Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

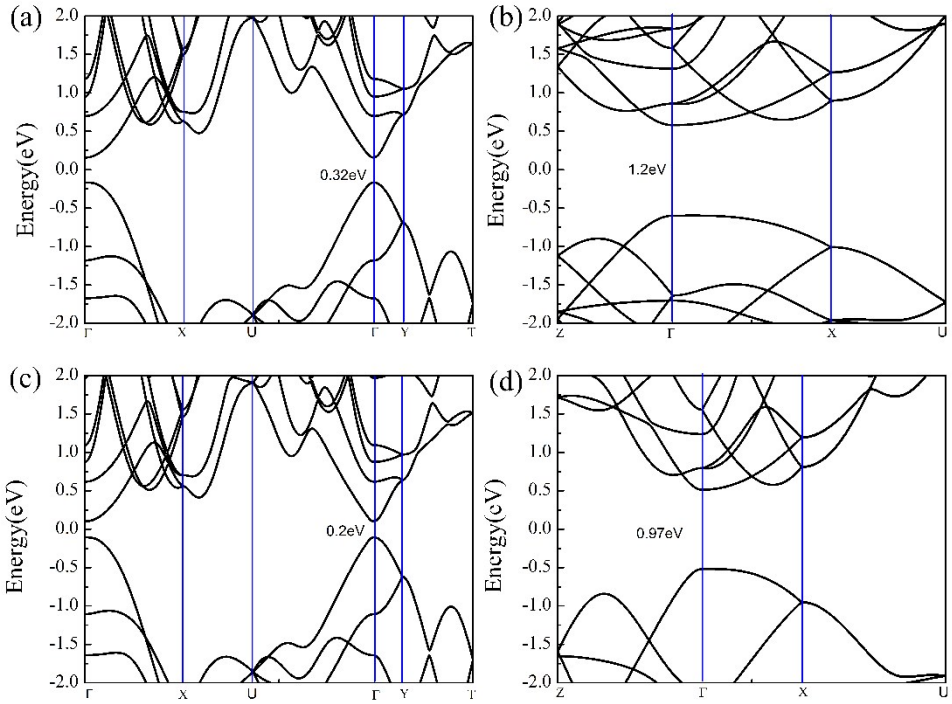

Fig.S1. calculated band structure of (a) bulk phosphorus by using MGGA, (b) single layer of bulk black phosphorene by using MGGA, (c) bulk phosphorus by using PBE and (d) single layer of bulk black phosphorus by using PBE. The Fermi-energy is set to 0 eV.

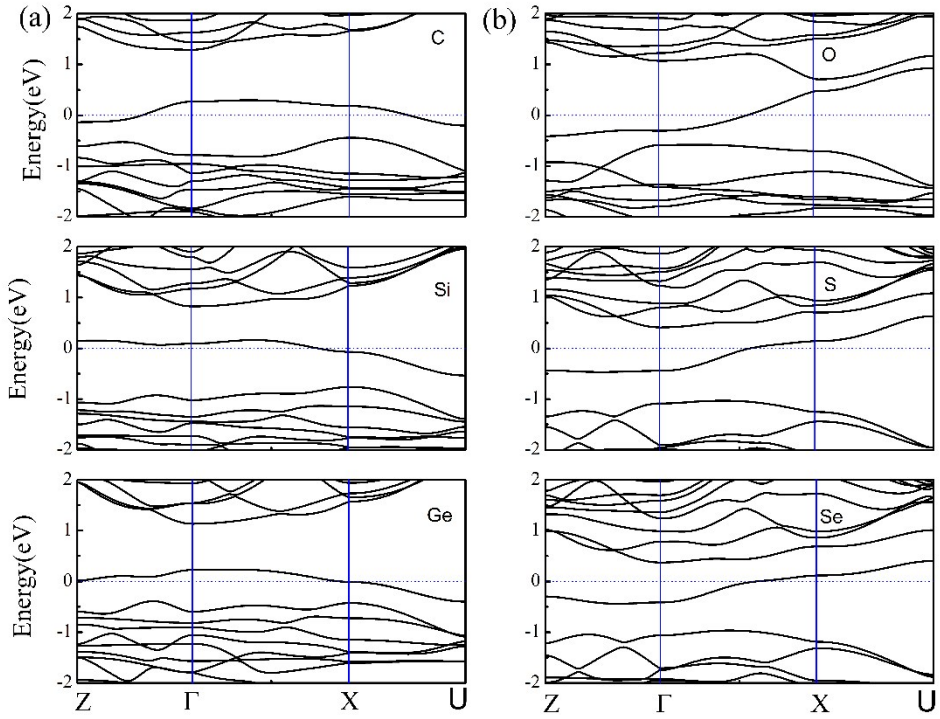

Fig.S2. Calculated band structure of doped phosphorene with (a) group IV and (b) group VI atoms, respectively.

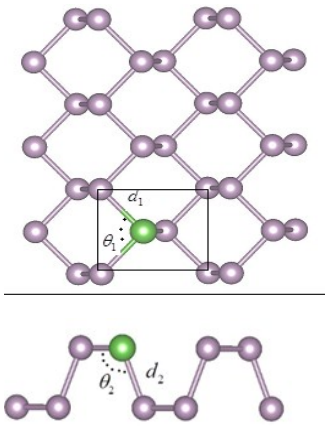

Figure S3: The schematic of phosphorene, (a) top view and (b) side view. The P tom substituted by a dopant atom is drawn with a dark circle. The bond lengths (d_1 and d_2) and bond angles (θ_1 and θ_2) are represented in Table S1.

Table S1: Calculated bond lengths (d_1 and d_2) and bond angles (θ_1 and θ_2) for 2×2 supercell of group Ⅲ to group Ⅵ elements doped phosphorene, respectively. Together with those of pure phosphorene, For comparison, previous theoretical results for pure phosphorene are also given.

Dopant atom	$d_1(\AA)$	$d_2(\AA)$	$\theta_1(°)$	$\theta_2(°)$
Pure[1]	2.25	2.26	96.9	102.3
pure	2.24163	2.26386	94.9955	103.1664
B	1.96005	1.87783	109.0278	122.9979
C	1.81992	1.80525	106.5523	121.8137
N	1.81247	1.82556	103.1496	119.7765
O	2.12179	1.80211	108.5768	118.5664
Al	2.35352	2.35096	91.9347	116.3683
Si	2.28013	2.29639	93.2899	108.8055
S	2.3477	2.31801	106.9744	113.1779
Ga	2.3228	2.32569	96.8235	120.3359
Ge	2.37262	2.41392	90.6851	103.266
As	2.36114	2.39683	92.3333	99.3
Se	2.48781	2.51966	104.1866	108.4787

Table S2: calculated lattice constants for supercell of group III to group VI elements doped phosphorene, respectively, together with those of pristine phosphorene.

Dopant atom	a (Å)	b(Å)	c(Å)
pristine	6.6272	11.3115	8.86485
B	6.60009	11.3082	8.87517

Al	6.74929	11.3652	8.44615
Ga	6.75325	11.362	8.46652
C	6.5919	11.3266	8.78562
Si	6.7198	11.4083	8.37851
Ge	6.76508	11.376	8.45446
N	6.5061	11.3295	8.76784
As	6.67666	11.291	8.87567
O	6.5499	11.374	8.7404
S	6.217	11.2997	8.91053
Se	6.67938	11.269	8.99964

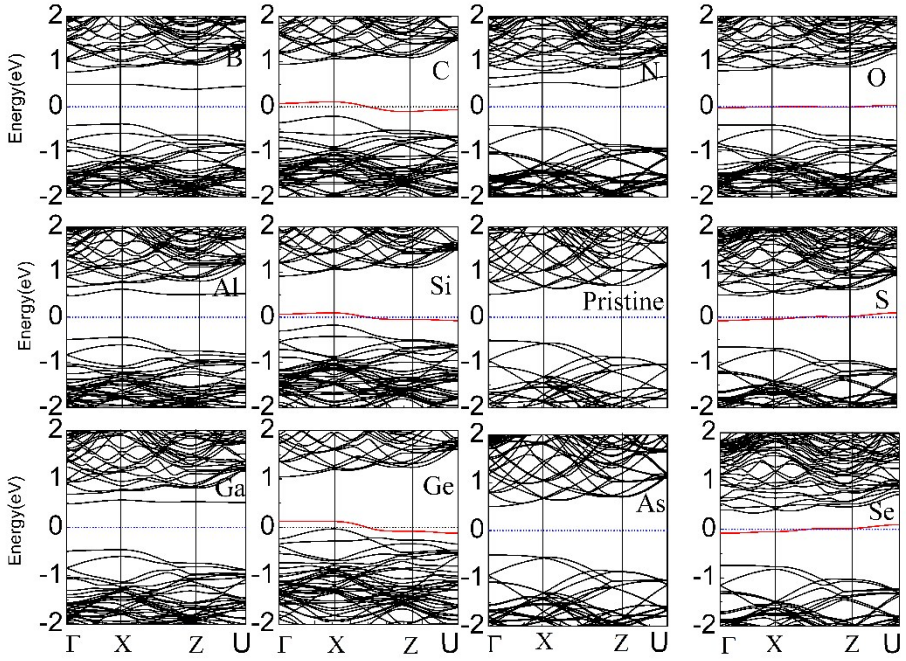

Figure S4. Calculated band structures for 4×4 supercell pristine phosphorene and doped with B, C, N, O, Al, Si, S, Ga, Ge, As, Se atoms, respectively. The energy zero represents the Fermi level.