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Essentials of Computational Chemistry - Christopher J. Cramer
2013-04-29

Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas. The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

Mathematics for Quantum Chemistry - Jay Martin Anderson
2012-12-13

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.

Molecular Electronic-Structure Theory - Trygve Helgaker 2014-08-11

Ab initio quantum chemistry has emerged as an important tool in chemical research and is applied to a wide variety of problems in chemistry and molecular physics. Recent developments of computational methods have enabled previously intractable chemical problems to be solved using rigorous quantum-mechanical methods. This is the first comprehensive, up-to-date and technical work to cover all the important aspects of modern molecular electronic-structure theory. Topics covered in the book include: * Second quantization with spin adaptation * Gaussian basis sets and molecular-integral evaluation * Hartree-Fock theory * Configuration-interaction and multi-configurational self-consistent theory * Coupled-cluster theory for ground and excited states * Perturbation theory for single- and multi-configurational states * Linear-scaling techniques and the fast multipole method * Explicitly correlated wave functions * Basis-set convergence and extrapolation *

Calibration and benchmarking of computational methods, with applications to molecular equilibrium structure, atomization energies and reaction enthalpies. Molecular Electronic-Structure Theory makes extensive use of numerical examples, designed to illustrate the strengths and weaknesses of each method treated. In addition, statements about the usefulness and deficiencies of the various methods are supported by actual examples, not just model calculations. Problems and exercises are provided at the end of each chapter, complete with hints and solutions. This book is a must for researchers in the field of quantum chemistry as well as for nonspecialists who wish to acquire a thorough understanding of ab initio molecular electronic-structure theory and its applications to problems in chemistry and physics. It is also highly recommended for the teaching of graduates and advanced undergraduates.

Modern Quantum Chemistry - Attila Szabo 1996-07-02

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.

Electronic Structure Calculations for Solids and Molecules - Jorge Kohanoff 2006-06-29

Electronic structure problems are studied in condensed matter physics and theoretical chemistry to provide important insights into the properties of matter. This 2006 graduate textbook describes the main theoretical approaches and computational techniques, from the simplest approximations to the most sophisticated methods. It starts with a detailed description of the various theoretical approaches to calculating the electronic structure of solids and molecules, including density-functional theory and chemical methods based on Hartree-Fock theory. The basic approximations are thoroughly discussed, and an in-depth overview of recent advances and alternative approaches in DFT is given.

The second part discusses the different practical methods used to solve the electronic structure problem computationally, for both DFT and Hartree-Fock approaches. Adopting a unique and open approach, this textbook is aimed at graduate students in physics and chemistry, and is intended to improve communication between these communities. It also serves as a reference for researchers entering the field.

Group Theory and Chemistry - David M. Bishop 2012-07-12

Concise, self-contained introduction to group theory and its applications to chemical problems. Symmetry, matrices, molecular vibrations, transition metal chemistry, more. Relevant math included. Advanced-undergraduate/graduate-level. 1973 edition.

Problems and Solutions in Quantum Chemistry and Physics -

Charles S. Johnson 2013-01-18

Unusually varied problems, with detailed solutions, cover quantum mechanics, wave mechanics, angular momentum, molecular spectroscopy, scattering theory, more. 280 problems, plus 139 supplementary exercises.

Quantum Mechanics for Chemists - David O. Hayward 2002

This book is designed to provide chemistry undergraduates with a basic understanding of the principles of quantum mechanics.

Modern Quantum Chemistry - Szabó Attila 1982

Introduction to Computational Chemistry - Frank Jensen 2016-12-14

Introduction to Computational Chemistry 3rd Edition provides a comprehensive account of the fundamental principles underlying different computational methods. Fully revised and updated throughout to reflect important method developments and improvements since publication of the previous edition, this timely update includes the following significant revisions and new topics: Polarizable force fields Tight-binding DFT More extensive DFT functionals, excited states and time dependent molecular properties Accelerated Molecular Dynamics methods Tensor decomposition methods Cluster analysis Reduced scaling and reduced prefactor methods Additional information is available at: www.wiley.com/go/jensen/computationalchemistry3

Introduction to Quantum Mechanics with Applications to Chemistry - Linus Pauling 2012-06-08

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. *Modern Quantum Chemistry* - Szabo A. 1996

Modern Electronic Structure Theory - D. R. Yarkony 1995

Modern Electronic Structure Theory provides a didactically oriented description of the latest computational techniques in electronic structure theory and their impact in several areas of chemistry. The book is aimed at first year graduate students or college seniors considering graduate study in computational chemistry, or researchers who wish to acquire a wider knowledge of this field.

Molecular Quantum Electrodynamics - D. P. Craig 2012-11-13

Self-contained, systematic introduction examines application of quantum electrodynamics to interpretation of optical experiments on atoms and molecules and explains the quantum theory of electromagnetic radiation and its interaction with matter.

Spins in Chemistry - Roy McWeeny 2004-06-18

Originally delivered as a series of lectures, this volume systematically traces the evolution of the "spin" concept from its role in quantum mechanics to its assimilation into the field of chemistry. Author Roy McWeeny presents an in-depth illustration of the deductive methods of quantum theory and their application to spins in chemistry, following the path from the earliest concepts to the sophisticated physical methods employed in the investigation of molecular structure and properties. Starting with the origin and development of the spin concept, the text advances to an examination of spin and valence; reviews a simple example of the origin of spin Hamiltonians; and explores spin density, spin populations, and spin correlation. Additional topics include nuclear hyperfine effects and electron spin-spin coupling, the g tensor, and chemical shifts and nuclear spin-spin coupling.

Electronic Structure and the Properties of Solids - Walter A. Harrison

2012-03-08

This text offers basic understanding of the electronic structure of covalent and ionic solids, simple metals, transition metals and their compounds; also explains how to calculate dielectric, conducting, bonding properties.

Handbook of Computational Quantum Chemistry - David B. Cook

2005-08-02

This comprehensive text provides upper-level undergraduates and graduate students with an accessible introduction to the implementation of quantum ideas in molecular modeling, exploring practical applications alongside theoretical explanations. Topics include the Hartree-Fock method; matrix SCF equations; implementation of the closed-shell case; introduction to molecular integrals; and much more. 1998 edition.

Quantum Mechanics in Chemistry - George C. Schatz 2012-04-30

Advanced graduate-level text looks at symmetry, rotations, and angular momentum addition; occupation number representations; and scattering theory. Uses concepts to develop basic theories of chemical reaction rates. Problems and answers.

Modern Quantum Chemistry - Attila Szabo 2012-06-08

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.

A Mathematical Introduction to Electronic Structure Theory - Lin Lin

2019-06-05

Based on first principle quantum mechanics, electronic structure theory

is widely used in physics, chemistry, materials science, and related fields and has recently received increasing research attention in applied and computational mathematics. This book provides a self-contained, mathematically oriented introduction to the subject and its associated algorithms and analysis. It will help applied mathematics students and researchers with minimal background in physics understand the basics of electronic structure theory and prepare them to conduct research in this area. The book begins with an elementary introduction of quantum mechanics, including the uncertainty principle and the Hartree-Fock theory, which is considered the starting point of modern electronic structure theory. The authors then provide an in-depth discussion of two carefully selected topics that are directly related to several aspects of modern electronic structure calculations: density matrix based algorithms and linear response theory. Chapter 2 introduces the Kohn-Sham density functional theory with a focus on the density matrix based numerical algorithms, and Chapter 3 introduces linear response theory, which provides a unified viewpoint of several important phenomena in physics and numerics. An understanding of these topics will prepare readers for more advanced topics in this field. The book concludes with the random phase approximation to the correlation energy. The book is written for advanced undergraduate and beginning graduate students, specifically those with mathematical backgrounds but without a priori knowledge of quantum mechanics, and can be used for self-study by researchers, instructors, and other scientists. The book can also serve as a starting point to learn about many-body perturbation theory, a topic at the frontier of the study of interacting electrons.

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