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Large scale molecular dynamics study of polymer-surfactant complex MONOJOY GOSWAMI, BOBBY SUMPTER, Oak Ridge National Laboratory, Oak Ridge, TN — In this work, we study the self-assembly of cationic polyelectrolytes mediated by anionic surfactants in dilute or semi-dilute and gel states. The understanding of the dilute system is a requirement for the understanding of gel states. The importance of polyelectrolyte with oppositely charged colloidal particles can be found in biological systems, such as immobilization of enzymes in polyelectrolyte complexes or nonspecific association of DNA with protein. With the same understanding, interaction of surfactants with polyelectrolytes shows intriguing phenomena that are important for both in academic research as well as industrial applications. Many useful properties of PE surfactant complexes come from the highly ordered structures of surfactant self-assembly inside the PE aggregate. We do large scale molecular dynamics simulation using LAMMPS to understand the structure and dynamics of PE-surfactant systems. Our investigation shows highly ordered ring-string structures that have been observed experimentally in biological systems. We will investigate many different properties of PE-surfactant complexation which will be helpful for pharmaceutical, engineering and biological applications.

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