Supplementary Information – pH-dependent Polyelectrolyte Bridging of Charged Nanoparticles

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Quenched vs. annealed

Figures showing the difference between quenched and annealed PEs for a larger number of distances, as well as bridge formation.

Influence of salt

Figures showing the influence of salt on the systems, where the salt has been included using the Debye-Hückel approximation. As can be seen, the addition of salt does not have a large effect at a concentration of 10 mM, while 100 mM diminishes the PE-NP interactions substantially. Note that the salt systems have a shorter run time than the corresponding systems with no salt, hence having more noisy density distributions and larger error bars in Fig. S6.

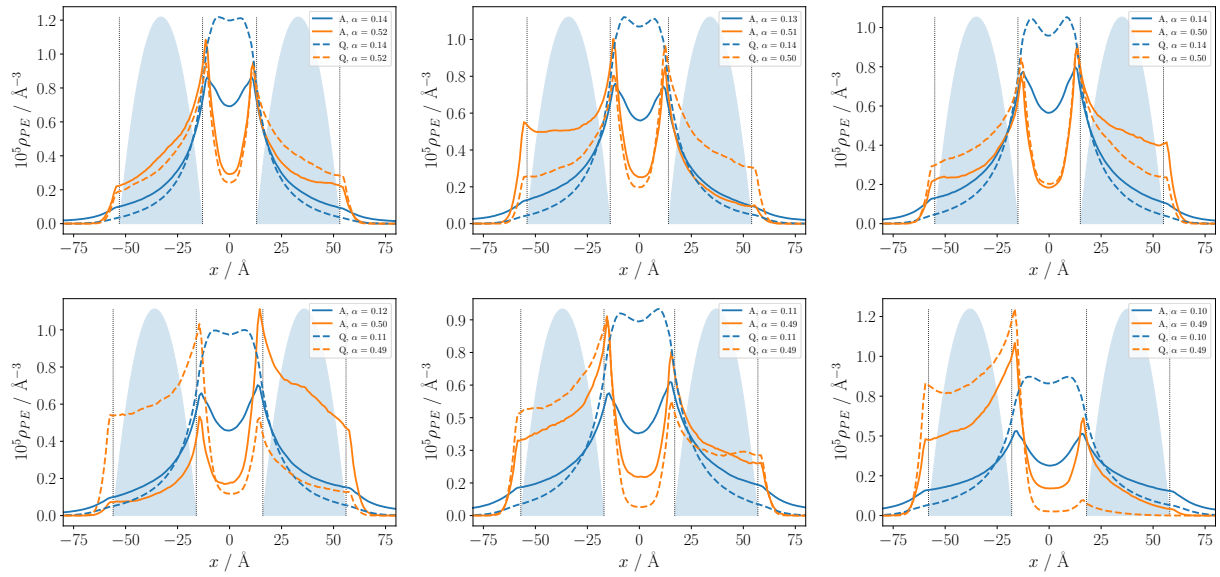

Figure S1: PE monomer density distribution for separation distances d = 26 (top left), 28 (top middle), 30 (top right), 32 (bottom left), 34 (bottom middle) and 36 (bottom right) Å. Line styles and colors are similar to those used in Fig. 6.

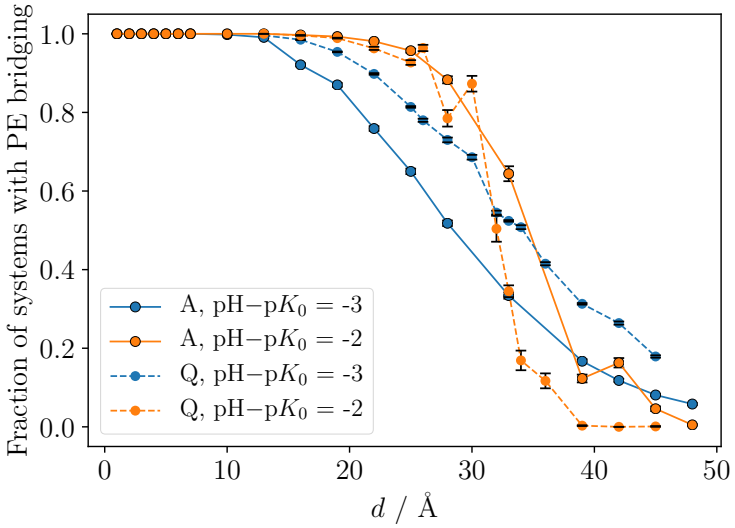

Figure S2: Fraction of sampled configurations where the PE is considered adsorbed to both NPs as a function of distance, for annealed and the corresponding quenched systems at pH−pK_0 = -3 and -2. Error bars show one standard deviation of the sample mean.

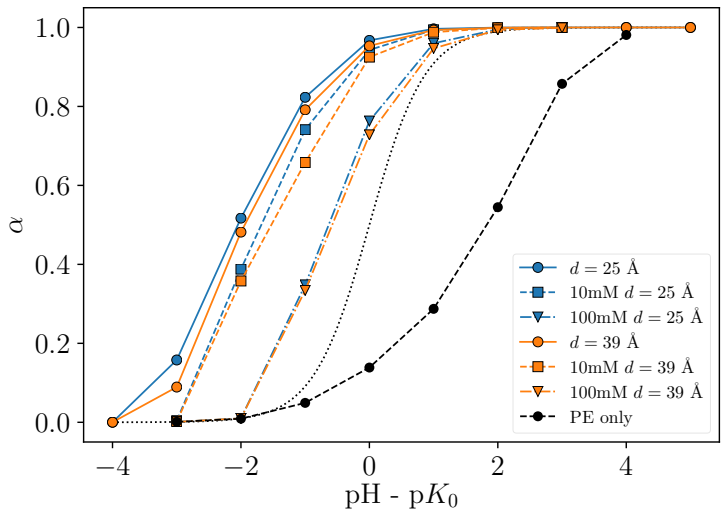

Figure S3: Titration curves for PE at distances $d = 25$ (blue) and 39 (orange) Å, without salt (circles, whole lines), and salt concentrations of 10 mM (squares, dashed lines) and 100 mM (triangles, dash-dotted lines). Dotted black line shows the ionization of a single monomer system.

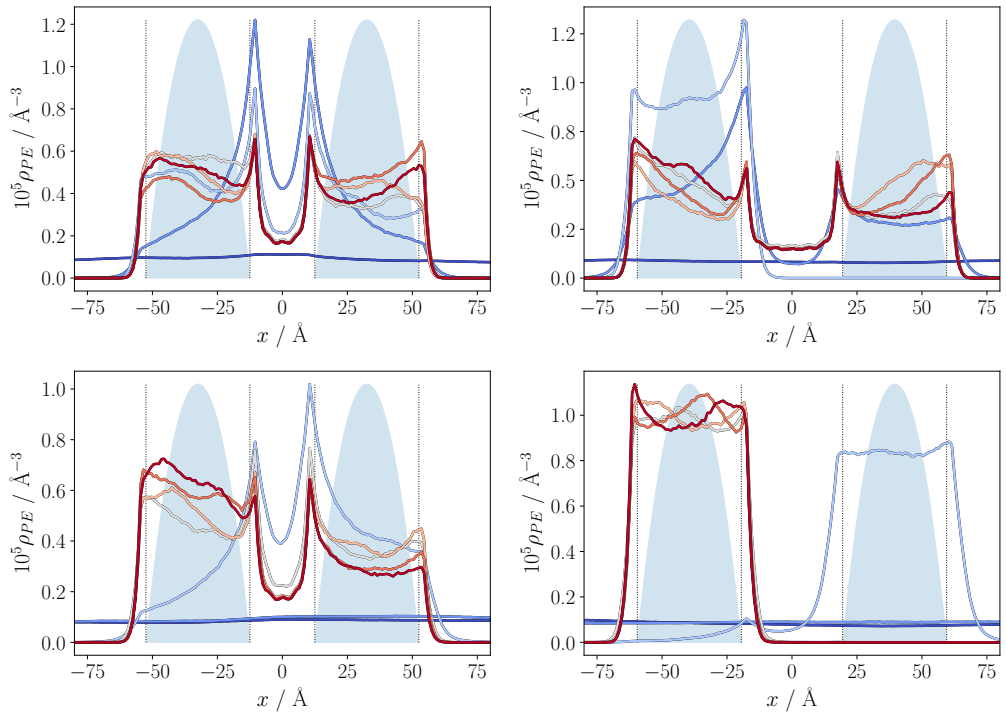

Figure S4: PE monomer density distribution for separation distances $d = 25$ (left) and 39 (right) Å with salt concentrations of 10mM (top) and 100 mM (bottom). pH$-$pK_0 ranging from -3 (dark blue) to 4 (dark red)

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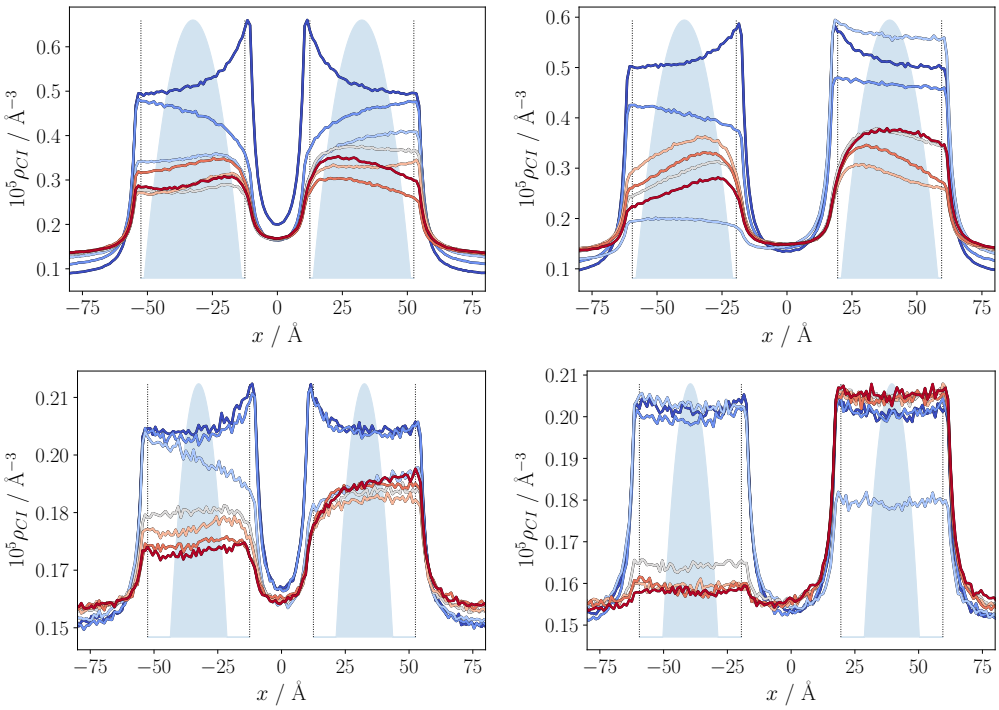

Figure S5: Counterion density distribution for separation distances $d = 25$ (left) and 39 (right) Å with salt concentrations of 10mM (top) and 100 mM (bottom). pH$-$pK_0 ranging from -3 (dark blue) to 4 (dark red)

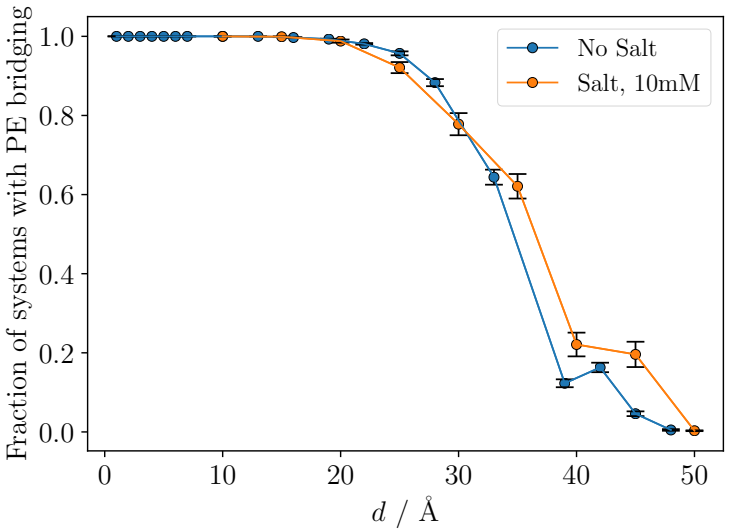

Figure S6: Fraction of sampled configurations where the PE is considered adsorbed to both NPs as a function of distance for systems with and without salt, at pH$-$p$K_0 = -2$. The curve for 100 mM is not included, as the PE remains neutral at that concentration, as seen in the titration curve, thus having no electrostatic interaction with the PE.