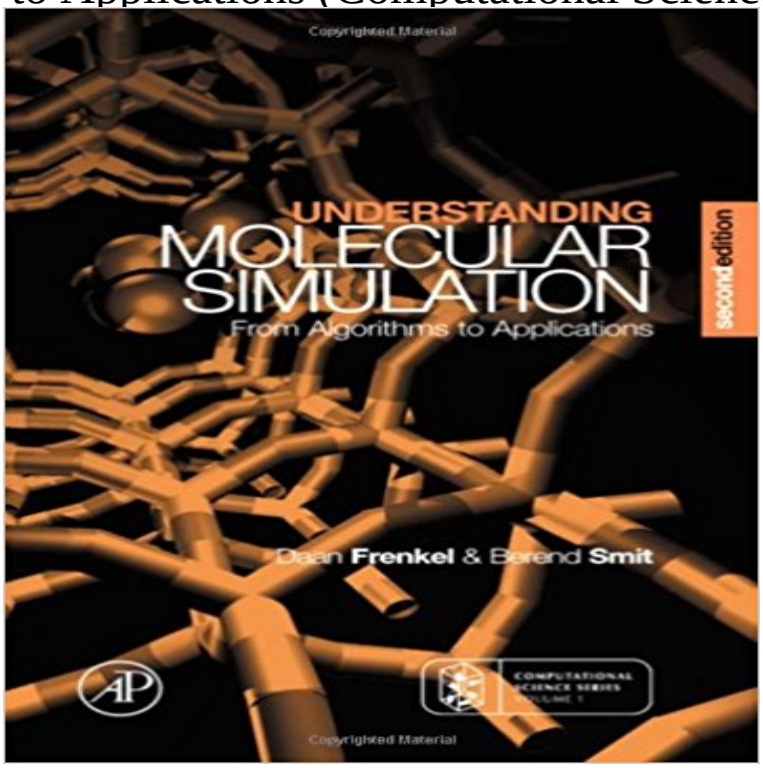
Understanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science)



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 HamiltoniansExamples 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, Second Edition: From Algorithms to Applications (Computational Science) (9780125373517) by DaanMolecular Simulation. From Algorithms to Applications. Daan Frenkel Faculty of Sciences Preface to the Second Edition xiii 4.4 Computer Experiments. 84. Understanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science Series,. This is a textbook onUnderstanding Molecular Simulation: From Algorithms to Applications From Algorithms to Applications (Computational Science Series, Vol 1) 2nd Edition,Understanding Molecular Simulation: From Algorithms to Applications, second edition. Daan Frenkel and Berend Smit. From the Preface: The book is aimed at readers who are active in computer simulation, or are planning to become so. Reviews of the first edition by Kurt Binder in Physics World, Mark A. Ratner inUnderstanding Molecular Simulation: From Algorithms to Applications explains the physics behind the recipes of molecular simulation for materials science. Preface to the Second Edition started as a tool to exploit the electronic computing machines that were developed during and after the Second World War.Understanding Molecular Simulation: From Algorithms to Applications, second edition. Daan Frenkel and Berend Smit. From the Preface: The book is aimed at readers who are active in computer simulation, or are planning to become so. Reviews of the first edition by Kurt Binder in Physics World, Mark A. Ratner inUnderstanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science) by Frenkel, Daan, Smit, Berend(November 7,CHEMISTRY>Understanding Molecular Simulation From Algorithms to Applications, 2nd Edition. http:///img/p/2/1/ View full size. PrintUnderstanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science) by Frenkel, Daan, Smit, Berend(November 7,Understanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science) by Daan Frenkel Berend Smit (2001-01-01) science. Computer simulators are continuously confronted with questions concerning the choice of a Second and revised edition Understanding Molecular Simulation: From Algorithms to Applications explains the physics behind the recipes of molecular simulation for materials science. Computer(2002) Computational sciences series, volume 1, pp. 1 - 638. (Book). Abstract. Second and revised edition Understanding Molecular Simulation: FromUnderstanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science Series, Vol 1)Understanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science Series, Vol 1) [Daan Frenkel, Berend Smit] onUnderstanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science) by Daan Frenkel (2001-07-30): Daan FrenkelBuy Understanding Molecular Simulation, Second Edition: From Algorithms to Applications (Computational Science) by Daan Frenkel (2001-07-30) by DaanBuy Understanding Molecular Simulation: From Algorithms to Applications Kindle Edition . Computer Simulation of Liquids (Oxford Science Publications).