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Electronic Supplementary Information

Surface tension effects on the phase transition of a DPPC bilayer with and without protein: A molecular dynamics simulation†

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Simulated annealing simulations

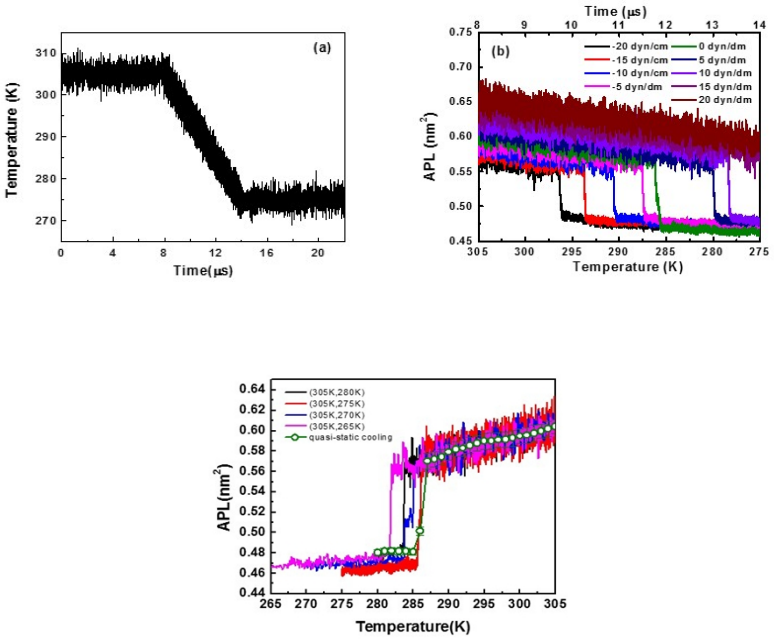

Fig. S1 Simulated annealling simulations were run to determine the range of temperature and surface tension among which the phase transition may occur. During a simulated annealing simulation, the system was first equilibrated for 8 μs under a higher temperature (305 K), at which the bilayer was in a liquid crystal phase. Then the coupling temperature was linearly reduced to 275 K within 6 μs to bring the lipid bilayer into a gel phase. Temperature change during a typical simulated annealing is shown in (a). (b) gives the change of area per lipid (APL) during the annealing period. (c) gives a comparasion of simulated annealing with different cooling speed and with the "quasi-static" cooling method proposed by Rodgers JM *et al* (ref 21 in main text). This shows the simulated annealing is capable of determining temperature range for the phase transition.

Summary for Equilibrium Simulations

Table S1 Simulation summary

	DPPC bilayer	AqpZ embedded DPPC bilayer
DPPC beads number	216	160
W beads number	3778	3759
AqpZ beads number	0	474
	6370	6153
Considered Temperatures (K)	275,280,285,290,295,300,305	
Considered Surface tension (dyn/cm)	±50, ±40, ±30, ±25,±20, ±15, ±10, ±5, 0	

RMSD of Protein

Table S2 RMSD of Protein backbone beads at temperature 290K

Surface tension (dyn/cm)	RMSD (nm)	Standard deviation(nm)
-50	0.21	0.02
-10	0.20	0.02
0	0.22	0.02
10	0.23	0.02
50	0.21	0.02