Supporting Information for

Phosphorene Nanoribbons, Phosphorus Nanotubes and van der Waals Multilayers

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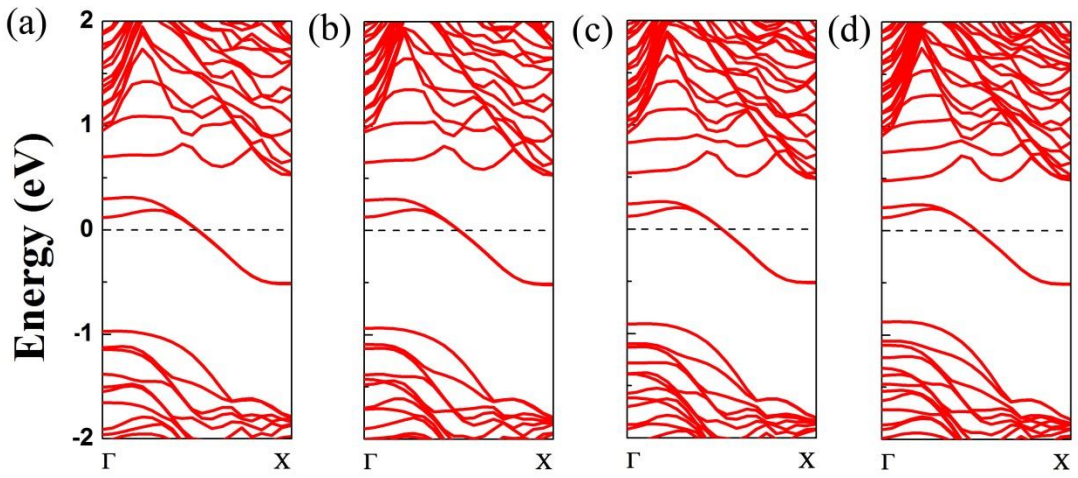

Figure S1. Computed band structures (PBE) of the edge-unpassivated (a) 7-, (b) 8-, (c) 9-, (d) 10-*z*-PNRs. The Fermi level is set to zero.

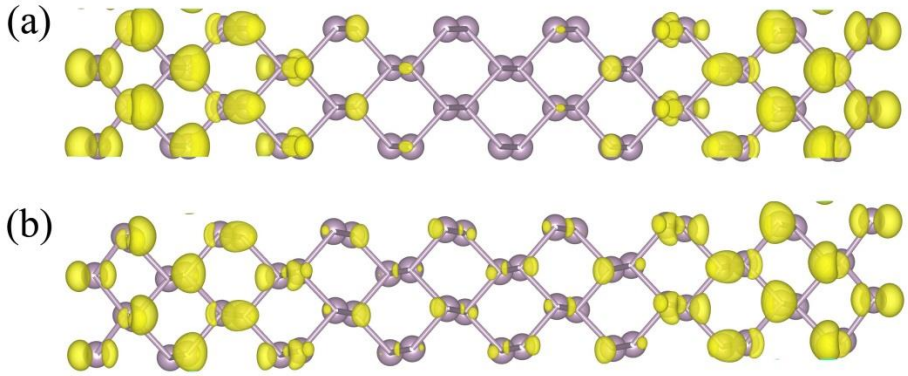

Figure S2. The partial charge density distribution corresponding to (a) α and (b) β band at the Γ point, respectively, for the edge-unpassivated 8-*z*-PNR.

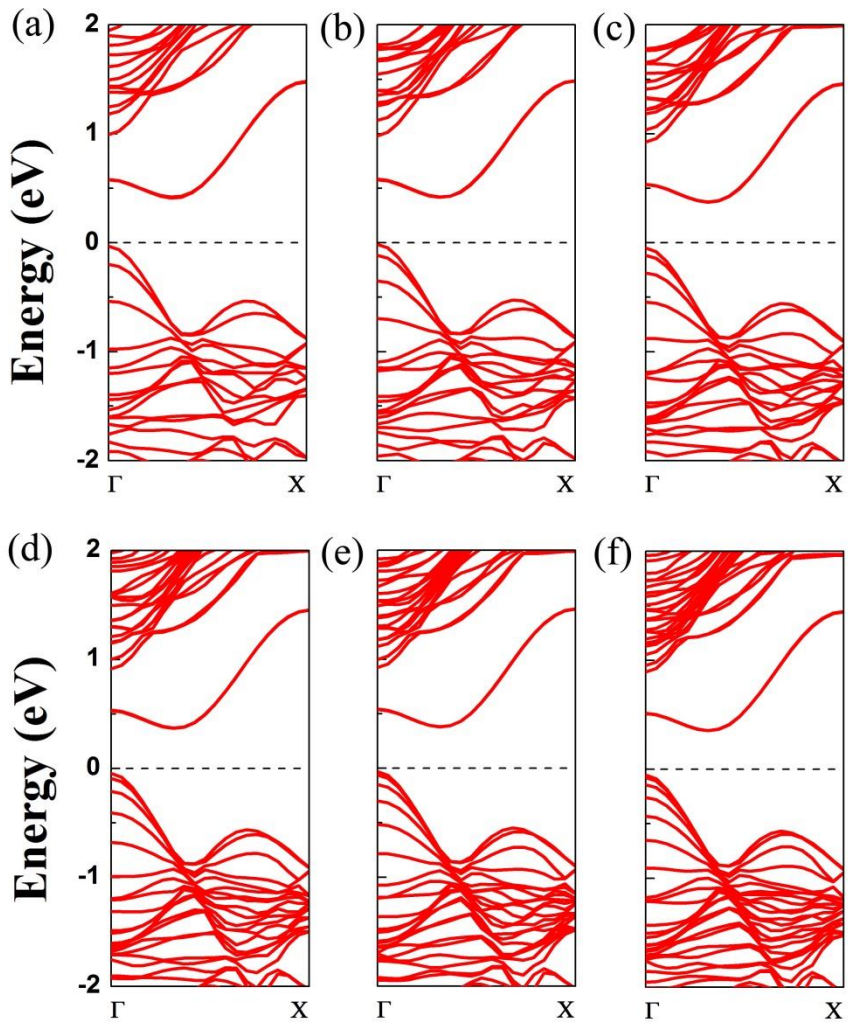

Figure S3. Computed band structures (PBE) of the edge-unpassivated (a) 7-, (b) 8-, (c) 9-, (d) 10, (e) 11-, and (f) 12-*a*-PNRs. The Fermi level is set to zero.

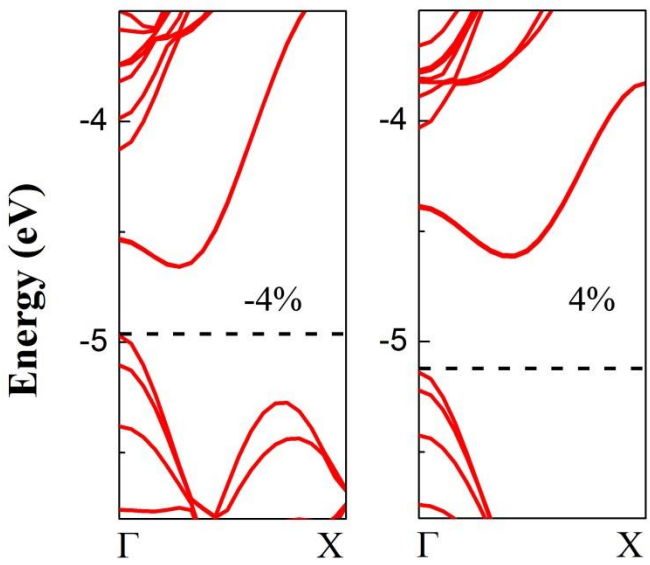

Figure S4. Computed band structures (PBE) of the edge-unpassivated 8-*a*-PNR at the strain of -4% and 4%. The vacuum level is set to zero. The dashed line denotes the Fermi level.

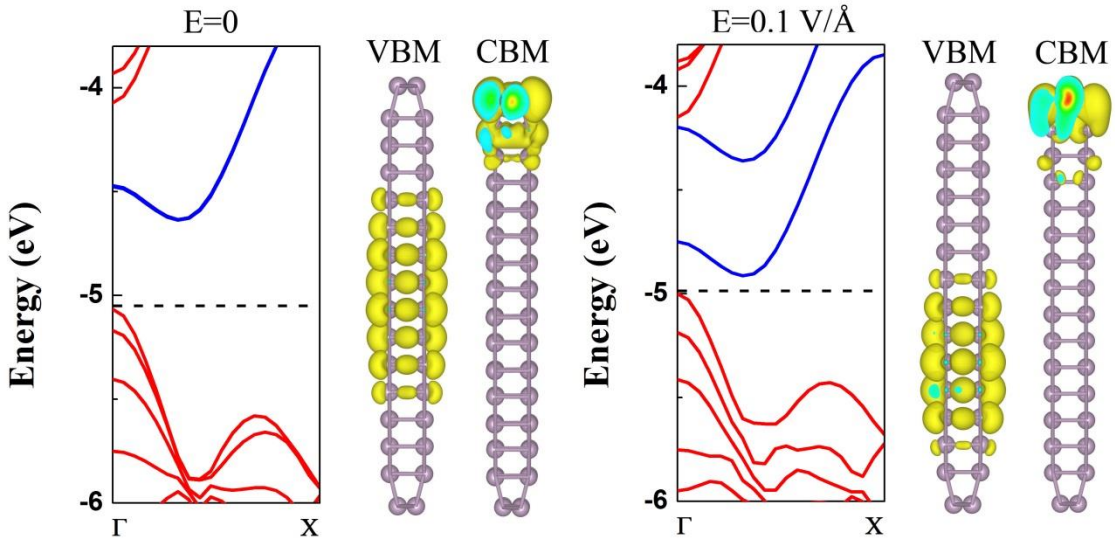

Figure S5. Computed band structures (PBE) and partial charge density distribution corresponding to the VBM and CBM for the edge-unpassivated 8-*a*-PNR at zero and an external in-plane transverse electric field of 0.1 V/Å, respectively. The vacuum level is set to zero. The dashed line denotes the Fermi level. The CBM corresponds to the edge-state and the corresponding bands are highlighted by blue lines.

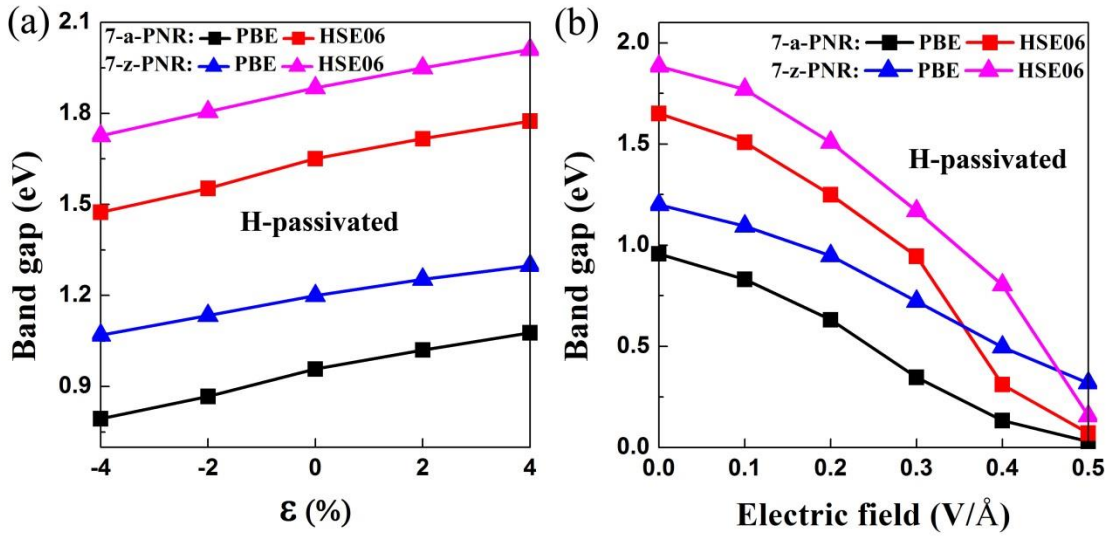

Figure S6. (a) Computed bandgaps of the edge-passivated 7-*a*-PNR and 7-*z*-PNR by hydrogen *versus* the tensile strain, ranging from -4% to 4%, "-" represents compression and "+" represents expansion. (b) Computed bandgaps versus in-plane transverse electric field for the edge-passivated 7-*a*-PNR and 7-*z*-PNR.

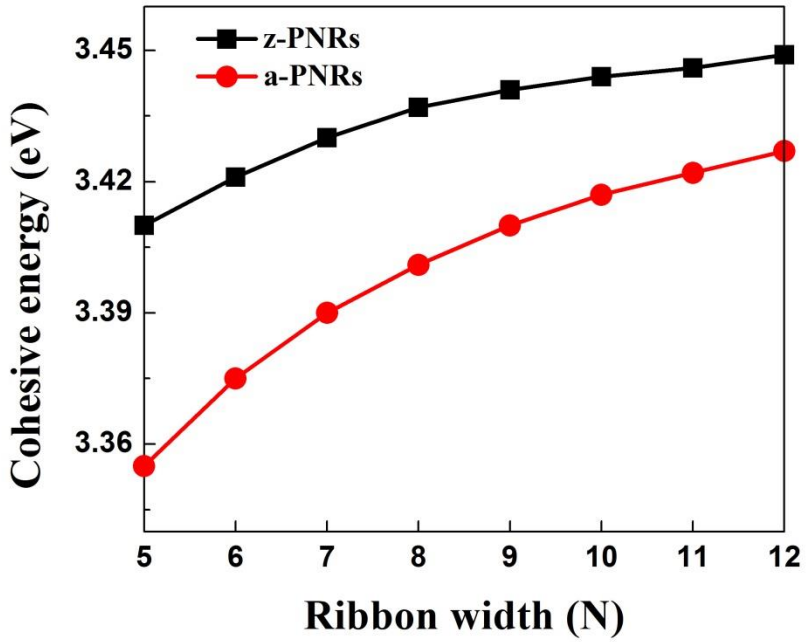

Figure S7. Computed cohesive energy per atom of the edge-unpassivated PNRs *versus* the ribbon width N ($5 \leq N \leq 12$).

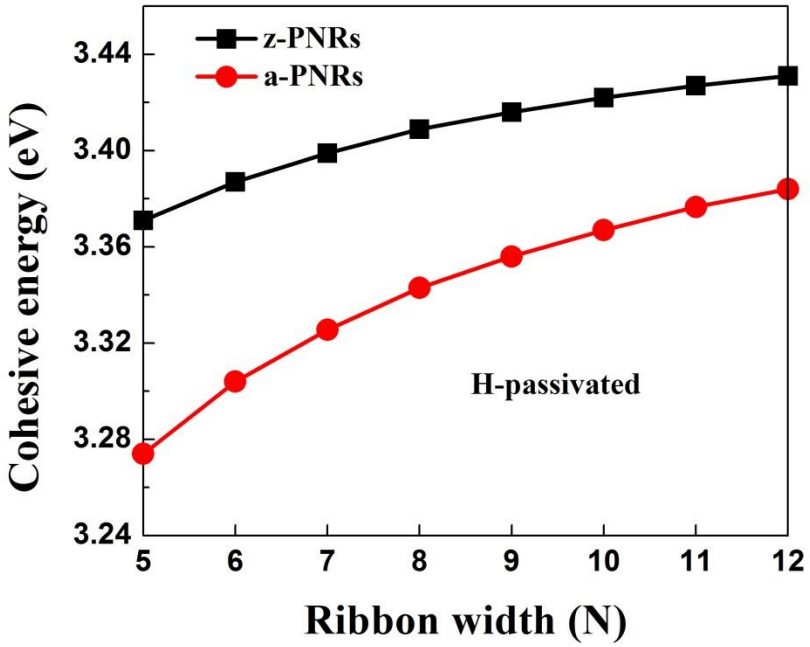

Figure S8. Computed cohesive energy per atom of the edge-passivated PNRs *versus* the ribbon width ($5 \leq N \leq 12$).

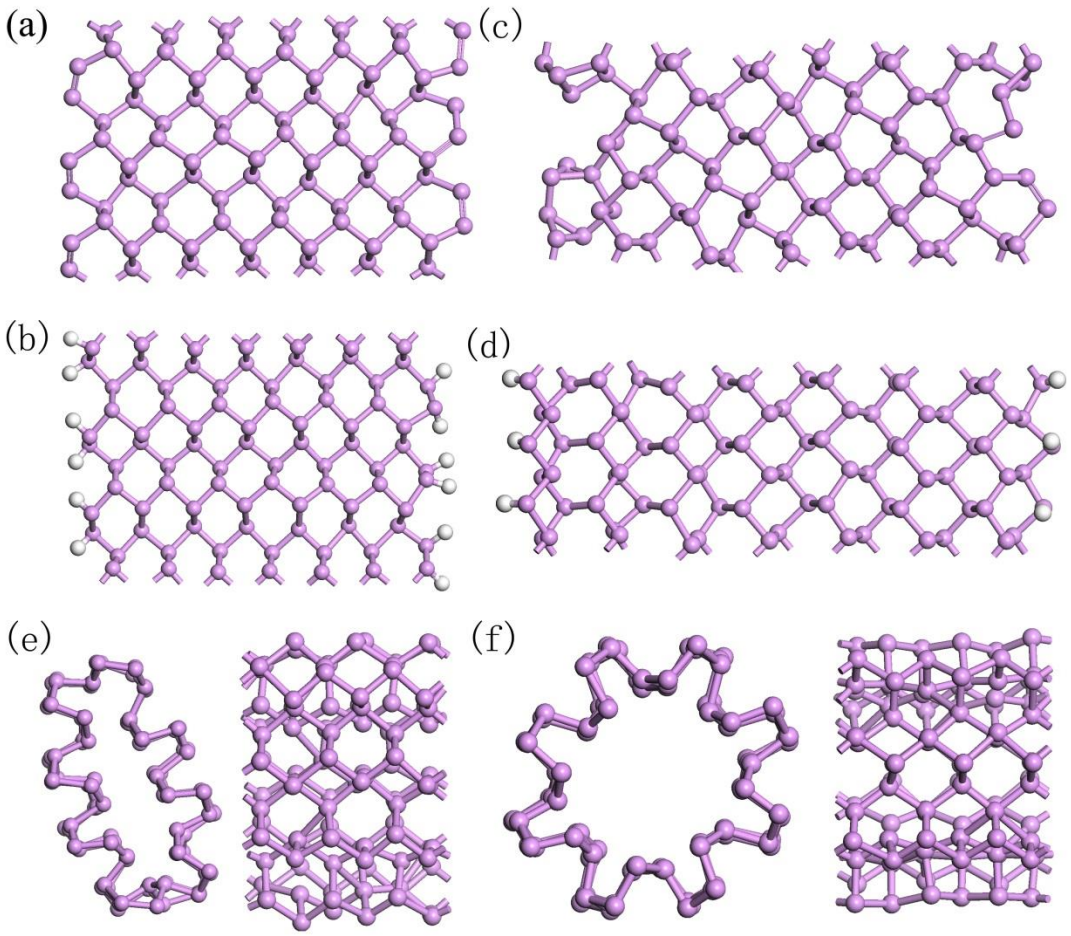

Figure S9. Snapshots of BOMD simulations at 8 ps for (a) the edge-unpassivated 7-*a*-PNR, (b) the edge H-passivated 7-*a*-PNR, (c) the edge-unpassivated 7-*z*-PNR, and (d) the edge H-passivated 7-*z*-PNR, as well as at 8 ps for (e) the armchair PNT (0, 8) [top view on the left and side view on the right], all with temperature controlled at 600 K. A snapshot of BOMD simulation at 8 ps for (f) the armchair PNT (0, 8) [top view on the left and side view on the right], with temperature controlled at 400 K.

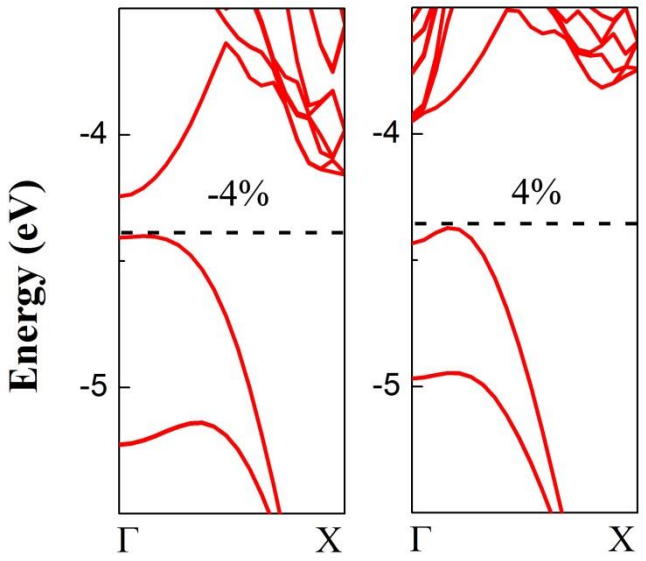

Figure S10. Computed band structures (PBE) of armchair PNT (0, 8) at strain of -4% and 4%. The vacuum level is set to zero. The dashed line denotes the Fermi level.

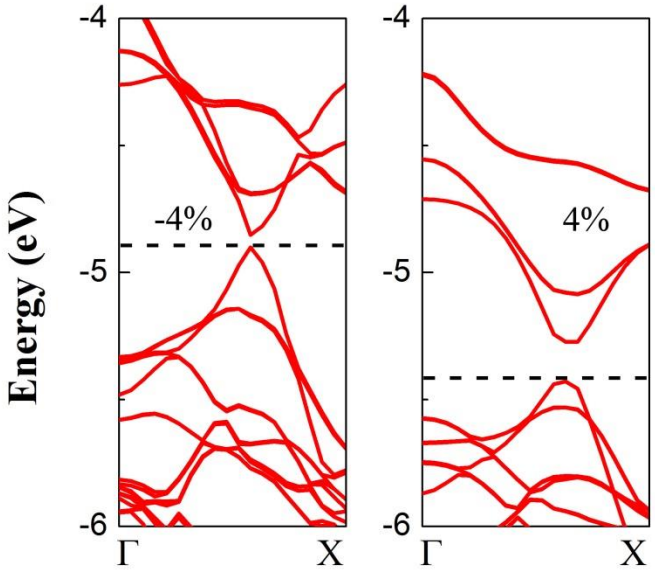

Figure S11. Computed band structures (PBE) of zigzag PNT (12, 0) at strain of -4% and 4%. The vacuum level is set to zero. The dashed line denotes the Fermi level.

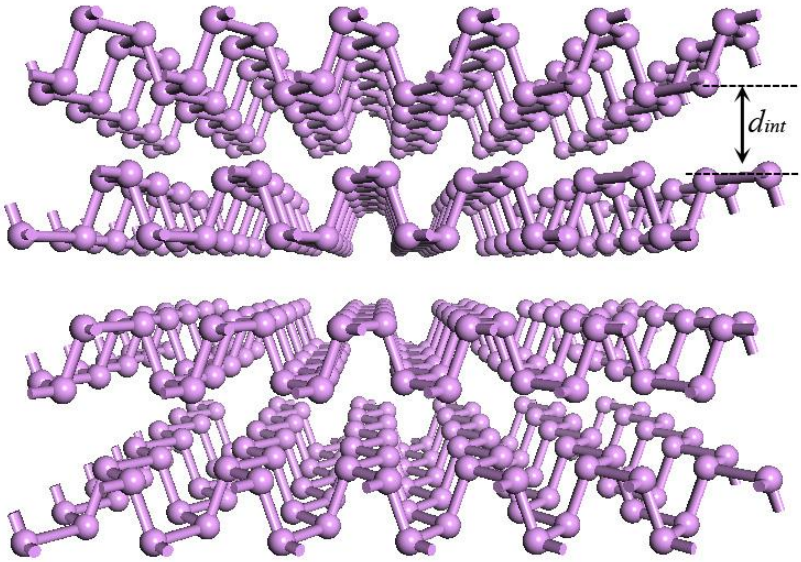

Figure S12. Geometric structure of multilayer phosphorene. d_{int} represents the interlayer spacing between two adjacent phosphorene monolayers.

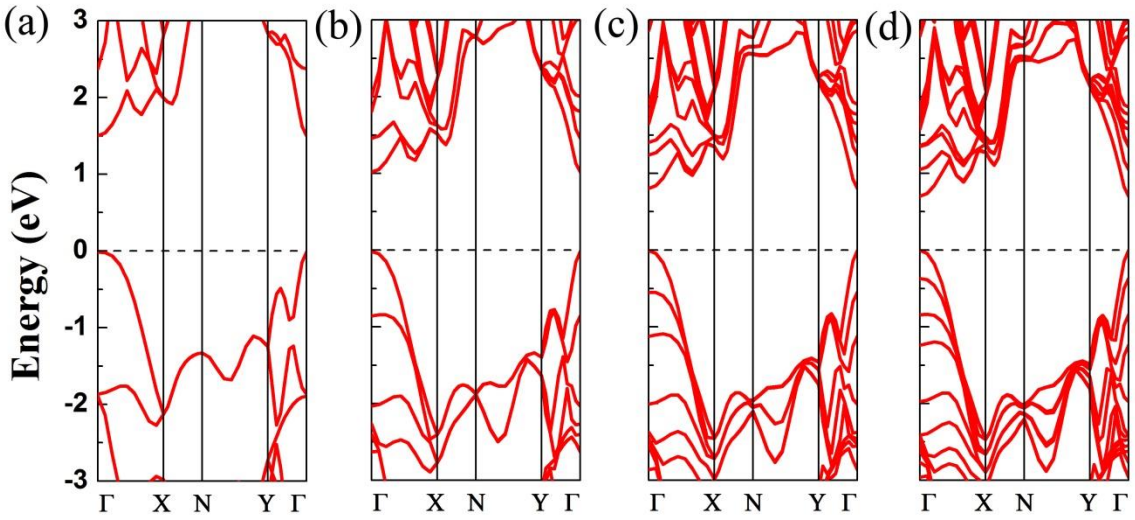

Figure S13. Computed band structures (HSE06) of (a) monolayer, (b) bilayer, (c) trilayer, (d) 4-layer phosphorene sheets. The Fermi level is set to zero.

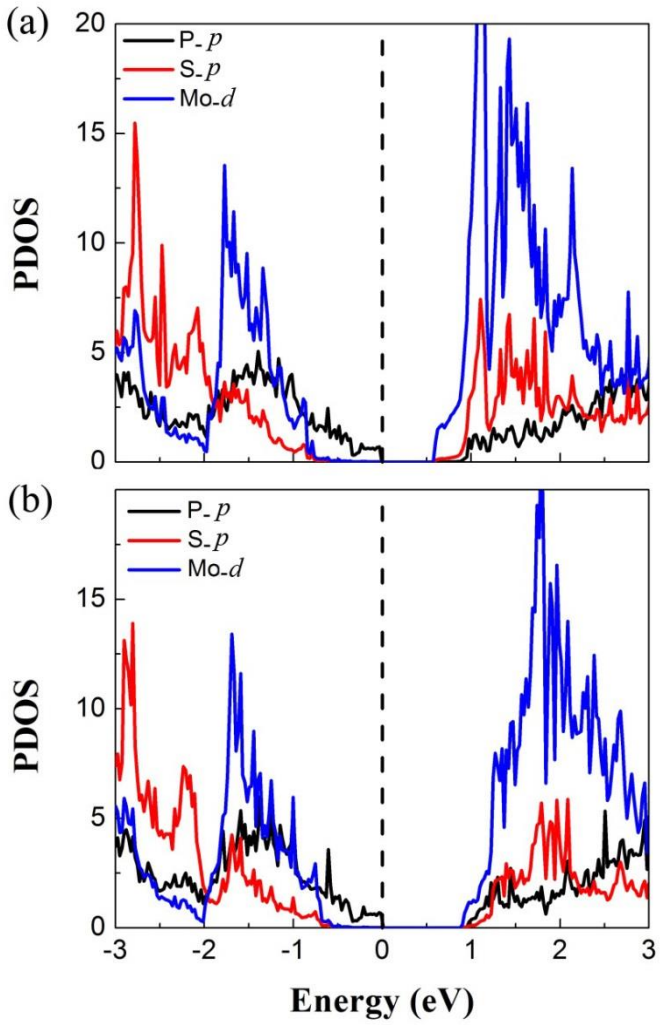

Figure S14. Computed partial density of states (PDOS) of (a) MoS_2/phosphorene and (b) WS_2/phosphorene heterobilayers. The Fermi level is set to zero.

Table S1: Cell parameter a_1 and a_2 (in Å) of multilayer phosphorene and the interlayer spacing between two adjacent phosphorene layers d_{int} (in Å).

	a_1	a_2	d_{int}
Monolayer	3.32	4.58	/
Bilayer	3.33	4.52	3.18
Trilayer	3.34	4.50	3.22
4-layer	3.34	4.50	3.23

Table S2. The charge transfer q (in unit of e) between the MoS_2 (or WS_2) and phosphorene layers with and without the electric field E (in V/ Å).

E	**0**	**0.2**	**0.4**
***q* (MoS_2/phosphorene)**	0.1	0.15	0.2
***q* (WS_2/phosphorene)**	0.07	0.11	0.15