PROJECT TITLE: Computing thermodynamic properties to search for descriptors of surfactant harshness

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Project Description

Surfactant molecules are characterized by their tendency to adsorb at surfaces and interfaces such as liquid-liquid, liquid-solid and, liquid-vapor. The driving force of this adsorption is the unique amphiphilic (meaning both) nature of their molecular constituent. All surfactant molecules consist of at least two parts, one which is soluble in water (Hydrophilic head group) and one which is insoluble (Hydrophobic tail group). This amphiphilic nature drives them to surfaces and interfaces to adsorb, and, as a result, the surface tension (or amount of work required to expand the interface) is reduced. Additionally, these amphiphilic molecules can associate into a variety of structures in aqueous solution by changing the solution conditions such as surfactant or electrolyte concentration, pH, or temperature. As an example, most single-chained surfactants containing 12-16 carbons per chain such as SDS (sodium dodecyl sulfate) self-aggregate to a spherical shape micelle structure which contained ~62 monomers at a concentration of ~80 mM (CMC) in pure aqueous solution in 25 °C.

Due to this intriguing ability of lowering interfacial tension, surfactants are widely used as wetting agents and this phenomenon is of fundamental importance to diverse applications that include, among others, detergents, coating technologies, enhance oil recovery, drug delivery and pharmacy. Much current concern is drawn to the dermatological problems related to exposure of unprotected skin to surfactant solutions which is currently poorly understood at the molecular level.

Recent experimental work at UC has examined a series of surfactants with head group spacers for their impact on harshness. Our group recently have examined single surfactant hydration thermodynamics to look for molecular descriptors...
that correlate with harshness using molecular dynamics simulations. Using this proposed research we determined to study the surfactant hydration and thermodynamic properties at higher monomer concentration levels such as CMC. First of all we will build and simulate the spherical micelle structure by using computational software packages and then we will compute the micelle-monomer solvent averaged potential of mean force (PMF) profile as a function of the relative distance between the monomer center-of-mass and the micelle center-of-mass. We will use the molecular dynamics simulation method for the PMF computation.