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Theoretical and Computational Studies of Biomacromolecule–Water Interactions

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Although it is conventional wisdom that water plays a very significant role in the structure, stability, dynamics and interactions of many biochemical systems, the operation of such solvent effects at the molecular level is very poorly understood. Any adequate theoretical or computational approach to *e.g.* the statics and dynamics of protein–solvent interactions at this microscopic level necessarily requires knowledge of the various interatomic potential functions. That such chosen functions should be realistic is underlined by the very marginal stability of native protein structures, their free energies being generally only around 10–20 kcal mol^{-1} lower than their denatured conformations; this represents the energy of only 2–4 hydrogen bonds.

Within this context, our recent work has been directed at (*a*) the effects of changes in water structure itself, and in solvent organisation around ions and macromolecules, as the model potentials are varied, and (*b*) the establishment of reliable potential functions, largely through quantum mechanical calculations. Particular stress is placed on a thorough testing of these potentials at relatively well-defined macromolecule–solvent interfaces, such as are found in protein crystals whose structures have been refined to *very* high (1.5 Å or better) resolution. Computer simulation and model-building studies of several suitable systems (*e.g.* insulin, pancreatic trypsin inhibitor, coenzyme B_{12}) will be described, and the current problems and possible solutions discussed. The particular importance of the cooperative nature of the hydrogen bond is emphasised, especially as it may seriously affect solvent–ion and solvent–macromolecule interactions.

An Experimentalist Point of View on Quantitative Elaboration of Theoretical Models

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In a number of problems of solute–solute–solvent interaction, information on the geometrical structure of solvent in the near neighbourhood of solute is now available. This was obtained from a variety of experiments as well as from numerical calculations. The present trend in computer simulation as well as in experimental techniques seems to appropriately be towards an extension of this information to include thermal disorder.

Despite these efforts, other aspects of solute–solute–solvent interaction do not seem likely to find exhaustive answers through a study of the geometrical configurations of solvent molecules around the solute.

More detailed calculations of inter- and intramolecular dynamical behaviour would not only add appreciably to our knowledge and description of the behaviour of water in the phase-space. It would also provide ampler grounds for comparison between theoretical expectations and experimental findings, now available in this area. In turn, this could hopefully provide a better insight on the possible role of solvent motional modes on solute–solute–solvent interaction.

Molecular Dynamics Simulations of Aqueous Electrolyte Solutions

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In the molecular dynamics simulations the classical equations of motion are solved numerically for a