Advances in Chemical Physics, Volume 93: New Methods in Computational Quantum Mechanics

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The use of quantum chemistry for the quantitative prediction of molecular properties has long been frustrated by the technical difficulty of carrying out the needed computations. In the last decade there have been substantial advances in the formalism and computer hardware needed to carry out accurate calculations of molecular properties efficiently. These advances have been sufficient to make quantum chemical calculations a reliable tool for the quantitative interpretation of chemical phenomena and a guide to laboratory experiments. However, the success of these recent developments in computational quantum chemistry is not well known outside the community of practitioners. In order to make the larger community of chemical physicists aware of the current state of the subject, this self-contained volume of Advances in Chemical Physics surveys a number of the recent accomplishments in computational quantum chemistry.

This stand-alone work presents the cutting edge of research in computational quantum mechanics. Supplemented with more than 150 illustrations, it provides evaluations of a broad range of methods, including:
* Quantum Monte Carlo methods in chemistry
* Monte Carlo methods for real-time path integration
* The Redfield equation in condensed-phase quantum dynamics
* Path-integral centroid methods in quantum statistical mechanics and dynamics
* Multiconfigurational perturbation theory-applications in electronic spectroscopy
* Electronic structure calculations for molecules containing transition metals
* And more

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