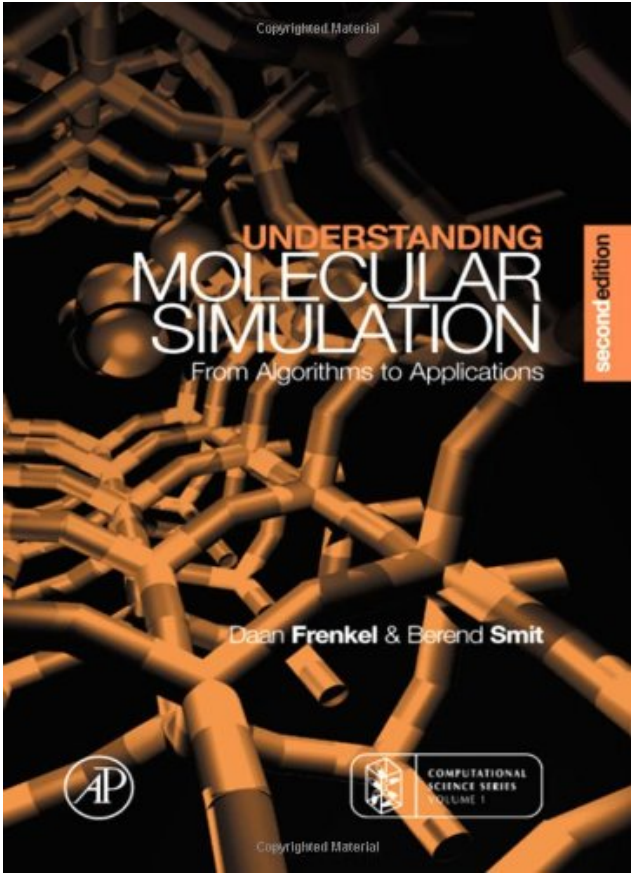

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Understanding Molecular Simulation-Daan Frenkel 2001-10-19 Understanding Molecular Simulation: From Algorithms to Applications

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.

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.

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.

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.

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

Molecular Simulations-Saman Alavi 2020-06-03 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.

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.

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

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.

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

Molecular Simulation of Fluids-Richard J. Sadus 2002-05-31 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.

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

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

Molecular Modeling and Simulation: An Interdisciplinary Guide-Tamar Schlick 2010-08-03 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

Molecular Dynamics Simulation of Nanostructured Materials-Snehanshu Pal 2020-04-28 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.

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

Molecular Dynamics-Ben Leimkuhler 2015-05-18 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.

Statistical Mechanics: Algorithms and Computations-Werner Krauth 2006-09-14 This book discusses the computational approach in modern statistical physics, adopting simple language and an attractive format of many illustrations, tables and printed algorithms. The discussion of key subjects in classical and quantum statistical physics will appeal to students, teachers and researchers in physics and related sciences. The focus is on orientation with implementation details kept to a minimum. - ;This book discusses the computational approach in modern statistical physics in a clear and accessible way and demonstrates its close relation to other approaches in theoretical physics. Individual chapters focus on subjects as diverse as the hard sphere liquid, classical spin models, single quantum particles and Bose-Einstein condensation. Contained within the chapters are in-depth discussions of algorithms, ranging from basic enumeration methods to modern Monte Carlo techniques. The emphasis is on orientation, with discussion of implementation details kept to a minimum. Illustrations, tables and concise printed algorithms convey key information, making the material very accessible. The book is completely self-contained and graphs and tables can readily be reproduced, requiring minimal computer code. Most sections begin at an elementary level and lead on to the rich and difficult problems of contemporary computational and statistical physics. The book will be of interest to a wide range of students, teachers and researchers in physics and the neighbouring sciences. An accompanying CD allows incorporation of the book's content (illustrations, tables, schematic programs) into the reader's own presentations. - ;'This book is the best one I have reviewed all year.' Alan Hinchliffe, Physical Sciences Educational Reviews -

Molecular Dynamics Simulations in Statistical Physics: Theory and Applications-Hiqmet Kamberaj 2020-03-20 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.

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.

Biomolecular and Bioanalytical Techniques-

Vasudevan Ramesh 2019-05-13 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.

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

Biological Modeling and Simulation-Russell Schwartz 2008-07-25 A practice-oriented survey of techniques for computational modeling and simulation suitable for a broad range of biological problems. There are many excellent computational biology resources now available for learning about methods that have been developed to address specific biological systems, but comparatively little attention has been paid to training aspiring computational biologists to handle new and unanticipated problems. This text is intended to fill that gap by teaching students how to reason about developing formal

mathematical models of biological systems that are amenable to computational analysis. It collects in one place a selection of broadly useful models, algorithms, and theoretical analysis tools normally found scattered among many other disciplines. It thereby gives the aspiring student a bag of tricks that will serve him or her well in modeling problems drawn from numerous subfields of biology. These techniques are taught from the perspective of what the practitioner needs to know to use them effectively, supplemented with references for further reading on more advanced use of each method covered. The text, which grew out of a class taught at Carnegie Mellon University, covers models for optimization, simulation and sampling, and parameter tuning. These topics provide a general framework for learning how to formulate mathematical models of biological systems, what techniques are available to work with these models, and how to fit the models to particular systems. Their application is illustrated by many examples drawn from a variety of biological disciplines and several extended case studies that show how the methods described have been applied to real problems in biology.

Computational Molecular Dynamics: Challenges, Methods, Ideas-Peter Deuflhard 2012-12-06 On May 21-24, 1997 the Second International Symposium on Algorithms for Macromolecular Modelling was held at the Konrad Zuse Zentrum in Berlin. The event brought together computational scientists in fields like biochemistry, biophysics, physical chemistry, or statistical physics and numerical analysts as well as computer scientists working on the advancement of algorithms, for a total of over 120 participants from 19 countries. In the course of the symposium, the speakers agreed to produce a representative volume that combines survey articles and original papers (all refereed) to give an impression of the present state of the art of Molecular Dynamics. The 29 articles of the book reflect the main topics of the Berlin meeting which were i) Conformational Dynamics, ii)

Thermodynamic Modelling, iii) Advanced Time-Stepping Algorithms, iv) Quantum-Classical Simulations and Fast Force Field and v) Fast Force Field Evaluation.

Foundations of Molecular Modeling and Simulation-Randall Q Snurr 2016-06-01 This book is a collection of select proceedings of the FOMMS 2015 conference. FOMMS 2015 was the sixth triennial FOMMS conference showcasing applications of theory of computational quantum chemistry, molecular science, and engineering simulation. The theme of the 2015 meeting was on Molecular Modeling and the Materials Genome. This volume comprises chapters on many distinct applications of molecular modeling techniques. The content will be useful to researchers and students alike.

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.

Innovations in Biomolecular Modeling and Simulations-Tamar Schlick 2012 The chemical and biological sciences face unprecedented opportunities in the 21st century. A confluence of factors from parallel universes - advances in experimental techniques in biomolecular structure determination, progress in theoretical modeling and simulation for large biological systems, and breakthroughs in computer technology - has opened new avenues of opportunity as never before. Now, experimental data can be interpreted and further analysed by modeling, and predictions from any approach can be tested and advanced through companion

methodologies and technologies. This two volume set describes innovations in biomolecular modeling and simulation, in both the algorithmic and application fronts. With contributions from experts in the field, the books describe progress and innovation in areas including: simulation algorithms for dynamics and enhanced configurational sampling, force field development, implicit solvation models, coarse-grained models, quantum-mechanical simulations, protein folding, DNA polymerase mechanisms, nucleic acid complexes and simulations, RNA structure analysis and design and other important topics in structural biology modeling. The books are aimed at graduate students and experts in structural biology and chemistry and the emphasis is on reporting innovative new approaches rather than providing comprehensive reviews on each subject.

Ab Initio Molecular Dynamics-

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.

Detectors for Particle Radiation-Konrad Kleinknecht 1998-12-10 A clear, concise, comprehensive review of detectors of high-energy particles and radiation; thoroughly revised and updated.

Monte Carlo Simulation for the Pharmaceutical Industry-Mark Chang 2010-09-29 Helping you become a creative,

logical thinker and skillful "simulator," Monte Carlo Simulation for the Pharmaceutical Industry: Concepts, Algorithms, and Case Studies provides broad coverage of the entire drug development process, from drug discovery to preclinical and clinical trial aspects to commercialization. It presents the theories and methods needed to carry out computer simulations efficiently, covers both descriptive and pseudocode algorithms that provide the basis for implementation of the simulation methods, and illustrates real-world problems through case studies. The text first emphasizes the importance of analogy and simulation using examples from a variety of areas, before introducing general sampling methods and the different stages of drug development. It then focuses on simulation approaches based on game theory and the Markov decision process, simulations in classical and adaptive trials, and various challenges in clinical trial management and execution. The author goes on to cover prescription drug marketing strategies and brand planning, molecular design and simulation, computational systems biology and biological pathway simulation with Petri nets, and physiologically based pharmacokinetic modeling and pharmacodynamic models. The final chapter explores Monte Carlo computing techniques for statistical inference. This book offers a systematic treatment of computer simulation in drug development. It not only deals with the principles and methods of Monte Carlo simulation, but also the applications in drug development, such as statistical trial monitoring, prescription drug marketing, and molecular docking.

Free Energy Calculations-Christophe Chipot 2007-01-08 Presenting an account of the concepts that underly different approaches devised for the determination of free energies, this book aims to give the reader, an insight into the theoretical and computational foundations of the subject. It is aimed at students and researchers having a background in chemistry, physics, engineering and physical biology.

Thermodynamics and Statistical Mechanics-M. Scott Shell 2015-04-16 Learn classical thermodynamics alongside statistical mechanics and how macroscopic and microscopic ideas interweave with this fresh approach to the subjects.

Biomolecular Simulations in Structure-Based Drug Discovery-Francesco L. Gervasio 2019-04-29 A guide to applying the power of modern simulation tools to better drug design Biomolecular Simulations in Structure-based Drug Discovery offers an up-to-date and comprehensive review of modern simulation tools and their applications in real-life drug discovery, for better and quicker results in structure-based drug design. The authors describe common tools used in the biomolecular simulation of drugs and their targets and offer an analysis of the accuracy of the predictions. They also show how to integrate modeling with other experimental data. Filled with numerous case studies from different therapeutic fields, the book helps professionals to quickly adopt these new methods for their current projects. Experts from the pharmaceutical industry and academic institutions present real-life examples for important target classes such as GPCRs, ion channels and amyloids as well as for common challenges in structure-based drug discovery. Biomolecular Simulations in Structure-based Drug Discovery is an important resource that: -Contains a review of the current generation of biomolecular simulation tools that have the robustness and speed that allows them to be used as routine tools by non-specialists -Includes information on the novel methods and strategies for the modeling of drug-target interactions within the framework of real-life drug discovery and development -Offers numerous illustrative case studies from a wide-range of therapeutic fields -Presents an application-oriented reference that is ideal for those working in the various fields Written for medicinal chemists, professionals in the pharmaceutical industry, and

pharmaceutical chemists, Biomolecular Simulations in Structure-based Drug Discovery is a comprehensive resource to modern simulation tools that complement and have the potential to complement or replace laboratory assays for better results in drug design.

Computer Simulations in Condensed Matter: From Materials to Chemical Biology-Mauro Ferrario 2007-03-09 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.

Machine Learning in Biomolecular Simulations-Gennady Verkhivker 2019-10-21 Machine learning methods such as neural networks, non-linear dimensionality reduction techniques, random forests and others meet in this research topic with biomolecular simulations. The authors of eight articles applied these methods to analyze simulation results, accelerate simulations or to make molecular mechanics force fields more accurate.

Particle Detectors-Claus Grupen 2011-09-22 The scope of the detection techniques in particle detectors is very wide, depending on the aim of the measurement. Detectors cover the measurement of energies from the very low to the highest of energies observed in cosmic rays. Describing the instrumentation for experiments in high energy physics and astroparticle physics, this edition describes track detectors, calorimeters, particle identification, neutrino detectors, momentum measurement, electronics, and data analysis. It also discusses applications of these detectors in other fields such as nuclear

medicine, radiation protection and environmental science. Problem sets have been added to each chapter and additional instructive material has been provided, making this an excellent reference for graduate students and researchers in particle physics.

Nonequilibrium Molecular Dynamics-Billy D. Todd 2017-03-10 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.

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

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.