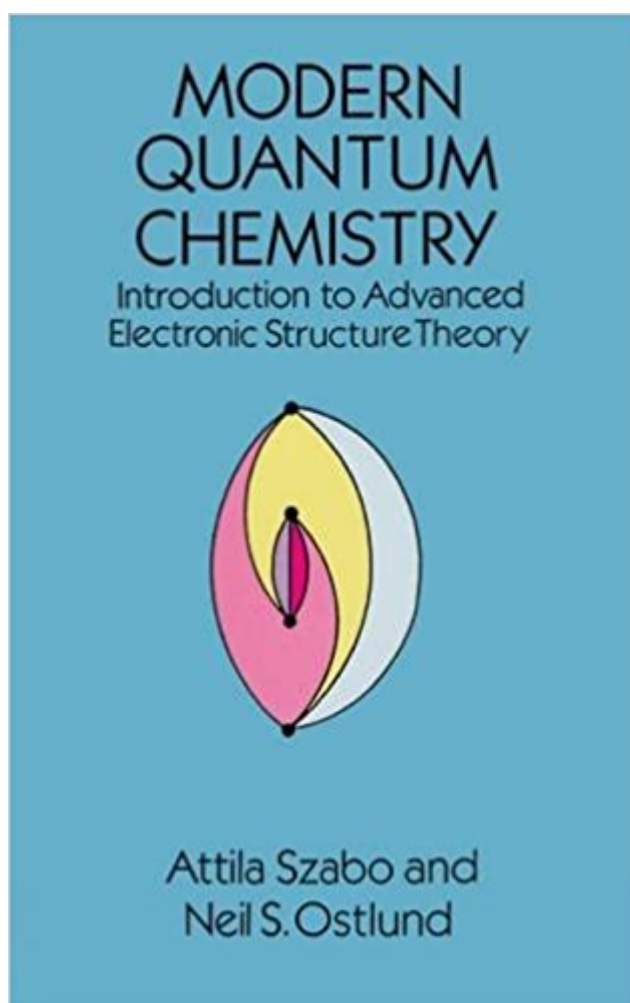


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Modern Quantum Chemistry: Introduction To Advanced Electronic Structure Theory (Dover Books On Chemistry)



Synopsis

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

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Customer Reviews

If you are someone just trying to learn computational chemistry and if you have some background from Quantum Mechanics this book is for you. It starts with 2 chapters of review of quantum mechanics including matrix notations, spin operators, many electron wf etc. If you have not seen these subjects in quantum mechanics you will probably cannot follow the subject. (If you do not have a background you can learn necessary quantum chemistry from Pilar's book) The most important chapter is the 3rd one- Hartree Fock which explains how does a HF calculation operate. Writers just take He^+ & H_2 and show how is the calculation done. You can learn what is electron density, exchange correlation and any other basic terms from this chapter. The next chapters are configuration interaction, pair theories, many body perturbation theory and Green's function. The chapter with perturbation theory is really good and explains most of the core of the subject. This book is always taken as a holy book because it is one of the first qc books that tries to exemplify what do the computer programs calculate in such long periods. It compares the methods their efficiencies in determining geometries, energies, etc. If you have a background and want to learn qc you should start from here. Another book in the same level that I can recommend is the Lecture Notes In Quantum Chemistry (Ed. Roos). If you do not know anything about computational chemistry probably the first book you have to read is Jensen. It becomes really annoying if you do not have any background when reading this book and learn nothing but you have to start somewhere and after you get familiar with the terminology you can circle around Jensen-Pilar-Szabo-Roos learn subject and feel confident to apply the methods.

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