

Supplementary Information for “Lateral electric field inhibits gel-to-fluid transition in lipid bilayers”

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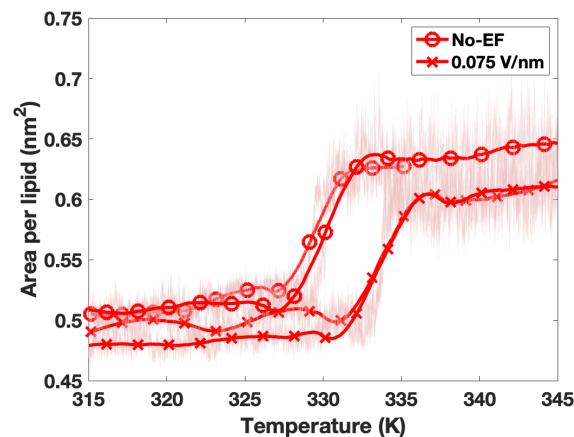
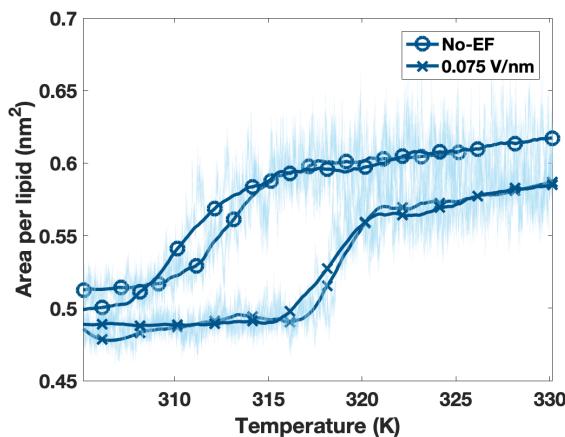


Figure S1: APL evolution obtained from repeat (a) cooling and (b) heating simulations of DPPC lipid bilayer. Details of the phase transition temperatures are provided in Table 3. Phase transition temperature was shifted by ~ 6 K and ~ 4.5 K in cooling and heating simulations, respectively upon application of 0.075 V/nm external electric field.

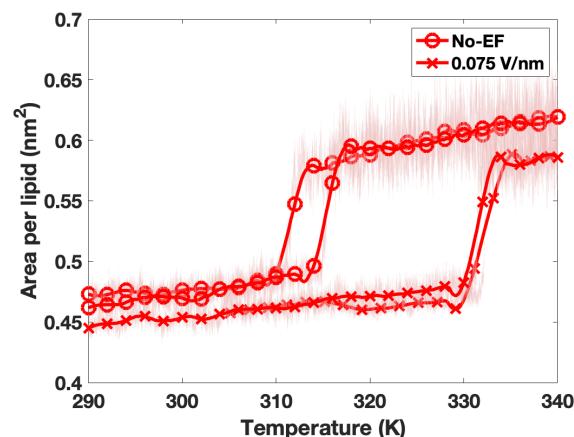
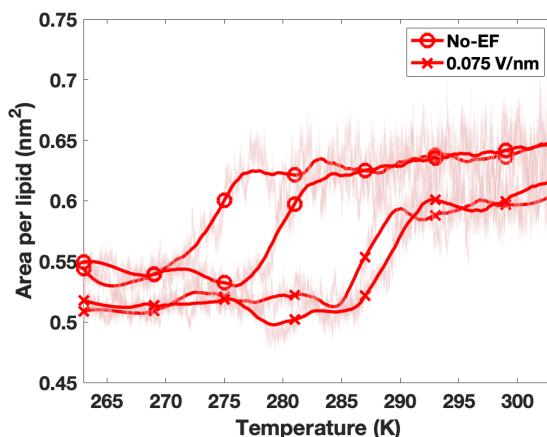


Figure S2: APL evolution obtained from repeat heating simulations of (a) POPC and (b) POPE lipid bilayers. Details of the phase transition temperatures are provided in Table 3. Phase transition temperature was shifted by ~ 13 K and ~ 16 K in POPC and POPE simulations, respectively upon application of 0.075 V/nm external electric field.

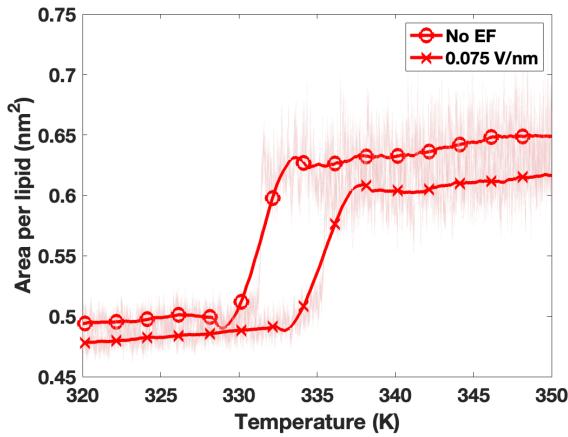


Figure S3: Phase transition temperature of DPPC bilayer system in the presence of 0.150 M KCl salt and lateral electric field. When 0.150 M KCl is added to the bilayer, the phase transition temperature was shifted by ~ 1.83 K to 331.43 K for system without electric field. Similarly, phase transition temperature of system with 0.150 M KCl and 0.075 V/nm lateral electric field was shifted by ~ 1.64 K to 335.43 K.

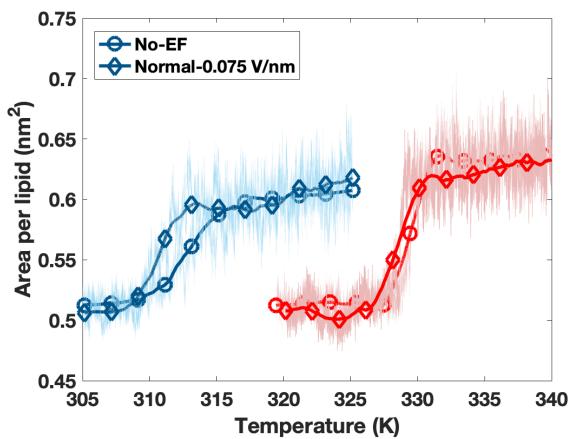


Figure S4: Normal electric field does not shift phase transition temperature in DPPC bilayers. The phase transition shift is uniquely induced by lateral electric field.

System	Lipids per leaflet	Time (ns)	Temperature (K)	EF (V/nm)
DPPC	48	300	293	0.0
DPPC	48	300	303	0.0
DPPC	48	300	313	0.0
DPPC	48	300	323	0.0
DPPC	48	300	333	0.0
DPPC	48	300	343	0.0
DPPC	48	300	293	0.05
DPPC	48	300	303	0.05
DPPC	48	300	313	0.05
DPPC	48	300	323	0.05
DPPC	48	300	333	0.05
DPPC	48	300	343	0.05
DPPC	48	300	293	0.075
DPPC	48	300	303	0.075
DPPC	48	300	313	0.075
DPPC	48	300	323	0.075
DPPC	48	300	333	0.075
DPPC	48	300	343	0.075
DPPC	48	300	293	0.10
DPPC	48	300	303	0.10
DPPC	48	300	313	0.10
DPPC	48	300	323	0.10
DPPC	48	300	333	0.10
DPPC	48	300	343	0.10
POPC	48	400	253	0.0
POPC	48	400	253	0.075
POPE	48	400	290	0.0
POPE	48	400	290	0.075
DPPC-Normal EF	48	400	345	0.0
DPPC-Normal EF	48	400	345	0.075

Table S1: Summary of equilibrium simulations at constant temperature. Electric field was applied laterally, parallel to the bilayer-water interface, except for Normal-EF systems in which electric field was applied perpendicular to the bilayer-water interface. More lipids were used in normal EF systems since smaller patches do not show electroporation associated with normal-EF.

System	Lipids per leaflet	Rate (K/ns)	Time (ns)	EF (V/nm)	Number of simulations
DPPC	48	+0.05	800	0.0	2
DPPC	48	+0.05	1000	0.075	2
DPPC	48	-0.05	800	0.0	2
DPPC	48	-0.05	1000	0.075	2
POPC	48	+0.05	1000	0.0	2
POPC	48	+0.05	1000	0.075	2
POPE	48	+0.05	1000	0.0	2
POPE	48	+0.05	1000	0.075	2
DPPE	48	+0.05	1000	0.0	2
DPPE	48	+0.05	1000	0.075	2
DPPC-Normal EF	48	+0.05	1000	0.075	2
DPPC-Normal EF	48	-0.05	1000	0.075	2
DPPC-(0.150 M KCl)	48	+0.05	1000	0.0	2
DPPC-(0.150 M KCl)	48	-0.05	1000	0.075	2

Table S2: Summary of heating (+ sign) and cooling (– sign) simulations. Electric field was applied laterally, parallel to the bilayer-water interface, except for Normal-EF systems in which electric field was applied perpendicular to the bilayer-water interface.