

## Adsorption and Desorption Behavior of Ionic and Nonionic Surfactants on Polymer Surfaces

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**Abstract :** Experimental and computational studies are combined to elucidate the adsorption properties of ionic and nonionic surfactants on hydrophobic polymer surface such as poly(styrene). To present these two types of surfactants, sodium dodecyl sulfate and poly(ethylene glycol)-block-poly(ethylene), commonly utilized in emulsion polymerization, are chosen. By applying quartz crystal microbalance with dissipation monitoring it is found that, at low surfactant concentrations, it is easier to desorb (as measured by rate) ionic surfactants than nonionic surfactants. From molecular dynamics simulations, the effective, attractive force of these nonionic surfactants to the surface increases with the decrease of their concentration, whereas, the ionic surfactant exhibits mildly the opposite trend. The contrasting behavior of ionic and nonionic surfactants critically relies on two observations obtained from the simulations. The first is that there is a large degree of interweavement between head and tails groups in the adsorbed layer formed by the nonionic surfactant (PEO/PE systems). The second is that water molecules penetrate this layer. In the disordered layer, these nonionic surfactants generate at the surface, only oxygens of the head groups present at the interface with the water phase or oxygens next to the penetrating waters can form hydrogen bonds. Oxygens inside this layer lose this favorable energy, with a magnitude that increases with the surfactants density at the interface. This reduced stability of the surfactants diminishes their driving force for adsorption. All that is shown to be in accordance with experimental results on the dynamics of surfactants desorption. Ionic surfactants assemble into an ordered structure and the attraction to the surface was even slightly augmented at higher surfactant concentration, in agreement with the experimentally determined adsorption isotherm. The reason these two types of surfactants behave differently is because the ionic surfactant has a small head group that is strongly hydrophilic, whereas the head groups of the nonionic surfactants are large and only weakly attracted to water.

**Keywords :** emulsion polymerization process, molecular dynamics simulations, polymer surface, surfactants adsorption

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