Electronic Supplementary Information

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

Xian Konga, Shanshan Qinb, Diannan Lu*a, Zheng Liua

a Department of Chemical Engineering, Tsinghua University, Beijing, 100084, China.
E-mail: *ludiannan@tsinghua.edu.cn; liuzheng@mail.tsinghua.edu.cn.
b Key Laboratory of Bioorganic Phosphorous Chemistry and Chemical Biology (Ministry of Education), Department of Chemistry, Tsinghua University, Beijing 100084, P. R. China.

Simulated annealing simulations

Fig. S1 Simulated annealing 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 comparison 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

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

**RMSD of Protein**

Table S2 RMSD of Protein backbone beads at temperature 290K

<table>
<thead>
<tr>
<th>Surface tension (dyn/cm)</th>
<th>RMSD (nm)</th>
<th>Standard deviation(nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-50</td>
<td>0.21</td>
<td>0.02</td>
</tr>
<tr>
<td>-10</td>
<td>0.20</td>
<td>0.02</td>
</tr>
<tr>
<td>0</td>
<td>0.22</td>
<td>0.02</td>
</tr>
<tr>
<td>10</td>
<td>0.23</td>
<td>0.02</td>
</tr>
<tr>
<td>50</td>
<td>0.21</td>
<td>0.02</td>
</tr>
</tbody>
</table>