Abstract

Studies presented in this work can be divided into two main topics. In the first part we considered the hydration of nonpolar solutes in a simple water model. Thermodynamical and structural properties of aqueous solutions were calculated via perturbation and integral equation theories. Theoretical predictions were compared to the values obtained by the computer simulation of a given model. We examined the range of thermodynamic parameters where a given model supposedly describes the real water at room temperature and atmospheric pressure. Within the considered model we have found a good agreement between theoretical calculations and results of computer simulation. We could not reproduce certain experimentally determined features of hydrophobic hydration. However, this is likely to be due to the failure of the model to describe the real water properties. The phase diagram of the simple water model is not yet known, so the range of thermodynamic parameters that we studied might not correspond to the real water at ambient conditions.

In the second part we examined the effect of water molecules' translational and rotational motion on the structure of water and aqueous solutions of simple solutes. We employed the modified molecular dynamics simulations, where we ascribed different values for rotational and translational kinetic energies to the water molecules. Formally, we established a non–equilibrium steady–state, where the rotational and translational temperatures were not equal. Starting from the equilibrium at ambient conditions, we determined structural changes in water and aqueous solutions. From a practical point of view, the situation where the rotational temperature exceeds the translational one could be used as a simple model for the study of non–thermal microwave effects on aqueous solutions. We have found that increased rotational temperature substantially reduces the number of hydrogen bonds in water, increases the order in aqueous solutions and induces the collapse of a hydrophobic chain. Increased rotational temperature affects hydration of cations and anions in an opposite way, and strongly promotes the association of ions. Elevated translational temperature practically always results in the reduction of interparticle correlations.