

Electronic Supplementary Information

Huge Rashba type spin orbit coupling in binary hexagonal PX nanosheets (X = As, Sb, and Bi)

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I. Phonon dispersion of the biaxially tensile-strained PBi nanosheet.

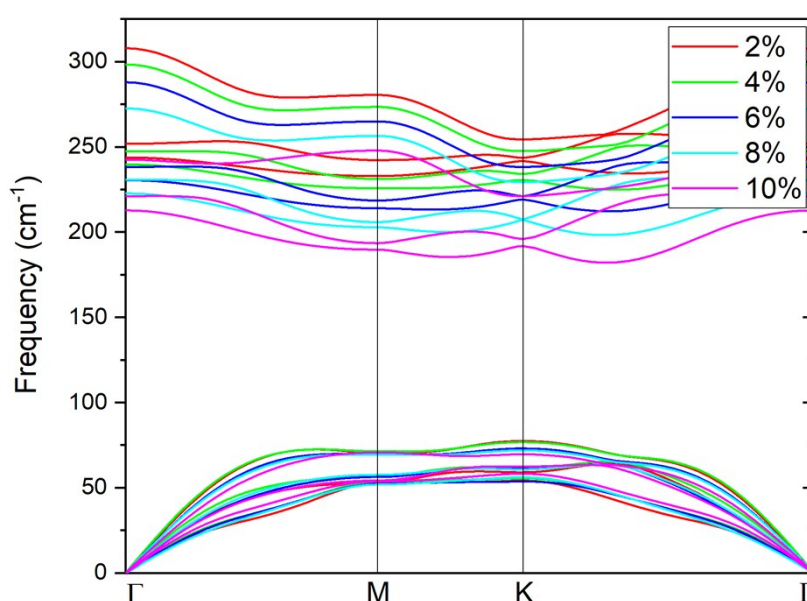


Figure S1. Phonon dispersion of the biaxially tensile-strained PBi nanosheet.

II. A positive correlation between Rashba coefficients and the net macroscopic electric fields.

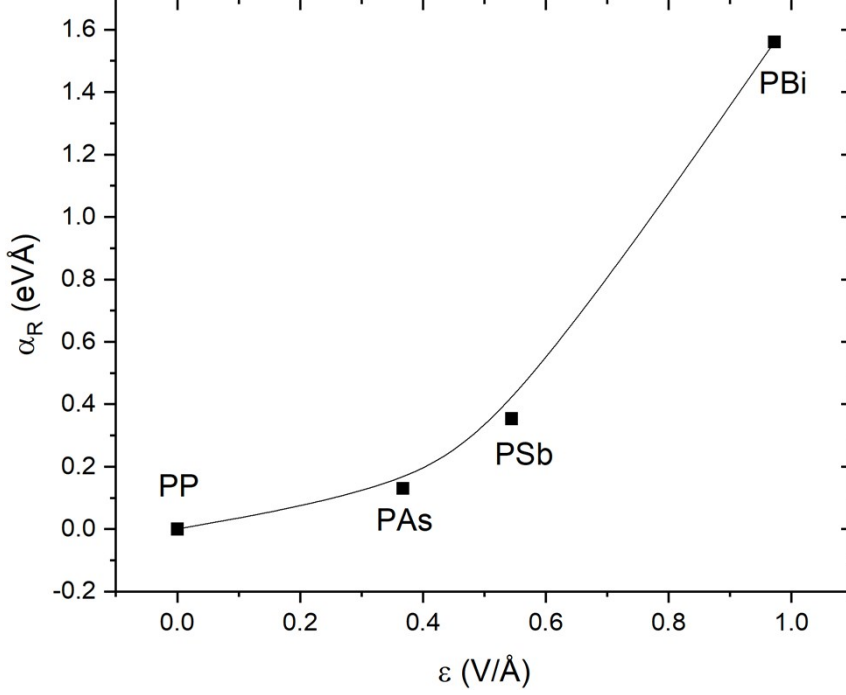


Figure S2. Rashba coefficients (α_R) versus net electric fields (ϵ).

III. Formation of band gap due to the inversion symmetry breaking and the SOC.

In single layer PP, the inversion symmetry is preserved due to the equivalence of two P atoms in a primitive cell. The lowest conduction band (CB1) and the next conduction band (CB2) belong to different irreducible representations, for example, the irreducible representations for the CB1 and CB2 at the M point are A_g and B_u , respectively. Thus, the two bands are allowed to cross each other, for instance, the two bands cross at around the middle point along the K-M path (see grey shaded regions in Fig. 2). However, the symmetry is lowered when one of sublayers is replaced by another type of pnictogen element. The two CBs now belong to the same irreducible representation. Hence, they avoid crossing each other. Such an anticrossing results in the gap formation, which could be simply understood from a two-level system.

For single layer PP, the effective Hamiltonian ($H(PP)$) for CB1 and CB2 at the band crossing point can be roughly expressed as

$$H(PP) = \begin{bmatrix} \langle p(P)|H|p(P) \rangle & 0 \\ 0 & \langle p(P)|H|p(P) \rangle \end{bmatrix} \equiv \begin{bmatrix} E_p(P) & 0 \\ 0 & E_p(P) \end{bmatrix}, \quad (S1)$$

where H in the matrix is just the single particle Hamiltonian, and $|p(\bullet)\rangle$ represents the linear superposition of valence p orbitals of the \bullet atom since the CB1 and CB2 are mainly contributed the p orbitals of atoms. The $E_p(P) \equiv \langle p(P)|H|p(P) \rangle$ is the band energy at the crossing point, which is mainly determined by the energy of valence p orbital of P atoms.

While in the binary system of PX, the effective Hamiltonian ($H(PX)$) is given by

$$H(PX) = \begin{bmatrix} \langle p(P)|H|p(P) \rangle & \langle p(P)|H|p(X) \rangle \\ \langle p(X)|H|p(P) \rangle & \langle p(X)|H|p(X) \rangle \end{bmatrix} \equiv \begin{bmatrix} E_p(P) & \Delta \\ \Delta^* & E_p(X) \end{bmatrix}. \quad (S2)$$

By diagonalizing this matrix, we can obtain the two eigenvalues,

$$E_{\pm} = \frac{1}{2}(E_p(P) + E_p(X)) \pm \sqrt{(E_p(P) - E_p(X))^2 + 4\Delta^2}. \quad (S3)$$

Apparently, the originally degenerated bands now split into two non-degenerated bands, and the energy splitting ($E_+ - E_-$) is determined by the energy difference between the energy difference of p orbitals between P and X atoms as well as the non-vanishing overlap between them. Intuitively, the energy of valence p orbital of X atoms will gradually decrease as the atomic number of X increases from As to Bi. Consequently, there is a band gap formed between the two CBs, and the magnitude of band gap gradually increases as the atomic number of X increases as shown in Fig. 2, which is consistent with the direct calculations of band structures (see Fig. 2).

But once the SOC is included, the CBs will further split into two bands due to the strong SOC interaction. Hence, the newly formed band gap between the two bands is narrowed.

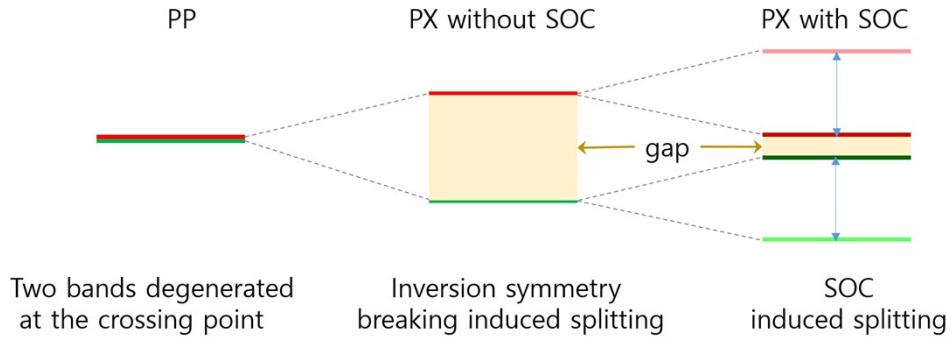


Figure S3. Underlying mechanism of gap formation between lowest two conduction bands.