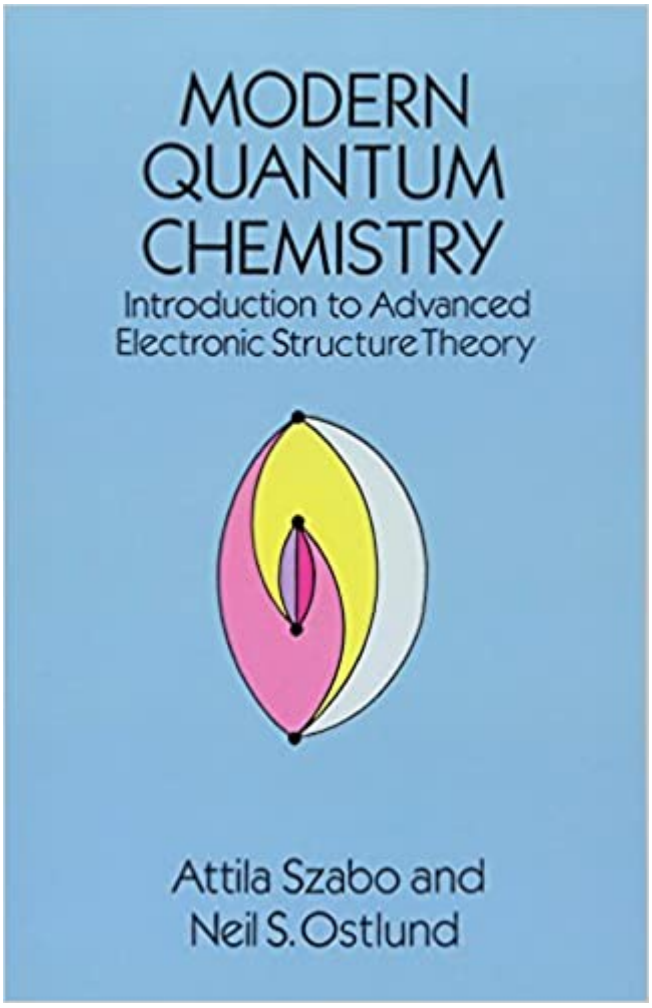
Modern Quantum Chemistry: Introduction To Advanced Electronic Structure Theory (Dover Books On Chemistry)



Synopsis

The aim of this graduate-level textbook is to present and explain, at other than a superficial level, modem 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 (Cl) 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

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Customer Reviews

This book can be pretty neatly divided into two part: 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 give 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-elctron wave functions and operators. This chapter developes 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 martix 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 mathmatics.

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 physic.

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.

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