Supplementary Materials: Polyelectrolyte-Nanoplatelet Complexation: Is it possible to predict the state diagram?

Maria Jansson [1,*] and Marie Skepö [1,2,*]

1. Composition of the PE-NP Complex

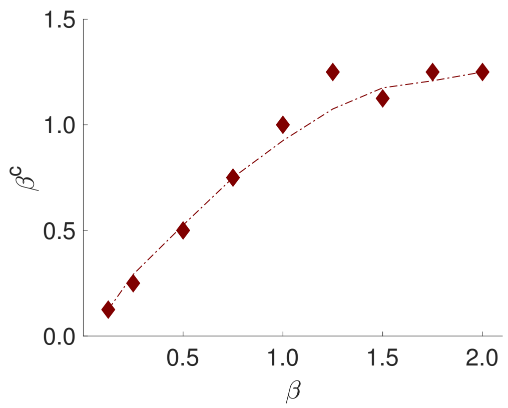


Figure S1. The complexed charge-ratio, β^c, as a function of the stoichiometric charge-ratio in the system, β. The dash-dotted line is an implemented smooth function.

2. Effect of PE Total Charge

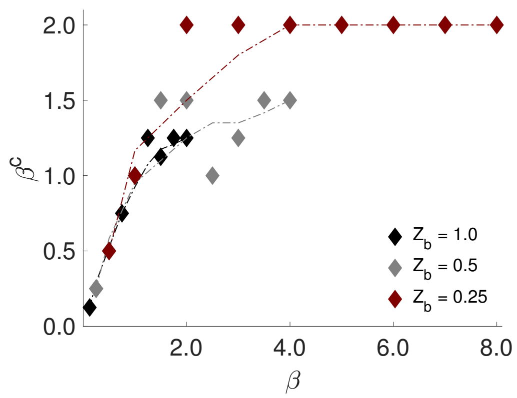


Figure S2. The complexed charge-ratio, β^c, as a function of the stoichiometric the charge-ratio, β, in the system. The dash-dotted lines are an implemented smooth function.

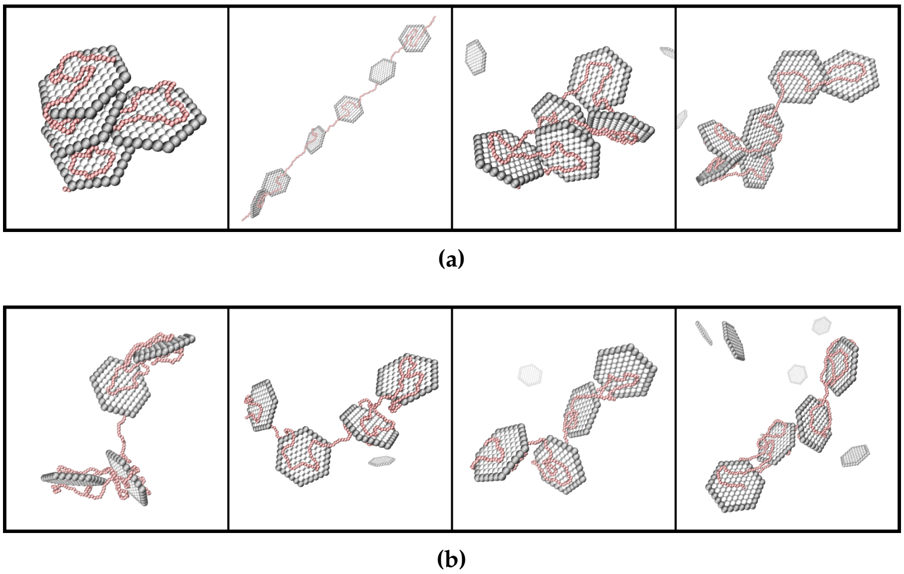


Figure S3. Representative snapshots of the structures with $\beta = 0.5$, 1.0, 1.5, and 2.0 (from left to right) for (a) $Z_b = 0.5$, and (b) $Z_b = 0.25$. The counterions are omitted for clarity, the NPs are shown in grey, and the PE is shown in red.

3. Effect of PE Flexibility

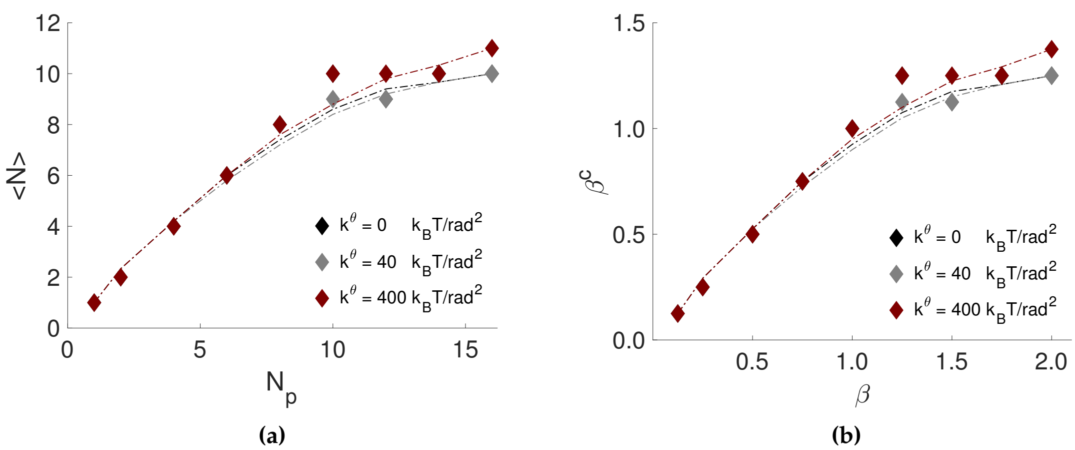
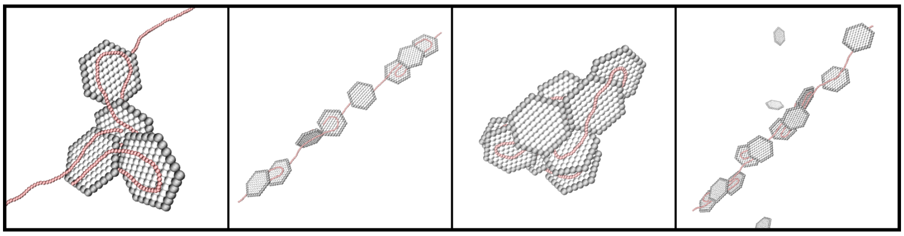


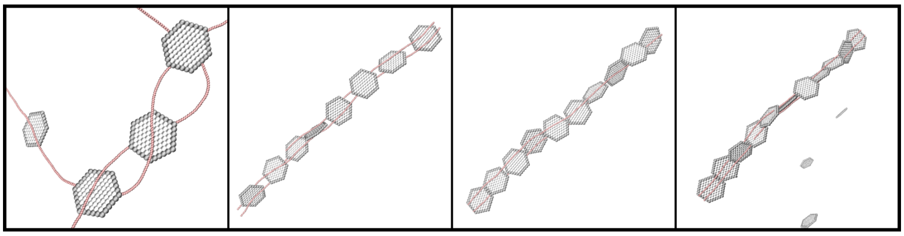
Figure S4. (a) The average number of NPs complexed to the PE, $\langle N \rangle$, as a function of the number of NPs, N_p. (b) The complexed charge-ratio, β^c, as a function of the stoichiometric charge-ratio, β, in the system. The dash-dotted lines are an implemented smooth function.

Table S1. Number of NPs, N_p, stoichiometric charge-ratio in the system, β, angular force constant, k^θ, complexed charge-ratio, β^c, average number of NPs complexed to the PE, $\langle N \rangle$, and normalised radii of gyration, R_g/R_g^0, for the effect of the PE flexibility. (The unit of k^θ is $k_\mathrm{B}T/\mathrm{rad}^2$).

N_p	β	k^θ	β^c	$\langle N \rangle$	R_g/R_g^0	k^θ	β^c	$\langle N \rangle$	R_g/R_g^0	k^θ	β^c	$\langle N \rangle$	R_g/R_g^0
1	0.13	0	0.13	1	0.89	40	0.13	1	0.94	400	0.13	1	0.92
2	0.25		0.25	2	0.77		0.25	2	0.83		0.25	2	0.81
4	0.50		0.50	4	0.66		0.50	4	0.62		0.50	4	0.76
6	0.75		0.75	6	0.66		0.75	6	0.61		0.75	6	0.60
8	1.00		1.00	8	0.13		1.00	8	0.60		1.00	8	1.03
10	1.25		1.25	10	0.65		1.13	9	0.15		1.25	10	1.02
12	1.50		1.13	9	0.13		1.13	9	0.17		1.25	10	1.03
14	1.75		1.25	10	0.65		1.25	10	0.61		1.25	10	1.03
16	2.00		1.25	10	0.65		1.25	10	0.66		1.38	11	1.01



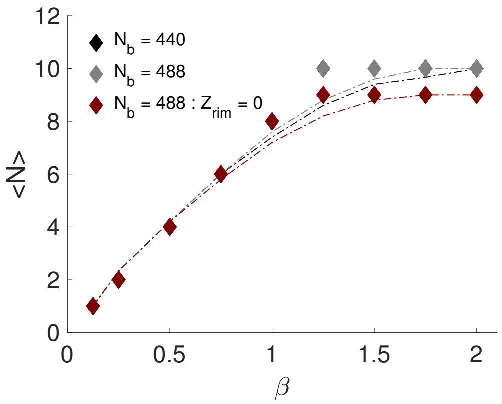
(a)



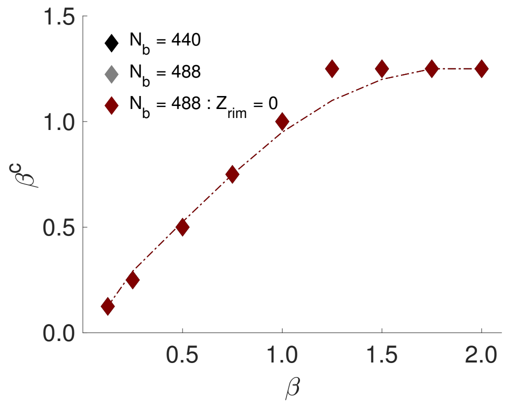
(b)

Figure S5. Representative snapshots of the structures with $\beta = 0.5$, 1.0, 1.5, and 2.0 (from left to right) for (a) $k^\theta = 40\ k_\mathrm{B}T/\mathrm{rad}^2$, and (b) $k^\theta = 400\ k_\mathrm{B}T/\mathrm{rad}^2$. The counterions are omitted for clarity, the NPs are shown in grey, and the PE is shown in red.

4. Effect of NP Charge and Rim



(a)



(b)

Figure S6. (a) The average number of NPs complexed to the PE, $\langle N \rangle$, as a function of the number of NPs, N_p. (b) The complexed charge-ratio, β^c, as a function of the stoichiometric the charge-ratio, β, in the system. The dash-dotted lines are an implemented smooth function.

Table S2. Number of NPs, N_p, stoichiometric charge-ratio in the system, β, complexed charge-ratio, β^c, number of PE beads, N_b, average number of NPs complexed to the PE, $\langle N \rangle$, and normalised radii of gyration, R_g/R_g^0, for the effect of the NP charge and rim.

N_p	β	β^c	N_b	$\langle N \rangle$	R_g/R_g^0	N_b	$\langle N \rangle$	R_g/R_g^0	N_b	$\langle N \rangle$	R_g/R_g^0
1	0.13	0.13	440	1	1.01	488	1	1.01	488	1	0.94
2	0.25	0.25		2	0.92		2	0.92	with $Z_\mathrm{rim} = 0$	2	0.78
4	0.50	0.5		4	0.53		4	0.53		4	0.38
6	0.75	0.75		6	0.34		6	0.34		6	0.16
8	1.00	1.00		8	0.14		8	0.14		8	0.12
10	1.25	1.25		10	0.13		10	0.13		9	0.12
12	1.50	1.25		9	0.13		10	0.13		9	0.12
14	1.75	1.25		10	0.13		10	0.13		9	0.12
16	2.00	1.25		10	0.13		10	0.13		9	0.13

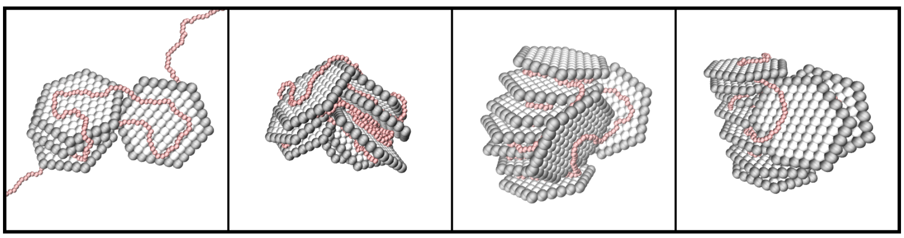


Figure S7. Representative snapshots of the structures with $\beta = 0.5$, 1.0, 1.5, and 2.0 (from left to right) for $N_\mathrm{b} = 488$ with $Z_\mathrm{rim} = 0$. The counterions are omitted for clarity, the NPs are shown in grey, and the PE is shown in red.