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Similarities between unfolded protein dynamics and polyelectrolyte dynamics

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Proteins are biological macromolecules built from a sequence of amino acids with varying characteristics as hydrophobicity, charge and side-group that determine their biological and physical properties. Unfolded proteins, like intrinsically disordered proteins (IDPs), share similarities with polymers in structure and dynamics. For thermal unfolded Ribonuclease A or the IDP myelin basic protein we showed already similarities to polymer dynamics reflected by Zimm-like dynamics with internal friction [1-3]. Also normal mode analysis based on explicit configurations resulted in improved description of the dynamics. Here we explore the dynamics of polystyrene sulfonic acid (PSS-H) and salt (PSS-Na) as a well-known polyelectrolyte well below the overlap concentration to examine the single chain conformation and dynamics. The aim is to observe the influence of the large charged sidechain onto the chain dynamics and to find similarities to the molecular dynamics of IDP that deviates from standard polymer dynamic models.
The structure of PSS-H can be described by a wormlike chain model with a finite thickness. A disclike cross-section indicating the extended side chains can be observed by SAXS due to the specific contrast conditions. Neutron Spin Echo, observing the molecular dynamics, clearly indicate a change of chain dynamics as a function of salt concentration and temperature. The dynamics shows a crossover between rigid body like behavior (stiff chains) to Zimm-like dynamics as expected for flexible polymer chains.

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