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Molecular Dynamics Simulations of Polyelectrolyte Solutions¹

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Polyelectrolytes are polymers with ionizable groups. In polar solvents, these groups dissociate releasing counterions into solution and leaving uncompensated charges on the polymer backbone. Examples of polyelectrolytes include biopolymers such as DNA and RNA, and synthetic polymers such as poly(styrene sulfonate) and poly(acrylic acids). In this talk I will discuss recent molecular dynamics simulations of static and dynamic properties of polyelectrolyte solutions. These simulations show that in dilute and semidilute polyelectrolyte solutions the electrostatic induced chain persistence length scales with the solution ionic strength as $I^{-1/2}$. This dependence of the chain persistence length is due to counterion condensation on the polymer backbone. In dilute polyelectrolyte solutions the chain size decreases with increasing the salt concentration as $R \sim I^{-1/5}$. This is in agreement with the scaling of the chain persistence length on the solution ionic strength, $l_p \sim I^{-1/2}$. In semidilute solution regime at low salt concentrations the chain size decreases with increasing polymer concentration, $R \sim c_p^{-1/4}$. While at high salt concentrations one observes a weaker dependence of the chain size on the solution ionic strength, $R \sim I^{-1/8}$. Analysis of the simulation data throughout the studied salt and polymer concentration ranges shows that there exist general scaling relations between multiple quantities $X(I)$ in salt solutions and corresponding quantities $X(I_0)$ in salt-free solutions, $X(I) = X(I_0)(I/I_0)^\beta$. The exponent $\beta = -1/2$ for chain persistence length l_p , $\beta = 1/4$ for solution correlation length, $\beta = -1/5$ and $\beta = -1/8$ for chain size R in dilute and semidilute solution regimes respectively. Furthermore, the analysis of the spectrum and of the relaxation times of Rouse modes confirms existence of the single length scale (correlation length) that controls both static and dynamic properties of semidilute polyelectrolyte solutions. These findings confirm predictions of the scaling model of polyelectrolyte solutions.

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