Electronic supplementary information for

Enhanced photocatalytic performance of black phosphorene by isoelectronic co-dopants

Xuhui Yang[1], Baisheng Sa[1,*], Chao Xu[2], Hongbing Zhan[1,**], Masakazu Anpo[3], and Zhimei Sun[4,***]

[1] *Key Laboratory of Eco-materials Advanced Technology, College of Materials Science and Engineering, Fuzhou University, Fuzhou 350108, P. R. China*

[2]*Xiamen Talentmats New Materials Science & Technology Co., Ltd., Xiamen 361015, P. R. China*

[3] *State Key Laboratory of Photocatalysis on Energy and Environment, Fuzhou University, Fuzhou 350116, P. R. China.*

[4]*School of Materials Science and Engineering, and Center for Integrated Computational Materials Science, International Research Institute for Multidisciplinary Science, Beihang University, Beijing 100191, P. R. China*

*To whom the correspondence should be addressed: bssa@fzu.edu.cn.
**To whom the correspondence should be addressed: hbzhan@fzu.edu.cn.
***To whom the correspondence should be addressed: zmsun@buaa.edu.cn.

Table S1. The calculated bond angels around the co-dopants in different isoelectronic co-doped black phosphorenes

Co-dopant		Bond angel (°)			
X	*Y*	P_1-*X*-P_2	P_1-*X*-Y	P_3-*Y*-*X*	P_3-*Y*-P_4
phosphorene		95.95	104.14	104.14	95.95
C	O	126.35	103.25	113.97	120.51
C	S	105.14	120.02	115.37	91.59
C	Se	107.26	117.61	110.76	91.48
C	Te	108.45	117.17	105.12	89.48
Si	O	93.29	103.59	117.28	109.28
Si	S	93.47	98.17	106.48	99.05
Si	Se	94.24	97.21	101.68	97.10
Si	Te	95.41	97.54	95.02	93.69
Ge	O	92.72	98.78	115.08	112.29
Ge	S	91.94	94.41	107.00	99.84
Ge	Se	92.44	93.51	102.20	97.67
Ge	Te	93.48	93.80	95.37	94.11
Sn	O	86.90	93.95	114.85	111.37
Sn	S	87.71	87.77	106.70	100.44
Sn	Se	88.18	86.52	102.39	98.15
Sn	Te	89.46	86.63	95.64	94.75
Pb	O	83.92	90.53	113.43	112.21
Pb	S	85.02	84.73	106.34	100.70
Pb	Se	85.39	83.39	102.30	98.30
Pb	Te	86.63	83.23	95.74	94.94

Fig. S1.

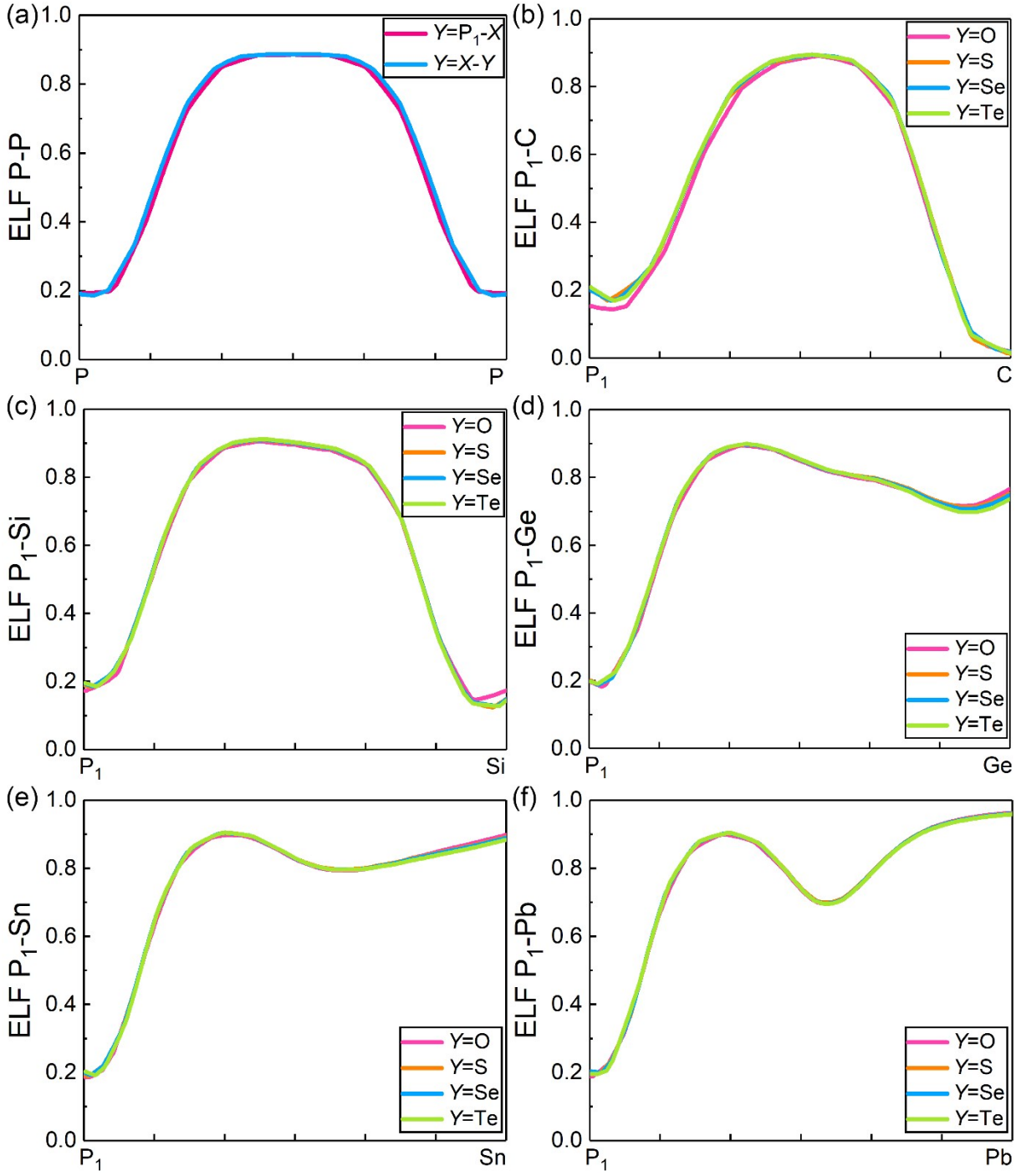

Figure S1. The electronic localization function 2D line profiles of the (a) intraplanar and interplanar P-P bonds in pure phosphorene, and the (b) P_1-C bonds, (c) P_1-Si bonds, (d) P_1-Ge bonds, (e) P_1-Sn bonds, (f) P_1-Pb bonds in different isoelectronic co-doped phosphorenes.

Fig. S2

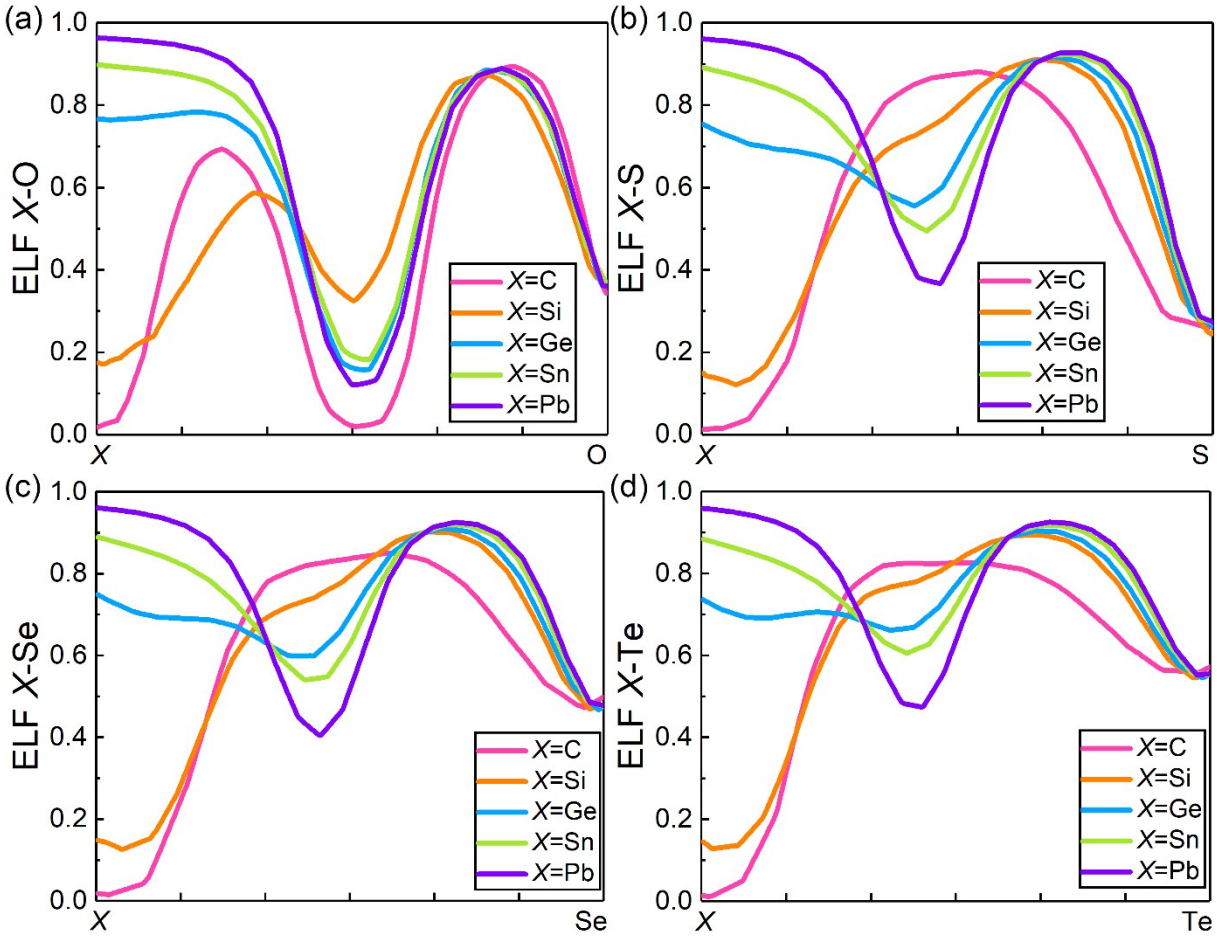

Figure S2. The electronic localization function 2D line profiles of the (a) *X*-O bonds, (b) *X*-S bonds, (c) *X*-Se bonds, and (d) *X*-Te bonds in different isoelectronic co-doped phosphorenes.

Fig. S3

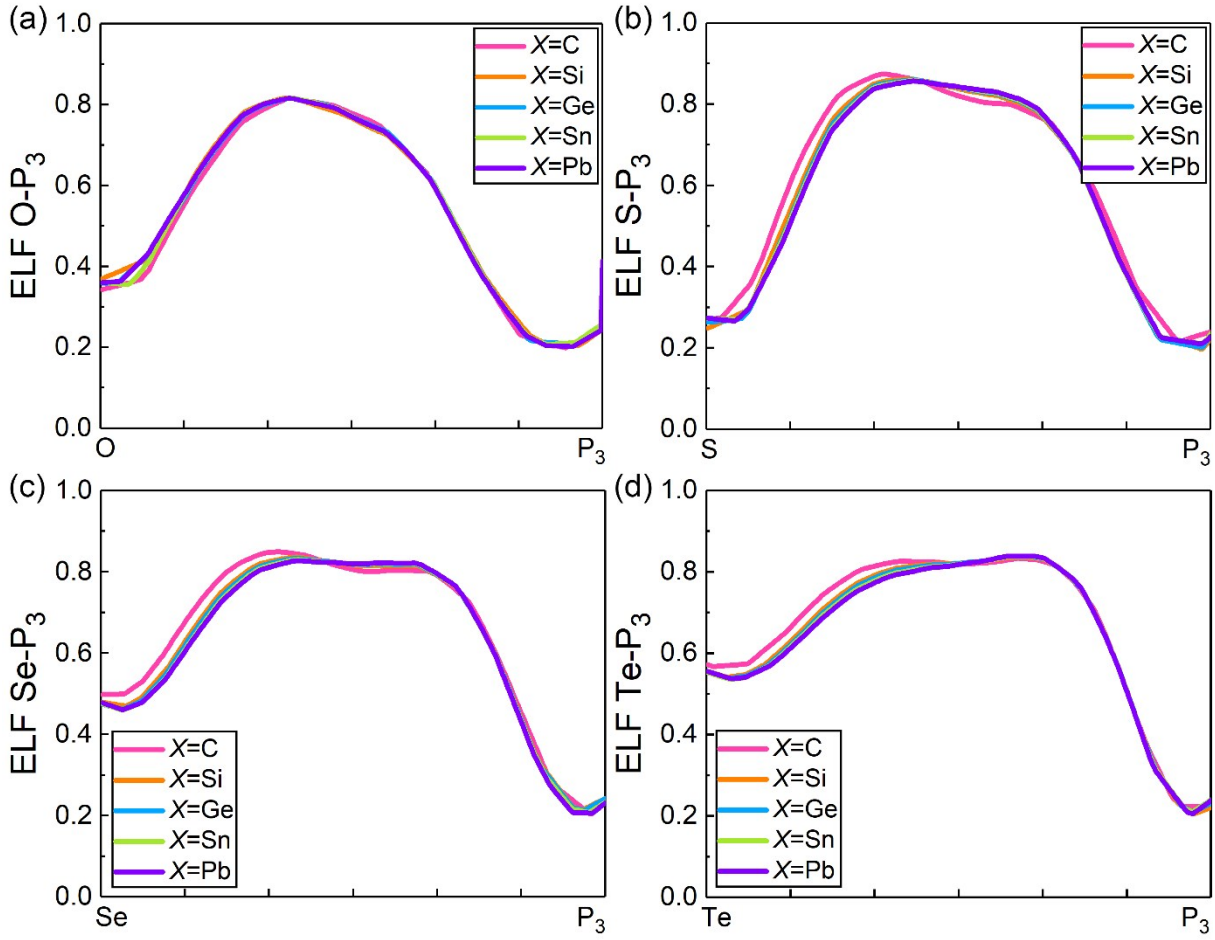

Figure S3. The electronic localization function 2D line profiles of the (a) O-P_3 bonds, (b) S-P_3 bonds, (c) Se-P_3 bonds, and (d) Te-P_3 bonds in different isoelectronic co-doped phosphorenes.

Fig. S4

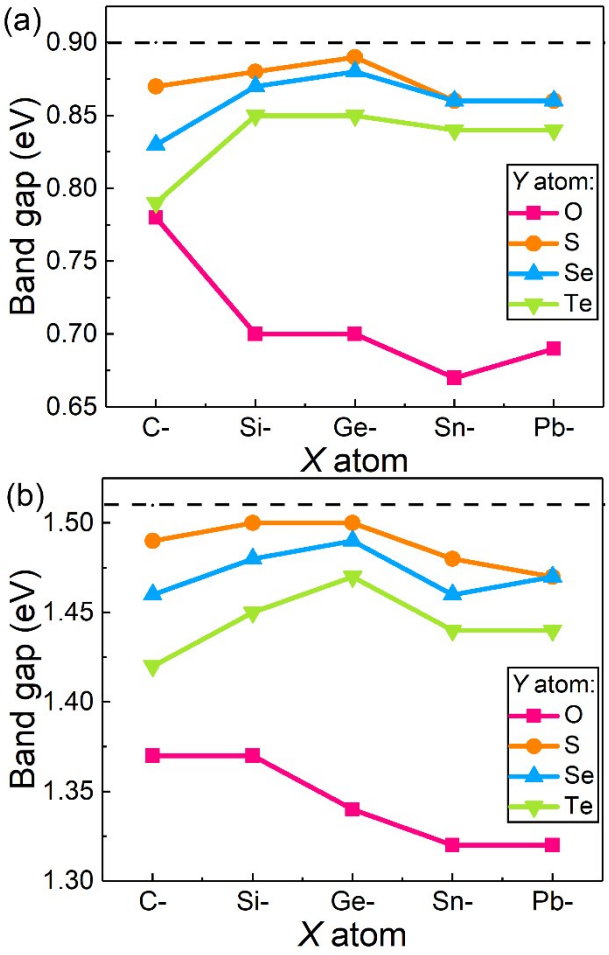

Figure S4. The (a) PBE and (b) HSE06 band gap of different isoelectronic co-doped phosphorenes, the black dash line marks the band gap of pure phosphorenes.

Fig. S5

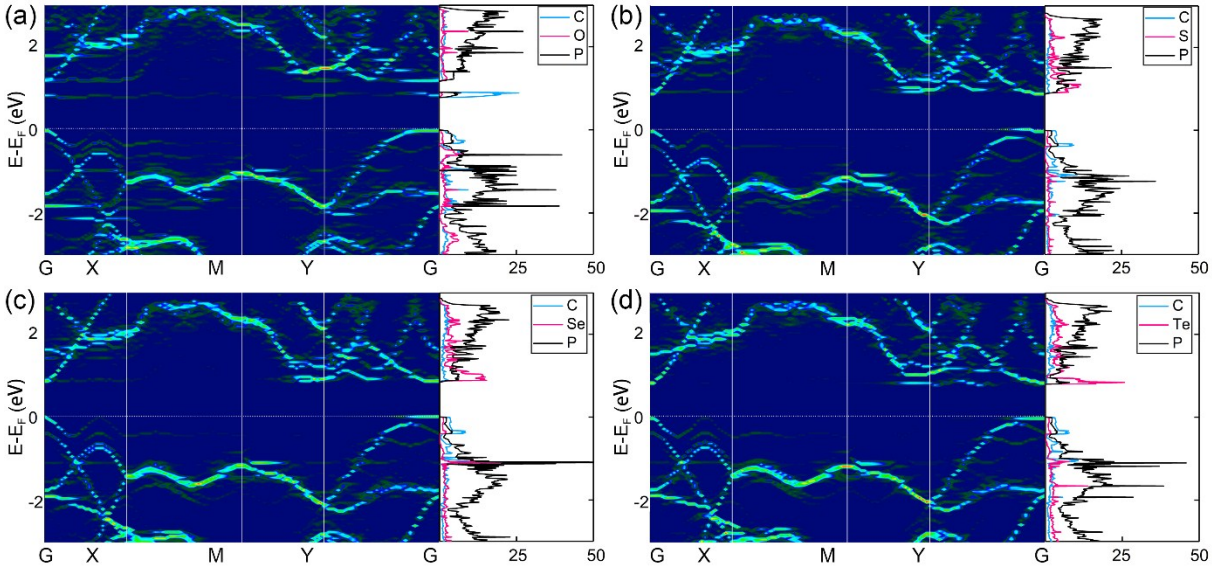

Figure S5. Unfolding PBE band structures and partial density of states of C-*Y* ((a) *Y*=O, (b) *Y*=S, (c) *Y*=Se, (d) *Y*=Te) isoelectronic co-doped phosphorenes. The partial density of states contribution from P, C and *Y* atoms are represented by black, blue and red lines, respectively.

Fig. S6

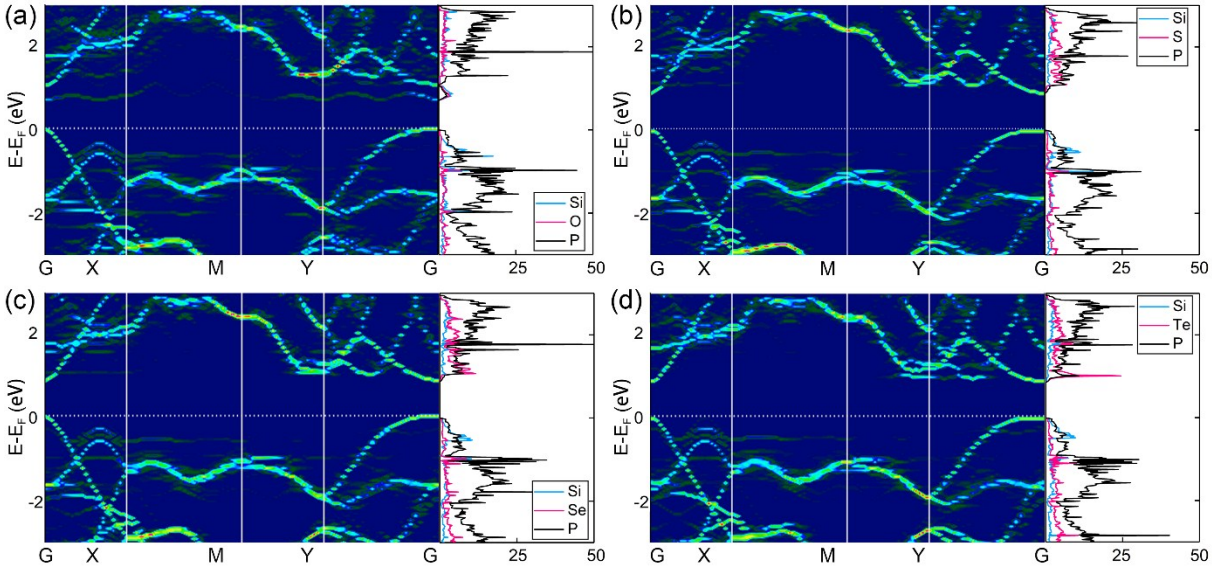

Figure S6. Unfolding PBE band structures and partial density of states of Si-*Y* ((a) *Y*=O, (b) *Y*=S, (c) *Y*=Se, (d) *Y*=Te) isoelectronic co-doped phosphorenes. The partial density of states contribution from P, Si and *Y* atoms are represented by black, blue and red lines, respectively.

Fig. S7

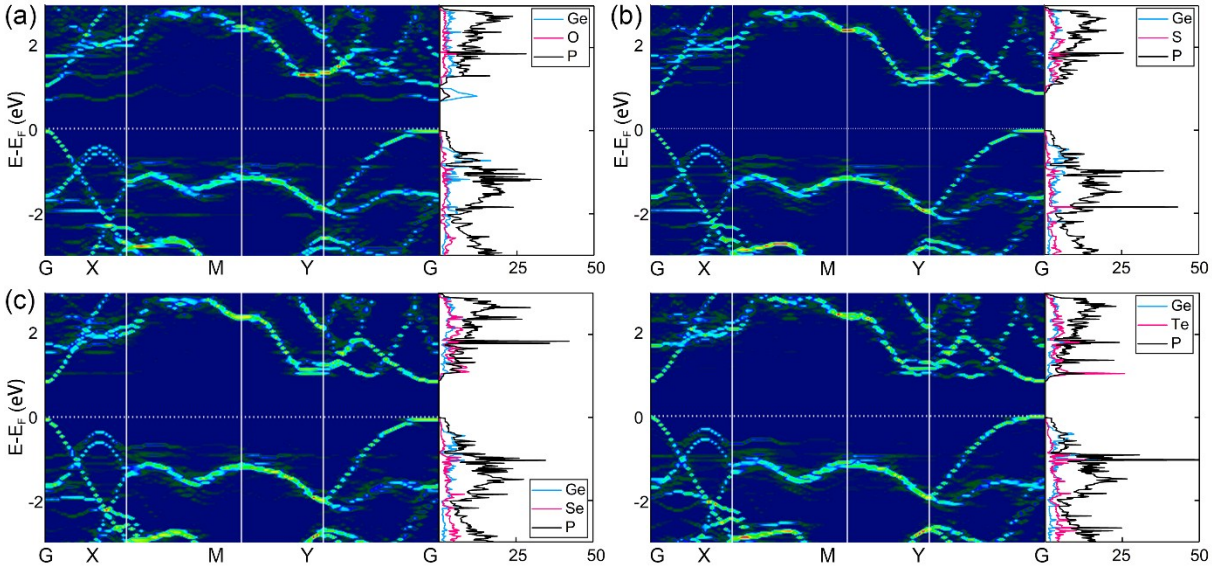

Figure S7. Unfolding PBE band structures and partial density of states of Ge-*Y* ((a) *Y*=O, (b) *Y*=S, (c) *Y*=Se, (d) *Y*=Te) isoelectronic co-doped phosphorenes. The partial density of states contribution from P, Ge and *Y* atoms are represented by black, blue and red lines, respectively.

Fig. S8

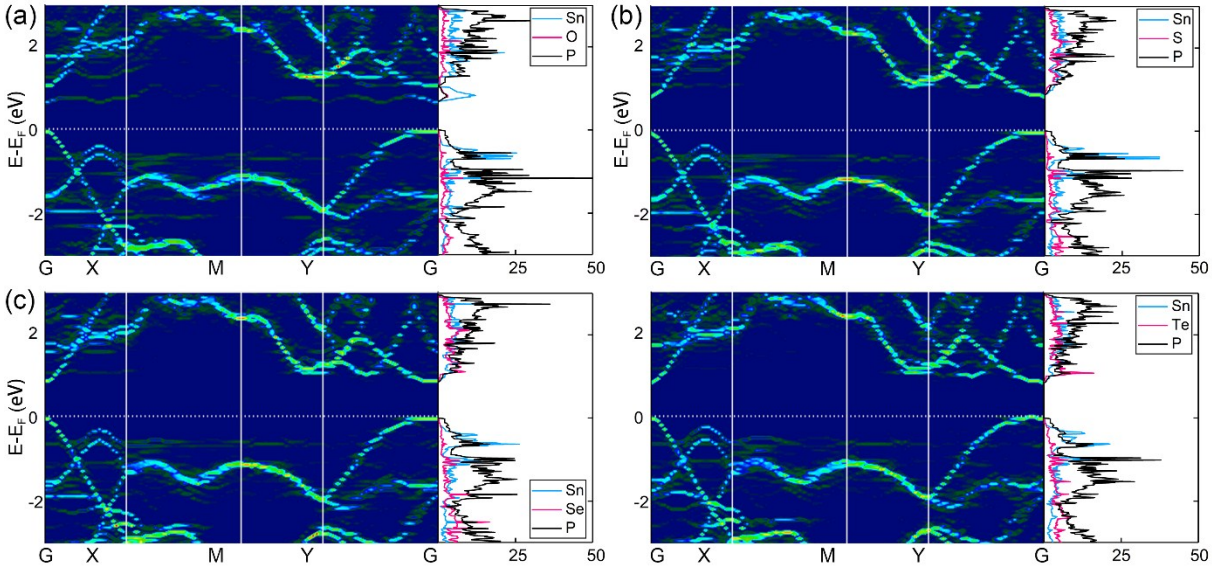

Figure S8. Unfolding PBE band structures and partial density of states of Sn-*Y* ((a) *Y*=O, (b) *Y*=S, (c) *Y*=Se, (d) *Y*=Te) isoelectronic co-doped phosphorenes. The partial density of states contribution from P, Sn and *Y* atoms are represented by black, blue and red lines, respectively.

Fig. S9

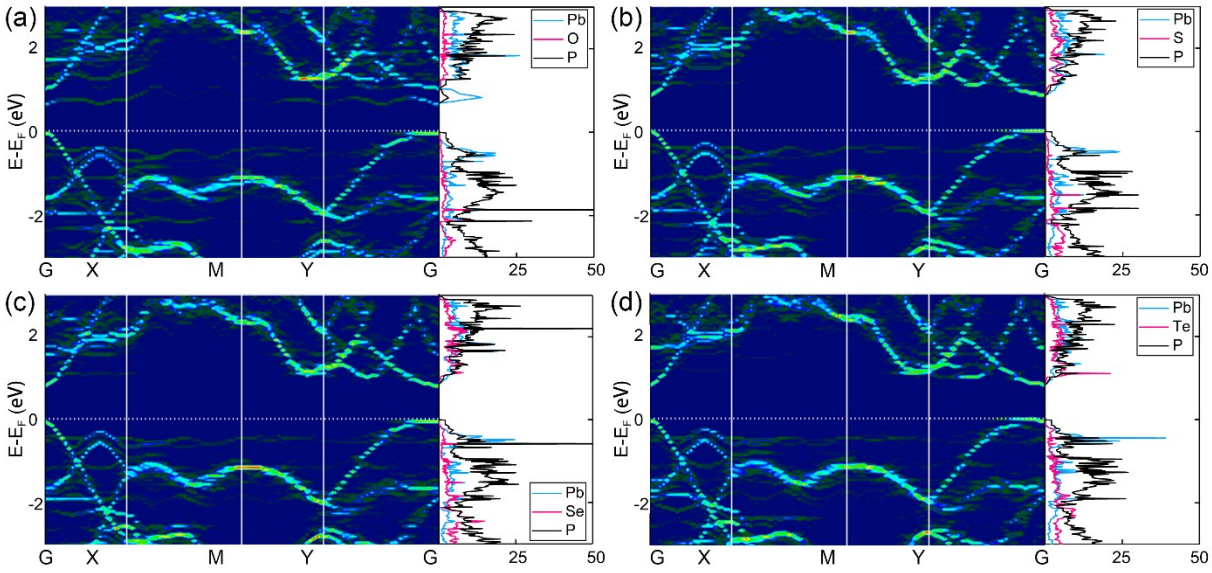

Figure S9. Unfolding PBE band structures and partial density of states of Pb-*Y* ((a) *Y*=O, (b) *Y*=S, (c) *Y*=Se, (d) *Y*=Te) isoelectronic co-doped phosphorenes. The partial density of states contribution from P, Pb and *Y* atoms are represented by black, blue and red lines, respectively.

Fig. S10

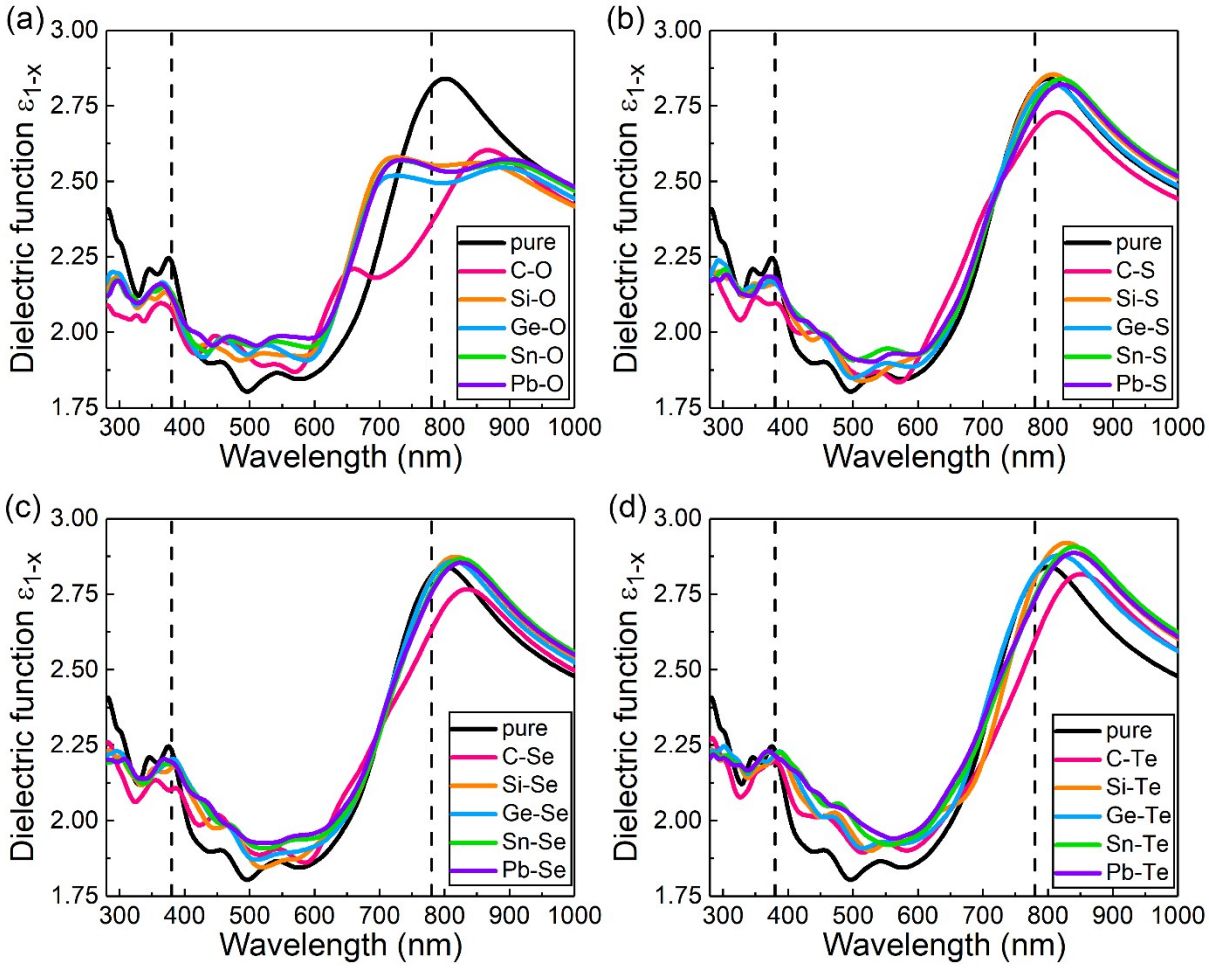

Figure S10. The real part of dielectric functions along the *x* direction of isoelectric co-doped phosphorenes.

Fig. S11

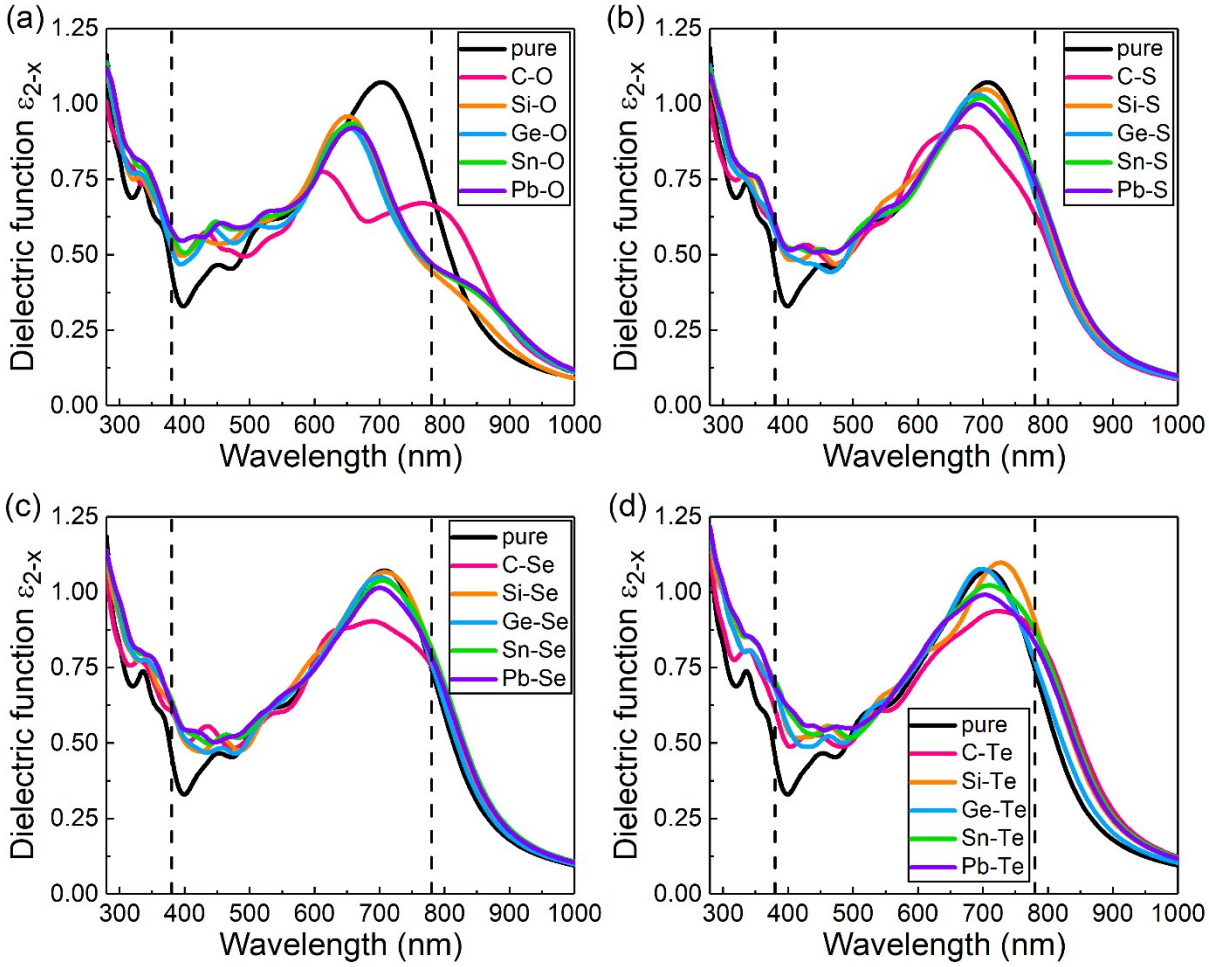

Figure S11. The imaginary part of dielectric functions along the *x* direction of isoelectric co-doped phosphorenes.

Fig. S12

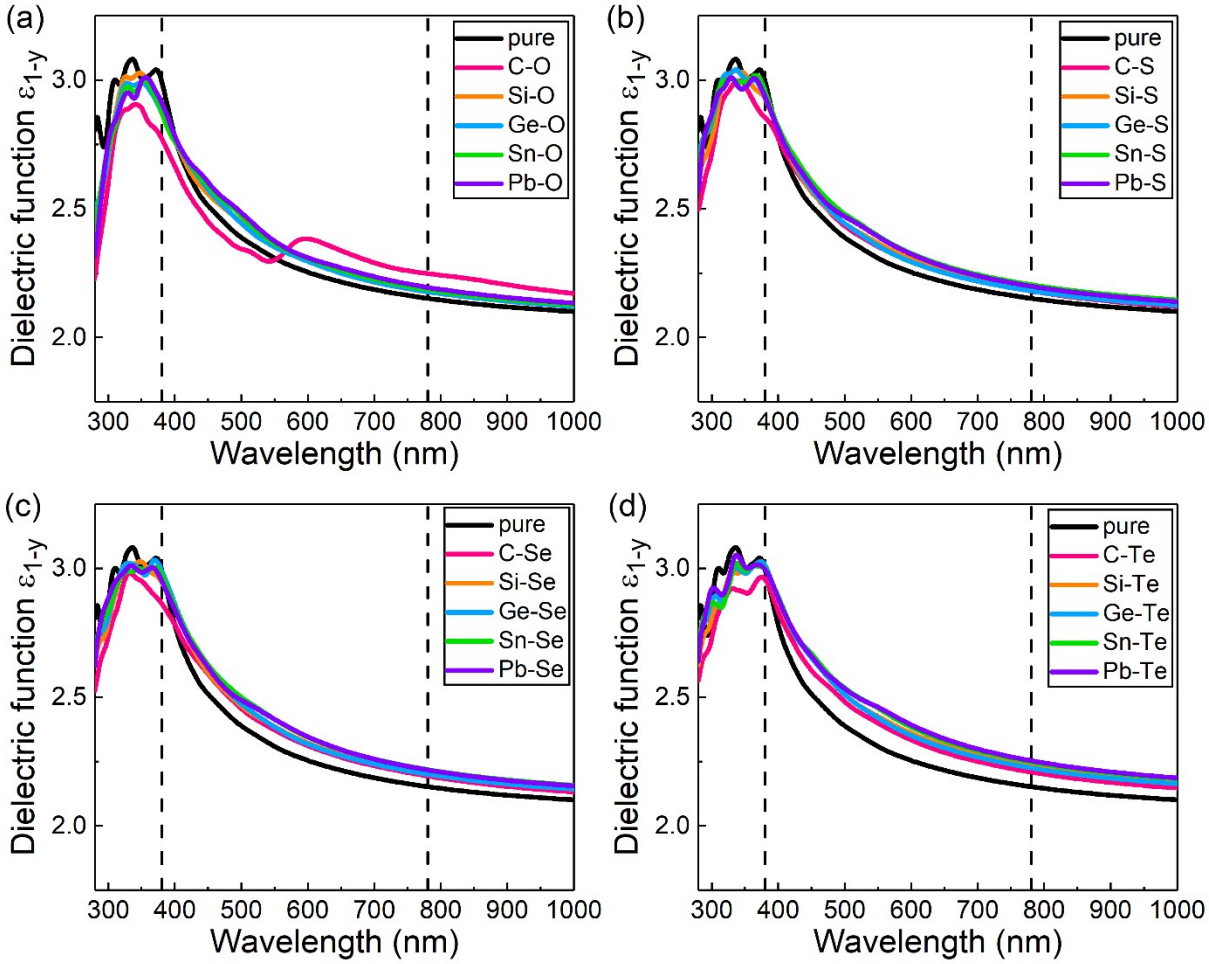

Figure S12. The real part of dielectric functions along the *y* direction of isoelectric co-doped phosphorenes.

Fig. S13

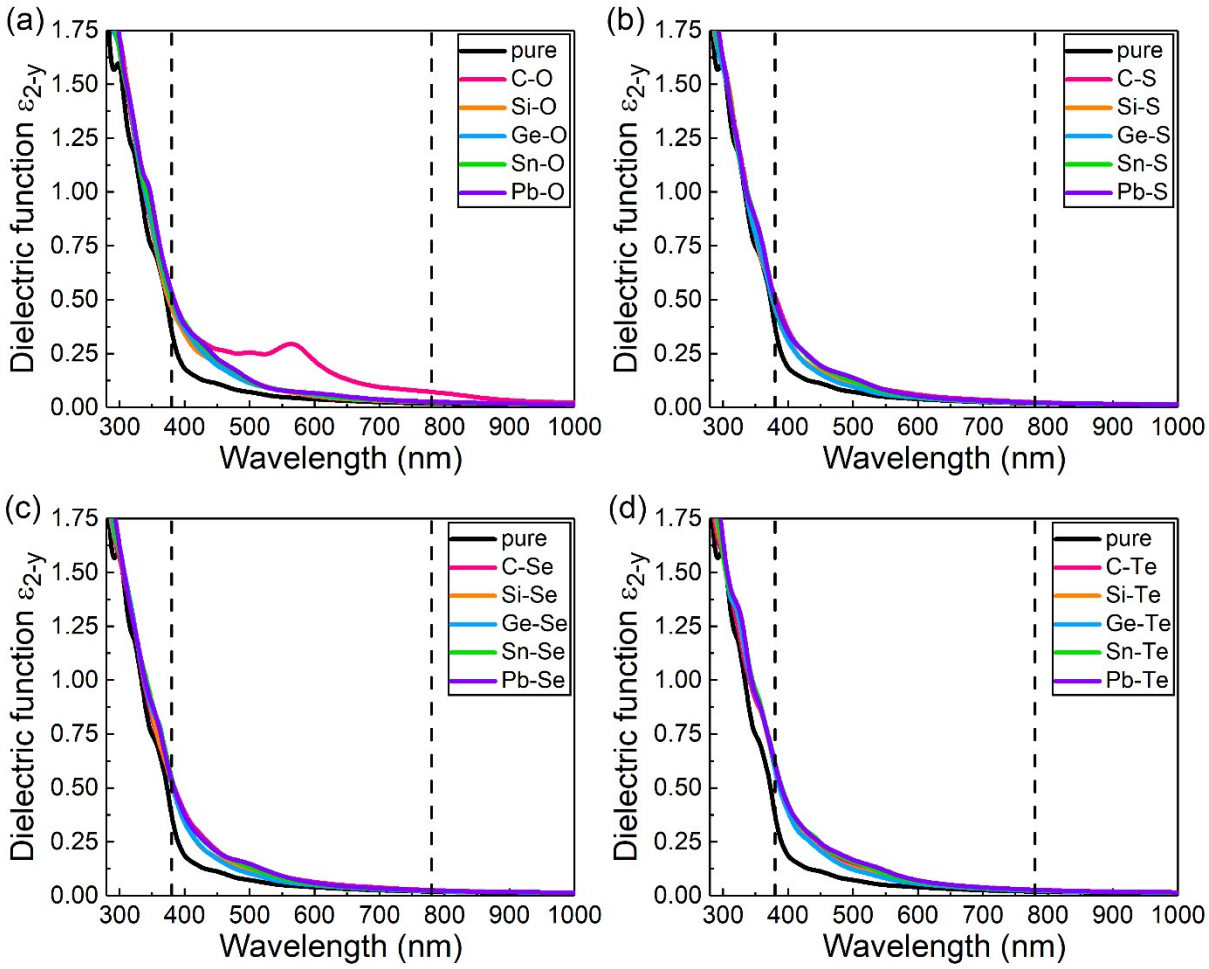

Figure S13. The imaginary part of dielectric functions along the *y* direction of isoelectric co-doped phosphorenes.

Fig. S14

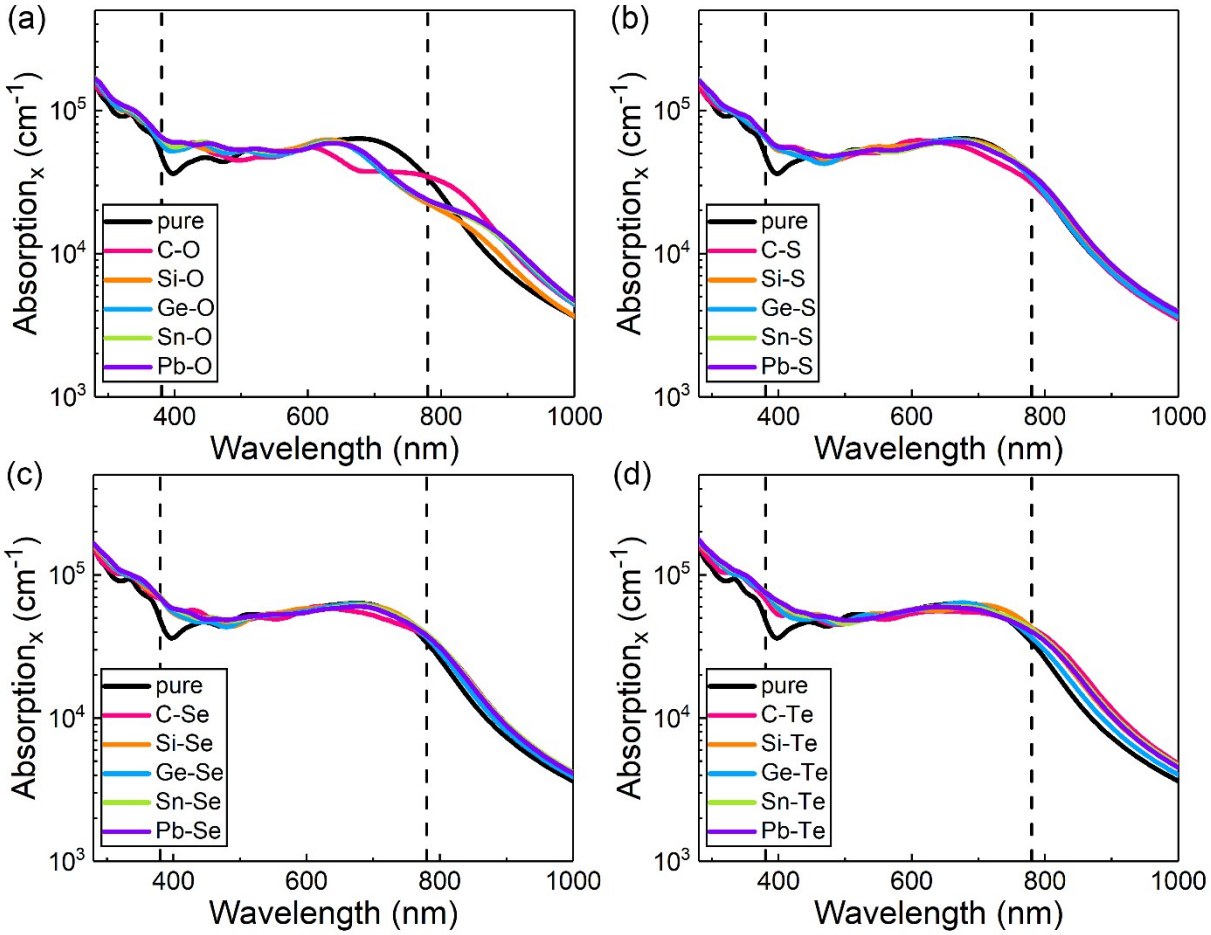

Figure S14. The absorption coefficients along the *x* direction of different isoelectronic co-doped phosphorenes from HSE06 calculations.

Fig. S15

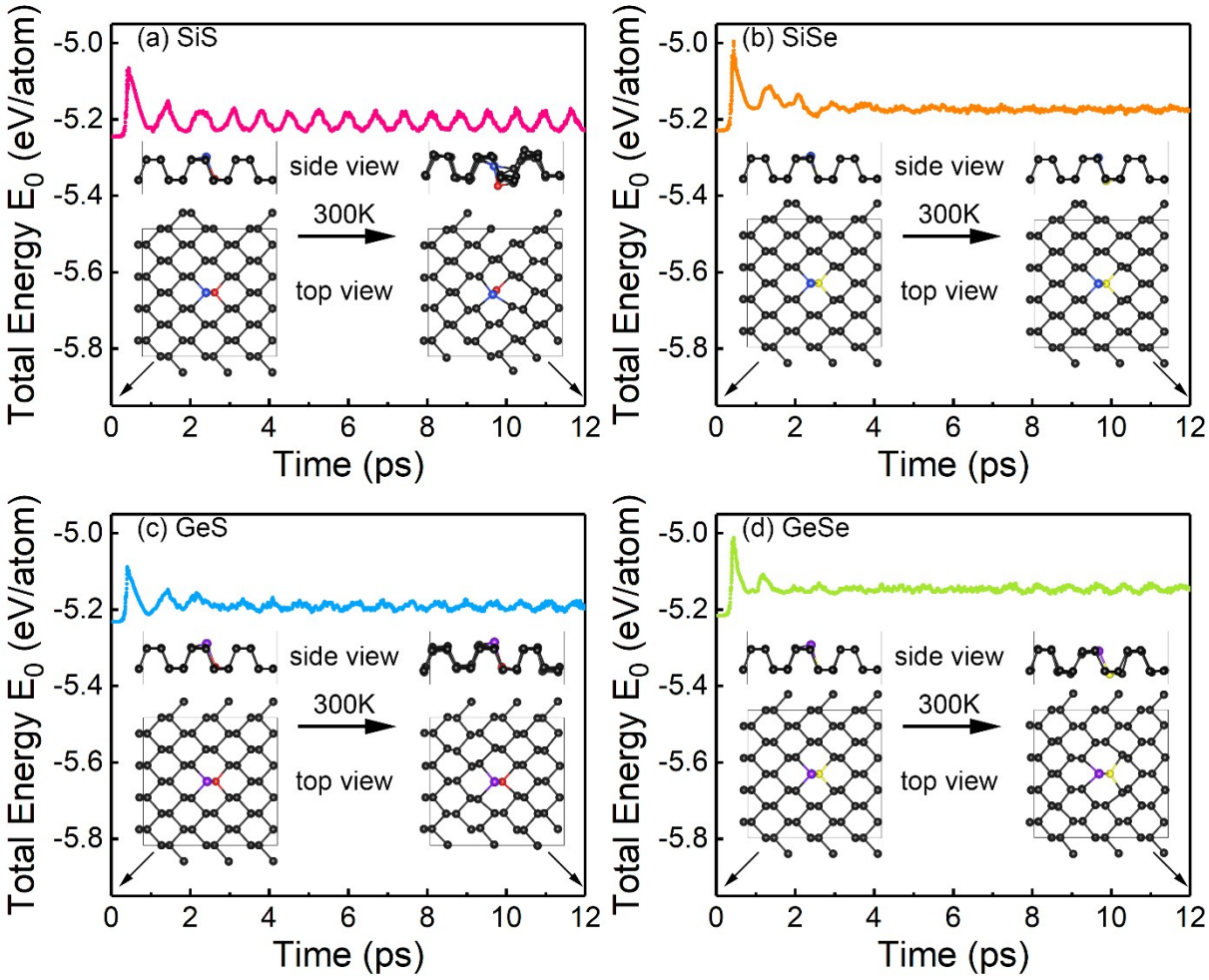

Figure S15. The evolution of total energy of (a)Si-S, (b)Si-Se, (c)Ge-S and (d)Ge-Se isoelectronic co-doped BPs.