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Sommario/riassunto	Density Functional Theory (DFT) is a powerful technique for calculating and comprehending the molecular and electrical structure of atoms, molecules, clusters, and solids. Its use is based not only on the capacity to calculate the molecular characteristics of the species of interest but also on the provision of interesting concepts that aid in a better understanding of the chemical reactivity of the systems under study. This book presents examples of recent advances, new perspectives, and applications of DFT for the understanding of chemical reactivity through descriptors forming the basis of Conceptual DFT as well as the application of the theory and its related computational procedures in the determination of the molecular properties of different systems of academic, social, and industrial interest.