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Self-assembly of polyelectrolyte surfactant complexes using large scale MD simulation MONOJOY GOSWAMI, BOBBY SUMPTER, Oak Ridge National Laboratory — Polyelectrolytes (PE) and surfactants are known to form interesting structures with varied properties in aqueous solutions. The morphological details of the PE-surfactant complexes depend on a combination of polymer backbone, electrostatic interactions and hydrophobic interactions. We study the self-assembly of cationic PE and anionic surfactants complexes in dilute condition. The importance of such complexes of PE with oppositely charged surfactants can be found in biological systems, such as immobilization of enzymes in polyelectrolyte complexes or nonspecific association of DNA with protein. Many useful properties of PE surfactant complexes come from the highly ordered structures of surfactant self-assembly inside the PE aggregate which has applications in industry. We do large scale molecular dynamics simulation using LAMMPS to understand the structure and dynamics of PE-surfactant systems. Our investigation shows highly ordered pearl-necklace structures that have been observed experimentally in biological systems. We investigate many different properties of PE-surfactant complexation for different parameter ranges that are useful for pharmaceutical, engineering and biological applications.

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