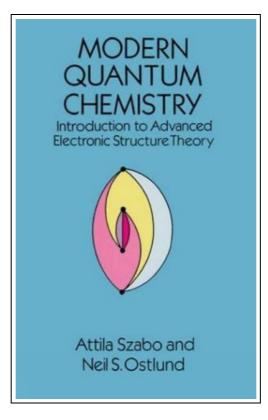
Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory



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Reviews

Great eBook and useful one. it was actually writtern really completely and useful. You are going to like the way the article writer publish this publication. (Prof. Ernestine Emard)

MODERN QUANTUM CHEMISTRY: INTRODUCTION TO ADVANCED ELECTRONIC STRUCTURE THEORY



Dover Publications Inc., United States, 1996. Paperback. Book Condition: New. New edition. 212 x 138 mm. Language: English . Brand New Book. 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.

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