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Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory

By Attila Szabo, Neil S. Ostlund

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, 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...



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