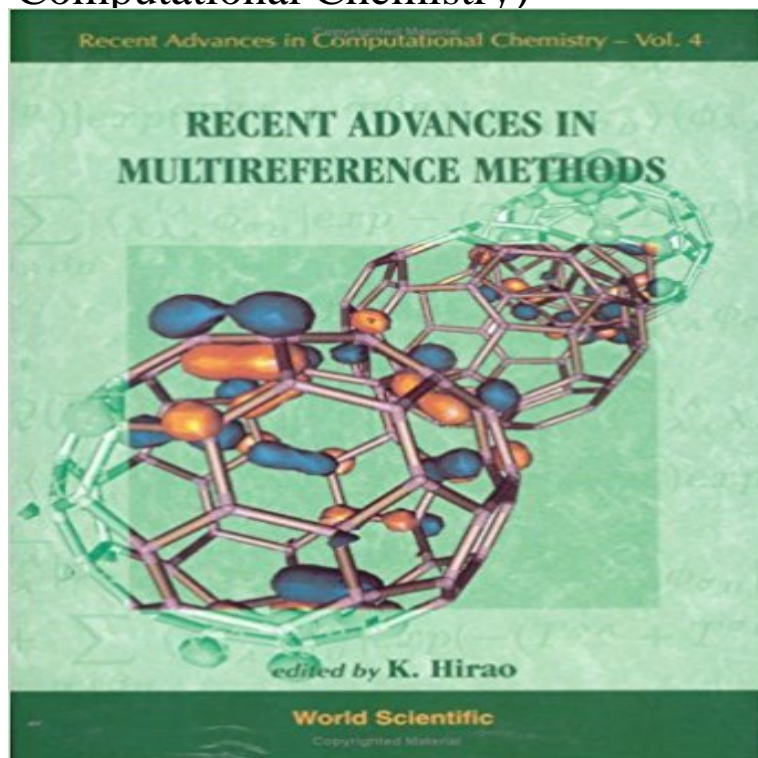


Recent Advances in Multireference Methods (Recent Advances in Computational Chemistry)



Recently, accurate ab initio quantum computational chemistry has evolved dramatically. In particular, the development of multireference-based approaches has opened up a whole new area and has also had a profound impact on the potential of theoretical chemistry. The multiconfigurational SCF (MCSCF)/CASSCF method is an attempt to generalize the Hartree-Fock (HF) model and to treat real chemical processes, where nondynamic correlation is important, while keeping the conceptual simplicity of the HF model as much as possible. Although MCSCF/CASSCF itself does not include dynamic correlations, it provides a good starting point for such studies. There are three approaches to handling dynamic correlations. Beginning with the MCSCF/CASSCF wave function, they are the variational (MRCI), perturbational (MRPT) and cluster expansion (MRCC) approaches. This important book presents the most recent and important developments in multireference-based approaches and their applications. Its main purpose is to highlight essential aspects of the frontiers of multireference theory and provide readers with the fundamental knowledge necessary for further development.

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