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Sampling + Scoring; Rigid-Body Docking; Flexible Docking; Example; Estimating the Extent of Conformational Change upon Binding Rigid-Body DockingFlexible Docking with Side-Chain Flexibility; Flexible Docking with Full Flexibility; Future Directions; Conclusions; References; 3. Spin-Orbit Coupling in Molecules; What It Is All About; The Fourth Electronic Degree of Freedom; The Stern-Gerlach Experiment; Zeeman Spectroscopy; Spin Is a Quantum Effect; Angular Momenta; Orbital Angular Momentum; General Angular Momenta; Spin Angular Momentum; Spin-Orbit Hamiltonians; Full One- and Two-Electron Spin-Orbit Operators; Valence-Only Spin-Orbit Hamiltonians; Effective One-Electron Spin-Orbit Hamiltonians; Symmetry Transformation Properties of the Wave FunctionTransformation Properties of the Hamiltonian; Matrix Elements; Examples; Summary; Computational Aspects; General Considerations; Evaluation of Spin-Orbit Integrals; Perturbational Approaches to Spin-Orbit Coupling; Variational Procedures; Comparison of Fine-Structure Splittings with Experiment; First-Order Spin-Orbit Splitting; Second-Order Spin-Orbit Splitting; Spin-Forbidden Transitions; Radiative Transitions; Nonradiative Transitions; Summary and Outlook; Acknowledgments; References; 4. Cellular Automata Models of Aqueous Solution Systems IntroductionCellular Automata; Historical Background; The General Structure; Cell Movement; Movement (Transition) Rules; Collection of Data; Aqueous Solution Systems; Water as a System; The Molecular Model; Significance of the Rules; Studies of Water and Solution Phenomena; A Cellular Automata Model of Water; The Hydrophobic Effect; Solute Dissolution; Aqueous Diffusion; Immiscible Liquids and Partitioning; Micelle Formation; Membrane Permeability; Acid Dissociation; Percolation; Solution Kinetic Models; First-Order Kinetics; Kinetic and Thermodynamic Reaction Control; Excited-State Kinetics Second-Order Kinetics

Sommario/riassunto

Computational chemistry is increasingly used in most areas of molecular science including organic, inorganic, medicinal, biological, physical, and analytical chemistry. Researchers in these fields who do molecular modelling need to understand and stay current with recent developments. This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Two chapters focus on molecular docking, one of which relates to drug discovery and cheminformatics and the other to proteomics. In addition, this volume contains tutorials on spin-orbit coupling and ce