

### Methods in Computational Molecular Physics (Nato Science Series C:)



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This NATO Advanced Study Institute was concerned with modern ab initio methods for the determination of the electronic structure of molecules. Recent years have seen considerable progress in computer technology and computer science and these developments have had a very significant influence on computational molecular physics. Progress in computer technology has led to increasingly larger and faster systems as well as powerful minicomputers. Simultaneous research in computer science has explored new methods for the optimal use of these resources. To a large extent develop ments in computer technology, computer science and computational molecular physics have been mutually dependent. The availability of new computational resources, particularly minicomputers and, more recently, vector processors, has stimulated a great deal of research in molecular physics. Well established techniques have been reformulated to make more efficient use of the new computer technology and algorithms which were previously computationally intractable have now been successfully implemented. This research has given a new and exciting insight into molecular structure and molecular processes by enabling smaller systems to be studied in greater detail and larger systems to be studied for the first time.

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