Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Understanding asymmetry effects at low grafting density on the self-assembly of polyion grafted nanoparticles

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Supplementary Information

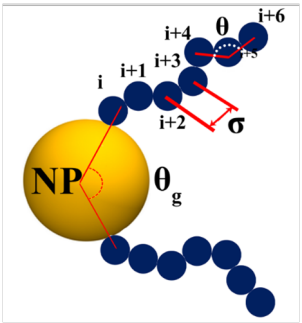

Figure S1: Pictorial representation of nanoparticles grafted with polyanions and polycations at grafting density $N_g = 2$. θ represents the angle between the i,i+1 and i+2 beads of the polyions which is internal to the grafted polymer. θ_g refers to the angle between the position of the tethers on the surface of the nanoparticle i.e it is the angle formed between the center of the first monomer of the graft, center of the NP and the first monomer of the second graft. There is no relationship between θ and θ_g

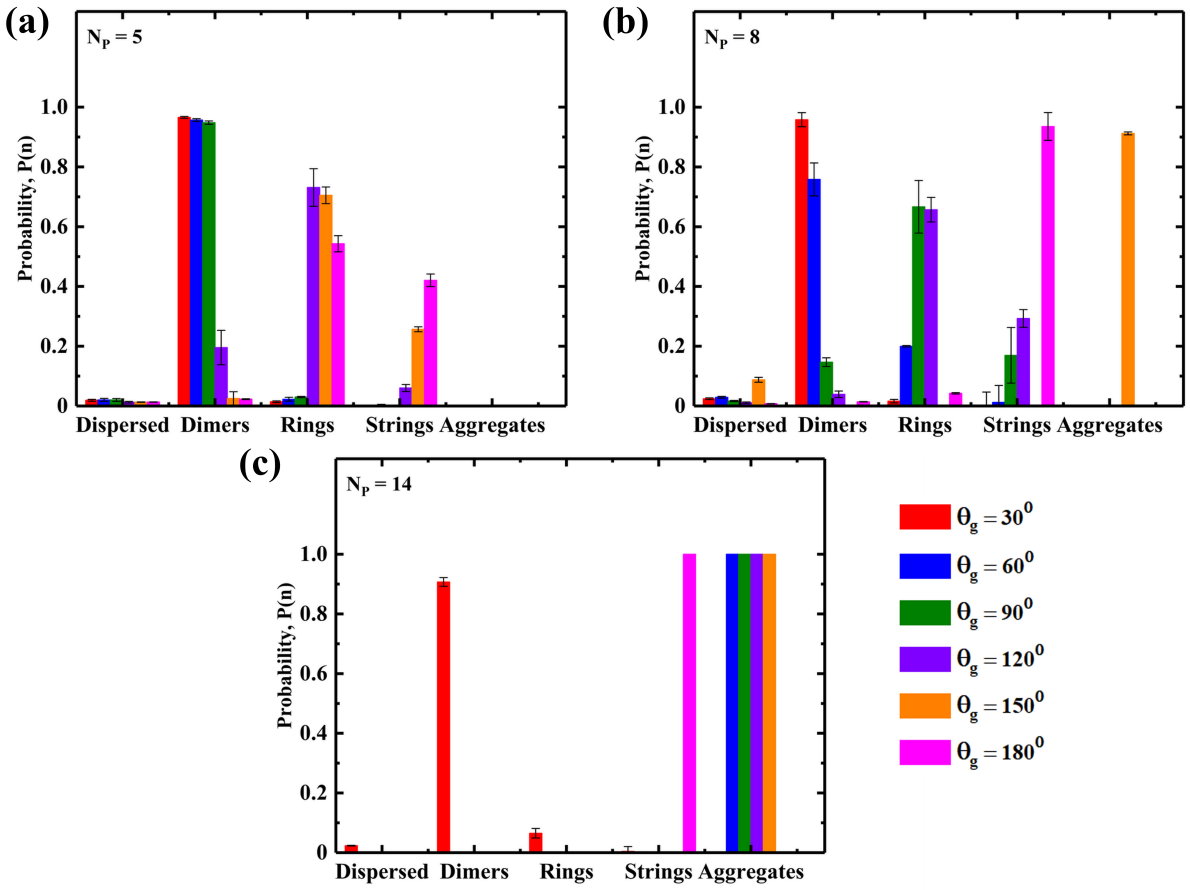

Figure S2: Probability of formation of various morphologies of the polyion grafted nanoparticle system at a grafting density $N_g = 2$ and chain stiffness $k_\theta = 20 k_B T/rad^2$ for graft polyion length (a) $N_P = 5$, (b) $N_P = 8$, and (c) $N_P = 14$

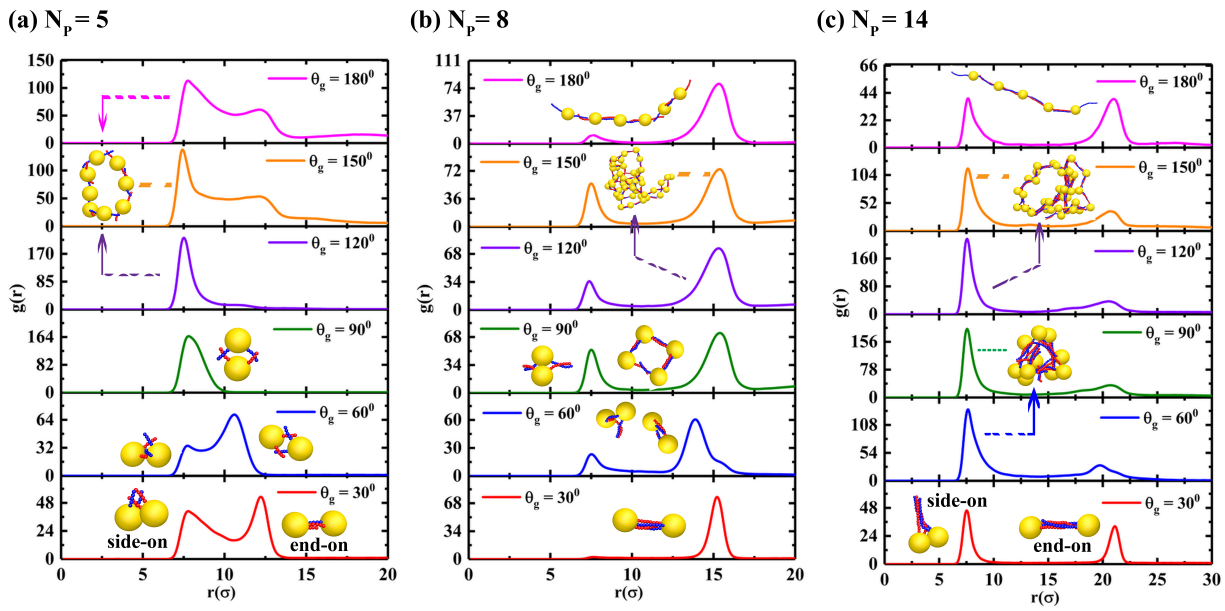

Figure S3: Pair correlation function ($g(r)$) between nanoparticles for grafting density $N_g = 2$ and chain stiffness $k_\theta = 20k_BT/rad^2$ at graft length (a) $N_P = 5$, (b) $N_P = 8$ and (c) $N_P = 14$.

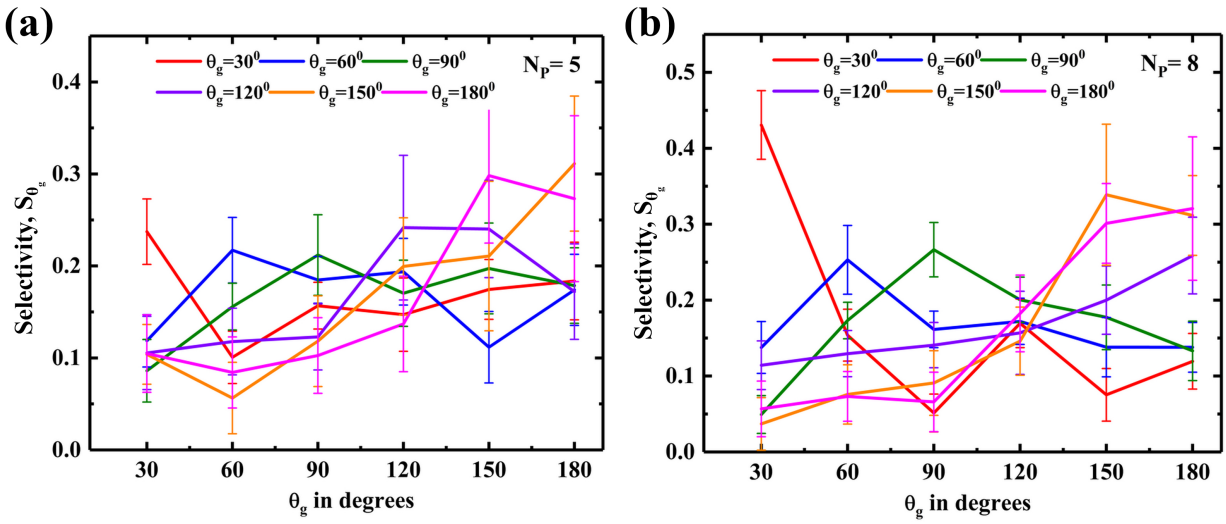

Figure S4: Selectivity data between nanoparticles for system containing an equimolar mixture of oppositely charged polyion grafted nanoparticles at different graft angles $\theta_g = 30°$, 60°, 90°, 120°, 150° and 180° at chain stiffness $k_\theta = 0$ for graft length (a) $N_P = 5$, and (b) $N_P = 8$.

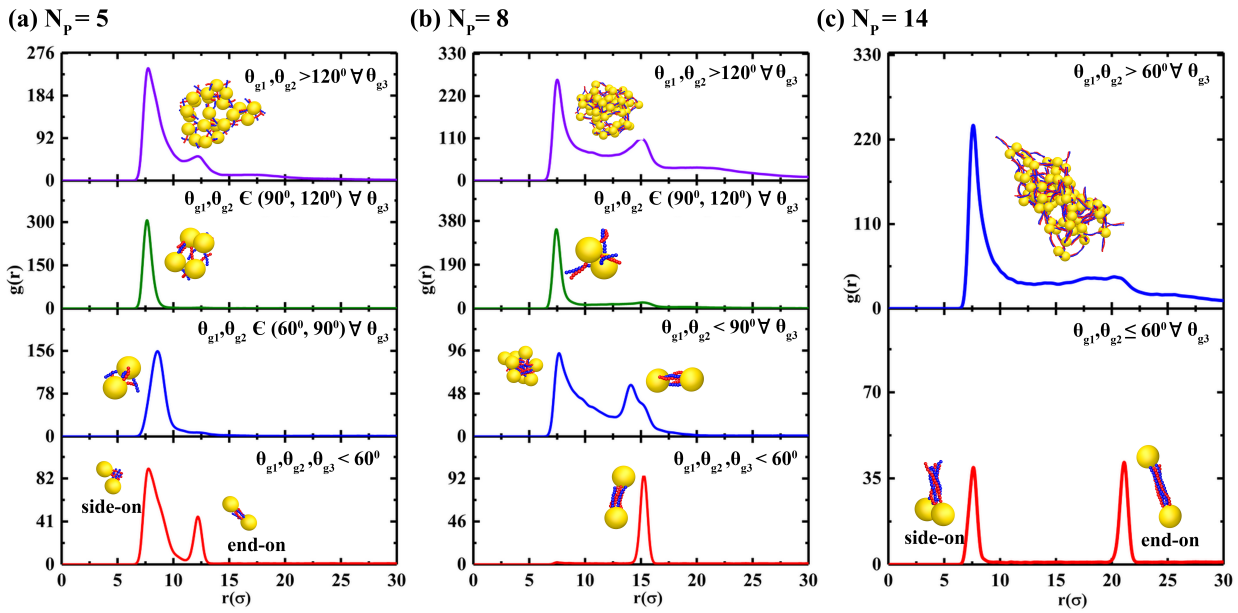

Figure S5: Pair correlation function ($g(r)$) between nanoparticles for grafting density $N_g = 3$ and chain stiffness $k_\theta = 20 k_B T/rad^2$ at graft length (a) $N_P = 5$, (b) $N_P = 8$ and (c) $N_P = 14$.

Quantifying morphologies using Python Code

The implementation of the algorithm is explained below

1. The first step involves calculating the number of nanoparticles that lie within the distance of $r_{cut} = 9.5\sigma$ from the center of the nanoparticle. Using this information we can classify the connected components into clusters containing different number of NPs

2. Morphologies containing only one nanoparticle (NP) i.e with zero neighbours within the cutoff distance r_{cut} are termed as dispersed

3. Morphologies containing only two NPs i.e. every NP in the morphology has only one neighbour within the cutoff distance (r_{cut}) are termed as 'dimers '.

4. Morphologies that contain even number of NPs with cluster size>2 where each of the NP possess only two neighbours within cutoff distance (r_{cut}) are termed as 'rings '

5. Morphologies that contain even/odd number of NPs with cluster size>2 where NPs present at the ends contain one neighbor and other NPs have two neighbours within cutoff distance (r_{cut}) are termed as Strings.

6. Morphologies that contain even/odd number of NPs with cluster size>2 which do not satisfy any of the above conditions are classified as 'aggregates '.

The code can be found on **GitHub** *Access here*[*]