Supporting Information: Formation Mechanism and Properties of Polyelectrolyte Multilayer-Supported Lipid Bilayers: A Coarse-Grained Molecular Dynamics Study

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Supporting Figures

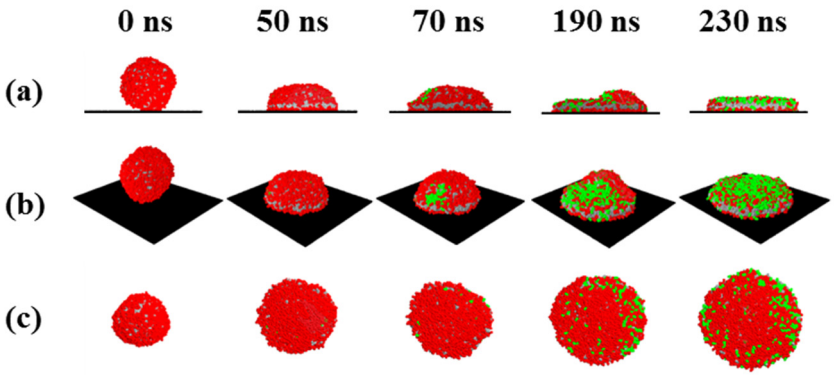

Figure S1. Snapshots of a vesicle composed of 1600 lipids spreading on a hydrophilic solid substrate via a receding-top mechanism, viewed from different directions: (a) side view, (b) top view, and (c) bottom view.

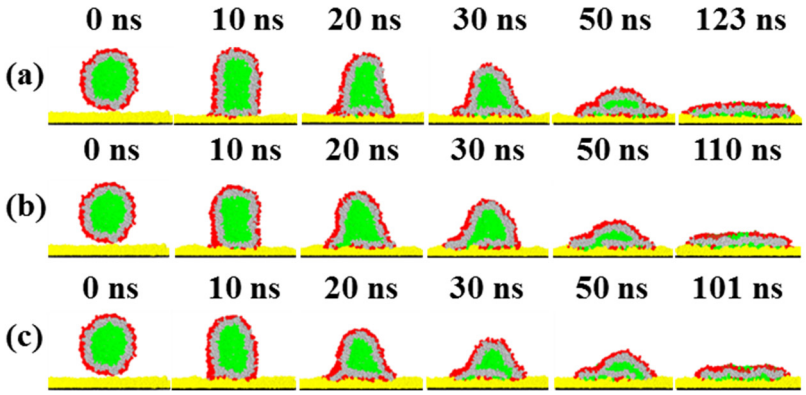

Figure S2. Time evolution of vesicles spreading on $(CHI/ALG)_2$-cushions composed of (a) 50, (b) 60, and (c) 70 CHI polymer chains and same amount of ALG chains. Half of the ALG chains are constrained to the solid surface via harmonic potentials.

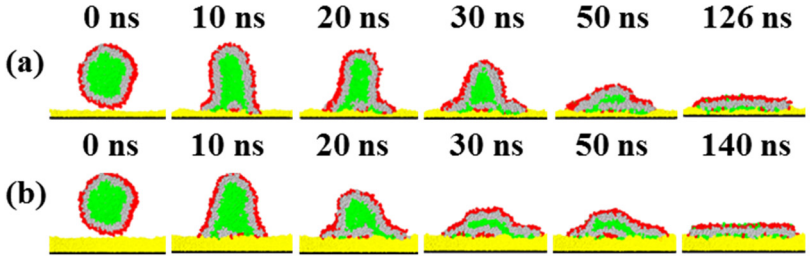

Figure S3. Time evolution of vesicles spreading on (a) one layered $(CHI/ALG)_1$-cushions and (b) three layered $(CHI/ALG)_3$-cushions. Each layer is composed of 35 CHI and 35 ALG polymer chains.

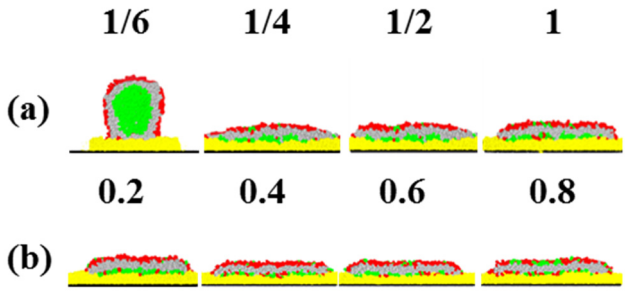

Figure S4. Outcomes of vesicles spreading on $(CHI/ALG)_2$-cushions with reduced charges. (a) The number of charged beads of both CHI and ALG polymer chains is reduced by a factor of 1/6, 1/4, 1/2, or 1 with each bead carrying one unit of charge. (b) The numbers of charged bead of CHI and ALG polymer chains are same but each bead carries a fractional charge of value 0.2, 0.4, 0.6, or 0.8.

Table S1. CG bead types and bond parameters of CHI and ALG polymers.

atoms(CHI)		bonds				angles				
i	type	i	j	length nm	K_{bond} kJ mol^{-1} nm^{-2}	i	j	k	angle	K_{angle} kJ mol^{-1}
1	P1	1	2	0.33	640	2	1	3	88.5	25
2	P2	1	3	0.28	640	1	2	3	41.5	25
3	Qd	2	3	0.43	640	1	3	2	49.5	25
4	P1	3	4	0.40	320	1	3	4	132.5	25
5	P2	4	5	0.37	640	2	3	4	83.5	25
6	Qd	4	6	0.28	640	3	4	5	66.5	25
		5	6	0.44	640	3	4	6	81.5	25
		6	7	0.40	320	5	4	6	91.5	25
		7	8	0.30	640	4	5	6	40.5	25
		7	9	0.27	640	4	6	5	50.5	25
		8	9	0.43	640	4	6	7	124.5	25
		9	10	0.40	320	5	6	7	91.5	25
		10	11	0.31	640	6	7	8	68.5	25
		10	12	0.27	640	6	7	9	152.5	25
		11	12	0.43	640	8	7	9	100.5	25
		12	13	0.39	320	7	8	9	38.5	25
		13	14	0.30	640	7	9	8	41.5	25
		13	15	0.27	640	7	9	10	126.5	25
						8	9	10	90.5	25
						9	10	11	68.5	25
						9	10	12	155.5	25
						11	10	12	91.5	25
						10	11	12	39.5	25
						10	12	11	49.5	25
						10	12	13	125.5	25
						11	12	13	90.5	25
						12	13	14	75.5	25
						12	13	15	153.5	25
						14	13	15	97.5	25
						13	14	15	39.5	25
						13	15	14	41.5	25
						13	15	16	114.5	25

atoms(ALG)		bonds				angles				
i	type	i	j	length nm	K_{bond} kJ mol^{-1} nm^{-2}	i	j	k	angle	K_{angle} kJ mol^{-1}
1	Qa	1	2	0.34	640	2	1	3	43.5	25
2	P4	1	3	0.29	640	1	2	3	57.5	25
3	P1	2	3	0.23	640	1	3	2	79.5	25
4	Qa	3	4	0.33	320	1	3	4	153.5	25
5	P4	4	5	0.35	640	2	3	4	100.5	25
6	P1	4	6	0.23	640	3	4	5	81.5	25
		5	6	0.28	640	3	4	6	110.5	25
		6	7	0.33	320	5	4	6	52.5	25
		7	8	0.35	640	4	5	6	42.5	25
		7	9	0.28	640	4	6	5	84.5	25
		8	9	0.23	640	4	6	7	103.5	25
		9	10	0.33	320	5	6	7	117.5	25
		10	11	0.35	640	6	7	8	71.5	25
		10	12	0.23	640	6	7	9	109.5	25
		11	12	0.28	640	8	7	9	41.5	25
		12	13	0.33	320	7	8	9	52.5	25
		13	14	0.34	640	7	9	8	84.5	25
		13	15	0.28	640	7	9	10	154.5	25
						8	9	10	124.5	25
						9	10	11	85.5	25
						9	10	12	110.5	25
						11	10	12	52.5	25
						10	11	12	41.5	25
						10	12	11	85.5	25
						10	12	13	154.5	25
						11	12	13	116.5	25
						12	13	14	71.5	25
						12	13	15	110.5	25
						14	13	15	41.5	25
						13	14	15	52.5	25
						13	15	14	85.5	25
						13	15	16	102.5	25