

Abstract Submitted
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Field-theoretic simulations of correlation effects in charged polymers JING CAO, ROBERT RIGGLEMAN, Univ of Pennsylvania — Dielectric properties of inhomogeneous soft materials have attracted great deal of attention over the last several decades. Polyelectrolyte block copolymers can demonstrate more rich features comparing to its “simple” homogeneous counterpart since the packing between bound-ions and surrounding counterions are complicated as well as the local dielectric constant can vary significantly between different domains. However, in the standard field-theoretical approach of treating charged systems, a uniform dielectric constant has been assumed through the system and packing effects are challenging to incorporate, leading to qualitative differences between theoretical predictions and experiments. We present here a molecularly statistical field theory model of inhomogeneous diblock copolymers with ionic junctions. We studied the tendency of phase separation due to strong correlations between bound-ions and counterions by using mean-field approximation and complex Langevin simulation technique. In addition, the results from our field-theoretical model were compared with the results from molecular dynamics simulations and experiments.

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