



Practical Aspects of Computational Chemistry I: An Overview of the Last Two Decades and Current Trends

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Practical Aspects of Computational Chemistry I: An Overview of the Last Two Decades and Current Trends gathers the advances made within the last 20 years by well-known experts in the area of theoretical and computational chemistry and physics. The title itself reflects the celebration of the twentieth anniversary of the “Conference on Current Trends in Computational Chemistry (CCTCC)” to which all authors have participated and contributed to its success.

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.

Practical Aspects of Computational Chemistry I: An Overview of the Last Two Decades and Current Trends is aimed at theoretical and computational chemists, physical chemists, materials scientists, and particularly those who are eager to apply computational chemistry methods to problem of chemical and physical importance. This book will provide valuable information to undergraduate, graduate, and PhD students as well as to established researchers.

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Charles Payne:

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