

Supplementary Material for
“Dirac-Weyl semimetal phase in noncentrosymmetric transition metal monochalcogenides MoTe and WTe”

Lijun Meng^{✉1,2,3}, Jiafang Wu¹, Yizhi Li¹, Jianxin Zhong^{✉1,2}

¹School of Physics and Optoelectronics, Xiangtan University, Xiangtan 411105, Hunan, People's Republic of China

²Hunan Key Laboratory for Micro-Nano Energy Materials and Devices, Hunan, People's Republic of China

³Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom

1. The thermal stability of the system and possible synthesis route

To verify the thermal stability of the optimized structures, we conducted a long-time first-principle molecular dynamics (FPMD) calculation based on $4 \times 4 \times 2$ supercell at 300K. A velocity Verlet algorithm, with a time step of $2fs$ and NVT ensemble, was adopted. The temperature and the total energy for both MoTe and WTe exhibit thermal fluctuation around average values up to $10ps$ as shown in Fig.1S. These results imply the thermal stability of structures at room temperature.

The synthesis strategies applied to prepare transition metal dichalcogenides (TMD) layered materials include solid-state reaction, molecular beam epitaxy (MBE), chemical vapor deposition (CVD) and chemical synthesis¹⁻⁴. The synthesis of different phases of TMD can be realized by flux-based solid-state reaction. The possible synthesis of MoTe and WTe may be realized by a rapid quench cooling under the assistance of small amount transport agency and the control of atomic composition¹.

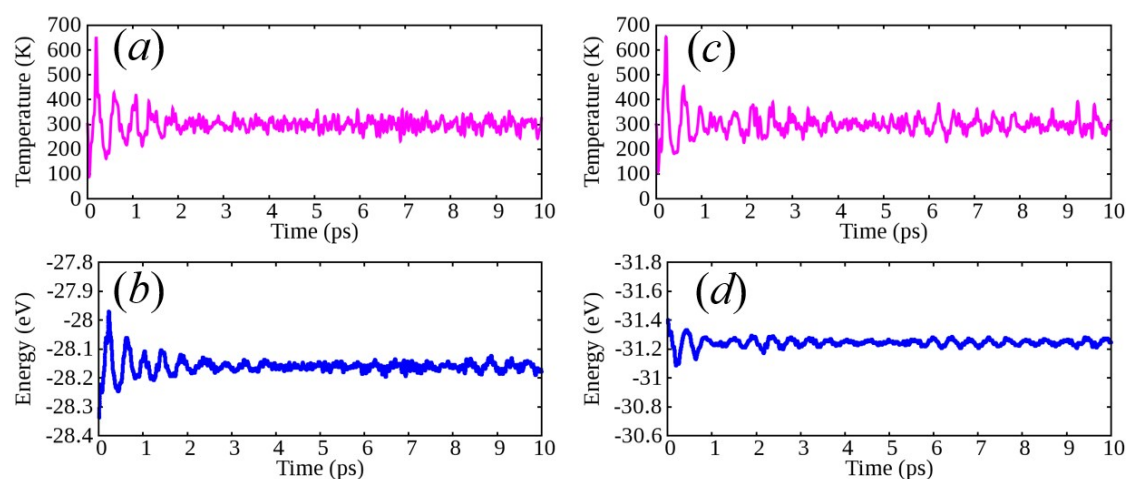


Fig.1S. The Temperature and total energy in FPMD simulation for MoTe ((a) (c)) and WTe ((c) (d))

✉ The corresponding author Email: lijmeng@xtu.edu.cn

✉ The corresponding author Email: jxzhong@xtu.edu.cn

2. The fitted parameters and bands along a line of going through Weyl points

Four parameters in low energy effective Hamiltonian (Eq.(1) in the main text) can be determined by the dispersions in point Γ and Dirac points and the results are listed in Table 1S. Other nine parameters are fitted through the DFT-based bands and the results are given in Table.2S.

Table 1S. The parameters of low energy effective Hamiltonian Eq. (1)

System	ε_0	m_0	ε_2	m_2
MoTe	0.0996	-0.1470	-0.1494	-1.6080
WTe	0.1815	-0.1385	-0.0234	-2.1638

Table 2S. The parameters of low energy effective Hamiltonian Eq. (1)

Parameters	MoTe	WTe	Parameters	MoTe	WTe
ε_1	-1.7461	-1.8803	g_3	0.2532	0.2424
m_1	-1.3298	-0.8182	g_2'	-0.2659	-0.5631
g_1'	-0.0348	0.0020	g_3'	-0.2409	-0.1564
g_1	-0.0061	-0.0062	g_3''	-0.2492	-0.1988
g_2	-0.2764	-1.0532			

We also calculated the bands along a non-high-symmetry line Γ -S which goes through one of Weyl points as shown in Fig.2S. The fitted bands of parameterized low effective Hamiltonian slightly deviate from the DFT-based bands near the point Γ as shown in Fig.2S (a) (b) for both MoTe and WTe. The bands along Γ -S line exhibits the band crossing between the conduction band and valence band, and captures the variation tendency of bands around the Weyl point. The deviation from DFT bands may come from the approximation of the k - p model which is only considered up to cubic order near the Γ point⁵.

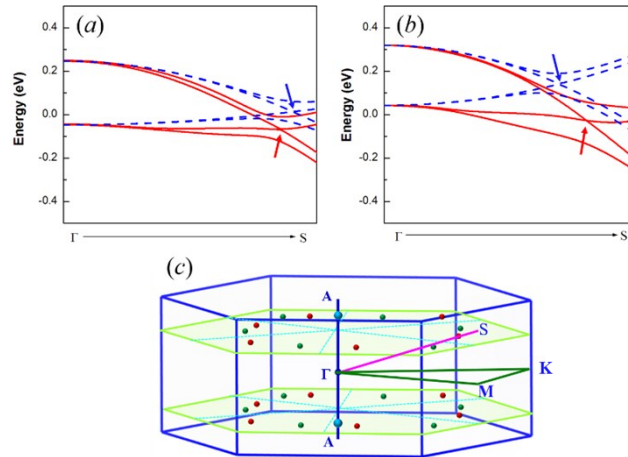


Fig.2S. The DFT-based bands (red solid lines) and Hamiltonian fitted bands (blue dash lines) along Γ -S for (a) MoTe and (b) WTe. The blue and red arrows indicate the Weyl points. (c) The twelve pairs of

Weyl points in the Brillouin zone. The pink line stands for the path of bands in the (a) (b). The red and blue points indicate the Weyl points with positive and negative chirality.

3. The evolution of Weyl points under strain

We plotted the perspectives and top views of all twenty-four Weyl points in Dirac-Weyl semimetal (DWS) phase under strain in Fig.3S. Note that the Weyl nodes with opposite chirality move close to the Γ -K line under both compression and tensile as shown in the right panel of Fig.3S. Interestingly, under larger strains, the pairs of Weyl points with opposite handedness meet on the Γ -K line and then annihilate each other for both MoTe and WTe. In our calculations, all Weyl points annihilate and disappear at compression strain around -6%(-8%) and tensile strain 8% (6%) for MoTe (WTe). The k_z -axis coordinates of Weyl points decrease monotonously as strain from compression to tensile as shown in Fig.7 in the main text. However, the Dirac points remain within strain range(-10%, 10%) and result in a phase transition from DWS to Dirac-semimetal (DS) phase. It is noted that the strain-induced annihilation of Weyl nodes was also discussed in the Type-II Weyl semimetals WTe₂⁶ and MoTe₂⁷⁻⁸.

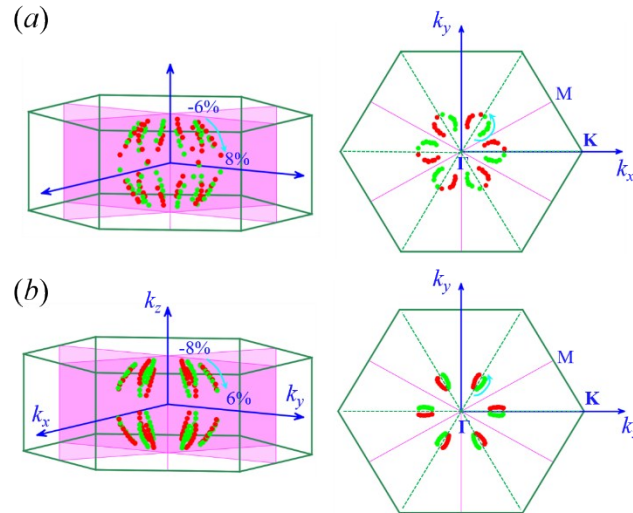


Fig.3S. (Color Online).The distribution of Weyl nodes under strain along c axis for (a) MoTe; (b) WTe in the presence of SOC. The red and green dots represent Weyl nodes with positive and negative chirality. The light blue arrow represents the change of strain from compressive to tensile strain. Here, the BZ corresponds to the BZ of strain-free MoTe and WTe.

References

1. Ma, J.; Deng, K.; Zheng, L.; Wu, S.; Liu, Z.; Zhou, S.; Sun, D., Experimental Progress on Layered Topological Semimetals. *2D Materials* **2019**, 6.
2. Li, J., et al., Synthesis of Ultrathin Metallic Mte2 (M = V, Nb, Ta) Single-Crystalline Nanoplates. *Adv Mater* **2018**, e1801043.
3. Han, G. H.; Duong, D. L.; Keum, D. H.; Yun, S. J.; Lee, Y. H., Van Der Waals Metallic Transition Metal Dichalcogenides. *Chem Rev* **2018**, 118, 6297-6336.
4. Das, P. K.; Sante, D. D.; Cilento, F., Electronic Properties of Type-II Weyl Semimetal Wte2 a Review Perspective.Pdf. *Electron. Struct.* **2019**.
5. Gao, H.; Kim, Y.; Venderbos, J. W. F.; Kane, C. L.; Mele, E. J.; Rappe, A. M.; Ren, W., Dirac-Weyl

Semimetal: Coexistence of Dirac and Weyl Fermions in Polar Hexagonal Abc Crystals. *Phys Rev Lett* **2018**, *121*, 106404.

6. Soluyanov, A. A.; Gresch, D.; Wang, Z.; Wu, Q.; Troyer, M.; Dai, X.; Bernevig, B. A., Type-II Weyl Semimetals. *Nature* **2015**, *527*, 495-8.

7. Sun, Y.; Wu, S.-C.; Ali, M. N.; Felser, C.; Yan, B., Prediction of Weyl Semimetal in Orthorhombic MnTe . *Physical Review B* **2015**, *92*.

8. Wang, Z.; Gresch, D.; Soluyanov, A. A.; Xie, W.; Kushwaha, S.; Dai, X.; Troyer, M.; Cava, R. J.; Bernevig, B. A., MnTe : A Type-II Weyl Topological Metal. *Phys Rev Lett* **2016**, *117*, 056805.