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Effect of Sodium Chloride Concentration and Degree of Neutralization on the Structure and Dynamics of Poly(Methacrylic Acid) (PMA) in Dilute Aqueous Solutions – a Molecular Dynamics Simulations Study

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Abstract : Atomistic Molecular Dynamics (MD) Simulations have been performed to study the effect of monovalent salt i.e. NaCl concentration (Cs) and chain degree of neutralization (f) on the structure and dynamics of anionic poly(methacrylic acid) (PMA) in dilute aqueous solutions. In the present study, the attention is to unveil the conformational structure, hydrogen-bonding, local polyion-counterion structure, h-bond dynamics, chain dynamics and thermodynamic enthalpy of solvation of a-PMA in dilute aqueous solutions as a function of salt concentration, Cs and f. The results have revealed that at low salt concentration, the conformational radius of gyration (Rg) increases and then decreases reaching a maximum in agreement with the reported light scattering experimental results. The Rg at f = 1 shows a continual decrease and acquire a plateau value at higher salt concentration in agreement with results obtained by light scattering experiments. The radial distribution functions between PMA, salt and water atoms has been computed with respect to atom and centre-of-mass to understand the intermolecular structure in detail. The results pertaining to PMA chain conformations and hydrogen bond autocorrelation function showcasing the h-bond dynamics will be presented. The results pertaining to chain dynamics will be presented. The results pertaining to counterion condensation on the PMA chain shows greater condensation of Na+ ions on to the carboxylate ions with increase in salt concentration. Moreover, the solvation enthalpy of the system as a function of salt concentration will be presented.

Keywords : conformations, molecular dynamics simulations, NaCl concentration, radial distribution functions
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