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Sommario/riassunto

Computational Quantum Chemistry removes much of the mystery of modern computer programs for molecular orbital calculations by showing how to develop Excel spreadsheets to perform model calculations and investigate the properties of basis sets. Using the book together with the CD-ROM provides a unique interactive learning tool. In addition, because of the integration of theory with working examples on the CD-ROM, the reader can apply advanced features available in the spreadsheet to other applications in chemistry, physics, and a variety of disciplines that require the solution