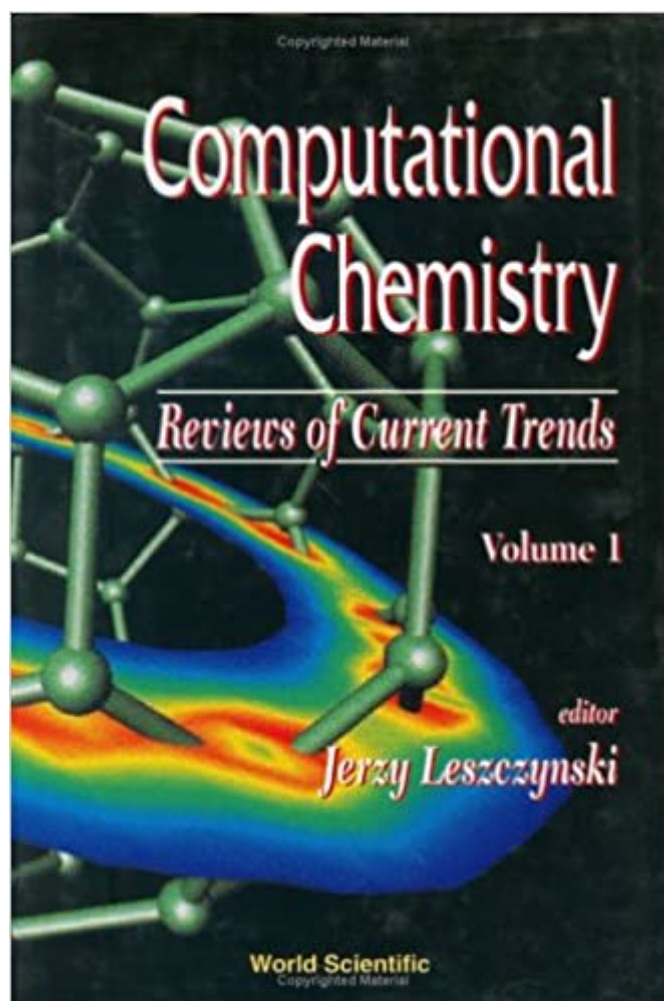The book was found

Computational Chemistry: Reviews Of Current Trends, Vol. 1

Synopsis

This book presents an overview of recent progress in computational techniques as well as examples of the application of existing computational methods in different areas of chemistry, physics, and biochemistry. Introductory chapters cover a broad range of fundamental topics, including: state-of-the-art basis set expansion methods for computing atomic and molecular electronic structures based on the use of relativistic quantum mechanics; the most recent developments in Hartree-Fock methods, particularly in techniques suited for very large systems; the current analysis of the solute-solvent free energy of interaction and the physical bases used to evaluate the electrostatic, cavitation, and dispersion terms; an introduction to the additive fuzzy electron density fragmentation scheme within various ab initio Hartree-Fock quantum-chemical computational schemes, which has provided the means for generating representative molecular fragment densities characteristic to their local environment within a molecule. This book also features a review of recent ab initio calculations on the structure and interactions of DNA bases, a chapter on computational approaches to the design of safer drugs and their molecular properties, and a systematic conceptual study on a route which allows one to stuff fullerenes.

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