Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Regimes of Conformational Transitions of Diblock Polyampholytes

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Regimes of electrostatically-driven conformational transitions of diblock polyampholytes are investigated by scaling theory and molecular dynamics simulations. The coil-globule transition of a symmetric diblock polyampholyte is found to consist of three regimes identified with increasing interaction strength: (i) the folding regime where the electrostatic attraction causes the diblock chain to to fold through the overlap of the two blocks, while each block is slightly stretched by self-repulsion; (ii) the weak association regime which is the classical collapse of the chain into a globule dominated by the fluctuation-induced attractions between oppositely charged chain sections; (iii) the strong association regime that starts with direct binding of oppositely charged monomers (dipole formation), followed by a cascade of multipole formation leading to multiplets. The conformation of a charge-asymmetric diblock polyampholyte changes from extended polyelectrolyte structure, to tadpole-shape with a globular head and a polyelectrolyte tail, and then to polyelectrolyte structure with the variation of the ratio between the charges of the two blocks.

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Date submitted: 30 Nov 2005

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