REBECCA RUTHERFORD, RACHEL VAN OSDOL, and ERICA HARVEY, Dept of Biology, Chemistry and Geoscience, Fairmont State University, Fairmont, WV, 26554, and SADEGH FARAMARZI and BLAKE MERTZ, Dept of Chemistry, West Virginia University, Morgantown, WV, 26506. Molecular dynamics simulations of detergent micelles.

Molecular Dynamics (MD) simulations are being used to model the aggregation of detergents into spherical assemblies called micelles. Detergent micelles can be used experimentally to study membrane proteins. In the present study, we are investigating micelle formation in dodecyl β-D-maltoside (DDM) detergents with a longer-term goal of understanding how the nature of the detergent micelle influences the properties of the membrane protein proteorhodopsin.

Proteorhodopsin captures sunlight and stores it in a proton gradient that the cell can use to directly drive ATP synthesis; in marine environments, this protein may be responsible for 10-15% of what was once thought to be photosynthesis. Nanoscale Molecular Dynamics (NAMD) and Visual Molecular Dynamics (VMD) software programs are being run on a high-speed Linux workstation at Fairmont State University and the High Performance Computing systems at West Virginia University. Simulation results are analyzed to generate quantitative data about the system, including aggregation number and radius of gyration. Current simulations to be reported on include random assemblies of 20, 60, 110 and 200 DDM molecules, pre-formed micelles of 150 and 220 DDM molecules, and a pre-formed inverted micelle of 110 DDM molecules.

Funding for the project was provided by the College of Science and Technology at Fairmont State University and the NASA WV Space Grant Consortium.