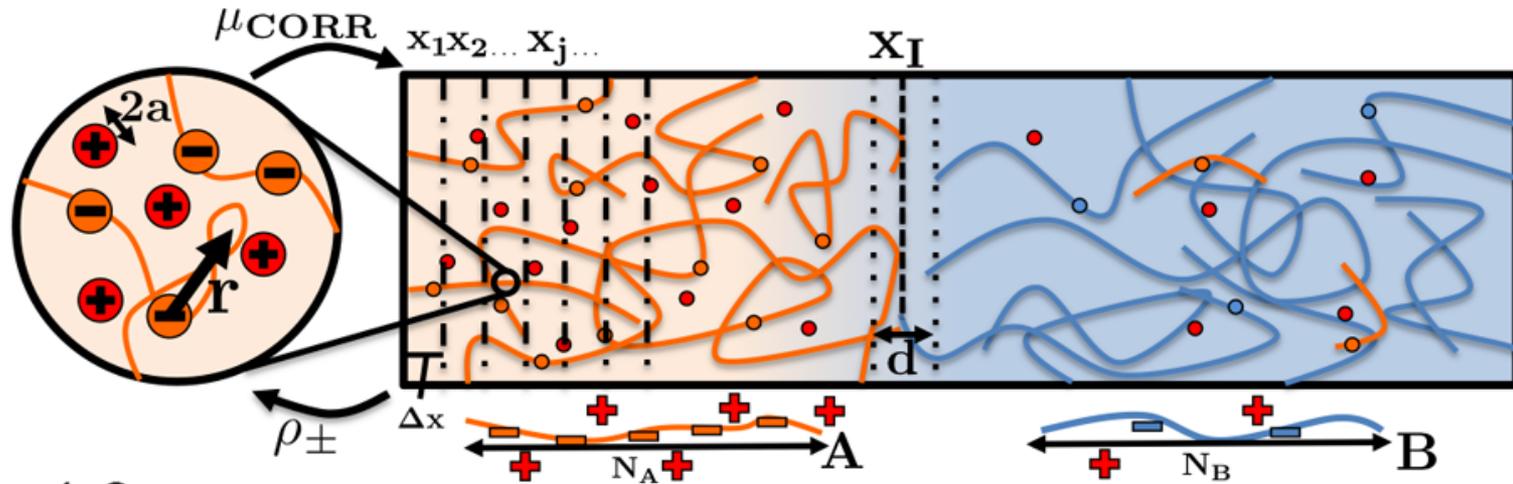


# Interfacial Behavior in Polyelectrolyte Blends: Hybrid Liquid-State Integral Equation and Self-Consistent Field Theory Study

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We present a novel method that is developed to understand the role of local charge-ordering effects in inhomogeneous polyelectrolyte systems. This method incorporates liquid-state integral equation theory, which describes local ion structure in a quantitative fashion, into larger-length scale self-consistent field theory calculations. Applied to polyelectrolyte blends, we demonstrate that the structure of the interface between a highly-charged polymer and a polymer with low charge can be strongly adjusted due to a combination of counterion entropy, hard sphere interactions, and Coulombic attraction effects; the latter two are not described using traditional Poisson-Boltzmann mean-field theory.



The above diagram describes our theoretical scheme; local structural information about ion correlations (left) is calculated with LS theory, and provides thermodynamic inputs into larger-scale structural calculations using SCFT (right), which in turn provides thermodynamic inputs into the original LS calculation. This work considers a blend of a highly-charged polyelectrolyte with a lightly-charged polyelectrolyte (bottom) that may be immiscible and therefore phase separate. In principle this approach could be extended to other inhomogeneous polyelectrolyte systems.

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