

Supplementary Materials

Structures of Cationic and Anionic Polyelectrolytes in Aqueous Solutions:

The Sign Effect

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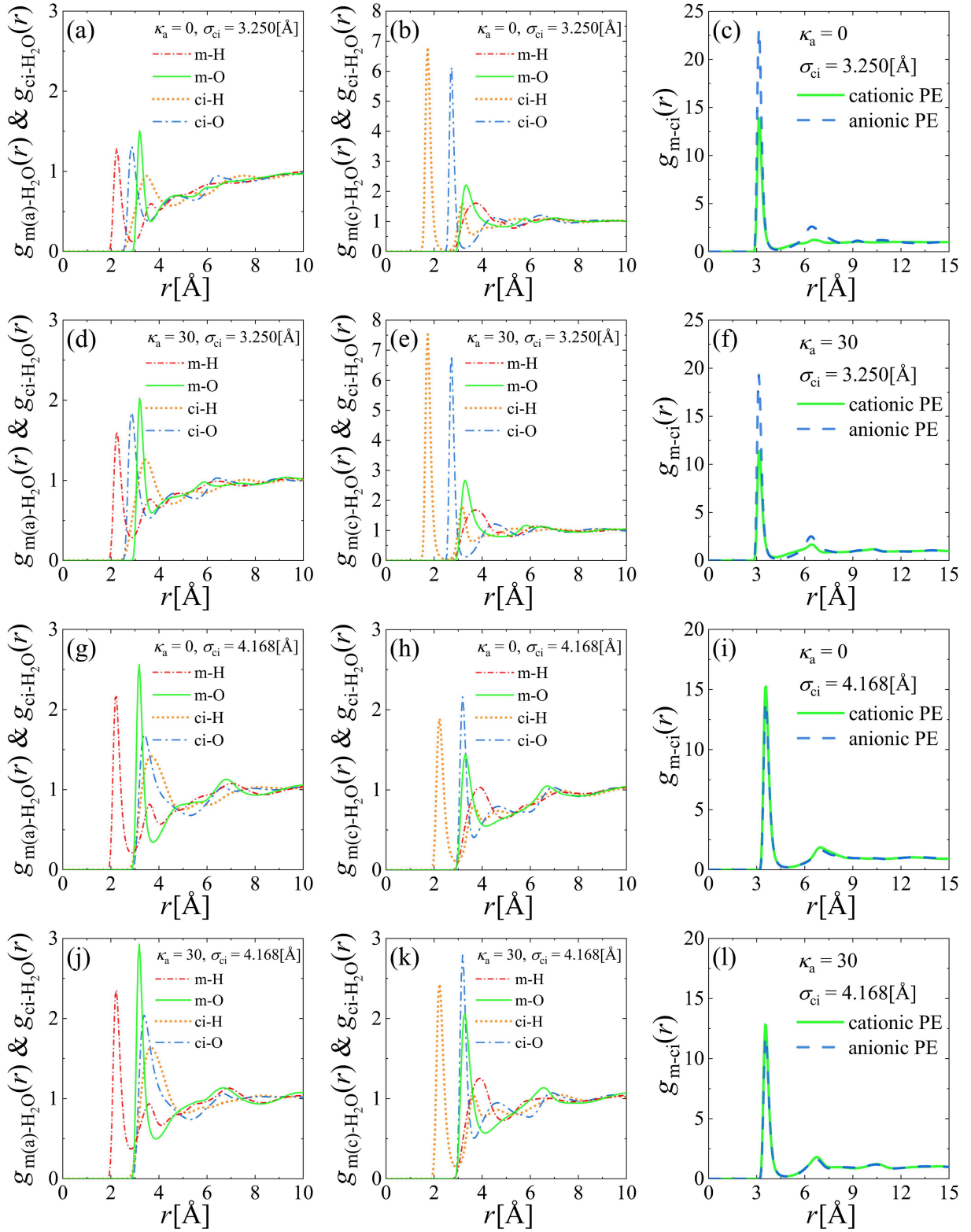


Fig. S1 Radial distribution functions of O and H in H_2O molecules around each monomer and counterion of (a) anionic and (b) cationic PEs [denoted as $g_{m(a)-O}(r)$, $g_{m(a)-H}(r)$, $g_{m(c)-O}(r)$, $g_{m(c)-H}(r)$, $g_{ci-O}(r)$, $g_{ci-H}(r)$], and counterions around each monomer of single (c) PEs [denoted as $g_{m(a)-ci}(r)$, $g_{m(c)-ci}(r)$] at $\kappa_a = 0$ and $\sigma_{ci} = 3.25[\text{\AA}]$. (d), (e) and (f) correspond to the results of (a), (b) and (c) at $\kappa_a = 30$ and $\sigma_{ci} = 3.25[\text{\AA}]$, respectively. (g), (h) and (i) correspond to the results of (a), (b) and (c) at $\kappa_a = 0$ and $\sigma_{ci} = 4.168 [\text{\AA}]$, respectively. (j), (k) and (l) correspond to the results of (a), (b) and (c) at $\kappa_a = 30$ and $\sigma_{ci} = 4.168 [\text{\AA}]$, respectively.

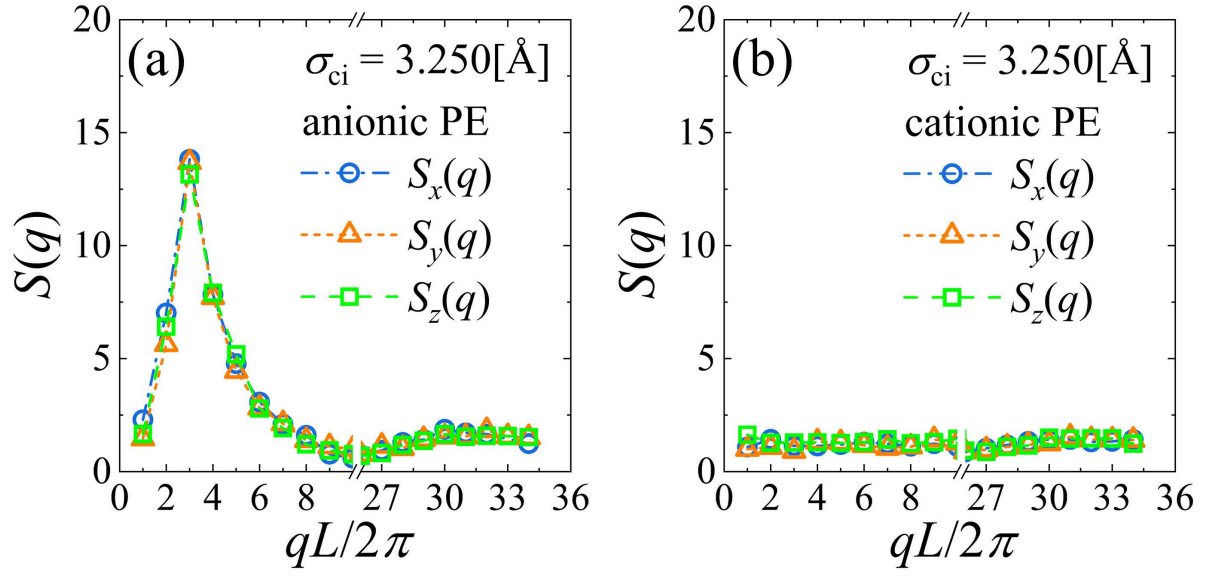


Fig. S2 Three components of $S(q)$ in Figure 6(c) along x , y , and z directions, for (a) anionic polyelectrolytes and counterions, and (b) cationic polyelectrolytes and counterions, at $\sigma_{ci} = 3.25 [\text{\AA}]$.