

Effects of Surface Energy of Substrate on Water Density Profile at a Solid Interface

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ABSTRACT

Achieving a proper knowledge of water/substrate interfaces at the molecular-scale is essential in numerous areas of science. Recently, several experimental studies have been performed on the water density profile at a solid interface. The uncertainties associated with experimental studies on water at a solid interface calls for numerical simulations, which can provide a detailed and reliable understanding of how varying parameters at molecular scales affect the water density profile at a solid interface. The aim of this work is to investigate the microscopic structure of water at a solid surface, using molecular dynamics simulations. In particular, the water density profile at a solid substrate as a function of the hydrophobicity or hydrophilicity of the surface, which is often associated with the surface energy of the substrate (SE_s), is investigated. The substrate material chosen is silver, which is originally a high energy material with surface energy equal to SE_{Ag} . The surface energy of the substrate is modified to adjust the strength of interaction energy between water and surface. The results show that the water density profile as a function of the vertical distance from the substrate ($+z$) depends on the surface energy of the substrate. There are two peaks in the water density profile at $z = 2.5 \text{ \AA}$ and $z = 5.5 \text{ \AA}$ for the unmodified silver substrate ($SE_s = SE_{Ag}$) indicating that the water molecules form a double-layer structure. The double-layer structure and the vertical distance of each layer from the substrate remains unchanged but the density of both layers decreases when SE_s decreases to 40% of its initial value. The second layer at $z = 5.5 \text{ \AA}$ disappears when SE_s is reduced to 20% of its original value. The layered structure disappears when SE_s reduces to 10% of its original value, and the water density becomes lower than its bulk value for $z < 3 \text{ \AA}$. The results indicate that on both hydrophobic and hydrophilic surfaces, interfacial water layers possess properties different from those of the bulk water. On hydrophobic surfaces, weakening of water-surface interaction strength results in dewetting and a water-vapor interfacial region. Instead, on a hydrophilic substrate, water is found to have a higher density than in the bulk, and it behaves like a solid water layer at room temperature.