The Origin of Long Range Attraction Between Hydrophobes in Water

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Introduction

When water-coated hydrophobic surfaces meet, direct contacts form between the surfaces, driving water out [1-4]. However long-range attractive forces first bring those surfaces close. This analysis reveals the source and strength of the long-range attraction between water-coated hydrophobic surfaces. The origin is in the strong correlation and coupling of the dipoles of the water molecules at the surfaces.

Recently [5], we analyzed the consequences of the dipole-dipole correlation of water molecules under hydrophobic confinement and formulated a statistical self-consistent approach describing the response behavior of such semi-confined water. The approach provides the background for our interpretation and quantification here of the physical effects that underlie the attraction between hydrophobes in water.

Methods and Materials

From basic principles we derive the polarization field in the region of correlated water molecules and show that this field induces long-range attractions between hydrophobic solutes.

Results

Our results show that hydrophobic aggregation begins with a step in which nonpolar solutes approach one another due to long range electrostatic forces. This precursor regime occurs before the entropy of releasing the water layers and the short-range van der Waals attraction provide enough driving force to "dry out" the contact surface. The results shed light on the way water mediates chemical and biological self-assembly, a long outstanding problem. The phenomenon should be observable in the transverse relaxation rates in water proton magnetic resonance, but some other experimental techniques can also be able to measure the effect, which will be discussed in my presentation.

Discussion

By employing basic molecular principles, we have shown how water molecules with depleted H-bonds and slow reorientation of their intrinsic molecular dipoles organize themselves around hydrophobic units and give rise to polarization fields which can set effective long range attractions between these hydrophobic units.

The analysis reveals that the mechanism of the hydrophobic interaction may involve an initial step stage in which nonpolar solutes approach one another via a long range electrostatic potential. This precursor regime occurs before the entropy of releasing the water layers may well provide enough driving force to "dry out" the contact surface. The present theory offers a practical way to quantify these hydrophobic interactions and to correlate the solvent effects to the effective interactions between biomolecules. In addition, the present theory predicts the consequences of confining water in nanoscale hydrophobic environments and offers a reliable way to describe them in a quantitative manner.

The present approach can be valuable in questions related to various engineering applications as, for example, controlling the formation of nanoparticles, improving the quality of surface catalysts, as well as designing synthetic molecular chaperones. Also, understanding essential features of the hydrophobic hydration opens new ways for using MR imaging to infer structural changes at the molecular level in cells and living tissues (e.g., deciphering MR images of biological tissues containing denaturated proteins), an initiative with immediate clinical applications

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