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

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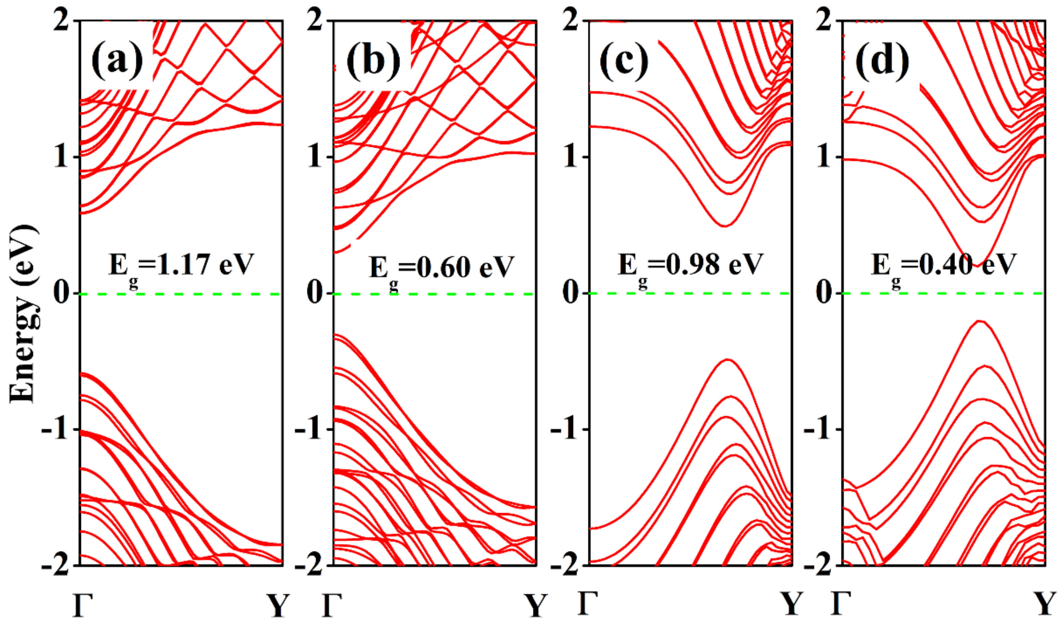

Fig. S1 Band structures of (a) armchair BP-BAs supercell, (b) armchair BAs-BSb supercell, (c) zigzag BP-BAs supercell, (d) zigzag BAs-BSb supercell at HSE06 level. The horizontal dash lines show the Fermi level.

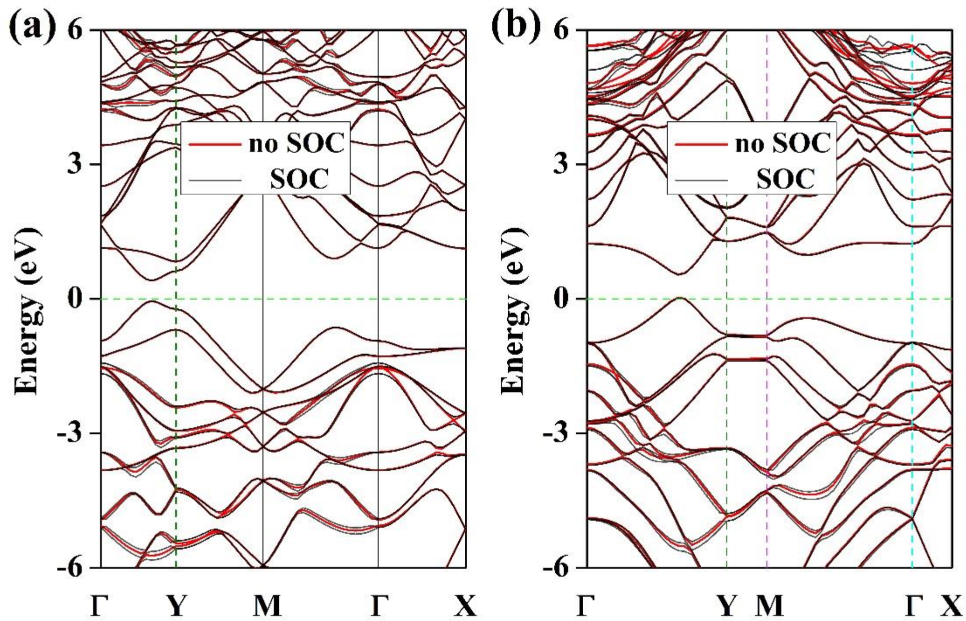

Fig. S2 Band structures of (a) armchair and (b) zigzag BAs-BSb LHSs with (black curves) and without (red curves) SOC effect.

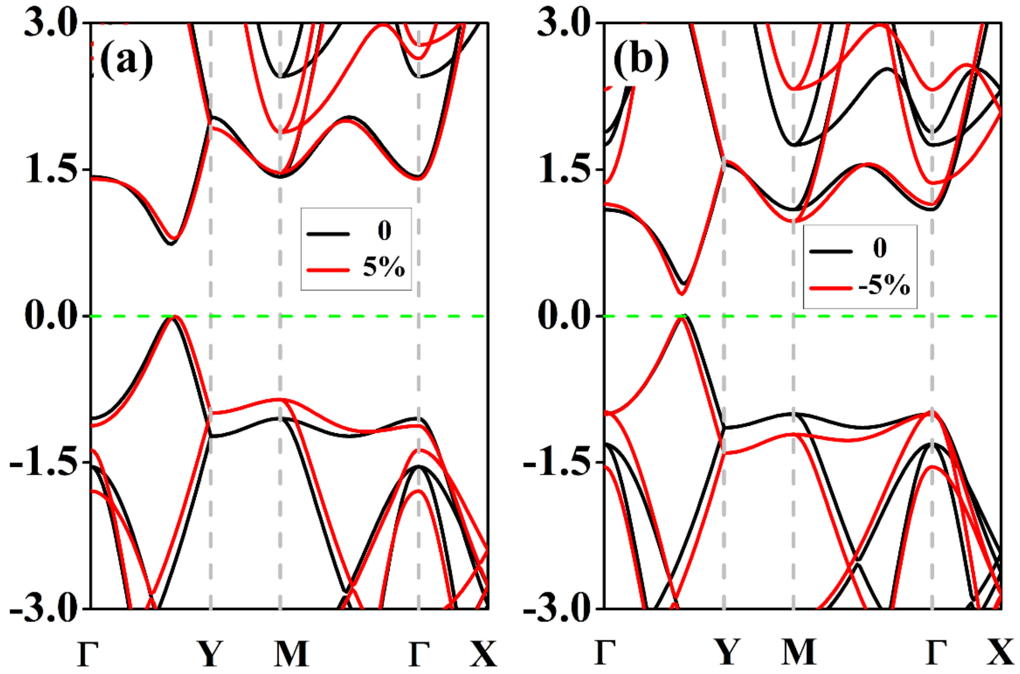

Fig. S3 Band structures of individual 2D BAs (a) and individual 2D BSb (b) with 5% or without scaling of lattice constant. 5% means the amplification of lattice constant, and -5% means the contraction of lattice constant.

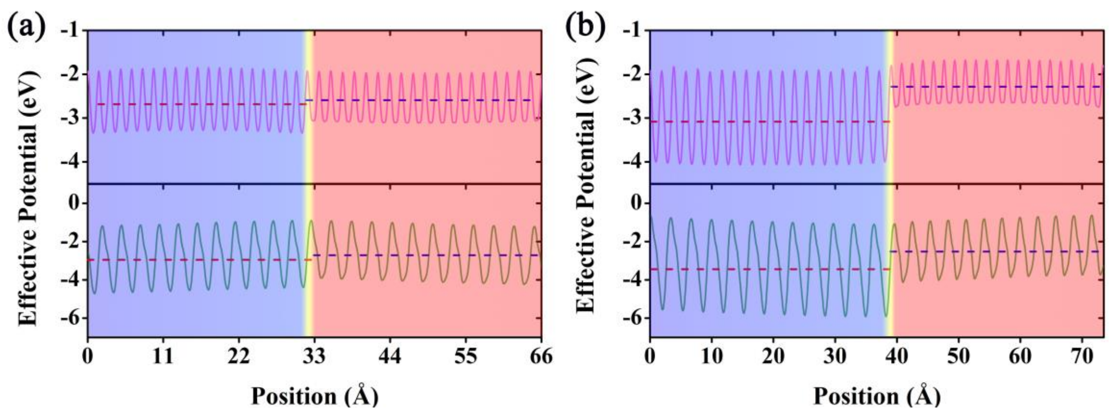

Fig. S4 (color online) Averaged effective potential profile along the transport direction for (a) BP-BAs and (b) BAs-BSb devices, where the top and bottom sides are for the armchair and zigzag interlines, respectively.

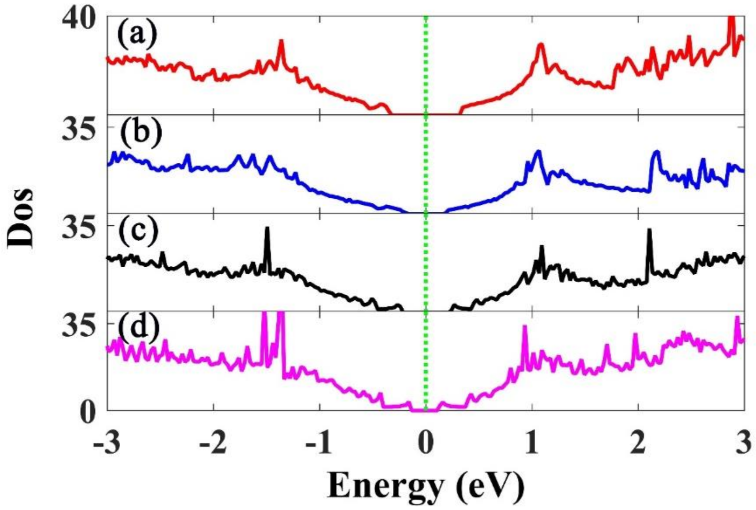

Fig. S5 (color online) The density of states (Dos) versus energy for the four LHS with (a) armchair BP-BAs interline, (b) armchair BAs-BSb interline, (c) zigzag BP-BAs interline, and (d) zigzag BAs-BSb interline. The green dash lines in each panel indicate the fermi levels.