1. Record Nr. UNISA996418179303316

Autore	Kamberaj Hiqmet
Titolo	Molecular Dynamics Simulations in Statistical Physics: Theory and Applications [[electronic resource] /] / by Hiqmet Kamberaj
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2020
ISBN	3-030-35702-3
Edizione	[1st ed. 2020.]
Descrizione fisica	1 online resource (XV, 463 p. 65 illus., 21 illus. in color.)
Collana	Scientific Computation, , 1434-8322
Disciplina	530.13
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
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
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. .

2. Record Nr. UNINA9910810924403321

Autore	Buck Pearl S (Pearl Sydenstricker), <1892-1973, >
Titolo	Peony / / Pearl S. Buck
Pubbl/distr/stampa	New York, New York : , : Open Road Media Integrated Media, , 2012 ©1948
ISBN	1-4532-6353-5
Descrizione fisica	1 online resource (339 p.)
Disciplina	813.54
Soggetti	Jews
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Sommario/riassunto	The Nobel Prizewinning author's perceptive fable of cross-cultural passions in nineteenth-century ChinaIn 1850s China, a young girl, Peony, is sold to work as a bondmaid for a rich Jewish family in Kaifeng. Jews have lived for centuries in this region of the country, but by the mid-nineteenth century, assimilation has begun taking its toll on their small enclave. When Peony and the family's son, David, grow up and fall in love with one another, they face strong opposition from every side. Tradition forbids the marriage, and the family already has a rabbi's daughter in mind for David.Long celebrated for its subtle and even-handed treatment of colliding traditions, Peony is an engaging coming-of-age story about love, identity, and the tragedy and beauty found at the intersection of two disparate cultures. This ebook features an illustrated biography of Pearl S. Buck including rare images from the author's estate.