Abstract

Hydrophobicity is a phenomenon with important meaning in many fields of science and has been the subject of research for several decades by many groups from around the world Hydrophobic interactions occur between nonpolar molecules or groups in water. Hydrophobic substances have a low affinity for the solvent. An important role of this interaction can be observed in many processes taking place in aqueous solutions, e.g. complexation, aggregation of surfactants, coagulation. They are also key drivers of processes such as micelle formation and protein folding.

In the presented doctoral dissertation, the influence of the ionic strength, temperature, shape and size of the studied particles on the hydrophobic interactions was investigated. Molecular dynamics (MD) simulations were carried out in the AMBER 16.0 force field of ten homodimers of compounds, namely: methane, neopentane, adamantane, fullerene, ethane, propane, butane, hexane, octane, decane. Based on the results of series of MD simulations, the potentials of mean force for all systems were determined, taking into account the ionic strengths equal to 0; 0.04; 0.08; 0.40 mol/dm^3, and additionally for two systems (adamantane and hexane), this range was extended by higher values: 1.0; 1.5; 2.0 mol/dm^3, exceeding its physiological value. The tested temperature range included the following values: 248, 273, 285, 298, 310, 323, 335, 348, 360, 373 K. In the first step, MD simulations were carried out at 298 K in two water models: TIP3P and TIP4PEW. Additionally, maps of the water density distribution function and the average number of hydrogen bonds between water molecules in two minima for hexane and adamantane at ionic strengths equal to 0 and 0.4 mol/dm^3 were determined. Changes in thermodynamic parameters of hydrophobic interactions, as Gibbs free energy, enthalpy, entropy and heat capacity, were also determined.

It was observed that the ionic strength has a different influence on the hydrophobic interactions depending on the shape and size of the particles, as well as the tested temperature. It influences also on the shape of potential of mean force curves.