On the hydration structure and dynamics near hydrophilic/hydrophobic group: A view from ab initio molecular dynamics simulation

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The structure and dynamics of interfacial water is of great importance in nature, since it is related to the wetting on the hydrophobic materials, stability of the aerosol in atmospheric chemistry, and designing and controlling the surface tension of the liquids. We perform *ab initio* MD (AIMD) simulations of the trimethylamine N-oxide (TMAO)-D_2O solution to elucidate the effects of hydrophilic/hydrophobic part of TMAO on the reorientational dynamics of water molecules [1]. In contrast with the previous results by experiment [2] and force field MD simulation [3] which claim slower reorientation motion of OH stretching near hydrophobic group compared with bulk water, we found very slow water dynamics near the hydrophilic group of TMAO. We attributed it to the strong directional hydrogen bond near the hydrophilic group through the sp3 orbital configuration. Furthermore, we developed an efficient algorithm based on the surface-specific velocity-velocity correlation function (ssVVCF) and calculated the SFG spectra at the water-air interface from the AIMD trajectory. The AIMD shows no 3100 cm^{-1} positive peak in contrast to the force field MD simulation [4], and is in good agreement with the very recent SFG measurement [5].

【References】

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