Highly-correlated Charges in Block Copolyelectrolytes: Charge as a Tool for Morphology Manipulation

CHARLES SING, JOS ZWANIKKEN, MONICA OLVERA DE LA CRUZ, Northwestern University — Block copolymers that include at least one charged block have been of great technological interest due to their use in materials for battery membranes. These materials are difficult to understand theoretically, however, due to the disparate length scale effects of charge correlation and chain conformation driving the microphase separation of these systems. Using a new theoretical approach that can account for both of these effects that is based of hybrid liquid state integral equation-self consistent field theory (LS-SCFT) calculations, we elucidate the fundamental physics underpinning the thermodynamics of these materials. In particular, we demonstrate four main effects that drive the phase behavior of block copolyelectrolytes: Coulombic cohesion, counterion entropy, excluded volume, and ion self energy effects. Tuning parameters such as charge fraction and dielectric constant can be used to explore different microphase-separated morphologies on an axis orthogonal to traditional routes of manipulating block copolymers (i.e. $\chi$, N and block fraction). This expands the palette of tools that can be used to tune this important class of polymeric materials.