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Counterion Condensation and Collapse of Sodium Polystyrene Sulfonate in Water: A Molecular Dynamics Study JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — Hydrophobic polyelectrolytes are known to form necklace-like structures of dense beads connected by strings of monomers. This structure appears as a result of optimization of electrostatic and short-range interactions. To elucidate the effect of counterion condensation on polyelectrolyte conformations we performed two sets of molecular dynamics simulations of sodium polystyrene sulfonate (NaPSS) chains with degree of polymerizations $N=16, 32$ and 64 and fraction of charged monomers $f=0.25, 0.33, 0.5$ and 1.0 in aqueous solutions; (1) water molecules were considered explicitly using TIP3P model and (2) water molecules were modeled as a dielectric continuum with dielectric constant 77.73 . Our simulations showed that with increasing f a polyelectrolyte chain adopts an elongated conformation. The transition between collapsed and elongated states does not show any features of abrupt transition due to the fact that only relatively short chains were considered. Furthermore, even for our longest chains ($N=64$) the necklace-like globule was not observed. Effect of the water-ion interactions on counterion condensation was analyzed by comparing the radial distribution function between the sulfonate groups and sodium counterions for chains with different f . It was found that in simulations with explicit water ionized groups are located at the globular surface.

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