1. Record Nr. UNINA9910143985803321

Titolo	Reviews in computational chemistry . Volume 12 [[electronic resource] /] / edited by Kenny B. Lipkowitz and Donald B. Boyd
Pubbl/distr/stampa	New York, : Wiley-VCH, 1998
ISBN	1-282-30848-3 9786612308482 0-470-12589-6 0-470-12616-7
Descrizione fisica	1 online resource (434 p.)
Collana	Reviews in computational chemistry ; ; 12
Altri autori (Persone)	LipkowitzKenny B BoydDonald B
Disciplina	542.85 542/.8
Soggetti	Chemistry - Data processing Chemistry - Mathematics
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	Reviews in Computational Chemistry Volume 12; Contents; Calculation of the Free Energy and the Entropy of Macromolecular Systems by Computer Simulation; Introduction; Statistical Mechanics of Fluids and Chain Systems; The Partition Function and the Boltzmann Probability Density; The Absolute Entropy and Free Energy as Ensemble Averages; Fluctuations; Entropy and Free Energy Differences by "Calorimetric" Thermodynamic Integration; The Kirkwood and Zwanzig Equations; Basic Sampling Theory and Simulation; Importance Sampling; The Monte Carlo and Molecular Dynamics Methods Application of the MC and MD Methods to Macromolecular SystemsDirect Methods for Calculating the Entropy of Proteins; The Harmonic Approximation; The Quasi-Harmonic Approximation; Free Energy from ; Applications of Integration and Importance Sampling Techniques; Calculations by Calorimetric Integration and Perturbation Methods; Umbrella Sampling and the Potential of Mean Force; Thermodynamic Cycles; Historical Perspective; Free Energy of Enzyme-Ligand Binding; Application of Thermodynamic Cycles; New

Perturbation-Related Procedures; Entropy from Linear Buildup Procedures
Step-by-Step Construction Methods for PolymersDirect Methods for Calculating the Entropy from MC and MD Samples; The Stochastic Models Method of Alexandrowicz and Its Implications; Additional Methods for Calculating the Entropy; The Multicanonical Approach; Calculation of Entropy by Adiabatic Switching; Four Additional Methods; Summary; Acknowledgments; References; Molecular Dynamics with General Holonomic Constraints and Application to Internal Coordinate Constraints; Introduction; The Analytical Method of Constraint Dynamics; Computation of the Forces of Constraints and Their Derivatives
Numerical Integration of the Equations of MotionError Analysis of the Analytical Method; Method of Edberg, Evans, and Morriss in Context; The Method of Undetermined Parameters; Computation of the Partially Constrained Coordinates; Computation of the Undetermined Parameters and the Constrained Coordinates; Error Analysis of the Method of Undetermined Parameters; Using the Method of Undetermined Parameters with the Basic Verlet Integration Algorithm; The Matrix Method; SHAKE; Physical Picture of SHAKE for Internal Coordinate Constraints; Method of Tobias and Brooks in Context Application to Internal Coordinate ConstraintsBond-Stretch Constraints; Angle-Bend Constraints; Torsional Constraints; Angle Constraint Versus Triangulation; Using the Method of Undetermined Parameters with the Velocity Verlet Integration Algorithm; RATTLE for General Holonomic Constraints; Application to Bond-Stretch, Angle-Bend, and Torsional Constraints; Further Developments and Future Prospects; Acknowledgments; References; Computer Simulation of Water Physisorption at Metal-Water Interfaces; Introduction; Modeling; Treatment of Water; Treatment of Metal-Water Interactions
Simulation Methods

Sommario/riassunto

VOLUME 12: REVIEWS IN COMPUTATIONAL CHEMISTRY Kenny B. Lipkowitz and Donald B. Boyd HOW DOES ONE COMPUTE FREE ENERGY AND ENTROPY FROM MOLECULAR SIMULATIONS? WHAT HAPPENS WHEN SIMULATIONS ARE RUN WITH CONSTRAINTS? HOW SHOULD SIMULATIONS BE PERFORMED TO MODEL INTERFACIAL PHENOMENA? HOW IS DENSITY FUNCTIONAL THEORY USED TO SIMULATE MATERIALS? WHAT QUANTUM MECHANICAL METHODS SHOULD BE USED TO COMPUTE NONLINEAR OPTICAL PROPERTIES OF MATERIALS? WHICH PARAMETERS ARE MOST INFLUENTIAL IN A MOLECULAR SIMULATION? HOW CAN CRYSTAL STRUCTURES BE PREDICTED? TUTORIALS PROVIDING ANSWERS TO THESE QUESTIONS