Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Strain-tunable magnetism and topological states in layered VBi_2Te_4

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Supplementary figures and captions

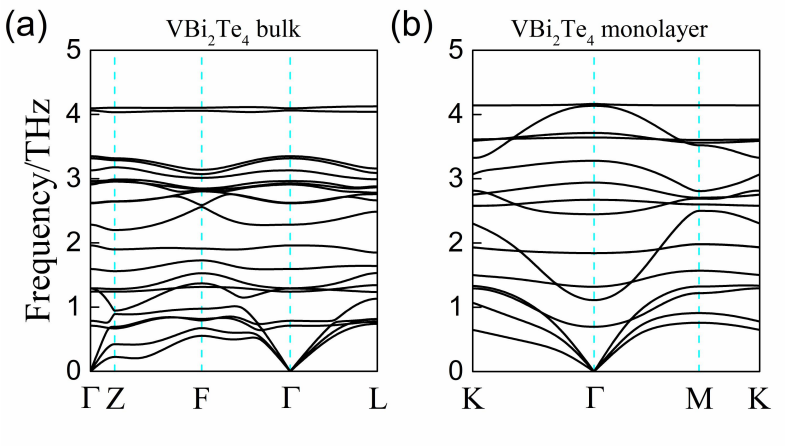

Fig. S1 Calculated phonon spectra of bulk (a) and monolayered (b) VBi_2Te_4 (VBT).

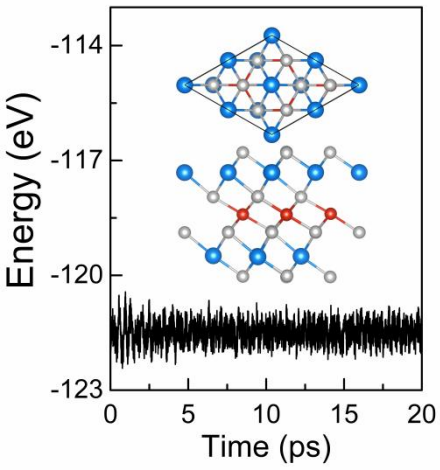

Fig. S2 Ab initio molecular dynamics simulations of a VBT monolayer at 300 K. The insets display the final structure after 20 ps.

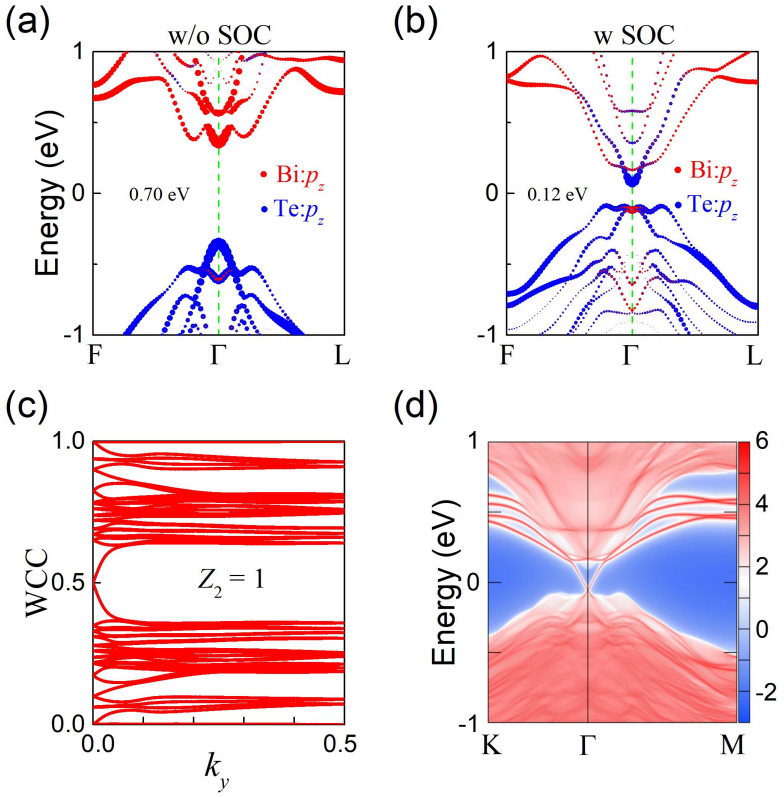

Fig. S3 Band structures of antiferromagnetic VBT, without (a) and with spin-orbit (SOC). Here, the projected bands of Bi-p_z and Te-p_z are also given. (c) The corresponding Z_2 invariant of $k_3 = 0.0$ plane. (d) Calculated edge states.

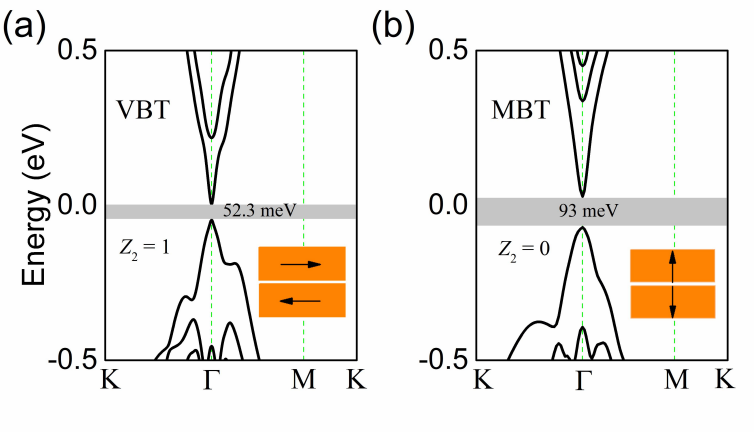

Fig. S4 The electronic band structures of antiferromagnetic VBT (a) and $MnBi_2Te_4$ (MBT) (b) calculated by HSE06 functional, respectively. Here, SOC is included, and the calculated Z_2 invariant of VBi_2Te_4 and $MnBi_2Te_4$ respectively are 1 and 0.

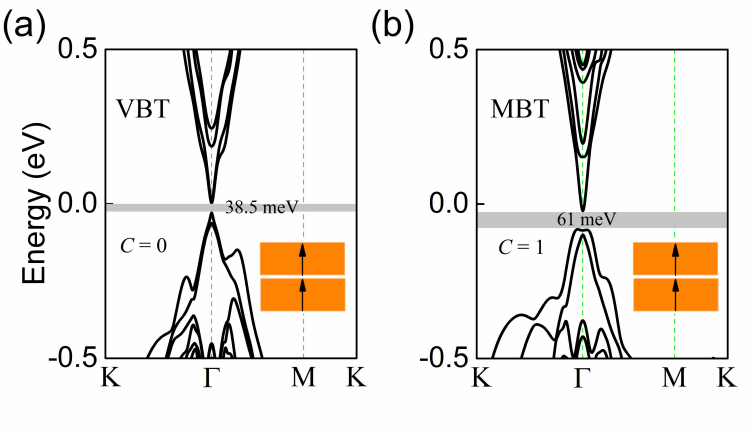

Fig. S5 The electronic band structures of ferromagnetic VBT (a) and MBT (b) calculated by HSE06 functional, respectively. The calculated Chern number (*C*) of VBT and MBT respectively are 0 and 1.

Table S1 Calculated the magnetic anisotropy energy (MAE), nearest magnetic coupling parameter J_N, and estimated Curie temperature (T_c) of VBT monolayer under strain. Here, "-" and "+" denote compressed and tensile strain, respectively. MAE is defined by MAE = $E_\perp$ - $E_\parallel$, with $E_\perp$ and $E_\parallel$ denoting the total energies associated with the magnetic moment perpendicular and parallel to the plane of the 2D materials, respectively.

VBT monolayer	MAE (meV)	J_N (meV)	T_c (K)
-5%	0.157	-0.171	8
-3%	0.115	-0.354	13
-1%	0.111	-0.586	20
0	0.181	-0.608	21
+1%	0.118	-0.795	26
+3%	0.125	-0.776	25
+5%	0.130	-0.819	28