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Molecular dynamics simulation studies of structure and dynamics of poly(acrylic) acid in semidilute concentration regime

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A detailed fully atomistic molecular dynamics (MD) simulation study was carried out with the aid of explicit specification of solvent molecules on poly(acrylic) acid (PAA) in salt free aqueous solution from dilute to semidilute concentration region at different degree of ionization (f) values viz. f = 0.2, 0.4, 0.7 and 1.0. The structural properties viz. Radius of gyration (Rg), end-to-end distance (R), hydrogen bonding (interchain, intrachain and intermolecular), intermolecular structure, bound water ratio, scattering structure factor, interchain distance, interchain contacts and dihedral angle distribution have been elucidated. The dynamic properties viz. hydrogen-bond dynamics and self diffusion coefficient of PAA and counterions have been reported and compared with experimental and model studies. The results have revealed that, conformation size (Rg and R) decreases with increase in polymer volume fraction (ϕP) which is in qualitative agreement with the experimental studies where, ionized PAA particle length decreases with increase in PAA concentration in the semidilute region. Moreover, this behavior is in agreement with the model studies that, demonstrated a decrease in conformational Rg with polymer concentration. The number of interchain and intrachain H- bonds show an increase with increase in ϕP. The self diffusion coefficient of PAA and sodium counterions showed a non-monotonic and monotonic decrease with increase in ϕP which, is in good agreement with the bead – spring polyelectrolyte model studies under fully ionized conditions. The details of analysis of properties will be presented.

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