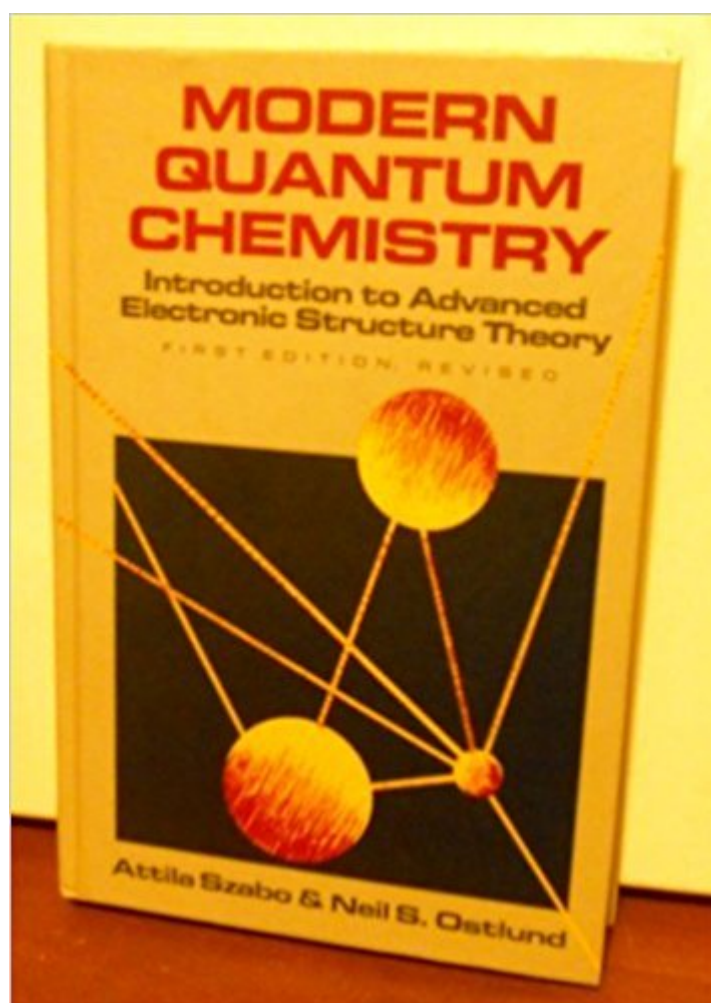




Ebook Directory
the best source of ebook

The book was found

Modern Quantum Chemistry: Introduction To Advanced Electronic Structure Theory



Synopsis

The aim of this graduate-level textbook is to present and explain, at other than a superficial level, modern ab initio approaches to the calculation of the electronic structure and properties of molecules. The first three chapters contain introductory material culminating in a thorough discussion of the Hartree-Fock approximation. The remaining four chapters describe a variety of more sophisticated approaches, which improve upon this approximation. Among the highlights of the seven chapters are (1) a review of the mathematics (mostly matrix algebra) required for the rest of the book, (2) an introduction to the basic techniques, ideas, and notations of quantum chemistry, (3) a thorough discussion of the Hartree-Fock approximation, (4) a treatment of configuration interaction (CI) and approaches incorporating electron correlation, (5) a description of the independent electron pair approximation and a variety of more sophisticated approaches that incorporate coupling between pairs, (6) a consideration of the perturbative approach to the calculation of the correlation energy of many-electron systems and (7) a brief introduction to the use of the one-particle many-body Green's function in quantum chemistry. Over 150 exercises, designed to help the reader acquire a working knowledge of the material, are embedded in the text. The book is largely self-contained and requires no prerequisite other than a solid undergraduate physical chemistry course; however, some exposure to quantum chemistry will enhance the student's appreciation of the material. Clear and well-written, this text is ideal for the second semester of a two-semester course in quantum chemistry, or for a special topics course.

Book Information

Hardcover: 480 pages

Publisher: McGraw-Hill (Tx); Revised edition (March 1989)

Language: English

ISBN-10: 0070627398

ISBN-13: 978-0070627390

Product Dimensions: 1 x 6.5 x 9.5 inches

Shipping Weight: 1.6 pounds

Average Customer Review: 4.6 out of 5 stars 38 customer reviews

Best Sellers Rank: #1,279,685 in Books (See Top 100 in Books) #60 in [Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry](#) #1112 in [Books > Science & Math > Physics > Quantum Theory](#) #3536 in [Books > Science & Math > Chemistry > General & Reference](#)

Customer Reviews

This book can be pretty neatly divided into two parts: the first three chapters which elucidate the Hartree-Fock approximation, and the remainder of the book which develops refinements of it. After a helpful preface, chapter 1 gives us a 38 page mathematical review. Section 1.1 is on linear algebra, and the reader should bring a solid background in this subject to this book. Dirac notation is introduced immediately and used throughout the book. Section 1.2 is on orthogonal functions, eigenfunctions, and operators. Section 1.3 is on the variational method for finding approximate solutions to eigenvalue problems and which find heavy use in quantum chemistry. Chapter 2 is a ~70 page treatment of many-electron wave functions and operators. This chapter develops all of the machinery necessary for the Hartree-Fock approximation. Section 2.1 introduces the electronic problem in general, discusses (but does not prove) the Born-Oppenheimer approximation and the basic antisymmetry condition for many-electron wave functions. Section 2.2 introduces us to spin and spatial orbitals, Hartree products, and Slater determinants. It then provides with our first peek at Hartree-Fock and introduces the minimal basis H₂ model which is used throughout the book as an aid. Section 2.3 is a heavy section which focuses on the evaluation of matrix elements for operators on many-electron wave functions. The contents of this section are absolutely key to the remainder of the book. Section 2.4 is an optional, but very good, section on second quantization techniques for evaluating matrix elements. Section 2.5 ends this chapter with a look at spin adapted configurations and unrestricted determinants. (Review to be completed later)

Great great great book for sophomore, junior students in chemistry to begin their journey in quantum chemistry. From basic algorithm, i.e. Hartree-Fock to advanced electron-correlation method, and ended up with Green function method, Szabo finds a fantastic way to organize various materials and illustrate mathematics.

I work in an electronic structure theory group the first thing anyone does when they join the group is read chapters 1-3 (and possibly work out the problems). The rest of the book might be worthwhile, but there are better, newer books available.

Excellent book for computational chemists

This is a must read book for quantum chemistry. It is written in a clearly way, and it goes from the very basic to the complex approaches in a very progressively.

This is a fundamental resource for understanding the quantum physics applications of the atom and molecular physics.

Look at the cover, haha. Some scientists were having fun in the 80s. If you want a good intro text in computational chemistry, this is it.

Brand new and fast delivery.

[Download to continue reading...](#)

Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory (Dover Books on Chemistry) Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory
Advanced Molecular Quantum Mechanics: An Introduction to Relativistic Quantum Mechanics and the Quantum Theory of Radiation (Studies in Chemical Physics) Quantum Nanoelectronics: An introduction to electronic nanotechnology and quantum computing Advanced Organic Chemistry: Part A: Structure and Mechanisms: Structure and Mechanisms Pt. A The Quantum Mechanics Solver: How to Apply Quantum Theory to Modern Physics Transition Metal Oxides: An Introduction to Their Electronic Structure and Properties (The International Series of Monographs on Chemistry) Covariant Loop Quantum Gravity: An Elementary Introduction to Quantum Gravity and Spinfoam Theory (Cambridge Monographs on Mathematical Physics) Recent Advances in the Theory of Chemical and Physical Systems: Proceedings of the 9th European Workshop on Quantum Systems in Chemistry and Physics ... in Theoretical Chemistry and Physics) Modern Chemistry Florida: Holt Chemistry and Modern Chemistry FCAT Standardized Test Preparation The Electronic Structure and Chemistry of Solids (Oxford Science Publications) Quantum Field Theory in Strongly Correlated Electronic Systems (Theoretical and Mathematical Physics) Molecular Electronic-Structure Theory Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics Introduction to Topological Quantum Matter & Quantum Computation The Nature of the Chemical Bond and the Structure of Molecules and Crystals: An Introduction to Modern Structural Chemistry Study Guide: Ace Organic Chemistry I - The EASY Guide to Ace Organic Chemistry I: (Organic Chemistry Study Guide, Organic Chemistry Review, Concepts, Reaction Mechanisms and Summaries) Ace General Chemistry I and II (The EASY Guide to Ace General Chemistry I and II): General Chemistry Study Guide, General Chemistry Review Group Theory in Chemistry and Spectroscopy: A Simple Guide to Advanced Usage (Dover Books on Chemistry) Medicinal Chemistry: The Modern Drug Discovery Process (Pearson Advanced Chemistry)

Contact Us

DMCA

Privacy

FAQ & Help