Supplementary Material

Elemental ferroelectric topological insulator in *ψ*-bismuthene

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Note 1

To confirm the nontrivial topological order in ψ-bismuthene, the $\mathbf{Z}_2$ invariant is obtained by tracking the evolution of the Wannier charge center (WCC).[1,2] The Wannier functions (WFs) with regard to the lattice vector R is written as: [3]

$$|Rn>=\frac{1}{2\pi}\int_{-\pi}^{\pi} dke^{-ik(R-x)}|u_{nk}>$$

The WFs depend on the gauge choice for the Bloch states $|u_{nk}>$. Following Soluyanov and Vanderbilt's description, to optimally localize the WFs, the WCCs are defined as the mean value of the position operator defined by the mean value of $\bar{x}_n = <0_n|\hat{X}|0_n>$, where the $\hat{X}$ represent the position operator and 0_n is the state corresponding to a WF in the cell with R = 0.[4] Then we obtain

$$\bar{x}_n=\frac{i}{2\pi}\int_{-\pi}^{\pi} dk<u_{nk}|\nabla_k|u_{nk}>$$

Taking into account that $\sum_{\alpha}\bar{x}_{\alpha}^{S}=\frac{1}{2\pi}\int_{BZ}A^{S}$ for S = I or II, the summation in α is the occupied states and A is Berry connection, yielding the $\mathbf{Z}_2$ invariant following

$$Z_2=\sum_{\alpha}[\bar{x}_{\alpha}^{I}\left(\frac{T}{2}\right)-\bar{x}_{\alpha}^{II}\left(\frac{T}{2}\right)]-\sum_{\alpha}[\bar{x}_{\alpha}^{I}(0)-\bar{x}_{\alpha}^{II}(0)]$$

here I and II are the Kramer partners. The identification of $\mathbf{Z}_2$ invariant can be obtained by counting the numbers of crossing between any arbitrary horizontal reference line and evolution of the WCCs, in which the odd number equals to $\mathbf{Z}_2$ =1, revealing the nontrivial topological nature.

Since the bands near the Fermi level are primarily contributed by the *p* orbitals of Bi atoms, these orbitals are selected as projections to construct the maximally localized Wannier functions (MLWFs).[4-

[6] A total of 48 bands, spanning discrete bands 17 to 64, along with 4 additional empty bands within the energy window of -6 to 6 eV relative to the Fermi level, are chosen for disentanglement, resulting in a set of well-localized WFs. Additionally, the spin Hall conductivity and Berry curvature calculations are performed using the Wannier interpolation method.[7,8]

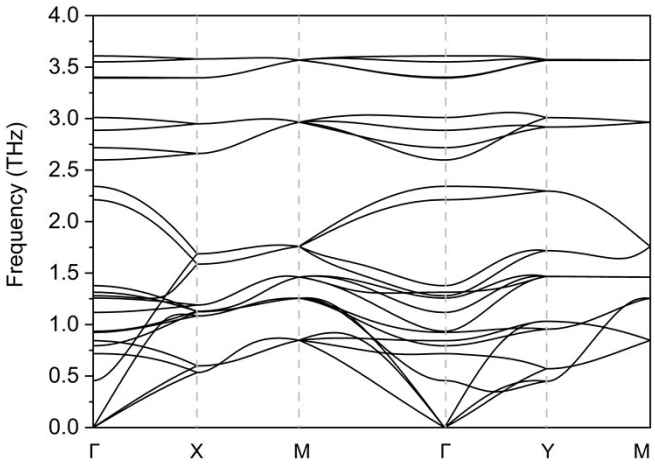

Fig. S1. Phonon spectrum for the 2D elemental ψ-bismuthene.

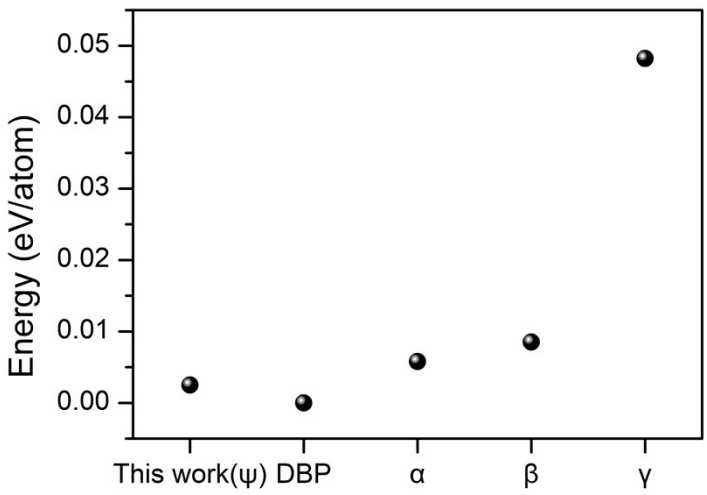

Fig. S2. Calculated binding energy difference between ψ, DBP, α, β, and γ bismuthene monolayers.

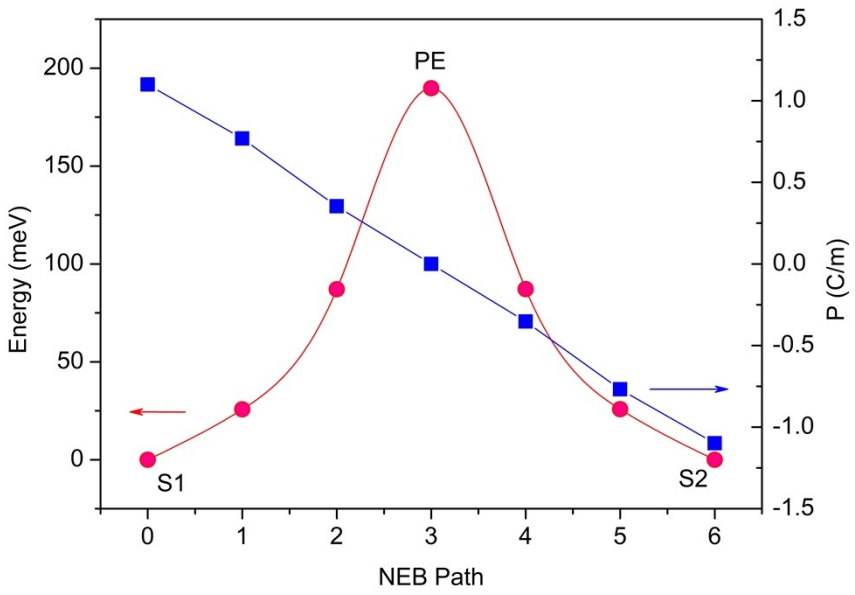

Fig. S3. The evolution of polarization P and energy landscape of the structural switching process between the energy-degenerate polarization states S1 and S2.

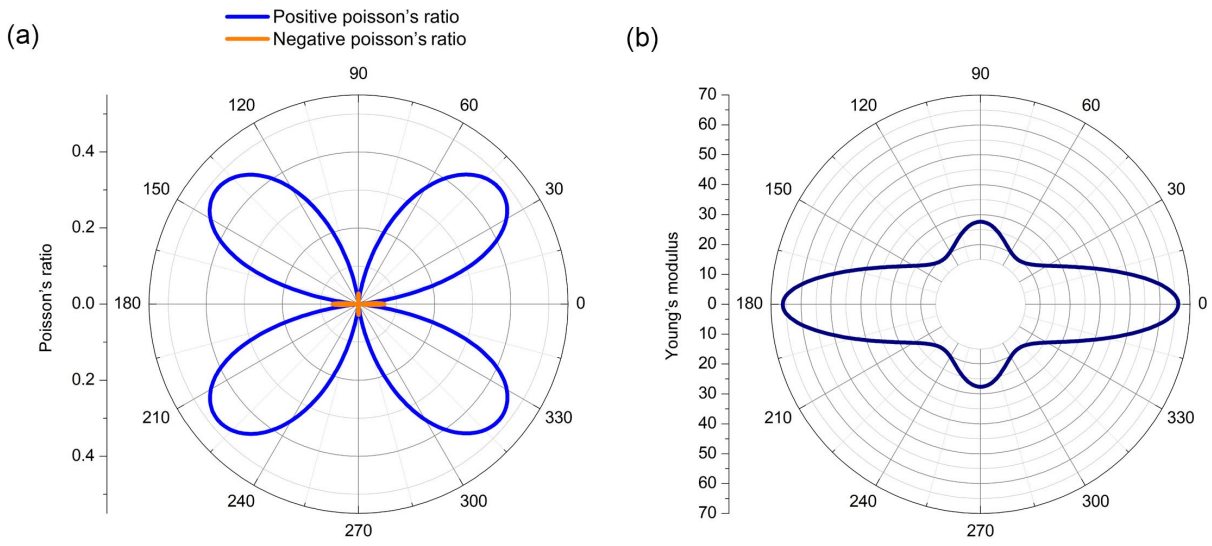

Fig. S4. (a) Poisson's ratio and (b) Young's modulus of *ψ*-bismuthene as a function of arbitrary angle.

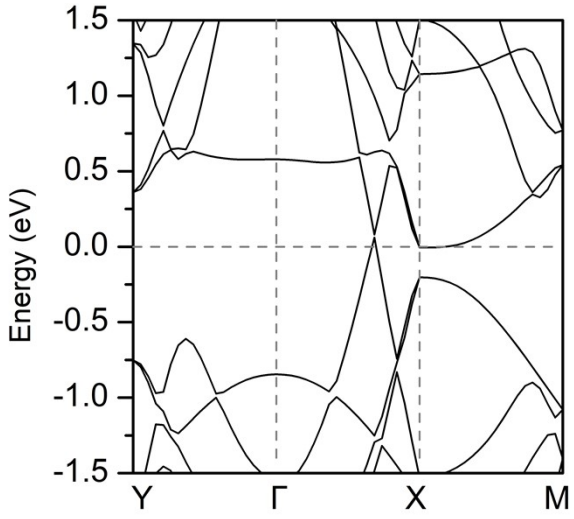

Fig. S5. Band structure of ψ-bismuthene calculated by Nanodcal using the mode-conservation pseudopotential and linear atomic orbit combination basis set.

References

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