Electronic Supplementary Information

Structure and Stability of Two Dimensional Phosphorene with =O or =NH Functionalization

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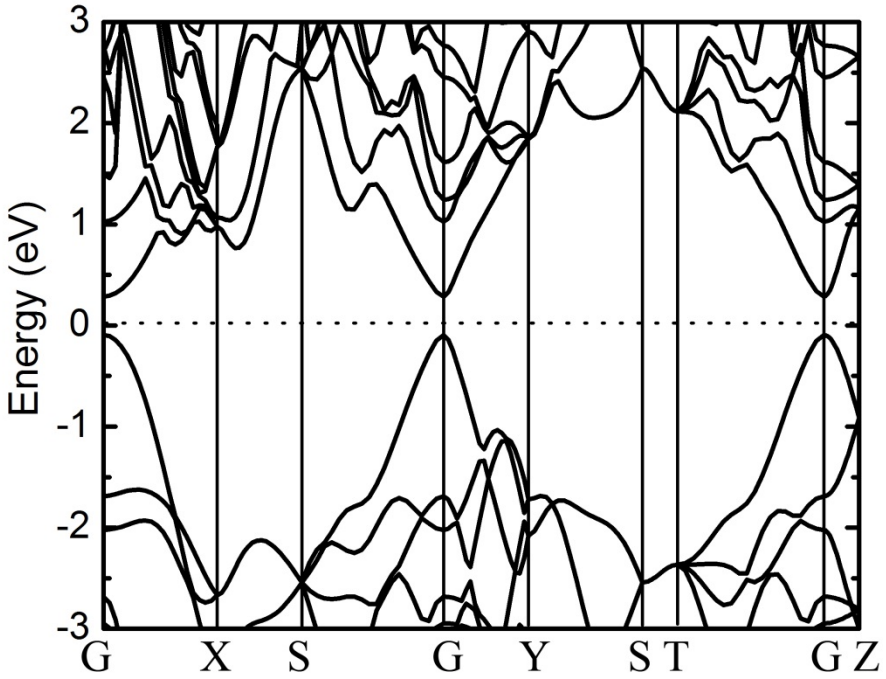

Figure S1. Computed band structures (HSE06) of bulk black phosphorus. G (0.0, 0.0, 0.0), X (0.0, 0.5, 0.0), S (0.5, 0.5, 0.00), Y (0.5, 0.0, 0.0), T (0.5, 0.5, 0.5) and Z (0.0, 0.0, 0.5) refer to special points in the first Brillouin zone.

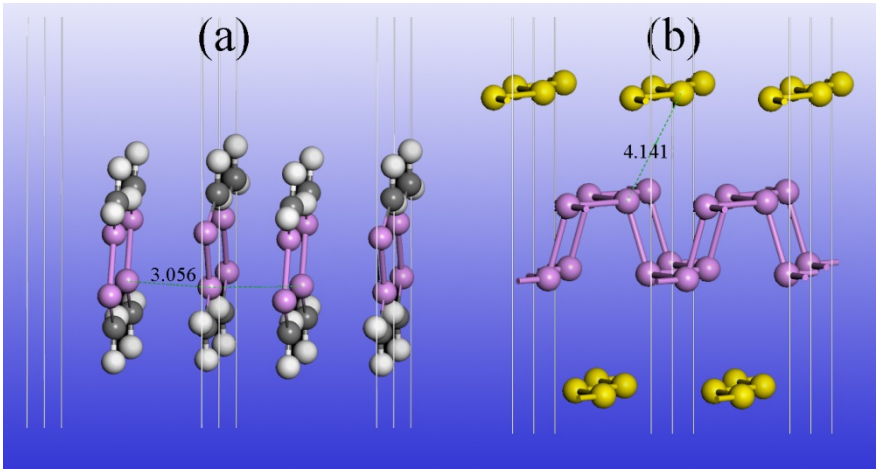

Figure S2. Optimized structures of $=CH_2$ and =S functionalized phosphorene, the pink, grey, white and yellow spheres denote the P, C, H and S atoms, respectively.

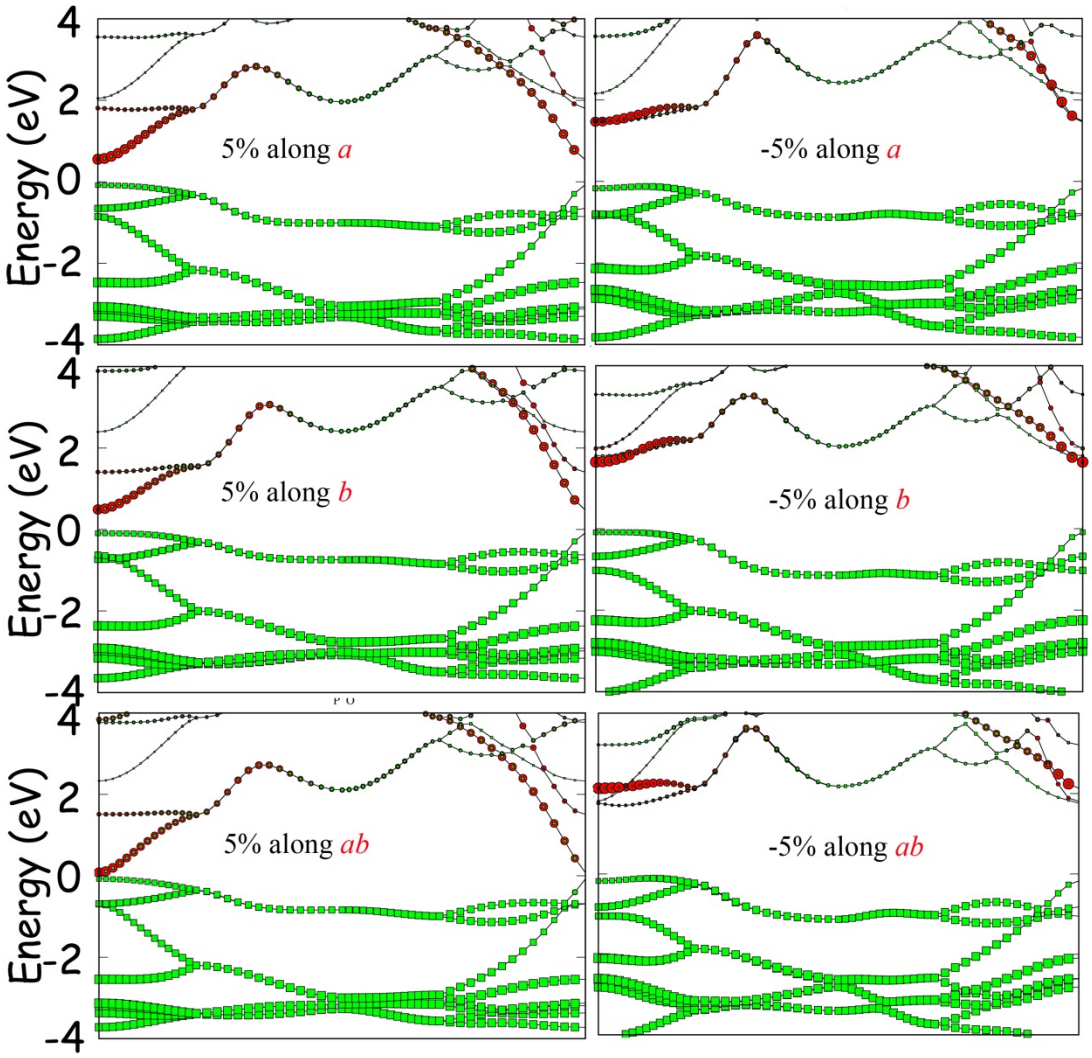

Figure S3 HSE06 band structures of P-O under uniaxial or biaxial strain of 5% or -5%.

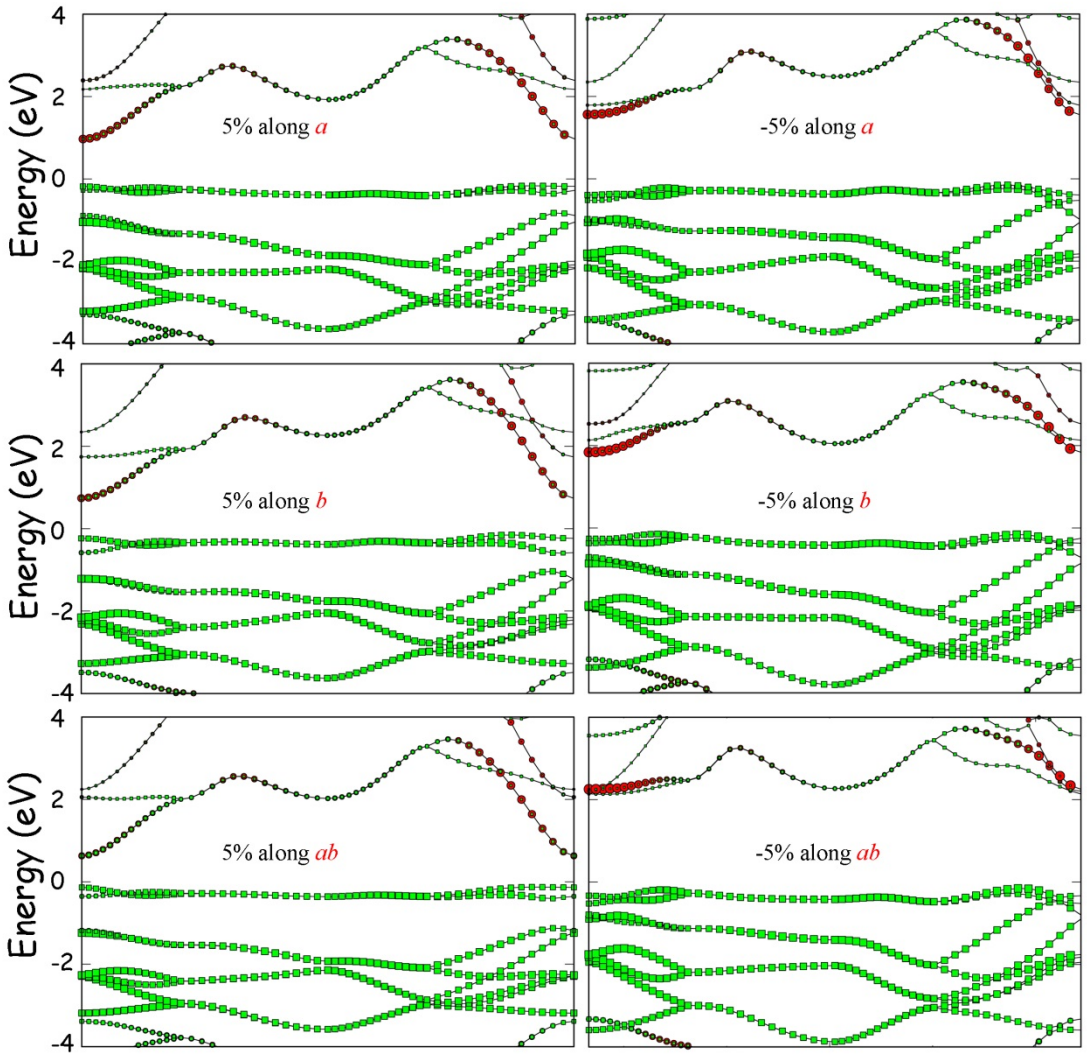

Figure S4 HSE06 band structures of P-NH under uniaxial or biaxial strain of 5% or -5%.

Table S1 Computed charge transfer for P-NH-half, P-NH, P-O-half and P-O based on Bader's charge analysis, P^1 denotes the phosphorus atoms with NH or O while P^2 denotes those without NH or O. The unit of the charge transfer is e^-, positive values indicate electron gain while negative values electron loss.

	P^1	*P^2*	*N*	*H*	*O*
P-NH-half	-1.15	+0.03	+1.64	-0.52	N/A
P-NH	-1.12	N/A	+1.64	-0.52	N/A
P-O-half	-1.29	+0.03	N/A	N/A	+1.26
P-O	-1.27	N/A	N/A	N/A	+1.27

Table S2 Computed formation energies (in eV/P) of P-O and P-NH with an uniaxial strain (along *a* or *b axis*) or a biaxial strain of +5% or -5%.

	+5%	0%	-5%
P-O uniaxial along *a*	-1.588	-1.612	-1.604
P-O uniaxial along *b*	-1.583	-1.612	-1.608
P-O biaxial along *a and b*	-1.562	-1.612	-1.591
P-NH uniaxial along *a*	-0.180	-0.212	-0.194
P-NH uniaxial along *b*	-0.181	-0.212	-0.211
P-NH biaxial along *a and b*	-0.145	-0.212	-0.195