

Future Directions in Physiochemical Modeling of the Thermodynamics of Polyelectrolyte Coacervates (PECs)

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Abstract

We review theories of polyelectrolyte (PE) coacervation, which is the spontaneous association of oppositely charged units of PEs and phase separation into a polymer-dense phase in aqueous solution. The simplest theories can be divided into “physics-based” and “chemistry-based” approaches. In the former, polyelectrolytes are treated as charged, long-chain, molecules, defined by charge level, chain length, and chain flexibility, but otherwise lacking chemical identity, with electrostatic interactions driving coacervation. The “chemistry-based” approaches focus on the local interactions between the species for which chemical identity is critical, and describe coacervation as the result of competitive local binding interactions of monomers and salts. In this article, we show how these approaches complement each other by presenting recent approaches that take both physical and chemical effects into account. Finally, we suggest future directions towards producing theories that are made quantitatively predictive by accounting for both long range electrostatic and local chemically specific interactions.

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