

Abstract Submitted
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Molecular Effects on Coacervate-Driven Block Copolymer Self Assembly TYER LYTLE, Univ of Illinois - Urbana, MITHUN RADHAKRISHNA, Indian Institute of Technology - Gandhinagar, CHARLES SING, Univ of Illinois - Urbana — Two oppositely charged polymers can undergo associative phase separation in a salt solution in a process known as complex coacervation. Recent work has used this as a motif to control the self-assembly behavior of a mixture of oppositely-charged block copolymers which form nanoscale structures. The materials formed from these complex coacervate-block copolymers (BCPs) have potential use as drug delivery systems, gels, and sensors. We have developed a hybrid Monte Carlo-Single Chain in a Mean Field (MC-SCMF) simulation method that is able to determine morphological phase diagrams for BCPs. This technique is an efficient way to calculate morphological phase diagrams and provides a clear link between molecular level features and self-assembly behaviors. Morphological phase diagrams showing the effects of polymer concentration, salt concentration, chain length, and charge-block fraction at large charge densities on self-assembly behavior have been determined. An unexpected phase transition from disorder to hexagonal packing at large salt concentrations has been observed for charge-block fractions equal to and larger than 0.5. This is attributed to the salt filling space stabilizing the morphology of the BCP.

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