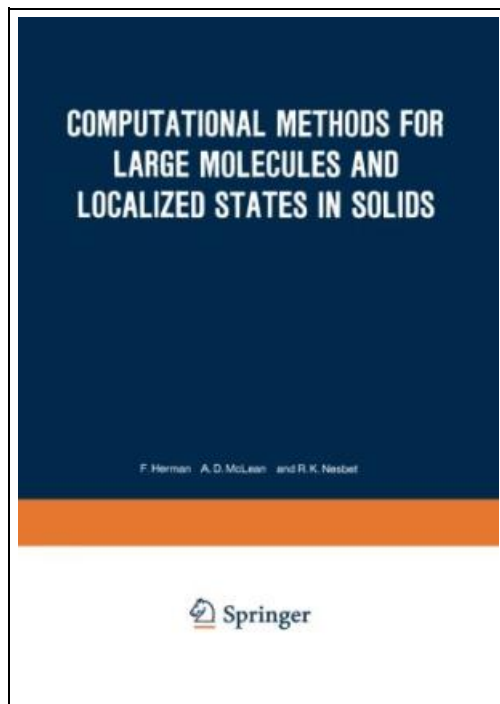


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Reviews

This written book is great. I am quite late in start reading this one, but better then never. You will not really feel monotony at at any moment of your time (that's what catalogues are for about when you check with me).

(Abe Reichel DDS)

COMPUTATIONAL METHODS FOR LARGE MOLECULES AND LOCALIZED STATES IN SOLIDS



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Book Condition: New. Publisher/Verlag: Springer, Berlin | Proceedings of a Symposium, Held May 15-17, 1972, at the IBM Research Laboratory, San Jose, California | During the past few years, there has been dramatic progress in theoretical and computational studies of large molecules and localized states in solids. Various semi-empirical and first-principles methods well known in quantum chemistry have been applied with considerable success to ever larger and more complex molecules, including some of biological importance, as well as to selected solid state problems involving localized electronic states. Increasingly, solid state physicists are adopting a molecular point of view in attempting to understand the nature of electronic states associated with (a) isolated structural and chemical defects in solids; (b) surfaces and interfaces; and (c) bulk disordered solids, most notably amorphous semiconductors. Moreover, many concepts and methods already widely used in solid state physics are being adapted to molecular problems. These adaptations include pseudopotentials, statistical exchange approximations, muffin-tin model potentials, and multiple scattering and cellular methods. In addition, many new approaches are being devised to deal with progressively more complex molecular and localized electronic state problems. | Welcoming Remarks.- 1. Scientific Challenges I.- Introductory Remarks.- Quantum Chemistry. Theory of Geometries and Energies of Small Molecules.- Organic Transition States.- Solid State Concepts in Radiation Chemistry and Biology.- Molecular Modeling by Computer.- 2. Scientific Challenges II.- Introductory Remarks.- Structural Characteristics and Electronic States of Hemoglobin.- Molecular Theory of Nucleation.- 3. Computational Methods I.- Approximations for Large-Molecule Calculations.- AB Initio Computation of Molecular Structures Through Configuration Interaction.- Approximate Methods in Quantum Chemistry.- LCAO-MO Cluster Model for Localized States in Covalent Solids.- Description of Molecules in Terms of Localized Orbitals.- 4. Computational Methods II.- Introductory Remarks.- The SCF-X? Scattered-Wave Method.- The Orbital Correction Method.- Panel Discussion on Computational Methods.- AB Initio...



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