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**Supplemental Information for:**

# Universal co-existence of photovoltaics and ferroelectricity from two-dimensional 3R bilayer BX (X=P, As, Sb)

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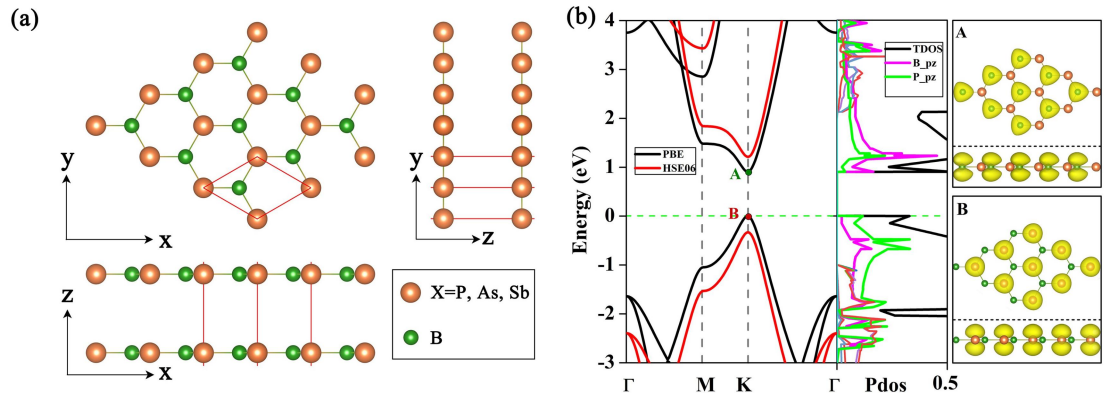


**Fig. S1 (color online) (a) Top and side views of the schematic structures of 2D bilayer 1T BX (X=P, As, Sb), where X and B atoms are labeled by orange and green balls and the smallest unit cell is marked with red lines, too. (b) Band structures (left panels), PDOS (middle panels), and Partial charge densities at the CBM and VBM (right panels) of monolayer BP.**

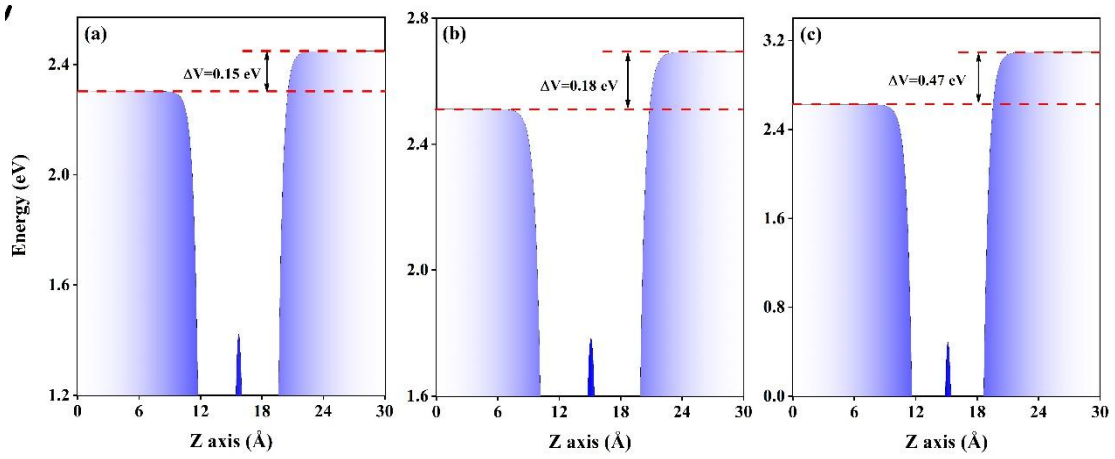


**Fig. S2 Plane averaged electrostatic potential of bilayer 2D 3R (a) BP, (b) BAs, and (c) BSb along the z direction. In each panel, the potential differences between top and bottom layers of the corresponding crystals are marked by ΔV.**

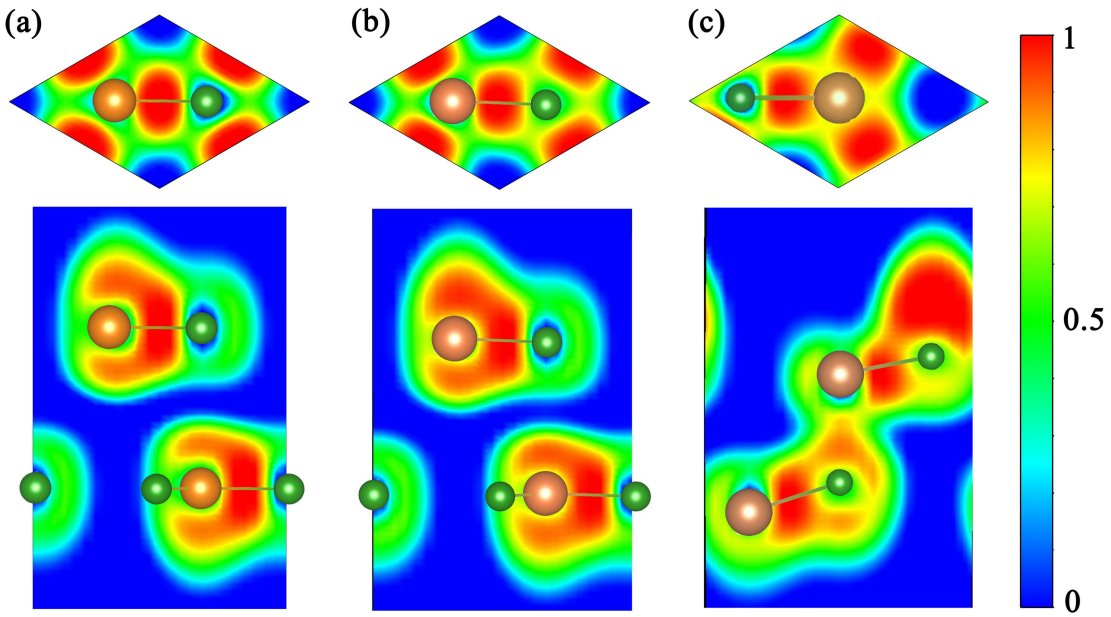


**Fig. S3 (color online) Top and side views of the ELF distributions along arbitrary in-plane directions of 2D bilayer 3R (a) BP, (b) BAs, and (c) BSb, respectively.**

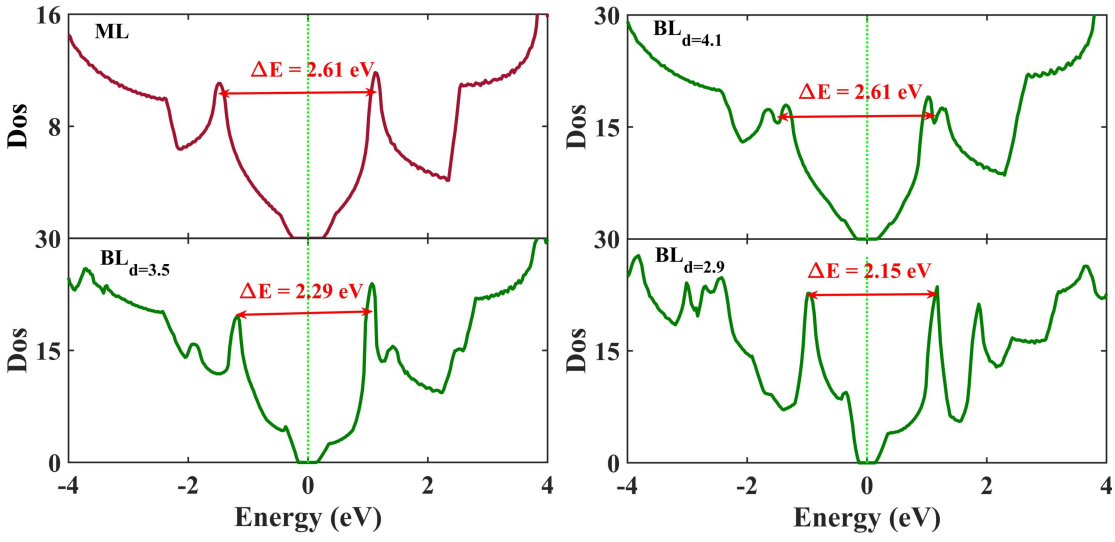


**Fig. S4 (color online) The density of states (Dos) versus energy for monolayer BP (a) and bilayer 3R BP devices with interlayer distance d is equal to 4.1Å (b) 3.5 Å (c) and 2.9 Å (d). The green dash lines in each panel indicate the fermi levels.**

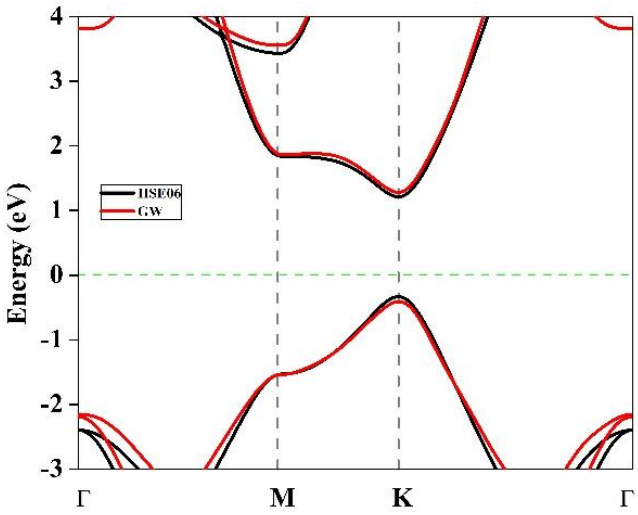


**Fig. S5 band structures of monolayer BP at HSE06 and $G_0W_0$ levels. For the $G_0W_0$ calculation, a vacuum thickness of 25 Å was added to eliminate the interaction between periodic slabs; The NBANDS=144 and ENCUTGW=200 were set, and the $20 \times 20 \times 1$ k-points samplings were employed for quasi-particle (PQ) calculations, where a combination of PBE and one-shot $G_0W_0$ correction was adopted.**