REBECCA RUTHERFORD[1], JACK JOHNSTON[1], ERICA HARVEY[1],and BLAKE MERTZ[2], [1]Dept. of Natural Sciences, Fairmont State University, Fairmont, WV, 26554, and, [2]Dept. of Chemistry, West Virginia University, Morgantown, WV, 26506. Modeling detergent applications using molecular dynamics.

The molecular dynamics group at Fairmont State University models detergent systems with interdisciplinary applications. Simulations currently underway include octane interacting with sodium dodecyl sulfate (SDS) in aqueous solution as well as micelle formation in systems of cetyltrimethylammonium bromide and chloride (CTAB and CTAC, respectively).

The simulation of octane and SDS in aqueous solution is designed to model the process of washing away grease with a detergent commonly found in dish soap. It is intended for use as a web-based educational tool to provide a dynamic visualization of micelle formation, e.g. in freshman chemistry classes.

CTAB was chosen as a target because of literature evidence that low concentrations of the detergent cause a 100-fold increase in fluorescence of a small organic molecule. This organic molecule is a localized photosensitizer, which is useful in improving photodynamic light therapy that is currently being used as treatment for some cancers. Bromide ion parameters were adapted from the well parameterized chloride ion in the CHARMM forcefield; the comparison is interesting because CTAC and CTAB are known to have different aggregation numbers. Initial simulation results indicate that micelle formation from a random assembly of detergent molecules (n=20-130) occurs rapidly for both species.

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