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Hydrophobicity; Introduction; Simulation Methods; Statistical Mechanics and Thermodynamics; Particle Insertion Methods; Perturbation Methods; Thermodynamic Integration; Free Energy and Structure; Entropy and Energy; Heat Capacity; Hydrophobic Hydration; Structure Hydration Free Energy Hydration Entropy and Energy; Hydration Heat Capacity; Water Mimics; Hydrophobic Interactions; Free Energy of Association; Entropy and Energy of Association; Heat Capacity of Association; Pressure Dependence of Hydrophobic Interactions; Outlook; Acknowledgments; References; 3. Born-Oppenheimer Direct Dynamics Classical Trajectory Simulations; Introduction; Classical Trajectory Simulations; Traditional Approach: Analytic Potential Energy Surfaces; Direct Dynamics Simulations; Born-Oppenheimer Direct Dynamics; Semiempirical Electronic Structure Theory Ab Initio Electronic Structure Theory QM+MM and QM/MM Methods; Integrating the Classical Equations of Motion; Cartesian Coordinates; Instantaneous Normal-Mode Coordinates; Trajectory Initial Conditions; Unimolecular Reactions; Bimolecular Reactions; Exciting the Transition State; Gas-Surface Collisions; Importance of Quantum Effects; Bimolecular Reactions; Intramolecular Dynamics and Unimolecular Reactions; Summary; Applications of Born-Oppenheimer Direct Dynamics; Cyclopropane Stereomutation; $\text{Cl}(-) + \text{CH}(3)\text{Cl}$ Central-Barrier Dynamics; $\text{OH}(-) + \text{CH}(3)\text{F}$ Exit-Channel Dynamics Protonated Glycine Surface-Induced Dissociation Concluding Remarks; Acknowledgments; References; 4. The Poisson-Boltzmann Equation; Introduction; State of the Field; Overview of the Chapter; A Brief History; The Poisson-Boltzmann Equation; Analytical Solutions to the Poisson-Boltzmann Equation; Planar Geometry: The Membrane Model; Curved Surfaces: Cylinders and Spheres; Cylindrical Geometry: The Polymer Model; Spherical Geometry: The Micelle Model; Mixed-Geometry Studies; Numerical Solutions to the Poisson-Boltzmann Equation; One-Dimensional Geometries Finite-Difference/Finite-Element Algorithms

Sommario/riassunto

The Reviews in Computational Chemistry series brings together leading authorities in the field. The chapters in this book series are written to teach the newcomer and update the expert. Topics include computational chemistry, molecular modeling, computer-assisted molecular design (CAMD), quantum chemistry, molecular mechanics and dynamics, and quantitative structure-activity relationships (QSAR). Detailed author and subject indices on each volume help the reader to quickly discover particular topics. The chapters are approached in a tutorial manner and written in a non-mathem
