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Complexation of Oppositely Charged Polyelectrolytes and Diblock Polyampholytes¹

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The conformational properties of both symmetric and asymmetric flexible diblock polyampholytes and oppositely charged polyelectrolytes are investigated by molecular dynamics simulations and scaling theory. The electrostatically driven coil-globule transition of a symmetric diblock polyampholyte consist of three regimes identified with increasing electrostatic interaction strength: the folding regime, the weak association regime dominated by the fluctuation-induced attractions between oppositely charged sections of the chains, and the ion binding regime that starts with direct binding of oppositely charged monomers (dipole formation), followed by a cascade of multipole formation leading to multiplets analogous to those found in ionomers. In asymmetric block polyampholytes we find the globule to tadpole transition with the increase of charge asymmetry. In the weak association regime this transition is controlled by the balance of net charge and surface tension of the complex and characterized by the ratio of the difference in the number of electrostatic “blobs” between oppositely charged blocks and one third power of the total number of electrostatic blobs. We find the maximum overcharging of the complexes formed by either asymmetric diblock polyampholytes or by pairs of oppositely charged polyelectrolytes is by 50% independent of system parameters. We use scaling theory to estimate the average size of the complex and the electrostatic correlation length as functions of chains length, strength of electrostatic interactions, charge fractions, and solvent quality. The theoretically predicted scaling laws of these conformational properties are in good agreement with our simulation results.

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