

Review

The quantum anomalous Hall effect in two-dimensional hexagonal monolayers studied by first-principles calculations

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SUMMARY

The quantum anomalous Hall effect (QAHE) demonstrates the potential for achieving quantized Hall resistance without the need for an external magnetic field, making it highly promising for reducing energy loss in electronic devices. Its realization and research rely heavily on precise first-principles calculations, which are essential for analyzing the electronic structures and topological properties of novel two-dimensional (2D) materials. This review article explores the theoretical progress of QAHE in 2D hexagonal monolayers with strong spin-orbit coupling and internal magnetic ordering. We summarize current strategies and methods for realizing QAHE in these monolayers, focusing on material selection and fine-tuning to achieve stable QAHE at room temperature. We hope that this review will provide new perspectives for theoretical studies and enable researchers to more accurately predict materials with superior QAHE properties. Meanwhile, we anticipate that these theoretical advancements will further drive breakthroughs in experimental studies and promote its broader application in low-power electronic devices and quantum information technology.

INTRODUCTION

The traditional quantum Hall effect (QHE) relies on the application of an external magnetic field, characterized by the quantization of Landau levels.¹ In contrast, the quantum anomalous Hall effect (QAHE) does not require an external magnetic field. It arises from the spontaneous magnetization and strong spin-orbit coupling (SOC) intrinsic to the material.^{2–4} In 1988, QAHE's theoretical model was first proposed by Haldane, considering a honeycomb lattice structure with staggered magnetic flux, thereby pioneering new directions for the study of novel quantum Hall phenomena.⁵ This pioneering model has recently been realized in ultracold Fermi atomic systems and is expected to be implemented in other systems in the future.⁶ A key feature of QAHE is the Berry curvature of electronic states in the system, where the integral over the entire Brillouin zone yields a topological invariant known as the Chern number. This invariant characterizes QAHE, and insulators displaying QAHE are termed Chern insulators (magnetic topological insulators).^{7–9}

Compared to traditional three-dimensional (3D) materials, the distinct electronic structures and tunable properties of two-dimensional (2D) materials, where electron motion is confined to a plane, enhance quantum effects and facilitate stable QAHE, especially when combined with SOC and spontaneous magnetization.^{10–12} Experimentally, QAHE has already been

realized in certain materials, such as magnetically doped (Bi,Sb)₂Te₃ films and HgTe/CdTe quantum wells.^{13–19} However, limitations such as low operating temperatures and narrow topological bandgaps hinder their practical applications.^{13,18} In this context, first-principles calculations provide a powerful tool for identifying new materials.^{20–22} Through theoretical predictions, researchers can not only estimate the electronic structure and topological properties of materials but also efficiently screen potential 2D candidates, reducing the cost and difficulty of experimental validation.^{20,22} Consequently, theoretical calculations play an indispensable role in QAHE research, offering critical guidance for experimental studies.

Among these 2D materials, tetragonal crystal systems have garnered attention due to their physical properties and electronic structures.^{23–28} For example, the ferromagnetic (FM) double exchange mechanism under the orbital-selective Mott phase of the tetragonal crystal MgFeP, in combination with SOC, causes MgFeP to exhibit quantum anomalous Hall (QAH) phase ($C = 2$).²³ Moreover, the non-trivial bandgap can be substantially enhanced by strain modulation to exploit the orbital selectivity, indicating the potential value of such monolayers for spintronics applications. QAHE have also been predicted in other tetragonal materials, such as V₂MX₄ ($M = W, Mo$; $X = S, Se$) monolayer, which exhibit large topological bandgap via d-orbital band inversion mechanisms.²⁴ Tetragonal KTiSb shows band inversion driven by crystal field and electron hopping effects, its SOC



effect introduces a gap at the Fermi level, providing a direction for further exploration.²⁵

Despite the promising potential of 2D tetragonal materials in QAHE research, 2D hexagonal materials offer additional advantages in realizing and optimizing topological quantum states.^{29–37} The high symmetry and simple structure of hexagonal materials not only simplify the complexity of first-principles calculations but also facilitate experimental implementation.^{29,30} This high degree of symmetry helps stabilize intrinsic Dirac cone states in the electronic band structure which, under the influence of SOC, can open non-trivial bandgap, laying the foundation for the realization of QAHE.^{31–33} Furthermore, hexagonal materials exhibit greater responsiveness to external tuning methods, such as electric fields, strain, and magnetic fields, making them more advantageous in stabilizing topological states and optimizing material performance.^{34–36,38}

For example, classic 2D hexagonal materials such as MnBi_2Te_4 family exhibit strong coupling between magnetism and topology due to their layered structure.^{14,39–45} MnBi_2Te_4 has been theoretically predicted as an ideal candidate for QAHE and has shown stability at low temperatures in experiments.^{39–41} Similarly, FeBi_2Te_4 exhibits trivial antiferromagnetic (AFM) semiconductor properties; QAHE can be observed in its bilayer FM state.⁴² MnSb_2Te_4 undergoes band inversion under enhanced SOC, transforming into an AFM topological insulator; uniaxial compressive strain along the z-direction can induce the same topological transition.⁴³ Furthermore, in $\text{NiVBi}_2\text{Te}_5$, QAHE with a Chern number of 1 is observed in six-layer and sixteen-layer configurations, while a non-trivial topological phase with a higher Chern number ($C = 2$) is realized in twenty-layer systems.⁴⁴

Compared to van der Waals heterostructures or multilayer structures (e.g., twisted Moiré superlattices), 2D hexagonal monolayers hold greater theoretical value.^{46–51} In multilayer structures, interlayer coupling and hybridization often complicate the electronic structure, diminishing topological properties; 2D hexagonal monolayers avoid these issues, offering clearer electronic behavior and facilitating a deeper understanding of the intrinsic mechanisms of QAHE.^{46–49} Additionally, this enhances the feasibility of achieving precise experimental control over high-quality quantum states.^{50,51} Therefore, 2D hexagonal monolayers, with their highly tunable topological properties and well-defined theoretical development, have emerged as ideal candidates for QAHE research.⁵²

This review summarizes recent progress in realizing QAHE in 2D hexagonal monolayers, with a particular emphasis on significant advances achieved through first-principles calculations. Due to their excellent electronic properties, topological properties, and tunability, 2D hexagonal monolayers have become ideal platforms for achieving high-performance QAHE. We categorize 2D hexagonal monolayers based on their elemental compositions, which facilitates systematic analysis of how different elements influence the electronic structure, magnetism, and topological properties of the monolayers, providing theoretical guidance for the design and screening of new materials. It is notable that Kagome-structured monolayers have great potential for applications due to the unique magnetic and topological properties they exhibit, which is therefore described separately.

Moreover, for practical applications of these theoretically predicted materials, precise external tuning of their electronic and topological properties is crucial. Therefore, we discuss various external modulation techniques, such as the application of vertical electric fields, adjustments in magnetic field directions, and biaxial strain effects on material properties. These tuning methods not only alter the electronic properties of the materials but also optimize their topological characteristics to meet different application requirements. In summary, whether involving classic 2D hexagonal monolayers or novel Kagome lattice structures, first-principles calculations provide new possibilities for achieving efficient QAHE and lay a solid theoretical foundation for the development of future low-power electronic devices and quantum information technologies.

THE QAHE IN CLASSIC 2D HEXAGONAL MONOLAYERS

The QAHE in AB hexagonal monolayers

The simplest of the 2D hexagonal monolayers with QAHE are the AB monolayers, based on elemental composition. Meanwhile AB monolayers can be categorized into two distinct types. The first category includes the d^0 orbital AB monolayers (Figure 1A) with space group $P\bar{6}M2$ (No. 187), which are composed of elements such as K, Rb, Cs (denoted as A) and N, P, As, Sb, Bi (denoted as B). These monolayers exhibit an FM state, with a preference for out-of-plane magnetization over in-plane magnetization. For example, in KBi, the maximum magnetic anisotropy energy (MAE) can reach up to 72.01 meV.⁵³ Many of these monolayers also have a Curie temperature (T_C) that exceeds room temperature. Without considering SOC, the band structure of these monolayers is fully spin-polarized due to the FM ordering, which breaks time-reversal symmetry. However, the introduction of SOC results in further splitting of the band system, leading to a range of electronic phases. These phases include metallic phase (Figure 1B), indirect bandgap insulator phase (Figure 1C), and direct bandgap insulator phase (Figures 1D and 1E).

In the case of CsSb, the bandgap can reach as high as 154.9 meV. This monolayer also exhibits a QAH phase with a Chern number of 1, which arises from band inversion between different p-orbitals. The interplay of SOC with the breaking of time-reversal and spatial inversion symmetries lifts the degeneracy between the K and K' valleys, enabling the valley quantum anomalous Hall effect (VQAHE).⁵³ In this system, both the valence and conduction bands show intrinsic valley polarization, resulting in a total valley polarization of 481.4 meV. Additionally, the QAH phase of these d_0 orbital AB monolayers can be tuned using the biaxial strain (Figure 1F). This strain not only modulates the bandgap but can also induce band inversion, as observed in CsBi, thereby triggering a topological phase transition (Figures 1G and 1H).

The second type of AB structures is characterized by a space group $P\bar{3}M1$ (No. 164). This configuration consists of a bilayer of metal atoms (A) sandwiched between halogen atoms (B), arranged in a honeycomb pattern (Figure 2A).⁵⁴ Due to their van der Waals layered nature, these materials exhibit the potential for exfoliation into monolayers.⁵⁵ The magnetic ground state of these systems is FM, with the magnetism primarily contributed

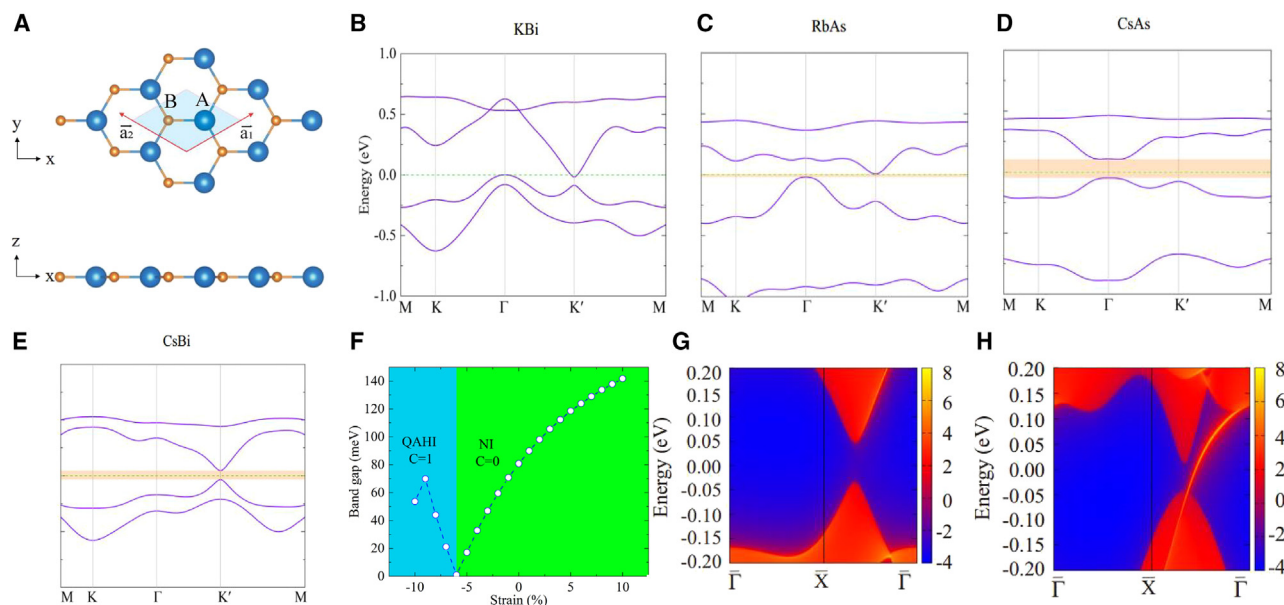


Figure 1. The electronic and topological properties of first type hexagonal AB monolayers

- (A) The top and side views of the first type of hexagonal AB structure.
 (B) The band structure of the hexagonal KBi when SOC is considered (metal).
 (C) The band structure of the hexagonal RbAs when SOC is considered (indirect bandgap insulator).
 (D) The band structure of energy of the hexagonal CsAs when SOC is considered (Γ point direct bandgap insulator).
 (E) The band structure of energy of the hexagonal CsBi when SOC is considered (K' point direct bandgap insulator).
 (F) The effect of biaxial strain to the phase in the hexagonal CsBi.
 (G) The edge state of hexagonal CsBi at 0% strain.
 (H) The edge state of hexagonal CsBi at 10% strain.

by the f and d electrons of the metal atoms A. For instance, the CeCl monolayer shows out-of-plane magnetization. In the absence of SOC, this system forms a Weyl nodal loop semimetal (Figures 2B and 2C).

However, when SOC is introduced, the system evolves into either a Weyl semimetal or a Chern insulator, generating a non-zero Berry curvature and transitioning into a QAHE phase.⁵⁶ The effect of mirror symmetry on the system depends on the direction of magnetization. By controlling the in-plane magnetization (Figure 2D), it is possible to switch between positive and negative Chern numbers. When the magnetization is aligned in the in-plane x-direction, the system behaves as a Weyl semimetal (Figures 2F and 2J). As the magnetization shifts from the x-direction to the y-direction, the Chern number changes, and the system becomes a Chern insulator with $C = -1$ (Figures 2G and 2K). On the other hand, out-of-plane magnetization generates a positive Berry curvature within the Brillouin zone, leading to a QAHE phase with $C = 1$ (Figures 2E and 2I). When the magnetization is in the out-of-plane direction, the C_{3z} symmetry is unbroken so that the bandgaps on the paths from Γ to three different M are the same. When the magnetization is in the in-plane x direction, the mirror symmetry parallel to it is broken, and the ring of Weyl nodes degenerates into a pair of Weyl points, with Γ having a bandgap of 0 to M_1 and the same bandgap to M (M_2). When rotating in the in-plane direction of the magnetization, all symmetries are broken, and all three paths have bandgaps.

The QAHE in AB_2 hexagonal monolayers

Classifying 2D hexagonal monolayers with QAHE based on their elemental composition, in addition to the two types of AB monolayers, also includes the AB_2 family, which encompasses H-phase, T-phase, and the corresponding Janus monolayers. Among these, H- AB_2 monolayers have recently attracted considerable attention (Figure 3A). These monolayers resemble the structure of H-phase transition metal dichalcogenides, featuring a hexagonal lattice with perpendicular mirror symmetry, where a layer of metal atom (A) is sandwiched between two monolayers of halogen atom (B). The A-B-A bond angles, approaching 90° , indicate that the FM in H- AB_2 originates from superexchange interactions.⁵⁷ The effective Coulomb interaction parameter (U_{eff}) influences the MAE, as observed in FeCl_2 (D_{3h}).⁵⁸ Meanwhile, in a U_{eff} range below 2 eV, robust AFM is maintained.⁵⁹ This magnetism results in spin polarization between spin-up and spin-down channels, with states near the Fermi level predominantly contributed by electrons in the spin-down channel. The inclusion of SOC and magnetic effects leads to the breaking of time-reversal and inversion symmetries, which induces spontaneous valley polarization.⁶⁰ The intrinsic QAHE is attributed to the strong SOC effects in transition metals and the significant exchange interactions, with chiral edge states between the conduction and valence band valleys topologically protected within the insulating gap.⁶¹ The external tensile strain can induce band inversion between the K' valley in the valence and conduction bands (Figure 3B), transitioning the system

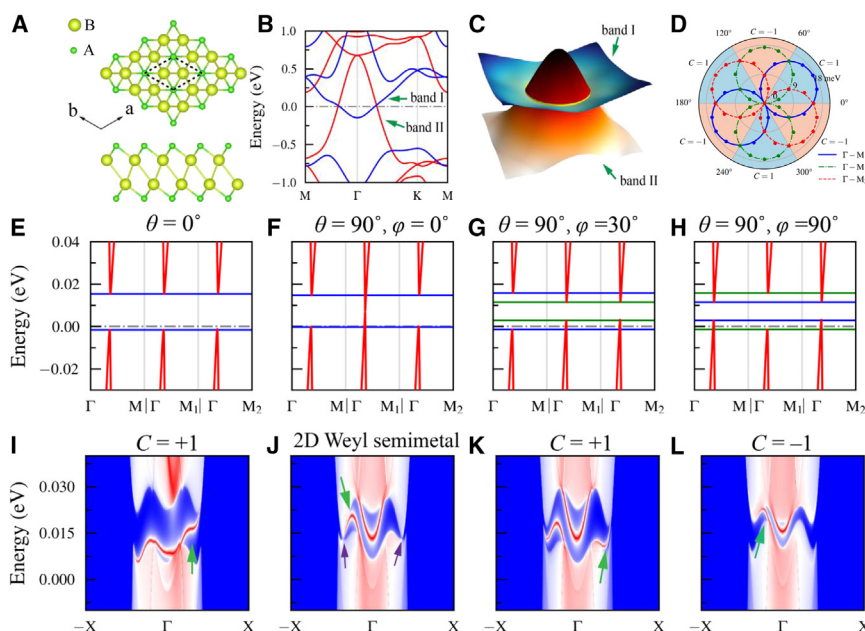


Figure 2. The electronic and topological properties of second type hexagonal AB monolayer (CeCl)

(A) The top and side views of the crystal structure. (B) The band structure when SOC is not considered, where the red (blue) line indicates spin up (spin down). (C) The three-dimensional band structure near the Fermi surface when SOC is not considered. (D) The bandgap and the Chern number are tuned with the direction of the in-plane magnetization. (E) The band structure when the magnetization is along the out-of-plane z-direction. (F) The band structure when the magnetization is along the in-plane x-direction. (G) The band structure when the magnetization is along the in-plane x-direction with a 30° rotation. (H) The band structure when the magnetization is along the in-plane y-direction. (I) The edge state when the magnetization is along the out-of-plane z-direction. (J) The edge state when the magnetization is along the in-plane x-direction. (K) The edge state when the magnetization is along the in-plane x-direction with a 30° rotation. (L) The edge state when the magnetization is along the in-plane y-direction.

from a non-trivial QAH insulator ($C = 1$) to a trivial FM insulator (Figures 3C and 3D). Conversely, compressive strain leads to gap is 0 and band inversion at the K point, transitioning to a higher-order topological insulator.⁶² In addition, under the influence of circularly polarized light and out-of-plane magnetization, the increase in light amplitude in FeI_2 not only induces a topological phase transition from a trivial state to a nontrivial state, but also leads to a topological phase transition where the chiral edge states change from one to two.⁶³

Moreover, Janus AB_2 monolayers (Figure 3E), which exhibit out-of-plane easy-axis magnetization, have been predicted to display the QAHE. In OsClBr ($P3m1$ space group), spontaneous valley polarization occurs due to strong SOC and intrinsic exchange interactions among localized d electrons (Figures 3F and 3G). Furthermore, band inversion among the d orbitals of metal atom Os triggers topological phase transitions between ferrovalley phase, ferrovalley half-metal phase, and valley quantum anomalous Hall phase (Figures 3H and 3I).⁶⁴ For VQAHE, the valley polarization is as high as 201 meV by replacing the non-metallic atoms on one side with hydroxyl groups. In the case of the RuOHCl , under compressive strain, changes in the interactions among the d orbitals of metal atom Ru preserve its FM state while shifting the easy magnetization axis from in-plane to out-of-plane.⁶⁵ The similar strain-induced topological phase transition occurs in the Janus TiTeCl monolayer, which exhibits an intrinsic QAH phase with a Chern number of -1 .⁶⁶ Concurrently, Janus ScClI is also an intrinsically magnetic monolayer. The tight-binding (TB) model incorporating multi-orbital coupling has been used to predict its tunable topological phase, transitioning from a second-order topological insulator (SOTI) to a QAH insulator, and then to a trivial FM insulator.⁶⁷ In the TB model, the topological phase transition can be achieved by adjusting the magnetic moment angle θ_z of the K-point valley and

the energy level difference between the d_{xy} and dz^2 orbitals. The θ_z angle mainly affects the valley, while the energy level difference influences the band inversion.

The QAHE in AB_2 structures is not limited to the H-phase but can also be observed in other phases.^{68–70} For instance, in the T-phase of PrN_2 (Figure 4A), theoretical studies predict that it exhibits the properties of a topological semimetal ($P\bar{3}M1$). The size of the nontrivial band gap and the formation of the QAH phase depend on the degree of the breaking of the C_2 symmetry. Its topological properties can be tuned by applying an external magnetic field. When the magnetization direction is parallel to the three 2-fold rotation axes, the C_2 symmetry is unbroken, Weyl points exist, and the nontrivial band gap is zero. When the magnetization direction is not parallel to the three 2-fold rotation axes, the Weyl points vanish, and a nontrivial band gap emerges. When the magnetization is aligned parallel to the plane, the Chern number can switch between ± 1 , with a maximum bandgap of 81.74 meV (Figure 4B). In contrast, when the magnetization is oriented out of the plane, the bandgap increases to 101.12 meV, and the Chern number rises to ± 3 , showcasing a high-Chern number QAHE (Figures 4C and 4D).⁷¹ On the other hand, people found that different stacking configurations can be designed to achieve non-trivial topological properties with a high Chern number ($C = 3$) in monolayer T-phase YN_2 by using GaSe as the substrate, thereby providing the feasibility for experimentally realizing the QAHE under T-phase conditions. Additionally, in the classical 1T-TMD AB_2 fluorinated structure (MoSe_2F_2) (Figure 4E), which also opens a non-trivial bandgap in the band structure (Figures 4F and 4G). It displays a QAHE with a high Chern number of -2 (Figure 4H). The Berry curvature in each valley contributes to a valley Chern number of -1 , with the bandgap reaching 117.2 meV.⁷²

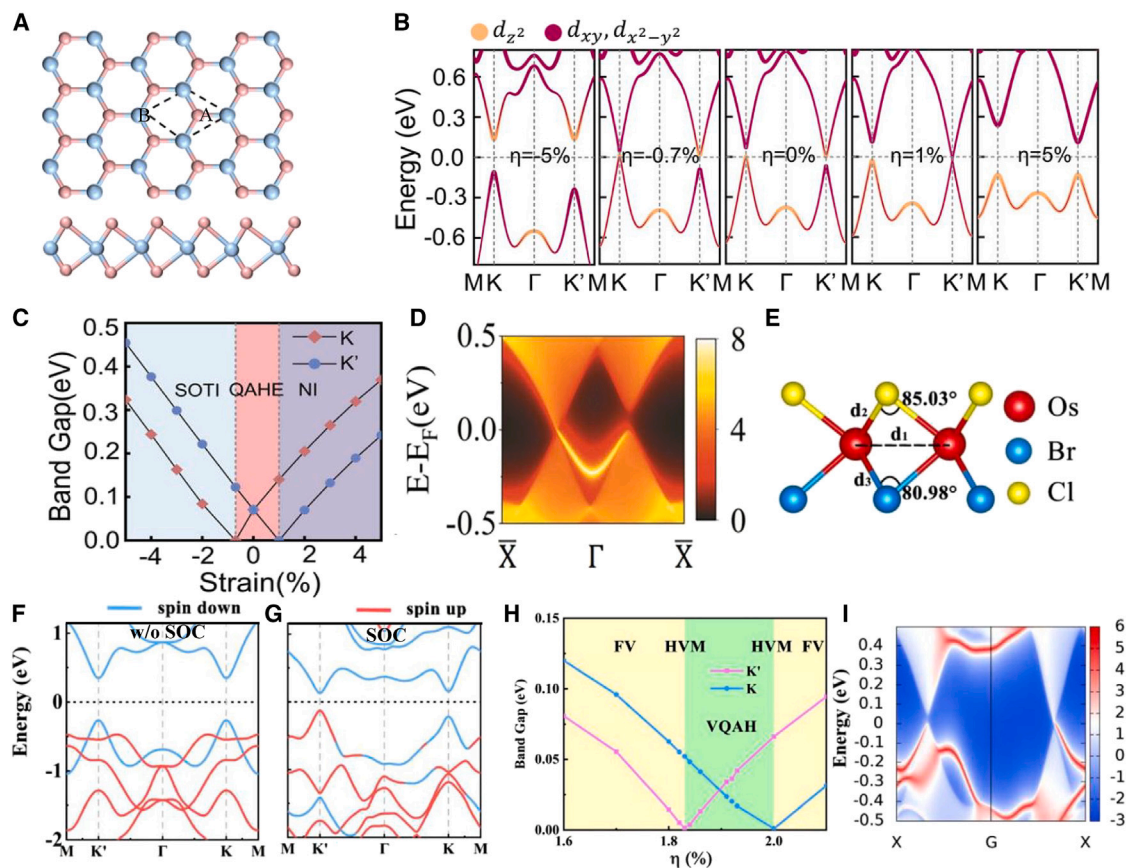


Figure 3. The electronic and topological properties of the hexagonal H-AB₂ monolayers

- (A) The top and side views of the hexagonal H-FeCl₂ monolayer.
 (B) The band structure of the H-FeCl₂ monolayer as a function of the biaxial strain modulation when SOC is considered.
 (C) The bandgap and the phase of the H-FeCl₂ monolayer under strain modulation when SOC is considered.
 (D) The edge state of the H-FeCl₂ monolayer.
 (E) The side view of the hexagonal OsClBr monolayer.
 (F) The band structure of the OsClBr monolayer when SOC is not considered.
 (G) The band structure of the OsClBr monolayer when SOC is considered.
 (H) The bandgap and the phase of OsClBr monolayer at K (K') are modulated by the tensile strain when SOC is considered.
 (I) The edge state of OsClBr.

The QAHE in AB₃ hexagonal monolayers

In the study of 2D topological materials, AB₃ monolayers belong to the $P\bar{3}M1$ space group (No.162).^{73,74} These AB₃ monolayers are characterized by a three-layer atomic structure, where metal atom A and non-metal atoms B alternate in sequence (Figure 5A). The A-B-A bond angles are approximately 90°, resulting in superexchange interactions mediated by the p-orbitals of the non-metal atoms B. This superexchange interaction leads the system to exhibit FM in its ground state.⁷⁵ In OsI₃, which has a T_c of 362 K, SOC effect arises due to contributions from both Os and I atoms. This effect results in a non-trivial bandgap, turning the system into a magnetic topological insulator (Figure 5B). The non-trivial property is manifested with the Chern number $C = 1$ (Figure 5C), which changes to -1 when the magnetization lies within the plane.⁷⁶ Furthermore, the energy of different magnetic states and the MAE increase with strain, indicating that the easy magnetization axis

and magnetic state retains robustness under these conditions (Figure 5D). In hole-doped CrI₃, a transition from semimetal to magnetic topological insulator can be effectively modulated through a combination of strain and the Hubbard parameter U . At 2% tensile strain, increasing U causes a band inversion at the M point, leading to a topological phase transition where the Chern number changes sequentially from 2 to 1, and then to 0 (Figures 5E and 5F).⁷⁷ Moreover, the QAHE is also observed in CrCl₃ when doped with alkali metals. Specifically, Na- and K-doped CrCl₃ exhibit a Chern number of 1, whereas Li-doped CrCl₃ shows QAHE with a Chern number of -2 (Figures 5G and 5H).⁷⁸

The substitution of atoms in 2D topological monolayers can also cause the QAHE. For example, Janus CrMnI₆ monolayer demonstrates a QAHE phase with a high Chern number, resulting from Cr and Mn atoms occupying two asymmetric positions (Figure 6A). The inclusion of SOC opens a topological bandgap

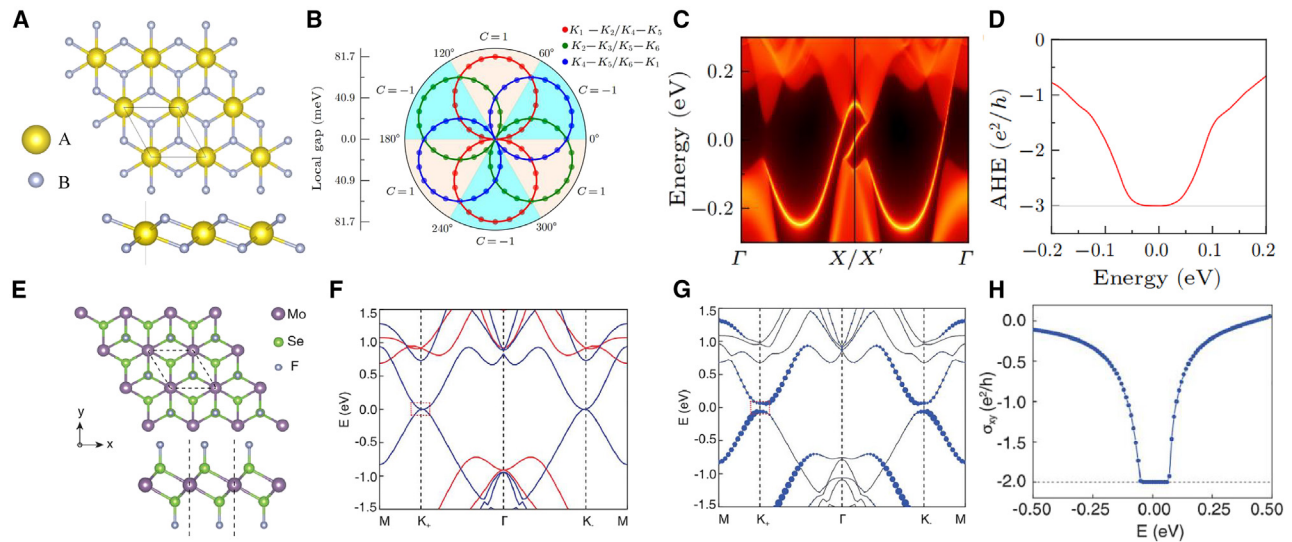


Figure 4. The electronic and topological properties of the hexagonal T-AB₂ monolayers

- (A) The top and side views of the hexagonal T-AB₂ (PrN₂) monolayer.
 (B) The bandgap and the Chern number are changed with the modulation of the in-plane magnetization direction.
 (C) The quantized anomalous Hall conductance of the hexagonal PrN₂ monolayer when the magnetization is along the out-of-plane z-direction.
 (D) The edge states of the hexagonal PrN₂ monolayer when the magnetization is along the out-of-plane z-direction.
 (E) The top and side views of the fluorinated hexagonal T-AB₂ (MoSe₂F₂) monolayer.
 (F) The band structure of the MoSe₂F₂ monolayer when SOC is not considered.
 (G) The band structure of the MoSe₂F₂ monolayer when SOC is considered.
 (H) The quantized anomalous Hall conductance of MoSe₂F₂.

in the band structure (Figures 6B and 6C). The Chern number of 2 can be established through the summation of six Dirac cones (each with a Chern number of 1/2) plus the Chern number of the

Γ point, which contributes -1 (Figure 6D).⁷⁹ The quantized anomalous conductance and corresponding edge states indicative of a high Chern number are also observed (Figures 6E and

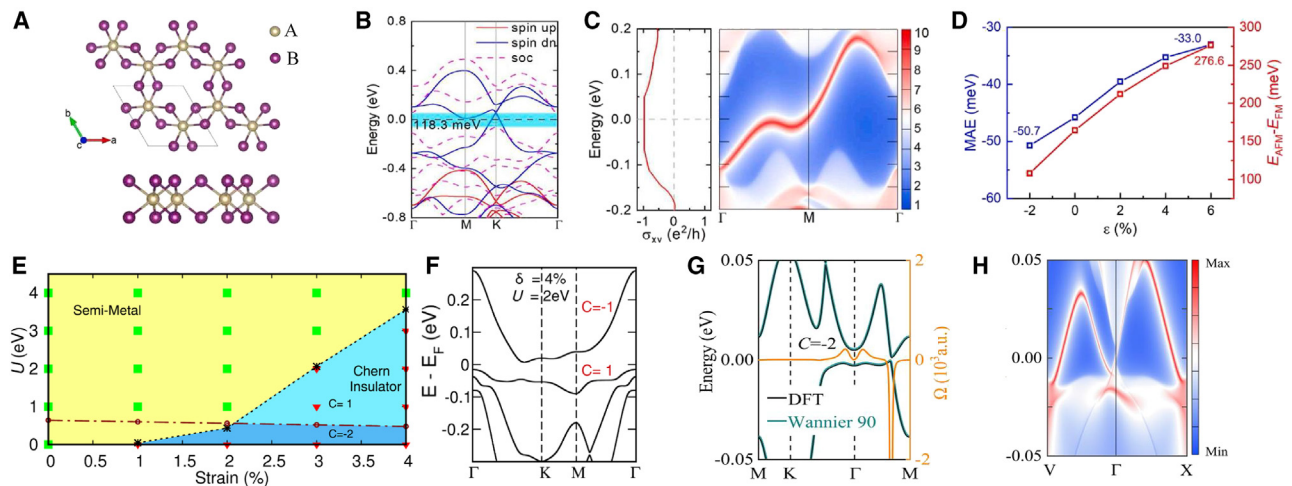


Figure 5. The electronic and topological properties of the hexagonal AB₃ monolayers

- (A) The top and side views of the hexagonal AB₃ monolayer.
 (B) The band structure of the OsI₃ monolayer.
 (C) The edge state and the quantized anomalous Hall conductance of the OsI₃ monolayer when SOC is considered.
 (D) The MAE and the energy difference between the FM and AFM states of the OsI₃ monolayer affected by the strain modulation.
 (E) The Chern number and the phase of the hole-doped CrI₃ monolayer at the different U and the tensile strain modulation when SOC is considered.
 (F) The band structure of the hole-doped CrI₃ monolayer at $U = 2\text{eV}$ and 4% tensile strain when SOC is considered.
 (G) The band structure of Li-doped CrCl₃ calculated by Wannier90 and DFT, respectively, when SOC is considered.
 (H) The corresponding edge states.

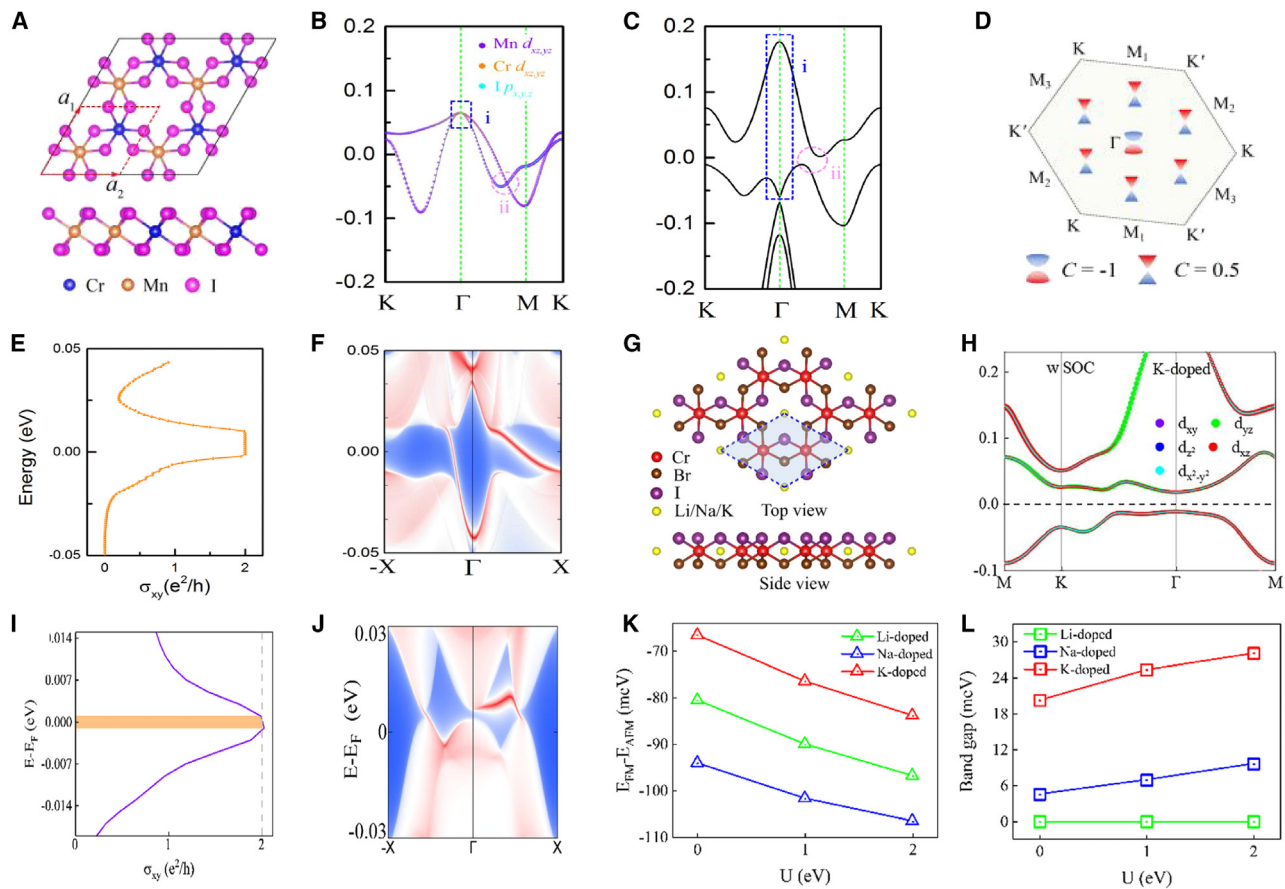


Figure 6. The electronic and topological properties of two types of the Janus hexagonal monolayers

- (A) The top and side views of the first type of Janus hexagonal $AA'B_6$ monolayer.
 (B) The band structure of the $CrMnI_6$ monolayer when SOC is not considered.
 (C) The band structure of the $CrMnI_6$ monolayer when SOC is considered.
 (D) The distribution of the Berry curvature in the first Brillouin zone of the $CrMnI_6$ monolayer when SOC is considered.
 (E) The quantized anomalous Hall conductance of the $CrMnI_6$ monolayer when SOC is considered.
 (F) The edge states of the $CrMnI_6$ monolayer when SOC is considered.
 (G) The top and side views of the second type of Janus hexagonal $A_2B_3B'_3$ monolayer.
 (H) The band structure of the K-doped $Cr_2Br_3I_3$ monolayer when SOC is considered.
 (I) The quantized anomalous Hall conductance of the K-doped $Cr_2Br_3I_3$ monolayer when SOC is considered.
 (J) The edge states of the K-doped $Cr_2Br_3I_3$ monolayer when SOC is considered.
 (K) The energy difference between the FM and AFM states of the alkali metal-doped $Cr_2Br_3I_3$ at the different U values.
 (L) The bandgap of the alkali metal-doped $Cr_2Br_3I_3$ at the different U values.

6F). Similarly, $RuCS_6$ has been identified to possess a topological gap as large as 336 meV, demonstrating that its topological properties are significantly robust against biaxial strain. The topological gap increases under strain, reaching 583 meV at 6% tensile strain.⁸⁰

Another interesting example involves the Janus $A_2B_3B'_3$, which is also composed of three atomic layers, with one metallic layer (A) sandwiched between two distinct non-metal layers (B and B') (Figure 6G). The difference between B and B' leads to asymmetric interlayer distances relative to the metal layer A, breaking the original symmetry of the AB_3 monolayers. In Janus $Mn_2Cl_3Br_3$, the Chern number and chiral edge currents can be controlled by changing the magnetization direction. Specifically, when the magnetization is oriented

along the in-plane x-direction, a bandgap of 32.49 meV opens, with a Chern number of -1 . Conversely, adjusting the magnetization to the out-of-plane z-direction results in a bandgap of 28.38 meV with a Chern number of 1 .⁸¹ Further research suggests that doping alkali metals into Janus $A_2B_3B'_3$ monolayers can realize QAH phase with high Chern number. For instance, introducing alkali metals induces a topological phase transition in Janus $Cr_2Br_3I_3$ from a semiconductor to a Dirac semimetal. Under the influence of SOC, $Cr_2Br_3I_3$ opens a non-trivial bandgap (Figure 6H), resulting in a QAH phase with a Chern number of 2 (Figures 6I and 6J). Additionally, the stability of the magnetic state is confirmed under different U values, with the topological properties remaining invariant (Figures 6K and 6L).⁸²

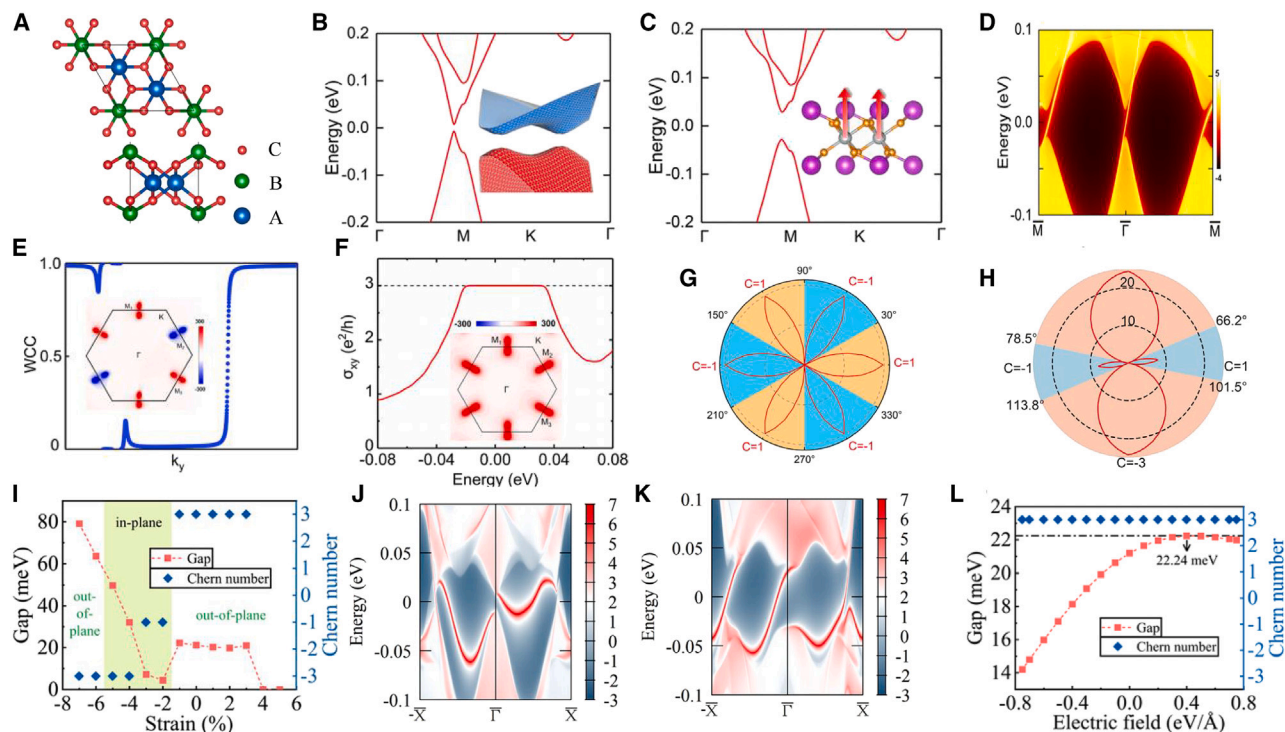


Figure 7. The electronic and topological properties of the hexagonal ABC_3 monolayers

- (A) The top and side views of the hexagonal ABC_3 structure.
 (B) The band structure of the $NiBiO_3$ monolayer when magnetization is along the in-plane direction.
 (C) The band structure of the $NiBiO_3$ monolayer when the magnetization is along the out-of-plane direction.
 (D) The edge states of the $NiBiO_3$ monolayer when the magnetization is along the out-of-plane direction.
 (E) The distribution of the Berry curvature in the first Brillouin zone and the Wannier Charge Center (WCC) of the $NiBiO_3$ monolayer when the magnetization is along the in-plane direction.
 (F) The distribution of the Berry curvature in the first Brillouin zone and the quantized anomalous Hall conductance of the $NiBiO_3$ monolayer when the magnetization is along the out-of-plane direction.
 (G) The bandgap and the Chern number of the $NiBiO_3$ monolayer changes with the modulation of the in-plane magnetization direction.
 (H) The bandgap and the Chern number changes of the $PdSbO_3$ monolayer with the modulation of the out-plane magnetization direction.
 (I) The bandgap, the direction of the easy magnetization axis and the variation of the Chern number of the $MnAsO_3$ monolayer are modulated by strain when SOC is considered.
 (J) The edge state of the hexagonal $MnAsO_3$ monolayer under the -1% compressive strain when the magnetization is along the out-of-plane direction.
 (K) The edge state of the hexagonal $MnAsO_3$ monolayer under the -6% compressive strain when the magnetization is along the out-of-plane direction.
 (L) The bandgap and the Chern number of the hexagonal $MnAsO_3$ monolayer modulated by the electric field when SOC is considered.

The QAHE in ABC_3 hexagonal monolayers

Another classification, ABC_3 crystals with the space group $P\bar{3}M1$, exhibit a layer stacking order of B-C-A-C-B (Figure 7A). This structure is classified as an FM semimetal, primarily due to the near 90° bond angles between A-C-A, which facilitate FM interactions. Owing to the system's C_3 symmetry and inversion symmetry, six Dirac points exist in the first Brillouin zone of $NiBiO_3$. When SOC is included, these Dirac points open a non-trivial bandgap, leading to the emergence of the QAHE (Figures 7B and 7C). Additionally, by tuning the magnetization direction from in-plane to out-of-plane, the system can achieve a QAHE phase with a high Chern number (Figure 7D).⁸³ In the in-plane magnetization condition, the system exhibits a Chern number $C = 1$, where two-thirds of the Berry curvature at high-symmetry points in the Brillouin zone are positive, and one-third is negative. Conversely, when $C = -1$, the Berry curvature distribu-

tion is inverted (Figure 7E). In the out-of-plane magnetization scenario, the Berry curvature at the K point becomes either all positive or all negative (Figure 7F).⁸⁴ The Chern number of $NiBiO_3$ varies with the direction of in-plane magnetization (Figure 7G), while the high Chern number of a $PdSbO_3$ can vary with the out-of-plane magnetization direction (Figure 7H). Notably, in the $PdSbO_3$ - MoS_2 heterostructure, the out-of-plane z-direction magnetization induces a non-trivial bandgap increase to 31.6 meV, while still preserving the QAHE with a high Chern number of -3 . $MnAsO_3$, has a relatively high T_c of 308 K, which surpasses that of $NiBiO_3$ (258 K). Furthermore, the FM ground state of $MnAsO_3$ demonstrates robustness over a range U_{eff} values. External modulation methods, such as applying biaxial strain, can effectively switch the direction of the easy magnetization (Figure 7I) and facilitate the achievement of QAHE phases with varying Chern numbers (Figures 7J and 7K).⁸⁵ Additionally, the

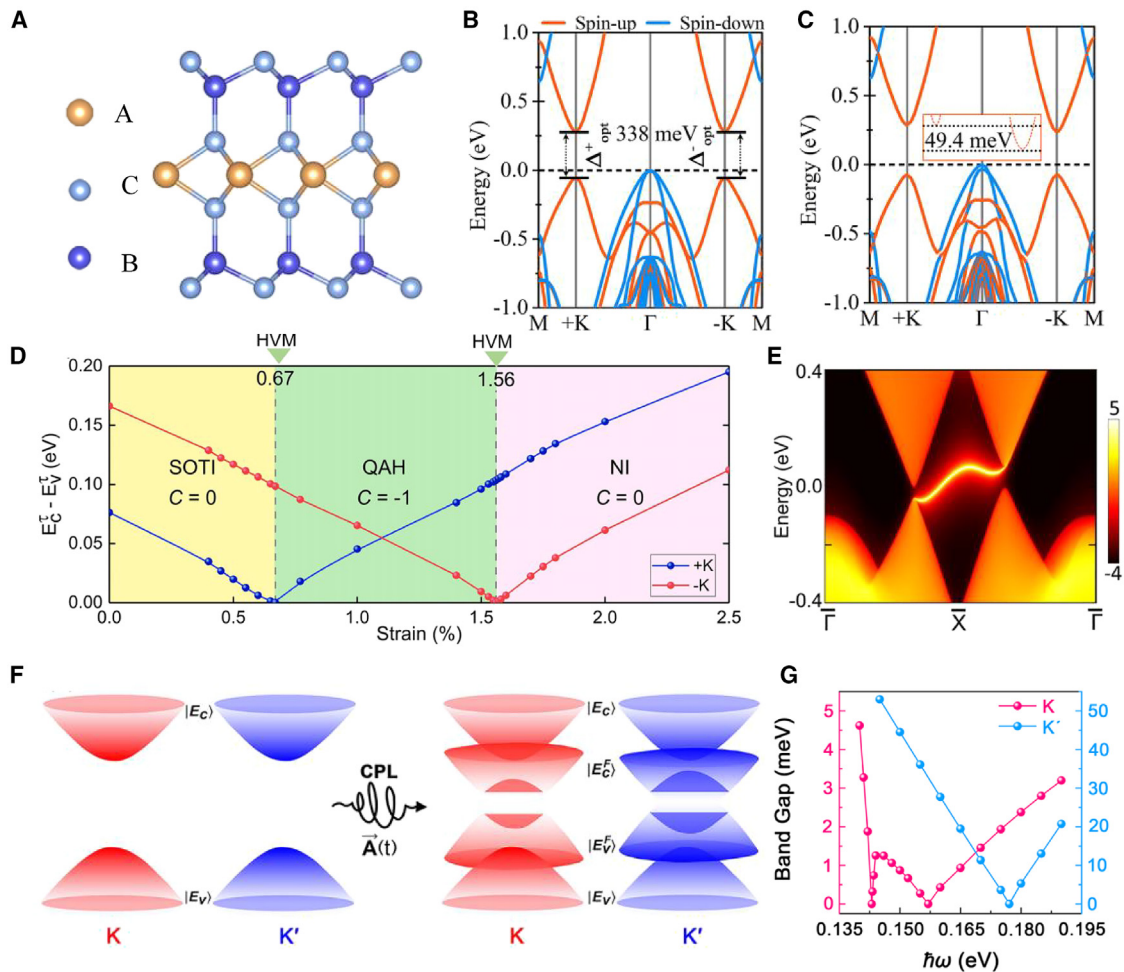


Figure 8. The electronic and topological properties of the hexagonal AB_2C_4 monolayers

- (A) The side view of the hexagonal AB_2C_4 structure.
 (B) The band structure of the VSi_2P_4 monolayer when SOC is not considered.
 (C) The band structure of the VSi_2P_4 monolayer when SOC is considered.
 (D) The bandgap and the phase of the VSi_2P_4 monolayer at K (K') are modulated by the tensile strain when SOC is considered.
 (E) The edge state of the hexagonal VSi_2P_4 monolayer under the 1.25% tensile strain.
 (F) The band inversion of the VSi_2N_4 monolayer is generated by irradiation of the circularly polarized light.
 (G) The bandgap of the VSi_2N_4 monolayer at K (K') is modulated by different photon energies.

application of a perpendicular electric field can further increase the non-trivial bandgap (Figure 7L).

The QAHE in AB_2C_4 hexagonal monolayers

In emerging classification with QAHE, AB_2C_4 monolayers, exhibit the space group $P\bar{6}M2$ and features a septuple-layer stacking sequence of C-B-C-A-C-B-C (Figure 8A). The near 90° bond angle between the metal atom A and the non-metallic atoms B promotes FM coupling, resulting in a stable FM ground state. In the case of VSi_2P_4 , the out-of-plane easy magnetization axis remains robust across a range of the U, whereas U significantly influences the band structure. Specifically, VSi_2P_4 with $U = 3\text{ eV}$ behaves as an FM semiconductor with intrinsic valley polarization, where the valley polarization between the conduction band (49.4 meV) and the valence band (3 meV) is driven by con-

tributions from different orbitals (Figures 8B and 8C). Under compressive strain, band inversion occurs at the K' point, triggering a topological transition to a magnetic topological insulator ($C = 1$).⁸⁶ Additionally, when $U = 2.4\text{ eV}$, VSi_2P_4 displays the zero-energy corner state and fractional charge for a SOTI phase (Figure 8D). With the application of tensile strain, the system maintains its FM state, whereas the energy difference between the two magnetic states decreases. The calculation of the Berry curvature reveals that the system transitions from SOTI to a magnetic topological insulator with $C = -1$, and finally to a valley-polarized FM insulator (Figure 8E).⁸⁷

In the VGe_2N_4 monolayer, in-plane MAE is observed. When SOC is considered, strain-induced band structure inversion at the K point leads to changes in the Berry curvature. These changes facilitate a transition from ferrovalley phase to

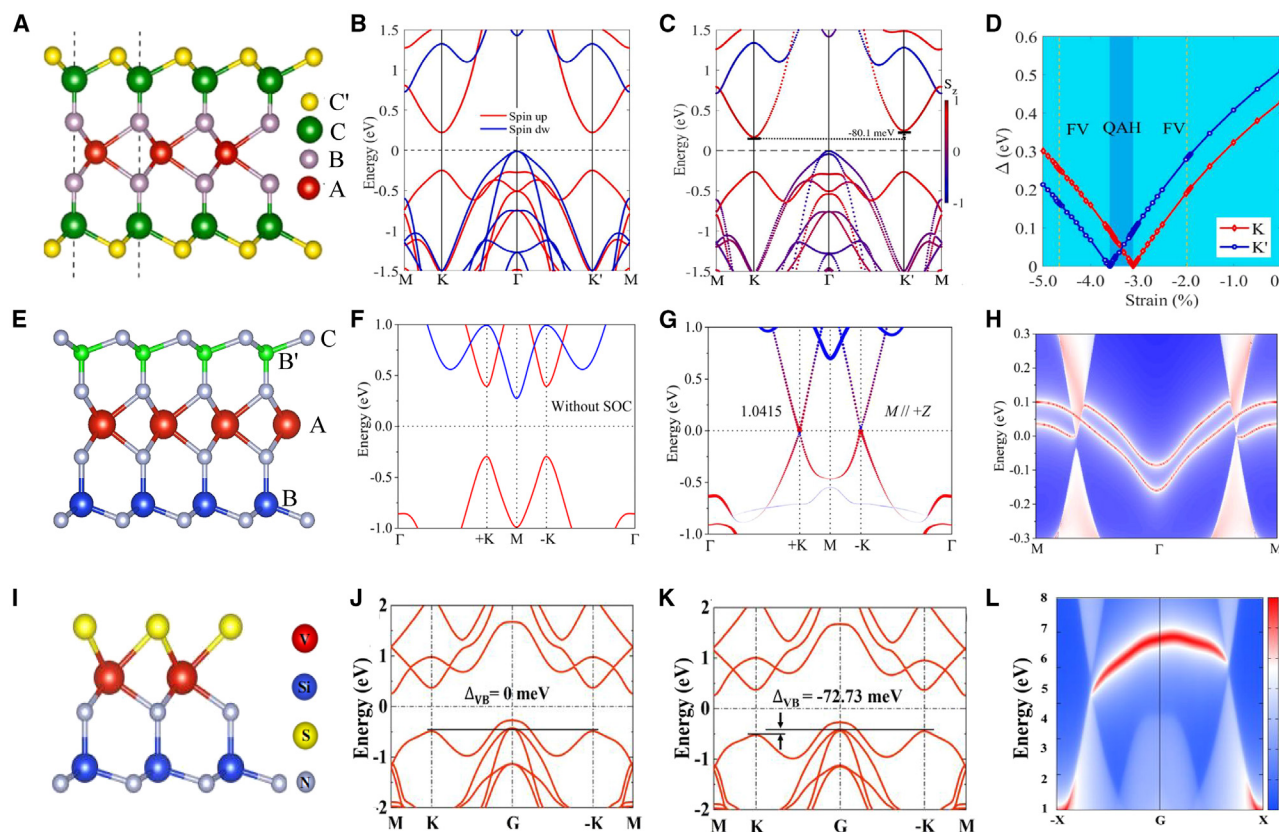


Figure 9. The electronic and topological properties of the three Janus AB_2C_4 monolayers

- (A) The side view of the first type of the Janus $AB_2C_2C'_2$ crystal structure.
 (B) The band structure of the Janus $VP_2Ga_2S_2$ monolayer when SOC is not considered.
 (C) The band structure of the Janus $VP_2Ga_2S_2$ monolayer when SOC is considered.
 (D) The bandgap and the phase of the Janus $VP_2Ga_2S_2$ monolayer at K (K') are modulated by the compressive strain when SOC is considered.
 (E) The side view of the second type of the Janus $ABB'C_4$ crystal structure.
 (F) The band structure of the Janus $VCSiN_4$ monolayer when SOC is not considered.
 (G) The energy band structure of the Janus $VCSiN_4$ monolayer under the 1.0415 tensile strain when the magnetization is along the out-of-plane z-direction.
 (H) The edge state of the Janus $VCSiN_4$ with 1.0415 tensile strain when the magnetization is along the out-of-plane z-direction.
 (I) The side view of the third type of the Janus $ABB'C_2$ ($VSSiN_2$) crystal structure.
 (J) The band structure of the Janus $VSSiN_2$ monolayer when the magnetization is along the in-plane direction.
 (K) The band structure of the Janus $VSSiN_2$ monolayer when the magnetization is along the out-of-plane z-direction.
 (L) The edge state of the Janus $VSSiN_2$ monolayer under the 5.7% tensile strain when the magnetization is along the out-of-plane z-direction.

ferrovalley half-metal phase, and ultimately to magnetic topological insulator state, displaying a quantized Hall conductivity of -1 , indicative of the QAHE.⁸⁸ Similarly, VSi_2N_4 exhibits in-plane easy-axis magnetization. By modulating the frequency and intensity of circularly polarized light (CPL), the bandgap can be closed and reopened, enabling highly tunable Chern numbers in the QAH phase, including $C = 1$, $C = 3$, and $C = 4$ (Figures 8F and 8G). Meanwhile, adjusting the chirality of CPL can modify both the sign of the Chern number and the chirality of the edge channels. This effect is attributed to light-induced trigonal warping and band inversion at the valleys.⁸⁹

Researchers have also explored various Janus structures within the AB_2C_4 family, such as $AB_2C_2C'_2$ (Figure 9A), $ABB'C_4$,⁹⁰ or the removal of one side as in $ABB'C_2$. For instance, in the $AB_2C_2C'_2$ structure, exemplified by $VP_2Al_2S_2$ and $VP_2Ga_2S_2$, the natural easy magnetization axis is out-of-plane.⁹¹

Without considering SOC, the band structure is spin-polarized, with the valence band maximum (VBM) located at the Γ point in the spin-down channel, while the conduction band minimum (CBM) is found at the $K(K')$ point in the spin-up channel. The resulting indirect bandgap is 0.22 eV (Figure 9B). When SOC is accounted for, valley degeneracy is lifted, leading to an energy difference between the K' and K valleys (Figure 9C). In the Janus $AB_2C_2C'_2$ structures are also capable of undergoing strain-controlled topological transitions (Figure 9D).⁹²

In the $ABB'C_4$ structure, such as $VGeN_4$ monolayer (Figure 9E), with increasing tensile strain, the MAE shows potential to switch to an out-of-plane orientation.⁹³ At the same time, the topological bandgap widens as the strain increases. $VCSiN_4$ also exhibits negative MAE, yet it remains ferromagnetic at high temperatures (up to 410 K).⁹⁴ Without considering SOC, $VCSiN_4$ is a bipolar FM semiconductor, with opposite spin

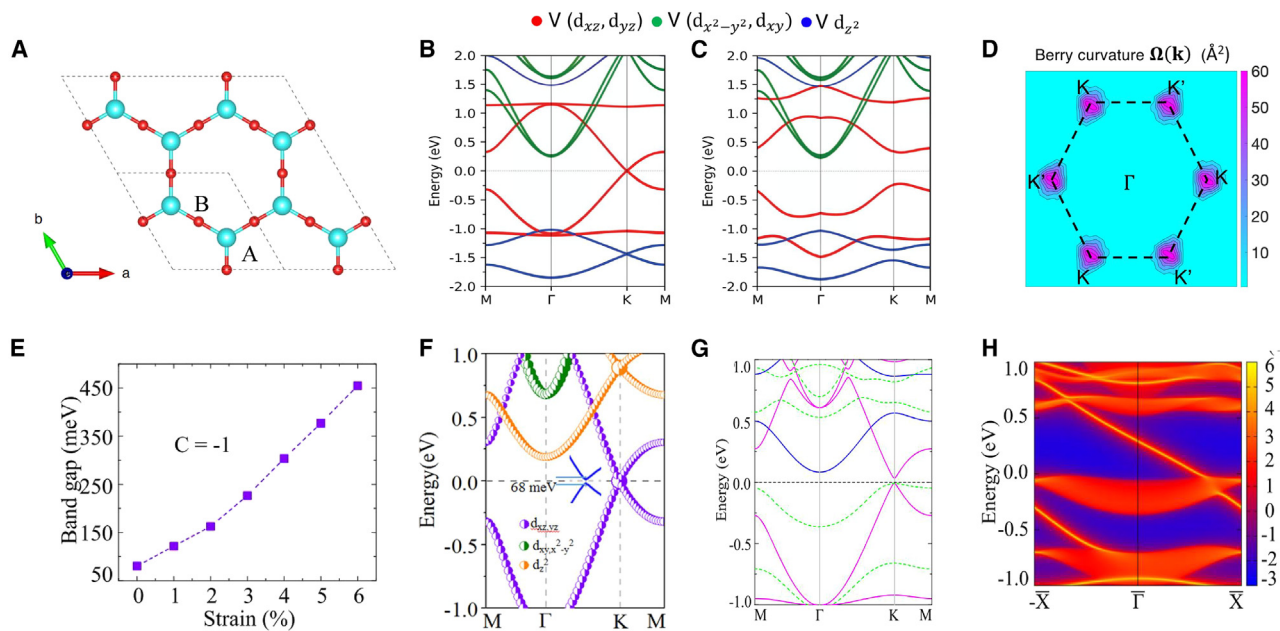


Figure 10. The electronic and topological properties of the Kagome A_2B_3 monolayers

- (A) The top view of the Kagome A_2B_3 crystal structure.
 (B) The band structure of the Kagome V_2O_3 monolayer when SOC is not considered.
 (C) The band structure of the Kagome V_2O_3 monolayer when SOC is considered.
 (D) The distribution of the Berry curvature in the first Brillouin zone of the Kagome V_2O_3 when SOC is considered.
 (E) The band gap of the Kagome Ta_2O_3 modulated by the tensile strain when SOC is considered.
 (F) The band structure of the Nb_2O_3/MoS_2 heterojunction when SOC is considered.
 (G) The band structure of the Ta_2O_3/h -BN heterojunction when SOC is considered.
 (H) The edge state of the Ta_2O_3/h -BN heterojunction when SOC is considered.

orientations in the valence and conduction bands, and a bandgap of 0.58 eV (Figure 9F). At the phase transition point, corresponding to a tensile strain of 1.0415, the system undergoes a band inversion (Figure 9G), and the presence of non-trivial edge states indicates a QAHE phase (Figure 9H).

For ABB'_2C_2 structures, such as $VSGeN_2$ and $VSSiN_2$ (Figure 9I), is FM valley semiconductor with in-plane easy magnetization. In $VSSiN_2$, there is no valley polarization when the magnetization is oriented in the in-plane direction (Figure 9J). However, when the magnetization aligns with the out-of-plane z -direction, the valley polarization in the conduction band becomes very small, while the valence band shows a significant polarization of -72.73 meV (Figure 9K). Furthermore, in this third type of Janus structures, strain-induced VQAHE is observed (Figure 9L).⁹⁵ The band structure of $VSGeN_2$ is strongly affected by biaxial strain, while the influence of a perpendicular electric field is minimal.⁹⁶

THE QAHE IN 2D KAGOME MONOLAYERS

The Kagome monolayer is a lattice structure composed of corner-sharing triangles, known for its unique geometric frustration and unusual electronic properties.^{97–101} Recently, Kagome monolayers with out-of-plane magnetization properties have emerged as promising platforms for studying QAHE.^{102,103} Therefore, we also discuss the QAHE of Kagome monolayers by classifying them according to their elemental composition.

The QAHE in A_2B_3 Kagome monolayers

For instance, inserting non-metal atoms (such as O, S, Se) into a honeycomb lattice formed by metal atoms (such as V, Nb, Ta) results in a five-atom A_2B_3 Kagome lattice (Figure 10A).¹⁰⁴ This structure retains the D_{6h} point group symmetry, similar to that of graphene. In terms of magnetic properties, the FM state in these systems is primarily driven by direct exchange interactions between metal atoms, which are positively correlated with electron hopping and help reduce the system's energy.⁹⁹ Furthermore, studies of external biaxial strain reveal that the FM state generally has lower energy and greater stability.¹⁰² The band structure calculations using the Perdew-Burke-Ernzerhof + U (PBE + U) method and the Heyd-Scuseria-Ernzerhof (HSE06) functional show several key features of these monolayers.¹⁰³ The spin-down channel presents a large bandgap, while the spin-up channel reveals a Dirac cone at high-symmetry K point near the Fermi level (Figures 10B and 10C). These topological properties are mainly derived from the d_{xz} and d_{yz} orbitals of the metal atoms.¹⁰⁰ When SOC is considered, the Berry curvature in the first Brillouin zone of Kagome V_2O_3 is concentrated at the K point (Figure 10D), resulting in a Chern number of 1, consistent with TB model calculations. For instance, Ta_2O_3 exhibits a non-trivial bandgap as large as 454.8 meV, which exceeds the energy scale at room temperature, and this gap increases with applied tensile strain (Figure 10E). This behavior is influenced not only by SOC but also by electron correlation

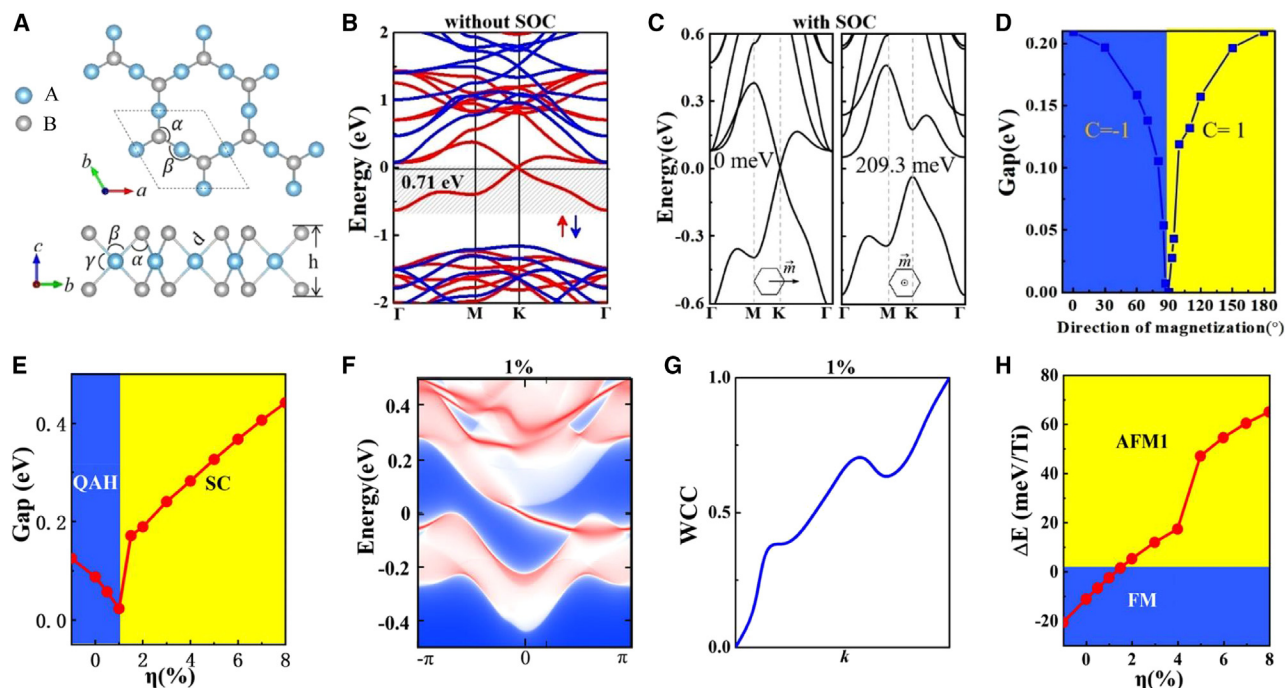


Figure 11. The electronic and topological properties of the Kagome A_3B_4 monolayers

- (A) The top and side views of the Kagome A_3B_4 crystal structure.
 (B) The band structure of the Kagome Ti_3Te_4 when SOC is not considered.
 (C) The band structure of the Kagome Ti_3Te_4 when the magnetization is along the in-plane y-direction and the out-of-plane z-direction, respectively.
 (D) The bandgap and the Chern number of the Kagome Ti_3Te_4 when the magnetization is shifted from the z-direction to the -z-direction.
 (E) The bandgap and the phase of the Kagome Ti_3Te_4 are changed by the tensile strain when SOC is considered.
 (F) The edge state of the Kagome Ti_3Te_4 under the 1% tensile strain when SOC is considered.
 (G) The WCC of the Kagome Ti_3Te_4 under the 1% tensile strain when SOC is considered.
 (H) The phase and the energy difference between the FM state and the AFM state of the Kagome Ti_3Te_4 are modulated by the tensile strain when SOC is considered.

effects. Strain tuning further reveals that these topological phases exhibit strong robustness, and the manipulation of the MAE is crucial for maintaining the QAH phase in 2D topological monolayers. A large MAE enables Ta_2O_3 to achieve a T_c of 392 K. In the A_2B_3 structure, the valley degeneracy at the K and K' points arise from C_3 rotational symmetry.¹⁰¹ To break this valley degeneracy, both inversion and time-reversal symmetries must be broken, and SOC plays a key role in this process. The electronic properties of these monolayers can also be tuned by introducing different metal atoms A or A'.¹⁰⁵ Additionally, when these monolayers are integrated into different substrates, specific van der Waals heterostructures are formed. For example, Ta_2O_3 on a hexagonal boron nitride (h-BN) substrate exhibits a minimal lattice mismatch of only 0.3% and weak van der Waals interactions, resulting in an interlayer spacing of 3.30 Å (Figure 10F). Similarly, the Nb_2O_3/MoS_2 heterostructure maintains an interlayer spacing of 3.51 Å while preserving both the Dirac cone near the Fermi level and the SOC-induced bandgap (Figure 10G), along with the retention of the QAHE (Figure 10H).

The QAHE in A_3B_4 Kagome monolayers

Building on the research of AB_3C_5 monolayers (A = K, Pb, Cs), 2D Kagome A_3B_4 (A = Ti, Cr, Te; B = Se, Te) monolayers have been

discovered (Figure 11A).^{106–109} In this structure ($P6/mmm$), the metal atoms (A) form a Kagome lattice, while two layers of non-metal atoms (B) form a honeycomb lattice. Magnetic analysis of these systems reveals that superexchange interactions between metal atoms, with bond angles close to 90°, facilitate the formation of an FM state. In the absence of SOC, the Fermi surface is primarily composed of spin-up electrons, displaying fully spin-polarized Weyl points (Figure 11B).

Upon the introduction of SOC, the existence of Weyl points becomes closely linked to the direction of magnetization (Figure 11C). When the magnetization is in-plane, C_{3z} and M_z symmetries are broken, while M_x (M_y) and P symmetries remain intact, preserving the Weyl points.¹⁰⁶ However, when the magnetization is out-of-plane, non-trivial bandgaps open near the Fermi level 209.3 meV and 227.5 meV for Ti_3Te_4 and Fe_3S_4 monolayers, respectively (Figure 11D). These bandgaps are a result of the enhanced SOC effects arising from the interaction between the metal d orbitals and the non-metal p orbitals. The topological properties of these systems exhibit robustness under biaxial strain (Figures 11E–11G). However, under specific conditions, such as compressive strains below -6% or tensile strains exceeding 2%, certain monolayers, including Cr_3Se_4 and Fe_3S_4 , undergo a phase transition to AFM semiconductor

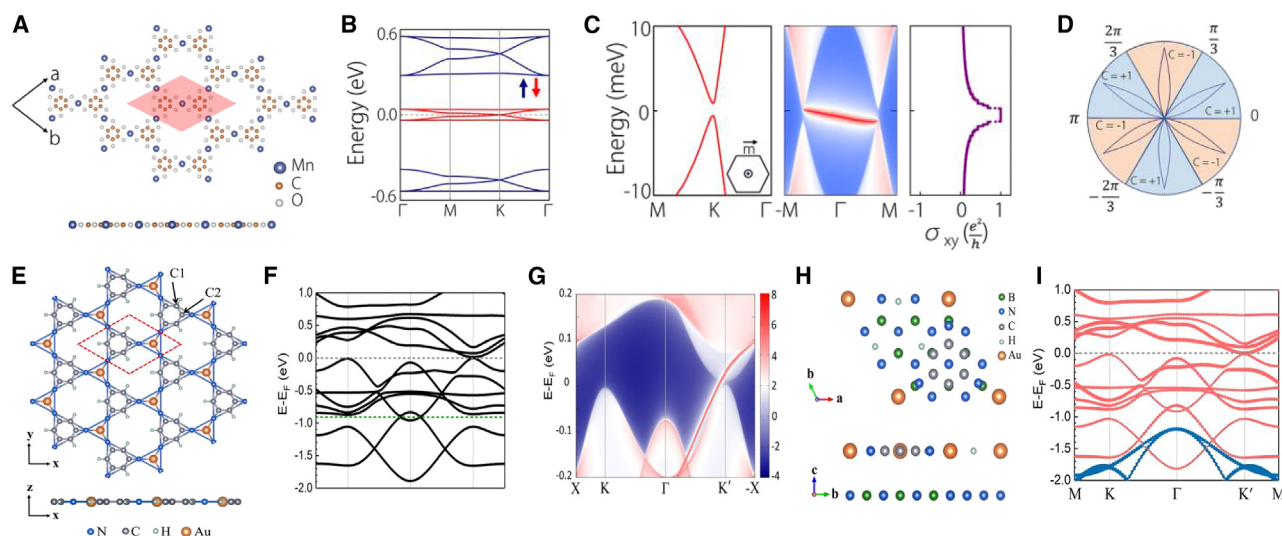


Figure 12. The electronic and topological properties of the MOF Kagome monolayers

- (A) The top and side views of the crystal structure of the $\text{Mn}_3(\text{C}_6\text{O}_6)_2$ monolayer.
 (B) The band structure of the $\text{Mn}_3(\text{C}_6\text{O}_6)_2$ monolayer when SOC is not considered.
 (C) The band structure with edge states and quantized anomalous Hall conductance of the $\text{Mn}_3(\text{C}_6\text{O}_6)_2$ monolayer when SOC is considered.
 (D) The Chern number of the Kagome $\text{Mn}_3(\text{C}_6\text{O}_6)_2$ is changed by the modulation of the in-plane magnetization direction.
 (E) The top and side views of the breathing Kagome $\text{C}_6\text{N}_3\text{H}_3\text{Au}$ crystal structure.
 (F) The band structure of the Kagome $\text{C}_6\text{N}_3\text{H}_3\text{Au}$ monolayer when SOC is considered.
 (G) The edge state of the Kagome $\text{C}_6\text{N}_3\text{H}_3\text{Au}$ monolayer when SOC is considered.
 (H) The top and side views of the Kagome $\text{C}_6\text{N}_3\text{H}_3\text{Au}$ crystal structure on the BN substrate.
 (I) The band structure of the $\text{C}_6\text{N}_3\text{H}_3\text{Au}/\text{BN}$ heterojunction when SOC is considered, where the pink and blue parts are the $\text{C}_6\text{N}_3\text{H}_3\text{Au}$ and BN substrates, respectively.

state. Additionally, Ti_3Te_4 transitions to an AFM state when subjected to tensile strains greater than 1.5% (Figure 11H).¹⁰⁷

The QAHE in MOF Kagome monolayers

The metal-organic frameworks (MOFs) demonstrate significant potential in quantum physics applications, particularly due to their structure containing transition metals, which can lead to phenomena such as topological Weyl semimetal state and the QAHE.^{110–114} Taking the FM MOF $\text{Mn}_3(\text{C}_6\text{O}_6)_2$ as an example, this monolayer features a Kagome lattice formed by Mn atoms in the same plane, with organic ligands consisting of C and O atoms, with a space group of $P6/mmm$ (No. 191) (Figure 12A). The calculations using generalized gradient approximation and local density approximation, across different U values, indicate that the FM is energetically favorable, suggesting that $\text{Mn}_3(\text{C}_6\text{O}_6)_2$ tends to form an FM-ordered. The Tc of this monolayer is 171 K, with an easy magnetization axis lying in the x-y plane. At the K point, the Weyl points arise entirely from spin-down state, making MOF $\text{Mn}_3(\text{C}_6\text{O}_6)_2$ a fully spin-polarized Weyl semimetal (Figure 12B). In the absence of SOC, the monolayer features fully spin-polarized Weyl points precisely at the Fermi level. Upon considering SOC, the spin-polarized Weyl points remain, but magnetization breaks vertical mirror symmetry (Figure 12C). When this symmetry is broken, the Weyl semimetal phase can transition into a QAH phase with a Chern number ($|C| = 1$). The Chern number of Kagome $\text{Mn}_3(\text{C}_6\text{O}_6)_2$ can be modulated by altering the direction of magnetization within the

plane (Figure 12D). Due to the fact that the bands near the Fermi level are predominantly contributed by C and O atoms, the SOC gap in the QAH phase of $\text{Mn}_3(\text{C}_6\text{O}_6)_2$ is relatively small, similar to other MOF-based QAHE, such as $\text{CuC}_{21}\text{N}_3\text{H}_{15}$ (2.2 meV) and $\text{XC}_{21}\text{N}_3\text{H}_{15}$ (X = Ti, Zr, Ag, Au) (7.1 meV).^{113,114}

Another proposed structure, the breathing MOF $\text{C}_6\text{N}_3\text{H}_3\text{Au}$, also exhibits interesting topological properties (Figure 12E). In this system, the anomalous valley Hall effect and the VQAHE coexist. When SOC is introduced, a non-trivial bandgap opens (Figure 12F). Berry curvature integration results indicate that this monolayer possesses a Chern number of $C = -1$, demonstrating its topological properties (Figure 12G). The monolayer shows a non-trivial bandgap of up to 269 meV and $E_K \neq E_{K'}$, implying that valley-polarized transport can be achieved by utilizing only the valleys from the K point. Valley splitting at the K and K' points reach up to 275 meV, significantly larger than the splitting observed in some transition metal dichalcogenides, highlighting this material's advantages in achieving VQAHE.¹¹¹ Additionally, the band structure of the $\text{C}_6\text{N}_3\text{H}_3\text{Au}/\text{BN}$ heterojunction reveals that the system is minimally affected by the substrate, similar to the behavior of $\text{C}_6\text{N}_3\text{H}_3\text{Au}$ alone (Figures 12H and 12I).

The QAHE in Yin-Yang Kagome monolayers

There exists a unique type known as the Yin-Yang Kagome monolayer, which features two enantiomorphic Kagome bands near the Fermi surface.^{115–118} Each of these bands comprises

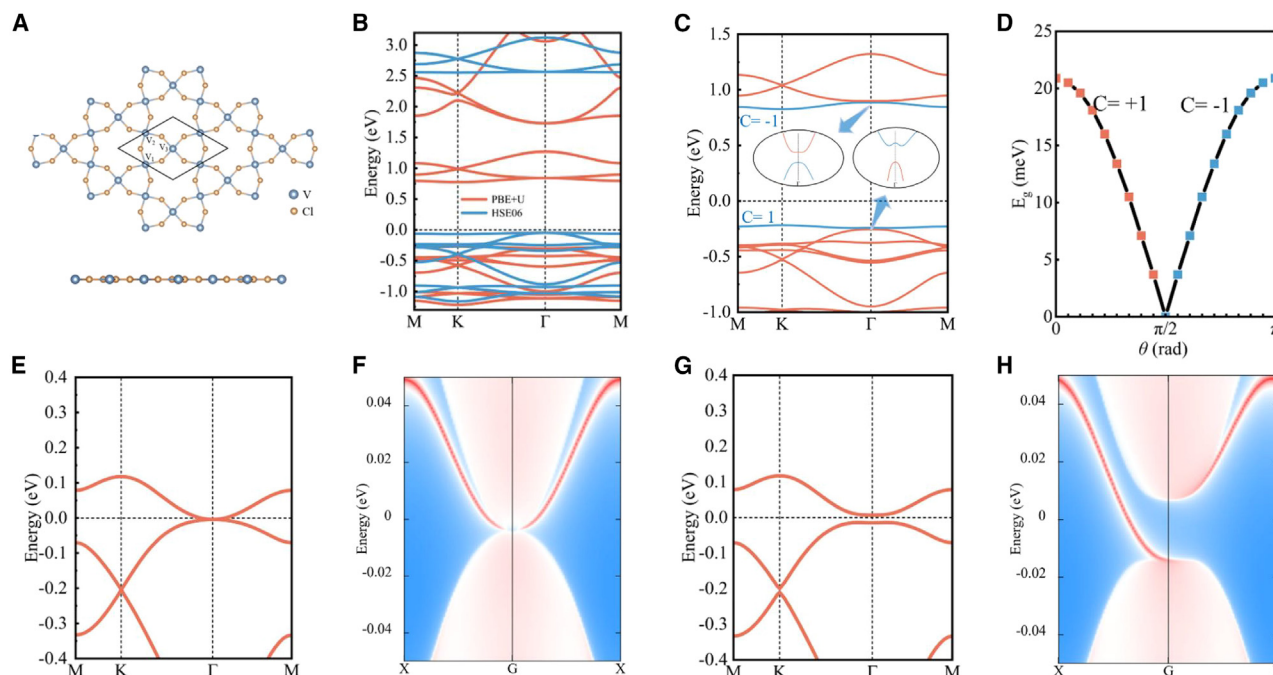


Figure 13. The electronic and topological properties of the Yin-Yang Kagome V_3Cl_6 monolayer

- (A) The top and side views of the Kagome crystal structure.
 (B) The band structure of the Kagome monolayer when SOC is not considered.
 (C) The band structure of the Kagome monolayer showing the Yin-Yang Kagome bands when SOC is considered.
 (D) The bandgap and the Chern number of the hole-doped Kagome when the magnetization is shifted from the z-direction to the -z-direction.
 (E) The band structure of the hole-doped Kagome when the magnetization is along the in-plane x-direction.
 (F) The edge state of the hole-doped Kagome when the magnetization is along the in-plane x-direction.
 (G) The band structure of the hole-doped Kagome when the magnetization is along the out-of-plane z-direction.
 (H) The edge state of the hole-doped Kagome when the magnetization is along the out-of-plane z-direction.

two Dirac bands and one flat band. A representative example of this class is the V_3Cl_6 monolayer. In this monolayer, each V atom is coordinated with four Cl atoms, forming a honeycomb Kagome lattice structure (Figure 13A). The monolayers belong to the $P6/mmm$ space group (No. 191). Band structure calculations using both the PBE+U and HSE06 methods indicate that the system behaves as a trivial FM semiconductor when SOC is not considered (Figure 13B). The V_3Cl_6 monolayer features enantiomorphic Kagome bands near the Fermi surface with identical spin orientations. Due to the differing coordination environments of the three V atoms in the V_3Cl_6 monolayer, the hopping between their two orthogonal d orbitals takes on opposite signs.¹¹⁵ This results in the yin-yang Kagome band structure near the Fermi level (Figure 13C). The MAE of 0.28 meV suggests that the easy axis of magnetization lies out-of-plane. As the magnetization direction gradually shifts from +z to -z, the non-trivial bandgap closes and then reopens, enabling the tuning of the QAH phase, through hole doping (Figure 13D). When the magnetization aligns along the x-direction, the V_3Cl_6 monolayer transitions to a semi-metallic state (Figure 13E). Further corresponding calculation of the edge state of V_3Cl_6 monolayer indicates that the system is a trivial stat phase (Figure 13F). However, when the magnetization is adjusted to the +z-direction, the monolayer exhibits a bandgap of approximately 20.9 meV

when doped with holes (Figure 13G) and QAH phase with a Chern number $C = 1$ (Figure 13H).

The QAHE in $Co_3B_3C_2$ Kagome monolayers

In contrast to the previously discussed Kagome structures, the $Co_3B_3C_2$ ($B = Sn, Pb$; $C = S, Se$) monolayers (Figure 14A) belong to the space group $P3m1$ (No. 164) and exhibit Weyl semimetal state in the absence of SOC. When SOC is taken into account, along the K to Γ path near the Fermi level, these monolayers display fully spin-polarized Weyl points, which are associated with a Chern number of 1/2 in the Berry curvature distribution (Figures 14B and 14C). Due to the C_3 inversion symmetry, the system contains six Weyl points, all carrying the same Chern number, resulting in a total Chern number of 3. An example of the tunability of these monolayers is the application of tensile strain, which can significantly increase the T_c , raising it from 46 K to 65 K. When SOC is considered, the $Co_3B_3C_2$ exhibits highly quantized anomalous Hall conductivity. This conductivity arises from edge states, indicating a high Chern number ($|C| = 3$). External factors like biaxial strain significantly influence the electronic properties of the monolayer. For instance, under compressive strain, the VBM at the Γ point increases, while the CBM at the K point decreases, leading to the gradual closure of the non-trivial bandgap (Figure 14D).¹¹⁹ In contrast, tensile strain

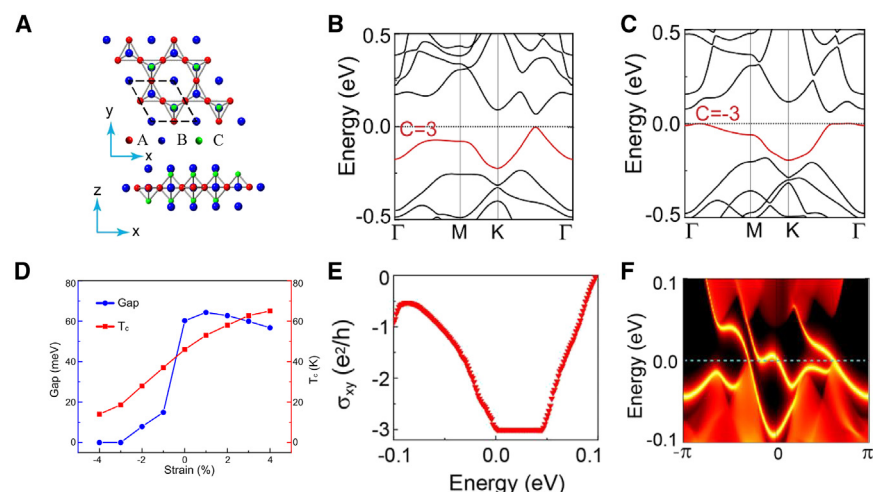


Figure 14. The electronic and topological properties of the Kagome $\text{Co}_3\text{B}_3\text{C}_2$ monolayers

(A) The top and side views of the Kagome $\text{Co}_3\text{B}_3\text{C}_2$ crystal structure. (B) The band structure and the Chern number of the Kagome $\text{Co}_3\text{Pb}_3\text{Se}_2$ when SOC is considered. (C) The band structure and the Chern number of the Kagome $\text{Co}_3\text{Sn}_3\text{Se}_2$ when SOC is considered. (D) The bandgap and the T_c of the Kagome $\text{Co}_3\text{Sn}_3\text{Se}_2$ modulated by the strain. (E) The quantized anomalous Hall conductance of the $\text{Co}_3\text{Sn}_3\text{Se}_2/\text{MoSe}_2$ heterojunction. (F) The edge states of the $\text{Co}_3\text{Sn}_3\text{Se}_2/\text{MoSe}_2$ heterojunction.

drives the VBM at the Γ point and the CBM at the K point in opposite direction, maintaining the non-trivial bandgap at approximately 60 meV. Furthermore, considering the effect of different substrates for practical applications, the $\text{Co}_3\text{Sn}_3\text{Se}_2/\text{MoSe}_2$ heterojunction demonstrates quantized anomalous Hall conductivity, with corresponding edge states (Figures 14E and 14F).

CONCLUSIONS

The discovery of the QAHE has opened new avenues for achieving quantized Hall resistance without the need for an external magnetic field, which is highly attractive both theoretically and practically. Notably, first-principles calculations provide a powerful tool for a deep understanding and prediction of the novel 2D topological monolayers. This review focuses on the latest theoretical advances in QAHE within hexagonal monolayers exhibiting strong SOC effect and internal magnetic ordering. Through precise first-principles calculations, we not only gain insights into the electronic structures and topological properties of these materials but also predict and design new materials that can realize QAHE. The realization of QAHE relies on the precise control of magnetic properties and electronic structures within the materials. We highlight the significance of external tuning methods, such as applying vertical electric fields, adjusting magnetization orientations, and introducing biaxial strain. These methods can effectively manipulate the topological properties of materials, tailoring them to meet specific application demands. With the continued advancements in materials science and nanotechnology, it is anticipated that more 2D materials with excellent QAHE will be developed. Research and application of these materials will offer new directions and possibilities for the design and realization of next-generation electronic and quantum devices.

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AUTHOR CONTRIBUTIONS

Conceptualization, L.Z. and H.C.; investigation, L.Z. and H.C.; writing—original draft preparation, L.Z. and H.C.; writing—review and editing, L.Z., H.C., J.R., and X.Y.

DECLARATION OF INTERESTS

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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