Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Molecular Mechanisms Underlying the Role of Puckered Surface in the Biocompatibility of Black Phosphorus

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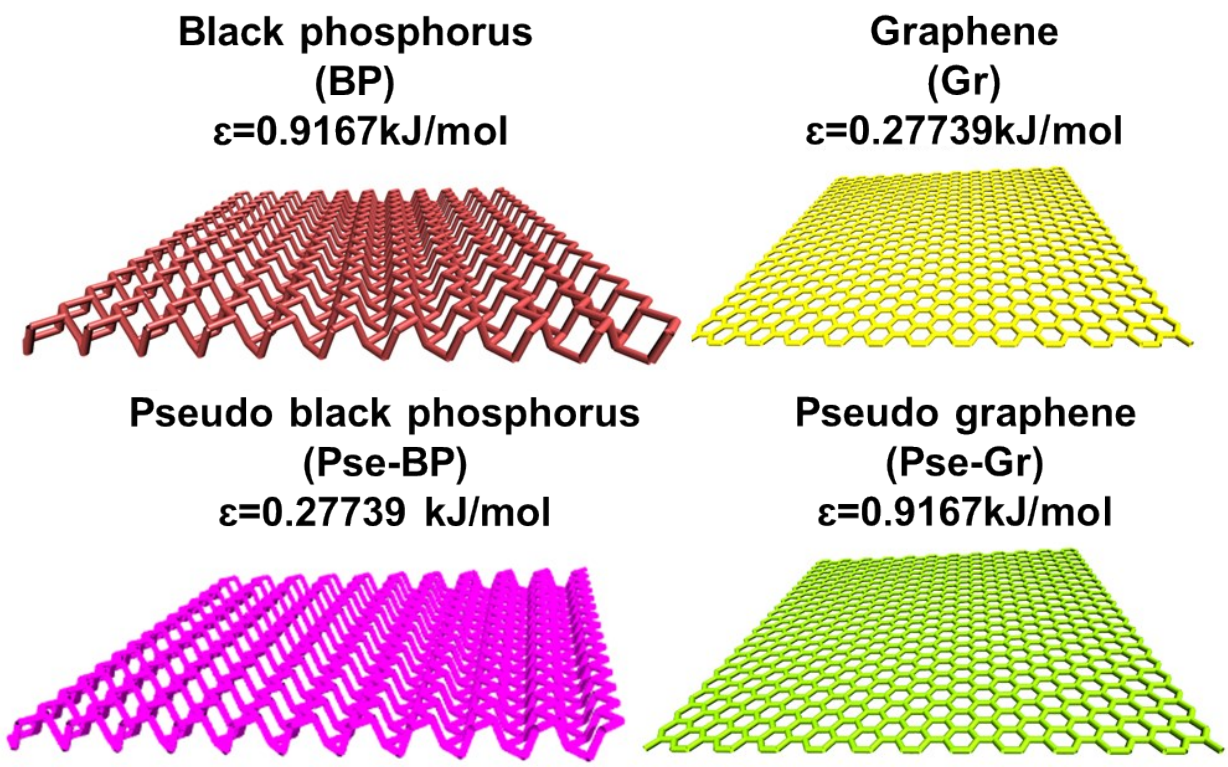

Fig. S1 Schematic illustration of the model for each type of nanosheet.

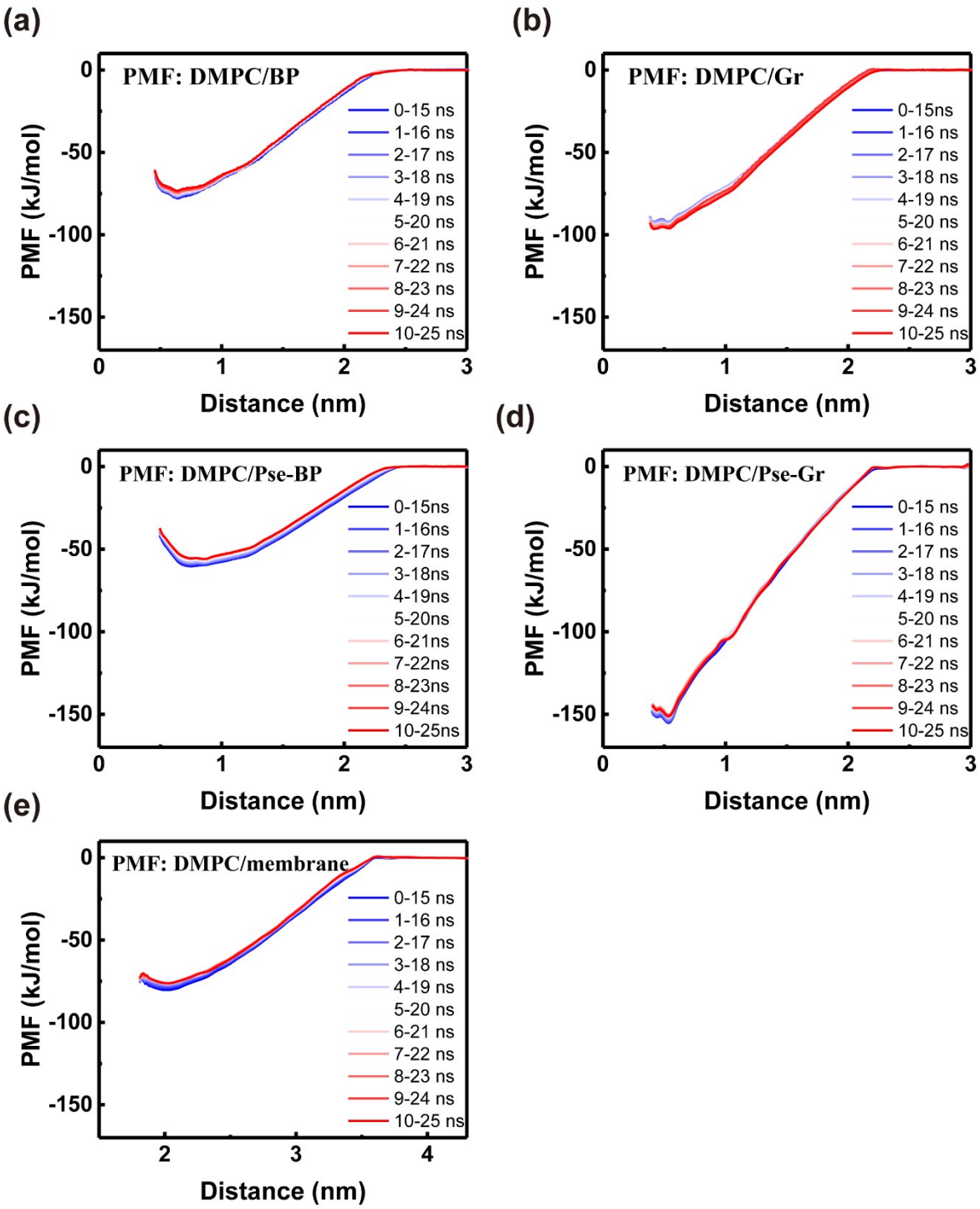

Fig. S2 Potential of mean force (PMF) convergence testing for pulling a lipid molecule away from the membrane and from the nanosheet surface. PMF profiles were calculated for 15 ns time intervals every 1 ns, and colored from blue to red. Evolution of PMF profiles shows that the results reached convergence at 10-25 ns. The distance (x-axis) between the pulled lipid molecule

and the membrane is the z distance from the center-of-mass of phosphorus atoms in upper leaflets of membranes to the pulled phosphorus atom. The distance between lipid molecule and the nanosheet surface is the z distance from the center-of-mass of nanosheet to the pulled phosphorus atom.

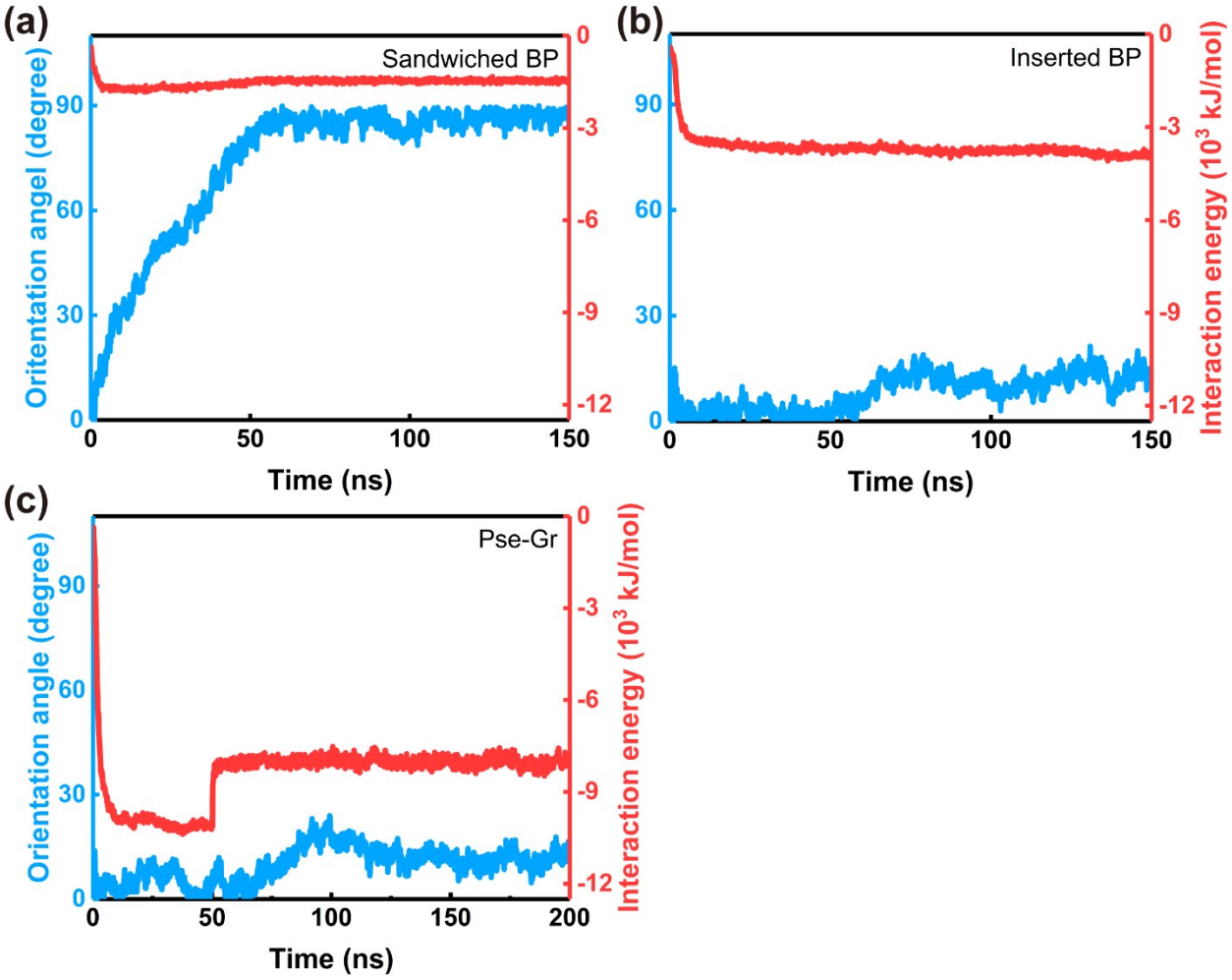

Fig. S3 Evolution of nanosheet orientation angle profiles and interaction energy profiles of each system with: (a) artificially inserted Pse-BP, (b) artificially inserted BP and (c) spontaneous inserted Pse-Gr during the penetration processes. (The blue lines represent the orientation angle profiles, while the red lines represent the interaction energy profiles.) The simulation duration for

each case varies according the convergence of the interaction energy profiles as well as the orientation of the nanosheet.

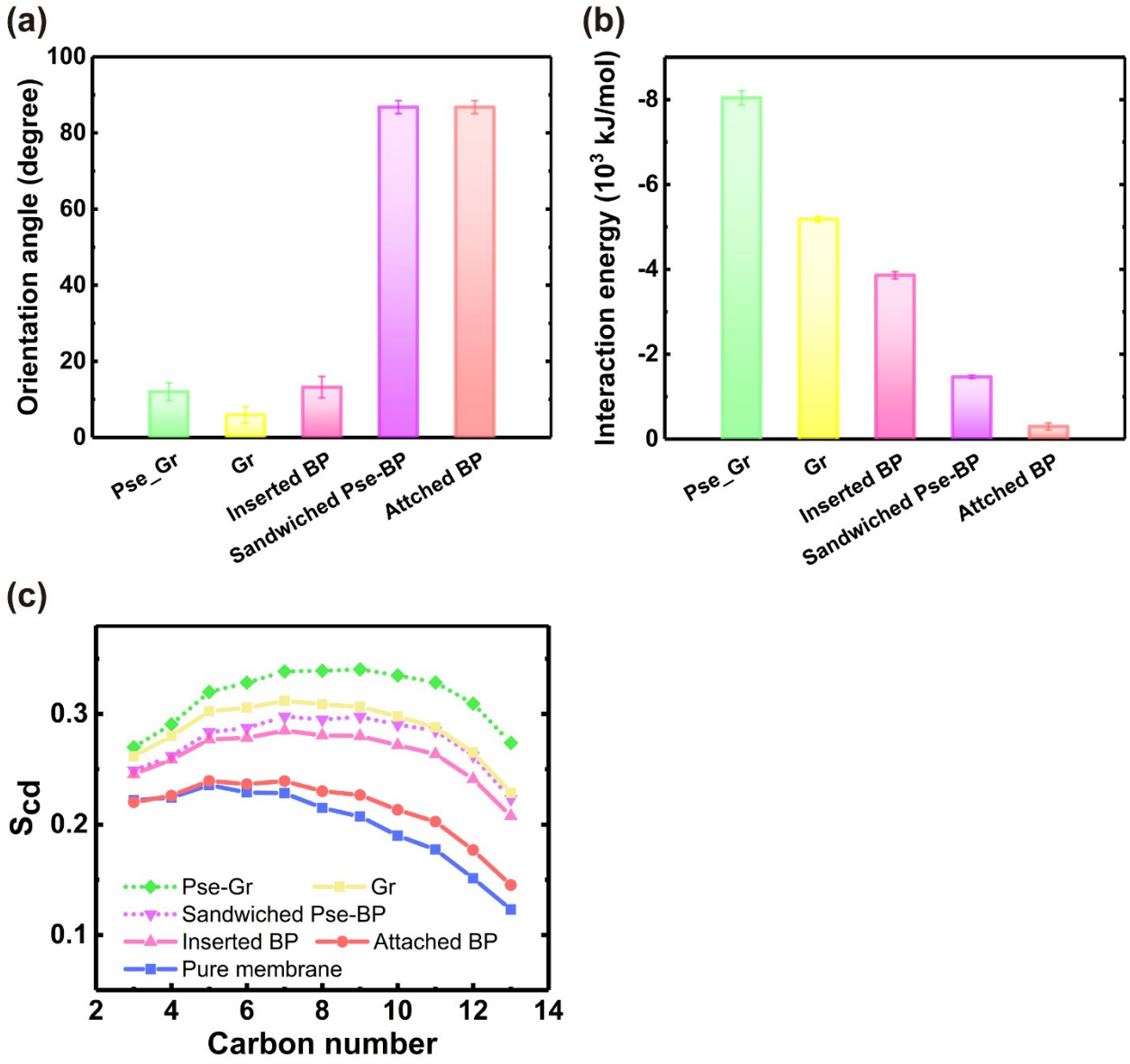

Fig. S4 (a) The convergence orientation angle of nanosheet. (b) The convergence interaction energy between nanosheet and the membrane. (c) Order parameter, S_{cd} in sn2. For clarity, only the S_{cd} of lipid tails in sn1 is shown in the manuscript, which shares the same trend with S_{cd} in sn2.