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Hydrophilic–hydrophobic interplay: from model systems to living systems

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Abstract

Water is a unique liquid, many of whose properties are critical for the continued support of life. In living systems, essential water-related phenomena occur in restricted geometries in cells, and at active sites of proteins and membranes or at their surface. The stability of biological systems is controlled by the subtle hydrophilic–hydrophobic interplay. It is well known that hydration water plays a prominent role in the relationship between structure, dynamics, and biological function. Various examples of systems developing either hydrophilic or hydrophobic interactions, or both, are presented. The static and transport properties of what is defined as confined or interfacial water are compared with those of bulk water. Finally, it is shown that there is some strong evidence that structural and dynamic properties of water close to a hydrophilic surface, at room temperature, are similar to that of bulk supercooled water. ***To cite this article: M.-C. Bellissent-Funel, C. R. Geoscience 337 (2005).***

Résumé

Interactions hydrophiles–hydrophobes : des systèmes modèles aux systèmes vivants. L'eau est un liquide unique, dont les propriétés sont cruciales pour les processus de la vie. Dans les systèmes vivants, les phénomènes essentiels ont lieu, en géométrie confinée, dans les cellules vivantes, et à proximité des sites actifs des protéines et des membranes ou à leur surface. La stabilité des systèmes biologiques est contrôlée par le jeu subtil entre les interactions hydrophiles et les interactions hydrophobes. Il est admis que l'eau d'hydratation joue un rôle prédominant dans la relation entre la structure, la dynamique et la fonction des systèmes biologiques. Dans cet article, nous présentons des exemples variés de systèmes qui sont le siège d'interactions hydrophiles ou hydrophobes ou des deux types d'interactions. Les propriétés statiques et de transport de l'eau confinée ou de l'eau interfaciale sont comparées à celles de l'eau en grand volume. Enfin, nous montrons que les propriétés structurales et dynamiques de l'eau, à température ambiante et au voisinage d'une surface hydrophile, sont comparables à celles de l'eau surfondue. ***Pour citer cet article : M.-C. Bellissent-Funel, C. R. Geoscience 337 (2005).***

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Mots-clés : Interaction hydrophile ; Interaction hydrophobe ; Verre poreux ; Solutions aqueuses ; Systèmes biologiques ; Structure ; Dynamique ; Eau confinée ; Eau d'hydratation ; Eau surfondue ; Transition vitreuse ; Diffusion de neutrons

1. Introduction

Water is the most abundant fluid on earth and the major constituent of organisms (70% of total weight in most cases). The understanding of hydrophilic and hydrophobic effects is of prime importance. These effects are related to the solvent properties of water and to the fact that some compounds are more or less soluble in water. The solvent abilities of water arise primarily from two properties: its tendency to form hydrogen bonds (very short characteristic lifetime, between 10^{-13} and 10^{-12} s) and its dipolar character [3]. The high dielectric constant ($\varepsilon \sim 80$), already alluded to, results from its dipolar character.

2. Hydrophilic interactions

2.1. Hydrogen-bond formers

Any molecules that carry groups capable of forming hydrogen bonds can do so with water; such groups will tend to make these molecules hydrophilic. Water readily dissolves hydroxyl compounds, amines, sulphydryl compounds, esters, ketones, and a wide variety of other organic compounds.

In the presence of a solid substratum, water may also form bonds. This is the case, for instance, of glasses where silanol groups Si–O–H are present at the interface water–silica. Let us mention porous materials [2], such as Vycor glass, silica gels, and zeolites.

2.2. Ionic compounds

Water is also an excellent solvent for ionic compounds. The explanation lies in the dipolar nature of the water molecules. Dipoles interact with ions such that cations and anions in aqueous solutions are surrounded with hydration shells. Careful neutron scattering experiments allowed us to determine the characteristics of the hydration shell around many ions, that is to say the distance between the ion and the water molecule, the tilt angle and the hydration number [16]. Around a cation, the water molecule is oriented with the oxygen close to the cation corresponding to a minimisation of the energy between the ion and the water dipole. Instead, around an anion, the hydrogen atoms are close to the ion. The hydration number, i.e. the number of water molecules inside the first hydration shell, and the lifetime of this shell depend on the nature of the solute and on its concentration. Layer-like clays minerals [32,36] have been the objects of many studies.

3. Hydrophobic interactions

The dipolar nature of the water molecule also contributes to dissolve non-ionic, but apolar molecules. Substances like hydrocarbon that are non-polar and non-ionic and cannot form hydrogen bonds show only limited solubility in water. Such hydrophobic molecules do not form hydration shells, as hydrophilic substances do. Instead, the regular water lattice forms 'cages' of ice-like clathrate structure about non-polar molecules, probably with some geometry close to that of polyhedra such as icosahedra [20].

4. Hydrophilic/hydrophobic interactions

Amphipathic molecules simultaneously exhibit both hydrophilic and hydrophobic properties. They have a head group that is strongly hydrophilic, coupled to a hydrophobic tail, usually a hydrocarbon. When one attempts to dissolve them in water, amphipathic substances form peculiar structures. Possible structures are a monolayer on the water surface, a micelle, and a bilayer vesicle, with water both inside and out. Examples of other structures that impose spatial restrictions on water molecules include polymer gels and micro-emulsions. In these cases, since the hydrophobic effect