Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Table S1. Comparison of the lattice parameters obtained for phosphorene using different functionals for the exchange and correlation energy. Lattice parameters are given in units of Å. Band gaps are given in units of eV. For comparison, we also include the experimental results for the bulk black phosphorus.

Method	*a* (Å)	*b* (Å)	*c* (Å)	*a*/*b*	E_g (eV)
PBE (this work)	3.30	4.63	-	0.76	0.91
LDA[1, 2]	3.26	4.35	-	0.74	0.72
PBE [1, 2]	3.30	4.60	-	0.76	0.90
PBEsol [1, 2]	3.28	4.45	-	0.71	0.71
Expt. (bulk) [3]	3.313	4.37	10.47	0.75	0.31

Table S2 Calculated lattice parameter (*a*, *b*), interlay distance (*d*) for bilayer phosphorene with different stacking types. Distances and lattice parameters are given in units of Å. Band gaps are given in units of eV.

System	*a* (Å)	*b* (Å)	*a*/*b*	*d* (Å)	E_g (eV)
AA	3.32	4.52	0.74	3.50	0.38
AB	3.33	4.52	0.74	3.05	0.42

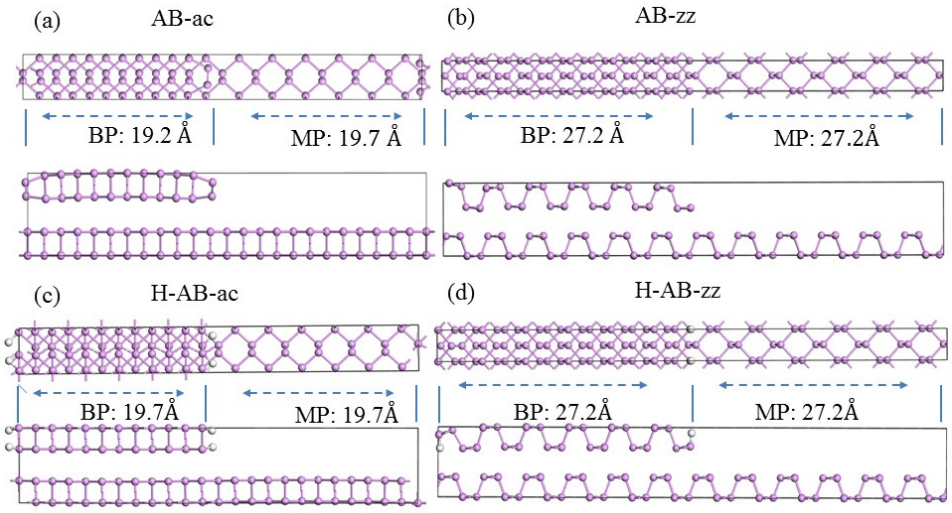

Figure S1. The structures of (6,6) BP/MP heterostructures from both top view and side view: (a) AB-ac, (b) AB-zz, (c) H-AB-ac and (d) H-AB-zz. The left and right represent the phosphorus atoms in the bilayer region and monolayer region, respectively.

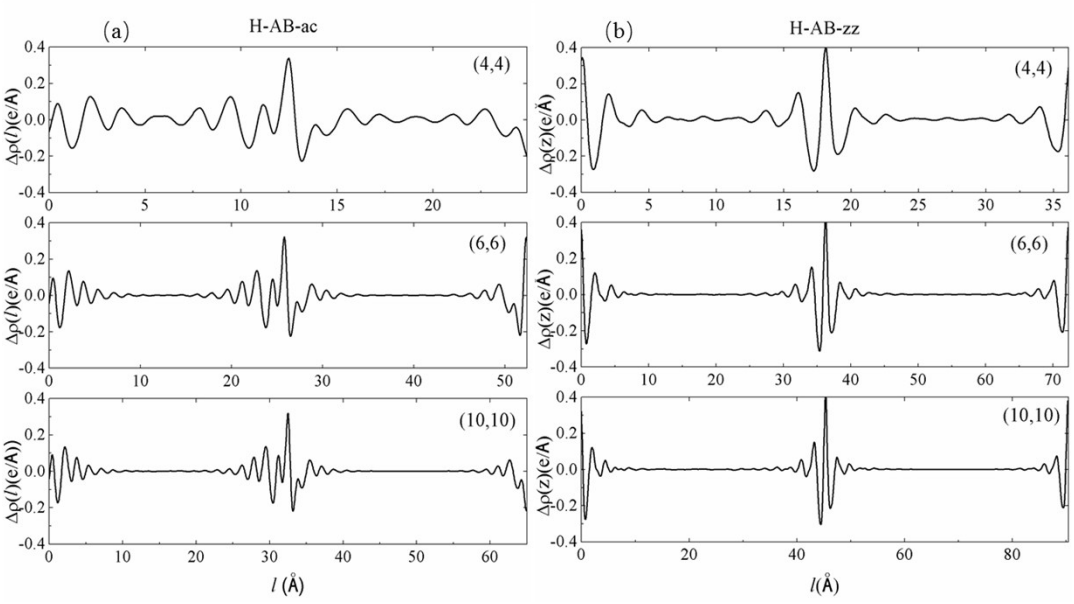

Figure S2. The plane-averaged electron density difference $\Delta\rho(l)$ for H-passivated AB-ac (a) and AB-zz (b) BP/MP heterostructures with different widths of (4, 4) (8, 8) and (10, 10).

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