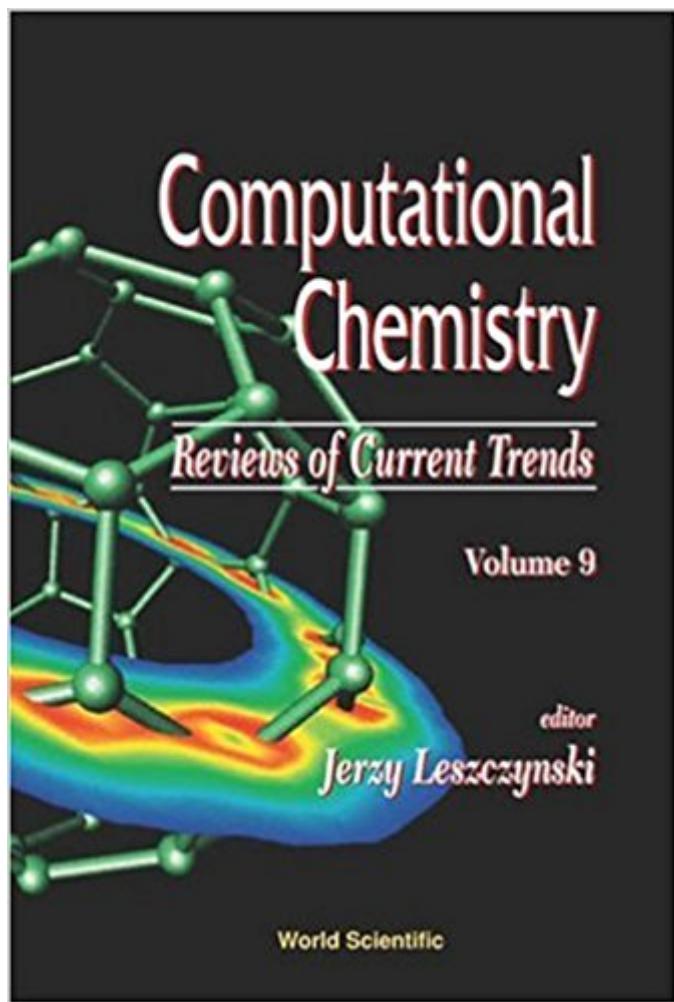


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Computational Chemistry: Reviews Of Current Trends



Synopsis

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 discuss the current advances in computational methodologies and their applications. The areas covered include materials science, nanotechnology, inorganic and biological systems. The major thrust of the book is to bring timely overviews of new findings and methods applied in the rapidly changing field of computational chemistry.

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.. " an excellent source of information not only for advanced specialists, but also for graduate and undergraduate students."

Stay current in computational chemistry with this text. The chapters summarise recent techniques and show the continuing influence of advances in computer hardware and software. Basically, the molecules that you can usefully simulate keep getting bigger. Several chapters discuss ab initio methods. Conceptually, these are always attractive, in enabling a first principles construction of molecules or reactions. There is extensive specific discussion of applying the methods towards DNA molecules. In part to predict various three dimensional structures. The book is ideal for a

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