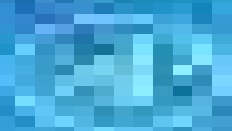


Computer-Controlled Quantum Chemistry

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Computational Quantum Chemistry An Interactive Introduction To Basis Set Theory

D. Michael P. Mingos



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Molecular Quantum Mechanics Peter W. Atkins, Ronald S. Friedman, 2011 This text unravels those fundamental physical principles which explain how all matter behaves It takes 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 molecules

50th Anniversary of Electron Counting Paradigms for Polyhedral Molecules D. Michael P. Mingos, 2022-01-01 The 50 Year Anniversary of the development of electron counting paradigms for polyhedral molecules is celebrated in two volumes of Structure and Bonding Volume 1 covers the historical development theoretical models and applications to boranes and metalloboranes

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Basis Sets in Computational Chemistry Eva Perlt, 2021-05-06 This book addresses the construction and application of the major types of basis sets for computational chemistry calculations In addition to a general introduction it includes mathematical basics and a discussion of errors arising from incomplete or inappropriate basis sets The different chapters introduce local orbitals and orbital localization as well as Slater type orbitals and review basis sets for special applications such as those for correlated methods solid state calculations heavy atoms and time dependent adaptable Gaussian bases for quantum dynamics simulations This detailed review of the purpose of basis sets their design applications possible problems and available solutions provides graduate students and beginning researchers with information not easily obtained from the available textbooks and offers valuable supporting material for any quantum chemistry or computational chemistry course at the graduate and or undergraduate level This book is also useful as a guide for researchers who are new to computational chemistry but are willing to extend their research tools by applying such methods

Computational Quantum Chemistry Charles M. Quinn, 2002

Computational Chemistry Errol G. Lewars, 2007-05-08 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 Hckel 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

Subject Guide

to Books in Print ,1991 *Computational Methods for the Description of Intermolecular Interactions and Molecular Motion in Confining Environments* Heribert Reis,Piotr Żuchowski,Sonja Grubisic,2022-06-23

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