Supporting Information

Mild Lipid Extraction and Anisotropic Cell Membrane Penetration of α-Phase Phosphorene Carbide Nanoribbons by Molecular Dynamics Simulation Studies

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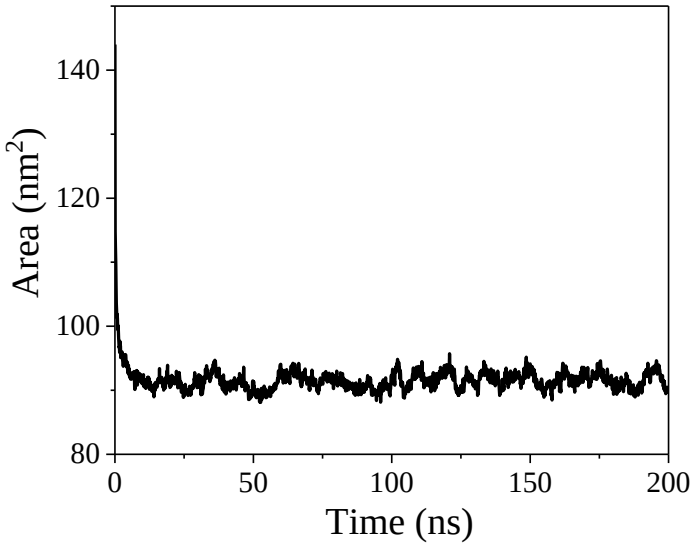

Figure S1. Time evolution of the cross section area of the membrane model. The membrane model reached good equilibration from around 10 ns.

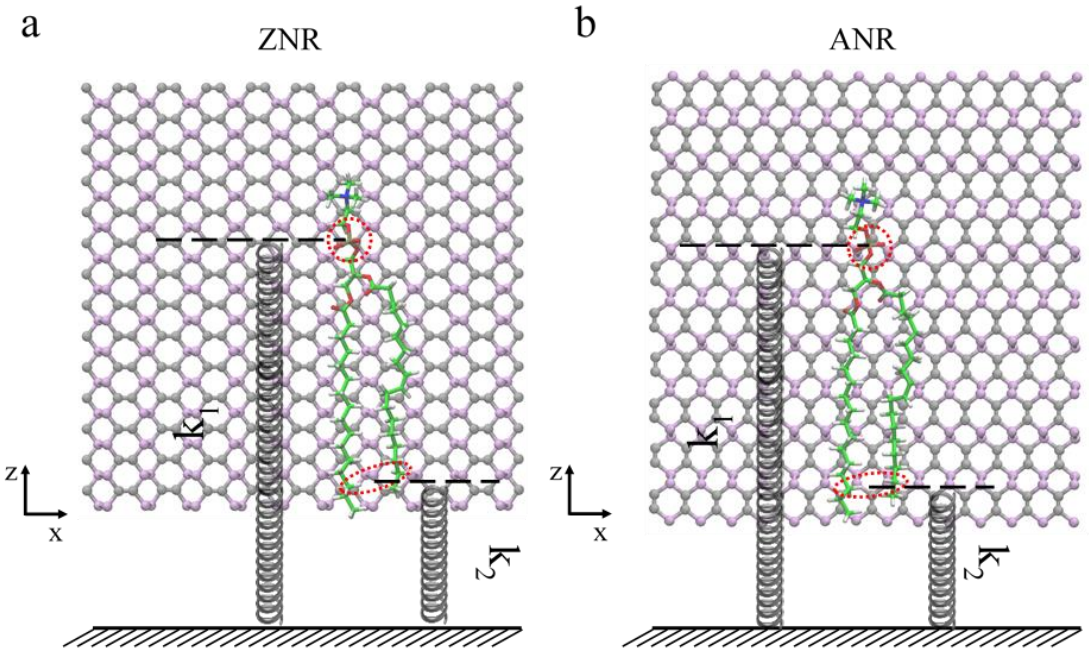

Figure S2. Umbrella sampling system setup for the (a) ZNR and (b) ANR system. In each system, two harmonic forces (k_1=k_2=1000 kJ/(mol·nm^2)) were applied to the phosphorus atom and the center of the mass of two carbon atoms from both tails of the lipid, respectively, to maintain its relative position to the lower edge of the α-PC sheet.

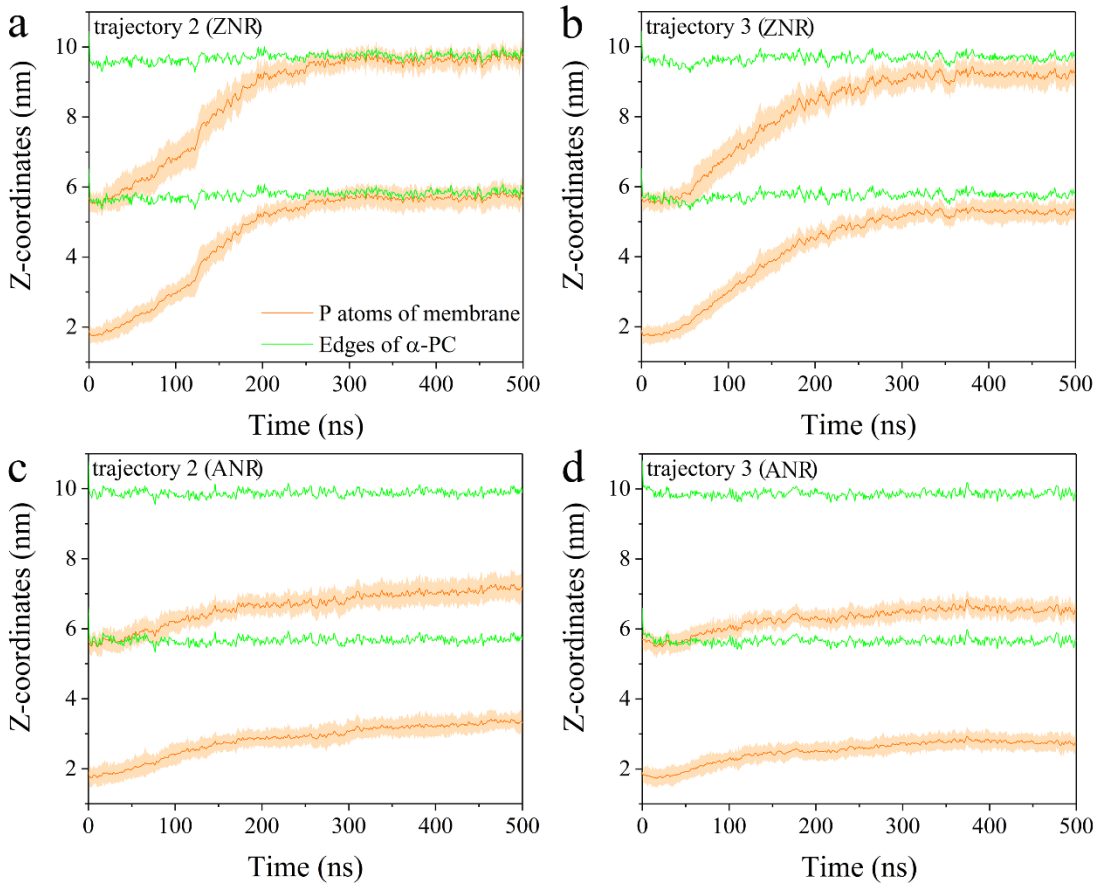

Figure S3. Different penetration dynamics of the α-PC sheet along two different directions in the parallel trajectories. (a, b) α-PC penetration through zigzag edge; (c, d) α-PC penetration through armchair edge. The green lines represent the top and bottom edges of the α-PC sheet. The orange lines indicate the upper and lower leaflets of the phosphorus head groups of membrane.

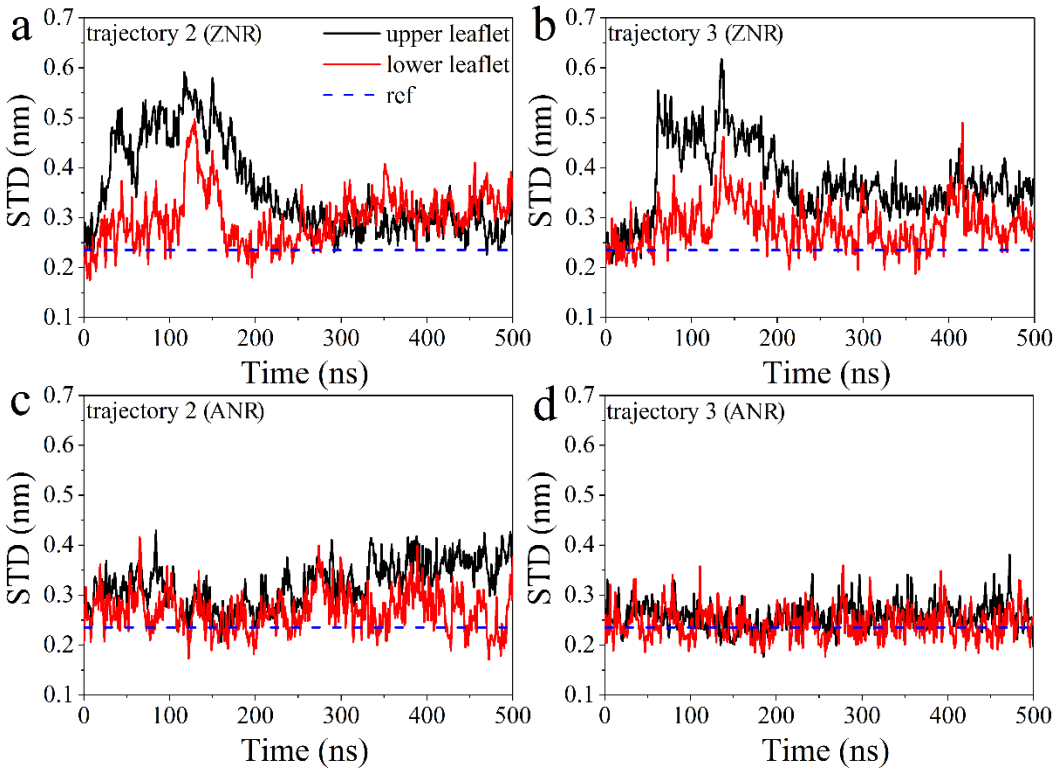

Figure S4. Standard deviation (STD) of the z-coordinates of the phosphorus atoms in each leaflet in parallel trajectories. (a, b) the ZNR system and (c, d) the ANR system. The blue line represents the STD value of pristine membrane.

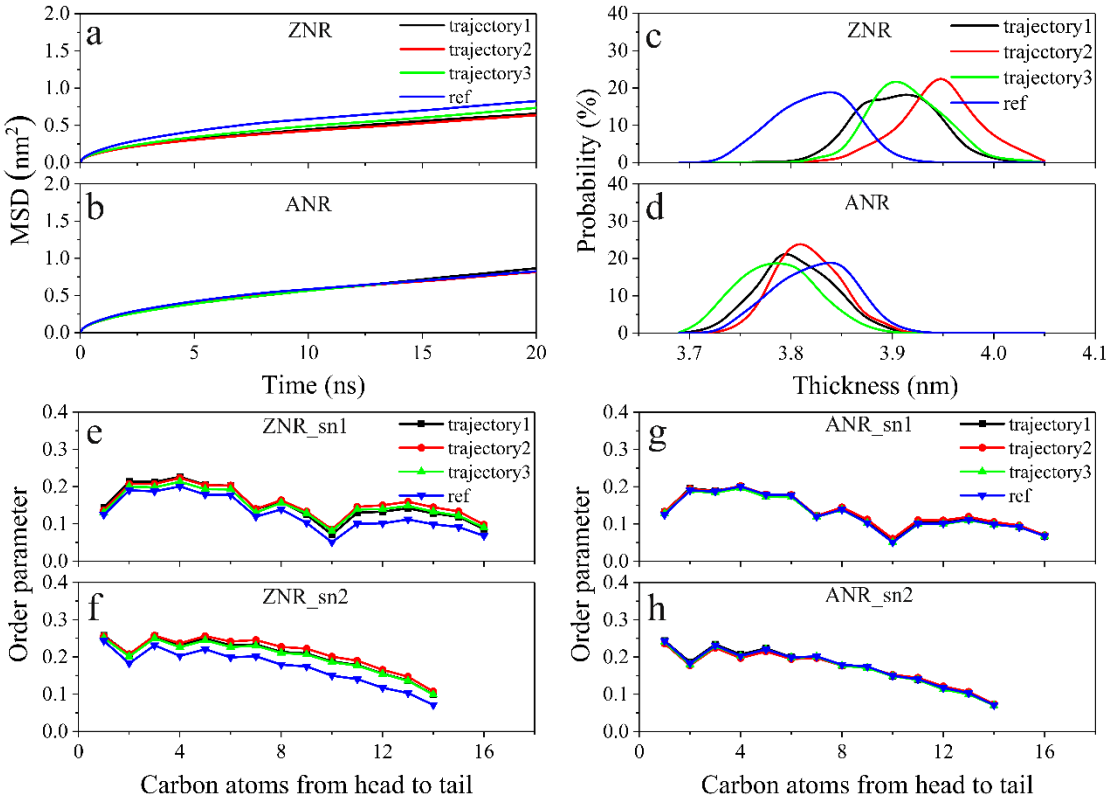

Figure S5. Variations of membrane properties after penetration of the α-PC sheet. Based on the last 50 ns trajectories of the ZNR and ANR systems, the mean square displacements (MSD) of the center of mass of lipids (a and b), the probability distributions of the membrane thickness (c and d), the order parameters (e, f, g and h) for the two lipid tails (sn1 and sn2) are calculated and compared to those in the control simulation. The thickness is calculated as the distance between the COM of phosphorus atoms in two leaflets. The order parameters S_z are calculated according to $S_z = \frac{3}{2}(cos^2\theta_z) - \frac{1}{2}$, where θ_z is the angle between the z-axis and the vector from carbon atom $C_z$to C_{z+1}.

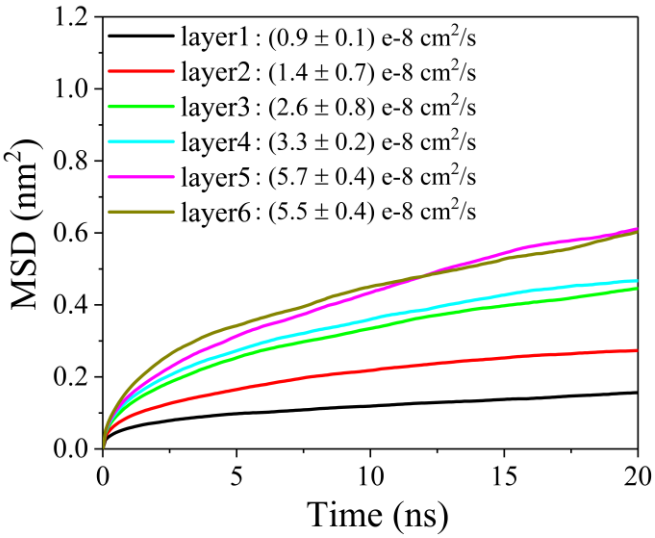

Figure S6. Mean squared displacement (MSD) of lipids in six binding layers around α-PC.