Supplemental Information for:

BX$_1$-BX$_2$ ($X_1$, $X_2$ = P, As, Sb) Lateral Heterostructure: Novel and Efficient Two-Dimensional Photovoltaic Materials with Ultra-high Carrier Mobilities

Qiang Wang,$^{a,b}$ Jianwei Li,$^b$ Yan Liang,$^{b,c}$ Bin Wang,*$^{b,d}$ and Yihang Nie,*$^a$

$^a$Institute of Theoretical Physics, State Key Laboratory of Quantum Optics and Quantum Optics Devices, Institute of Opto-Electronics, Shanxi University, Taiyuan 030006, People’s Republic of China

$^b$Shenzhen Key Laboratory of Advanced Thin Films and Applications, College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, 518060, People’s Republic of China

$^c$School of Physics, State Key Laboratory of Crystal Materials, Shandong University, 250100 Jinan, People’s Republic of China

$^d$Center for Quantum Computing, Peng Cheng Laboratory, Shenzhen, 518055, People's Republic of China.

Corresponding Authors:

*E-mail: nieyh@sxu.edu.cn

binwang@szu.edu.cn
Fig. S1 Band structures of (a) armchair BP-BAs supercell, (b) armchair BAs-BSb supercell, (c) zigzag BP-BAs supercell, (d) zigzag BAs-BSb supercell at HSE06 level. The horizontal dash lines show the Fermi level.

Fig. S2 Band structures of (a) armchair and (b) zigzag BAs-BSb LHSs with (black curves) and without (red curves) SOC effect.
Fig. S3 Band structures of individual 2D BAs (a) and individual 2D BSb (b) with 5% or without scaling of lattice constant. 5% means the amplification of lattice constant, and -5% means the contraction of lattice constant.

Fig. S4 (color online) Averaged effective potential profile along the transport direction for (a) BP-BAs and (b) BAs-BSb devices, where the top and bottom sides are for the armchair and zigzag interlines, respectively.
Fig. S5 (color online) The density of states (Dos) versus energy for the four LHS with (a) armchair BP-BAs interline, (b) armchair BAs-BSb interline, (c) zigzag BP-BAs interline, and (d) zigzag BAs-BSb interline. The green dash lines in each panel indicate the fermi levels.