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Molecular simulations (introduction) Molecular dynamics MD Monte carlo MC

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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 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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Understanding Molecular Simulation: From Algorithms to Applications, second edition Daan Frenkel and Berend Smit. From the Preface: "The book is aimed at readers who are active in computer simulation, or are planning to become so. Computer simulators are continuously confronted with questions concerning the choice of technique, because there is ...

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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
Understanding Molecular Simulation: From Algorithms to Applications (Computational Science Series, Vol 1) 2nd Edition, Kindle Edition by Daan Frenkel (Author)

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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 simulaterare events · Dissipative particle dynamic as a course-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 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.

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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.

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.

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.

Molecular Driving Forces, Second Edition E-book is an introductory statistical thermodynamics text that describes the principles and forces that drive chemical and biological processes. It demonstrates how the complex behaviors of molecules can result from a few simple physical processes, and how simple models provide surprisingly accurate insights into the workings of the molecular world. Widely adopted in its First Edition, Molecular Driving Forces is regarded by teachers and students as an accessible textbook that illuminates underlying principles and concepts. The Second Edition includes two brand new chapters: (1) "Microscopic Dynamics" introduces single molecule experiments; and (2) "Molecular Machines" considers how nanoscale machines and engines work. "The Logic of Thermodynamics" has been expanded to its own chapter and now covers heat, work, processes, pathways, and cycles. New practical applications, examples, and end-of-chapter questions are integrated throughout the revised and updated text, exploring topics in biology, environmental and energy science, and nanotechnology. Written in a clear and reader-friendly style, the book provides an excellent introduction to the subject for novices while remaining a valuable resource for experts.

This book presents the most important and main concepts of the molecular and microsimulation techniques. It enables readers to improve their skills in developing simulation programs by providing physical problems and sample simulation programs for them to use. Provides tools to develop skills in developing simulations programs Includes sample simulation programs for the reader to use Appendix explains Fortran and C languages in simple terms to allow the non-expert to use them

Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas. The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

Addressing the need of chemistry, biology and engineering students to understand and perform their own molecular simulations, the author introduces the fundamentals of molecular modeling for a broad, practice-oriented audience and presents versatile practical applications. The book presents a thorough overview of the underlying concepts.