Understanding Molecular Simulation From Algorithms To Applications

Computational Materials Science provides the theoretical basis necessary for understanding atomic surface phenomena and processes of phase transitions, especially crystallization, is given. The most important information concerning computer simulation by different methods and simulation techniques for modeling of physical systems is also presented. A number of results are discussed regarding modern studies of surface processes during crystallization. There is sufficiently full information on experiments, theory, and simulations concerning the surface roughening transition, kinetic roughening, nucleation kinetics, stability of crystal shapes, thin film formation, imperfect structure of small crystals, size dependent growth velocity, distribution coefficient at growth from alloy melts, superstructure ordering in the intermetallic compound. Computational experiments described in the last chapter allow visualization of the course of many processes and better understanding of many key problems in Materials Science. There is a set of practical steps concerning computational procedures presented. Open access to executable files in the book make it possible for everyone to understand better phenomena and processes described in the book. Valuable reference book, but also helpful as a supplement to courses Computer programs available to supplement examples Presents several new methods of computational materials science and clearly summarizes previous methods and results
"In the opening chapter of An Introduction to Molecular Dynamics, the method of statistical geometry, based on the construction of a Voronoi polyhedral, is applied to the pattern recognition of atomic environments and to the investigation of the local order in molecular dynamics-simulated materials. Next, the authors discuss the methodology of bimolecular simulations and their advancements, as well as their applications in the field of nanoparticle-biomolecular interactions. The theory of molecular dynamics simulation and some of the recent molecular dynamics methods such as steered molecular dynamics, umbrella sampling, and coarse-grained simulation are also discussed. The use of auxiliary programs in the cases of modified cyclodextrins is discussed. Additionally, results from molecular dynamics studies on cases of inclusion compounds of molecules of different sizes and shapes encapsulated in the same host cyclodextrin have been examined and compared. In closing, the authors discuss the methodology of molecular dynamics simulation with a non-constant force field. In the context of molecular simulations, the term "force field" refers to a set of equations and parameters for the calculation of forces acting on the particles of the system and its potential energy"--
Understand the LAMMPS source code and modify it to meet your research needs, and run simulations for bespoke applications involving forces, thermostats, pair potentials and more with ease Key FeaturesUnderstand the structure of the LAMMPS source codeImplement custom features in the LAMMPS source code to meet your research needsRun example simulations involving forces, thermostats, and pair potentials based on implemented featuresBook Description LAMMPS is one of the most widely used tools for running simulations for research in molecular dynamics. While the tool itself is fairly easy to use, more often than not you'll need to customize it to meet your specific simulation requirements. Extending and Modifying LAMMPS bridges this learning gap and helps you achieve this by writing custom code to add new features to LAMMPS source code. Written by ardent supporters of LAMMPS, this practical guide will enable you to extend the capabilities of LAMMPS with the help of step-by-step explanations of essential concepts, practical examples, and self-assessment questions. This LAMMPS book provides a hands-on approach to implementing associated methodologies that will get you up and running and productive in no time. You'll begin with a short introduction to the internal mechanisms of LAMMPS, and gradually transition to an overview of the source code along with a tutorial on modifying it. As you advance, you'll understand the structure, syntax, and organization of LAMMPS source code, and be able to write your own source code extensions to LAMMPS that implement features beyond the ones available in standard downloadable versions. By the end of this book, you'll have learned how to add your own extensions and modifications to the LAMMPS source code that can implement features that suit your simulation requirements. What you will learnIdentify how LAMMPS input script commands are parsed within the source codeUnderstand the architecture of the source codeRelate source code elements to simulated quantitiesLearn how stored quantities are accessed within the source codeExplore the mechanisms controlling pair styles, computes, and fixesModify the source code to implement custom features in LAMMPSWho this book is for This book is for students, faculty members, and researchers who are currently using LAMMPS or considering switching to LAMMPS, have a basic knowledge of how to use LAMMPS, and are looking to extend LAMMPS source code for research purposes. This book is not a tutorial on using LAMMPS or writing LAMMPS scripts, and it is assumed that the reader is comfortable with the basic LAMMPS syntax. The book is geared toward users with little to no experience in source code editing. Familiarity with C++ programming is helpful but not necessary.
First time paperback of successful physics monograph. Copyright © Libri GmbH. All rights reserved.
Nonequilibrium Gas Dynamics and Molecular Simulation
Molecular Dynamics Simulation of Nanostructured Materials
Biomolecular and Bioanalytical Techniques

Computational Materials Science
An Understanding of Mechanical Behavior

The aim of the book is to provide an understanding of the current science underpinning Carbon Capture and Sequestration (CCS) and to provide students and interested researchers with sufficient background on the basics of Chemical Engineering, Material Science, and Geology that they can understand the current state of the art of the research in the field of CCS. In addition, the book provides a comprehensive discussion of the impact of CCS on the energy landscape, society, and climate as these topics govern the success of the science being done in this field. The book is aimed at undergraduate students, graduate students, scientists, and professionals who would like to gain a broad multidisciplinary view of the research that is being carried out to solve one of greatest challenges of our generation. Contents:Energy and ElectricityThe Atmosphere and Climate ModelingThe Carbon CycleIntroduction to Carbon CaptureAbsorptionAdsorptionMembranesIntroduction to Geological SequestrationFluids and RocksLarge-Scale Geological Carbon SequestrationLand Use and Geo-EngineeringList of SymbolsCredits Readership: Students taking courses on environmental sciences and research level individuals who are interested in environmental issues related to CCS. Key Features:The first comprehensive textbook on Carbon Capture and Sequestration (CCS)A comprehensive discussion on the science of CCS and its impact on society and climateA multidisciplinary approach to CCS by the leading US research centers on CCSKeywords:Carbon Capture;Carbon Storage;Carbon Sequestration;Gas Separations
Protein folding is a process by which a protein structure assumes its functional shape of conformation, and has been the subject of research since the publication of the first software tool for protein structure prediction. Protein folding in silico approaches this issue by introducing an ab initio model that attempts to simulate as far as possible the folding process as it takes place in vivo, and attempts to construct a mechanistic model on the basis of the predictions made. The opening

chapters discuss the early stage intermediate and late stage intermediate models, followed by a discussion of structural information that affects the interpretation of the folding process. The second half of the book covers a variety of topics including ligand binding site recognition, the "fuzzy oil drop" model and its use in simulation of the polypeptide chain, and misfolded proteins. The book ends with an overview of a number of other ab initio methods for protein structure predictions and some concluding remarks. Discusses a range of ab initio models for protein structure prediction Introduces a unique model based on experimental observations Describes various methods for the quantitative assessment of the presented models from the viewpoint of information theory

An essential guide to biomolecular and bioanalytical techniques and their applications Biomolecular and Bioanalytical Techniques offers an introduction to, and a basic understanding of, a wide range of biophysical techniques. The text takes an interdisciplinary approach with contributions from a panel of distinguished experts. With a focus on research, the text comprehensively covers a broad selection of topics drawn from contemporary research in the fields of chemistry and biology. Each of the internationally reputed authors has contributed a single chapter on a specific technique. The chapters cover the specific technique's background, theory, principles, technique, methodology, protocol and applications. The text explores the use of a variety of analytical tools to characterise biological samples. The contributors explain how to identify and quantify biochemically important molecules, including small molecules as well as biological macromolecules such as enzymes, antibodies, proteins, peptides and nucleic acids. This book is filled with essential knowledge and explores the skills needed to carry out the research and development roles in academic and industrial laboratories. A technique-focused book that bridges the gap between an introductory text and a book on advanced research methods Provides the necessary background and skills needed to advance the research methods Features a structured approach within each chapter Demonstrates an interdisciplinary approach that serves to develop independent thinking Written for students in chemistry, biological, medical, pharmaceutical, forensic and biophysical sciences, Biomolecular and Bioanalytical Techniques is an in-depth review of the most current biomolecular and bioanalytical techniques in the field.

Capitalist Nigger is an explosive and jarring indictment of the black race. The book asserts that the Negroid race, as naturally endowed as any other, is culpably a non-productive race, a consumer race that depends on other communities for its culture, its language, its feeding and its clothing. Despite enormous natural resources, blacks are economic slaves because they lack the 'devil-may-care' attitude and the 'killer instinct' of the Caucasian, as well as the spider web mentality of the Asian. A Capitalist Nigger must embody ruthlessness in pursuit of excellence in his drive towards achieving the goal of becoming an economic warrior. In putting forward the idea of the Capitalist Nigger, Chika Onyeani charts a road to success whereby black economic warriors employ the 'Spider Web Doctrine' – discipline, self-reliance, ruthlessness – to escape from their victim mentality. Born in Nigeria, Chika Onyeani is a journalist, editor and former diplomat.

Capitalist Nigger

Molecular Modeling and Simulation

A pragmatic guide to extending LAMMPS as per custom simulation requirements

Thermodynamics and Statistical Mechanics

Computational Pharmaceutics

Nonequilibrium Molecular Dynamics

Introduction to Computational Chemistry 3rd Edition provides a comprehensive account of the fundamental principles underlying different computational methods. Fully revised and updated throughout to reflect important method developments and improvements since publication of the previous edition, this timely update includes the following significant revisions and new topics: Polarizable force fields Tight-binding DFT More extensive DFT functionals, excited states and time dependent molecular properties Accelerated Molecular Dynamics methods Tensor decomposition methods Cluster analysis Reduced scaling and reduced prefactor methods Additional information is available at: www.wiley.com/go/jensen/computationalchemistry3

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.

"The book is divided into two parts based on the overall goals, with the first part focusing on fundamental considerations, and the second part dedicated to describing computer simulation methods. The first section covers three different areas: (1) kinetic theory, (2) quantum mechanics, and (3) statistical mechanics. Important results from these three areas are then brought together to allow analysis of nonequilibrium processes in a gas based on molecular level considerations. Chapter 1 covers kinetic theory, in which the basic idea is to develop techniques to relate the properties and behavior of particles, representing atoms and molecules, to the fluid mechanical aspects of a gas at the macroscopic level. This requires us to provide a basic definition by what is meant by a particle, and how these particles interact with one another through the mechanism of inter-molecular collisions. This leads us into a discussion of modeling of macroscopic molecular transport processes, such as viscosity and thermal conductivity, that represents one of the first key successes of kinetic theory. We will find that kinetic theory relies on the use of statistical analysis techniques, such as probability density functions, due to the very large volumes of information involved in tracking the behavior of every single particle in a real gas flow"--

The Monte Carlo method is now widely used and commonly accepted as an important and useful tool in solid state physics and related fields. It is broadly recognized that the technique of "computer simulation" is complementary to both analytical theory and experiment, and can significantly contribute to ad vancing the understanding of various scientific problems. Widespread applications of the Monte Carlo method to various fields of the statistical mechanics of condensed matter physics have already been reviewed in two previously published books, namely Monte Carlo Methods in Statistical Physics (Topics Curro Phys. , Vol. 7, 1st edn. 1979, 2ndedn. 1986) and Applications of the Monte Carlo Method in Statistical Physics (Topics Curro Phys. , Vol. 36, 1st edn. 1984, 2nd edn. 1987). Meanwhile the field has continued its rapid growth and expansion, and applications to new fields have appeared that were not treated at all in the above two books (e. g. studies of irreversible growth phenomena, cellular automata, interfaces, and quantum problems on lattices). Also, new methodic aspects have emerged, such as aspects of efficient use of vector com puters or parallel computers, more efficient analysis of simulated systems con figurations, and methods to reduce critical slowing down at i>hase transitions.

Taken together with the extensive activity in certain traditional areas of research (simulation of classical and quantum fluids, of macromolecular materials, of spin glasses and quadrupolar glasses, etc.

Introduction to Practice of Molecular Simulation

Computational Many-Particle Physics

Surfaces, Interfaces, Crystallization

Application of Molecular Modeling in Drug Delivery

AB INITIO Molecular Orbital Theory

An Integrated Approach

This book details the necessary numerical methods, the theoretical background and foundations and the techniques involved in creating computer particle models, including linked-cell method, SPME-method, tree codes, amd multipol technique. It illustrates modeling, discretization, algorithms and their parallel implementation with MPI on computer systems with distributed memory. The text offers step-by-step explanations of numerical simulation, providing illustrative code examples. With the description of the algorithms and the presentation of the results of various simulations from fields such as material science, nanotechnology, biochemistry and astrophysics, the reader of this book will learn how to write programs capable of running successful experiments for molecular dynamics.

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.

Looking for the real state of play in computational many-particle physics? Look no further. This book presents an overview of state-of-the-art numerical methods for studying interacting classical and quantum many-particle systems. A broad range of techniques and algorithms are covered, and emphasis is placed on their implementation on modern high-performance computers. This excellent book comes complete with online files and updates allowing readers to stay right up to date.

Molecular Dynamic Simulation: Fundamentals and Applications explains the fundamentals of MD simulation and explores recent developments in advanced modeling approaches based on the MD method. The improvements in efficiency and accuracy delivered by this new research are explained to help readers apply them to a wide range of tasks. Details of the implementation of MD simulation are illustrated by presenting the applications of MD simulation in various aspects of materials study including mechanical, thermal, mass transportation, and absorption/desorption problems. Innovative methods of using MD to explore the mechanics of nano/micromaterials, and for the characterization of crystalline, amorphous and liquid materials are also presented. The rich research experience of the authors in molecular dynamic simulation will ensure that readers are provided with both an in-depth understanding of this method and clear technical guidance. Examines applications of MD to simulation of mechanics of nano/micromaterials, and characterization of crystalline, amorphous and liquid materials Provides a thorough overview of the theory behind molecular dynamics simulation Applies Molecular dynamic simulation to a broad range of mechanical, thermal, and mass transport problems

From Algorithms to Applications

Extending and Modifying LAMMPS Writing Your Own Source Code

Protein Folding in Silico

Statistical Mechanics: Theory and Molecular Simulation
A Practical Introduction to the Simulation of Molecular Systems
Understanding Molecular Simulation

This book clearly explains the principles of in silico tools of molecular docking and molecular dynamics. It provides examples of algorithms and procedures proposed by different software programs for visualizing and identifying potential interactions in complexes of biochemical interest. The book is structured in six chapters, each of which discusses different molecular simulation methodologies and provides concrete examples of complexes interactions. In each chapter authors give an overview of the treated subject, a description of the methodologies used, and a discussion of the results. The authors describe computational ways to achieve a rational design of bioactive compounds with various therapeutic applications, including antitumoral agents, antitubercular drugs, nonsteroidal anti-inflammatory drugs, and radiopharmaceuticals.

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.

This comprehensive collection of lectures by leading experts in the field introduces and reviews all relevant computer simulation methods and their applications in condensed matter systems. Volume 1 is an in-depth introduction to a vast spectrum of computational techniques for statistical mechanical systems of condensed matter. Volume 2 is a collection of state-of-the-art surveys on numerical experiments carried out for a great number of systems.

Learn classical thermodynamics alongside statistical mechanics and how macroscopic and microscopic ideas interweave with this fresh approach to the subjects.

An Interdisciplinary Guide
The Monte Carlo Method in Condensed Matter Physics
Computer Simulations in Condensed Matter: From Materials to Chemical Biology. Volume 1
Theory, Algorithms and Applications
Molecular Docking and Molecular Dynamics
Numerics, Algorithms, Parallelization, Applications

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.

This book discusses the computational approach in modern statistical physics, adopting simple language and an attractive format with many illustrations, tables and printed algorithms. The style will appeal to students, teachers and researchers in the physical sciences. The focus is on orientation, with implementation details kept to a minimum.

This book provides an introduction to Monte Carlo simulations in classical statistical physics and is aimed both at students beginning work in the field and at more experienced researchers who wish to learn more about Monte Carlo methods. The material covered includes methods for both equilibrium and out of equilibrium systems, and common algorithms like the Metropolis and heat-bath algorithms are discussed in detail, as well as more sophisticated ones such as continuous time Monte Carlo, cluster algorithms, multigrid methods, entropic sampling and simulated tempering. Data analysis techniques are also explained starting with straightforward measurement and error-estimation techniques and progressing to topics such as the single and multiple histogram methods and finite size scaling. The last few chapters of the book are devoted to implementation issues, including discussions of such topics as lattice representations, efficient implementation of data structures, multispin coding, parallelization of Monte Carlo algorithms, and random number generation. At the end of the book the authors give a number of example programmes demonstrating the applications of these techniques to a variety of well-known models.

Studies of surfaces and interactions between dissimilar materials or phases are vital for modern technological applications. Computer simulation methods are indispensable in such studies and this book contains a substantial body of knowledge about simulation methods as well as the theoretical background for performing computer experiments and analyzing the data. The book is self-contained, covering a range of topics from classical statistical mechanics to a variety of simulation techniques, including molecular dynamics, Langevin dynamics and Monte Carlo methods. A number of physical systems are considered, including fluids, magnets, polymers, granular media, and driven diffusive systems. The computer simulation methods considered include both standard and accelerated versions. The simulation methods are clearly related to the fundamental principles of thermodynamics and statistical mechanics.

Adsorption and Diffusion
Molecular Dynamics
Fundamentals and Applications
Computer Simulations of Surfaces and Interfaces
Molecular Dynamics, Monte Carlo, Brownian Dynamics, Lattice Boltzmann and Dissipative Particle Dynamics
The Art of Molecular Dynamics Simulation

Molecular modeling techniques have been widely used in drug discovery fields for rational drug design

and compound screening. Now these techniques are used to model or mimic the behavior of molecules, and help us study formulation at the molecular level. Computational pharmaceutics enables us to understand the mechanism of drug delivery, and to develop new drug delivery systems. The book discusses the modeling of different drug delivery systems, including cyclodextrins, solid dispersions, polymorphism prediction, dendrimer-based delivery systems, surfactant-based micelle, polymeric drug delivery systems, liposome, protein/peptide formulations, non-viral gene delivery systems, drug-protein binding, silica nanoparticles, carbon nanotube-based drug delivery systems, diamond nanoparticles and layered double hydroxides (LDHs) drug delivery systems. Although there are a number of existing books about rational drug design with molecular modeling techniques, these techniques still look mysterious and daunting for pharmaceutical scientists. This book fills the gap between pharmaceutics and molecular modeling, and presents a systematic and overall introduction to computational pharmaceutics. It covers all introductory, advanced and specialist levels. It provides a totally different perspective to pharmaceutical scientists, and will greatly facilitate the development of pharmaceutics. It also helps computational chemists to look for the important questions in the drug delivery field. This book is included in the Advances in Pharmaceutical Technology book series.

This book describes the mathematical underpinnings of algorithms used for molecular dynamics simulation, including both deterministic and stochastic numerical methods. Molecular dynamics is one of the most versatile and powerful methods of modern computational science and engineering and is used widely in chemistry, physics, materials science and biology. Understanding the foundations of numerical methods means knowing how to select the best one for a given problem (from the wide range of techniques on offer) and how to create new, efficient methods to address particular challenges as they arise in complex applications. Aimed at a broad audience, this book presents the basic theory of Hamiltonian mechanics and stochastic differential equations, as well as topics including symplectic numerical methods, the handling of constraints and rigid bodies, the efficient treatment of Langevin dynamics, thermostats to control the molecular ensemble, multiple time-stepping, and the dissipative particle dynamics method.

This book addresses the formulation of theoretical molecular orbital models starting from quantum mechanics, and compares them to experimental results. It draws on a series of models that have already received widespread application and are available for new applications.

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.

Molecular Simulations

Computer Simulation of Liquids

Introduction to Carbon Capture and Sequestration

Statistical Mechanics: Algorithms and Computations

Monte Carlo Methods in Statistical Physics

Molecular Dynamics Simulation

"Molecular Sieves - Science and Technology" covers, in a comprehensive manner, the science and technology of zeolites and all related microporous and mesoporous materials. The contributions are grouped together topically in such a way that each volume deals with a specific sub-field. Volume 7 treats fundamentals and analyses of adsorption and diffusion in zeolites including single-file diffusion. Various methods of measuring adsorption and diffusion are described and discussed.

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

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

"Provides a lot of reading pleasure and many new insights." -Journal of Molecular Structure "This is the most entertaining, stimulating and useful book which can be thoroughly recommended to anyone with an interest in computer simulation." -Contemporary Physics "A very useful introduction . . . more interesting to read than the often dry equation-based texts." -Journal of the American Chemical Society Written especially for the novice, Molecular Dynamics Simulation demonstrates how molecular dynamics simulations work and how to perform them, focusing on how to devise a model for specific molecules and then how to simulate their movements using a computer. This book provides a collection of methods that until now have been scattered through the literature of the last 25 years. It reviews elements of sampling theory and discusses how modern notions of chaos and nonlinear dynamics explain the workings of molecular dynamics. Stresses easy-to-use molecules * Provides sample calculations and figures * Includes four complete FORTRAN codes

Elementary Methods

Molecular Simulation of Fluids

Molecular Dynamics Simulations in Statistical Physics: Theory and Applications

With Deterministic and Stochastic Numerical Methods

Numerical Simulation in Molecular Dynamics

Introduction to Computational Chemistry

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.

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.

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.

Understanding Molecular SimulationFrom Algorithms to ApplicationsElsevier

Simulation Methods for Polymers

Fundamentals and Practice

Theory, Methodology and Applications

An Introduction to Molecular Dynamics

Protein Folding Versus Protein Structure Prediction

The Road To Success – A Spider Web Doctrine

This text offers a logical sequence of polymer physics background, methods, calculations and application guidelines - including coverage of recently developed techniques and algorithms for modelling and simulation.

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.

Written by two specialists with over twenty-five years of experience in the field, this valuable text presents a wide range of topics within the growing field of nonequilibrium molecular dynamics (NEMD). It introduces theories which are fundamental to the field - namely, nonequilibrium statistical mechanics and nonequilibrium thermodynamics - and provides state-of-the-art algorithms and advice for designing reliable NEMD code, as well as examining applications for both atomic and molecular fluids. It discusses homogenous and inhomogenous flows and pays considerable attention to highly confined fluids, such as nanofluidics. In addition to statistical mechanics and thermodynamics, the book covers the themes of temperature and thermodynamic fluxes and their computation, the theory and algorithms for homogenous shear and elongational flows, response theory and its applications, heat and mass transport algorithms, applications in molecular rheology, highly confined fluids (nanofluidics), the phenomenon of slip and how to compute it from basic microscopic principles, and generalized hydrodynamics.

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.