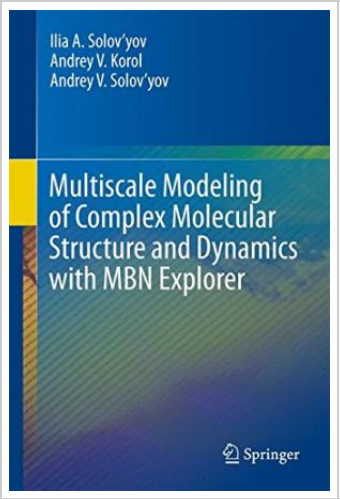

Multiscale Simulations of Complex Molecular Structure and Dynamics with the MBN Explorer

By Andrey Korol

Springer. Hardcover. Condition: New. 480 pages. This book introduces readers to MesoBioNano (MBN) Explorer a multi-purpose software package designed to model molecular systems at various levels of size and complexity. In addition, it presents a specially designed multi-task toolkit and interface the MBN Studio which enables the set-up of input files, controls the simulations, and supports the subsequent visualization and analysis of the results obtained. The book subsequently provides a systematic description of the capabilities of this universal and powerful software package within the framework of computational molecular science, and guides readers through its applications in numerous areas of research in bio- and chemical physics and material science ranging from the nano- to the meso-scale. MBN Explorer is particularly suited to computing the systems energy, to optimizing molecular structure, and to exploring the various facets of molecular and random walk dynamics. The package allows the use of a broad variety of interatomic potentials and can, e. g. , be configured to select any subset of a molecular system as rigid fragments, whenever a significant reduction in the number of dynamical degrees of freedom is required for computational practicalities. MBN Studio enables users to easily construct initial geometries for the molecular,...

Reviews

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