



Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory (Dover Books on Chemistry)

Attila Szabo, Neil S. Ostlund

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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.

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