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Computational Chemistry: Reviews of Current Trends

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This volume comprises six chapters which explore the development and applications of the methods of computational chemistry. The first chapter is on developments in coupled-cluster (CC) theory. The homotopy method is used to obtain complete sets of solutions of nonlinear CC equations. The correspondence between multiple solutions to the CCSD, CCSDT, and full CI equations is established, and the applications of the new approach in modelling molecular systems are discussed. The second chapter reviews the computational theory for the time-dependent calculations of a solution to the Schrodinger equation for two electrons and focuses on the development of propagators to the solution. The next chapter features a discussion on a new self-consistent field for molecular interactions (SCF-MI) scheme for modifying Roothaan equations in order to avoid basis set superposition errors (BSSE). This method is especially suitable for computations of intermolecular interactions. Details of the theory, along with examples of applications to nucleic acid base pair complexes, are given. This chapter is complemented by the following chapter, which reports the status of computational studies of aromatic stacking and hydrogen bonding interactions among nucleic acid bases. The next chapter reveals the possibility of calculating the kinetics of chemical reactions in biological systems from the first principles. The last chapter reviews the results of rigorous "ab initio" studies of the series of derivatives of methane, silane, and germane. The presented molecular and vibrational parameters complement experimental data for these systems. In addition, the theoretical approach allows the prediction of the effects of halogenosubstitutions on their structures and properties.

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