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Langevin Dynamics Simulations of Counterion-mediated Complexation of Polyelectrolytes ZHAOYANG OU, UMass, Amherst, M. MUTHUKUMAR, UMass, Amherst — We have used the Langevin dynamics simulation to study the complexation of oppositely charged flexible polyelectrolytes in salt free solutions. Two uniformly charged chains with condensed counterions are separated in space initially, and allowed to move and interact with each other. The chain size, Coulomb energy and the release of counterions are monitored. The simulations are carried out at different temperatures and electrostatic interaction strengths. We have found in simulations that while the release of the counterions dominates at lower temperatures, the electrostatic attraction between two chains takes over at higher temperatures.

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