

MATH, PHYSICS, AND COMPUTER SCIENCE DEPARTMENT
UNIVERSITY OF CINCINNATI BLUE ASH COLLEGE

SUMMER RESEARCH OPPORTUNITIES FOR UNDERGRADUATE WOMEN

APPLICATION DEADLINE: 03/01/2020

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

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Project Description

An effective computational protocol to understand and predict hydration thermodynamic properties of surfactant molecules is a crucial asset in any experimental research group who design, synthesize, and characterize novel candidates with desired properties. Computational modelling helps reveal molecular descriptors that can correlate with bulk solution properties such as skin harshness, thickening, and formulation. Due to the intriguing ability of lowering surface and interfacial tension, surfactants are widely used as wetting agents in a range of consumer products, including soaps and shampoos. Products with strong cleaning characteristics and gentle effects on skin and other tissues are desired.

While many anionic surfactants such as sodium dodecyl sulfate (SDS), commonly used in consumer products, are harsh on skin, they provide these products with excellent foaming and lather characteristics that are desired by consumers. Alternatively, sulfate-free natural surfactants, including sugar-based, amino acid-based (SLSar) and plant-based materials, are sustainable and readily biodegradable commodities have excellent skin mildness, yet are difficult to incorporate into personal cleansing formulations because of their impact on formulation stability, thickening and rheology. In particular, they change micelle structure in a way that markedly impacts wormlike micelle formation and entanglement, which are traditionally controlled by addition of salt and/or amphoteric surfactants. Hence, thickening of formulations containing these materials to levels suitable for personal care products is problematical. This phenomenon is widely recognized in the industry, but a structural/dynamic explanation and robust solutions to the problem remain to be developed.

Our goal for this WISE proposal is to employ and strive to improve first principle Molecular Dynamics Simulation methods conjunction with statistical thermodynamic techniques to characterize structure and dynamics of surfactant molecules to elucidate the hydration thermodynamics properties of single molecule and micellar systems comprised of these two types of materials. The impact of this research includes if successful proposed computational protocols could provide rapid screening of new surfactant candidates, insights into the mechanism of micellar self-assembly and dynamics, aspects of the computational analysis will benefit broader interpretations of both polymer and surfactant soft matter compositions, among others to the broader society.