Molecular Dynamic Simulation Study of Water Interactions with Hydrophilic and Hydrophobic Membranes

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Abstract

The goal of the present study is to understand the interactions occurring between water molecules and the hydrophilic and hydrophobic membranes using Density-functional theory (DFT), since a comprehensive study of the reasons for water and membrane interactions will help to design new approaches for enhancing membrane hydrophilicity. In order to achieve this, molecular dynamics simulations of Polyvinylidene fluoride (PVDF) and Polyacrylonitrile (PAN) membranes in aqueous solution were investigated, as hydrophobic and hydrophilic type membranes, respectively. DFT using B3LYP and UB3LYP functional and split-valance 6-311+G∗∗ basis sets were applied in order to optimize PAN, PVDF, and their various complexes with water molecules (from 1 to 6). The effects of geometrical parameters of the hydrogen bridge of PAN, PVDF, and the changes in the frequency of valence vibrations of the bonds directly participating in hydrogen bond formation on the number of water molecules were analyzed. The results indicated that the hydrogen bonds of PAN, in an isolated state and water solution, energy, dipole moments, and the hydrogen bridge parameters at room temperature were comparable to the hydrophobic PVDF. Two models were developed and they allowed to further study the reasons for the hydrophobicity of PVDF and hydrophilicity of PAN. The frequencies and intensities of absorption bands corresponding to stretching vibrations of the CN…H bond of PAN, and F…H bond of PVDF, in complexes with water were compared with the isolated states for applications of both models. In all of the study's calculations, the solvent effects were considered with the aid of a polarized continuum model (PCM). Furthermore, the hydrophilicity of the membranes and their interactions were confirmed experimentally using several analytical techniques discussed in the study. The experimental data obtained using PVDF and PAN working at the same operating conditions will likewise be compared and discussed.