

Access Free Elementary  
Molecular Quantum Mechanics

# Elementary Molecular Quantum Mechanics

These notes summarize in part  
lectures held regularly at the

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University of Zurich and, in the Summer of 1974, at the Seminario Latinoamericano de QUimica Cuantica in Mexico. I am grateful to those who have encouraged me to publish these lectures or have

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contributed to them by their suggestions. In particular, I wish to thank Professor J. Keller of the Universidad Nacional Autonoma in Mexico, Professor H. Labhart and Professor H. Fischer of the University of

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Zurich, as well as my former students Dr. J. Kuhn, Dr. W. Hug and Dr. R. Geiger. The aim of these notes is to provide a summary and concise introduction to elementary molecular orbital theory, with

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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.

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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

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mainly lies in a semiquantitative classification of electronic properties and in the search for regularities within given classes of larger molecules. The reader is supposed to have had some

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previous basic instruction in quantum mechanics, such as is now offered in many universities to chemists in their third or fourth year of study. The bibliography should encourage the reader to



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consult other texts, in particular also selected publications in scientific journals.

A readable little book assisting the student in understanding, in a nonmathematical way, the

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essentials of the different bonds occurring in chemistry. Starting with a short, self-contained, introduction, Chapter 1 presents the essential elements of the variation approach to either

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total or second-order molecular energies, the system of atomic units (au) necessary to simplify all mathematical expressions, and an introductory description of the electron distribution in molecules. Using mostly 2x2

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Hückel secular equations,  
Chapter 2, by far the largest  
part of the book because of the  
many implications of the  
chemical bond, introduces a  
model of bonding in  
homonuclear and

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heteronuclear diatomics,  
multiple and delocalized bonds  
in hydrocarbons, and the  
stereochemistry of chemical  
bonds in polyatomic molecules,  
in a word, a model of the  
strong first-order interactions

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originating the chemical bond. In Chapter 3 the Hückel model of the linear polyene chain is used to explain the origin of band structure in the 1-dimensional crystal. Chapter 4 deals with a simple two-state

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model of weak interactions, introducing the reader to understand second-order electric properties of molecules and VdW bonding between closed shells. Lastly, Chapter 5 studies the structure of H-

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bonded dimers and the nature of the hydrogen bond, which has a strength intermediate between a VdW bond and a weak chemical bond. Besides a qualitative MO approach based on HOMO-LUMO charge



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transfer from an electron donor to an electron acceptor molecule, a quantitative electrostatic approach is presented yielding an electrostatic model working even at its simplest pictorial

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level. A list of alphabetically ordered references, author and subject indices complete the book.

Non-covalent Interactions in  
Quantum Chemistry and  
Physics: Theory and

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Applications provides an entry point for newcomers and a standard reference for researchers publishing in the area of non-covalent interactions. Written by the leading experts in this field, the

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book enables experienced researchers to keep up with the most recent developments, emerging methods, and relevant applications. The book gives a comprehensive, in-depth overview of the available

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quantum-chemistry methods for intermolecular interactions and details the most relevant fields of application for those techniques. Theory and applications are put side-by-side, which allows the reader

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to gauge the strengths and weaknesses of different computational techniques. Summarizes the state-of-the-art in the computational intermolecular interactions field in a comprehensive work

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Introduces students and researchers from related fields to the topic of computational non-covalent interactions, providing a single unified source of information Presents the theoretical foundations of

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current quantum mechanical methods alongside a collection of examples on how they can be applied to solve practical problems

The field of crystal engineering concerns the design and



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synthesis of molecular crystals with desired properties. This requires an in-depth understanding of the intermolecular interactions within crystal structures. This new book brings together the

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latest information and theories about intermolecular bonding, providing an introductory text for graduates. The book is divided into three parts. The first part covers the nature, physical meaning and methods

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for identification and analysis of intermolecular bonds. The second part explains the different types of bond known to occur in molecular crystals, with each chapter written by a specialist in that specific bond

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type. The final part discusses the cooperativity effects of different bond types present in one solid. This comprehensive textbook will provide a valuable resource for all students and researchers in

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the field of crystallography,  
materials science and  
supramolecular chemistry.

Fundamentals of Quantum  
Chemistry

From Theory to Applications

Introduction to Quantum

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Mechanics with Applications to  
Chemistry

An Introduction to Electronic  
Molecular Structure

Introduction to the Theory and  
Applications of Molecular and  
Quantum Mechanics

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with Solutions

*Elementary Methods of  
Molecular Quantum  
Mechanics shows the  
methods of molecular  
quantum mechanics for  
graduate University*

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*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*



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*preliminary step before  
using commercial  
programmes doing quantum  
chemistry calculations.  
This book aims to bridge  
the gap between the  
classic Coulson's Valence,*

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*where application of wave  
mechanical principles to  
valence theory is  
presented in a fully non-  
mathematical way, and  
McWeeny's Methods of  
Molecular Quantum*

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*Mechanics, where recent advances in the application of quantum mechanical methods to molecular problems are presented at a research level in a full*

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*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*

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*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*

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

*This textbook introduces  
the molecular and quantum  
chemistry needed to*

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*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*

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*experimental and  
theoretical fundamentals  
for students in physics  
and physical and  
theoretical chemistry. The  
new edition treats new  
developments in areas such*



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*as high-resolution two-  
photon spectroscopy,  
ultrashort pulse  
spectroscopy,  
photoelectron  
spectroscopy, optical  
investigation of single*

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*molecules in condensed phase, electroluminescence, and light-emitting diodes. Quantum mechanics, shortly after invention, obtained applications in different*

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*area of human knowledge.  
Perhaps, the most  
attractive feature of  
quantum mechanics is its  
applications in such  
diverse area as,  
astrophysics, nuclear*

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*physics, atomic and  
molecular spectroscopy,  
solid state physics and  
nanotechnology,  
crystallography,  
chemistry, biotechnology,  
information theory,*

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*electronic engineering...  
This book is the result of  
an international attempt  
written by invited authors  
from over the world to  
response daily growing  
needs in this area. We do*

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*not believe that this book can cover all area of application of quantum mechanics but wish to be a good reference for graduate students and researchers.*

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*Elementary Molecular  
Quantum  
Mechanics Mathematical  
Methods and  
Applications Elsevier  
Elementary Molecular  
Quantum Mechanics*

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*Introduction to Molecular  
Energy Transfer  
Models for Bonding in  
Chemistry  
Molecular Physics and  
Elements of Quantum  
Chemistry*



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*Problems in Structural  
Inorganic Chemistry  
Quantum Mechanics For  
Organic Chemists*

New textbooks at all levels of chemistry appear with great regularity. Some fields like basic biochemistry, organic

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reaction mechanisms, and chemical thermodynamics are well represented by many excellent texts, and new or revised editions are published sufficiently often to keep up with progress in research. However, some areas of chemistry, especially many of

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those taught at the graduate level, suffer from a real lack of up-to-date textbooks. The most serious needs occur in fields that are rapidly changing. Textbooks in these subjects usually have to be written by scientists actually involved in the research which

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is advancing the field. It is not often easy to persuade such individuals to set time aside to help spread the knowledge they have accumulated. Our goal, in this series, is to pinpoint areas of chemistry where recent progress has outpaced what is covered in any

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available textbooks, and then seek out and persuade experts in these fields to produce relatively concise but instructive introductions to their fields. These should serve the needs of one semester or one quarter graduate courses in chemistry and biochemistry.

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In some cases, the availability of texts in active research areas should help stimulate the creation of new courses. New York, New York CHARLES R. CANTOR Preface This book is not a traditional quantum chemistry textbook. Instead, it represents a

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concept that has evolved from teaching graduate courses in quantum chemistry over a number of years, and encountering students with diverse backgrounds.

This book consists of over 422 problems and their acceptable answers

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on structural inorganic chemistry at the senior undergraduate and beginning graduate level. The central theme running through these questions is symmetry, bonding and structure: molecular or crystalline. A wide variety of topics are covered, including



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Electronic States and Configurations of Atoms and Molecules, Introductory Quantum Chemistry, Atomic Orbitals, Hybrid Orbitals, Molecular Symmetry, Molecular Geometry and Bonding, Crystal Field Theory, Molecular Orbital Theory, Vibrational Spectroscopy,

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Crystal Structure, Transition Metal Chemistry, Metal Clusters: Bonding and Reactivity, and Bioinorganic Chemistry. The questions collected here originate from the examination papers and take-home assignments arising from the teaching of courses in

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Chemical Bonding, Elementary Quantum Chemistry, Advanced Inorganic Chemistry, and X-Ray Crystallography by the book's two senior authors over the past five decades. The questions have been tested by generations of students taking

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these courses. The questions in this volume cover essentially all the topics in a typical course in structural inorganic chemistry. The text may be used as a supplement for a variety of inorganic chemistry courses at the senior undergraduate level. It also

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serves as a problem text to accompany the book *Advanced Structural Inorganic Chemistry*, co-authored by W.-K. Li, G.-D. Zhou, and T. C. W. Mak (Oxford University Press, 2008).

Computational chemistry has become extremely important in the last decade,

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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

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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

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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



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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

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students and academic and industrial researchers.

Providing a unified account of nonrelativistic quantum mechanics, *Fundamentals of Quantum Mechanics* covers the principles and formalism of quantum mechanics and the

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development and application of general techniques for the solution of quantum mechanical problems. The author has done everything possible to make the math in this book accessible. The b  
Elementary Quantum Mechanics  
Advanced Molecular Quantum

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Mechanics

Mathematical Methods and

Applications

Methods of Molecular Quantum

Mechanics

Elementary Quantum Chemistry

Elementary Quantum Chemistry,

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## Second Edition

This book is primarily intended for graduate chemists and chemical physicists. Indeed, it is based on a graduate course that I give in

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the Chemistry Department of Southampton University. Nowadays undergraduate chemistry courses usually include an introduction to quantum mechanics with

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particular reference to molecular properties and there are a number of excellent textbooks aimed specifically at undergraduate chemists. In valence theory and

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molecular spectroscopy  
physical concepts are  
often encountered that  
are normally taken on  
trust. For example,  
electron spin and the  
anomalous magnetic



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moment of the electron  
are usually accepted as  
postulates, although  
they are well understood  
by physicists. In  
addition, the advent of  
new techniques has led

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to experimental situations that can only be accounted for adequately by relatively sophisticated physical theory. Relativistic corrections to molecular

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orbital energies are needed to explain X-ray photo electron spectra, while the use of lasers can give rise to multiphoton transitions, which are not easy to

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understand using the classical theory of radiation. Of course, the relevant equations may be extracted from the literature, but, if the underlying physics

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is not understood, this is a practice that is at best dissatisfying and at worst dangerous. One instance where great care must be taken is in the use of

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spectroscopically  
determined parameters to  
test the accuracy of  
electronic wave  
functions.

Quantum mechanics is a  
general theory of the

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motions, structures,  
properties, and  
behaviors of particles  
of atomic and subatomic  
dimensions. While  
quantum mechanics was  
created in the first

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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



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great number of people working on a vast range of problems in wide areas of science and technology. Basic Molecular Quantum Mechanics introduces

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quantum mechanics by  
covering the  
fundamentals of quantum  
mechanics and some of  
its most important  
chemical applications:  
vibrational and

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rotational spectroscopy  
and electronic structure  
of atoms and molecules.  
Thoughtfully organized,  
the author builds up  
quantum mechanics  
systematically with each

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chapter preparing the student for the more advanced chapters and complex applications. Additional features include the following:  
This book presents

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rigorous and precise  
explanations of quantum  
mechanics and  
mathematical proofs. It  
contains qualitative  
discussions of key  
concepts with

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mathematics presented in the appendices. It provides problems and solutions at the end of each chapter to encourage understanding and application. This

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book is carefully  
written to emphasize its  
applications to  
chemistry and is a  
valuable resource for  
advanced undergraduates  
and beginning graduate

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students specializing in chemistry, in related fields such as chemical engineering and materials science, and in some areas of biology.



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This book is designed for a one-semester course, for undergraduates, not necessarily chemistry majors, who need to know something about physical

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chemistry. The emphasis is not on mathematical rigor, but subtleties and conceptual difficulties are not hidden. It covers the essential topics in

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physical chemistry,  
including the state of  
matter, thermodynamics,  
chemical kinetics, phase  
and chemical equilibria,  
introduction to quantum  
theory, and molecular

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spectroscopy.

Supplementary materials  
are available upon  
request for all  
instructors who adopt  
this book as a course  
text. Please send your

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request to  
sales@wspc.com.

Fundamentals of Quantum  
Mechanics, Third Edition  
is a clear and detailed  
introduction to quantum  
mechanics and its

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applications in  
chemistry and physics.  
All required math is  
clearly explained,  
including intermediate  
steps in derivations,  
and concise review of

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the math is included in the text at appropriate points. Most of the elementary quantum mechanical models—including particles in boxes,

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rigid rotor, harmonic oscillator, barrier penetration, hydrogen atom—are clearly and completely presented. Applications of these models to selected “real



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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

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complexes (including applications to ligand field theory), and small molecules of astrophysical interest. Accessible style and colorful illustrations

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make the content  
appropriate for  
professional researchers  
and students alike  
Presents results of  
quantum mechanical  
calculations that can be

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performed with readily  
available software  
Provides exceptionally  
clear discussions of  
spin-orbit coupling and  
group theory, and  
comprehensive coverage

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of barrier penetration  
(quantum mechanical  
tunneling) that touches  
upon hot topics, such as  
superconductivity and  
scanning tunneling  
microscopy Problems

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given at the end of each  
chapter help students to  
master concepts

An Introduction to  
Relativistic Quantum  
Mechanics and the  
Quantum Theory of

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Radiation

Intermolecular

Interactions in Crystals

Molecules for

Innovations

Molecular Driving Forces

Multiscale Modeling in

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Nanophotonics

Basic Principles and  
Techniques of Molecular  
Quantum Mechanics

***Pedagogical classic and  
essential reference focuses on  
mathematics of detailed***



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***vibrational analyses of  
polyatomic molecules,  
advancing from application of  
wave mechanics to potential  
functions and methods of  
solving secular determinant.  
This book focuses on current***

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***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***

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***helping to understand  
experimental observations in  
fields like heterogeneous  
catalysis, photochemistry,  
reactive scattering, optical  
spectroscopy, or femto- and  
attosecond chemistry and***

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***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,***

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***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***

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***quantum mechanical effects, including phenomena like tunneling, zero point energy effects, or non-adiabatic transitions. Being important to correctly understand many observations in chemical,***

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***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***

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***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***



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***"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***

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***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***

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***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.***

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***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***

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***fields, and generally for anyone interested in the exciting world of molecular quantum dynamics. Quantum Mechanics for Organic Chemists is based on the author's first-year graduate course on quantum mechanics***

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***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***

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***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-***

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***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***



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***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.  
Useful introductory course and***

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***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.***

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***1990 edition.***

***Understanding Properties of  
Atoms, Molecules and Materials  
Non-covalent Interactions in  
Quantum Chemistry and Physics  
Elementary Physical Chemistry  
Introduction to Experiments and***

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***Theory***

***Quantum Chemistry***

***Introduction to Elementary***

***Molecular Orbital Theory and to***

***Semiempirical Methods***

Molecules, small structures composed of atoms, are essential substances for lives.

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However, we didn't have the clear answer to the following questions until the 1920s: why molecules can exist in stable as rigid networks between atoms, and why molecules can change into different types of molecules. The most important event for solving the puzzles is the discovery of the quantum mechanics. Quantum

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mechanics is the theory for small particles such as electrons and nuclei, and was applied to hydrogen molecule by Heitler and London at 1927. The pioneering work led to the clear explanation of the chemical bonding between the hydrogen atoms. This is the beginning of the quantum chemistry. Since then, quantum chemistry

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has been an important theory for the understanding of molecular properties such as stability, reactivity, and applicability for devices. This book is devoted for the theoretical foundations and innovative applications in quantum chemistry.

The last twenty years have seen

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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



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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

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quantization, unitary group, propagators  
all developed assuming no previous  
knowledge)

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

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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.

This second edition of an extremely well-received book presents more than 250

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nonrelativistic quantum mechanics problems of varying difficulty with the aim of providing students didactic material of proven value, allowing them to test their comprehension and mastery of each subject. The coverage is extremely broad, from themes related to the crisis of classical physics through achievements

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within the framework of modern atomic physics to lively debated, intriguing aspects relating to, for example, the EPR paradox, the Aharonov-Bohm effect, and quantum teleportation. Compared with the first edition, a variety of improvements have been made and additional topics of interest included, especially focusing on

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elementary potential scattering. The problems themselves range from standard and straightforward ones to those that are complex but can be considered essential because they address questions of outstanding importance or aspects typically overlooked in primers. The book offers students both an excellent tool for

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independent learning and a ready-reference guide they can return to later in their careers.

Materials and Simulations

Basic Molecular Quantum Mechanics

Molecular Quantum Dynamics

Computational Chemistry

Fundamentals of Crystal Engineering

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Molecular Spectroscopy and Modern  
Electronic Structure Computations

*The second edition of  
Elementary Molecular  
Quantum Mechanics shows  
the methods of molecular  
quantum mechanics for*



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*graduate University  
students of Chemistry and  
Physics. This readable  
book teaches in detail the  
mathematical methods  
needed to do working  
applications in molecular*

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*quantum mechanics, as a preliminary step before using commercial programmes doing quantum chemistry calculations. This book aims to bridge the gap between the*

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*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*

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*Molecular Quantum  
Mechanics, where recent  
advances in the  
application of quantum  
mechanical methods to  
molecular problems are  
presented at a research*

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*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.*

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*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*

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*Simplifies all  
mathematical formulae for  
the reader Provides  
educational training in  
basic methodology  
As quantum theory enters  
its second century, it is*

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*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*



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*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*

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*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*

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*and their component systems, physical chemists began the foray into the study of larger, molecular systems. Quantum theory predictions of these systems were first*

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*verified through  
experimental spectroscopic  
studies in the  
electromagnetic spectrum  
(microwave, infrared and  
ultraviolet/visible), and,  
later, by nuclear magnetic*

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*resonance (NMR)  
spectroscopy. Over two  
generations these studies  
were hampered by two major  
drawbacks: lack of  
resolution of  
spectroscopic data, and*

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*the complexity of calculations. This powerful theory that promised understanding of the fundamental nature of molecules faced formidable challenges. The following*

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*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*

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*as simple as ketene was a  
four to five year  
dissertation project.*

*In a technology driven  
civilization the quest for  
new and smarter materials  
is everlasting. They are*



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*required as platforms for  
developing new  
technologies or for  
improving an already  
existing technology. The  
discovery of a new  
material is no longer*

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*chance driven or  
accidental, but is based  
on careful reasoning  
structured by deep  
understanding of the  
microconstituents of  
materials - the atoms and*

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*molecules in isolation or  
in an assembly. That  
requires fair amount of  
exposure to quantum and  
statistical mechanics.*

*`Understanding Properties  
of Atoms, Molecules and*

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*Materials' is an effort (perhaps the first ever) to bring all the necessary theoretical ingredients and relevant physical information in a single volume. The book*

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*introduces the readers  
(first year graduates) or  
researchers in material  
chemistry/engineering to  
elementary quantum  
mechanics of atoms,  
molecules and solids and*

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*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.*

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*The basic concepts are introduced with clarity and illustrated with easy to grasp examples, thus preparing the readers for an exploration through the world of materials - the*

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*exotic and the mundane.  
The emphasis has been on  
the phenomena and what  
shapes them at the  
fundamental level. A  
comprehensive description  
of modern designing*



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*principles for materials with examples is a unique feature of the book. The highlights of the book are comprehensive introduction and analysis of Quantum states of atoms and*

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*molecules The  
translational symmetry and  
quantum states in periodic  
and amorphous solids Band  
structure and tuning  
Classical and quantum  
statistics with*

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*applications to ideal  
gases (photons, phonons  
and electrons, molecules)  
Quantum states in type-I  
and type-II  
superconductors  
(elementary theory*

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*included) Magnetic materials, materials with GMR and CMR Shape memory effects in alloys and materials 2D materials (graphene and graphene analogus) NLO and*

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*photovoltaic materials  
Hydrogen storage material  
for mitigating the looming  
energy crisis Quantum  
states in low and high  
band gap semiconductors  
Semimetals Designer*

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*materials, etc. The volume is designed and organized to create interest in the science of materials and the silent revolution that is redefining the goals and boundaries of*

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*materials science  
continuously.*

*Ideas of Quantum Chemistry  
shows how quantum  
mechanics is applied to  
chemistry to give it a  
theoretical foundation.*

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*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*



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*needed for understanding  
specific aspects of the  
subject matter.*

*Interspersed throughout  
the text are short  
biographies of key  
scientists and their*

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*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*

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*digestable sections with each chapter following the same structure. It answers frequently asked questions and highlights the most important conclusions and the essential mathematical*

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*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.*

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*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.*

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*\* 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 \**

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*Informal language  
facilitates the  
understanding of difficult  
topics*

*Elementary Methods of  
Molecular Quantum  
Mechanics*

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*The Theory of Infrared and  
Raman Vibrational Spectra*

*Molecular Quantum  
Mechanics*

*Molecular Vibrations*

*Theory and Applications*

*Some Applications of*



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*Quantum Mechanics*

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

*This book deals with a central topic at the interface of chemistry and physics - the understanding of how the*

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*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*

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*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*

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*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*

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*to chemical problems.*

*Classic undergraduate text explores wave functions for the hydrogen atom, perturbation theory, the Pauli exclusion principle, and the structure of simple and complex molecules.*

*Numerous tables and figures.*

*Molecular Driving Forces, Second*

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*Edition E-book is an introductory statistical thermodynamics text that describes the principles and forces that drive chemical and biological processes. It demonstrates how the complex behaviors of molecules can result from a few simple physical processes, and how simple models*

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*provide surprisingly accurate insights into the workings of the molecular world. Widely adopted in its First Edition, Molecular Driving Forces is regarded by teachers and students as an accessible textbook that illuminates underlying principles and concepts. The Second Edition includes two*

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*brand new chapters: (1) "Microscopic Dynamics" introduces single molecule experiments; and (2) "Molecular Machines" considers how nanoscale machines and engines work. "The Logic of Thermodynamics" has been expanded to its own chapter and now covers heat, work, processes,*



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*pathways, and cycles. New practical applications, examples, and end-of-chapter questions are integrated throughout the revised and updated text, exploring topics in biology, environmental and energy science, and nanotechnology. Written in a clear and reader-friendly style, the book*

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*provides an excellent introduction to the subject for novices while remaining a valuable resource for experts.*

*Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience*

*Ideas of Quantum Chemistry*

*Brief Review of Elementary Quantum*

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*Chemistry*

*The Microscopic Foundation of  
Chemical Kinetics*

*Fundamentals of Quantum Mechanics*

This text unravels those  
fundamental physical  
principles which explain how  
all matter behaves. It takes

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us from the foundations of quantum mechanics, through quantum models of atomic, molecular, and electronic structure, and on to discussions of spectroscopy, and the electronic and magnetic properties of

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molecules.

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

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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

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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

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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.



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The idea of theoretically predicting the useful properties of various materials using multiscale simulations has become popular in recent years. Of special interest are nanostructured, organic

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functional materials, which have a hierarchical structure and are considered materials of the future because of their flexibility and versatility. Their functional properties are inherited from the molecule

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that lies at the heart of the hierarchical structure. On the other hand, the properties of this functional molecule, in particular its absorption and emission spectra, strongly depend on its

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interactions with its  
molecular environment.  
Therefore, the multiscale  
simulations used to predict  
the properties of organic  
functional materials should  
be atomistic, that is, they  
should be based on classical

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and/or quantum methods that explicitly take into account the molecular structure and intermolecular interactions at the atomic level. This book, written by well-known specialists in theoretical chemistry, focuses on the

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basics of classical  
mechanics, quantum chemistry  
methods used for molecular  
disordered materials,  
classical methods of  
molecular simulations of  
disordered materials,  
vibronic interactions, and

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applications (presented as multiscale strategies for atomistic simulations of photonic materials). It has been edited by Professor Mikhail Alfimov, a renowned Russian scientist, a full member of the Russian

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Academy of Sciences, Russia,  
and the founder, first  
director, and now research  
supervisor of the  
Photochemistry Center of the  
Russian Academy of Science,  
Russia. Professor Alfimov's  
main research interests are



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in the field of  
photochemistry and  
photophysics of molecular  
and supramolecular systems.  
The book is a great  
reference for advanced  
undergraduate- and graduate-  
level students of

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nanotechnology and molecular science and researchers in nano- and molecular science, nanotechnology, chemistry, and physical chemistry, especially those with an interest in functional materials.

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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

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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,

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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

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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

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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.

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A Molecular Espectral  
Corroboration of Elementary  
Operator Quantum Mechanics  
Theories of Molecular  
Reaction Dynamics  
Problems in Quantum  
Mechanics