

# Supplementary Materials for “Berry Curvature Engineering by Gating Two-Dimensional Antiferromagnets”

Shiqiao Du,<sup>1</sup> Peizhe Tang,<sup>2\*</sup> Jiaheng Li,<sup>1</sup> Zuzhang Lin,<sup>3</sup> Yong Xu,<sup>1,4,5†</sup> Wenhui Duan,<sup>1,3,4‡</sup> Angel Rubio,<sup>2,6,7§</sup>

<sup>1</sup>*State Key Laboratory of Low-Dimensional Quantum Physics,  
Department of Physics, Tsinghua University, Beijing 100084, China,*

<sup>2</sup>*Max Planck Institute for the Structure and Dynamics of Matter,  
Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany.*

<sup>3</sup>*Institute for Advanced Study, Tsinghua University, Beijing 100084, China*

<sup>4</sup>*Collaborative Innovation Center of Quantum Matter, Beijing 100084, China*

<sup>5</sup>*RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan*

<sup>6</sup>*Nano-Bio Spectroscopy Group, Departamento de Física de Materiales,  
Universidad del País Vasco UPV/EHU, 20018 San Sebastián, Spain. and*

<sup>7</sup>*Center for Computational Quantum Physics, Flatiron Institute, 162 Fifth Avenue, New York, NY 10010, USA.*

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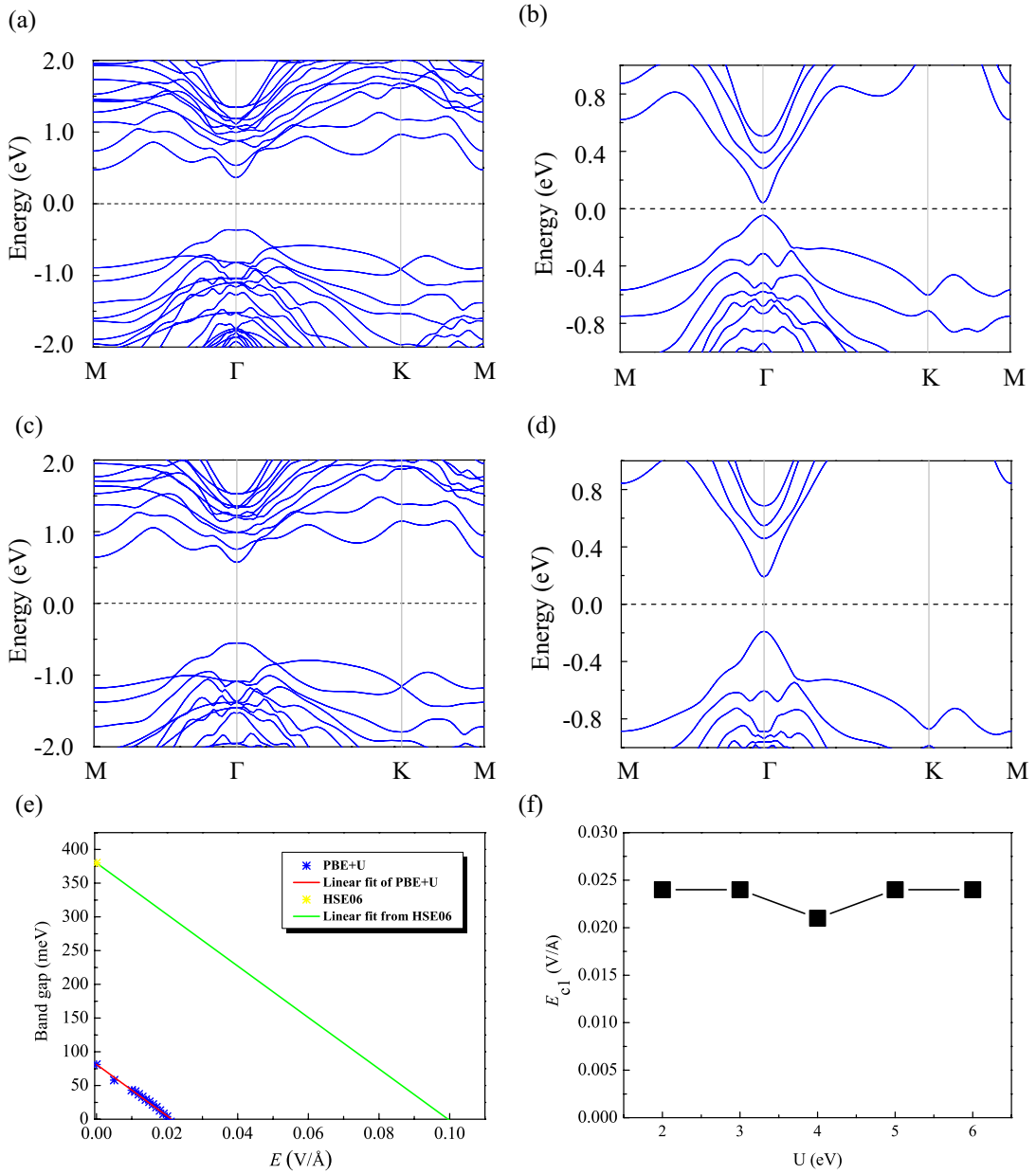
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\* Email: peizhe.tang@mpsd.mpg.de

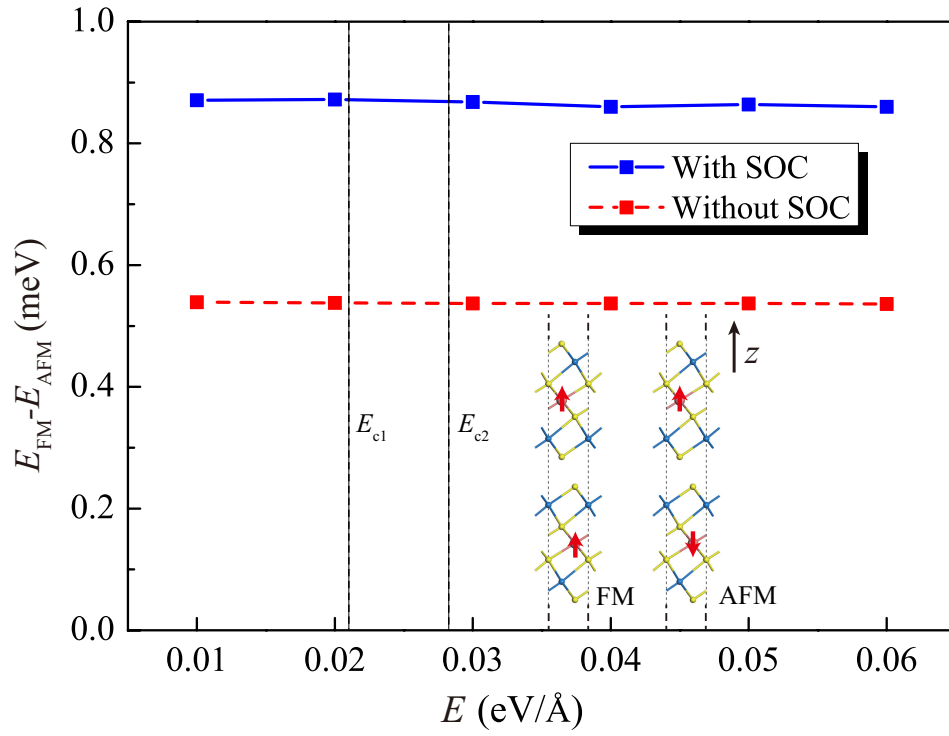
† Email: yongxu@mail.tsinghua.edu.cn.

‡ Email: dwh@phys.tsinghua.edu.cn.

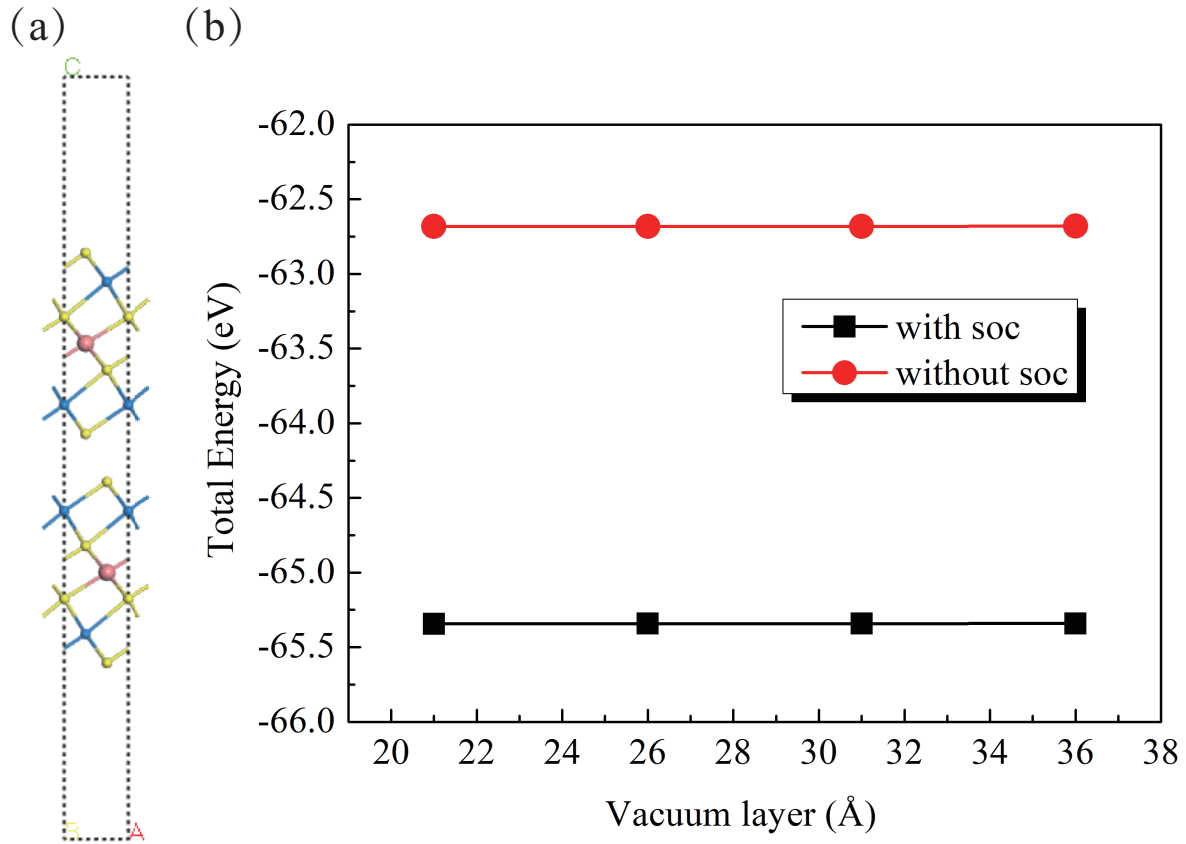
§ Email: angel.rubio@mpsd.mpg.de.



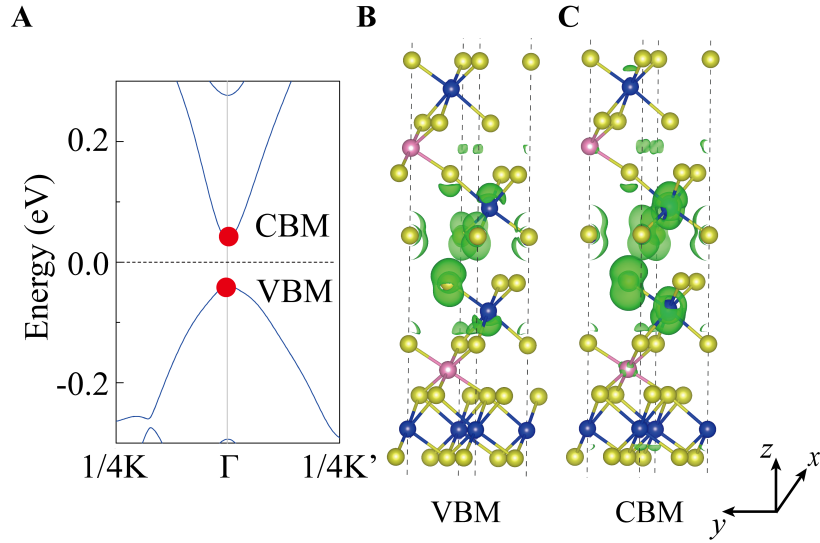
**FIG. S1: Intrinsic band structures of double-SL  $\text{MnBi}_2\text{Te}_4$  thin films using different exchange correlation functionals with and without SOC. (A) PBE+ $U$  without SOC; (B) PBE+ $U$  with SOC; (C) HSE06 without SOC; and (D) HSE06 with SOC. The Fermi level is set to zero and the band structures are doubly degenerated at each  $k$  point protected by the  $\mathcal{PT}$  symmetry. (e) Band gaps of DFT calculations with different exchange-correlation functionals response to the change of electric fields. The blue stars represent the results by using from PBE+ $U$  functional and the red line is the linear fit of that. The yellow star represents the result by using HSE06 functional and the green line is a linear function share the same slope with red line cross the yellow star. (f) The critical field  $E_{c1}$  (V/Å) depends on the choice of Hubbard  $U$  in PBE+ $U$  calculations.**



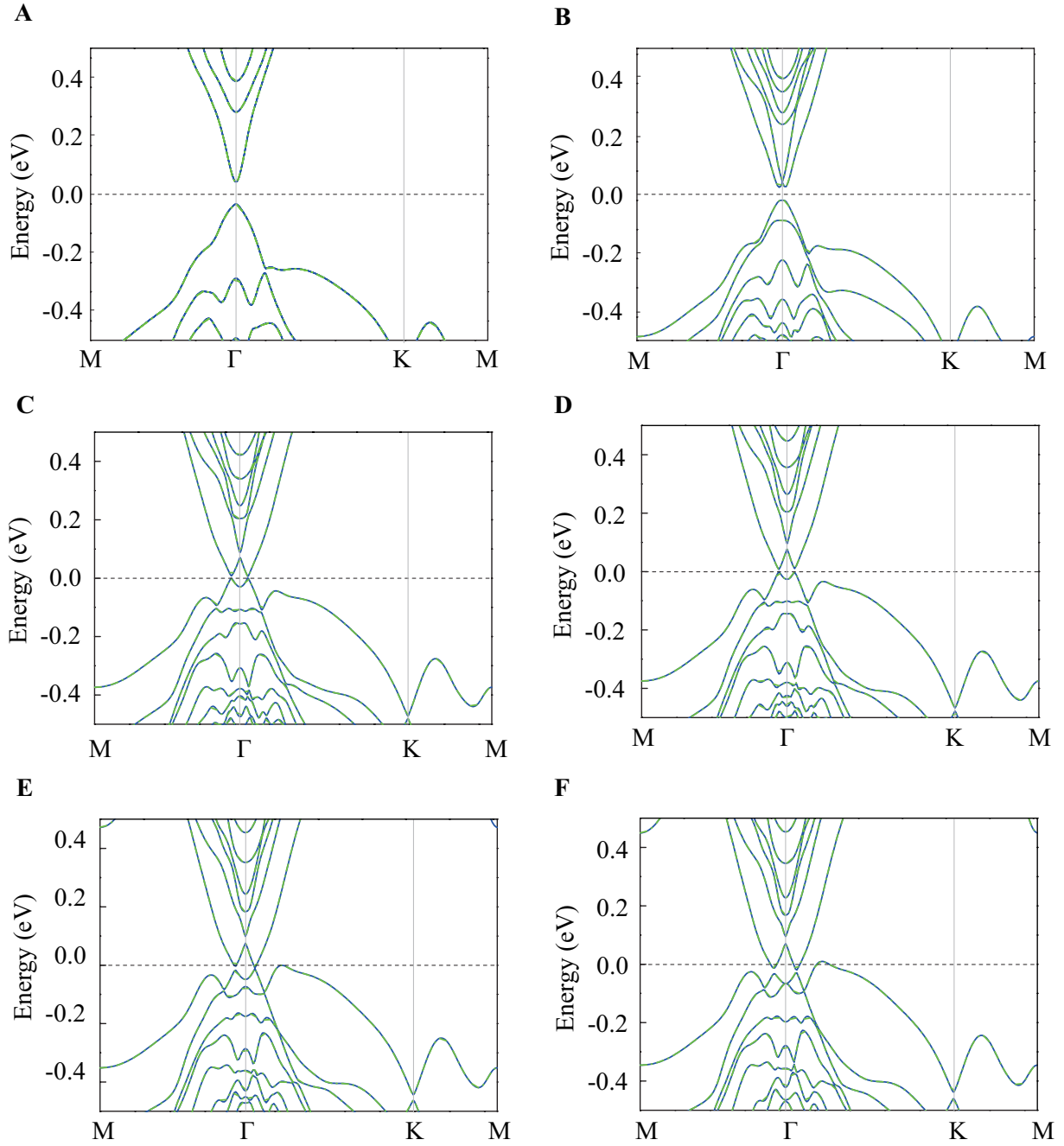
**FIG. S2: The magnetic order in double-SL  $\text{MnBi}_2\text{Te}_4$  thin film under electric field.** The total energies difference per cell of double-SL  $\text{MnBi}_2\text{Te}_4$  thin films under electric field between the intralayer FM order ( $E_{\text{FM}}$ ) and AFM order ( $E_{\text{AFM}}$ ). The blue and red lines are obtained from DFT calculations with SOC and without SOC, respectively. Insets show the FM and AFM orders in double-SL  $\text{MnBi}_2\text{Te}_4$  thin films. The system keeps AFM order as the ground state under a finite electric field. The black dash lines mark the critical electric field  $E_{c1}$  and  $E_{c2}$ .



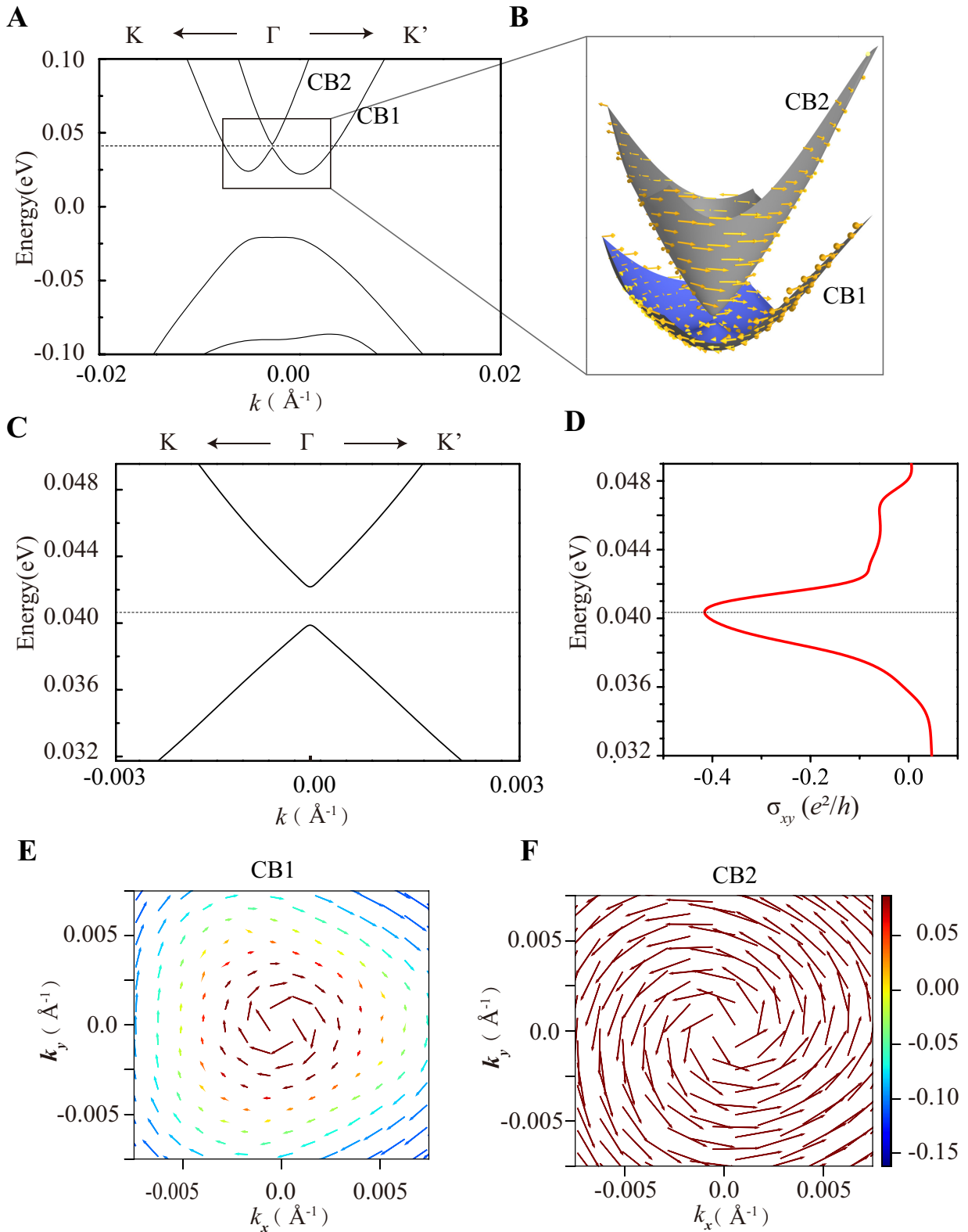
**FIG. S3: Convergence test for the thickness of the vacuum layer.** (a) The unit cell used in our calculations. (b) The total energies of the double-SL MnBi<sub>2</sub>Te<sub>4</sub> thin films vary with vacuum layer.



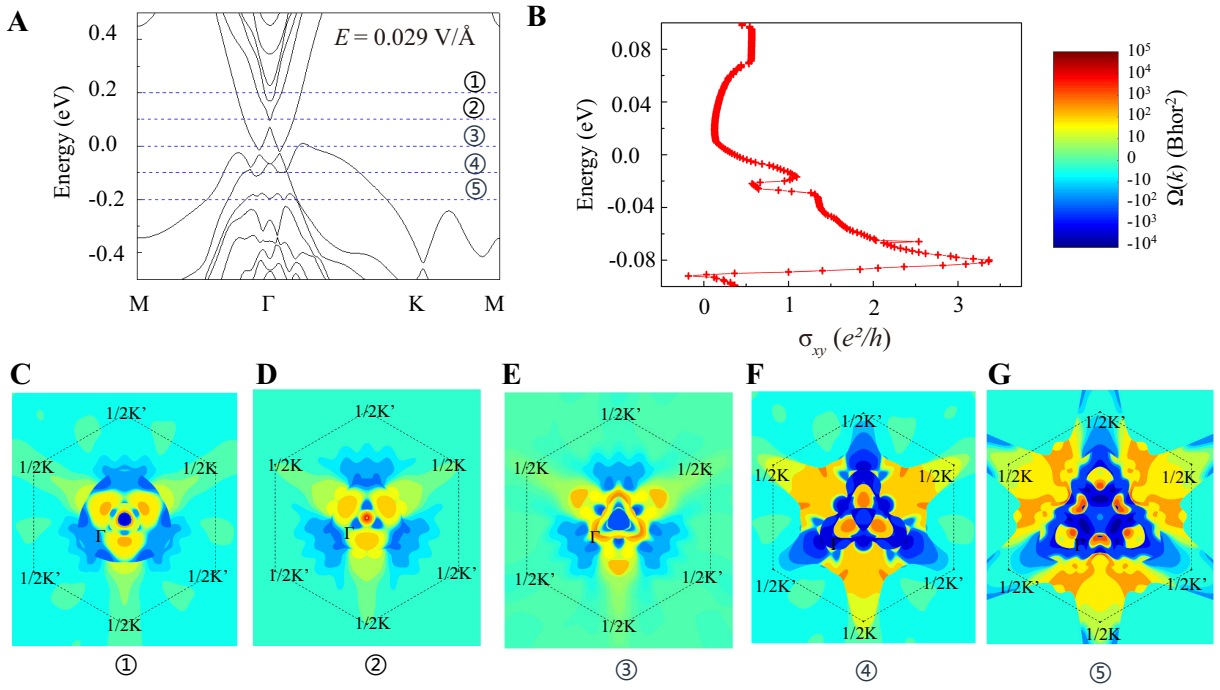
**FIG. S4: Partial charge density at band edges of double-SL  $\text{MnBi}_2\text{Te}_4$  thin film.** (A) Intrinsic band structure of double-SL  $\text{MnBi}_2\text{Te}_4$  thin film. Red solid points mark the doubly degenerate valence band maximum (VBM) and conduction band minimum (CBM). The Fermi level is set to zero. (B) Charge density at VBM plotted in green. The isosurface value is  $0.0014 \text{ e}\text{\AA}^{-3}$ . (C) Charge density at CBM plotted in green. The isosurface value is  $0.001 \text{ e}\text{\AA}^{-3}$ . The red, blue and yellow balls represent Mn, Bi and Te atoms respectively. As shown in (B) and (C), VBM is mainly contributed by the out-of-plane orbitals around Te atoms and in-plane orbitals around Bi atoms while the CBM is mainly contributed by the out-of-plane orbitals around Te atoms.



**FIG. S5: Wannier interpolated band structures of double-SL MnBi<sub>2</sub>Te<sub>4</sub> thin film under different electric fields  $E$ .** Blue solid lines: the band structures from DFT calculations. Green dash lines: the Wannier-interpolated band structures. The Fermi level is set to zero. **(A-F)** The band structures of double-SL MnBi<sub>2</sub>Te<sub>4</sub> thin film with different electric fields, the magnitudes of electric fields are 0, 0.010, 0.021, 0.023, 0.027, 0.029 V/Å, respectively.

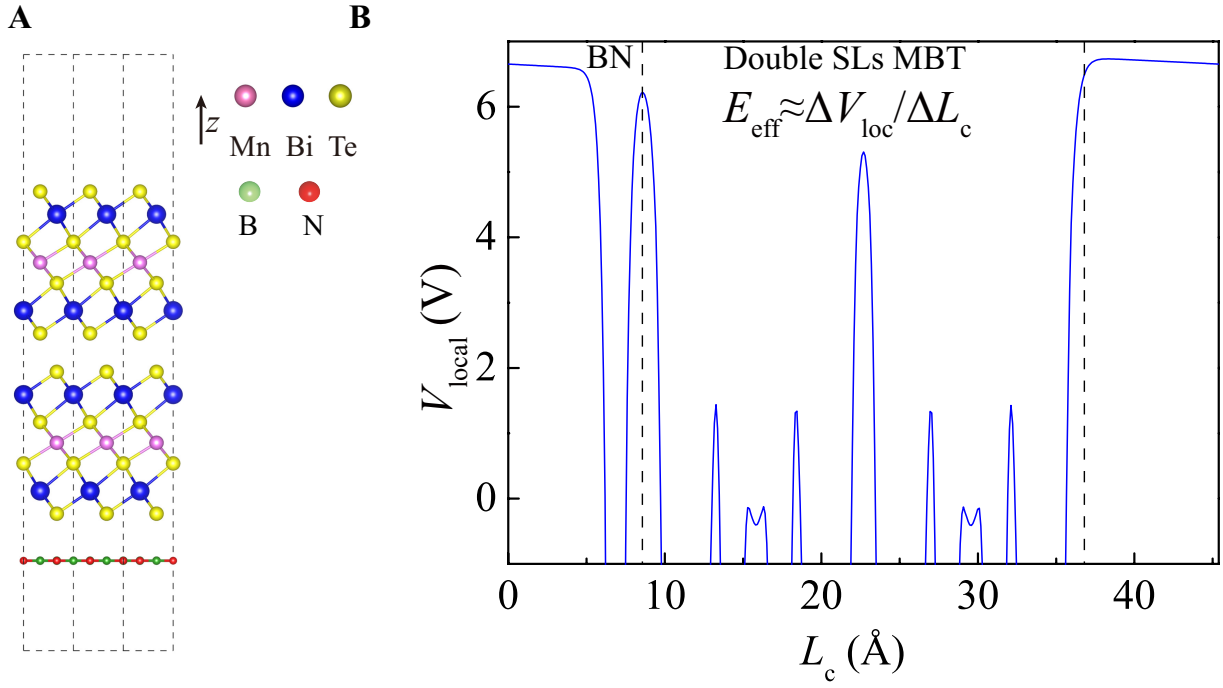


**FIG. S6: Spin textures of double-SL  $\text{MnBi}_2\text{Te}_4$  thin film with  $E=0.010 \text{ V/\AA}$ .** (A) Band structure of double-SL  $\text{MnBi}_2\text{Te}_4$  thin film under  $E=0.010 \text{ V/\AA}$ . The energy bands at the anti-crossing point are labeled as CB1 and CB2. (B) The spin textures for CB1 and CB2. The yellow arrows indicated the spin polarizations. It is noted that the directions of spin polarization is opposite for CB1 and CB2. (C) The electronic bands for CB1 and CB2 around the anti-crossing point. (D) AH conductance as a function of chemical potential. The black dashed line shows the energy level that corresponds to the negative AH effect in the Fig. 3b in the main text. (E-F) 2D schemes of spin-textures for CB1 and CB2. The arrows represent in-plane spin component whose length stands for the magnitude of corresponding spin polarization, and the color shows out-of-plane spin component. The magnitude of each spin vector is normalized.

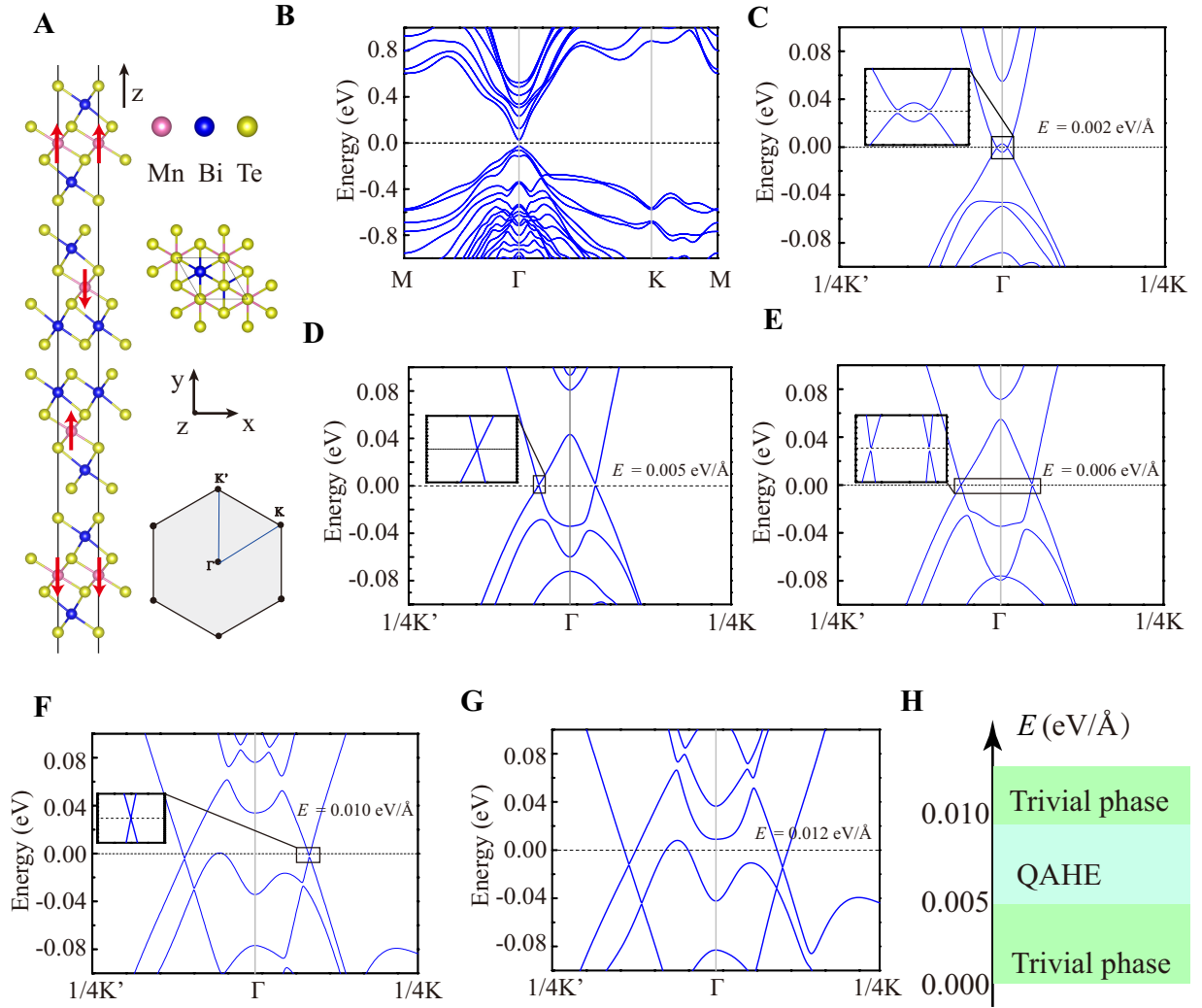


**FIG. S7: Berry curvature in the first BZ for double-SL MnBi<sub>2</sub>Te<sub>4</sub> thin film with  $E = 0.029 \text{ V/Å}$ .** (A) The band structure when  $E = 0.029 \text{ V/Å}$ . Under such electric field, the double-SL MnBi<sub>2</sub>Te<sub>4</sub> is a trivial AFM metal. (B) AH conductance with as a function of chemical potentials in double-SL MnBi<sub>2</sub>Te<sub>4</sub> thin film with  $E = 0.029 \text{ V/Å}$ . (C-G) The Berry curvature distributions in first BZ at different energy positions as marked in (A). It notes that the AH signal increases rapidly as the energy position shifts downwards.





**FIG. S8: Effective electric field induced by the substrate.** (A) Lattice structure of double-SL MnBi<sub>2</sub>Te<sub>4</sub> thin film on substrate of BN. (B) Local potential distribution along the  $z$  direction when double-SL MnBi<sub>2</sub>Te<sub>4</sub> thin film is on the substrate of BN. Black dash lines show the interface between the BN and double-SL MnBi<sub>2</sub>Te<sub>4</sub> thin film, and the boundary between double-SL MnBi<sub>2</sub>Te<sub>4</sub> thin film and vacuum region. The potential difference  $\Delta V_{\text{loc}} \approx 0.46$  V, correspondingly,  $\Delta L_c \approx 45$  Å, so the effective electric field  $E_{\text{eff}} \approx \Delta V_{\text{loc}} / \Delta L_c \approx 0.010 \text{ V}/\text{Å}$ .



**FIG. S9: Band structures and topological phase transitions for four-SL  $\text{MnBi}_2\text{Te}_4$  thin film under electric field** (A) Lattice structure of four-SL  $\text{MnBi}_2\text{Te}_4$  thin film and its first BZ. (B) Intrinsic band structure of four-SL  $\text{MnBi}_2\text{Te}_4$  thin film. (C-G) Band structures of four-SL  $\text{MnBi}_2\text{Te}_4$  thin film under different electric fields. From (C-G), the magnitudes of electric fields are 0.002, 0.005, 0.006, 0.010, 0.012  $\text{V/\AA}$ , respectively. The Fermi levels are set to be zero. All of results are calculated from PBE+U with SOC. (H) Schematic diagram of topological phase transitions in four-SL  $\text{MnBi}_2\text{Te}_4$  thin film under electric field. The first critical point is  $E=0.005 \text{ V/\AA}$ , the band crossing points are on lines of  $\Gamma$ - $\text{K}'$ , as shown in the inset of (D). Correspondingly, the system transforms from a trivial phase to the QAHE phase. The second critical point is  $E=0.010 \text{ V/\AA}$ , the band crossing points are on lines of  $\Gamma$ - $\text{K}$ , as shown in the inset of (F). At this time, the system becomes a trivial AFM metal.