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Self-Assembly of Gemini Surfactants ARUN YETHIRAJ, University of Wisconsin, JAGANNATH MONDAL, Columbia University, MAHESH MAHANTHAPPA, University of Wisconsin — The self-assembly behavior of Gemini (dimeric or twin-tail) dicarboxylate disodium surfactants is studied using molecular dynamics simulations. This gemini architecture, in which two single tailed surfactants are joined through a flexible hydrophobic linker, has been shown to exhibit concentration-dependent aqueous self-assembly into lyotropic phases including hexagonal, gyroid, and lamellar morphologies. Our simulations reproduce the experimentally observed phases at similar amphiphile concentrations in water, including the unusual ability of these surfactants to form gyroid phases over unprecedentedly large amphiphile concentration windows. We demonstrate quanitative agreement between the predicted and experimentally observed domain spacings of these nanostructured materials. Through careful conformation analyses of the surfactant molecules, we show that the gyroid phase is electrostatically stabilized related to the lamellar phase. By starting with a lamellar phase, we show that decreasing the charge on the surfactant headgroups by carboxylate protonation or use of a bulkier tetramethyl ammonium counterion in place of sodium drives the formation of a gyroid phase.

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