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Molecular Structure and Sequence in Complex Coacervates CHARLES SING, TYLER LYTLE, JASON MADINYA, MITHUN RADHAKRISHNA, University of Illinois at Urbana-Champaign — Oppositely-charged polyelectrolytes in aqueous solution can undergo associative phase separation, in a process known as complex coacervation. This results in a polyelectrolyte-dense phase (coacervate) and polyelectrolyte-dilute phase (supernatant). There remain challenges in understanding this process, despite a long history in polymer physics. We use Monte Carlo simulation to demonstrate that molecular features (charge spacing, size) play a crucial role in governing the equilibrium in coacervates. We show how these molecular features give rise to strong monomer sequence effects, due to a combination of counterion condensation and correlation effects. We distinguish between structural and sequence-based correlations, which can be designed to tune the phase diagram of coacervation. Sequence effects further inform the physical understanding of coacervation, and provide the basis for new coacervation models that take monomer-level features into account.

Charles Sing
University of Illinois at Urbana-Champaign

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