

Abstract Submitted
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Puzzle of the Electrostatic Persistence Length¹ A.V. DOBRYNIN, J.-M.Y. CARRILLO, University of Connecticut — Electrostatic interactions play an important role in controlling properties of synthetic and biological polyelectrolytes. The change in the ionic environment in such systems can significantly influence their conformational properties. For semiflexible polyelectrolyte chains with ionic groups interacting via the screened Debye-Huckel potential the electrostatic contribution to the chain persistence length scales quadratically with the Debye screening length (OSF model). However, recent computer simulations of flexible polyelectrolyte chains with explicit counterions and salt ions show that in the wide interval of the solution ionic strengths the electrostatic contribution to chain persistence length is proportional to the Debye screening length, r_D . To understand the crossover between flexible and semiflexible chain behavior and elucidate the effect of explicit ions on chain conformations we performed molecular dynamics of polyelectrolyte chains with degree of polymerization $N = 300$ and different values of the chain bending rigidity varying between $K = 1$ and $K = 160$. Our simulations have shown that the bond-bond correlation function describing chain's orientational memory can be approximated by a sum of two exponential functions manifesting the existence of the two characteristic length scales. One describes the chain's bending rigidity at the distances along the polymer backbone shorter than r_D while another controls the long-length scale chain's orientational correlations. The long-length scale bending rigidity is proportional to r_D for chains with bending rigidity smaller than a crossover bending rigidity K^* .

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