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Influence of Higher Valence Ions on Flexible Polyelectrolytes Stiffness and Counter-ion Distribution[1] ALEXANDROS CHREMOS, JACK F. DOUGLAS, NIST - Natl Inst of Stds Tech — We investigate the influence of counter-ion valency on the flexibility of highly charged flexible polymer chains by molecular dynamics simulations that include both salt and an explicit solvent. A theoretical understanding of solutions of these molecules (e.g., DNA, RNA, and sulfonate polyestyrene) has been slow to develop due to the complex coupling between the polyelectrolyte conformation and the ionic species in solution due to their long range Coulomb interactions. As observed experimentally, we find that divalent counter-ions greatly reduce the chain persistence length, in comparison to monovalent counter-ions, an effect correlated with the tendency of the polyelectrolyte chain to become distorted by divalent counter-ions. We rationalize these results by with the substantial increase of counter-ion population at the interface with the polyelectrolyte, which not only leads to a more effective screening of the bare charge, but also leads to charge inversion in the trivalent counter-ion case. These conformational changes with counter-ion valency are also associated with a drastic increase of the number of contacts the counter-ions have at the interface with polyelectrolyte, an effect associated with polyelectrolyte chain coiling around the counter-ions.

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