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Nota di contenuto	Introduction: Condensed Matter Theory by Computer Simulation -- Transition Path Sampling Methods -- Sampling Kinetic Protein Folding Pathways using All-Atom Models -- Calculation of Classical Trajectories with Boundary Value Formulation -- Transition Path Theory -- Multiscale Modelling in Molecular Dynamics: Biomolecular Conformations as Metastable States -- Transport Coefficients of Quantum-Classical Systems -- Linearized Path Integral Methods for Quantum Time Correlation Functions -- Ensemble Optimization Techniques for Classical and Quantum Systems -- The Coupled Electron-Ion Monte Carlo Method -- Path Resummations and the Fermion Sign Problem -- to Cluster Monte Carlo Algorithms -- Generic Sampling Strategies for Monte Carlo Simulation of Phase Behaviour -- Simulation Techniques for Calculating Free Energies -- Waste-Recycling Monte Carlo -- Equilibrium Statistical Mechanics, Non-Hamiltonian Molecular Dynamics, and Novel Applications from Resonance-Free Timesteps to Adiabatic Free Energy Dynamics -- Simulating Charged Systems with ESPResSo -- Density Functional Theory Based Ab Initio Molecular Dynamics Using the Car-Parrinello Approach -- Large Scale Condensed Matter Calculations using the

Gaussian and Augmented Plane Waves Method -- Computing Free Energies and Accelerating Rare Events with Metadynamics.

Sommario/riassunto

This extensive and comprehensive collection of lectures by world-leading experts in the field introduces and reviews all relevant computer simulation methods and their applications in condensed matter systems. Volume 1 is an in-depth introduction to a vast spectrum of computational techniques for statistical mechanical systems of condensed matter. It will enable the graduate student and both the specialist and nonspecialist researcher to get acquainted with the tools necessary to carry out numerical simulations at an advanced level. Volume 2 published as LNP 704 (ISBN 3-540-35283-X) is a collection of state-of-the-art surveys on numerical experiments carried out for a great number of systems, ranging from materials sciences to chemical biology.