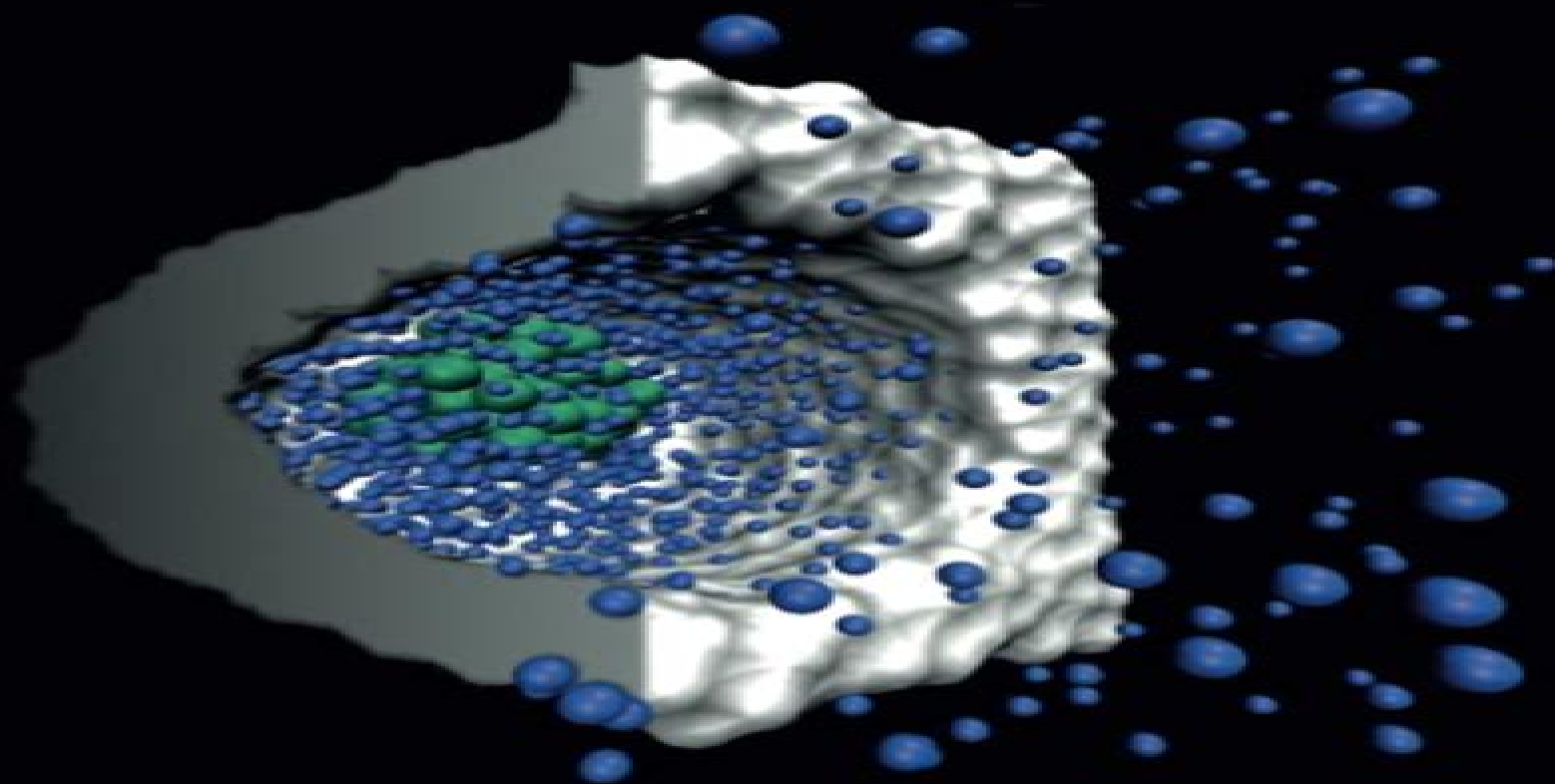


UNDERSTANDING MOLECULAR SIMULATION

From Algorithms to Applications

Third Edition



Daan Frenkel
Berend Smit



Understanding Molecular Simulation From Algorithms To Applications

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Understanding Molecular Simulation From Algorithms To Applications:

Understanding Molecular Simulation Daan Frenkel, Berend Smit, 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 simulate rare events. Dissipative particle dynamics as a coarse grained simulation technique. Novel schemes to compute the long ranged forces. Hamiltonian and non Hamiltonian dynamics in the context of 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, Berend Smit, 2025

Computational Many-Particle Physics Holger Fehske, Ralf Schneider, Alexander Weiße, 2007-12-07 Looking for the real state of play in computational many particle physics. Look no further. This book presents an overview of the 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. *Encyclopedia of Chemical Processing (Online)* Sunggyu Lee, 2005-11-01 This second edition *Encyclopedia* supplies nearly 350 gold standard articles on the methods, practices, products and standards influencing the chemical industries. It offers expertly written articles on technologies at the forefront of the field to maximize and enhance the research and production phases of current and emerging chemical manufacturing practices and techniques. This collecting of information is of vital interest to chemical, polymer, electrical, mechanical and civil engineers as well as chemists and chemical researchers. A complete reconceptualization of the classic reference series the *Encyclopedia of Chemical Processing and Design* whose first volume published in 1976. This resource offers extensive A-Z treatment of the subject in five simultaneously published volumes with comprehensive indexing of all five volumes in the back matter of each tome. It includes material on the design of key unit operations involved with chemical

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