Bipolarized Weyl semimetals and quantum crystal valley Hall effect in two-dimensional altermagnetic materials

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Magnetism and topology are two major areas of condensed matter physics. The combination of magnetism and topology gives rise to more novel physical effects, which have attracted strongly theoretical and experimental attention. Recently, the concept of altermagnetism has been introduced, characterized by a dual nature: real-space antiferromagnetism and reciprocal-space anisotropic spin polarization. The amalgamation of altermagnetism with topology may lead to the emergence of previously unobserved topological phases and the associated physical effects. In this study, utilizing a four-band lattice model that incorporates altermagnetism and spin group symmetry, we demonstrate that type-I, type-II, and type-III bipolarized Weyl semimetals can exist in altermagnetic systems. Through the first-principles electronic structure calculations, we predict four ideal twodimensional type-I alternagnetic bipolarized Weyl semimetals Fe₂WTe₄ and Fe₂MoZ₄ (Z=S,Se,Te). More significantly, we introduce the quantum crystal valley Hall effect, a phenomenon achievable in three of these materials namely Fe₂WTe₄, Fe₂MoS₄, and Fe₂MoTe₄, when spin-orbit coupling is considered. Furthermore, these materials have the potential to transition from a quantum crystal valley Hall phase to a Chern insulator phase under strain. In contrast, Fe₂MoSe₄ remains to be a Weyl semimetal under spin-orbit coupling but is distinguished by possessing only a single pair of Weyl points. Additionally, the position, polarization, and number of Weyl points in Fe₂WTe₄ and Fe_2MoZ_4 can be manipulated by adjusting the direction of the Néel vector. Consequently, Fe_2WTe_4 and Fe_2MoZ_4 emerge as promising experimental platforms for investigating the distinctive physical attributes of various altermagnetic topological phases.

Introduction. The topological Weyl semimetals have attracted much attention due to their novel physical properties, such as topological protected Fermi arc, chiral zero sound, chiral anomaly, large magnetoresistance effect, large intrinsic anomalous Hall effect [1-13], etc. Since Weyl points are formed by linear crossing of two nondegenerate energy bands, Weyl semimetals can only exist in the materials without the joint symmetry of time reversal and space inversion. The Weyl points of nonmagnetic or conventional antiferromagnetic Weyl semimetals have no spin polarization (Fig. 1(a)), while the Weyl points of ferromagnetic Weyl semimetals have only spinup or spin-down polarization (Fig. 1(b)). This then raises an intriguing question: Can a Weyl semimetal accommodate both spin-up and spin-down polarized Weyl points simultaneously? (Fig. 1(c)).

Recently, based on spin group theory, a new magnetic phase, namely altermagnetism, which is different from ferromagnetism and conventional antiferromagnetism, has been proposed [14–20]. Due to the duality of real-space antiferromagnetism and reciprocal-space anisotropic spin polarization similar to ferromagnetism, the altermagnetic materials show many novel physical effects, including spin-splitting torque [21–24], giant magnetoresistance (GMR) effect [25], tunneling magnetoresistance (TMR) effect [25, 26], piezomagnetic effect [27], nontrivial superconductivity [28, 29], time-reversal odd anomalous effect [15, 30–35], quantum anomalous Hall effect [36], higher-order topological states [37], altermagnetic ferroelectricity [38], strong spin-orbit coupling effect in light element altermagnetic materials [39] and so on. Moreover, the already predicted altermagnetic materials cover metals, semimetals, and insulators, which provides a guarantee for the realization of many novel physical effects in experiments [40–47]. Meanwhile, the reciprocal-space anisotropic spin polarization of altermagnetism also provides possibility to realize a topological Weyl semimetal with both spin-up and spin-down polarized Weyl points. Here, we term this class of Weyl semimetals as bipolarized Weyl semimetals.

In this work, based on spin group symmetry analysis, lattice model, and the first-principles electronic structure calculations, we not only demonstrate that type-I, type-II, and type-III bipolarized Weyl semimetal can be realized in altermagnetic systems, but also predict four ideal two-dimensional type-I bipolarized Weyl semimetals Fe₂WTe₄ and Fe₂MoZ₄ (Z=S,Se,Te). Furthermore, we find quantum crystal valley Hall effect in Fe₂WTe₄, Fe₂MoS₄, and Fe₂MoSe₄. And they can transform from quantum crystal valley Hall phase to Chern insulator phase under strain. In contrast, Fe₂MoTe₄ remains to be a Weyl semimetal with only one pair of Weyl points under spin-orbit coupling (SOC).

Lattice Model. We consider a square lattice containing

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FIG. 1. The schematic diagrams of three different Weyl semimetal phases. (a) Nonmagnetic (NM) or antiferromagnetic (AFM) Weyl semimetal; (b) Ferromagnetic (FM) semimetal; (c) bipolarized altermagnetic (AM) semimetal. The gray cones represent Weyl points without spin polarization. The red and blue cones represent spin-up and spin-down polarized Weyl points, respectively.

two sites (labeled by sublattice index $\alpha = 1, 2$) within a unit cell (Fig. 2(a)). The corresponding tight-binding (TB) model is

$$H = \sum_{d_{i,j}} \left[t^{d} C^{\dagger}_{1,j} C_{2,j+d_{i}} + h.c. \right]$$

+
$$\sum_{\alpha,j} \left[t^{x}_{\alpha} C^{\dagger}_{\alpha,j} C_{\alpha,j+\mathbf{x}} + t^{y}_{\alpha} C^{\dagger}_{\alpha,j} C_{\alpha,j+\mathbf{y}} + h.c. \right]$$

+
$$\sum_{\alpha,j} \mathbf{m}_{\alpha} \cdot \boldsymbol{\sigma} \ C^{\dagger}_{\alpha,j} C_{\alpha,j}$$
(1)

where $C_{\alpha,j}^{\dagger} = \left(C_{\alpha,j\uparrow}^{\dagger}, C_{\alpha,j\downarrow}^{\dagger}\right)$ and $C_{\alpha,j} = (C_{\alpha,j\uparrow}, C_{\alpha,j\downarrow})$ represent electron creation and annihilation operators, respectively. The terms containing t^d and $t_{\alpha}^{x,y}$ represent the nearest and next nearest hopping, respectively. As illustrated in Fig. 2(a), $d_{1,4} = \pm \frac{1}{2}(\mathbf{x}+\mathbf{y}), d_{2,3} = \pm \frac{1}{2}(\mathbf{x}-\mathbf{y})$ and $\mathbf{x} = a_1 \hat{x}, \mathbf{y} = a_2 \hat{y}$ denote the direction of hopping, where a_1, a_2 are the lattice constants along the unit vectors \hat{x}, \hat{y} . The σ_0 and $\boldsymbol{\sigma}$ are identity matrix and Pauli matrix, respectively. The $\mathbf{m}_1 = -\mathbf{m}_2 = \mathbf{m}$ stands for the static collinear AFM order, which couples to the electron spin as a Zeeman field. Due to the two opposite spin sites located at the space-inversion invariant position, the collinear AFM order breaks spin symmetry $\{C_2^{\perp}||I\}$. Moreover, since $t_1^{x,y} \neq t_2^{x,y}$ breaks the spin symmetry $\{C_2^{\perp}||\tau\}$ but $t_1^{x,y} = t_2^{y,x}$ preserves spin symmetry $\{C_2^{\perp}||C_{4z}\}$. Thus, this lattice model is a *d*-wave altermagnetism.

After performing the Fourier transformation, the TB Hamiltonian can be rewritten as $H = \sum_k \psi_k^{\dagger} H_0 \psi_k$ in momentum space with basis $\psi^{\dagger} = \left(C_{1k\uparrow}^{\dagger}, C_{1k\downarrow}^{\dagger}, C_{2k\uparrow}^{\dagger}, C_{2k\downarrow}^{\dagger}\right)$, where H_0 reads

$$H_0 = \Gamma_k^+ \tau_0 \sigma_0 + \Gamma_k^{12} \tau_x \sigma_0 + \Gamma_k^- \tau_z \sigma_0 + \tau_z \mathbf{m} \cdot \boldsymbol{\sigma} \qquad (2)$$

in which Pauli matrix $\boldsymbol{\tau}$ is the pseudospin matrix in lattice space. The auxiliary functions $\Gamma_k^{12} = 4t^d \cos \frac{k_x}{2} \cos \frac{k_y}{2}$ and $\Gamma_k^{\pm} = (t_1 \pm t_2) \cos k_x + (t_2 \pm t_1) \cos k_y$ with $t_{\alpha}^x = t_{\alpha}$ are related to inter-and intra-sublattice hoppings, respectively. Altermagnetism leads to anisotropic



FIG. 2. Two-dimensional lattice model with altermagnetism. (a) The schematic illustration for the hoppings between lattice sites for the Hamiltonian Eq. (1). The red and blue arrows represent spin-up and spin-down magentic moments, respectively. (b-d) The band structure of lattice model in certain parameters. (b), type-I bipolarized Weyl semimetal; (c), type-II bipolarized Weyl semimetal;(d), type-III bipolarized Weyl semimetal. The red and blue represent spin-up and spin-down bands, respectively. The 1 and -1 represent eigenvalues of the spin symmetry $\{E||C_{2x}\}$ or $\{E||C_{2y}\}$.

spin splitting, so what does the size of spin splitting depend on? The lattice model analysis shows the size of spin splitting is determined by the strength of anisotropic hopping $|t_1 - t_2|$ (Detailed calculations and analyses are presented in the supplementary materials (SM)).

When $2|t_1 - t_2| > |\mathbf{m}|$, the band crossing occurs, which is a necessary condition for the realization of bipolarized Weyl semimetals. Further symmetry analysis shows that there are two crossing points with spin-up polarization and another two crossing points with spin-down polarization protected by the spin symmetry $\{E||C_{2y}\}$ and $\{E||C_{2x}\}$, respectively. Therefore, a bipolarized Weyl semimetal can be realized in an altermagnetic system. Interestingly, by adjusting the hopping terms t_1 and t_2 , we are able to achieve type-I, type-II, and type-III bipolarized Weyl semimetals which are shown in Fig. 2(b), (c), and (d), respectively.

Candidate materials. Monolayer Fe_2XZ_4 (Fe_2WTe_4 and Fe_2MoZ_4) takes a square lattice structure with the symmorphic space group P-42m (No.111) symmetry and the corresponding point group is D_{2d} with generators S_{4z} and C_{2x} . Monolayer Fe_2XZ_4 contains three atomic layers where Fe_2X atomic layer is sandwiched by two Z atomic layers as shown in Fig. 3(a) and (b), and the corresponding BZ is shown in Fig. 3(c). Moreover, the dynamical stability of monolayer Fe₂XZ₄ is confirmed by the phonon calculations (Fig. S3) [48]. Since the crystal structure of monolayer Fe₂XZ₄ is proposed based on the already synthesized layered Cu₂XZ₄ (Z=S,Se) [49–53] and Ag₂WS₄ [54], monolayer Fe₂XZ₄ may be synthesized experimentally in a similar way.

To determine the magnetic ground states of monolayer Fe₂XZ₄, we consider three likely magnetic structures including one ferromagnetic and two antiferromagnetic ones (Fig. S4). The calculated results show that the AFM1 is always magnetic ground state for the four materials Fe₂XZ₄, as shown in Table. S2. From Fig. 3(a), the magnetic and crystal primitive cells are identical, thus Fe₂XZ₄ has no $\{C_2^{\perp} || \tau\}$ spin symmetry. And due to the lack of space-inversion symmetry, Fe₂XZ₄ must not have $\{C_2^{\perp} || I\}$ spin symmetry. Meanwhile, the Fe₂XZ₄ has $\{C_2^{\perp} || I\}$ spin symmetry. Thus, all the Fe₂XZ₄ are *d*-wave altermagnetic materials. In the following, we present nontrivial topological states with Fe₂WTe₄ as a representative material, while the calculated results of other three materials are presented in the SM.

For monolayer Fe_2WTe_4 , the W atom is at the corner of primitive cell and there is no W atom in the center, which leads to a strongly anisotropic polarized charge density around the magnetic Fe atom as shown in Fig. 3(d). The strongly anisotropic polarized charge density makes x- or y-directional two hopping interactions of the next nearest Fe atoms very different, which can lead to the large spin splitting in the non-relativistic case according to our lattice model analysis. Just like our analysis, the spin splitting caused by the exchange interactions in altermagnetic Fe_2WTe_4 is very large. The spins of these bands along the Γ -X and Γ -Y are opposite, reflecting the characteristics of *d*-wave altermagnetism (Fig. 3(e)). More significantly, altermagnetic Fe_2WTe_4 is a perfect semimetal with only four doubly degenerat crossing points at the Fermi level (Fig. 3(c) and (e)). These crossing points can be considered as a valley degree of freedom, similar to the case of graphene. Manipulating this valley degree of freedom will give rise to novel effects as shown below. The further orbital weight analysis shows that the two crossing bands along the Γ -Y direction are respectively contributed by the e_g and d_{yz} orbitals of Fe atoms (Fig. 3(f)). Since the e_g orbital is invariable but the d_{yz} orbital changes to $-d_{yz}$ under the $\{E \mid \mid C_{2y}\}$ operation, the corresponding eigenvalues of the two crossing bands are 1 and -1, respectively. Thus, the two crossing points on the Γ -Y direction are the Weyl points protected by $\{E || C_{2y}\}$ spin symmetry. Likewise, the two crossing points on the $\Gamma\text{-}X$ direction are also the Weyl points protected by $\{E || C_{2x}\}$ spin symmetry. Interestingly, the two Weyl points on the Γ -Y direction have spin-up polarization, while the two Weyl points in the Γ -X direction have spin-down polarization (Fig. 3(e)). Thus, the monolayer altermagnetic Fe_2WTe_4 is a bipolarized Weyl semimetal.



FIG. 3. Crystal and magnetic structures of monolayer Fe₂XZ₄ and electronic properties of monolayer Fe₂WTe₄. (a) and (b) represent the top and side views of crystal and magnetic structure of Fe₂XZ₄, respectively. The red and blue arrows represent spin-up and spin-down magnetic moments, respectively. (c) The Brillouin zone (BZ) of Fe₂XZ₄ where the high-symmetry points are labeled. The red and blue points represent spin-up and spin-down polarized Weyl points, respectively. (d) The polarization charge density of Fe₂WTe₄ without SOC (red: spin-up, blue:spin-down).The electronic structure along the high-symmetry directions without SOC (e) and with SOC (f). The e_g represents the d_{z^2} and $d_{x^2-y^2}$ orbitals of Fe element. The Spectral function of monolayer Fe₂WTe₄ with a semi-infinite termination left (g) and right (h) edges.

With SOC, monolayer Fe_2WTe_4 changes from spin group symmetry to magnetic group symmetry. According to our magnetic anisotropy calculations, the direction of the Néel vector is along the z-axis, which has magnetic point group symmetry $2S_{4z}T$, C_{2z} , $C_{2x}T$, $C_{2y}T$, and $2\sigma_d$. The symmetry of Γ -Y axis changes from the $\{E \mid \mid C_{2y}\}$ spin symmetry to the $C_{2x}T$ symmetry. Both e_q and d_{yz} orbitals are invariant under the C_{2x} operation, so the two crossing bands in the Γ -Y direction have the same irreducible representation, thus opening a gap (2.5 meV) (inset of Fig. 3(f)). Likewise, the two Weyl points in the Γ -X direction also open a gap of 2.5 meV. Due to the C_{2z} symmetry, the two Weyl points in the Γ -X or Γ -Y direction contribute the same Berry curvature, but the two pairs of Weyl points in the Γ -X and Γ -Y directions contribute the opposite Berry curvature due to the $S_{4z}T$ symmetry (Fig. 4(a)). We know that a twodimensional linear Weyl point has π Berry curvature, so one pair of Weyl points in the Γ -X (Γ -Y) direction contributes -2π (2π) Berry curvature, which corresponds to the Chern number -1 (1). Furthermore, the anisotropy Chern number may lead to nontrivial chiral edge states, which have been confirmed by the calculations of edge states (Fig. 3(g) and (h)). On the other hand, under the strain in the x direction, the band inversion of Fe₂WTe₄ in the Γ -X direction disappears, but the band inversion in the Γ -Y direction still remains (Fig. S9). Thus, monolayer altermagnetic Fe₂WTe₄ transforms into a Chern insulator with quantum anomalous Hall effect under strain.

Quantum crystal valley Hall effect. As is well known, under in-plane longitudinal electric field, an intrinsic Berry curvature can induce an anomalous Hall velocity for the Bloch electrons in two-dimensional materials $(v \sim E \times \Omega(k))$ [55]. For monolayer Fe₂WTe₄, there are four valleys originating from the Weyl points (Fig. 4 (a)). From Fig. 4(a), the valley electrons in the Γ -X and Γ -Y directions for Fe₂WTe₄ have opposite Berry curvature, resulting in opposite anomalous Hall velocities under the in-plane longitudinal electric field (Fig. 4(b)). Moreover, these valley electrons maintain opposite spin polarization under SOC (Fig. 4(a)), thus altermagnetic Fe₂WTe₄ can generate polarized spin currents perpendicular to the electric field, akin to the valley Hall effect in monolayer MoS_2 [56, 57]. For monolayer MoS2, the timereversal symmetry guarantees opposite Berry curvature and angular momentum for the valley electrons with opposite momentum, which results in the valley Hall effect. In comparison, Fe_2WTe_4 breaks the time-reversal symmetry, but the $S_{4z}T$ symmetry ensures opposite Berry curvature and spin polarization for the valley electrons in both Γ -X and Γ -Y directions. Due to the valley Hall effect deriving from crystal symmetry, the valley Hall effect in monolayer altermagnetic Fe₂WTe₄ can be called crystal valley Hall effect. More importantly, the two pairs of valley electrons in the Γ -X and Γ -Y directions contribute opposite Chern numbers, thus the valley Hall effect in monolayer altermagnetic Fe_2WTe_4 can be further called quantum crystal valley Hall effect, which is similar to the quantum valley Hall effect in two-dimensional nonmagnetic materials [12, 58].

On the other hand, our calculations show that the other three two-dimensional altermagnetic materials are also bipolarized Weyl semimetals without SOC. The directions of the Néel vector of both Fe_2MoS_4 and Fe_2MoS_4 are the same as that of Fe_2WTe_4 under SOC, so the quantum crystal valley Hall effect can also be realized in both Fe_2MoS_4 and Fe_2MoSe_4 (Fig. S6 and S7). Meanwhile, both Fe_2MoS_4 and Fe_2MoSe_4 also transform from quantum crystal valley Hall insulator phase to Chern insulator phase under strain (Fig. S9).

Different from the case of Fe₂MoS₄, Fe₂MoSe₄ and Fe₂WTe₄, the direction of Néel vector of Fe₂MoTe₄ is along the x- or y-axis due to the S_4 symmetry of crystal. When the Néel vector is along the x-axis, because there is no any symmetry for the Γ -Y axis, the pair of spinup polarized Weyl points in Fe₂MoTe₄ open gap, while



FIG. 4. (a) Top panel: the electronic band structure of monolayer Fe₂WTe₄ with the spin projection s_z ; bottom panel: the corresponding berry curvature along the high-symmetry line. (b) The schematic diagram of the topological valley Hall effect in monolayer Fe₂WTe₄. The *E* and *e* represent external electric field and electrons, respectively. The red and blue arrows represent up and down spins, respectively.

the two spin-down polarized Weyl points in the Γ -X axis remain stable protected by the C_{2x} symmetry. Therefore, monolayer altermagnetic Fe₂MoTe₄ is still a Weyl semimetal under SOC (Fig. S5(f)). Similarly, Fe₂MoTe₄ has also only one pair of Weyl points, but the pair of Weyl points have spin-up polarization when the Néel vector is along the y-axis. If the Néel vector is along the xydirection, the Γ -X and Γ -Y axes do not have any symmetry, thus the two pairs of Weyl points of Fe_2MoTe_4 open gap (Fig. S8). However, the $C_{2z}T$ symmetry is always present for the Néel vector in the xy plane, which results in the Berry curvature $\Omega_z(\mathbf{k})$ to be zero in the whole BZ, thus the quantum crystal valley Hall effect can not be realized in Fe_2MoTe_4 . According to the above analysis, the position, polarization, and number of Weyl points of Fe₂MoTe₄, as well as Fe₂MoS₄, Fe₂MoSe₄ and Fe₂WTe₄ (Fig. S8), can be manipulated by controlling the Néel vector.

In conclusion, our research, grounded in symmetry analysis, lattice modeling, and first-principles electronic structure calculations, not only confirms the theoretical feasibility of realizing a bipolarized Weyl semimetal in two-dimensional altermagnetic systems but also identifies four ideal candidates: Fe_2WTe_4 and Fe_2MoZ_4 (Z=S.Se.Te). Most notably, we propose that the quantum crystal valley Hall effect can be induced in the monolayer altermagnetic materials Fe_2WTe_4 , Fe_2MoS_4 , and Fe_2MoSe_4 when subject to spin-orbit coupling. These materials can further transition from a quantum crystal valley Hall insulator phase to a Chern insulator phase Unlike the other materials mentioned, under strain. Fe_2MoTe_4 retains its Weyl semimetal nature with a single pair of Weyl points even under SOC. Furthermore, the position, polarization, and number of Weyl points in Fe_2WTe_4 and Fe_2MoZ_4 (Z=S,Se,Te) can be manipulated by adjusting the direction of the Néel vector. Consequently, Fe₂WTe₄ and Fe₂MoZ₄ offer a promising experimental platform for exploring the distinctive physical properties associated with multiple altermagnetic topological phases.

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