

1. Record Nr.	UNINA9910144265503321
Titolo	Monte Carlo methods in chemical physics [[electronic resource] /] / edited by David M. Ferguson, J. Ilja Siepmann, Donald G. Truhlar
Pubbl/distr/stampa	New York, : J. Wiley, c1999
ISBN	1-282-68203-2 9786612682032 0-470-14164-6 0-470-14217-0
Descrizione fisica	1 online resource (574 p.)
Collana	Advances in chemical physics ; ; v. 105
Altri autori (Persone)	FergusonDavid M SiepmannJ. Ilja TruhlarDonald G. <1944->
Disciplina	539 541.305 541/.08
Soggetti	Monte Carlo method Chemistry, Physical and theoretical Electronic books.
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 and indexes.
Nota di contenuto	MONTE CARLO METHODS IN CHEMICAL PHYSICS; CONTENTS; AN INTRODUCTION TO THE MONTE CARLO METHOD FOR PARTICLE SIMULATIONS; RANDOM NUMBER GENERATORS FOR PARALLEL APPLICATIONS; BETWEEN CLASSICAL AND QUANTUM MONTE CARLO METHODS:"VARIATIONAL" QMC; MONTE CARLO EIGENVALUE METHODS IN QUANTUM MECHANICS AND STATISTICAL MECHANICS; ADAPTIVE PATH-INTEGRAL MONTE CARLO METHODS FOR ACCURATE COMPUTATION OF MOLECULAR THERMODYNAMIC PROPERTIES; MONTE CARLO SAMPLING FOR CLASSICAL TRAJECTORY SIMULATIONS; MONTE CARLO APPROACHES TO THE PROTEIN FOLDING PROBLEM; ENTROPY SAMPLING MONTE CARLO FOR POLYPEPTIDES AND PROTEINS MACROSTATE DISSECTION OF THERMODYNAMIC MONTE CARLO INTEGRALSSIMULATED ANNEALING-OPTIMAL HISTOGRAM METHODS; MONTE CARLO METHODS FOR POLYMERIC SYSTEMS;

THERMODYNAMIC-SCALING METHODS IN MONTE CARLO AND THEIR APPLICATION TO PHASE EQUILIBRIA; SEMIGRAND CANONICAL MONTE CARLO SIMULATION; INTEGRATION ALONG COEXISTENCE LINES; MONTE CARLO METHODS FOR SIMULATING PHASE EQUILIBRIA OF COMPLEX FLUIDS; REACTIVE CANONICAL MONTE CARLO; NEW MONTE CARLO ALGORITHMS FOR CLASSICAL SPIN SYSTEMS; AUTHOR INDEX; SUBJECT INDEX

Sommario/riassunto

In Monte Carlo Methods in Chemical Physics: An Introduction to the Monte Carlo Method for Particle Simulations J. Ilja Siepmann Random Number Generators for Parallel Applications Ashok Srinivasan, David M. Ceperley and Michael Mascagni Between Classical and Quantum Monte Carlo Methods: "Variational" QMC Dario Bressanini and Peter J. Reynolds Monte Carlo Eigenvalue Methods in Quantum Mechanics and Statistical Mechanics M. P. Nightingale and C.J. Umrigar Adaptive Path-Integral Monte Carlo Methods for Accurate Computation of Molecular Thermodynamic Properties Robert Q. Topper Monte Carlo Sampli
