1. Record Nr. UNISA990001232160203316

Record Nr.	UNISA990001232160203316
Autore	ARETINO, Pietro
Titolo	2: Teatro / Pietro Aretino ; a cura di Giorgio Petrocchi
Pubbl/distr/stampa	[Milano], : Mondadori, 1971
Descrizione fisica	XII, 907 p. ; 18 cm.
Collana	I Classici Mondadori
Disciplina	858.3
Collocazione	VI.3. Coll.27/ 13/2 (V A coll. 17/13 II)
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia

2. Record Nr. UNINA9910458817003321

Record Nr.	UNINA9910458817003321
Autore	Frenkel Daan <1948->
Titolo	Understanding molecular simulation : from algorithms to applications / / Daan Frenkel, Berend Smit
Pubbl/distr/stampa	San Diego, : Academic Press, c2002
ISBN	1-281-01974-7 9786611019747 0-08-051998-9
Edizione	[2nd ed.]
Descrizione fisica	1 online resource (661 p.)
Collana	Computational science series ; ; 1
Altri autori (Persone)	SmitBerend <1962->
Disciplina	539/.6/0113
Soggetti	Intermolecular forces - Computer simulation Molecules - Mathematical models
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references (p. [589]-617) and index.
Nota di contenuto	Front Cover; Understanding Molecular Simulation: From Algorithms to Applications; Copyright Page; Contents; Preface to the Second Edition;

Preface; List of Symbols; Chapter 1. Introduction; Part I: Basics; Chapter 2. Statistical Mechanics; 2.1 Entropy and Temperature; 2.2 Classical Statistical Mechanics; 2.3 Questions and Exercises; Chapter 3. Monte Carlo Simulations; 3.1 The Monte Carlo Method; 3.2 A Basic Monte Carlo Algorithm; 3.3 Trial Moves; 3.4 Applications; 3.5 Questions and Exercises; Chapter 4. Molecular Dynamics Simulations; 4.1 Molecular Dynamics: The Idea
4.2 Molecular Dynamics: A Program4.3 Equations of Motion; 4.4 Computer Experiments; 4.5 Some Applications; 4.6 Questions and Exercises; Part II: Ensembles; Chapter 5. Monte Carlo Simulations in Various Ensembles; 5.1 General Approach; 5.2 Canonical Ensemble; 5.3 Microcanonical Monte Carlo; 5.4 Isobaric-Isothermal Ensemble; 5.5 Isotension-Isothermal Ensemble; 5.6 Grand-Canonical Ensemble; 5.7 Questions and Exercises; Chapter 6. Molecular Dynamics in Various Ensembles; 6.1 Molecular Dynamics at Constant Temperature; 6.2 Molecular Dynamics at Constant Pressure; 6.3 Questions and Exercises
Part III: Free Energies and Phase EquilibriaChapter 7. Free Energy Calculations; 7.1 Thermodynamic Integration; 7.2 Chemical Potentials; 7.3 Other Free Energy Methods; 7.4 Umbrella Sampling; 7.5 Questions and Exercises; Chapter 8. The Gibbs Ensemble; 8.1 The Gibbs Ensemble Technique; 8.2 The Partition Function; 8.3 Monte Carlo Simulations; 8.4 Applications; 8.5 Questions and Exercises; Chapter 9. Other Methods to Study Coexistence; 9.1 Semigrand Ensemble; 9.2 Tracing Coexistence Curves; Chapter 10. Free Energies of Solids; 10.1 Thermodynamic Integration; 10.2 Free Energies of Solids
10.3 Free Energies of Molecular Solids10.4 Vacancies and Interstitials; Chapter 11. Free Energy of Chain Molecules; 11.1 Chemical Potential as Reversible Work; 11.2 Rosenbluth Sampling; Part IV: Advanced Techniques; Chapter 12. Long-Range Interactions; 12.1 Ewald Sums; 12.2 Fast Multipole Method; 12.3 Particle Mesh Approaches; 12.4 Ewald Summation in a Slab Geometry; Chapter 13. Biased Monte Carlo Schemes; 13.1 Biased Sampling Techniques; 13.2 Chain Molecules; 13.3 Generation of Trial Orientations; 13.4 Fixed Endpoints; 13.5 Beyond Polymers; 13.6 Other Ensembles; 13.7 Recoil Growth
13.8 Questions and ExercisesChapter 14. Accelerating Monte Carlo Sampling; 14.1 Parallel Tempering; 14.2 Hybrid Monte Carlo; 14.3 Cluster Moves; Chapter 15. Tackling Time-Scale Problems; 15.1 Constraints; 15.2 On-the-Fly Optimization: Car-Parrinello Approach; 15.3 Multiple Time Steps; Chapter 16. Rare Events; 16.1 Theoretical Background; 16.2 Bennett-Chandler Approach; 16.3 Diffusive Barrier Crossing; 16.4 Transition Path Ensemble; 16.5 Searching for the Saddle Point; Chapter 17. Dissipative Particle Dynamics; 17.1 Description of the Technique; 17.2 Other Coarse-Grained Techniques
Part V: Appendices

Sommario/riassunto

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 practic