

Electronic Supplementary Information

Coarse-grained simulation studies of the adsorption of polyelectrolyte complexes upon lipid membranes

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Table S1 Conformational characteristics of the free PECs

β	N_{PA}	N_{PC}	$R_{g,c}/nm$	$A_{r,c}$
0.83	250	300	2.66 ± 0.02	0.87 ± 0.01
1.0	250	250	2.57 ± 0.01	0.92 ± 0.01
1.2	300	250	2.74 ± 0.03	0.89 ± 0.01
1.4	350	250	2.95 ± 0.03	0.83 ± 0.01

- the average and standard errors are not affected by the initial polyion configurations in the simulation run.

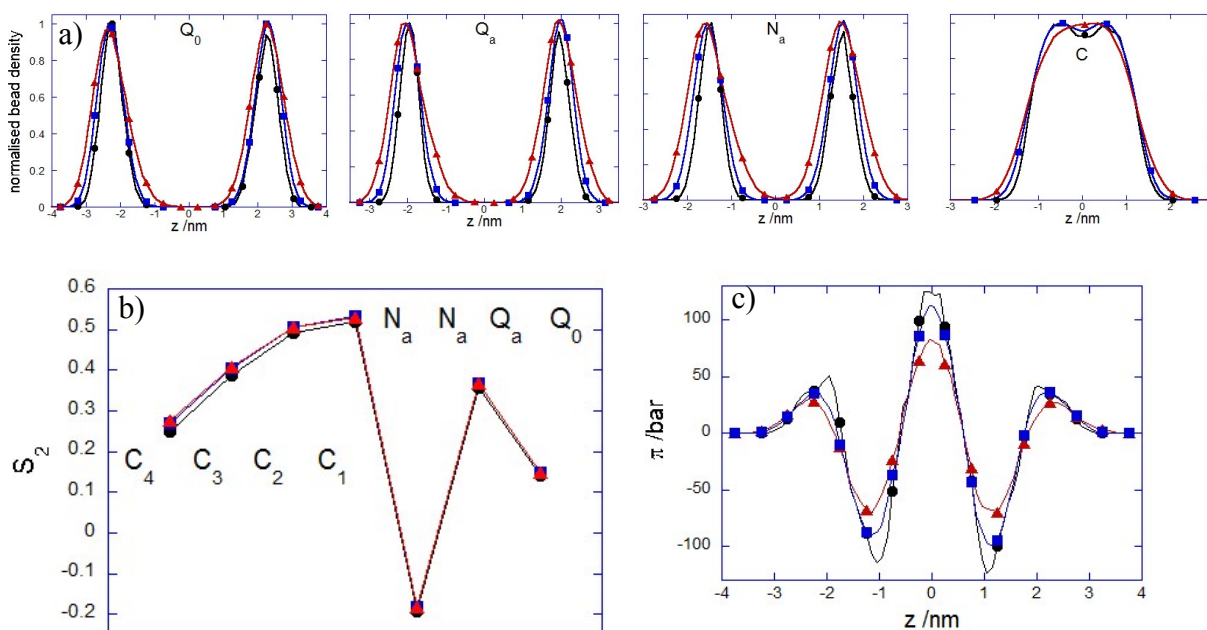


Fig. S1. a) Normalised densities of Q_0 , Q_a , N_a and C beads, b) S_2 order parameter and c) lateral pressure profile π for bilayer I (●), II (■) and III (□).

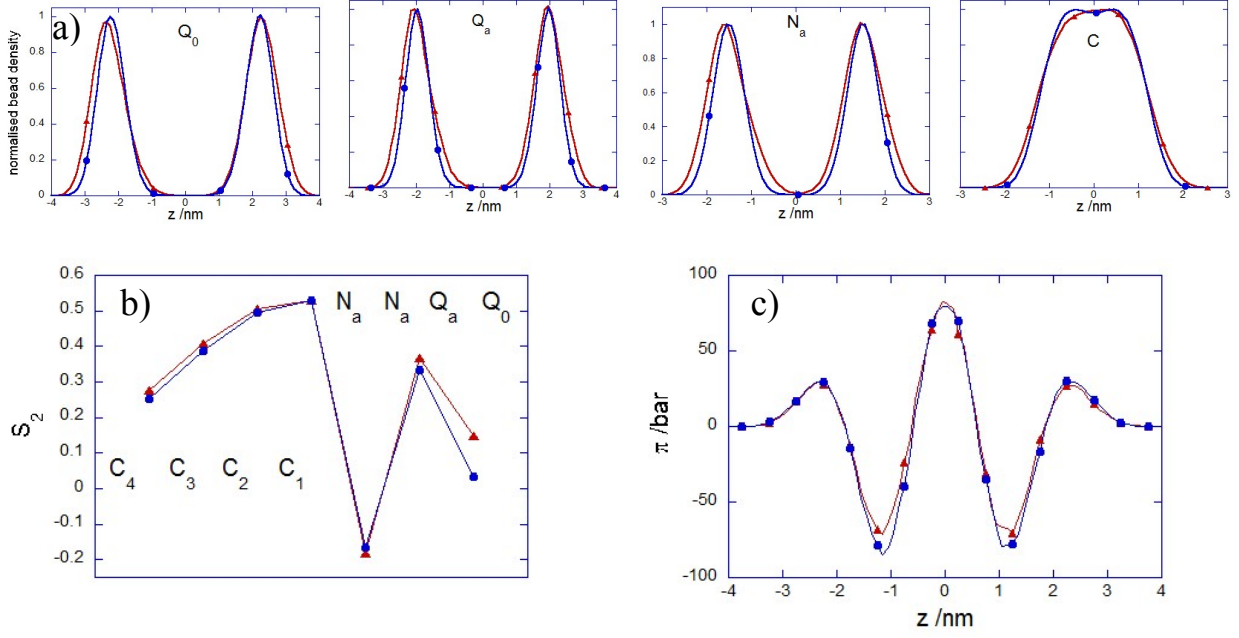


Fig. S2. Comparison of a) normalised densities of Q_0 , Q_a , N_a and C beads, b) orientational order parameter and c) lateral pressure profile of bilayer III at $r_{\text{cut,el}} = (\square)$ 15 and $(\bullet)$ 25 nm.

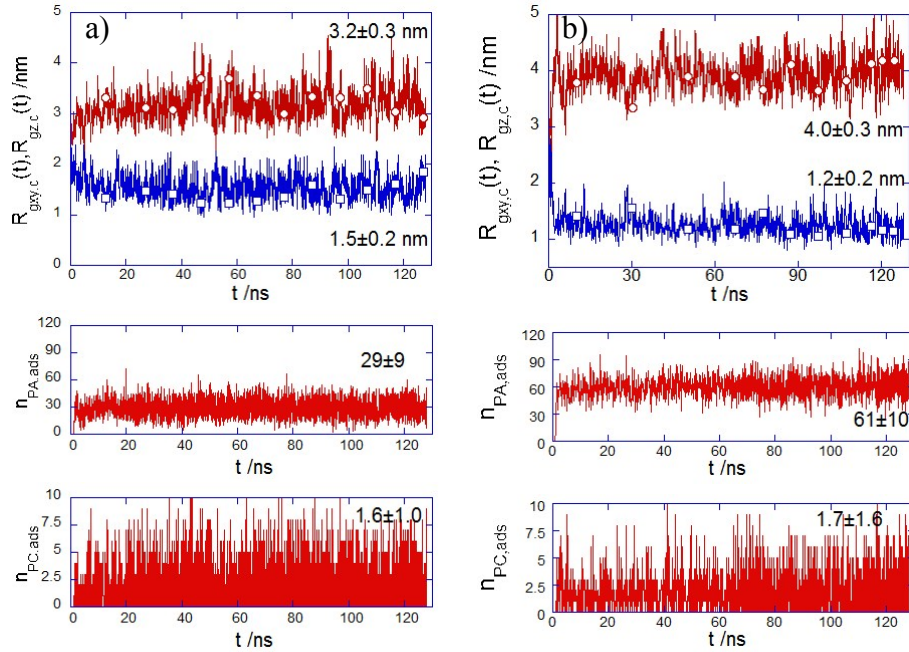


Fig. S3. $(\circ)R_{\text{gy},c}$ and $(\square)R_{\text{gz},c}$ projections of the radius of gyration and number of bound beads $n_{\text{PA,ads}}$ and $n_{\text{PC,ads}}$ for PEC with $\beta =$ a) 1.2 and b) 1.4 at $r_{\text{cut,el}} = 2.5$ nm. Averaged values over the last 40 ns time interval are given.

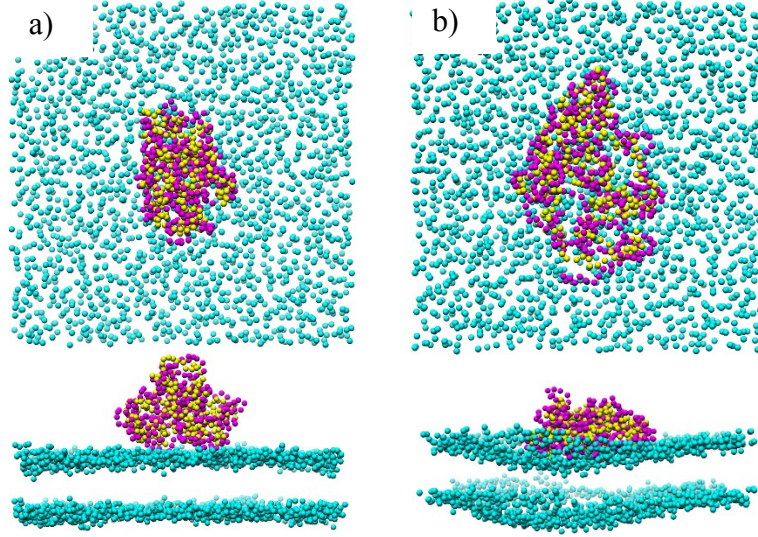


Fig. S4. Top and side-view snapshots of the final configuration of PEC with $\beta = 1.2$ and polyion 1.4 at $r_{\text{cut,el}} = 2.5$ nm; for clarity sake, only Q_0 group of DPPC is illustrated only and the color code is same as in Fig. 1

File: Movie S1.mp4

An animation created for the configuration of PEC with $\beta = 1.0$ bound to the bilayer **III** at $t = 11.0$ ns; Q_a , N_a and C beads of DPPC and all bonds are omitted.

File: Movie S2.mp4

An animation created for the configuration of PEC with $\beta = 1.2$ bound to the bilayer **III** at $t = 127.1$ ns; Q_a , N_a and C beads of DPPC and all bonds are omitted.

File: Movie S3.mp4

An animation created for the configuration of PEC with $\beta = 1.4$ bound to the bilayer **III** at $t = 127.9$ ns; Q_a , N_a and C beads of DPPC and all bonds are omitted.