

Kaoru Yamanouchi

Quantum Mechanics of Molecular Structures

Quantum Mechanics Of Molecular Structures

Pasquale De Marco



Quantum Mechanics Of Molecular Structures:

Quantum Mechanics of Molecular Structures Kaoru Yamanouchi, 2015-03-07 At a level accessible to advanced undergraduates this textbook explains the fundamental role of quantum mechanics in determining the structure dynamics and other properties of molecules Readers will come to understand the quantum mechanical basis for harmonic oscillators angular momenta and scattering processes Exercises are provided to help readers deepen their grasp of the essential phenomena

Quantum Mechanical/Molecular Mechanical Approaches for the Investigation of Chemical Systems – Recent Developments and Advanced Applications Thomas S. Hofer, Sam P. de Visser, 2018-11-28 The QM MM method short for quantum mechanical molecular mechanical is a highly versatile approach for the study of chemical phenomena combining the accuracy of quantum chemistry to describe the region of interest with the efficiency of molecular mechanical potentials to represent the remaining part of the system Originally conceived in the 1970s by the influential work of the the Nobel laureates Martin Karplus Michael Levitt and Arieh Warshel QM MM techniques have evolved into one of the most accurate and general approaches to investigate the properties of chemical systems via computational methods Whereas the first applications have been focused on studies of organic and biomolecular systems a large variety of QM MM implementations have been developed over the last decades extending the range of applicability to address research questions relevant for both solution and solid state chemistry as well Despite approaching their 50th anniversary in 2022 the formulation of improved QM MM methods is still an active field of research with the aim to i extend the applicability to address an even broader range of research questions in chemistry and related disciplines and ii further push the accuracy achieved in the QM MM description beyond that of established formulations While being a highly successful approach on its own the combination of the QM MM strategy with other established theoretical techniques greatly extends the capabilities of the computational approaches For instance the integration of a suitable QM MM technique into the highly successful Monte Carlo and molecular dynamics simulation protocols enables the description of the chemical systems on the basis of an ensemble that is in part constructed on a quantum mechanical basis This eBook presents the contributions of a recent Research Topic published in *Frontiers in Chemistry* that highlight novel approaches as well as advanced applications of QM MM method to a broad variety of targets In total 2 review articles and 10 original research contributions from 48 authors are presented covering 12 different countries on four continents The range of research questions addressed by the individual contributions provide a lucid overview on the versatility of the QM MM method and demonstrate the general applicability and accuracy that can be achieved for different problems in chemical sciences Together with the development of improved algorithms to enhance the capabilities of quantum chemical methods and the continuous advancement in the capacities of computational resources it can be expected that the impact of QM MM methods in chemical sciences will be further increased already in the near future

Equilibrium Molecular Structures Jean Demaison, James E. Boggs, Attila G. Csaszar, 2016-04-19 Molecular

structure is the most basic information about a substance determining most of its properties Determination of accurate structures is hampered in that every method applies its own definition of structure and thus results from different sources can yield significantly different results Sophisticated protocols exist to account for these

Molecular Structure Norman L. Allinger, 2010-12-15 A guide to analyzing the structures and properties of organic molecules Until recently the study of organic molecules has traveled down two disparate intellectual paths the experimental or physical method and the computational or theoretical method Working somewhat independently of each other these disciplines have guided research for decades but they are now being combined efficiently into one unified strategy Molecular Structure delivers the essential fundamentals on both the experimental and computational methods then goes further to show how these approaches can join forces to produce more effective analysis of the structure and properties of organic compounds by Looking at experimental structures electron neutron X ray diffraction and microwave spectroscopy as well as computational structures ab initio semi empirical molecular orbital and molecular mechanics calculations Discussing various electronic effects particularly stereoelectronic effects including hyperconjugation negative hyperconjugation the Bohlmann and anomeric effects and how and why these cause changes in structures and properties of molecules Illustrating complex carbohydrate effects such as the gauche effect the delta two effect and the external anomeric torsional effect Covering hydrogen bonding the CH bond and how energies especially heats of formation can be affected Using molecular mechanics to tie all of these things together in the familiar language of the organic chemist valence bond pictures Authored by a founding father of computational chemistry Molecular Structure broadens the scope of the subject by serving as a pioneering guide for workers in the fields of organic biological and computational chemistry as they explore new possibilities to advance their discoveries This work will also be of interest to many of those in tangential or dependent fields including medicinal and pharmaceutical chemistry and pharmacology

Quantum Modeling of Complex Molecular Systems Jean-Louis Rivail, Manuel Ruiz-Lopez, Xavier Assfeld, 2015-10-13 This multi author contributed volume includes methodological advances and original applications to actual chemical or biochemical phenomena which were not possible before the increased sophistication of modern computers The chapters contain detailed reviews of the developments of various computational techniques used to study complex molecular systems such as molecular liquids and solutions particularly aqueous solutions liquid gas solid gas interphase and biomacromolecular systems Quantum modeling of complex molecular systems is a useful resource for graduate students and fledgling researchers and is also an excellent companion for research professionals engaged in computational chemistry material science nanotechnology physics drug design and molecular biochemistry

Methods of Molecular Quantum Mechanics Valerio Magnasco, 2009-10-29 Methods of Molecular Quantum Mechanics 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

Lectures On Chemical Bonding And Quantum Chemistry Sambhu N Datta,2019-02-25 The concept of a chemical bond evolved from a variety of experimental observations It became useful to understand at times even predict the molecular structure reactivity and mechanism of chemical reactions Every aspect of the concept of bonding received a quantitative interpretation from the advent of quantum mechanics and its application to chemistry In Lectures on Chemical Bonding and Quantum Chemistry the reader will find a comprehensive discourse on the basic interpretation of the chemical bond as well as current understanding in terms of a dancing molecule that not only travels rotates and pulsates around an equilibrium molecular structure but also interacts and collides with other molecules thereby transferring linear and angular momentum characteristics and adjusting total energies One will also find a thorough survey of quantum mechanical methodologies for calculation of molecular characteristics in specific states and their changes under spectroscopic transitions tunneling electron and proton transfer phenomena and so on Guides to more advanced levels of theory are also provided

Nuclear Magnet: The Enigma of Molecular Structures Pasquale De Marco,2025-08-15 Embark on a captivating journey into the realm of molecular structures and dynamics with Nuclear Magnet The Enigma of Molecular Structures This comprehensive guide unveils the principles applications and advanced techniques of nuclear magnetic resonance NMR spectroscopy a powerful tool that has revolutionized our understanding of matter Delve into the depths of NMR spectroscopy unraveling the mysteries of nuclear spins relaxation processes and the intricate dance of atoms and molecules Discover how NMR spectra provide a wealth of information about molecular structure chemical environments and molecular interactions Explore the diverse applications of NMR spectroscopy across scientific disciplines Witness the power of NMR in chemistry where it aids in the identification and characterization of compounds elucidates reaction mechanisms and unlocks the secrets of molecular architecture Delve into the world of physics where NMR probes the properties of materials revealing their atomic level structures and magnetic behaviors Journey into the realm of biology where NMR unveils the intricate structures and dynamic motions of proteins nucleic acids and other biomolecules providing insights into their functions and interactions Discover the applications of NMR in medicine where it enables non invasive imaging of the human body and holds promise for targeted drug delivery and novel therapies Nuclear Magnet The Enigma of Molecular Structures is an invaluable resource for students researchers and professionals in chemistry physics biology and medicine Its clear explanations comprehensive coverage and

engaging style make it an essential guide for anyone seeking to harness the power of NMR spectroscopy in their research endeavors If you like this book write a review Fundamentals of Molecular Structural Biology Subrata Pal,2019-08-15
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