Ions at Aqueous Interfaces: From Water Surface to Hydrated Proteins

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Surfaces of aqueous solutions are traditionally viewed as devoid of inorganic ions. Molecular simulations and surface selective spectroscopic techniques show, however, that large polarizable anions and hydronium cations can be found (and even enhanced) at the surface and are involved in chemistry at the air/water interface. Here, we present recent studies of ions at the water/vapor interface and compare from this perspective more complex aqueous interfaces, such as those of hydrated proteins. We critically examine the suitability of dielectric models for the description of the protein/water interface in analogy to the water/vapor interface. Little correlation is found between these two interfaces in terms of ion segregation. Therefore, a local picture of pairing of ions from the solution with charged and polar groups at the protein surface is advocated and combined with a model for segregation of large soft ions at hydrophobic patches of the protein surface.