https://doi.org/10.1007/s11467-023-1262-x

RESEARCH ARTICLE

Two-dimensional rectangular bismuth bilayer: A novel dual topological insulator

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Received November 7, 2022; accepted January 15, 2023

Supporting Information

Note 1

The $\mathbb{Z}_2$ invariant is determined based on the evolution of the Wannier center of charges (WCCs) method which is proposed by Soluyanov and Vanderbilt. The Wannier functions (WFs) with regard to lattice vector **R** is described as

$$\left|R,n\right\rangle = \frac{i}{2\pi}\int_{-\pi}^{\pi} dk e^{ik(R-x)}\left|u_{nk}\right\rangle.$$

The WFs depend on a gauge choice for the Bloch states $\left|u_{nk}\right\rangle$. Following Marzari and Vanderbilt's description, to optimally localize the WFs, the WCCs are defined as the mean value of the position operator $\bar{x} = \left\langle 0n\right|\hat{X}\left|0n\right\rangle$. In the limit of an infinite lattice, $\mathbb{Z}_2$ can be written as

$$\mathbb{Z}_2 = \left[\sum_\alpha \bar{x}^I_\alpha(TRIM_1) - \bar{x}^{II}_\alpha(TRIM_1)\right] - \left[\sum_\alpha \bar{x}^I_\alpha(TRIM_2) - \bar{x}^{II}_\alpha(TRIM_2)\right],$$

where TRIM represents the time-reversal invariant momentum; α is a band index of the occupied states and I and II are the Kramer partners. The identification of $\mathbb{Z}_2$ 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 Z_2 = 1, revealing the nontrivial topological nature.

Note 2

To confirm the topological crystalline insulator phase, the mirror Chern number, defined as $C_M = (C_{+i} - C_{-i})/2$, is calculated. The C_{+i} and C_{-i} are Chern numbers for mirror eigenvalues +i and -i,

$$C_{\pm i} = \frac{1}{2\pi}\int_{BZ}\Omega(k)d^2k.$$

Here, $\Omega(k)$ is the Berry curvature of all occupied bands, which can be obtained by the relations,

$$\Omega(k) = \sum_{m,n<E_F}\sum_{m\neq n} 2\,\mathrm{Im}\frac{\left\langle\psi_{nk}\right|\upsilon_x\left|\psi_{mk}\right\rangle\left\langle\psi_{mk}\right|\upsilon_y\left|\psi_{nk}\right\rangle}{(\varepsilon_{mk}-\varepsilon_{nk})^2},$$

where *m* and *n* are band indices, $\psi_{m/nk}$ and $\varepsilon_{m/nk}$ are the Bloch wave functions and corresponding eigenvalues of band m/n, respectively, and $\upsilon_{x/y}$ are the velocity operators.

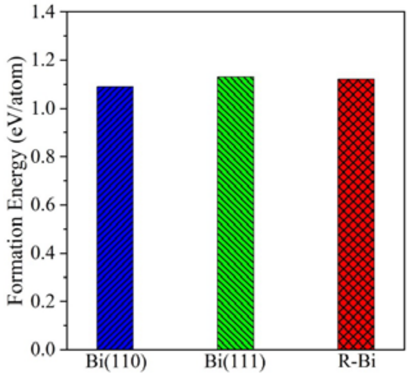

Fig. S1 Comparison of formation energy for Bi (110) film, Bi (111) film, and R-Bi bilayer.

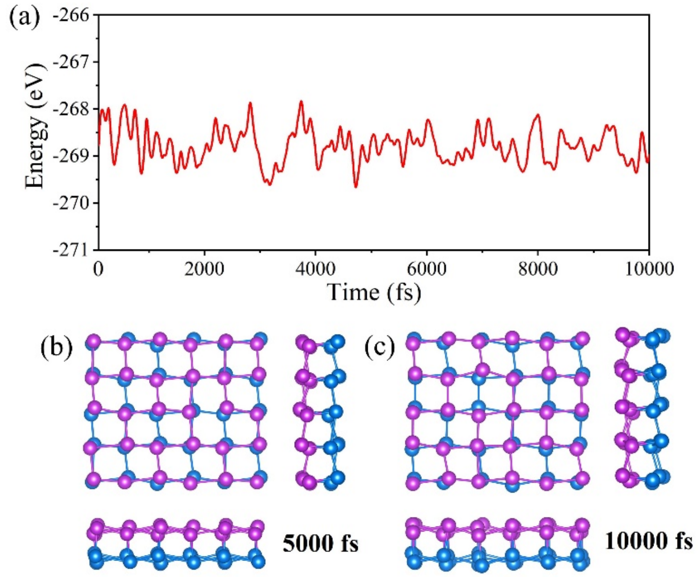

Fig. S2 (a) Variation of energy as a function of time for R-Bi bilayer obtained from AIMD simulation. **(b, c)** The snapshots of structure at 5000fs and 10000fs.

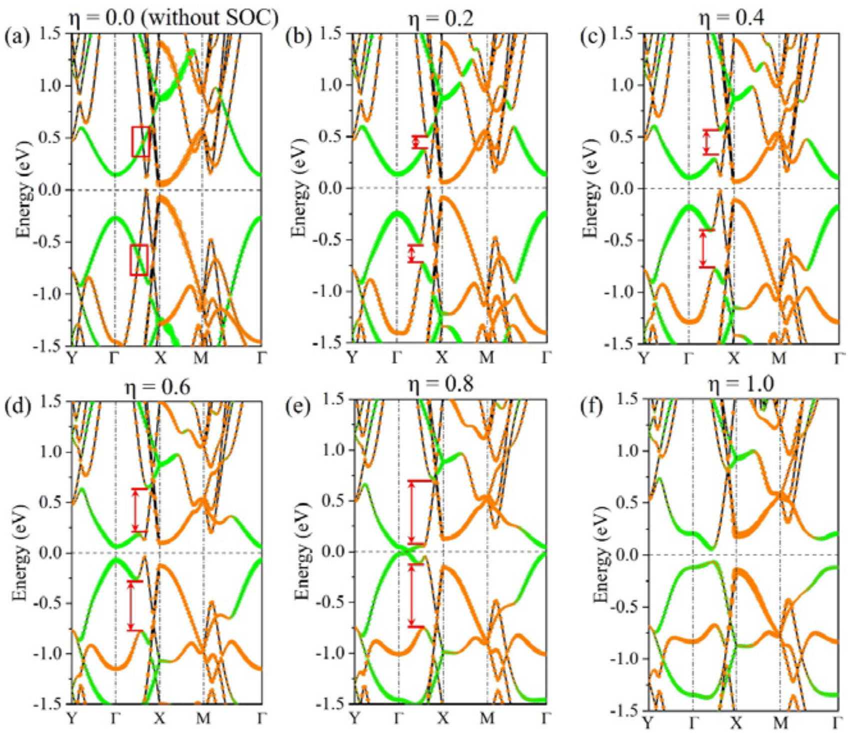

Fig. S3 Calculated band structures of R-Bi bilayer with different η.

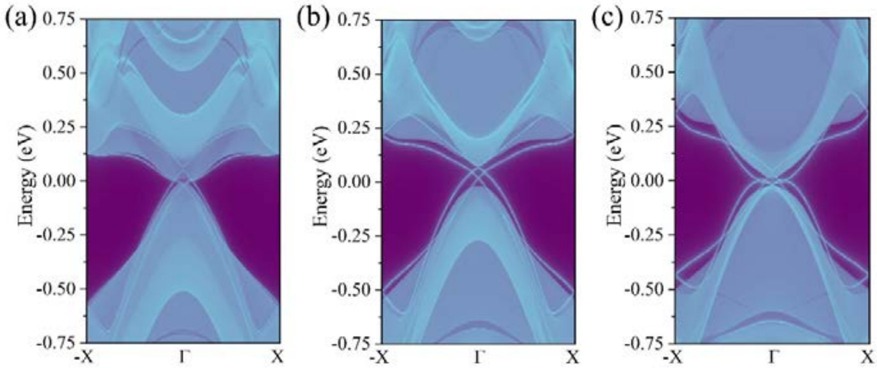

Fig. S4 Calculated edge states of R-Bi bilayer with η = 0.3 **(a)**, η = 0.6 **(b)**, and η = 0.9 **(c)**, respectively.

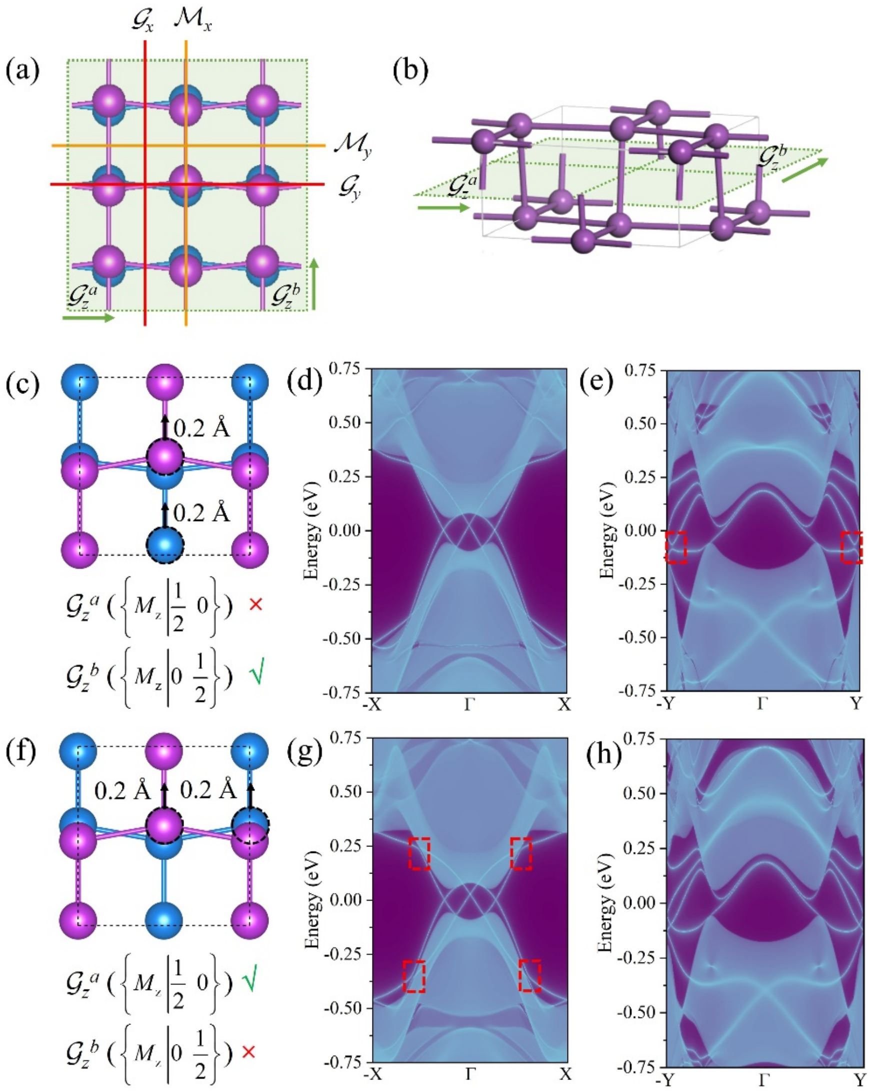

Fig. S5 (a, b) Six mirror symmetry operations in R-Bi bilayer. **(c-e)** Structural schematic of R-Bi bilayer with Γ_z^a breaking induced by atomic deviation and calculated edge states along *a* and *b* directions. **(f-h)** Structural schematic of R-Bi bilayer with Γ_z^b breaking induced by atomic deviation and calculated edge states along *a* and *b* directions.

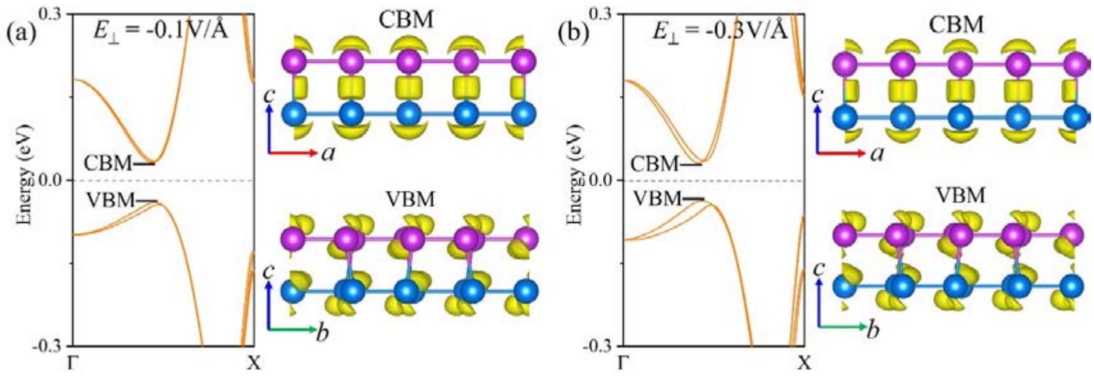

Fig. S6 Band structures and charge density distributions of CBM and VBM for R-Bi bilayer under the $E_\perp$ of -0.1 V/Å **(a)** and -0.3 V/Å **(b)**, respectively.

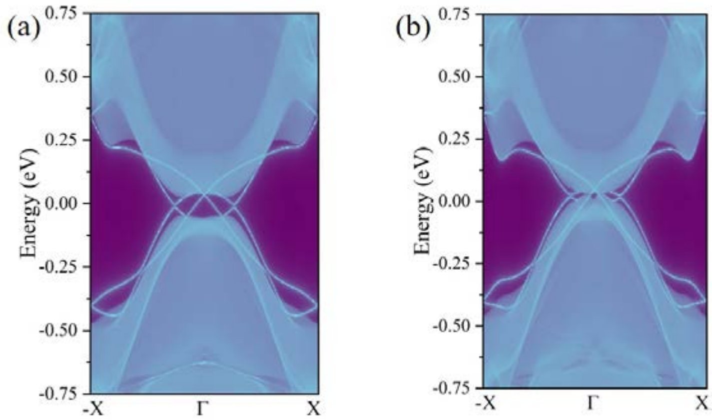

Fig. S7 Calculated edge states of R-Bi bilayer under the $E_\perp$ of -0.1 V/Å **(a)** and -0.3 V/Å **(b)**, respectively.

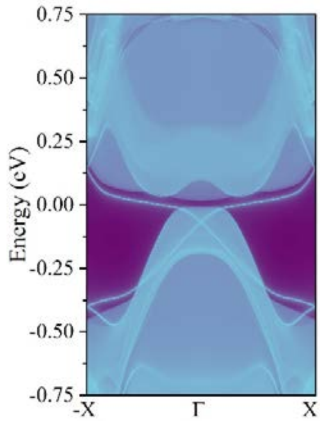

Fig. S8 Calculated edge states of vdW heterostructure composed of R-Bi bilayer and KBr(110) surface.

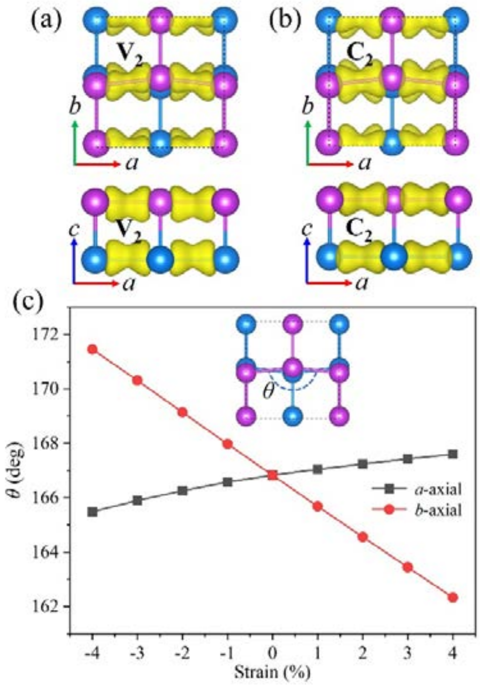

Fig. S9 (a, b) Calculated charge density distribution of V_2 and C_2 for R-Bi bilayer. **(c)** Variation of θ as a function of *a*-axial and *b*-axial strains. The inset is the schematic diagram of angle θ.

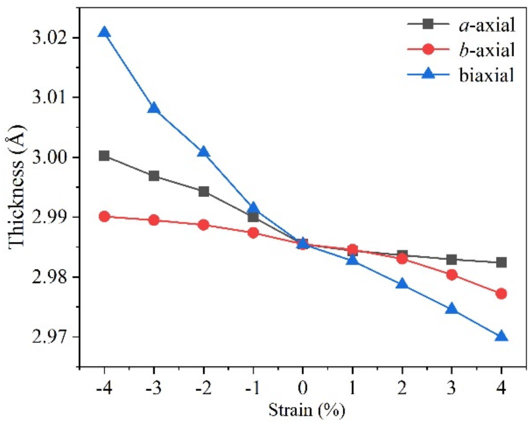

Fig. S10 Variation of thickness for R-Bi bilayer as a function of *a*-axial, *b*-axial and biaxial strains.