Practical aspects of computational chemistry I : an overview of the last two decades and current trends

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This volume poses (and answers) important questions of interest to the computational chemistry community and beyond. What is the historical background of the "structural chemistry"? Is there any way to avoid the problem of intruder state in the multi-reference formulation? What is the recent progress on multi-reference coupled cluster theory? Starting with a historical account of structural chemistry, the book focuses on the recent advances made in promising theories such as many body Brillouin-Wigner theory, multireference state-specific coupled cluster theory, relativistic effect in chemistry, linear and nonlinear optical properties of molecules, solution to Kohn-Sham problem, electronic structure of solid state materials, development of model core potential, quantum Monte Carlo method, nano and molecular electronics, dynamics of photodimerization and excited states, intermolecular interactions, hydrogen bonding and non-hydrogen bonding interactions, conformational flexibility, metal cations in zeolite catalyst and interaction of nucleic acid bases with minerals.