Efficient and Accurate Simulation of Surfactant Properties in Aqueous Solutions

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Surfactants are an ubiquitous class of chemical compounds, found in many areas of everyday life. Their function ranges from use in cleaning agents and emulsifiers/stabilizers in cosmetics and food industries, to more specialized applications in pharmaceutical industries. Surfactants are generally composed of a hydrophobic part, showing affinity to non-polar (oil) phases, and a hydrophilic part, showing affinity to polar (aqueous) phases. The polar part of a surfactant can either be neutral or ionic, where ionic surfactants are commonly further classified in anionic and cationic surfactants. Due to their specific structure, surfactants can adsorb at air-liquid or liquid-liquid interfaces and lower surface/interface tensions. Additionally, surfactants show self-assembling behavior into micellar structures. The minimum concentration at which micelles are formed, the critical micelle concentration, is a valuable key property of every industrial surfactant.

We want to provide researchers with a method, that can reliably predict key properties of any surfactant, based on physical principles that apply to all members of this extremely versatile class of compounds. COSMO-RS theory[1], as implemented in the BIOVIA COSMOtherm software package[2], allows for the efficient and accurate computation of physico-chemical properties of homogeneous liquid mixtures and is based on the generally valid principles of statistical thermodynamics. The recently introduced COSMOplex[3] approach generalizes COSMO-RS to inhomogeneous systems, paving the way to investigations of complex, self-organizing systems such as biomembranes, micelles and enriched surfaces.

In this contribution, we present benchmark results of experimentally accessible key properties such as critical micelle concentration and surface tension, computed for single- and multicharged cationic and anionic surfactants, neutral surfactants, and complex mixtures of multiple differently charged species. Additionally, surface related properties of biodegradable cleavable surfactants are investigated before and after degradation. Predicted observables are compared to available experimental results.

References

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