Understanding Molecular Simulation Second Edition From Algorithms To Applications Computational Science Series Vol 1

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Statistical Physics of Biomolecules - Daniel M. Zuckerman 2010-06-02
From the hydrophobic effect to protein-ligand binding, statistical physics is relevant in almost all areas of molecular biophysics and biochemistry, making it essential for modern students of molecular behavior. But traditional presentations of this material are often difficult to penetrate. Statistical Physics of Biomolecules: An Introduction brin

Simulation Methods for Polymers - Michael Kotelyanskii 2004-03-15
Synthetic Lubricants and High-Performance Functional Fluids, Second Edition offers state-of-the-art information on all the major synthetic fluids, describing established products as well as highly promising experimental fluids with commercial potential. This second edition contains chapters on polyinternalolefins, polymer esters, refrigeration lube

The Art of Molecular Dynamics Simulation - D. C. Rapaport 2004-04
First time paperback of successful physics monograph. Copyright © Libri GmbH. All rights reserved.

Extending and Modifying LAMMPS Writing Your Own Source Code - Dr. Shafat Mubin 2021-02-19
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.

Introduction to Carbon Capture and Sequestration - Berend Smit 2014-01-10
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

A Practical Introduction to the Simulation of Molecular Systems - Martin J. Field 2007-07-19
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 Simulations - Saman Alavi 2020-06-29
Provides hands-on knowledge enabling students of and researchers in chemistry, biology, and engineering to perform molecular simulations This book introduces the fundamentals of molecular simulations for a broad, practice-oriented audience and presents a thorough overview of the underlying concepts. It covers classical mechanics for many-molecule systems as well as force-field models in classical molecular dynamics; introduces probability concepts and statistical mechanics; and analyzes numerous simulation methods, techniques, and applications. Molecular Simulations: Fundamentals and Practice starts by covering Newton's equations, which form the basis of classical mechanics, then continues on to force-field methods for modelling potential energy surfaces. It gives an account of probability concepts before subsequently introducing readers

to statistical and quantum mechanics. In addition to Monte-Carlo methods, which are based on random sampling, the core of the book covers molecular dynamics simulations in detail and shows how to derive critical physical parameters. It finishes by presenting advanced techniques, and gives invaluable advice on how to set up simulations for a diverse range of applications. -Addresses the current need of students of and researchers in chemistry, biology, and engineering to understand and perform their own molecular simulations -Covers the nitty-gritty ? from Newton's equations and classical mechanics over force-field methods, potential energy surfaces, and probability concepts to statistical and quantum mechanics -Introduces physical, chemical, and mathematical background knowledge in direct relation with simulation practice -Highlights deterministic approaches and random sampling (eg: molecular dynamics versus Monte-Carlo methods) -Contains advanced techniques and practical advice for setting up different simulations to prepare readers entering this exciting field Molecular Simulations: Fundamentals and Practice is an excellent book benefitting chemist, biologists, engineers as well as materials scientists and those involved in biotechnology.

Computational Materials Science - June Gunn Lee 2016-11-25

This book covers the essentials of Computational Science and gives tools and techniques to solve materials science problems using molecular dynamics (MD) and first-principles methods. The new edition expands upon the density functional theory (DFT) and how the original DFT has advanced to a more accurate level by GGA+U and hybrid-functional methods. It offers 14 new worked examples in the LAMMPS, Quantum Espresso, VASP and MedeA-VASP programs, including computation of stress-strain behavior of Si-CNT composite, mean-squared displacement (MSD) of ZrO2-Y2O3, band structure and phonon spectra of silicon, and Mo-S battery system. It discusses methods once considered too expensive but that are now cost-effective. New examples also include various post-processed results using VESTA, VMD, VTST, and MedeA.

Molecular Modeling Applications in Crystallization - Allan S. Myerson 2005-09-08

Crystallization is an important purification process used in a broad range of industries, including pharmaceuticals, foods, and bulk chemicals. In recent years, molecular modeling has emerged as a useful tool in the analysis and solution of problems associated with crystallization. Modeling allows more focused experimentation based on structural and energetic calculations instead of intuition and trial and error. This book offers a general introduction to molecular modeling techniques and their application in crystallization. After explaining the basic concepts of molecular modeling and crystallization, the book discusses how modeling techniques are used to solve a variety of practical problems related to crystal size, shape, internal structure, and properties. With chapters written by leading experts and an emphasis on problem solving, this book will appeal to scientists, engineers, and graduate students involved in research and the production of crystalline materials.

Nonequilibrium Gas Dynamics and Molecular Simulation - Iain D. Boyd 2017-03-23

7.1 Introduction -- 7.2 Rotational Energy Exchange Models -- 7.2.1 Constant Collision Number -- 7.2.2 The Parker Model -- 7.2.3 Variable Probability Exchange Model of Boyd -- 7.2.4 Nonequilibrium Direction Dependent Model -- 7.2.5 Model Results -- 7.3 Vibrational Energy Exchange Models -- 7.3.1 Constant Collision Number -- 7.3.2 The Millikan-White Model -- 7.3.3 Quantized Treatment for Vibration -- 7.3.4 Model Results -- 7.4 Dissociation Chemical Reactions -- 7.4.1 Total Collision Energy Model -- 7.4.2 Redistribution of Energy Following a Dissociation Reaction -- 7.4.3 Vibrationally Favored Dissociation Model -- 7.5 General Chemical Reactions -- 7.5.1 Reaction Rates and Equilibrium Constant -- 7.5.2 Backward Reaction Rates in DSMC -- 7.5.3 Three-Body Recombination Reactions -- 7.5.4 Post-Reaction Energy Redistribution and General Implementation -- 7.5.5 DSMC Solutions for Reacting Flows -- 7.6 Summary -- Appendix A: Generating Particle Properties -- Appendix B: Collisional Quantities -- Appendix C: Determining Post-Collision Velocities -- Appendix D: Macroscopic Properties -- Appendix E: Common Integrals -- References -- Index

The Graduate Student's Guide to Numerical Analysis '98 - Mark Ainsworth 2012-12-06

Detailed lecture notes on six topics at the forefront of current research in numerical analysis and applied mathematics, with each set of notes presenting a self-contained guide to a current research area and supplemented by an extensive bibliography. In addition, most of the notes contain detailed proofs of the key results. They start from a level suitable for first year graduates in applied mathematics, mathematical analysis or numerical analysis, and proceed to current research topics. Readers will thus quickly gain an insight into the important results and techniques in each area without recourse to the large research literature. Current (unsolved) problems are also described, and directions for future research given.

Statistical Mechanics: Theory and Molecular Simulation - Mark Tuckerman 2010-02-11

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 Dynamics Simulation - J. M. Haile 1997-03-14

"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

A Guide to Monte Carlo Simulations in Statistical Physics - David P. Landau 2000-08-17

This book describes all aspects of Monte Carlo simulation of complex physical systems encountered in condensed-matter physics and statistical mechanics, as well as in related fields, such as polymer science and lattice gauge theory. The authors give a succinct overview of simple sampling methods and develop the importance sampling method. In addition they introduce quantum Monte Carlo methods, aspects of simulations of growth phenomena and other systems far from equilibrium, and the Monte Carlo Renormalization Group approach to critical phenomena. The book includes many applications, examples, and current references, and exercises to help the reader.

Computer Simulation of Liquids - M. P. Allen 1989

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.

Statistical Mechanics: Algorithms and Computations - Werner Krauth 2006-09-14

CD-ROM contains more than one hundred pseudocode programs and close to 300 figures, line drawings, and tables contained in the book.

Simulating Hamiltonian Dynamics - Benedict Leimkuhler 2004

Publisher Description

Molecular Dynamics Simulation - Kun Zhou 2022-02-10

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

Adsorption and Diffusion - Hellmut G. Karge 2008-06-17

"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.

Numerical Simulation in Molecular Dynamics - Michael Griebel 2007-08-16

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.

Free Energy Calculations - Christophe Chipot 2007-01-08

Free energy constitutes the most important thermodynamic quantity to understand how chemical species recognize each other, associate or react. Examples of problems in which knowledge of the underlying free energy behaviour is required, include conformational equilibria and molecular association, partitioning between immiscible liquids, receptor-drug interaction, protein-protein and protein-DNA association, and protein stability. This volume sets out to present a coherent and comprehensive account of the concepts that underlie different approaches devised for the determination of free energies. The reader will gain the necessary insight into the theoretical and computational foundations of the subject and will be presented with relevant applications from molecular-level modelling and simulations of chemical and biological systems. Both formally accurate and approximate methods are covered using both classical and quantum mechanical descriptions. A central theme of the book is that the wide variety of free energy calculation techniques available today can be understood as different implementations of a few basic principles. The book is aimed at a broad readership of graduate students and researchers having a background in chemistry, physics, engineering and physical biology.

Molecular Modelling: Principles And Applications, 2/E - Leach 2009-09

Computer Simulation Using Particles - R.W Hockney 2021-03-24

Computer simulation of systems has become an important tool in scientific research and engineering design, including the simulation of systems through the motion of their constituent particles. Important examples of this are the motion of stars in galaxies, ions in hot gas plasmas, electrons in semiconductor devices, and atoms in solids and liquids. The behavior of the system is studied by programming into the computer a model of the system and then performing experiments with this model. New scientific insight is obtained by observing such computer experiments, often for controlled conditions that are not accessible in the laboratory. Computer Simulation using Particles deals with the simulation of systems by following the motion of their constituent particles. This book provides an introduction to simulation using particles based on the NGP, CIC, and P3M algorithms and the programming principles that assist with the preparations of large simulation programs based on the OLYMPUS methodology. It also includes case study examples in the fields of astrophysics, plasmas, semiconductors, and ionic solids as well as more detailed mathematical treatment of the models, such as their errors, dispersion, and optimization. This resource will help you understand how engineering design can be assisted by the ability to predict performance using the computer model before embarking on costly and time-consuming manufacture.

Modeling Materials - Ellad B. Tadmor 2011-11-24

Material properties emerge from phenomena on scales ranging from Angstroms to millimeters, and only a multiscale treatment can provide a complete understanding. Materials researchers must therefore understand fundamental concepts and techniques from different fields, and these are presented in a comprehensive and integrated fashion for the first time in this book. Incorporating continuum mechanics, quantum mechanics, statistical mechanics, atomistic simulations and multiscale techniques, the book explains many of the key theoretical ideas behind multiscale modeling. Classical topics are blended with new techniques to demonstrate the connections between different fields and highlight current research trends. Example applications drawn from modern research on the thermo-mechanical properties of crystalline solids are used as a unifying focus throughout the text. Together with its companion book, Continuum Mechanics and Thermodynamics (Cambridge University Press, 2011), this work presents the complete fundamentals of materials modeling for graduate students and researchers in physics, materials science, chemistry and engineering.

Understanding Molecular Simulation - Daan Frenkel 1996

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.

Computational Materials Science - A.M. Ovrutsky 2013-11-19

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

Introduction to Computational Materials Science - Richard LeSar 2013-03-28

Emphasising essential methods and universal principles, this textbook provides everything students need to understand the basics of simulating materials behaviour. All the key topics are covered from electronic structure methods to microstructural evolution, appendices provide crucial background material, and a wealth of practical resources are available online to complete the teaching package. Modelling is examined at a broad range of scales, from the atomic to the mesoscale, providing students with a solid foundation for future study and research. Detailed, accessible explanations of the fundamental equations underpinning materials modelling are presented, including a full chapter summarising essential mathematical background. Extensive appendices, including essential background on classical and quantum mechanics, electrostatics, statistical thermodynamics and linear elasticity, provide the background necessary to fully engage with the fundamentals of computational modelling. Exercises, worked examples, computer codes and discussions of practical implementations methods are all provided

online giving students the hands-on experience they need.
Molecular Theory of Capillarity - J. S. Rowlinson 2013-04-26
History of surface phenomena offers critical and detailed examination and assessment of modern theories, focusing on statistical mechanics and application of results in mean-field approximation to model systems. 1989 edition.
Essentials of Computational Chemistry - Christopher J. Cramer 2013-04-29
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.
The Selfish Gene - Richard Dawkins 1989
An ethologist shows man to be a gene machine whose world is one of savage competition and deceit
Introduction to Practice of Molecular Simulation - Akira Satoh 2010-12-17
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
Protein Folding in Silico - Irena Roterman-Konieczna 2012-10-04
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
The Proceedings of International Conference on High Performance Computing in Asia-Pacific Region - 2018

Molecular Simulation of Fluids - Richard J. Sadus 2002-05-17
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.
An Introduction to Molecular Dynamics - Mark S. Kemp 2019
"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"--
Nonequilibrium Molecular Dynamics - Billy D. Todd 2017-03-10
This coherent collection of theory, algorithms, and illustrative results presents the field of nonequilibrium molecular dynamics in detail.
Computational Soft Matter: from Synthetic Polymers to Proteins - Norbert Attig 2004

Understanding Molecular Simulation - Daan Frenkel 2001-10-19
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 Modelling for Beginners - Alan Hinchliffe 2005-12-17
Presenting a concise, basic introduction to modelling and computational chemistry this text includes relevant introductory material to ensure greater accessibility to the subject. Provides a comprehensive introduction to this evolving and developing field Focuses on MM, MC, and MD with an entire chapter devoted to QSAR and Discovery Chemistry. Includes many real chemical applications combined with worked problems and solutions provided in each chapter Ensures that up-to-date treatment of a variety of chemical modeling techniques are introduced.
Molecular Modeling and Simulation - Tamar Schlick 2013-04-18
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