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Description. Understanding Molecular Simulation: From Algorithms to Applications explains the physics behind the "recipes" of molecular simulation for materials science. Computer simulators are continuously confronted with questions concerning

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the choice of a particular technique for a given application. A wide variety of tools exist, so the choice of technique requires a good understanding of the basic principles.

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Book: Understanding Molecular Simulation. This is a textbook on molecular simulations Daan Frenkel and I wrote in 1996 the first edition and 2002 the second edition. Daan and I were unhappy with the notion that a molecular simulation program is nothing more than a set of recipes.

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Understanding ... | Berend Smit
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DataGrid - Nagy Daniel E.V.

I have several other MD books, including Haile's Molecular Dynamics Simulation: Elementary Methods, Tuckerman's Statistical Mechanics: Theory and Molecular Simulation (Oxford Graduate Texts), Frenkel&Smit's Understanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science Series, Vol 1), and Rapaport's The Art of Molecular Dynamics Simulation. I have learned nothing from Rapaport and very little from Frenkel&Smit, but a lot from Haile, Tuckerman, and ...

Understanding Molecular Simulation: From Algorithms to Applications explains the physics behind the "recipes" of molecular simulation for materials science. Computer simulators are continuously confronted with questions concerning the choice of a particular technique for a given application. A wide variety of tools exist, so the choice of technique requires a good understanding of the basic principles. More importantly, such understanding may greatly improve the efficiency of a simulation program. The implementation of simulation methods is illustrated in pseudocodes and their practical use in the case studies used in the text. Since the first edition only five years ago, the simulation world has changed significantly -- current techniques have matured and new ones have appeared. This new edition deals with these new developments; in particular, there are sections on:

- Transition path sampling and diffusive barrier crossing to simulates rare events
- Dissipative particle dynamic as a coarse-grained simulation technique
- Novel schemes to compute the long-ranged forces
- Hamiltonian and non-Hamiltonian dynamics in the context constant-temperature and constant-pressure molecular dynamics simulations
- Multiple-time step algorithms as an alternative for constraints
- Defects in solids
- The pruned-enriched Rosenbluth sampling, recoil-growth, and concerted rotations for complex molecules
- Parallel tempering for glassy Hamiltonians

Examples are included that highlight current applications and the codes of case studies are available on the World Wide Web. Several new examples have been added since the first edition to illustrate recent applications. Questions are included in this new edition. No prior knowledge of computer simulation is assumed.

This book explains the physics behind the "recipes" of molecular simulation for materials science. Computer simulators are continuously confronted with questions concerning the choice of a particular technique for a given application. Since a wide variety of computational tools exists, the choice of technique requires a good understanding of the basic principles. More importantly, such understanding may greatly improve the efficiency of a simulation program. The implementation of simulation methods is illustrated in pseudocodes and their practical use in the case studies used in the text. Examples are

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included that highlight current applications, and the codes of the case studies are available on the World Wide Web. No prior knowledge of computer simulation is assumed.

Complex systems that bridge the traditional disciplines of physics, chemistry, biology, and materials science can be studied at an unprecedented level of detail using increasingly sophisticated theoretical methodology and high-speed computers. The aim of this book is to prepare burgeoning users and developers to become active participants in this exciting and rapidly advancing research area by uniting for the first time, in one monograph, the basic concepts of equilibrium and time-dependent statistical mechanics with the modern techniques used to solve the complex problems that arise in real-world applications. The book contains a detailed review of classical and quantum mechanics, in-depth discussions of the most commonly used ensembles simultaneously with modern computational techniques such as molecular dynamics and Monte Carlo, and important topics including free-energy calculations, linear-response theory, harmonic baths and the generalized Langevin equation, critical phenomena, and advanced conformational sampling methods. Burgeoning users and developers are thus provided firm grounding to become active participants in this exciting and rapidly advancing research area, while experienced practitioners will find the book to be a useful reference tool for the field.

Molecular simulation is a powerful tool in materials science, physics, chemistry and biomolecular fields. This updated edition provides a pragmatic introduction to a wide range of techniques for the simulation of molecular systems at the atomic level. The first part concentrates on methods for calculating the potential energy of a molecular system, with new chapters on quantum chemical, molecular mechanical and hybrid potential techniques. The second part describes methods examining conformational, dynamical and thermodynamical properties of systems, covering techniques including geometry-optimization, normal-mode analysis, molecular dynamics, and Monte Carlo simulation. Using Python, the second edition includes numerous examples and program modules for each simulation technique, allowing the reader to perform the calculations and appreciate the inherent difficulties involved in each. This is a valuable resource for researchers and graduate students wanting to know how to use atomic-scale molecular simulations. Supplementary material, including the program library and technical information, available through www.cambridge.org/9780521852524.

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Computer simulation is an essential tool in studying the chemistry and physics of liquids. Simulations allow us to develop models and to test them against experimental data. This book is an introduction and practical guide to the molecular dynamics and Monte Carlo methods.

Very broad overview of the field intended for an interdisciplinary audience; Lively discussion of current challenges written in a colloquial style; Author is a rising star in this discipline; Suitably accessible for beginners and suitably rigorous for experts;

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Features extensive four-color illustrations; Appendices featuring homework assignments and reading lists complement the material in the main text

The aim of this book is to examine some of the important aspects of recent progress in the use of molecular simulation for investigating fluids. It encompasses both Monte Carlo and molecular dynamic techniques providing details of theory, algorithms and implementation.

Molecular dynamics simulation is a significant technique to gain insight into the mechanical behavior of nanostructured (NS) materials and associated underlying deformation mechanisms at the atomic scale. The purpose of this book is to detect and correlate critically current achievements and properly assess the state of the art in the mechanical behavior study of NS material in the perspective of the atomic scale simulation of the deformation process. More precisely, the book aims to provide representative examples of mechanical behavior studies carried out using molecular dynamics simulations, which provide contributory research findings toward progress in the field of NS material technology.

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