Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Self Assembly of Phospholipids on Model Supports

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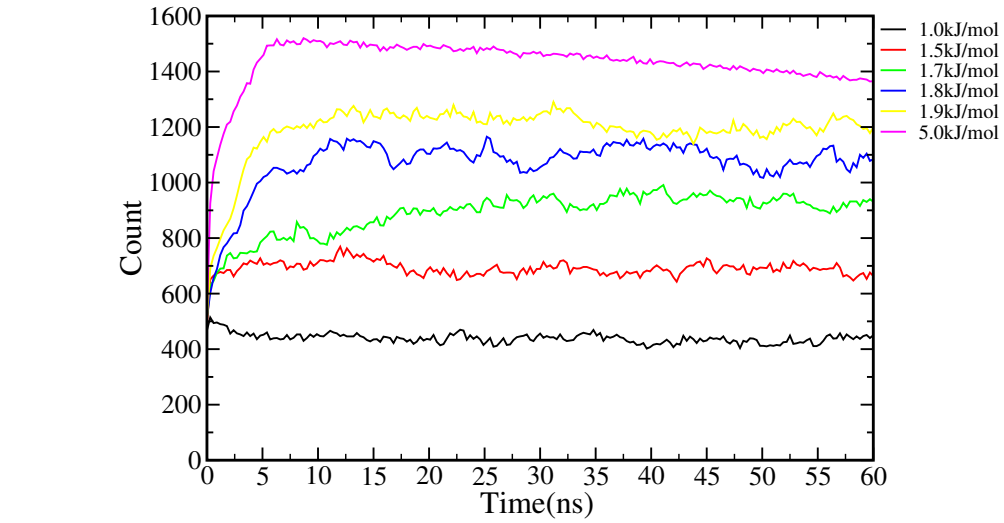
Table S 1: Non-bonded interaction strength (ϵ_{ij} in kJ/mol) between the particles for system Hb3.

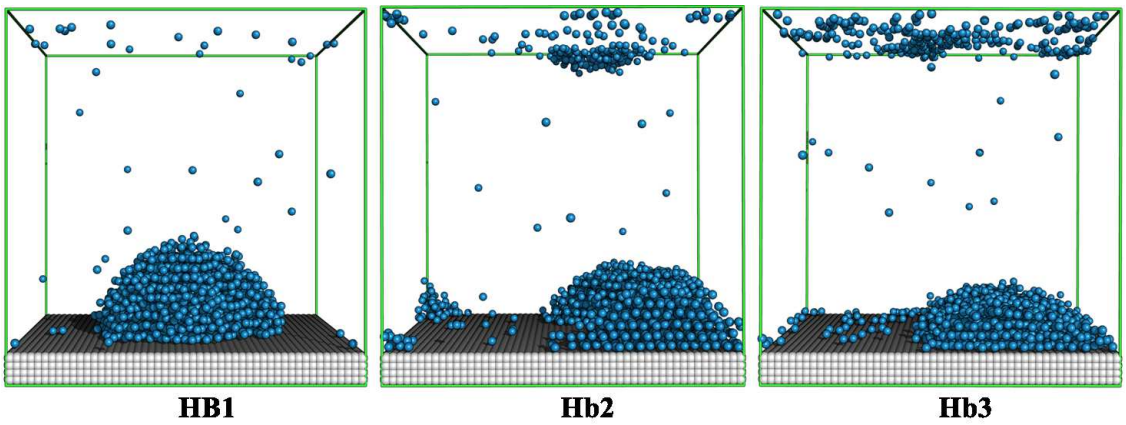
System	Support	Water	Head	Tail
Support	-	1.7	1.42	3.5
Water	1.7	3.8	5	2
Head	1.42	5	3.5	2
Tail	3.5	2	2	3.5

Table S 2: Diffusion coefficient

	DPPC $\times 10^{-7}\ cm^2/s$	$NC3_{lower}$ $\times 10^{-7}\ cm^2/s$	$NC3_{upper}$ $\times 10^{-7}\ cm^2/s$
Hb1	1.21±0.16	1.05±0.18	1.27±0.08
Hb2	1.10±0.20	1.02±0.17	1.13±0.18
Hb3	1.09±0.25	0.95±0.15	1.17±0.11
Hl1	0.95±0.21	0.64±0.28	1.11±0.18
Hl2	0.81±0.15	0.451±0.09	1.01±0.12
Hl3	0.59±0.07	0.23±0.05	0.82±0.11
Mhl1	0.70±0.11	0.437±0.10	0.80±0.09
Mhl2	0.55±0.06	0.20±0.03	0.74±0.05



(a)



(b)

Figure S 1: a) Water beads count near the support b) final snapshots after 60 ns simulation .

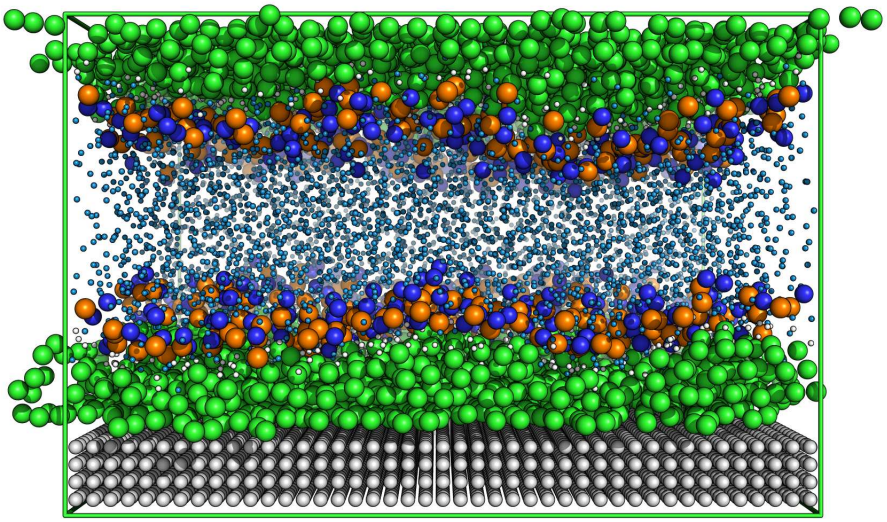
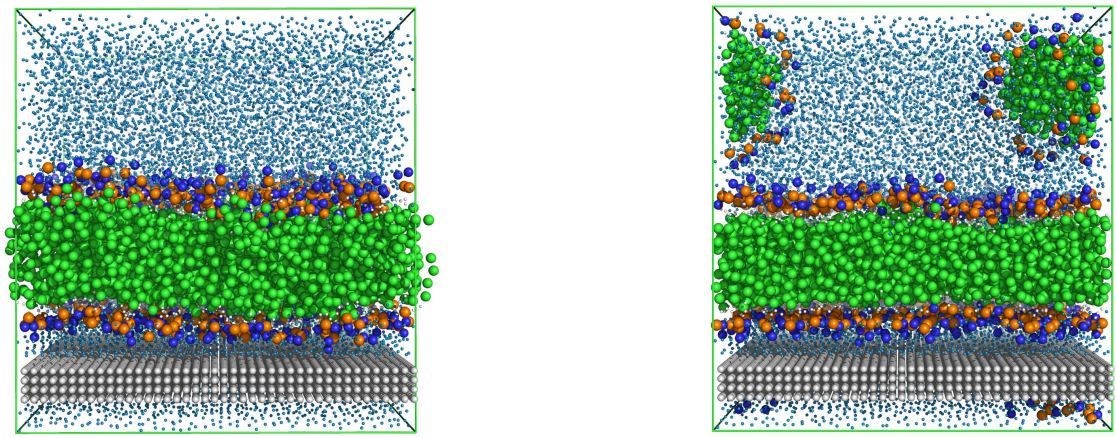


Figure S 2: Final snapshots after 1μs simulation.



(a) (b)

Figure S 3: Snapshots of a) initial and b) final configurations after 500 ns.

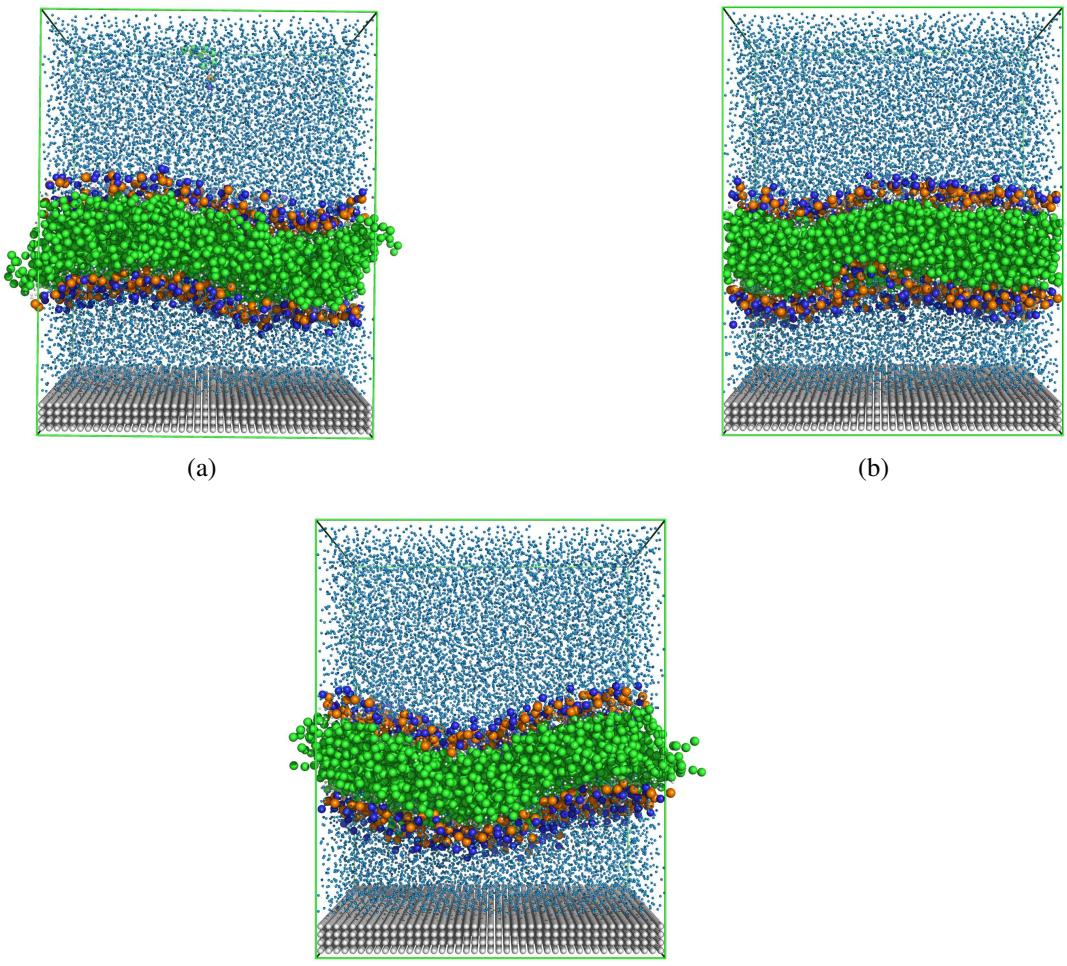


Figure S 4: Snapshots after 80ns for the systems a) Hl1, b)Hl2 and c) Hl3 respectively.

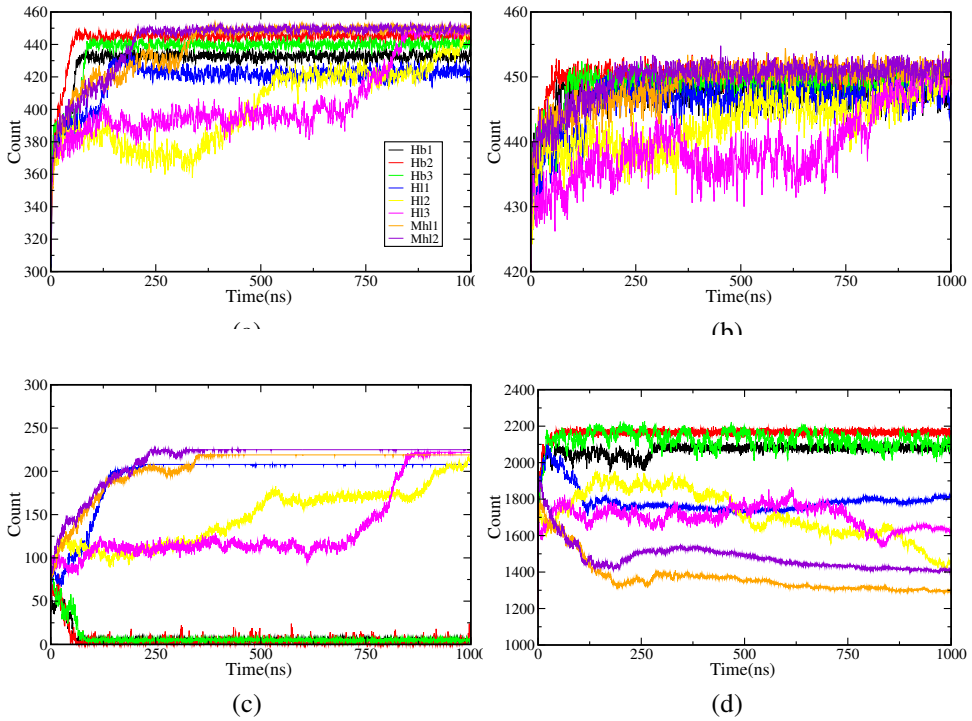


Figure S 5: Number of beads within 0.9 nm distance cut-off of intra a) NC3 bead and b) C1 beads distances as a function of simulation time. Figure c and d shows the number of NC3 and W beads near the support respectively.

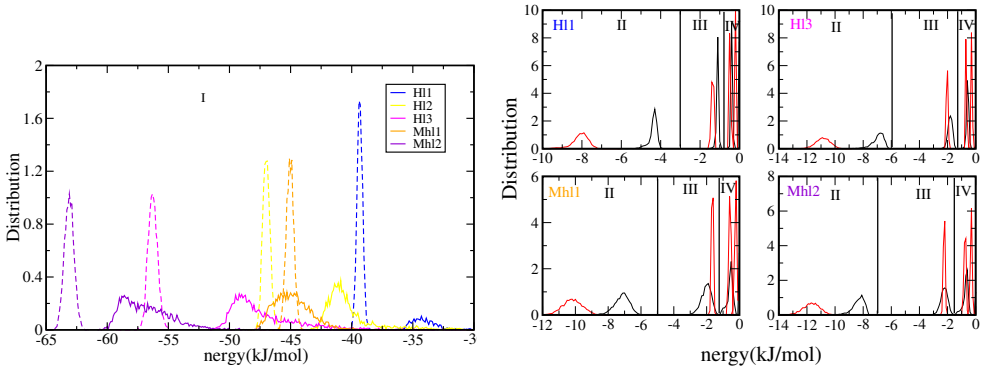


Figure S 6: Potential energies between water-water beads. a) Potential energies between the water beads falling in region I of 0-0.5 nm from support surface. Dotted and solid lines represents W-S and NC3-S interaction energies respectively and colors blue, yellow, magenta, orange and violet represents Hl1, Hl2, Hl3,Mhl1 and Mhl2 systems respectively b) Potential energy within regions II, III and IV. Color red is W-S and black is NC3-S LJ energies.

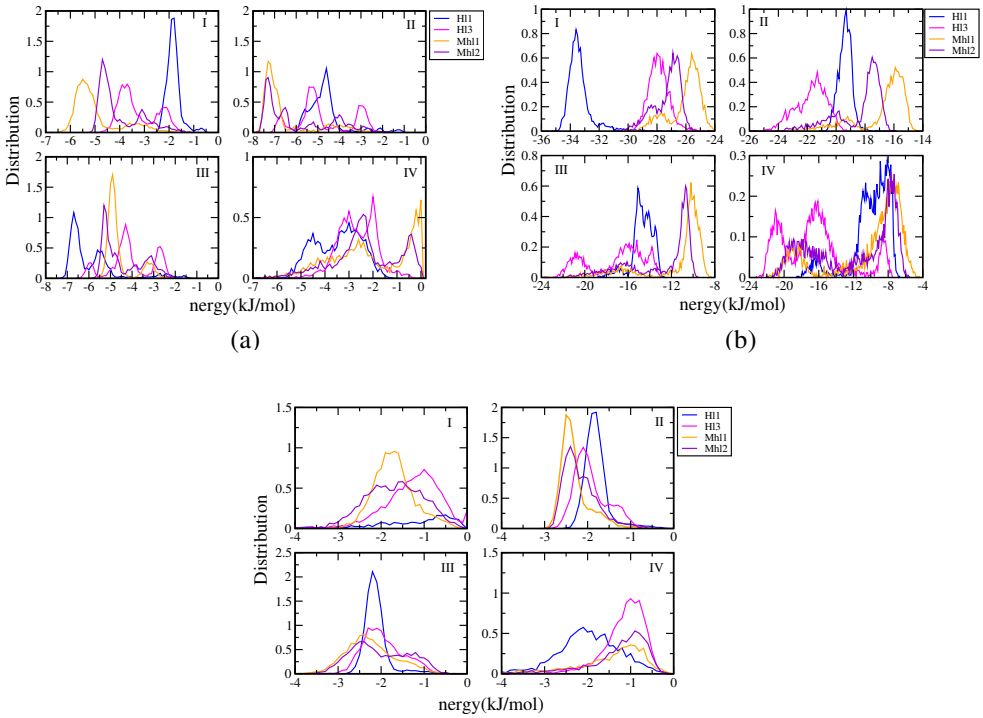


Figure S 7: Potential energy between a) NC3-water beads, b) water-water beads and c) NC3-NC3 beads respectively. Colors blue, magenta, orange and violet represents systems Hl1, Hl3, Mhl1 and Mhl2 respectively