

Synergistic and Antagonistic Effects Experienced by Surface-Active Compounds

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Most commercial products, pharmaceutical formulations, as well as consumer products are complex systems that contain multiple surface-active compounds. Formulating these products require extensive and expensive trial-and-error procedures because such compounds can compete for access to interfaces in ways that are difficult to predict. For example, simple ions are known to increase the surface tension of water while most surfactants are known to reduce it. Both synergistic and antagonistic effects are possible, depending on system conditions. For example, it has been observed that mixing ionic and non-ionic surfactants leads to stronger reductions in surface tension compared to using only one of the two compounds. Molecular simulations offer the opportunity of systematically changing the properties of the chemicals considered, although of course they require significant amount of computing time, depend in their accuracy on the reliability of the force fields, and might be limited in their ability to probe systems that contain chemicals at very low concentration. Towards developing systematic quantitative observations that could lead to the prediction of the interfacial properties of realistic formulations, simulation results are presented here for systems that contain surfactants and alcohols, different surfactants, as well as surfactants and other surface-active compounds interacting with water-air and water-oil interfaces, as well as with more complex interfacial systems such as phospholipid bilayers.

Keywords:

Molecular Simulations, Ion-Specific Effects, Self-Assembly, Surface Tension, Interfacial Tension