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Titolo	Molecular kinetics in condensed phases : theory, simulation, and analysis / / Ron Elber, Dmitrii E. Makarov, Henri Orland
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ISBN	1-119-17679-4 1-119-17678-6 1-119-17680-8
Descrizione fisica	1 online resource (292 pages) : illustrations
Disciplina	541.394
Soggetti	Chemical kinetics - Mathematical models Stochastic processes - Mathematical models Molecular structure
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	The Langevin equation and stochastic processes -- The Fokker-Planck equation -- The Schrodinger representation -- Discrete systems : the master equation and kinetic Monte Carlo -- Path integrals -- Barrier crossing -- Sampling transition paths -- The rate of conformational change : definition and computation -- Zwanzig-Caldeiga-Leggett model for low-dimensional dynamics -- Escape from a potential well in the case of dynamics obeying the generalized Langevin equation : general solution based on the Zwanzig-Caldeira-Leggett Hamiltonian -- Diffusive dynamics on a multidimensional energy landscape -- Quantum effects in chemical kinetics -- Computer simulations of molecular kinetics : foundation -- The master equation as a model for transitions between macrostates -- Direct calculation of rate coefficients with computer simulations -- A simple numerical example of rate calculations -- Rare events and reaction coordinates -- Celling -- An example of the use of cells : alanine dipeptide.
Sommario/riassunto	"Modern approaches to the study of kinetics routinely combine the use of computer simulations with analytic analysis. This book is focused on the theory, algorithms, simulations methods, and analysis of molecular kinetics in condensed phases. It provides a detailed and comprehensive

description of modern theories and simulation methods to model molecular events. Emphasis is placed on rigorous stochastic modeling of molecular processes and the use of the mathematical models to reproduce experimental observations, such as rate coefficients, mean first passage times, and transition times. Simulations focus on atomically detailed modeling of molecules in action and the connections of these simulations to theory and experiment. Applications are described that range from simple intuitive examples of one- and two-dimensional systems to complex solvated macromolecules. The book is divided into five sections and topics covered include: Introduction: Langevin dynamics, Fokker Planck equation, path integrals, generalized Langevin equation, generalized master equation, theory of optimal pathways. Kinetic Theory: Transition state theory, transmission coefficient, duration of transition path, Kramers theory, Grote-Hynes theory, generalized Langevin equation and transition state theory, diffusion controlled reactions, quantum effects on reaction rates. Simulations: Molecular dynamics simulations, Monte Carlo method, accelerated dynamics approaches for kinetics, calculations of reaction pathways. Analysis: Committors, transition path theory, kinetic networks, Markov state models. Examples: One and two-dimensional models, simulations of biological macromolecules, models of protein folding, molecular machines, transport processes"--