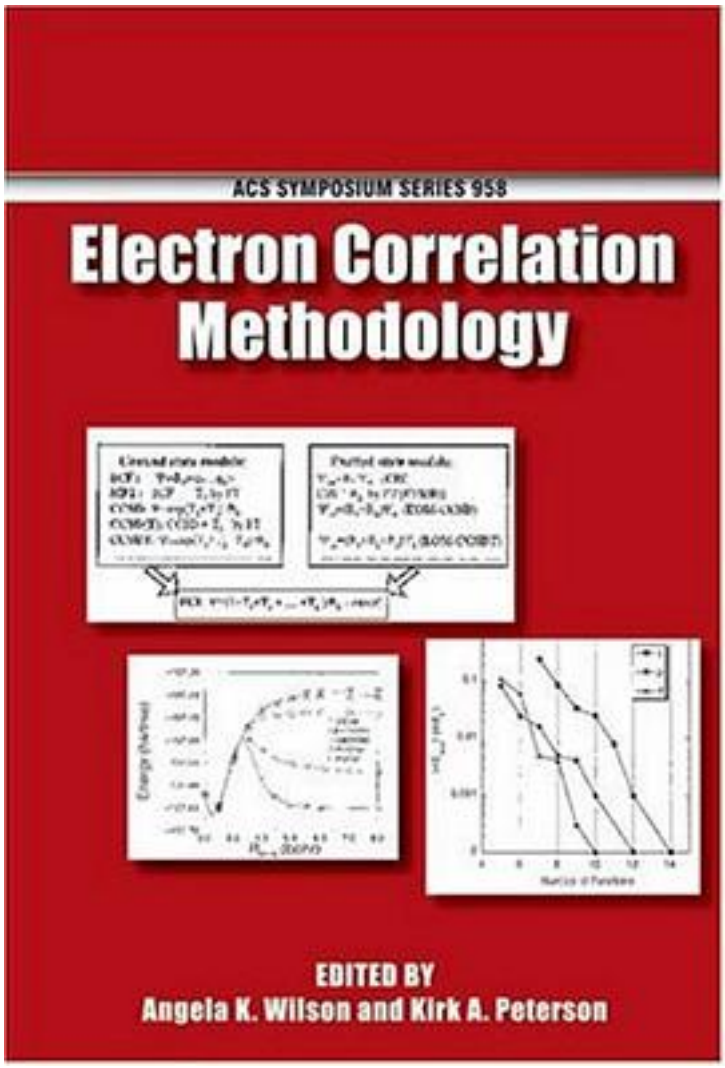
Recent Advances In Electron Correlation Methodology



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著者:Wilson, Angela K. (EDT)/ Peterson, Kirk A. (EDT)

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Modeling is becoming a significant component in the design and analysis of chemical systems in areas such as catalysis, nanomaterials, and biological systems. With rapidly advancing technology, there is an increasing need to model molecules that are quite large and complex, and to model such systems with reasonable accuracy. However, computational methods are generally more numerous and reliable for lighter, smaller molecules since calculations on smaller molecules are less computationally demanding than for larger molecules, and can take advantage of high accuracy, but prohibitively expensive, computational approaches. Two widely used approaches for chemical modeling are ab initio correlated methods and density functional theory. Though there is great interest in using these methods for high accuracy calculations on increasingly larger and more complex chemical systems, each approach currently has limitations. Ab initio methods suffer from a high "N-scaling" problem, where the N-scaling represents the computational cost (memory, disk space, and time requirements of the calculations), thus making high accuracy calculations. Density functional methods have a much lower N-scaling, and thus calculations can be done on much larger molecules. Unfortunately, density functional calculations are generally not as reliable as ab initio approaches, and sometimes, at best can only provide a qualitative description of properties of interest. This volume brings together researchers from throughout the world to assess recent progress in the field of electronic structure methodology, focusing upon ab initio and density functional developments, and to discuss future direction. This publication will impact a number of fields including computational chemistry, organic chemistry, and inorganic chemistry. It will help to provide a closer commonality of ab initio and density functional approaches, as it brings together many of the top senior and junior scientists in both fields to address a common problem: high accuracy modeling of larger chemical systems.

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