

# Hydrophobic surface enhances electrostatic interaction in water

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A high dielectric constant is one of the peculiar properties of liquid water, indicating that the electrostatic interaction between charged substances is largely reduced in water. Interestingly, a recent experimental study suggested that the electrostatic attraction in water is strengthened near the hydrophobic surface [1]. By conducting molecular dynamics simulation, we investigated the dielectric constant of water around hydrophobic surfaces by using the Onsager-Kirkwood-Fröhlich formula [2] and by the Stern-Feller formula [3]. We found that the dielectric constant of water is decreased near the hydrophobic surface (Fig. 1) and that the decrease in the dielectric constant was found to be due to both the decreased water density and the reduced water dipole correlation in the direction perpendicular to the surface. Furthermore, it was demonstrated that electrostatic interaction in water is actually strengthened near the hydrophobic surface. We finally discuss the relevance of our results to the biological molecules such as proteins; charged amino-acids on protein surfaces are often surrounded by hydrophobic ones, indicating that proteins utilize their hydrophobic surfaces to restrengthen the electrostatic interaction attenuated by water.

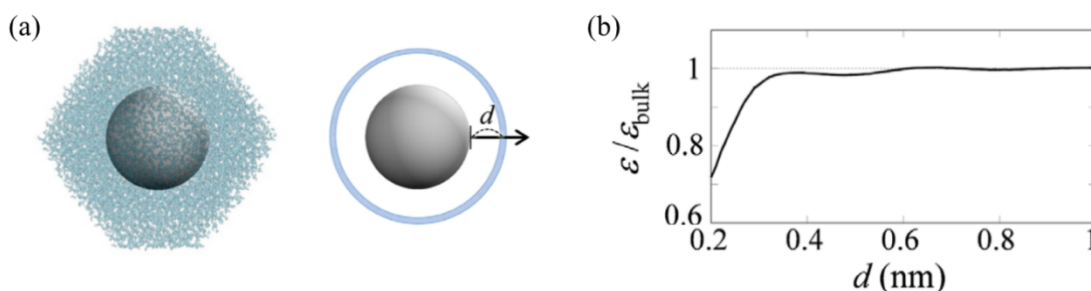


Fig. 1. (a) Hydrophobic particle-water system. The hydrophobic particle interacts with water molecules only via the Weeks-Chandler-Andersen potential with a purely repulsive term. (b) Dielectric constant,  $\epsilon$ , of water which was calculated using the Onsager-Kirkwood-Fröhlich formula as a function of the distance from the hydrophobic surface in the radial direction (denoted by  $d$ ). The values are normalized by the averages in the bulk water region.

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[2] T. Sato, T. Sasaki, J. Ohnuki, K. Umezawa, M. Takano, *Phys. Rev. Lett.* **121**, 206002 (2018).

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# **Promotion of homogeneous ice nucleation by polyvinyl alcohol**

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Polyvinyl alcohol (PVA) is well known for its ability to inhibit ice growth, which make it an excellent inhibitor of ice recrystallization. Nevertheless, at low concentrations PVA also promotes the nucleation of ice. It has been proposed that the enhancement is due to heterogeneous nucleation. However, PVA is a flexible coil and does not form a template or surface that would sustain a critical ice nucleus. We use molecular simulations to investigate the crystallization of water in the presence of PVA oligomers of various degrees of polymerizations as a function of concentration. The simulations reproduce the concentration dependence evolution of the freezing temperatures of the experiments. We find that PVA does not stabilize the ice nucleus. It promotes ice crystallization through destabilization of liquid water in the solution. On increasing PVA concentration, the colligative effects outwin the non-ideal mixing effects and the ice freezing efficiency decreases again. To our knowledge this is the first reported increase of homogeneous ice nucleation temperatures due to addition of solutes.

# **Coordinated analysis of protein hydration water by neutron crystallography, small-angle scattering, and quasielastic neutron scattering**

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In aqueous environments where proteins function, proteins constantly interact with surrounding water molecules. Water molecules on the protein surface thus have different properties from bulk water. This hydration water is a necessary constituent of proteins, which plays an important role in functions. Ultimate understanding of the mechanisms of the protein functions requires characterization of hydration water. Various techniques have been used to characterize hydration water. Among them, crystallography can provide the high-resolution hydration structure by directly locating the hydration water molecules. On the other hand, small-angle scattering provide the average hydration structure. Furthermore, quasielastic neutron scattering directly measures the dynamics of hydration water. To see if a consistent picture of hydration water emerges from the information obtained from these complementary techniques, we systematically apply these techniques to characterization of the structure and dynamics of hydration water around a protein. As an example, we characterized the hydration water around one of the typical globular proteins, RNase A. It was found that in addition to the water molecules located on the protein surface, the water molecules that cannot be located by crystallography provide significant contributions to the hydration structure.

# The influence of twist-bend coupling on the statistical mechanics of DNA

Enrico Carlon

*KU Leuven*

The Twistable Wormlike chain (TWLC) is considered a standard model of DNA mechanics. This model is characterized by uncoupled bending and torsional deformations and captures some of the essential features of DNA elasticity as observed in single molecule experiments.

The TWLC is however incomplete as it neglects an important interaction term which couples twist and bending degrees of freedom. Such twist-bend coupling follows from simple symmetry arguments about the structure of the double helix.

In this talk we will review some recent works analyzing the influence of twist-bend coupling on the mechanics and statistical mechanics of DNA, in particular two cases will be discussed in detail: (1) the structure of nucleosomal DNA (which is wrapped around histone proteins) and (2) DNA torsional elasticity as measured from Magnetic Tweezers experiments. We will show that twist-bend coupling offer a very natural explanation of several experimental results and discuss some open issues.

## References

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# **Self-assembly and ordering of anisotropic colloidal particles**

**Yasutaka Iwashita**

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We have experimentally studied how the anisotropy of colloidal particles affects their self-assembly and phase behavior by tuning the anisotropy in two ways; anisotropy in surface-surface interaction by producing patchy colloidal particles and in shape by producing arbitrary-designed particles by photolithography. For one-patch colloidal particles in a two dimensional system, we elucidated that their condensation transition becomes continuous in different from that of isotropic particles when the attraction between one-patch particles works only between the patches. I will also talk about some other results such as orientational order in patchy particles and geometric effect of amphiphilic particles' shape in emulsification.

# **Neutron Scattering**

## **– tools for structure and dynamics for biomacromolecules in solution-**

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Neutron scattering has several features which X-ray scattering does not have: the first one is a high penetration power, the second one is low irradiation damage for a sample, the third one is an isotope effect, and the fourth one is spin effect. Even though neutron intensity is weaker than that of X-ray, these features give neutron scattering special measuring techniques. In this talk, I would like to introduce scattering techniques for investigation on structure and dynamics for biomacromolecules in solution utilizing the third neutron feature and the fourth one. The isotope effect in neutron scattering is distinguished in the case of hydrogen: scattering lengths of proton and deuteron are  $-3.74$  fm and  $+6.67$  fm, respectively. We can make the target domain and/or protein in a complex labelled by selective deuteration. This technique is a powerful tool to observe the partial structure of a complex in solution coupled with Small-Angle Neutron Scattering (SANS). Utilizing neutron spin, namely Neutron Spin Echo (NSE), we can observe inelastic scattering ranging in  $\mu\text{eV}$ . This technique allows us to access the inner domain motion of protein.

In the presentation, I would like to introduce the scattering techniques and also the recent results.