

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Field Theoretic Simulations of Self-Coacervation Phenomena in Block Polyampholytes SCOTT DANIELSEN, KRIS DELANEY, RACHEL SEGALMAN, GLENN FREDRICKSON, Univ of California - Santa Barbara — Polyelectrolyte complexation is a common phenomenon in natural polymers and has been applied to synthetic materials systems for coatings, adhesives, and encapsulants. Single-component polyelectrolyte complexes are formed when block polyampholytes exhibit self-coacervation, phase separating into a dense liquid coacervate phase rich in the polaympholyte coexisting with a dilute supernatant phase. Using fully fluctuating field theoretic simulations, we explore the phase behavior of block polyampholytes in solution to understand the structure and thermodynamics of the self-coacervate. Results are shown concerning the effects of block architecture, excluded volume, and explicit counterions on the phase diagram. Simple analytical and random phase approximation (RPA) expressions are used to discuss scaling relationships.

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Date submitted: 09 Nov 2016

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