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Simulation Studies of LCST-like Phase Transitions in Elastin-like Polypeptides (ELPs) and Conjugates of ELP with Rigid Macromolecules[1]

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— We use atomistic (AA) and coarse-grained (CG) molecular dynamics simulations to elucidate the thermodynamic driving forces governing lower critical solution temperature (LCST)-like phase transition exhibited by elastin-like peptides (ELPs) and conjugates of ELP with other macromolecules. In the AA simulations, we study ELP oligomers in explicit water, and mark the transition as the temperature at which they undergo a change in "hydration" state. While AA simulations are restricted to small systems of short ELPs and do not capture the chain aggregation observed in experiments of ELPs, they guide the phenomenological CG model development by highlighting the solvent induced polymer-polymer effective interactions with changing temperature. In the CG simulations, we capture the LCST polymer aggregation by increasing polymer-polymer effective attractive interactions in an implicit solvent. We examine the impact of conjugating a block of LCST polymer to another rigid unresponsive macromolecular block on the LCST-like transition. We find that when multiple LCST polymers are conjugated to a rigid polymer block, increased crowding of the LCST polymers shifts the onset of chain aggregation to smaller effective polymer-polymer attraction compared to the free LCST polymers. These simulation results provide guidance on the design of conjugated bio-mimetic thermoresponsive materials, and shape the fundamental understanding of the impact of polymer crowding on phase behavior in thermoresponsive LCST polymer systems.

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