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Nota di contenuto	Protein Folding -- Sidechain Dynamics and Protein Folding -- Applications of Statistical Mechanics to Biological Systems -- A Coarse Grain Model for Lipid Monolayer and Bilayer Studies -- Polymer Structure and Dynamics -- Variable-Connectivity Monte Carlo Algorithms for the Atomistic Simulation of Long-Chain Polymer Systems -- Bridging the Time Scale Gap: How Does Foldable Polymer Navigate Its Conformation Space? -- Multiscale Computer Simulations for Polymeric Materials in Bulk and Near Surfaces -- Complex and Mesoscopic Fluids -- Effective Interactions for Large-Scale Simulations of Complex Fluids -- Slow Dynamics and Reactivity -- Simulation of Models for the Glass Transition: Is There Progress? -- Lattice Models -- Monte Carlo Methods for Bridging the Timescale Gap -- Go-with-the-Flow Lattice Boltzmann Methods for Tracer Dynamics -- Multiscale Modelling in Materials Science -- Atomistic Simulations of Solid Friction -- Methodological Developments in MD and MC -- Bridging the Time Scale Gap with Transition Path Sampling -- The Stochastic Difference Equation as a Tool to Compute Long Time Dynamics -- Numerical Simulations of Molecular Systems with Long Range Interactions -- Perpectives in ab initio MD -- New Developments in Plane-Wave Based ab initio Calculations -- Time and Length Scales in ab initio Molecular Dynamics -- Quantum Simulations -- A Statistical Mechanical Theory

	of Quantum Dynamics in Classical Environments -- The Coupled Electronic-Ionic Monte Carlo Simulation Method.
Sommario/riassunto	The behaviour of many complex materials extends over time- and lengthscales well beyond those that can normally be described using standard molecular dynamics or Monte Carlo simulation techniques. As progress is coming more through refined simulation methods than from increased computer power, this volume is intended as both an introduction and a review of all relevant modern methods that will shape molecular simulation in the forthcoming decade. Written as a set of tutorial reviews, the book will be of use to specialists and nonspecialists alike.