both research and pedagogic levels. This is the main aim of our presentation here.

This advanced text introduces to the advanced undergraduate and graduate student the mathematical foundations of the methods needed to carry out practical applications in electronic molecular quantum mechanics, a necessary preliminary step before using commercial programmes to carry out quantum chemistry calculations. Major features of the book include: Consistent use of the system of atomic units, essential for simplifying all mathematical formulae Introductory use of density matrix techniques for interpreting properties of many-body systems An introduction to valence bond methods with an explanation of the origin of the chemical bond A unified presentation of basic elements of atomic and molecular interactions The book is intended for advanced undergraduate and first-year graduate students in chemical physics, theoretical and quantum chemistry. In addition, it is relevant to students from physics and from engineering sub-disciplines such as chemical engineering and materials sciences.

This book focuses on current applications of molecular quantum dynamics. Examples from all main subjects in the field, presented by the internationally renowned experts, illustrate the importance of the domain. Recent success in helping to understand experimental observations in fields like heterogeneous catalysis, photochemistry, reactive scattering, optical spectroscopy, or femto- and attosecond chemistry and spectroscopy underline that nuclear quantum mechanical effects affect many areas of chemical and physical research. In contrast to standard quantum chemistry calculations, where the nuclei are treated classically, molecular quantum dynamics can cover quantum mechanical effects in their motion. Many examples, ranging from fundamental to applied problems, are known today that are impacted by nuclear quantum mechanical effects, including phenomena like tunneling, zero point energy effects, or non-adiabatic transitions. Being important to correctly understand many observations in chemical, organic and biological systems, or for the understanding of molecular spectroscopy, the range of applications covered in this book comprises broad areas of science: from astrophysics and the physics and chemistry of the atmosphere, over elementary processes in chemistry, to biological processes (such as the first steps of photosynthesis or vision). Nevertheless, many researchers refrain from entering this domain. The book "Molecular Quantum Dynamics" offers them an accessible introduction. Although the calculation of large systems still presents a challenge - despite the considerable power of modern computers - new strategies have been developed to extend the studies to systems of increasing size. Such strategies are presented after a brief overview of the historical background. Strong emphasis is put on an educational presentation of the fundamental concepts, so that the reader can inform himself about the most important concepts, like eigenstates, wave packets, quantum mechanical resonances, entanglement, etc. The chosen examples highlight that high-level experiments and theory need to work closely together. This book thus is a must-read both for researchers working experimentally or theoretically in the concerned fields, and generally for anyone interested in the exciting world of molecular quantum dynamics.

Introduction to problems of molecular structure and motion covers calculus of orthogonal functions, algebra of vector spaces, and Lagrangian and Hamiltonian formulation of classical mechanics. Answers to problems. 1966 edition.

A course in angular momentum techniques is essential for quantitative study of problems in atomic physics, molecular physics, nuclear physics and solid state physics. This book has grown out of such a course given to the students of the M. Sc. and M. Phil. degree courses at the University of Madras. An elementary knowledge of quantum mechanics is an essential pre-requisite to undertake this course but no knowledge of group theory is assumed on the part of the readers. Although the subject matter has group-theoretic origin, special efforts have been made to avoid the gro- theoretical language but place emphasis on the algebraic formalism dev- oped by Racah (1942a, 1942b, 1943, 1951). How far I am successful in this project is left to the discerning reader to judge. After the publication of the two classic books, one by Rose and the other by Edmonds on this subject in the year 1957, the application of angular momentum techniques to solve physical problems has become so common that it is found desirable to organize a separate course on this subject to the students of physics. It is to cater to the needs of such students and research workers that this book is written. A large number of questions and problems given at the end of each chapter will enable the reader to have a clearer understanding of the subject.

This graduate-level text explains the modern in-depth approaches to the calculation of electronic structure and the properties of molecules. Largely self-contained, it features more than 150 exercises. 1989 edition.

Originally published in 1934, this reference guide provides introductory and principle knowledge of the theory of quantum mechanics.

Includes bibliographical references.

Over recent decades, the increase in computational resources, coupled with the popularity of competitive quantum mechanics alternatives (particularly DFT), has promoted the widespread penetration of quantum mechanics calculations into a variety of fields targeting the reactivity of molecules. This book presents a selection of original research papers and review articles illustrating diverse applications of quantum mechanics in the study of problems involving molecules and their reactivity.

Elementary Methods of Molecular Quantum Mechanics shows the methods of molecular quantum mechanics for graduate University students of Chemistry and Physics. This readable book teaches in detail the mathematical methods needed to do working applications in molecular quantum mechanics, as a preliminary step before using commercial programmes doing quantum chemistry calculations. This book aims to bridge the gap between the classic Coulson’s Valence, where application of wave mechanical principles to valence theory is presented in a fully non-mathematical way, and McWeeny’s Methods of Molecular Quantum Mechanics, where recent advances in the application of quantum mechanical methods to molecular problems are presented at a research level in a full mathematical way. Many examples and mathematical points are given as problems at the end of each chapter, with a hint for their solution. Solutions are then worked out in detail in the last section of each Chapter. * Uses clear and simplified examples to demonstrate the methods of molecular quantum mechanics

* Simplifies all mathematical formulae for the reader * Provides educational training in basic methodology

These notes summarize in part lectures held regularly at the University of Zurich and, in the Summer of 1974, at the Semi nario Latinoamericano de QUimica Cuantica in Mexico. I am grateful to those who have encouraged me to publish these lec tures or have contributed to them by their suggestions. In particular, I wish to thank Professor J. Keller of the Univer sidad Nacional Autonoma in Mexico, Professor H. Labhart and Professor H. Fischer of the University of Zurich, as well as my former students Dr. J. Kuhn, Dr. W. Hug and Dr. R. Geiger. The aim of these notes is to provtde a summary and concise introduction to elementary molecular orbital theory, with an emphasis on semiempirical methods. Within the last decade the development and refinement of ab initio computations has tended to overshadow the usefulness of semiempirical methods. However, both approaches have their justification. Ab initio methods are designed for accurate predictions, at the expense of greater computational labor. The aim of semiempirical 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 have had some previous basic instruc tion in quantum mechanics, such as is now offered in many uni versities to chemists 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.