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| Nota di contenuto       | <ul> <li>Modeling Solvent Environments: Applications to Simulations of<br/>Biomolecules; Contents; Preface; List of Contributors; 1: Biomolecular<br/>Solvation in Theory and Experiment; 1.1 Introduction; 1.2 Theoretical<br/>Views of Solvation; 1.2.1 Equilibrium Thermodynamics of Solvation;<br/>1.2.2 Radial Distribution Functions; 1.2.3 Integral Equation Formalisms;<br/>1.2.4 Kirkwood-Buff Theory; 1.2.5 Kinetic Effects of Solvation; 1.3<br/>Computer Simulation Methods in the Study of Solvation; 1.3.1<br/>Molecular Dynamics and Monte Carlo Simulations; 1.3.2 Water Models;<br/>1.3.3 Solvent Structure and Dynamics from Simulations</li> <li>1.3.4 Free Energy Simulations1.4 Experimental Methods in the Study of<br/>Solvation; 1.4.1 X-Ray/Neutron Diffraction and Scattering; 1.4.2<br/>Nuclear Magnetic Relaxation; 1.4.3 Optical Spectroscopy; 1.4.4<br/>Dielectric Dispersion; 1.5 Hydration of Proteins; 1.5.1 Protein Folding<br/>and Peptide Conformations in Aqueous Solvent; 1.5.2 Molecular<br/>Properties of Water Near Protein Surfaces; 1.5.3 Water Molecules at<br/>Protein-Ligand and Protein-Protein Interfaces; 1.6 Hydration of Nucleic<br/>acids; 1.7 Non-Aqueous Solvation; 1.7.1 Alcohols; 1.7.2 Urea; 1.7.3<br/>Glycerol; 1.8 Summary; References</li> <li>2: Model-Free "Solvent Modeling" in Chemistry and Biochemistry Based</li> </ul> |

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|                    | on the Statistical Mechanics of Liquids2.1 Introduction; 2.2 Outline of<br>the RISM and 3D-RISM theories; 2.3 Partial Molar Volume of Proteins;<br>2.4 Detecting Water Molecules Trapped Inside Protein; 2.5 Selective Ion<br>Binding by Protein; 2.6 Water Molecules Identified as a Substrate for<br>Enzymatic Hydrolysis of Cellulose; 2.7 CO Escape Pathway in<br>Myoglobin; 2.7.1 Effect of Protein Structure on the Distribution of Xe;<br>2.7.2 Partial Molar Volume Change Through the CO Escape Pathway of<br>Myoglobin; 2.8 Perspective; References<br>3: Developing Force Fields From the Microscopic Structure of Solutions:<br>The Kirkwood-Buff Approach3.1 Introduction; 3.2 Biomolecular Force<br>Fields; 3.3 Examples of Problems with Current Force Fields; 3.4<br>Kirkwood-Buff Theory; 3.5 Applications of Kirkwood-Buff Theory; 3.6<br>The General KBFF Approach; 3.7 Technical Aspects of the KBFF<br>Approach; 3.8 Results for Urea and Water Binary Solutions; 3.9<br>Preferential Interactions of Urea; 3.10 Conclusions and Future<br>Directions; Acknowledgments; References; 4: Osmolyte Influence on<br>Protein Stability: Perspectives of Theory and Experiment; 4.1<br>Introduction<br>4.2 Denaturing Osmolytes4.2.1 Does Urea Weaken Water Structure?;<br>4.2.2 Effect of Urea on Hydrophobic Interactions; 4.2.3 Direct |
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|                    | Interaction of Urea with Proteins; 4.3 Protecting Osmolytes; 4.3.1 Do<br>Protecting Osmolytes Increase Water Structure?; 4.3.2 Effect of<br>Protecting Osmolytes on Hydrophobic Interactions; 4.4 Mixed<br>Osmolytes; 4.5 Conclusions; Acknowledgments; References; 5:<br>Modeling Aqueous Solvent Effects through Local Properties of Water;<br>5.1 The Role of Water and Cosolutes on Macromolecular<br>Thermodynamics; 5.2 Forces Induced by Water in Aqueous Solutions<br>5.2.1 Interactions in Water-Accessible Regions of Proteins   |
| Sommario/riassunto | A comprehensive view of the current methods for modeling solvent<br>environments with contributions from the leading researchers in the<br>field. Throughout, the emphasis is placed on the application of such<br>models in simulation studies of biological processes, although the<br>coverage is sufficiently broad to extend to other systems as well. As<br>such, this monograph treats a full range of topics, from statistical<br>mechanics-based approaches to popular mean field formalisms,<br>coarse-grained solvent models, more established explicit, fully atomic<br>solvent models, and recent advances in applying ab initio me   |