

Supporting Information

Directional Extraction and Penetration of Phosphorene Nanosheets to Cell Membranes

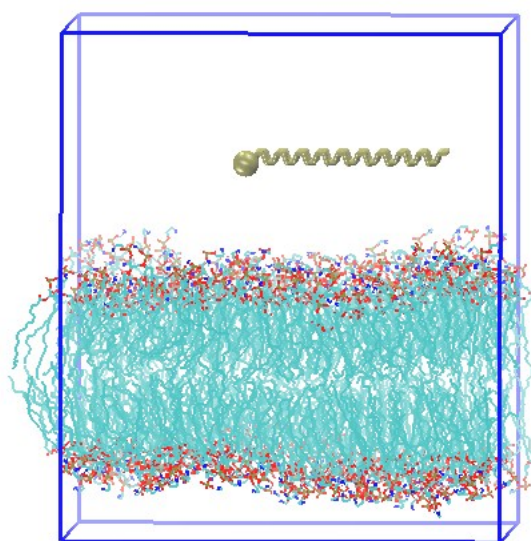


Figure S1. Side view of the configuration of one example system (the phosphorene shown as a tan-bonded sheet above the membrane). The large sphere marked at one corner is the restrained phosphorous atom. For clarity the water molecules are not shown.

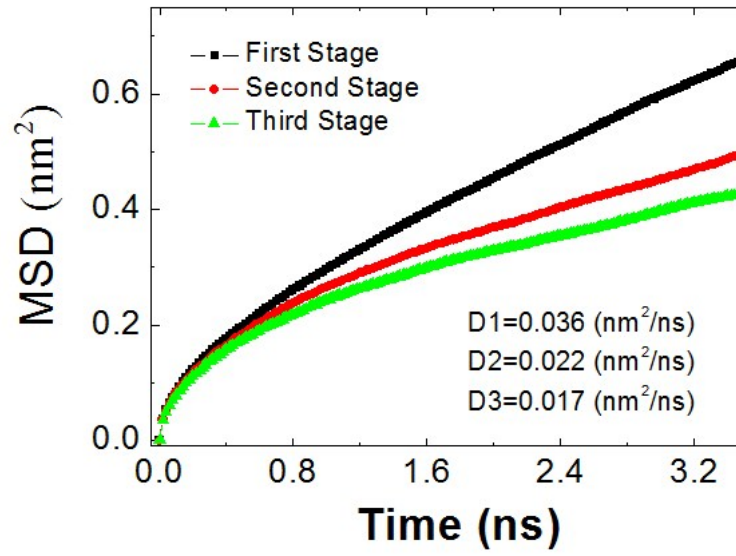
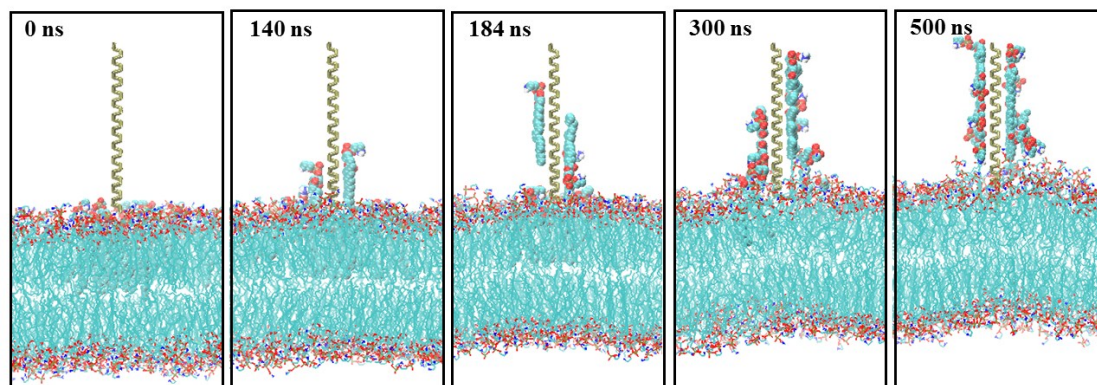


Figure S2. The lateral mean square displacement (MSD) and the lateral diffusion coefficient of lipid molecules in the first, second and third stages.

The relationship between lateral MSD and the lateral diffusion coefficient D_{lat} of lipid molecules is $MSD = 4D_{lat}t$. The lateral diffusion coefficient D_{lat} can be obtained from the slope of the lateral MSD versus time: $D_{lat} = MSD/4t$. We calculated the lateral diffusion coefficient D_{lat} of lipid molecules using the lateral MSD data ranging from 1.6ns to 3.3ns.

(a)



(b)

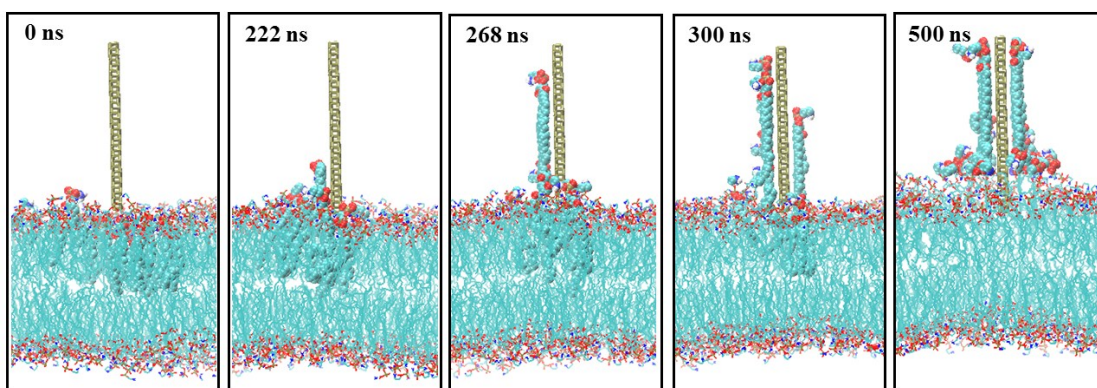


Figure S3. Two representative simulated trajectories of lipid extraction by strained phosphorene for (a) Model I and (b) Model II. The snapshot times are shown in the top left corner of each panel. Extracted lipid molecules are shown as larger spheres. The phosphorene sheet is shown as a tan-bonded sheet. For clarity the water molecules are not shown.

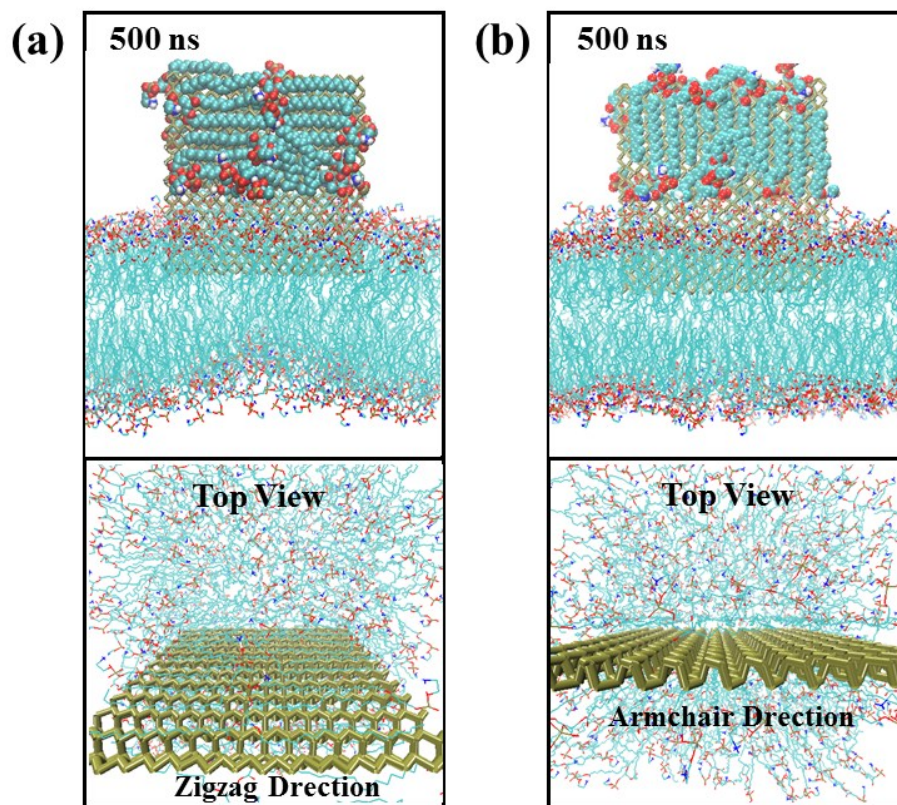


Figure S4. Lipid extraction by larger strained phosphorene whose (a) zigzag and (b) armchair direction are placed in a direction parallel to the surface of the membrane.

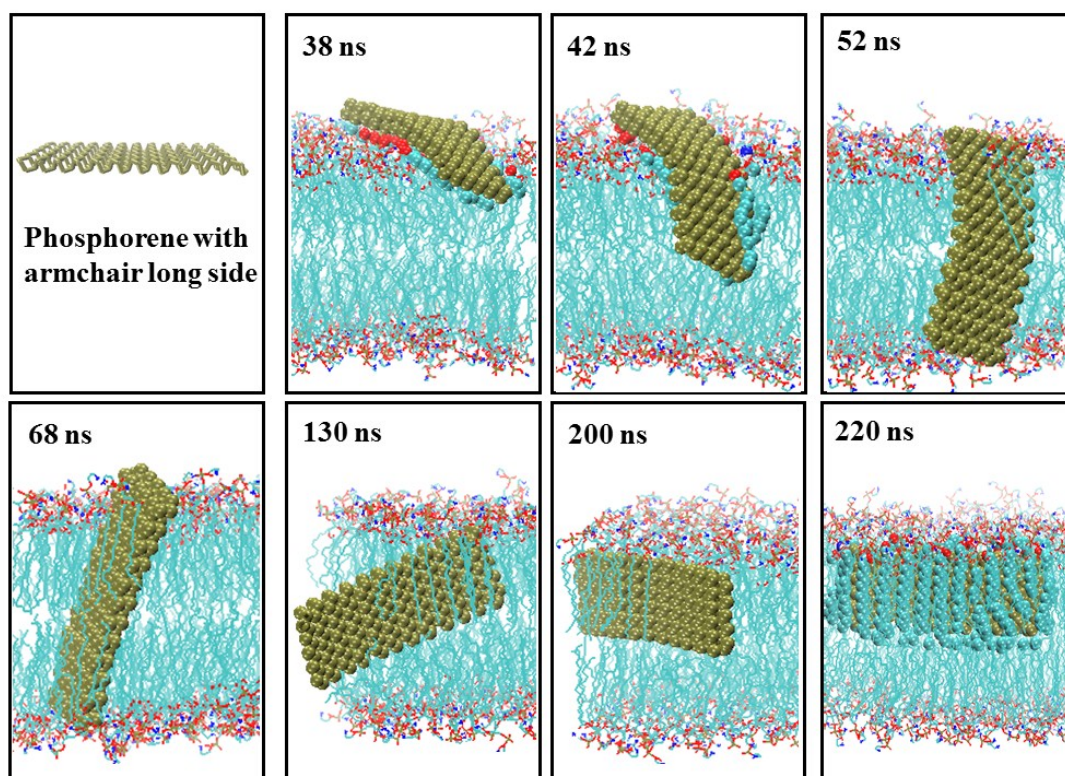


Figure S5. The representative simulated trajectories of insertion into the membrane of a rectangular phosphorene nanosheet with armchair long side.

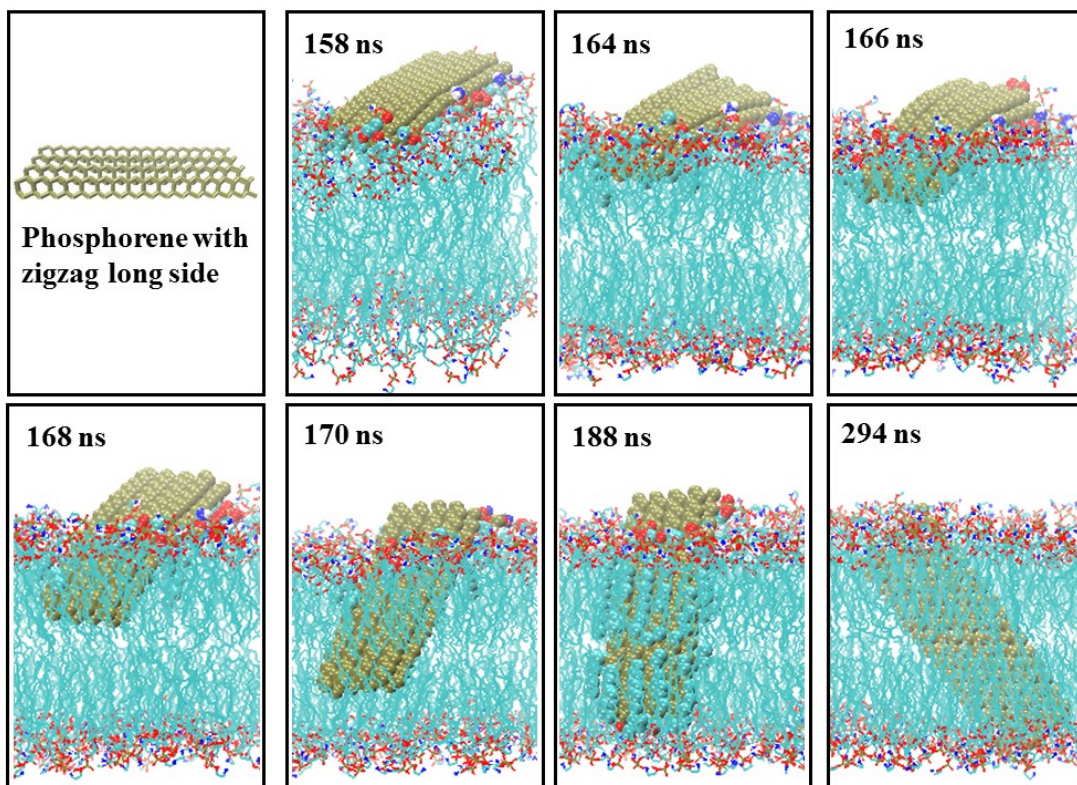


Figure S6. The representative simulated trajectories of insertion into the membrane of a rectangular phosphorene nanosheet with zigzag long side.

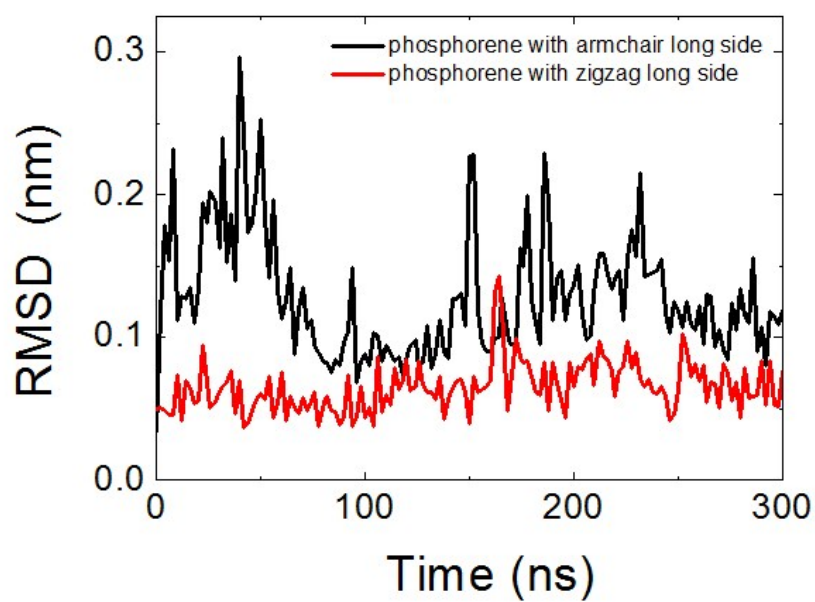


Figure S7. Time evolution of the RMSD of phosphorene with armchair and zigzag long side.

Figure S7 shows that the RMSD of phosphorene nanosheet with armchair long side is larger than that with zigzag long side, indicating that the former has a softer surface.