Solvent effects and their influence on the dynamic and static properties of macromolecules

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The properties of the solvent play a crucial role in most biological and chemical processes concerning the solvation of macromolecules and their static and dynamic behavior. In this talk, recent results of computer simulations will be discussed that illustrate the importance of the solvent for several effects at the nano- and the mesoscale.
As a first example, the influence of compatible solutes on the properties of DPPC lipid bilayers will be presented [1]. It will be shown that small zwitterionic molecules like hydroxyectoine are able to systematically vary the surface tension of a membrane by changing the solvation free energy of lipids due to solvent-mediated interactions. This is specifically of importance for extremophilic microbacteriae which synthesize these low-weight organic compounds to protect their cell metabolism under harsh environmental conditions like high salinity.
As a second example, stable conformations of a cytosine-rich single-stranded DNA i-motif will be discussed by the results of biased all-atom Molecular Dynamics simulations [2]. DNA i-motifs are specific non-Watson-Crick like structures that often occur at the telomeric and the centromeric region of the chromosome. The simulations indicate the presence of stable hairpin configurations whose occurrence can be explained by a variation of the solvent entropy within the unfolding process due to an increased influence of hydrogen bonds [3].
Regarding larger scales, we have investigated the coat thickness dependent adsorption of hydrophobic proteins at polymer brushes in a poor solvent. The results of Dissipative Particle Dynamics simulations in combination with experimental findings [4] significantly indicate different adsorption strengths for varying brush heights. The simulations as well as analytical considerations are able to explain the main mechanism which is related to a hydrophobic collapse of the brush.
In the last part, electrokinetic flow phenomena in micro- and nanochannes caused by the presence of ions in solution and external electric fields [5] will illustrate the influence of the hydrodynamic boundary conditions on the electrophoresis of macromolecules [6,7]. We were able to identify the influence of wall slippage on the migration properties of polyelectrolytes [6]. In addition, recent results will be discussed that demonstrate the possibility of a chiral separation of enantiomeres due to asymmetric solvent flow patterns [7].

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