

1. Record Nr.	UNISA996466852303316
Autore	Nakasako Masayoshi
Titolo	Hydration structures of proteins : atomic details / / Masayoshi Nakasako
Pubbl/distr/stampa	Tokyo, Japan : , : Springer, , [2021] ©2021
ISBN	4-431-56919-7
Descrizione fisica	1 online resource (321 pages)
Collana	Soft and Biological Matter
Disciplina	541.372
Soggetti	Hydration Proteins Hydratation
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Intro -- Preface -- Acknowledgements -- Contents -- About the Author -- Glossary of Symbols -- 1 Introduction -- 1.1 Water: The Cradle of Life -- 1.2 Structure and Interaction of Water Molecules -- 1.2.1 Structure of Water Molecules -- 1.2.2 Interactions Between Water Molecules -- 1.2.3 Hydrogen Bond Between Water Molecules -- 1.3 Phase Diagram of Water -- 1.3.1 Three Phases of Water -- 1.3.2 Hexagonal Ice and Amorphous Ice -- 1.4 Properties of Liquid Water -- 1.4.1 Unusual Physical Properties -- 1.4.2 Brownian Motion in Liquid Water -- 1.4.3 Structure of Liquid Water -- 1.5 Hydration -- 1.5.1 Solvation -- 1.5.2 Hydration -- 1.5.3 Hydration of Hydrophobic Molecules -- 1.6 Hydration Structures of Proteins -- 1.6.1 Proteins -- 1.6.2 Hydration Structures of Proteins -- 1.7 Scope of This Monograph -- References -- 2 Biophysical Methods to Investigate Hydration Structures of Proteins -- 2.1 Introduction -- 2.2 X-Ray Crystallography at Cryogenic Temperatures -- 2.2.1 Outline -- 2.2.2 Crystallographic Structure Refinement -- 2.2.3 Difference Fourier Map -- 2.2.4 X-Ray Crystallography at Cryogenic Temperatures -- 2.3 Cryogenic Electron Microscopy -- 2.3.1 Outline -- 2.3.2 Specimen Preparation and Image Collection -- 2.3.3 Image Processing and Single-Particle Analysis -- 2.4 Time-Resolved Fluorescence Measurement -- 2.4.1 Outline -- 2.4.2 Up-conversion Method -- 2.5 Molecular Dynamic Simulation --

2.5.1 Outline -- 2.5.2 Force Field -- References -- 3 Hydration Structures Inside Proteins -- 3.1 Introduction -- 3.2 Water Molecules Inside Proteins -- 3.2.1 Tightly Bound Water Molecules -- 3.2.2 Water Molecules Confined Inside Proteins -- 3.3 Hydration Water Molecules as Glue in Protein Complexes -- 3.3.1 Hydration at the Subunit Interface of a Protein Complex -- 3.3.2 Hydration Sites Conserved in Protein Families.

3.4 Hydration Water Molecules as Lubricant at the Protein Interface -- 3.5 Hydration Water Molecules in the Ligand-Binding Sites -- References -- 4 Hydration Layer Around Proteins -- 4.1 Introduction -- 4.2 Hydration Layer -- 4.2.1 First- and Second-Layer Classes -- 4.2.2 Distance Distribution and Positional Fluctuation -- 4.2.3 Monolayer Hydration -- 4.2.4 Contact Class -- 4.3 Local Patterns in Protein Hydration -- 4.3.1 Patterns on Hydrophilic Surfaces -- 4.3.2 Hydration Patterns on Hydrophobic Surfaces -- 4.3.3 Tetrahedral Hydrogen Bond Geometry of Water Molecules -- 4.4 Hydration Structures in Molecular Dynamics Simulation -- 4.4.1 Computation of Solvent Density -- 4.4.2 Characteristics of Solvent Density -- References -- 5 Structural Characteristics in Local Hydration -- 5.1 Introduction -- 5.2 Empirical Hydration Distribution Around Polar Atoms -- 5.2.1 Construction -- 5.2.2 Distribution Around Polar Protein Atoms -- 5.2.3 Hydration of Aromatic Acceptors -- 5.2.4 Characteristics and Benefits of the Empirical Hydration Distributions -- 5.2.5 Tetrahedral Hydrogen Bond Geometry -- 5.3 Assessment of Force Fields of Polar Protein Atoms -- 5.3.1 Models of Water Molecule Suitable for Simulation -- 5.3.2 Hydration of Deprotonated Polar Atoms in sp²-Hybridization -- 5.3.3 Hydration of Protonated Nitrogen Atoms in sp²- or sp³-Hybridization -- 5.3.4 Hydration of Protonated Oxygen Atoms in sp²- or sp³-Hybridization -- 5.3.5 Molecular Dynamics Simulation of Proteins Using Force Field with Lone-Pair Electrons -- References -- 6 Prediction of Hydration Structures -- 6.1 Introduction -- 6.2 Computation of Probability Distribution of Hydration Water Molecules [19] -- 6.3 Prediction for Soluble Protein [19] -- 6.3.1 On Solvent-Exposed Surfaces and in Cavities -- 6.3.2 At Interface in Protein Complex -- 6.4 Prediction for Membrane Proteins.

6.4.1 For Surfaces of Membrane Proteins -- 6.4.2 For Channels in Transmembrane Regions -- 6.5 Accuracy of Prediction -- 6.6 Comparison of the Prediction with Theory of Liquids -- 6.7 Utilization of Probability Distribution in Structure Analysis -- 6.7.1 Assessment on Hydration Water Sites -- 6.7.2 Probability Distribution-Weighted Electron Density Map [55] -- 6.8 Prediction of Hydration Structures on Hydrophobic Surfaces -- References -- 7 Network of Hydrogen Bonds Around Proteins -- 7.1 Introduction -- 7.2 Network of Hydrogen Bonds -- 7.2.1 Chain Connection of Hydrogen Bonds -- 7.2.2 Percolation Property -- 7.3 Probability of Hydrogen Bond Formation -- 7.4 Network of Hydrogen Bonds in Simulation Trajectory -- 7.5 Influence of Networks of Hydrogen Bonds on Protein Motions -- References -- 8 Dipole-Dipole Interactions in Hydration Layer -- 8.1 Introduction -- 8.2 Orientational Ordering of Hydration Water Molecules -- 8.2.1 Coherent Patterns of Time-Averaged Water Dipoles -- 8.2.2 Solvent Dipole and Network of Hydrogen Bonds -- 8.2.3 Solvent Dipole in Drug Design -- 8.2.4 Poisson-Boltzmann Equation and Orientation Ordering of Water Molecules -- 8.3 Fluorescence from Tryptophan Side Chains Exposed to Solvent -- 8.3.1 Fluorescence from Photo-Excited Tryptophan of Protein -- 8.3.2 Interpretation of Dynamic Stokes Shift -- 8.3.3 Orientation Ordering of Water Molecules Around Tryptophan Side Chains -- 8.3.4 Origin of Dynamic Stokes Shift -- References -- 9 Hydration Structure Changes

of Proteins at Work -- 9.1 Introduction -- 9.2 Experimental Evidence on Hydration-Regulated Protein Motion -- 9.2.1 Domain Motion in Glutamate Dehydrogenase -- 9.2.2 Hydration Structure Changes in Domain Motion -- 9.2.3 Model for Hydration Coupled Domain Motion -- 9.3 Molecular Mechanism in Hydration-Coupled Domain Motion -- 9.3.1 Domain Motion Observed in Simulation. 9.3.2 Simultaneous Changes in Conformation and Hydration -- 9.3.3 Hydration Changes in the Hydrophobic Pocket -- 9.3.4 Drying Transition in the Hydrophobic Pocket -- 9.3.5 Hydration Changes in the Hydrophilic Crevice -- 9.3.6 Mechanism of Hydration Regulated Domain Motion -- 9.4 Manipulation of Conformation and Hydration of Proteins in the Crystals -- 9.4.1 Conformational Changes of Protein in Different Molecular Packing -- 9.4.2 Hydration Changes in Different Molecular Packing -- References -- 10 Energy Landscape and Hydration of Proteins -- 10.1 Introduction -- 10.1.1 Protein Conformation Manifold and Energy Landscape -- 10.2 X-Ray Diffraction Imaging -- 10.2.1 Structure Analysis Using X-Ray Diffraction Imaging -- 10.2.2 X-Ray Diffraction Imaging Using X-Ray Laser -- 10.3 Cryogenic Electron Microscopy -- 10.3.1 Classification of Protein Structures -- 10.3.2 Energy Landscape in Protein Motions -- 10.3.3 Prediction of Hydration Structures Using Neural Networks -- 10.4 Future Prospects -- References -- Appendix A -- Appendix B X-Ray Diffraction by a Crystal -- B.1 Thomson Scattering [B1] -- B.2 Interference of X-Rays Emitted by Electrons -- B.3 Diffraction From a Crystal [B3] -- B.4 The Ewald Sphere -- References -- Appendix C The Image Obtained by Electron Microscopy -- C1. Electron Scattering by a Weak-Phase Object [C1, C2] -- C2. Contrast Transfer Function [C1, C2] -- References -- Appendix D The Principle of the Up-Conversion Method -- D.1 Higher-Order Dielectric Polarization -- D.2 Radiation by Nonlinear Dielectric Polarization [D2, D3] -- D.3 The Phase-Matching Condition and Birefringence [D2, D3] -- References -- Appendix E The Symplectic Integrator -- Appendix F The Geometries of the Polar Groups in Amino Acid Residues -- Reference. Appendix G Examples of Force Field Parameters Incorporating Lone-Pair Electrons for Deprotonated Oxygen and Nitrogen Atoms in the sp²-Hybridization -- Reference -- Appendix H Energy Relaxation of Perturbed System -- Reference -- Appendix I Surface Topography of Protein Crystals by Atomic Force Microscopy -- References -- Appendix J The Phase Retrieval Algorithm Used in X-Ray Diffraction Imaging -- References -- Appendix K Derivation of the Formula to Determine Appearance Frequencies of Model Structures in Electron Micrographs -- Reference -- Index.
