

Computational Chemistry: Reviews of Current Trends



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Vast progress in the area of computational chemistry has been achieved in the last decade. Theoretical methods such as quantum mechanics, molecular dynamics and statistical mechanics have been successfully used to characterize chemical systems and to design new materials, drugs and chemicals. The reviews presented in this volume look at the current advances in computational methodologies and applications within the areas of material science and nanotechnology, quantum-chemical methods, as well as bonding in inorganic and biological systems. The major thrust of the book is to bring timely overviews of new findings and applications in the rapidly changing field of computational chemistry.



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