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Descrizione fisica	1 online resource (XV, 463 p. 65 illus., 21 illus. in color.)
Collana	Scientific Computation, , 1434-8322
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Soggetti	Physics Chemistry, Physical and theoretical Bioinformatics Atomic structure Molecular structure Materials science Physical chemistry Numerical and Computational Physics, Simulation Theoretical and Computational Chemistry Computational Biology/Bioinformatics Atomic/Molecular Structure and Spectra Characterization and Evaluation of Materials Physical Chemistry
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Principles of Classical Mechanics -- Principles of Classical Thermodynamics -- Principles of Statistical -- Thermodynamics of Biological Phenomena -- Free Energy Calculation Methods Used in Computer Simulations -- Molecular Dynamics Methods in Simulations of Macromolecules -- Slow Collective Variables of Macromolecular Systems -- Information Theory and Statistical Mechanics -- Practical Aspects of Molecular Dynamics Simulations -- Sympletic and Time Reversible Integrator -- Index.
Sommario/riassunto	This book presents computer simulations using molecular dynamics

techniques in statistical physics, with a focus on macromolecular systems. The numerical methods are introduced in the form of computer algorithms and can be implemented in computers using any desired computer programming language, such as Fortran 90, C/C++, and others. The book also explains how some of these numerical methods and their algorithms can be implemented in the existing computer programming software of macromolecular systems, such as the CHARMM program. In addition, it examines a number of advanced concepts of computer simulation techniques used in statistical physics as well as biological and physical systems. Discussing the molecular dynamics approach in detail to enhance readers understanding of the use of this method in statistical physics problems, it also describes the equations of motion in various statistical ensembles to mimic real-world experimental conditions. Intended for graduate students and research scientists working in the field of theoretical and computational biophysics, physics and chemistry, the book can also be used by postgraduate students of other disciplines, such as applied mathematics, computer sciences, and bioinformatics. Further, offering insights into fundamental theory, it as a valuable resource for expert practitioners and programmers and those new to the field. .