

## A Molecular Dynamics Study of SDS and C12E6 Surfactants at the Silica-Water and Air-Water Interfaces

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Molecular dynamics simulations will be reported for the adsorption of sodium dodecyl sulfate (SDS) and hexaethylene glycol monododecyl ether (C12E6) surfactants at the silicon dioxide-water and water-air interfaces. The surface hydrophobicity was varied by changing the number of hydroxyl groups on the surface. Three different number densities of hydroxyl groups were chosen that correspond to (1) pH approximately equal to the isoelectric point of the silica surface, (2) pH less than the isoelectric point (acidic solution), and (3) pH greater than isoelectric point. We will discuss how the surface properties affect the molecular adsorption of surfactants on the three surfaces by presenting results for density profiles, planar radial distribution functions, and mean square displacement of both water and surfactants. The results will be compared to those of pure water at the SiO<sub>2</sub> surface in the absence of surfactants. This comparison will allow us to understand whether or not the equilibrium surfactant adsorption is influenced by hydrogen bonding within the water layers and/or by the local dielectric constant. The simulations at the water-air interface will be compared to experimental data obtained as a function of the density of surfactant molecules per unit interfacial surface area. The goal of this research is to compare the molecular structure of the self-assembled structures formed at the air-water compared to those formed at the silica-water interface.