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Nota di contenuto	Reviews in Computational Chemistry 27; Preface; Contents; Contributors; Contributors to Previous Volumes; CHAPTER 1 Brittle Fracture: From Elasticity Theory to Atomistic Simulations; INTRODUCTION; ESSENTIAL CONTINUUM ELASTICITY THEORY; Conceptual Layout; The Concept of Strain; The Concept of Stress; The Formal Structure of Elasticity Theory; Constitutive Equations; The Isotropic and Homogeneous Elastic Body; Governing Equations of Elasticity and Border Conditions; Elastic Energy; MICROSCOPIC THEORY OF ELASTICITY; Conceptual Layout; Triangular Lattice with Central Forces Only Triangular Lattice with Two-Body and Three-Body InteractionsInteratomic Potentials for Solid Mechanics; Atomic-Scale Stress; LINEAR ELASTIC FRACTURE MECHANICS; Conceptual Layout; Stress Concentration; The Griffith Energy Criterion; Opening Modes and Stress Intensity Factors; Some Three-Dimensional Configurations; Elastic Behavior of Multi Fractured Solids; Atomistic View of Fracture; ATOMISTIC INVESTIGATIONS ON BRITTLE FRACTURE; Conceptual

Layout; Griffith Criterion for Failure; Failure in Complex Systems; Stress Shielding at Crack-Tip; ACKNOWLEDGMENTS; APPENDIX: NOTATION; REFERENCES
CHAPTER 2 Dissipative Particle DynamicsINTRODUCTION; FUNDAMENTALS OF DPD; Mathematical Formulation; Units in DPD; Thermostat and Schmidt Number; Integration Algorithms; Boundary Conditions; EXTENSIONS OF DPD; DPD with Energy Conservation; Fluid Particle Model; DPD for Two-Phase Flows; Other Extensions; APPLICATIONS; Polymer Solutions and Melts; Binary Mixtures; Amphiphilic Systems; Red Cells in Microcirculation; SUMMARY; REFERENCES; CHAPTER 3 Trajectory-Based Rare Event Simulations; INTRODUCTION; Simulation of Rare Events; Rare Event Kinetics from Transition State Theory
The Reaction Coordinate ProblemAccelerating Dynamics; Trajectory-Based Methods; Outline of the Chapter; TRANSITION STATE THEORY; Statistical Mechanical Definitions; Rate Constants; Rate Constants from Transition State Theory; Variational TST; The Harmonic Approximation; REACTIVE FLUX METHODS; The Bennett-Chandler Procedure; The Effective Positive Flux; The Ruiz-Montero-Frenkel-Brey Method; TRANSITION PATH SAMPLING; Path Probability; Order Parameters; Sampling the Path Ensemble; Shooting Move; Sampling Efficiency; Biasing the Shooting Point; Aimless Shooting; Stochastic Dynamics Shooting Move
Shifting MoveFlexible Time Shooting; Which Shooting Algorithm to Choose?; The Initial Pathway; The Complete Path Sampling Algorithm; Enhancement of Sampling by Parallel Tempering; Multiple-State TPS; Transition Path Sampling Applications; COMPUTING RATES WITH PATH SAMPLING; The Correlation Function Approach; Transition Interface Sampling; Partial Path Sampling; Replica Exchange TIS or Path Swapping; Forward Flux Sampling; Milestoning; Discrete Path Sampling; MINIMIZING THE ACTION; Nudged Elastic Band; Action-Based Sampling; Transition Path Theory and the String Method
IDENTIFYING THE MECHANISM FROM THE PATH ENSEMBLE

Sommario/riassunto

This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Volume 27 covers brittle fracture, molecular detailed simulations of lipid bilayers, semiclassical bohmian dynamics, dissipative particle dynamics, trajectory-based rare event simulations, and understanding metal/metal electrical contact conductance from the atomic to continuum scales. Also included is a chapter on career opportunities in computational chemistry and an appendix listing the e-mail addresses of more than 2500 people in that discipline. FROM REVIEWS OF THE S