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Polyelectrolytes in Salt Solutions: Molecular Dynamics Simulations ANDREY DOBRYNIN, JAN-MICHAEL CARRILLO, University of Connecticut — We performed MD simulations of polyelectrolyte solutions in the presence of salt. Polyelectrolyte solutions were modeled as an ensemble of chains of charged LJ particles with explicit counterions and salt ions. Our simulations have shown that in dilute and semidilute polyelectrolyte solutions the electrostatic chain persistence length scales with ionic strength as $I^{-1/2}$. This is due to counterion condensation on the polymer backbone. In dilute polyelectrolyte solutions the chain size decreases with increasing salt concentration as $R \propto I^{-1/5}$, which is in line with the scaling of the persistence length on the ionic strength, $l_p \propto I^{-1/2}$. In semidilute solution at low salt concentrations the chain size decreases with increasing polymer concentration, $R \propto c_p^{-1/4}$, while at high salt concentrations it is, $R \propto I^{-1/8}$. Our simulations confirmed that the peak position in the polymer scattering function scales with the polymer concentration in dilute polyelectrolyte solutions as $c_p^{1/3}$. In semidilute polyelectrolyte solutions at low salt concentrations the peak shifts towards larger values of $q^* \propto c_p^{1/2}$ while at high salt concentrations the peak location depends on the ionic strength as $I^{-1/4}$. The simulations confirmed a general scaling relations between a quantity $X(I)$ in salt solutions and corresponding quantity $X(I_0)$ in salt-free solutions,$X(I) = X(I_0)(I/I_0)^{\beta}$ with exponents; β=-1/2 for persistence length l_p, β=1/4 for solution correlation length, β=-1/5 and β=-1/8 for chain size R in dilute and semidilute solution, respectively.

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