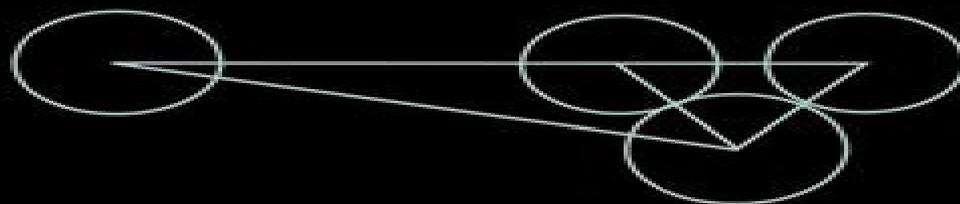


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Simulations in Nanobiotechnology Kilho Eom, 2011-10-19. Until the late 20th century computational studies of biomolecules and nanomaterials had considered the two subjects separately. A thorough presentation of state of the art simulations for studying the nanoscale behavior of materials. *Simulations in Nanobiotechnology* discusses computational simulations of biomolecules and nanomaterials together. **Th Computational Molecular Dynamics: Challenges, Methods, Ideas** Peter Deuffhard, 1999. 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. 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.

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Computer Simulation of Biomolecular Systems W.F. van Gunsteren,P.K. Weiner,A.J. Wilkinson,1994-01-31 The long range goal of molecular approaches to biology is to describe living systems in terms of chemistry and physics Over the last fifty years great progress has been made in applying the equations representing the underlying physical laws to chemical problems involving the structures and reactions of small molecules Corresponding studies of mesoscopic systems have been undertaken much more recently Molecular dynamics simulations which are the primary focus of this volume represent the most important theoretical approach to macromolecules of biological interest Now that molecular dynamics of macromolecules is a flourishing field serious questions have to be asked concerning what more can be done with the methodology What is the present and the future role of molecular dynamics in the development of our knowledge of macromolecules of biological interest How does the methodology need to be improved to make it applicable to important problems The present volume is concerned with providing some answers with its primary focus on the methodology and its recent developments

Physical Review,2000-09

International Symposium of Exotic Nuclei Yu E. Penionzhkevich,E.A. Cherepanov,2007-06-06 This book is a collection of talks presented at the International Symposium on Exotic Nuclei EXON2006 held in Khanty Mansiysk Russia

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