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Structure and dynamics of polyelectrolytes in water solution

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Intrinsically disordered proteins (IDP) challenge the classical structure function paradigm in structural biology as they have specific function without fixed structure. Specifically, the dynamics of flexible chains seems to be of great importance for fast response to environmental conditions. Since proteins and, in particular, IDPs have properties of charged polymer chains, polyelectrolytes (PE) can be used as model system to study response of charged chains to environmental changes.
We explore structure and dynamics of polystyrene sulfonic acid (PSSH) and salt (PSSNa) as a well-known polyelectrolyte in solution with low to high ion concentration (H+ and NaCl). The concentration of PE is well below the overlap concentration to examine the single chain regime. For single PE chains a transition from coils to globules is observed. Moreover, at some conditions ion condensation leads to pearl necklace conformation.
To elucidate the structure and form factor of PSSH SAXS and SANS (MLZ) measurements were conducted. Their combined analysis performed over a large Q-range allows us to examine the NaCl contribution and determine the details of intrachain structure.
NSE experiment (ILL) clearly shows change of polyelectrolyte dynamics as a function of salt concentration. Analysis of relaxation dynamics shows a change from a rigid body behavior (collapsed chains) to Zimm like dynamics as expected for strongly screened flexible polymer chains. The effect is temperature dependent.

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