

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Molecular Connectivity and Correlation Effects in Polymeric Complex Coacervates** MITHUN RADHAKRISHNA, CHARLES SING, University of Illinois at Urbana-Champaign — Complex Coacervation is a liquid-liquid phase separation induced by oppositely charged species and is a complicated process influenced by many factors like the solution pH, temperature, salt concentration, charge size and valency of the salt. Because of this inherent tunability complex coacervates have garnered a significant amount of attention as materials for under water adhesives, drug delivery platforms and self assembled structures. Most theoretical studies to address the complex coacervate materials to date have relied on the use of Poisson-Boltzmann theory (or extensions thereof). While these thermodynamic studies capture the phase behavior of complex coacervates in a qualitative sense, most of these theories neglect some of the important factors such as the effect of polyion-driven connectivity correlations and excluded volume interactions between the ions in the solution. In the current work we study the effect of these factors on the phase behavior of complex coacervates through molecular simulations coupled to thermodynamic models for phase separation. We demonstrate that these neglected molecular features (connectivity, finite polymer and ion size) profoundly impact the thermodynamics, and by articulating them in theoretical or simulation models, we can start to understand how to design coacervate materials at a molecular level.

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Date submitted: 13 Nov 2014

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