Visualizing the interplay of Dirac mass gap and magnetism at nanoscale in intrinsic magnetic topological insulators

Mengke Liu, Chao Lei, Hyunsue Kim, Yanxing Li, Lisa Frammolinno, Jiaqiang Yan, Allan H. Macdonald, and Chih-Kang Shih

In intrinsic magnetic topological insulators, Dirac surface-state gaps are prerequisites for quantum anomalous Hall and axion insulating states. Unambiguous experimental identification of these gaps has proved to be a challenge, however. Here, we use molecular beam epitaxy to grow intrinsic MnBi₂Te₄ thin films. Using scanning tunneling microscopy/spectroscopy, we directly visualize the Dirac mass gap and its disappearance below and above the magnetic order temperature. We further reveal the interplay of Dirac mass gaps and local magnetic defects. We find that, in high defect regions, the Dirac mass gap collapses. Ab initio and coupled Dirac cone model calculations provide insight into the microscopic origin of the correlation between defect density and spatial gap variations. This work provides unambiguous identification of the Dirac mass gap in MnBi₂Te₄ and, by revealing the microscopic origin of its gap variation, establishes a material design principle for realizing exotic states in intrinsic magnetic topological insulators.

In magnetic topological insulators (MTIs), time-reversal symmetry breaking opens a surface-state Dirac mass gap that is a prerequisite for realizing quantum anomalous Hall (QAH) and axion insulator ground states (1–3). QAH states support spin-momentum locked dissipationless edge states that hold great promise in advancing electronic and spintronic device applications. Early materials design was based on doping topological insulators with magnetic elements (4, 5); however, dopant disorder (6, 7) is significant and considered to be the main cause for quantized edge states being observed only at extremely low temperatures, ~30 mK in chromium-doped (Bi,Sb)₂Te₃ (5). Recently, a new family of intrinsic MTIs based on layered van der Waals material MnBi₂Te₄ has emerged, in which an ordered Mn magnetic layer is incorporated stoichiometrically in the middle of each van der Waals layer (8–14), suppressing the disorder effect. Indeed, the QAH effect has been observed in MnBi₂Te₄ at a significantly higher temperature of 1.4 K (15). However, the QAH effect is not always observed, even in samples that appear similar (16–20). Moreover, observations of the Dirac mass gap, a prerequisite for the QAH effect and a direct consequence of exchange coupling between the Dirac surface state and the spontaneous magnetization (21, 22), has proven to be challenging. Here, we report the direct observation of the Dirac mass gap. We further reveal microscopically the essential role of native magnetic antisite defects in controlling the formation of the Dirac mass gap. Our work provides unambiguous evidence of a Dirac mass gap in MnBi₂Te₄ thin film and identifies magnetic defects as an important parameter in designing the topological quantum material.

Significance

Intrinsic magnetic topological insulators (MTIs) MnBi₂Te₄ have recently emerged as a new frontier of topological quantum materials. Theoretical predicted exotic quantum phases of its thin-film form, such as Chern and axion insulator states, both have Dirac mass gaps in their surface states. However, direct observation of the Dirac mass gap has proved challenging. Here, we report the direct observation of the Dirac mass gap. We further reveal microscopically the essential role of native magnetic antisite defects in controlling the formation of the Dirac mass gap. Our work provides unambiguous evidence of a Dirac mass gap in MnBi₂Te₄ thin film and identifies magnetic defects as an important parameter in designing the topological quantum material.

Author contributions: M.L. and C.-K.S. designed research; M.L., C.L., H.K., Y.L., U.F., and C.-K.S. performed research; J.Y. contributed new reagents/analytic tools; M.L., C.L., H.K., A.H.M., and C.-K.S. analyzed data; and M.L., C.L., A.H.M., and C.-K.S. wrote the paper.

Competing interest statement: We acknowledge that J.Y. has coauthored papers with both reviewers. J.Y. developed the protocol of flux growth of MnBi₂Te₄ single crystals, and this protocol has been widely used by the community to produce high-quality single crystals of MnBi₂Te₄ and related compounds. In this work, MnBi₂Te₄ single crystals provided by J.Y. have been used to reveal the contrasting behaviors between bulk single crystals and MBE-grown ultra-thin films.

Copyright © 2022 The Author(s). Published by PNAS. This article is distributed under Creative Commons Attribution-NonCommercial-NoDerivatives License 4.0 (CC BY-NC-ND).

1To whom correspondence may be addressed. Email: macdpc@physics.utexas.edu or shih@physics.utexas.edu.

This article contains supporting information online at http://www.pnas.org/lookup/suppl/doi:10.1073/pnas.2207681119/-/DCSupplemental.

Published October 10, 2022.
the microscopic origin of the gap variation. It further establishes magnetic defect as a critical tuning knob in controlling the topological phases of MTI for QAH and axion insulator–based device applications.

**Bulk Crystals versus MBE-Grown Thin Films**

MnBi₂Te₄ is a layered van der Waals material consisting of Te–Bi–Te–Mn–Te–Bi–Te septuple layers (SLs), in which the Mn atomic layer is coupled ferromagnetically within the SL and antiferromagnetically with neighboring SLs. The lattice illustration shown in Fig. 1A includes two commonly observed native defects, MnBi and BiTe antisites. STM images taken on the cleaved bulk crystals (Fig. 1B) show ∼5% MnBi antisites, which appear as dark triangular depressions (39), and ∼0.2% of BiTe antisites, which appear as bright circular protrusions (39). The abundance of the BiTe antisites is related to the Te content during the growth (40). The broad background fluctuation may reflect an inhomogeneous distribution of the BiMn antisite, the most common n-type dopant (40), located at the Mn layer and is too far from the surface to be directly imaged by STM. But its high concentration is expected from the internal strain energy in the middle Mn layer (40) and can be inferred from the heavily degenerate n-type nature of the sample. As shown in Fig. 1C, we find that $E_F$ is 0.28 eV above the Dirac point in bulk samples, consistent with previous angle-resolved photoemission spectroscopic results (9, 23–25). However, the Dirac gap signature is smeared and difficult to quantify.

We succeed in growing MnBi₂Te₄ thin films on the HOPG and the graphene substrates. The STM/S results reported here are primarily carried out on samples grown on HOPG substrate. A typical STM image of our MBE-grown MnBi₂Te₄ flakes, shown in Fig. 1D, demonstrates SL-by-SL growth of high-quality MnBi₂Te₄ thin film. A topographic section across the flakes (Fig. 1E) allows us to determine the thickness in terms of the number of SLs. This thickness determination is crucial because it eliminates the possibility of Bi₂Se₃ or MnTe₂ intermixing, which would lead to different layer thicknesses (additional topographic images of MBE grown samples can be found in SI Appendix, Fig. S1). Fig. 1D, Inset shows the corresponding atomic image, exhibiting ∼4% of MnBi antisites and no bright BiTe antisites. The disappearance of BiTe antisites is due to a Te-rich growth ambient, which also reduces the BiMn antisites (40). Most importantly, in the ultra-thin regime, the internal energy in the Mn layer may not yet build up significantly, thus delaying the strain compensation effect through BiMn antisites (40). The clean and flat background of the atomic image reflects a considerably reduced amount of BiMn antisites. The SL-by-SL MBE growth of MnBi₂Te₄ films with low defect density we report provides access to the rich electronic properties of MnBi₂Te₄ thin films.

**Direct Observation of Dirac Mass Gaps**

We start with the 4-SL film, thick enough that its topological surface state is well developed. Fig. 2A shows a typical tunneling spectrum acquired at 4.3 K at a relatively high setpoint bias of 0.6 V. In this spectrum, there exists a sizeable low-conductance bias range from −0.3 V to +0.4 V, marked by the blue and orange arrows. This low-conductance region is due to a significantly reduced density of states (DOS). We find that, with a lower setpoint bias, as shown in Fig. 2B, for which the tip-to-sample distance is reduced, states near $E_F$ can be well resolved. The behavior of bias-dependent tip-to-sample distance can be found in SI Appendix, Fig. S2, and the tunneling junction characteristics (barrier height) at different biases can be found in SI Appendix, Fig. S3. In Fig. 2B, which focuses on states near the Fermi energy, one can observe a clear exchange gap of ∼120 meV, with $E_F$ located 20 meV below the conduction band edge.

We further carried out the STS measurement at 77 K, a temperature above the Neel temperature. At a high setpoint bias
(Fig. 2C), the spectrum exhibits a low-conductance region from −0.3 V to 0.4 V, similar to that acquired in Fig. 2A. With a low setpoint bias (Fig. 2D), the electronic states near the Fermi level can be clearly observed. However, the gap disappears. This direct comparison further affirms that the observed gap at 4.3 K is the Dirac mass gap due to the exchange interaction of the Dirac surface states with the spontaneous magnetization below the Neel temperature.

Fig. 2E shows theoretical projected DOS curves for the top four atomic layers of a defect-free, 4-SL MnBi₂Te₄ thin film. These results show an ∼0.45 eV low DOS energy range (marked between the blue and orange arrows), in agreement with our experimental observed low-conductance region of 0.7 eV. The true theoretical Dirac mass gap within which the DOS vanishes is only 48 meV for a 4-SL film. Fig. 2F summarizes the STS-measured (See SI Appendix, Fig. S4 for 1- to 3-SL STS) and the density functional theory (DFT)-calculated (SI Appendix, Fig. S5) energy gaps as a function of the film thickness, which shows excellent overall agreement, given the known tendency toward bandgap under-estimation in DFT. Our gap determinations have been cross-checked by obtaining STS data at different temperatures and in several different measurement modes (SI Appendix, Figs. S2 and S3). This provides unambiguous evidence of the Dirac mass gap in intrinsic MTIs, resolving current debates (9, 21, 23–28).

**Role of Magnetic Antisite Defects**

The thickness-dependent STS measurements discussed above were carried out in low defect areas, where STS shows consistent uniform gap values. We next discuss how defects impact the local electronic structure. Fig. 3A shows a region with low MnBi antisites (<4%) on 4-SL MnBi₂Te₄. Fig. 3B displays spatial-dependent tunneling spectra. Depending on their specific locations, the tunneling peak features show intensity variation. However, the spectra exhibit a uniform gap value with E_F located within the gap. Note that the intrinsic nature of this sample suggests a similar amount of BiMn antisite (n-type dopant) and MnBi antisite (p-type dopant). This situation changes drastically in high defective areas. Fig. 3C shows the atomic image of the defective area on 3-SL MnBi₂Te₄, exhibiting high concentrations of MnBi (∼9%). In such areas, locally “defect-free” regions on the scale of 2 nm by 4 nm can be found. Fig. 3D shows a sequence of spectra from points between the locally defect-free region (position No. 1) and the defective area. The spectrum at position No. 1 exhibits a finite Dirac gap, whose tunneling features are similar to those on the clean area (SI Appendix, Fig. S4C). As one progresses to a defective area, the Dirac gap decreases (position No. 2) and eventually collapses (No. 3 to No. 6) with a V-shape DOS suggesting the recovery of the linear Dirac dispersion. Interestingly, in the spectra acquired in the defective region (No. 3 to No. 6), one observes an additional zero-bias anomaly, characterized by a dip at zero bias and two peaks at ±6 meV. We attribute this zero-bias anomaly to inelastic scattering due to spin excitations, similar to those reported previously in other systems (41–43), further confirming the magnetic nature of the MnBi antisites. The evolution of the Dirac mass gap observed here strongly suggests the significance of defects concentration, particularly magnetic antisites, in suppressing the exchanging coupling between the Dirac surface states and the magnetic moments.

**Ab Initio DFT and Coupled Dirac Cone Model Calculations**

Motivated by our experimental observations, we performed DFT supercell calculation to account for the role of defects and interpreted them using a simplified Dirac-cone model (22) of the MnBi₂Te₄ electronic structure. Fig. 4A illustrates the magnetic moments and exchange couplings present in our model calculation. The MnBi antisites moments have been shown to be antiparallel to those in the central Mn layer (31). Exchange interactions between Fermi-level electrons and these moments
partially cancel those from the central Mn layer, reducing the same-layer and neighboring-layer exchange couplings $J_s$ and $J_D$ (see SI Appendix, Fig. S6 for detailed definition.). To estimate the change of $J_s$ and $J_D$ as a function of magnetic antisites density, we perform DFT supercell calculations for bulk MnBi$_2$Te$_4$ crystals that have a ferromagnetic spin configuration and varying antisite defect configurations. A $4 \times 4 \times 1$ superstructure with one MnBi antisite per 16 Bi atoms is used to simulate 6% MnBi (see SI Appendix, Fig. S7 for more superstructure configuration information). To keep the chemical potential within the gap, we choose to compensate the MnBi antisite with a BiMn antisite by substituting the Bi atom with its next nearest-neighbor Mn atom, as illustrated in Fig. 4A. This antisite pair configuration has the lowest formation energy (31). The presence of BiMn antisites also decreases $J_5$ by reducing the magnetic moment in the Mn layer. As shown in Fig. 4B, bulk MnBi$_2$Te$_4$ with a ferromagnetic spin configuration is a topological Weyl semimetal (red curve). This topological phase is destroyed by 6% MnBi, leading to a trivial insulating state (black curve).

We also calculate other defect concentrations to learn the evolution of electronic structure as defect density varies. Fig. 4C (red curve) summarizes the DFT-calculated $\Gamma$ point energy gap as a function of defect density, showing a gap closing at around 2% MnBi, at which a topological phase transition from a Weyl semimetal to a trivial insulating state (black curve).

Using the parameters extracted from DFT, we performed coupled Dirac cone model calculations for thin films with antiferromagnetic spin configurations. Fig. 4D summarizes the calculated $\Gamma$ point energy gaps for both spin-aligned bulk and antiferromagnetic thin film cases. The bulk results (dashed black line) agree well with the DFT results (gold diamonds), confirming the validity of our model. For antiferromagnetic thin films, such as 4 and 6 SLs, gaps can be suppressed by half with less than 6% MnBi. As is expected (44) (see SI Appendix, Fig. S8 for detailed discussion), this effect is even more dramatic for odd SLs, as exemplified by the 3 and 5 SLs results in Fig. 4D. In that case, gap values show a linear dependence on the defect density, and a topological phase transition occurs at around 1% for 3-SL and 6% for 5-SL thin films. A turning point occurs at about 9% due to the exchange coupling contributed by the MnBi overtaking that by the central Mn layer. This eventually leads to a second gap crossing zero accompanied by a trivial insulator to Chern insulator transition with the opposite relationship between Chern number and magnetization. The gap-quenching defect concentration (1%) is small for

---

**Fig. 3.** Dirac mass gap variation as a function of defect distribution. (A) Atomic image taken on low-defect 4-SL region (setpoint bias: 0.3 V). (B) Spatial-dependent STS distribution with spatial locations marked in A. Horizontal black dashed lines mark zero. (C) Atomic image taken on high-defect 3-SL region (setpoint bias: $-0.35$ V). (D) Spatial-dependent STS distribution with spatial locations marked in C. Black arrows mark the Dirac point. Vertical black dashed lines on STS No. 3 to No. 6 mark the zero-bias tunneling anomaly.
MnBi defects suppress the Dirac mass gap. Local surface states are gapped. STS spatial mapping across bound-
ary planes (16, 17, 19, 20, 46). Our experimental STM/S study of intrinsic MBE-grown MnBi2Te4 thin films provides unambiguous evidence for a Dirac mass gap in regions with low magnetic antisite defect density and resolves the current debate as to whether or not the topological surface states are gapped. STS spatial mapping across boundaries between pristine and defective regions directly reveals how MnBi defects suppress the Dirac mass gap. *Ab initio* DFT and coupled Dirac cone model calculations unveil the microscopic mechanism for this correlation. The model calculations predict critical antisite densities above which the QAH effect cannot be observed in the antiferromagnetic MnBi2Te4 thin films (~6% for 5-SL films). By demonstrating the microscopic origin of the Dirac mass gap variation in MnBi2Te4, our work establishes magnetic defect as an important parameter in controlling the topological quantum phases.

**Materials and Methods**

**Sample Growth and STM/S Measurements.** MnBi2Te4 thin films were grown in a home-built MBE chamber with base pressure at ~10^-10 Torr. HOPG substrates were cleaved in air and immediately transferred into the MBE chamber. HOPG substrates were outgassed at ~300 °C overnight before the growth of MnBi2Te4. High-purity Mn (99.99%), Bi (99.999%), and Te (99.999%) were evaporated from standard Knudsen cells. Samples were grown at 240 °C and postannealed at the growth temperature in a Te ambient. Samples were transferred from the MBE chamber into the STM chamber, with base pressure ~10^-11 Torr, through a transfer vessel, with base pressure ~10^-10 Torr, to maintain the cleanliness of the film. STM/S measurements were conducted at 4.3 K. The W tip was prepared by electrochemical etching and then cleaned by in situ electron-beam heating. STM dI/dV spectra were measured using a standard lock-in technique with feedback loop off, whose modulation frequency is 490 Hz.

**Ab Initio DFT Calculations.** DFT calculations were performed using Vienna *Ab Initio* Simulation Package (VASP) (47), in which generalized gradient approxima-
tions of Perdew-Burke-Emzerhof (48) have been adopted for exchange-correlation potential. On-site correlation on the Mn 3d states is treated by an on-site correlation potential. HOPG substrates were outgassed at ~300 °C overnight before the growth of MnBi2Te4. High-purity Mn (99.99%), Bi (99.999%), and Te (99.999%) were evaporated from standard Knudsen cells. Samples were grown at 240 °C and postannealed at the growth temperature in a Te ambient. Samples were transferred from the MBE chamber into the STM chamber, with base pressure ~10^-11 Torr, through a transfer vessel, with base pressure ~10^-10 Torr, to maintain the cleanliness of the film. STM/S measurements were conducted at 4.3 K. The W tip was prepared by electrochemical etching and then cleaned by in situ electron-beam heating. STM dI/dV spectra were measured using a standard lock-in technique with feedback loop off, whose modulation frequency is 490 Hz.

**Supplementary Information**

SI Appendix, Fig. S7, one MnBi antisite per 16 Bi atoms in a 4 × 4 × 1 supercell corresponds to MnBi density of 1/16, one MnBi antisite per nine Bi atoms in a 3 × 3 × 1 supercell corresponds to MnBi density of 1/9, and two MnBi antisites per 16 atoms in a 4 × 4 × 1 supercell corresponds to MnBi density of 1/8. The global break condition for the electronic self-consistency loop is set to be 10^-7 eV, and the plane wave energy cutoff is set to be 600 eV. DOSs in Fig. 2E are calculated on a 16 × 16 × 1 Γ-centered k-point integration grid with a Gaussian broadening factor of 50 meV.

**Data, Materials, and Software Availability.** All data are included in the manuscript and/or SI Appendix.
ACKNOWLEDGMENTS. This work was primarily supported by the NSF through the Center for Dynamics and Control of Materials: an NSF Materials Research Science and Engineering Centers under cooperative agreement no. DMR-1720595 and the US Air Force grant no. FA2386-21-1-0401. Other supports were from NSF grant nos. DMR-1808751, DMR-2219610, and the Welch Foundation F-1672. Work at Oak Ridge National Laboratory was supported by the US Department of Energy.

1. R. Li, J. Wang, X.-L. Qi, S.-C. Zhang, Dynamical axion field in topological magnetic insulators. Nat. Phys. 6, 284–288 (2010).
2. R. S. K. Mong, A. M. Essin, J. E. Moore, Antiferromagnetic topological insulators. Phys. Rev. B 81, 245209 (2010).
3. Y. Tokura, K. Yasuda, A. Tsukazaki, Magnetic Topological Insulators. Nat. Rev. Phys. 1, 126 (2019).
4. R. Yu et al., Quantized anomalous Hall effect in magnetic topological insulators. Science 329, 61–64 (2010).
5. C. Z. Chang et al., Experimental observation of the quantum anomalous Hall effect in a magnetic topological insulator. Science 340, 167–170 (2013).
6. I. Lee et al., Imaging Dirac mass disorder from magnetic dopant atoms in the ferromagnetic topological insulator CrB6S8(001), Proc. Natl. Acad. Sci. U.S.A. 112, 1316–1321 (2015).
7. Y. S. Hor et al., Development of ferromagnetism in the doped topological insulator Bi2xMnTe2. Phys. Rev. B 81, 195203 (2010).
8. M. M. Otrokov et al., Highly ordered wide bandgap materials for quantized anomalous Hall and magnetoelectric effects. 2D Mater. 4, 025082 (2017).
9. M. M. Otrokov et al., Prediction and observation of an antiferromagnetic topological insulator. Nature 576, 416–422 (2019).
10. J. Li et al., Intrinsic magnetic topological insulators in van der Waals layered MnBi2Te4 family materials. Sci. Adv. 5, eaax5685 (2019).
11. W. Ning, Z. Mao, Recent advancements in the study of intrinsic magnetic topological insulators and magnetic Weyl semimetals. APL Mater. 8, 090701 (2020).
12. C. Hu et al., A van der Waals antiferromagnetic topological insulator with weak interlayer magnetic coupling. Nat. Commun. 11, 97 (2020).
13. C. Liu et al., Robust axion insulator and Chern insulator phases in a two-dimensional antiferromagnetic topological insulator. Nat. Mater. 19, 522–527 (2020).
14. J. Ge et al., High-Chern-number and high-temperature quantum Hall effect without Landau levels. Natl. Sci. Rev. 7, 1280–1287 (2020).
15. Y. Deng et al., Quantum anomalous Hall effect in intrinsic magnetic topological insulator MnB2Te4. Science 367, 895–900 (2020).
16. Y. F. Zhao et al., Even-odd layer-dependent anomalous Hall effect in topological magnet MnB2Te4 thin films. Nano Lett. 21, 7691–7698 (2021).
17. L. Tai et al., Distinguishing two-component anomalous Hall effect from topological Hall effect in magnetic topological insulator MnB2Te4. Phys. Rev. B 89, 155125 (2019).
18. D. Ovchinnikov et al., Intertwined topological and magnetic orders in atomically thin Chern insulator MnB2Te4. Nat. Commun. 12, 4467 (2021).
19. M. M. Otrokov et al., Unique thickness-dependent properties of the van der Waals interlayer antiferromagnetic MnB2Te4 films. Phys. Rev. Lett. 122, 107202 (2019).
20. C. Lee, S. Chen, A. H. MacDonald, Magnetized topological insulator multilayers. Proc. Natl. Acad. Sci. U.S.A. 117, 27224–27230 (2020).
21. Y. J. Chen et al., Topological electronic structure and its temperature evolution in antiferromagnetic topological insulator MnB2Te4. Phys. Rev. X 9, 041040 (2019).
22. Y. J. Hao et al., Gapless surface Dirac cone in antiferromagnetic topological insulator MnB2Te4. Phys. Rev. X 9, 041038 (2019).
23. X. Wu et al., Distinct topological surface states on the two terminations of MnB2Te4. Phys. Rev. X 10, 031013 (2020).
24. Y. Yuan et al., Electronic states and magnetic response of MnB2Te4 by scanning tunneling microscopy and spectroscopy. Nano Lett. 20, 3271–3277 (2020).
25. M. P. Sisak, J. Kim, D. Vandenbult, J. Yan, W. Wu, Robust A-type order and spin-flop transition on the surface of the antiferromagnetic topological insulator MnB2Te4. Phys. Rev. Lett. 123, 037201 (2020).
26. Z. Li et al., Mapping Dirac fermions in the intrinsic antiferromagnetic topological insulators (MnB2Te4)(Bi2Te3)n (n = 0,1). Phys. Rev. B 102, 161115 (2020).
27. D. Nevala et al., Coexistence of surface ferromagnetism and a gapless topological state in MnB2Te4. Phys. Rev. Lett. 125, 117205 (2020).
28. B. Li et al., Competing magnetic interactions in the antiferromagnetic topological insulator MnB2Te4. Phys. Rev. Lett. 124, 167204 (2020).
29. Y. Liu, L. Ke, J. Yan, R. D. McDonald, R. J. McGuirey, Defect-driven ferromagnetism and hidden magnetization in MnB2Te4. Phys. Rev. B 103, 184429 (2021).
30. Y. Liu et al., Site mixing for engineering magnetic topological insulators. Phys. Rev. X 11, 021033 (2021).
31. M. Garnica et al., Native point defects and their implications for the Dirac point gap at MnBi2Te4(001). NPJ Quantum Mater. 7, 2 (2022).
32. T. Hirahara et al., Large-gap magnetic topological heterostructure formed by subsurface incorporation of a Ferromagnetic layer. Nano Lett. 17, 3493–3500 (2017).
33. E. D. L. Rienks et al., Large magnetic gap at the Dirac point in Bi2Te3/MnBi2Te4 heterostructures. Nature 576, 423–428 (2019).
34. S. Wimmer et al., Mn-Rich MnSb2Te4. A topological insulator with magnetic gap closing at high curie temperatures of 45–50 K. Adv. Mater. 33, e2102935 (2021).
35. P. Kippers et al., Probing the magnetic band gap of the ferromagnetic topological insulator MnBi2Te4. arXiv [Preprint] arXiv: 2202.11540 (2021).
36. D. S. Lee et al., Crystal structure, properties and nanostructuring of a new layered chalcogenic semiconductor, Bi3MnTe4, CrystEngComm 15, 5532 (2013).
37. Z. Huang, M. H. Du, J. Yan, W. Wu, Native defects in antiferromagnetic topological insulator MnBi2Te4. Phys. Rev. Mater. 4, 121202 (2020).
38. M. H. Du, J. Yan, V. R. Cooper, M. Eisenbach, Tuning Fermi levels in intrinsic antiferromagnetic topological insulators MnBi2Te4 and MnBi2Te6 by defect engineering and chemical doping. Adv. Funct. Mater. 31, 2006516 (2021).
39. A. A. Khajetoorians et al., Detecting excitation and magnetization of individual dopants in a semiconductor. Nature 567, 1084–1087 (2019).
40. A. A. Khajetoorians et al., Spin excitations of individual Fe atoms on Pt(111): impact of the site-dependent giant substrate polarization. Phys. Rev. Lett. 111, 157204 (2013).
41. Y. F. Hinjebhein, C. P. Lutz, A. J. Heinrich, Spin coupling in engineered atomic structures. Science 312, 1021–1024 (2006).
42. C. Lee, A. H. MacDonald, Gate-tunable quantum anomalous Hall effects in MnBi2Te4 thin films. Phys. Rev. Mater. 5, 055201 (2021).
43. J. Q. Yan et al., Crystal growth and magnetic structure of MnB2Te4. Phys. Rev. Mater. 3, 064202 (2019).
44. J. Yan, The elusive quantum anomalous Hall effect in MnB2Te4: a materials perspective. arXiv [Preprint] arXiv: 2112.09702 (2021).
45. G. Kresse, J. Hafner, Ab initio molecular dynamics for liquid metals. Phys. Rev. B Condens. Matter 48, 1447–1456 (1993).
46. J. Yan, The elusive quantum anomalous Hall effect in MnB2Te4: a materials perspective. arXiv [Preprint] arXiv: 2112.09702 (2021).
47. G. Kresse, J. Hafner, Ab initio molecular dynamics for liquid metals. Phys. Rev. B Condens. Matter 48, 1447–1456 (1993).