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Effects of the dielectric inhomogeneity in polyelectrolyte solution

ISSEI NAKAMURA, ZHEN-GANG WANG, Division of Chemistry and Chemical Engineering, California Institute of Technology — We study the effects of dielectric inhomogeneity on the statistical properties of polyelectrolyte in solution, developing a new lattice Monte Carlo method based on the bond fluctuation model with a local algorithm for computing the electrostatic interactions. Our theory accounts for the difference in the dielectric properties between the polymer backbone and the solvent. Taking the coil-globule transition of a single polyelectrolyte in solvent as an example, we show that the chain conformation and the degree of counterion condensation are substantially affected by the electrostatic response of the polymer backbone.

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