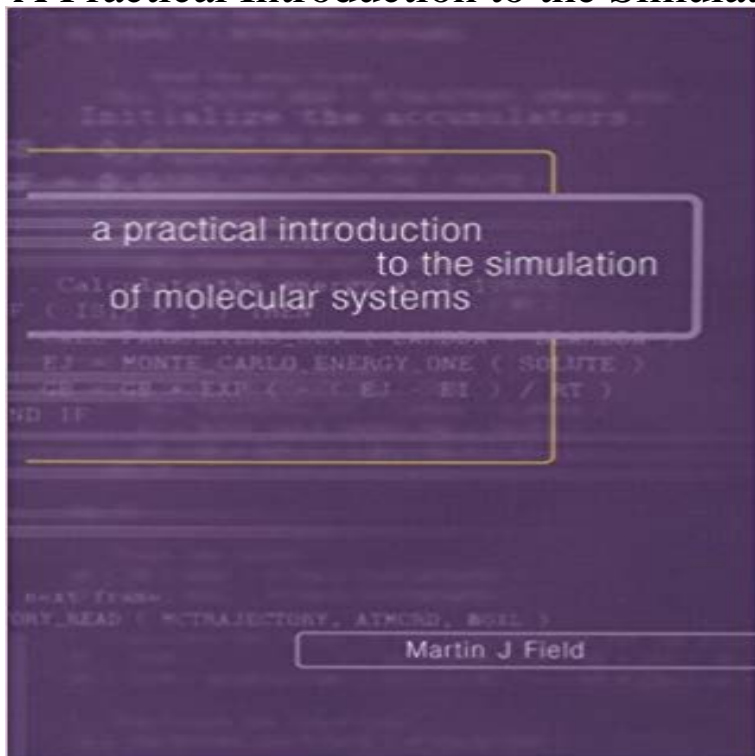


A Practical Introduction to the Simulation of Molecular Systems



In this vital resource, Martin Field provides a practical introduction to the range of different techniques available for the simulation of molecular systems. The text includes a library of program modules written in Fortran 90 with which the simulations discussed were performed. Each chapter describes a general class of methods or algorithms, and then illustrates their use with example programs, written using the module library. Topics covered include energy functions, geometry optimization and reaction path location techniques, normal mode analysis, molecular dynamics and Monte Carlo simulations and free energy calculations. This book will be of interest to advanced undergraduates, graduate students and researchers who use molecular simulation techniques, particularly in theoretical and computational chemistry, biophysics, and computational molecular physics.

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