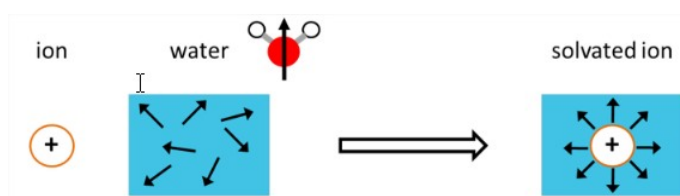


4.1: Solvation

Solvation describes the intermolecular interactions of a molecule or ion in solution with the surrounding solvent, which for our purposes will refer to water. Aqueous solvation influences an enormous range of problems in molecular biophysics, including (1) charge transfer and charge stabilization; (2) chemical and enzymatic reactivity; (3) the hydrophobic effect; (4) solubility, phase separation, and precipitation; (5) binding affinity; (6) self-assembly; and (7) transport processes in water. The terms solute and solvent commonly apply to dilute mixtures in the liquid phase in which the solute (minor component) is dispersed into the solvent (major component). For this reason, the concept of solvation is also at times extended to refer to the influence of any surrounding environment in which a biomolecule is embedded, for instance, a protein or membrane.

There are numerous types of interactions and dynamical effects that play a role in solvation. Typically, solute–solvent interactions are dominated by electrostatics (interactions of charges, dipoles, and induced dipoles), as well as hydrogen bonding and repulsion (both of which have electrostatic components). Therefore there is a tendency to think about solvation purely in terms of these electrostatic interaction energies. A common perspective—polar solvation—emphasizes how the dipoles of a polar liquid can realign themselves to energetically stabilize solute charges, as illustrated here for the case of ion solvation in water. The extent of solute stabilization in the liquid is the reorganization energy.



Unlike most solvents, the presence of water as a solvent for biological molecules fundamentally changes their properties and behavior from the isolated molecule. This means that water influences the conformation of flexible molecules, and sometimes hydrogen bonding interactions with water can be strong enough that it is hard to discern where the boundary of solute ends and water begins. But there is also a significant energetic cost to disrupting water's hydrogen bonding network in order to insert a solute into the liquid. Furthermore, the fluctuating hydrogen bond network of water introduces a significant entropy to the system which can be competitive or even the dominant contributor to the free energy of solvation. As a result, there are competing interactions involving both solute and water that act to restructure the solute and solvent relative to their isolated structures.

It is also important to remember that solvation is a highly dynamical process. Solvation dynamics refers to the time-dependent correlated motions of solute and solvent. How does a solvent reorganize in response to changes in solute charge distribution or structure? Conversely, how do conformational changes to the intermolecular configuration of the solvent (i.e., flow) influence changes in structure or charge distribution in the solute? The latter perspective views the solute as "slaved" to the solvent dynamics. These coupled processes result in a wide variety of time-scales in the solvation of biological macromolecules that span timescales from 10^{-14} to 10^{-7} seconds.

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