



Concepts and Methods in Modern Theoretical Chemistry: Electronic Structure and Reactivity (Atoms, Molecules, and Clusters)

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Concepts and Methods in Modern Theoretical Chemistry: Electronic Structure and Reactivity, the first book in a two-volume set, focuses on the structure and reactivity of systems and phenomena. A new addition to the series *Atoms, Molecules, and Clusters*, this book offers chapters written by experts in their fields. It enables readers to learn how concepts from *ab initio* quantum chemistry and density functional theory (DFT) can be used to describe, understand, and predict electronic structure and chemical reactivity.

This book covers a wide range of subjects, including discussions on the following topics:

- DFT, particularly the functional and conceptual aspects
- Excited states, molecular electrostatic potentials, and intermolecular interactions
- General theoretical aspects and application to molecules
- Clusters and solids, electronic stress, and electron affinity difference
- The information theory and the virial theorem
- New periodic tables
- The role of the ionization potential

Although most of the chapters are written at a level that is accessible to a senior graduate student, experienced researchers will also find interesting new insights in these experts' perspectives. This comprehensive book provides an invaluable resource toward understanding the whole gamut of atoms, molecules, and clusters.



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