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Understanding self-assembly of charged–neutral block copolymer (BCP) and surfactant complexes using molecular dynamics (MD) simulation[1] MONOJOY GOSWAMI[2], BOBBY SUMPTER[3], Oak Ridge National Laboratory, MICHAEL KILBEY[4], University of Tennessee, Knoxville — Here we report the formation of phase separated BCP-surfactant complexes resulting from the electrostatic self-assembly of charge-neutral block copolymers with oppositely charged surfactants. Complexation behaviors of oppositely charged polyelectrolytes has gained considerable attention in the field of soft condensed matter physics due to their potential application as functional nanomaterials for batteries, wastewater treatment and drug delivery systems. Numerous experiments have examined the self-assembled structures resulting from complexation of charge-neutral BCP and surfactants, however, there is a lack of comprehensive understanding at the fundamental level. To help bridge this gap, we use, MD simulations to study self-assembly and dynamics of the BCP-surfactant complex at the molecular level. Our results show an overcharging effect in BCPs with hydrophobic neutral blocks and a formation of core-shell colloidal structure. Hydrophilic neutral blocks, on the other hand, show stable, hairy colloidal structures with neutral blocks forming a loosely-bound, fuzzy outer layer. Our results qualitatively agree with previous SANS and SAXS experiments.

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