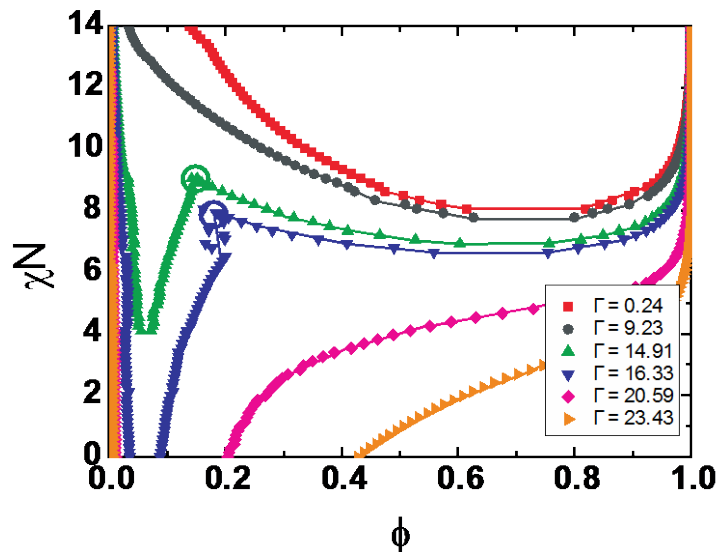


Theoretical analysis of multiple phase coexistence in polyelectrolyte blends

Ha-Kyung Kwon, Jos W. Zwanikken, Kenneth R. Shull, and Monica Olvera de la Cruz

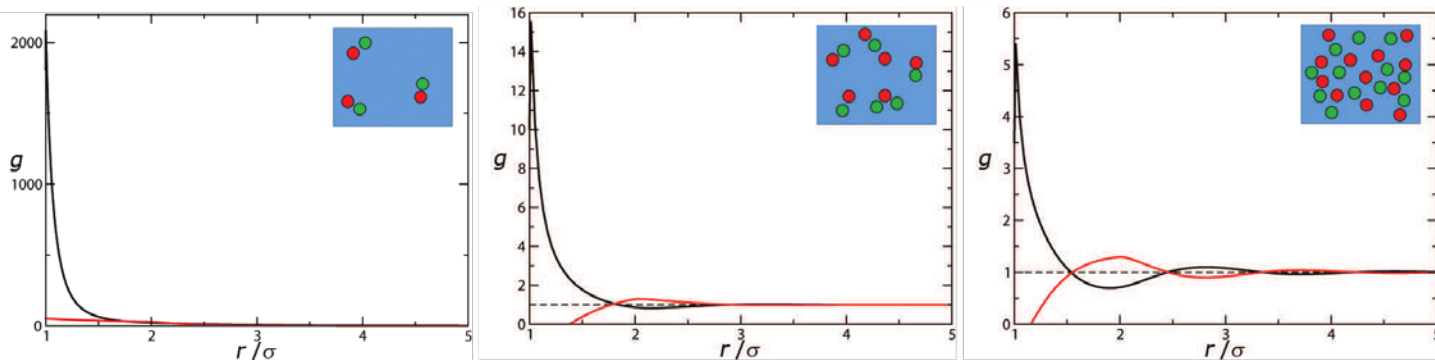


Significance

- Polymer charge has been identified as an important tuning parameter that can drastically change the structure and functionality of the polyelectrolyte
- The method described in the study, which combines Flory-Huggins theory with liquid state methods, can accurately capture the effects of electrostatic molecular interactions, providing an understanding of the competing effects that determine phase behavior of a polyelectrolyte blend at multiple length scales

Findings

- Ionic correlations between the charged backbone and counterions can significantly enhance phase separation, especially in blends dilute in charge
- A strong coupling strength Γ , set by the dielectric properties of the polymer, can result in a phase separation in blends even at $\chi N = 0$.
- By tuning parameters Γ and χN , one can find triple phase separation, where the coexisting phases show different ion morphologies



Above: Effect of Γ on the phase diagram of symmetric polyelectrolyte blends with $N = 40$, and charge fraction of 0.2. At the triple point (hollow circles), the coexisting phases consist of ion pairs, ion clusters, and liquid-like ordering of charges (below)

Macromolecules, 48, 6008-6015 (2015); DOI: 10.1021/acs.macromol.5b00901