Electronic Supplementary Material (ESI) for Soft Matter.

Understanding the stimuli responsive behavior of polyion grafted nanoparticles in the presence of salt and polyelectrolytes

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Supplementary information

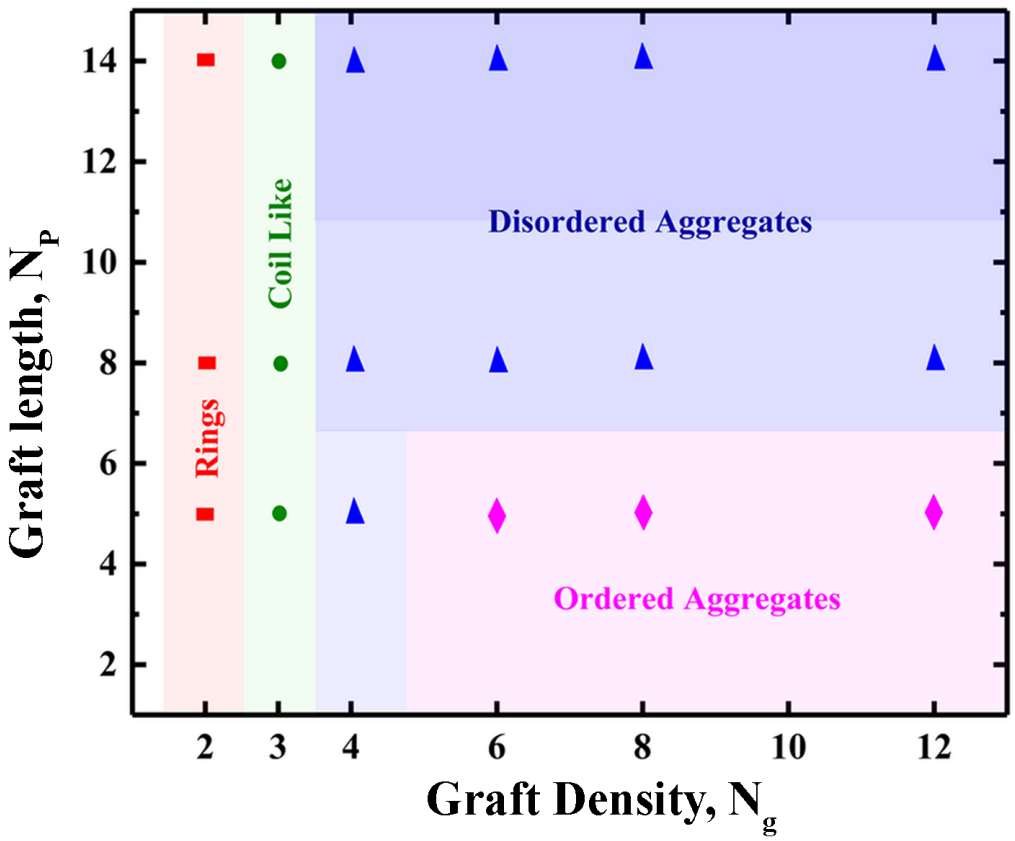

Figure S1: Phase morphology of electrostatic-driven self-assembly of nanoparticles grafted with oppositely charged polyions in an implicit solvent (water) at a temperature $T^* = 1.0$ as a function of graft density (N_g) and graft length (N_P) at $\lambda_B = 2\sigma$, "Reprinted (adapted) with permission from " Charge-Driven Self-Assembly of Polyelectrolyte-Grafted Nanoparticles in Solutions, Rajesh Pavan Pothukuchi, Vinod Kumar Prajapat, and Mithun Radhakrishna, Langmuir 2021 37 (41), 12007-12015, DOI: 10.1021/acs.langmuir.1c01571". Copyright 2021 American Chemical Society."

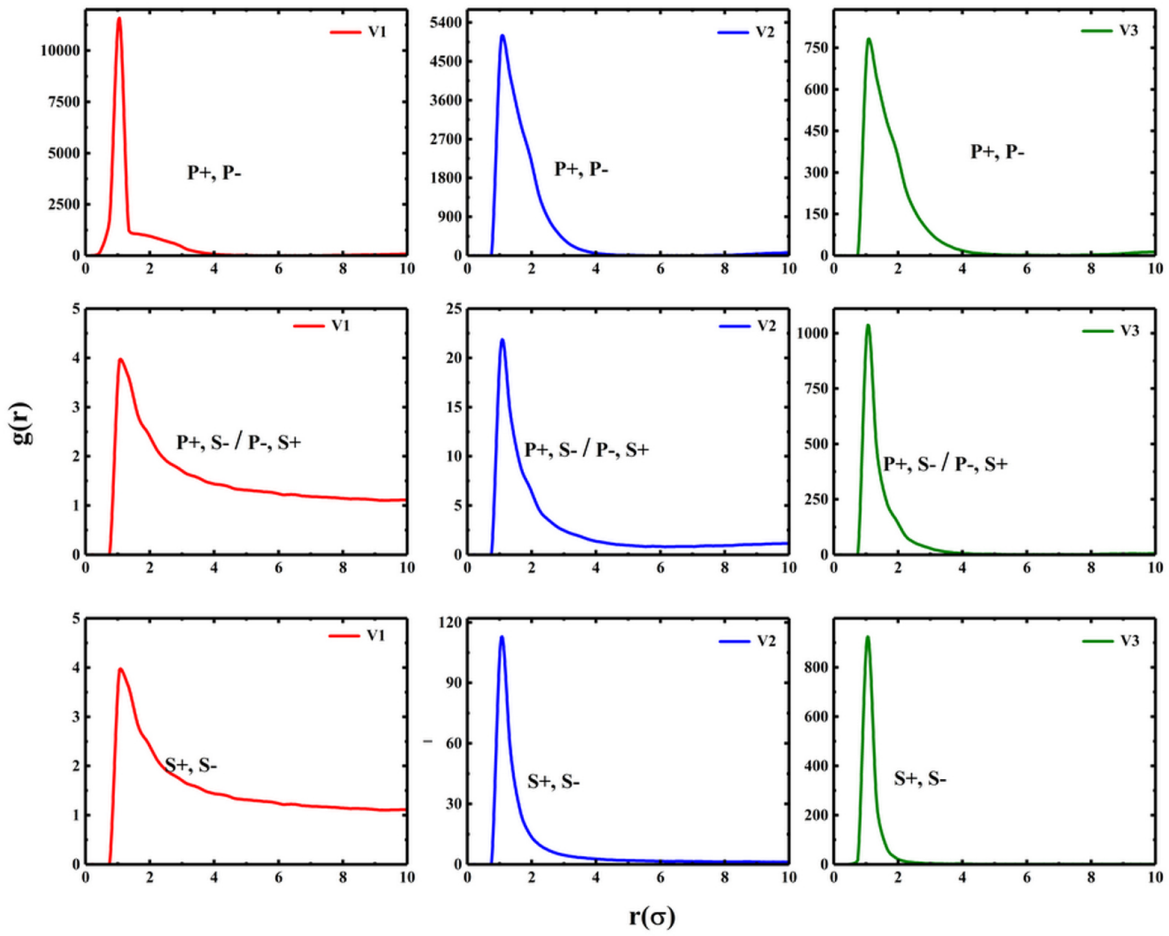

Figure S2: Radial distribution (pair correlation) functions between polycation,polyanion (P+,P-); salt cation, salt anion (S+,S-) and polyion and the oppositely charged salt ions (P+,S-/P-,S+) at different salt valency for the polyion grafted nanoparticle system at a grafting density $N_g = 2$ at a salt concentration of $C_S = 2.5$ mM and diameter $\sigma_S = \sigma$ for chain length $N_P = 8$. V1, V2 and V3 represent system with univalent, divalent and trivalent salt ions.

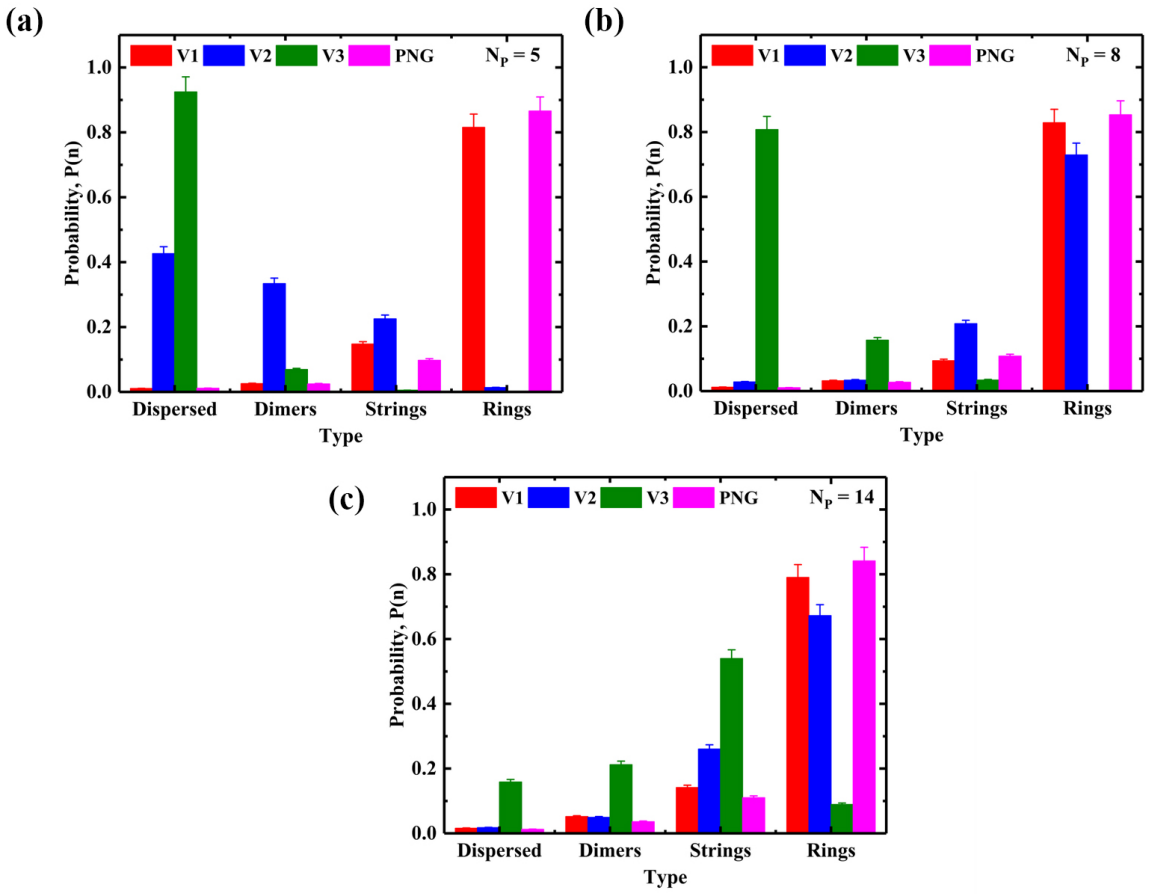

Figure S3: Probability distribution of various morphologies of the polyion grafted nanoparticle system at a grafting density $N_g = 2$ at a salt concentration of $C_S = 5$ mM when $\sigma_S = \sigma$ a) $N_P = 5$ b)$N_P = 8$ and c) $N_P = 14$. V1, V2 and V3 represent system with univalent, divalent and trivalent salt ions. $\lambda_B = 2\sigma$. PNG represents the primary nanoparticle graft system in the absence of salt

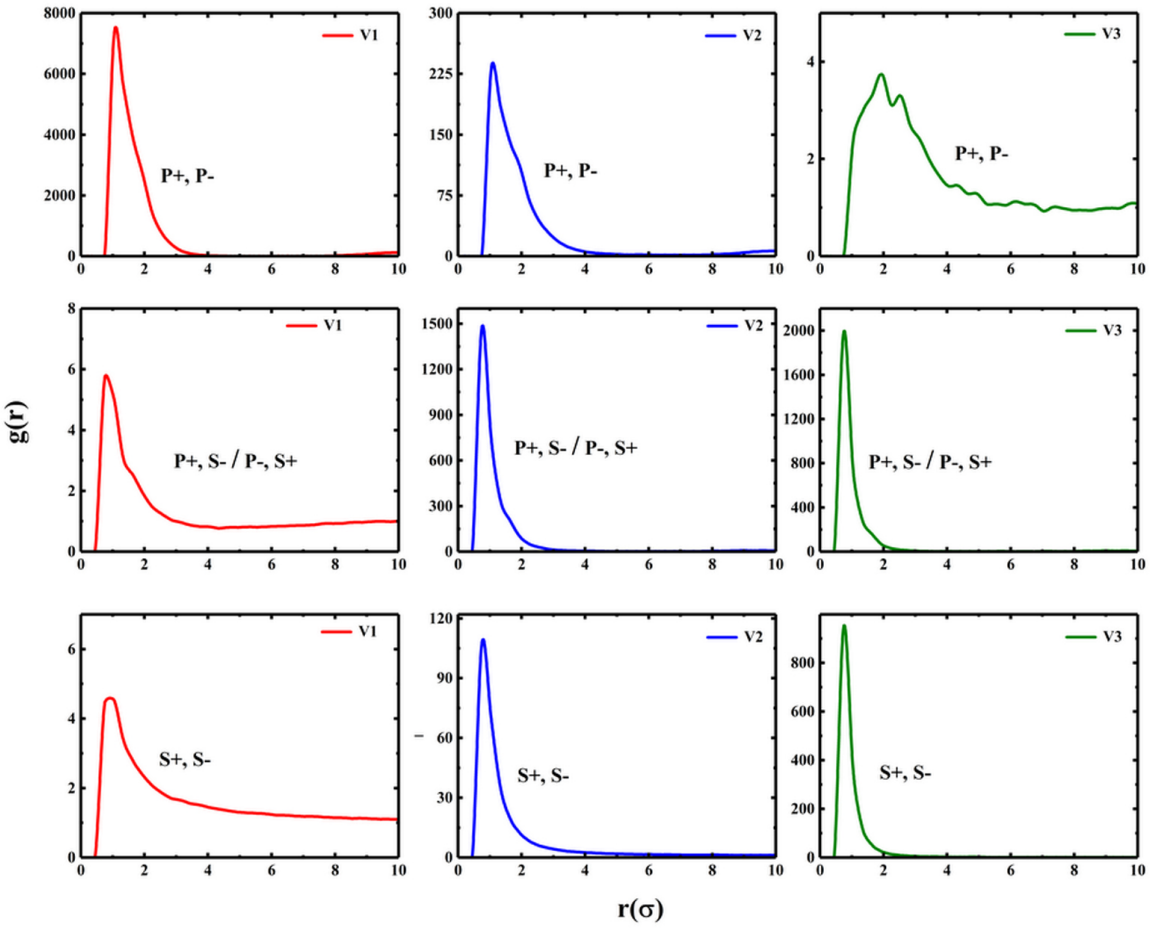

Figure S4: Radial distribution (pair correlation) functions between polycation,polyanion (P+,P-); salt cation,salt anion (S+,S-) and polyion and the oppositely charged salt ions (P+,S-/P-,S+) at different salt valency for the polyion grafted nanoparticle system at a grafting density $N_g = 2$ at a salt concentration of $C_S = 2.5$ mM and diameter $\sigma_S = 0.5\sigma$ for chain length $N_P = 5$. V1, V2 and V3 represent system with univalent, divalent and trivalent salt ions.

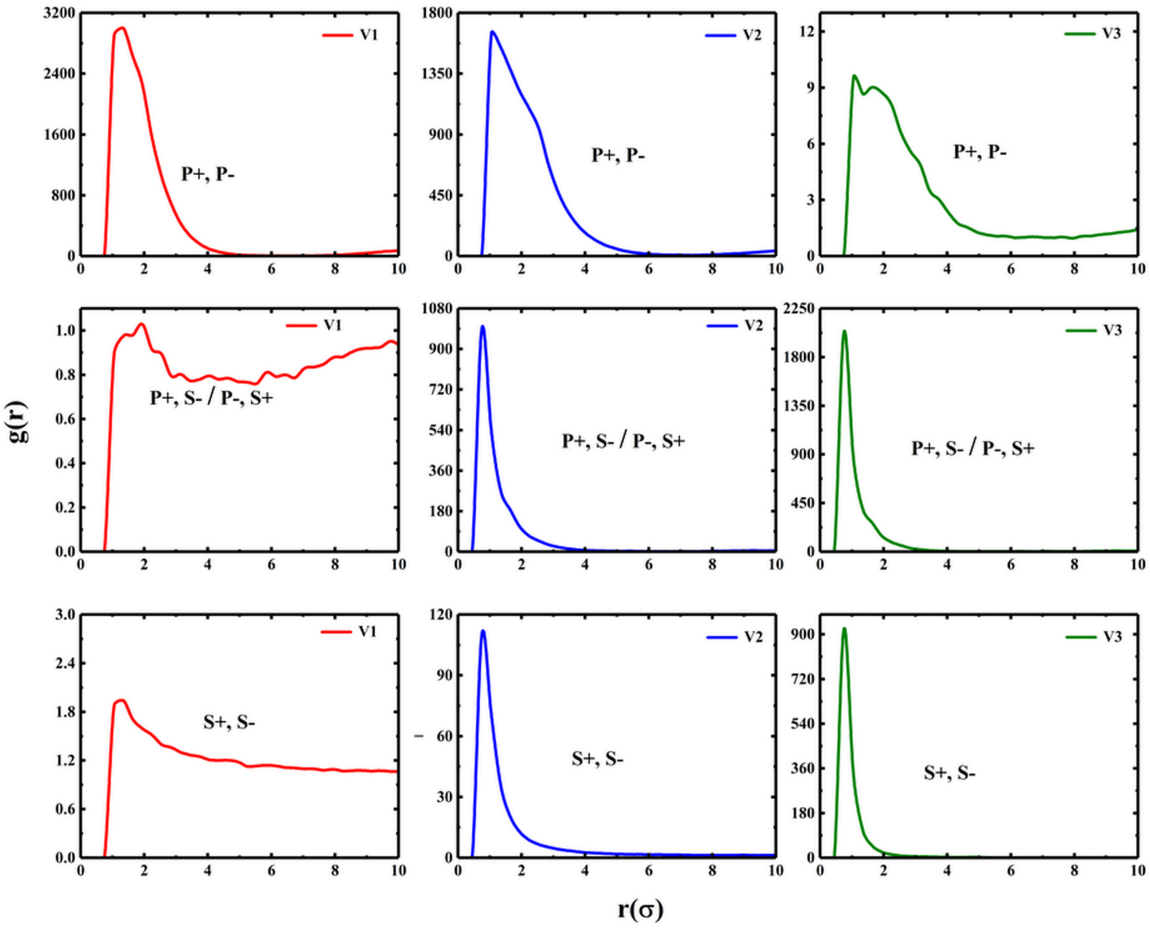

Figure S5: Radial distribution (pair correlation) functions between polycation,polyanion (P+,P-); salt cation, salt anion (S+,S-) and polyion and the oppositely charged salt ions (P+,S-/P-,S+) at different salt valency for the polyion grafted nanoparticle system at a grafting density $N_g = 2$ at a salt concentration of $C_S = 2.5$ mM and diameter $\sigma_S = 0.5\sigma$ for chain length $N_P = 8$. V1, V2 and V3 represent system with univalent, divalent and trivalent salt ions.

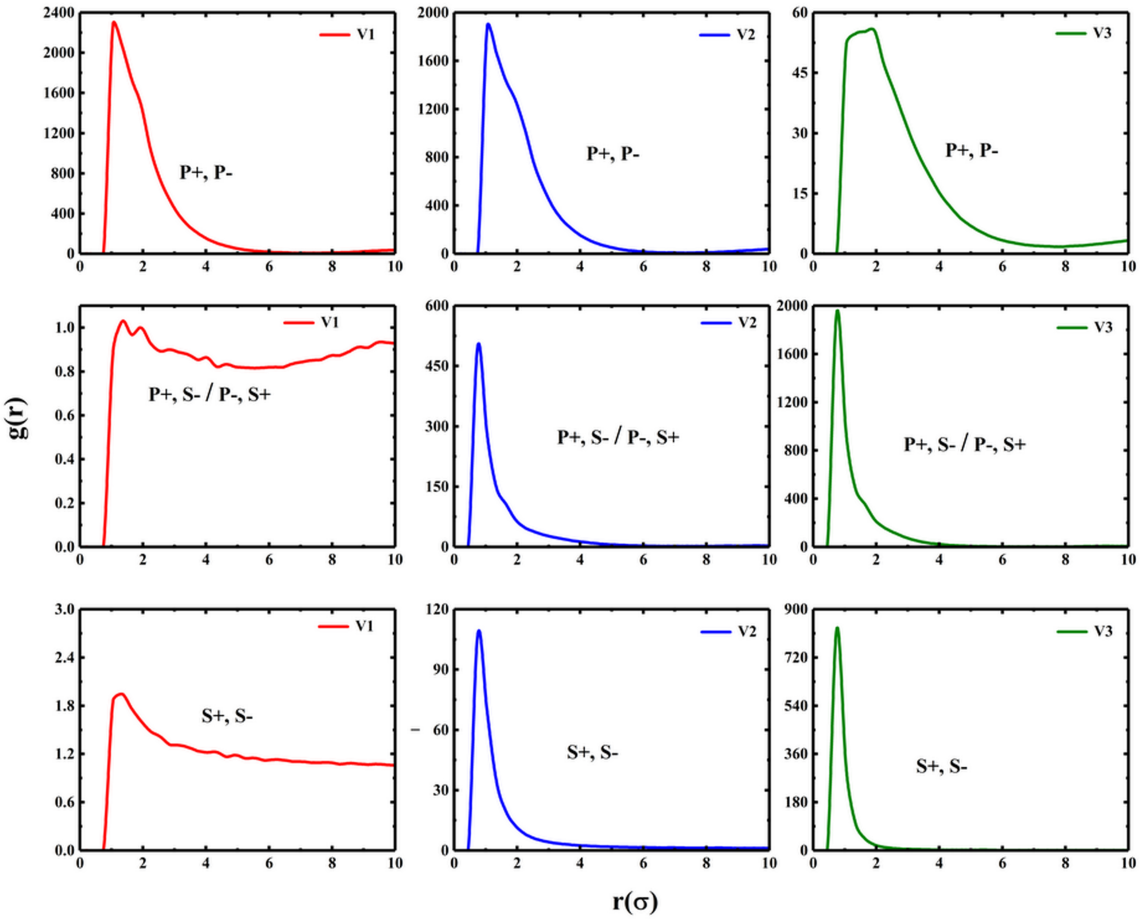

Figure S6: Radial distribution (pair correlation) functions between polycation,polyanion (P+,P-); salt cation, salt anion (S+,S-) and polyion and the oppositely charged salt ions (P+,S-/P-,S+) at different salt valency for the polyion grafted nanoparticle system at a grafting density $N_g = 2$ at a salt concentration of $C_S = 2.5$ mM and diameter $\sigma_S = 0.5\sigma$ for chain length $N_P = 14$. V1, V2 and V3 represent system with univalent, divalent and trivalent salt ions.

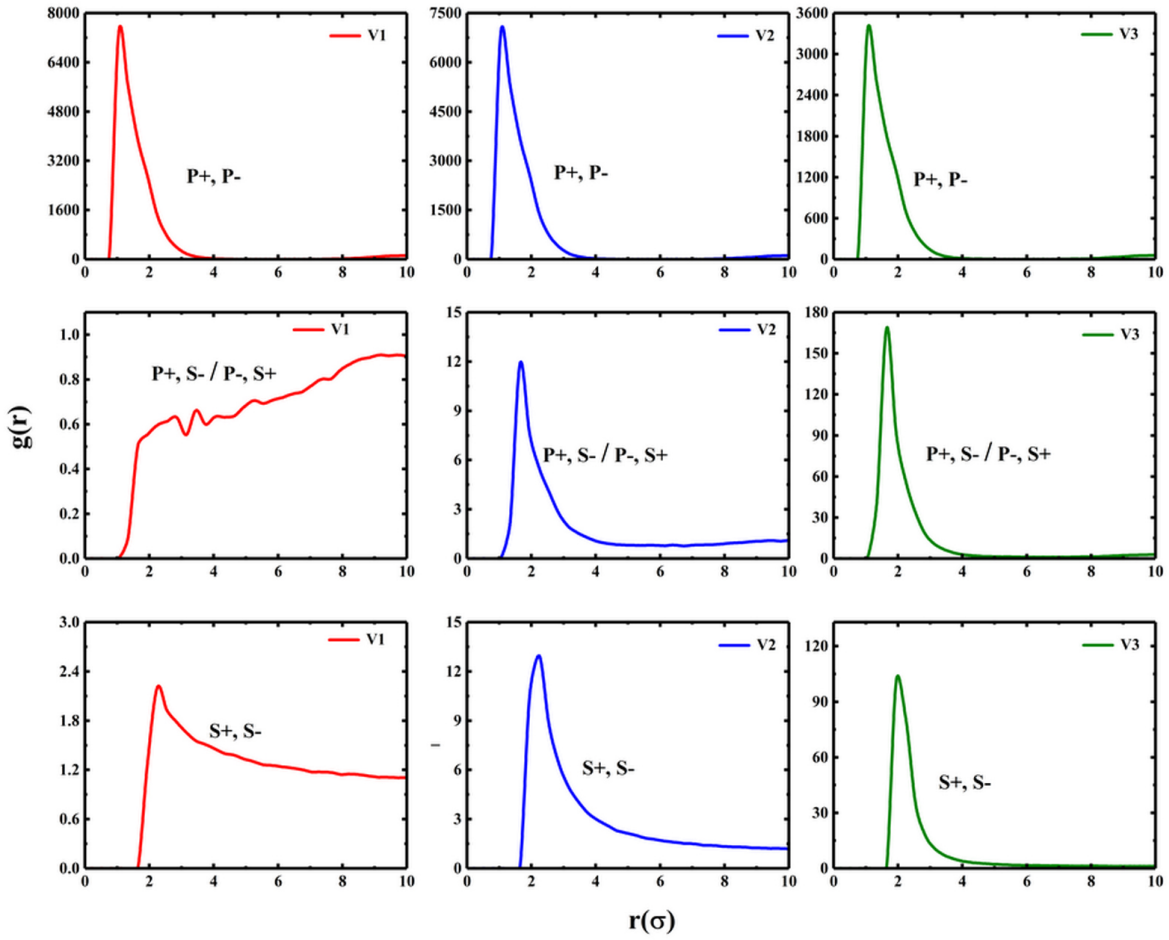

Figure S7: Radial distribution (pair correlation) functions between polycation,polyanion (P+,P-); salt cation,salt anion (S+,S-) and polyion and the oppositely charged salt ions (P+,S-/P-,S+) at different salt valency for the polyion grafted nanoparticle system at a grafting density $N_g = 2$ at a salt concentration of $C_S = 2.5$ mM and diameter $\sigma_S = 2\sigma$ for chain length $N_P = 5$. V1, V2 and V3 represent system with univalent, divalent and trivalent salt ions.

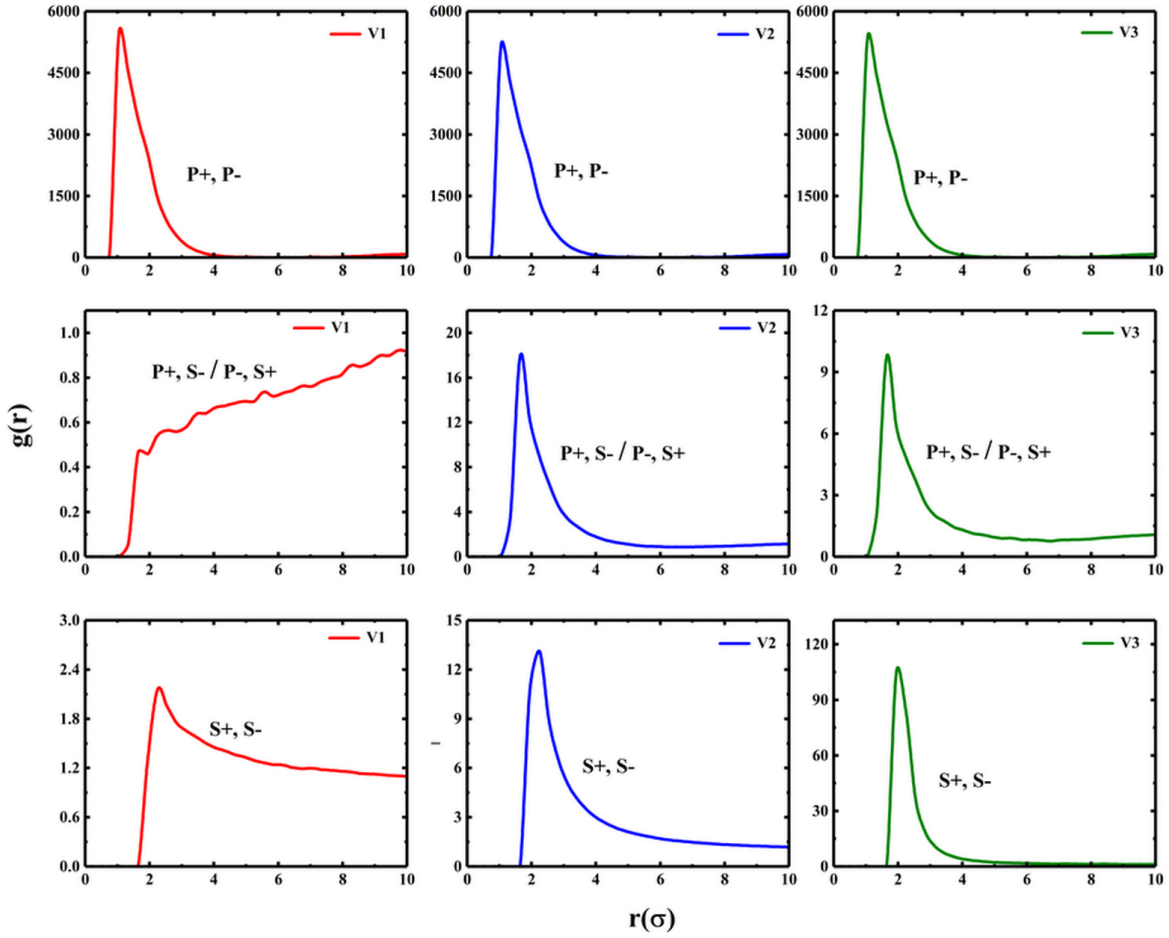

Figure S8: Radial distribution (pair correlation) functions between polycation,polyanion (P+,P-); salt cation,salt anion (S+,S-) and polyion and the oppositely charged salt ions (P+,S-/P-,S+) at different salt valency for the polyion grafted nanoparticle system at a grafting density $N_g = 2$ at a salt concentration of $C_S = 2.5$ mM and diameter $\sigma_S = 2\sigma$ for chain length $N_P = 8$. V1, V2 and V3 represent system with univalent, divalent and trivalent salt ions.

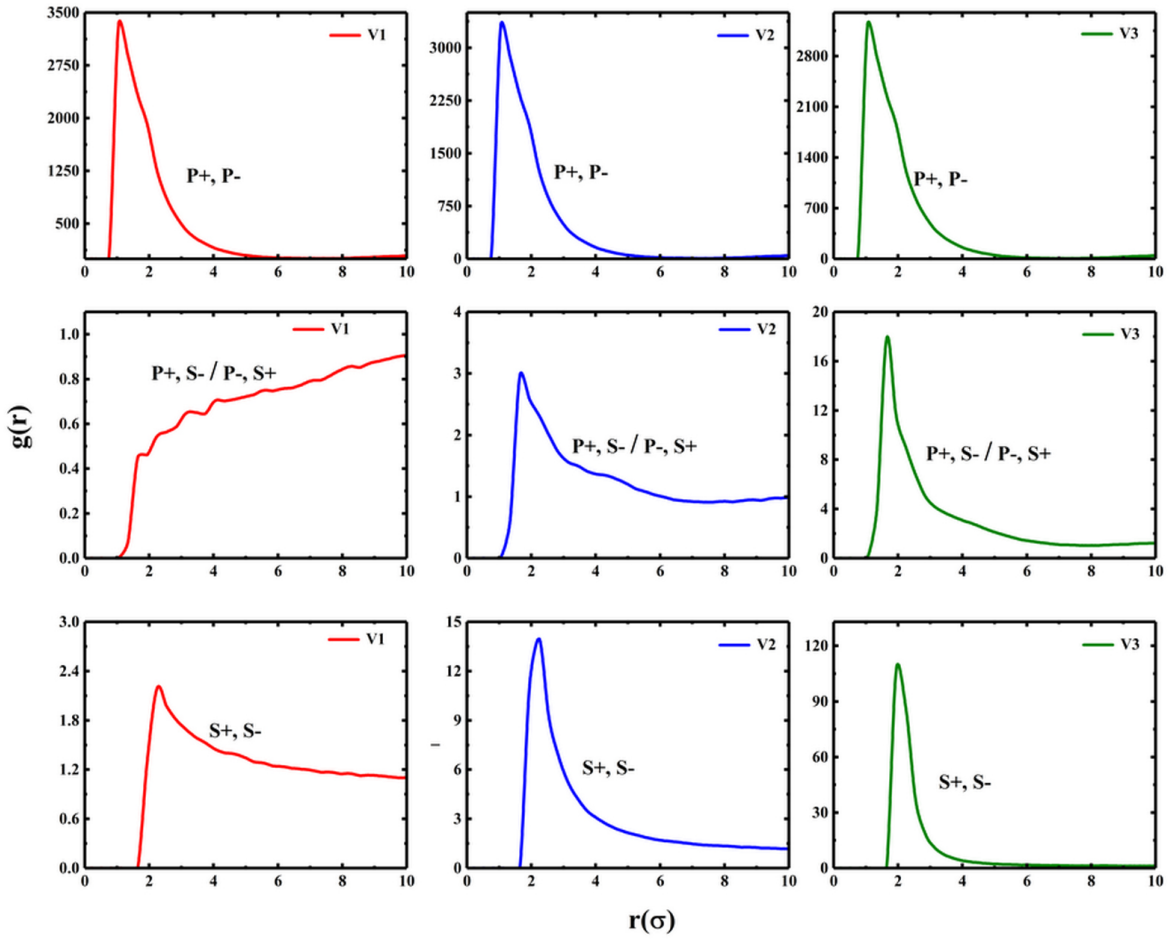

Figure S9: Radial distribution (pair correlation) functions between polycation,polyanion (P+,P-); salt cation,salt anion (S+,S-) and polyion and the oppositely charged salt ions (P+,S-/P-,S+) at different salt valency for the polyion grafted nanoparticle system at a grafting density $N_g = 2$ at a salt concentration of $C_S = 2.5$ mM and diameter $\sigma_S = 2\sigma$ for chain length $N_P = 14$. V1, V2 and V3 represent system with univalent, divalent and trivalent salt ions.