Ion Correlation-Induced Phase Separation in Polyelectrolyte Blends

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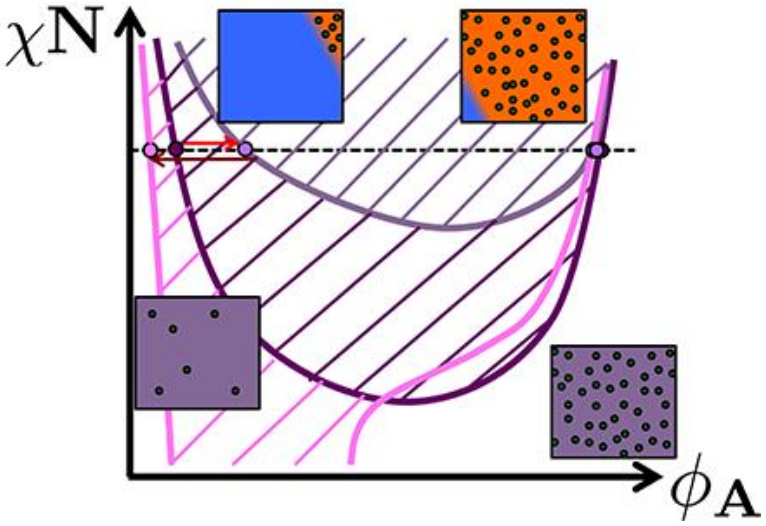
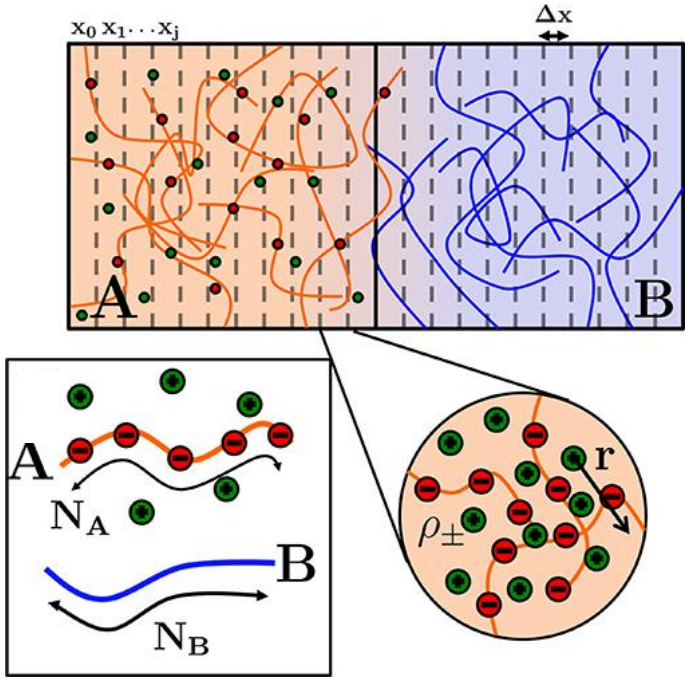
ACS Macro Letters, 2 ,1042-1046 (2013) DOI: 10.1021/mz400511r

Polymer blends exhibit technologically advantageous properties for adhesives and fuel cell membranes and serve as an ideal model system to study more complicated behaviors in polyelectrolyte materials. We go beyond traditional self-consistent field theory (SCFT) which only reproduces Poisson-Boltzmann behavior due to mean-field assumptions. We have developed a way to couple SCFT with liquid state (LS) integral equation theory, which can calculate ion correlations in a quantitative fashion. This permits the articulation of ion effects in very low dielectric regimes relevant to polymer blends. These correlations can give rise to marked enhancement of phase separation, even when the two polymers are fully miscible.





(Above) SCFT calculations occur on a grid, where each grid point can contain some local charge order, which is described by LS theory. This is used to understand the mixing of a charged A polymer and an uncharged B polymer. (Left) Mixtures can phase separate in vastly different ways when charges are included and depending on the strength of the charge coupling.

The authors acknowledge support from NSF grant number DMR-0907781, International Institute for Nanotechnology Postdoctoral Fellowship, DDR&E and the AFOSR under Award no. FA9550-10-1-0167