Supporting Information

The Electronic Structure, Mechanical Flexibility and Carrier Mobility of Black Arsenic-Phosphorus monolayer: A First Principles Study

Jie Sun,^a Na Lin,^{a,*} Hao Ren,^b Cheng Tang,^a Letao Yang,^a Xian Zhao^{a,*}

^a State Key Laboratory of Crystal Materials, Shandong University, 250100 Jinan, Shandong, PR China

^b State Key Laboratory of Heavy Oil Processing & Center for Bioengineering and Biotechnology, China University of Petroleum (East China), 266580 Qingdao, PR China

*Corresponding authors: <u>linnakth@gmail.com</u>, <u>xianzhao@sdu.edu.cn</u>.



Section 1. The constructed structures of b-AsP systems for each composition.

(a)



 $As_{0.5}P_{0.5}$

(b)



(c)

Figure S1. The constructed structures of b-AsP systems for (a) $As_{0.33}P_{0.67}$ (b) $As_{0.5}P_{0.5}$ (c) $As_{0.67}P_{0.33}$

Section 2. The typical As-As, As-P and P-P bond lengths for different Arsenic compositions.

		In plane			Out plane	
	P-P(Å)	As-P(Å)	As-As(Å)	P-P(Å)	As-P(Å)	As-As(Å)
BP	2.22	-	-	2.25	-	-
As _{0.33} P _{0.67}	2.22~2.25	2.35~2.38	2.45~2.46	2.23~2.24	2.40~2.42	2.51~2.52
As _{0.5} P _{0.5}	2.24~2.25	2.37~2.39	2.46~2.47	2.22~2.23	2.38	2.49~2.52
$As_{0.67}P_{0.33}$	2.23~2.25	2.37~2.39	2.47~2.50	2.23	2.36~2.39	2.50~2.52

Table S1. The typical As-As, As-P and P-P bond lengths for different Arsenics compositions.

Section 3. The cleavage energies of b-AsP systems with PBE+D3 method.



Figure S2. Cleavage energies Ecl in J/m^2 (full symbol curve) and their derivatives σ in GPa (empty symbol curve) as a function of the separation distance d for a fracture in bulk b-AsP systems.

Section 4. The in-plane and out-plane bond variation of b-AsP systems from the stable state to the instability point state.

To estimate the stability of P-P and P-As bond in the b-AsP systems, we calculate the in-plane and out-plane bond variation of b-AsP systems from the stable state to the instability point state and a statistic results are shown in Figure S3 (a)-(d). Figure 3(a) and 3(b) show the in-plane bond variation of b-AsP systems under critical strain along the armchair and zigzag, respectively. We can see that the contraction of P-P bond is larger than that of P-As bond under critical strain along the armchair direction, which indicates the P-As bond is more stable than P-P bond in this case. As applying the critical strain along the zigzag direction, the elongation of the As-P bond is larger than that of P-P bond, demonstrating the P-P bond is more stable than P-As bond in this case. Similarly, the out-plane P-P bond is more stable than P-As bond under critical strain along the armchair direction (Figure S3 (c)), while P-As bond is much more stable under critical strain along the zigzag direction (Figure S3 (d)).



Figure S3. (a) and (b) are in-plane bond variations of b-AsP systems under critical strain along the armchair and zigzag directions, respectively. (c) and (d) are out-plane bond variations under critical strain along the armchair and zigzag directions, respectively.



Section 5. The electronic band structures of b-AsP systems with HSE06.

Figure S4. The electronic band structures of b-AsP systems with HSE06.

Section 6. The electronic band structures of b-AsP systems are calculated by PBE with SOC.



Figure S5. The electronic band structures of b-AsP systems calculated by PBE with SOC. Insets provide a magnification to show the SOC effects on the band structure.

Section 7. Band structures of b-AsP systems under uniaxial strain. Positive strain indicates expansion, while negative corresponds to compression. The position of the CBM and VBM are labeled with circles. The same colors of two circles represent the direct band gap and different colors represent the indirect band gap.



Figure S6. Band structures of pure BP under strain along the armchair direction.



Figure S7. Band structures of pure BP under strain along the zigzag direction.



Figure S8. Band structures of $As_{0.33}P_{0.67}$ under strain along the armchair direction.



Figure S9. Band structures of $As_{0.33}P_{0.67}$ under strain along the zigzag direction.



Figure S10. Band structures of $As_{0.5}P_{0.5}$ under strain along the armchair direction.



Figure S11. Band structures of $As_{0.5}P_{0.5}$ under strain along the zigzag direction.



Figure S12. Band structures of $As_{0.67}P_{0.33}$ under strain along the armchair direction.



Figure S13. Band structures of $As_{0.67}P_{0.33}$ under strain along the zigzag direction.

Section 8. The linear fit of the band energy shifts of the VBM and the highest CBM as a function of strain along the armchair and zigzag directions.





Figure S14. Shifts of conduction band and valence band under uniaxial strain: (a) valence and (b) conduction band along the armchair direction, (c) valence and (d) conduction band along the zigzag direction. The black dashed line is the linear fitting. The inset table shows the deformation potential E_1 and the standard fitting error.