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Descrizione fisica	1 online resource (X, 146 p. 31 illus., 19 illus. in color.)
Disciplina	541.2
Soggetti	Chemistry, Physical and theoretical Physical biochemistry Biophysics Biomolecules Biology - Technique Enzymology Theoretical Chemistry Biophysical Chemistry Molecular Biophysics Biophysical Methods
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Introduction -- Phenomenological description -- Statistical mechanics of molecular liquids -- Irreversible statistical mechanics of molecular liquids -- Conformational and density fluctuation in biomolecular system -- Chemical reactions of biomolecules in solutions -- Transitions among equilibrium states driven by fluctuations.
Sommario/riassunto	This book describes molecular processes taking place in living cells, in which "water" or "solvation" play essential roles. The molecular processes include conformational stability, fluctuation, relaxation, self-organization, molecular recognition, and chemical reactions. In all those processes, so-called solvation free-energy, and its first and second derivatives with respect to the atomic coordinates of biomolecules play key roles. Such derivatives of the free energy may not be calculated by any method of molecular simulation, because the calculation requires an analytical formula of the solvation free energy

as a function of the atomic coordinates of a biomolecule. In this book, the theory is applied to analyze phenomena closely related to the conformational and density fluctuation of biomolecular systems, including the entropy and spectroscopy of both biomolecules and solvents. The theory is further developed to give microscopic expressions to the well-regarded phenomenological theories of chemical reactions, including the Michaelis–Menten theory of the enzymatic reaction, and the theory of the electron-transfer reaction by R. Marcus. Also clarified in the book is physical basis of Anfinsen's hypothesis concerning the protein folding. This book is beneficial for graduate students and researchers in the field of life science and technology, especially for those studying pharmaceutical design and biomimetic technology such as artificial enzymes.

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