Molecular Dynamics Simulations of Water Droplets On Hydrophilic Silica Surfaces

Wetting is essential and ubiquitous in a variety of natural and technological processes. Silicon dioxides-water systems are abundant in nature and play fundamental roles in a vast variety of novel science and engineering activities such as silicon based devices, nanoscale lab on a chip systems and DNA microarrays technologies. Although extensive experimental, theoretical and computational work has been devoted to study the nature of the interaction between silica and water, at the molecular level a complete understanding of silica-water systems has not been reached. Contact angle computations of water droplets on silica surfaces offers a useful fundamental and quantitative measurement in order to study chemical and physical properties of water-silica systems. For hydrophobic systems the static and dynamic properties of the fluid-solid interface are influenced by the presence of air. Hence, nanobubbles have been observed and proposed as the origin of long range "hydrophobic" forces even for hydrophilic silica-water interfaces unusual phenomena related to nanobubbles have been observed. In this work we study the role of air on the wetting of amorphous silica-water systems. We conduct molecular dynamics (MD) simulations of a hydrophilic air-water-silica system using the MD package FASTTUBE. We employ quantum chemistry calculation to obtain air-silica interaction parameters for the simulations. Our simulations are based in the following force fields: i) The silica-silica interaction is based on the potential model developed by Guissani et al. ii) The water-water interaction is simulated based on the classical rigid SPC/E water model. iii) The silica-water interaction is based on the force field model developed by Hassanali et al. iv) The air-silica interaction is simulated using a Lennard-Jones (LJ) 12-6 potential, parameterised using two different approaches therefore from quantum chemistry computations, and from Lorentz-Berhelot (LB) mixing rules with values obtained from the universal force field (UFF) and from Guissani et al. v) The water-air interaction is simulated using a LJ 12-6 potential with parameters obtained using LB mixing rules and values obtained from Jiang et al. for nitrogen and air oxygen and from Werder et al. for water oxygen.

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