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Connectivity and Excluded Volume Effects in Polymeric Complex Coacervates CHARLES SING, MITHUN RADHAKRISHNA, University of Illinois at Urbana-Champaign — Oppositely-charged polyelectrolytes in salt solutions can undergo phase separation to form complex coacervates. This charge-driven phase behavior is the basis for emerging motifs in self-assembly. Traditional uses for coacervates are in food and personal care products, while applications in technologies for drug delivery and sensory materials are being developed. One of the primary theories driving understanding of complex coacervates is the Voorn-Overbeek (V-O) theory, which is a precursor to more sophisticated field theories. We present both theory and simulation that provides an alternate picture of coacervates, specifically addressing the limitations of V-O. Our theoretical approach is based on PRISM, which is a liquid-state theory that specifically accounts for connectivity. This is compared with Monte Carlo-based simulations, which likewise provide a molecular picture of coacervation. We demonstrate that a combination of connectivity-based correlations and excluded volume has a profound effect on coacervation phase behavior, suggesting that favorable comparison of V-O to experiment benefits from a cancellation of errors. The influence of connectivity on coacervate phase behavior hints at new opportunities for molecular-based design in electrostatically-driven self-assembly.

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