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ISBN: 9780471184393

"Provides a lot of reading pleasure and many new insights." -Journal of Molecular Structure

"This is the most entertaining, stimulating and useful book which can be thoroughly recommended to anyone with an interest in computer simulation." -Contemporary Physics

"A very useful introduction . . . more interesting to read than the often dry equation-based texts." -Journal of the American Chemical Society

Written especially for the novice, Molecular Dynamics Simulation demonstrates how molecular dynamics simulations work and how to perform them, focusing on how to devise a model for specific molecules and then how to simulate their movements using a computer. This book provides a collection of methods that until now have been scattered through the literature of the last 25 years. It reviews elements of sampling theory and discusses how modern notions of chaos and nonlinear dynamics explain the workings of molecular dynamics.