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# First-principles study of transition-metal doped GaBiCl<sub>2</sub> monolayers as magnetic topological insulators

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Magnetic topological insulators (MTIs) offer a pathway to dissipationless quantum and spintronic devices, but to date, their realization has been limited to extremely low temperatures. Therefore, identifying MTIs with sizable band gaps is crucial for raising the operating temperature toward practical applications. Through first-principles calculations, we present the first systematic study of transition-metal-doped GaBiCl<sub>2</sub> monolayers (X = Cu, Mn, Cr, and Mo) as a platform for high-temperature topological phases. We find that Cr doping induces a magnetic topological semimetal (MTSM), where strong Cr-3d/host hybridization collapses the global gap. In contrast, Mo doping stabilizes a ferromagnetic MTI with a nontrivial  $\mathbb{Z}_2 = 1$  invariant and a robust spin-orbit coupling-induced band gap of 41.3 meV, indicating its potential for room temperature applications. The preservation of the nontrivial gap arises from relatively weak p-d hybridization between Mo-4d and host Bi-p states, which suppresses the impurity-driven gap closure seen with other dopants. These results make Mo-doped GaBiCl<sub>2</sub> a promising candidate for room temperature MTIs and a versatile platform for exploring the quantum anomalous Hall effect and next-generation spintronic devices.

## 1. Introduction

Harnessing quantum phenomena for next-generation technology requires materials that enable robust, energy-efficient information processing at practical temperatures.<sup>1–3</sup> Topologically protected phases offer dissipationless conduction channels resilient to local perturbations, making them ideal for scalable quantum and spintronic devices. Materials exhibiting the quantum anomalous Hall effect (QAHE), in particular, support topologically protected edge states suitable for low-power applications.<sup>4,5</sup> Achieving the QAHE at practical temperatures could thus unlock a new generation of quantum devices. However, realizing the QAHE at higher temperatures remains a grand challenge due to the lack of materials that combine robust ferromagnetism with a sizable topological band gap.<sup>6</sup> Magnetic topological insulators (MTIs), which combine topological properties with intrinsic magnetism to break time-reversal symmetry while preserving nontrivial band topology,<sup>7–17</sup> represent a promising route. There were many attempts to realize the QAHE in 3-dimensional (3D) MTIs, including MnBi<sub>2</sub>Te<sub>4</sub><sup>18</sup> and MnBi<sub>2</sub>Te<sub>4</sub> thin flakes,<sup>19,20</sup> Cr-doped (Bi,Sb)<sub>2</sub>Te<sub>3</sub> films,<sup>21</sup> MnBi<sub>4</sub>Te<sub>7</sub>, MnBi<sub>6</sub>Te<sub>10</sub>, and EuSn<sub>2</sub>As<sub>2</sub>,<sup>22</sup> all of which failed to be applicable beyond 2 K, with global band gaps of the aforementioned materials being limited below 0.2 eV. Thus, the search for magnetic topological insulators,<sup>23–26</sup> particularly

those with sufficient bulk gaps, has emerged as a key objective in the field of topological material research. The most notable progress in 3D MTIs has been seen in MnBi<sub>2</sub>Te<sub>4</sub>-based heterostructures, where inserting a topological insulator spacer induces interlayer ferromagnetism with a predicted Curie temperature of up to 42 K and a nontrivial band gap of about 0.2 eV.<sup>27,28</sup> Recently, however, researchers have increasingly turned to two-dimensional (2D) materials as monolayer MTIs are more promising than their 3D counterparts for several reasons. In 2D systems, the reduced dimensionality enables robust edge states with quantized conductance, which are protected by topological invariants and less prone to backscattering or localization compared to the surface states, and they do not face challenges such as increased complexity of surface state manipulation and sensitivity to bulk defects.<sup>29,30</sup> This enhanced stability is critical for achieving dissipationless transport channels ideal for spintronic and quantum computing applications.

2D MTIs have garnered attention due to their unique electronic properties and promising applications. Monolayer materials such as transition metal dichalcogenides (TMDs) and halides exhibit robust topological phases, making them strong candidates for dissipationless transport.<sup>31–33</sup> In 2018, Baidya *et al.* demonstrated that monolayer CrI<sub>3</sub> can host tunable Chern insulating states.<sup>34</sup> The QAHE has also been realized in various monolayer systems, including the V<sub>2</sub>MX<sub>4</sub> (M = W and Mo; X = Se and S) family,<sup>35</sup> and honeycomb-Kagome vanadium oxides,<sup>36</sup> which exhibit sizable topological band gaps and high Curie temperatures,

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making them viable for practical applications.<sup>30,37–39</sup> However, these materials face challenges in either experimental realization, magnetic stability, or synthesis. Overall, progress in 2D MTIs has been limited, primarily due to their small band gaps, the lack of extensive research on their ferromagnetic properties and the lack of intrinsically magnetic 2D MTIs.

Recent efforts have been directed at addressing these limitations by engineering 2D materials with both large topological band gaps and robust ferromagnetism. Numerous studies have explored 2D topological insulators (TIs) with large band gaps to enable their viability for room-temperature applications, including silicene,<sup>40</sup> germanene,<sup>41</sup> and stanene,<sup>42</sup> with reported nontrivial band gaps ranging from 1 meV to 0.3 eV. Theoretical predictions have proposed several candidates for magnetic topological insulators, such as FeBr<sub>3</sub><sup>43</sup> and Janus monolayers;<sup>44</sup> however, few showed the potential for realistic applications. A major breakthrough came with the theoretical prediction of a V<sub>2</sub>O<sub>3</sub> monolayer as an intrinsic magnetic topological insulator, exhibiting a sizable nontrivial band gap (0.45 eV) as a room temperature MTI.<sup>36</sup> These developments set the stage for introducing our proposed material. The GaBiCl<sub>2</sub> monolayer was theoretically predicted to be a large gap topological insulator in 2015, but the effect of ferromagnetism on this material is yet to be investigated.<sup>45</sup>

First-principles calculations predict that GaBiCl<sub>2</sub> hosts a large nontrivial band gap (~0.65 eV) and stability due to the absence of under-coordinated atoms, making it a promising platform for higher-temperature applications.<sup>45</sup> A subsequent theoretical work by Maciel *et al.* demonstrated that GaBiCl<sub>2</sub> exhibits out-of-plane ferroelectric polarization with a switchable direction, enabling bistable electronic states.<sup>46</sup> They also found that the bandgap of GaBiCl<sub>2</sub> can be tuned by external electric fields, allowing for control over its semiconducting properties and making it suitable for applications in non-volatile memory and nanoelectronic devices. Importantly, Hangyu Li and Zhongyao Li predicted quantum edge states in GaBiCl<sub>2</sub> nanoribbons and found that vacancies in chloridized gallium bismuthide (GaBiCl<sub>2</sub>) nanoribbons, especially those at the center of the nanoribbon, induce quasi-periodic scattering of these states, which may serve as a distinctive signature for defect identification.<sup>47</sup> Its large intrinsic band gap makes GaBiCl<sub>2</sub> an ideal platform for transition metal doping, offering the potential to break time-reversal symmetry and realize magnetic topological insulating phases. However, the effects of transition metal (TM) doping on its electronic and topological properties are yet to be investigated, prompting us to examine the TM-doped GaBiCl<sub>2</sub> monolayer.

In this study, we used density functional theory (DFT) to investigate the electronic, magnetic, and topological properties of GaBiCl<sub>2</sub> monolayers doped with transition metals (Cu, Mn, Cr, and Mo). We calculated the band structures and computed the  $\mathbb{Z}_2$  topological invariant of these compounds. Finally, we compared our results to other similar research and discussed future work.

## 2. Methodology

We performed first-principles calculations based on density functional theory (DFT) using the projector augmented-wave (PAW)

method,<sup>48,49</sup> as implemented in the ABINIT software package,<sup>50</sup> which solves the Kohn–Sham equations.<sup>51</sup> The exchange–correlation interaction was modeled using the Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA)<sup>52</sup> and the pseudopotential in projector augmented wave (PAW) method.<sup>48,49</sup>

The plane-wave energy cutoff, vacuum, and *k*-point mesh were converged for each system. For TM-doped GaBiCl<sub>2</sub>, the kinetic energy cutoffs for the individual components, namely, GaBiCl<sub>2</sub> and bulk TM, were determined separately, and the larger was implemented. The self-consistent field (SCF) convergence criterion was set such that the difference in total energy between two consecutive iterations was less than  $1.0 \times 10^{-10}$  Ha twice. The convergence parameters were converged until the energy difference between successive datasets did not exceed  $1.0 \times 10^{-4}$  Ha twice.

Structural optimization was carried out using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization method. For unit cell calculations, Brillouin zone integration was sampled using an  $8 \times 8 \times 1$  *k*-point grid, with a shift of (0, 0, 1/2). Atomic positions were relaxed until forces on all atoms fell below  $5.0 \times 10^{-5}$  Ha Bohr<sup>-1</sup>.

Using the relaxed structures, spin-polarized calculations (SPCs) were performed to compute spin-up and spin-down band structures and total magnetization, except for pristine GaBiCl<sub>2</sub> as it is nonmagnetic. Additionally, band structures incorporating and not incorporating spin–orbit coupling (SOC) were evaluated for all materials. Fig. 1(a) shows the honeycomb crystal structure of GaBiCl<sub>2</sub>, and its Brillouin zone marked with chosen high-symmetry points is shown in Fig. 1(b). Doping of GaBiCl<sub>2</sub> was performed *via* substitutional doping, as shown in Fig. 1(c) and (d), where a single Cl atom was replaced with the dopant (X = Cu, Mn, Cr, and Mo) atom in a  $2 \times 2$  supercell. We selected the Cl site for substitution since replacing an anion preserves the Ga–Bi framework and minimizes structural disruption, while effectively introducing carriers and magnetism without destabilizing the host lattice. The global band gap was defined as the energy difference between the conduction band minimum and the valence band maximum. Bands were plotted through the selected high-symmetry *k*-points in the reciprocal space, *M* (1/2, 0, 0),  $\Gamma$  (0, 0, 0), *K* (2/3, 1/3, 0), and back to  $\Gamma$  (0, 0, 0) in the first Brillouin zone of reciprocal space. The  $\mathbb{Z}_2$  topological invariant was computed using Z2Pack<sup>53,54</sup> based on maximally localized Wannier functions obtained from ABINIT using Wannier90.<sup>55</sup>

## 3. Results

We computed the band structures of TM-doped GaBiCl<sub>2</sub> with SOC, without SOC, with SPC, and with partial density of states (DOS) under relaxed lattice parameters and examined their atomic and electronic properties. Then, we used the band structure with SOC and  $\mathbb{Z}_2$  calculations to evaluate their topological characteristics.

### 3.1. GaBiCl<sub>2</sub>

Fig. 1(c) shows the crystal structure of pristine monolayer GaBiCl<sub>2</sub>. The fully relaxed optimized structure has an optimized







Fig. 2 The band structure of GaBiCl<sub>2</sub> (a) without SOC and (b) with SOC. (c) Time evolution of Wannier charge centers (WCCs) at  $k_z = 0$  and  $k_z = 0.5$ . The Fermi level is set to 0 eV (dashed line). SOC opens a substantial nontrivial band gap at the  $\Gamma$  point and the band structure displays band inversion.



Fig. 3 Cu-doped GaBiCl<sub>2</sub>'s (a) atomic structure, top view (top) and side view (bottom), with green, pink, grey, and brown representing Cl, Ga, Bi, and Cu, respectively; (b) band structure without SOC; and (c) spin-polarized band structure. Black and purple lines denote spin-up and spin-down bands, respectively. The Fermi level is set to 0 eV (dashed line). Cu doping introduced no magnetism.

as confirmed by  $\mathbb{Z}_2 = 0$  from WCC analysis shown in Fig. 4(f). This trivialization likely stems from strong p-d hybridization that collapses the inverted gap.

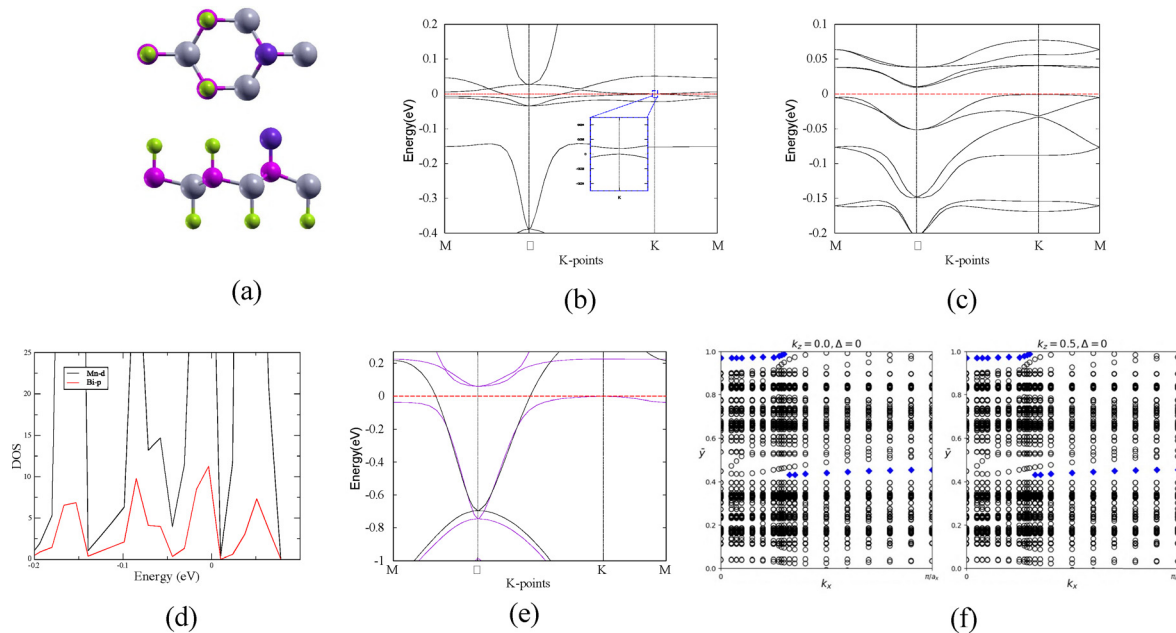
Table 2 Each TM-doped GaBiCl<sub>2</sub> system's magnetization, in  $\mu_B$ , global band gap under SOC ( $E_g$ ) in eV, and classification

Dopant	Total magnetic moment ( $\mu_B$ )	$E_g$ (eV)	Classification
Mo	5.09	0.041	MTI
Cr	4.92	0.000	MTSM
Mn	4.52	0.011	Trivial insulator
Cu	0.00	—	Trivial insulator
None	0.00	0.647	TI

### 3.4. Cr-doped GaBiCl<sub>2</sub>

Cr-doped GaBiCl<sub>2</sub> also demonstrated little structural deviation from the pristine system, as shown in Fig. 5(a), with electronic structures demonstrating similar characteristics to the Mn-doped system. This can be attributed to the comparable 3d orbital occupancies of Cr and Mn, which lead to analogous exchange splitting and hybridization with surrounding p-orbitals of Bi, as shown in Fig. 5(d). However, unlike the Mn-doped system, Cr-doped GaBiCl<sub>2</sub> exhibits a semimetallic state under SOC, where the conduction band, although not crossing with the valence bands, dips below the Fermi level for band structures both with and without SOC, as shown in Fig. 5(b)





**Fig. 4** Mn-doped GaBiCl<sub>2</sub>'s (a) atomic structure, top view (top) and side view (bottom), with green, pink, grey, and purple representing Cl, Ga, Bi, and Mn, respectively; (b) band structure without SOC; (c) band structure with SOC; (d) projected partial DOS on the dopant and the neighboring Bi atom; (e) spin-polarized band structure; and (f) time evolution of Wannier charge centers (WCCs) at  $k_z = 0$  and  $k_z = 0.5$ . The Fermi level is set to 0 eV (dashed line). Black and purple lines denote the spin-up and spin-down bands, respectively.

and (c). Notably, after the inclusion of SOC, band degeneracies are preserved only at the  $\Gamma$  point. This localized degeneracy is a direct consequence of the underlying crystalline symmetry and remaining inversion symmetry at that high-symmetry point. Away from  $\Gamma$ , the degeneracies are lifted likely due to the

combined effects of ferromagnetic exchange interactions and SOC, indicating that TRS is broken across the Brillouin zone. Like Mn-doped GaBiCl<sub>2</sub>, band narrowing can be attributed to strong p-d hybridization between Bi-p and Cr-d orbitals, which was also seen in Cr-doped Bi<sub>2</sub>Se<sub>3</sub>.<sup>65</sup> In addition, the collapse of



**Fig. 5** Cr-doped GaBiCl<sub>2</sub>'s (a) atomic structure, top view (top) and side view (bottom), with green, pink, grey, and blue representing Cl, Ga, Bi, and Cr, respectively; (b) band structure without SOC; (c) band structure with SOC; (d) projected partial DOS on the dopant and the neighboring Bi atom; (e) spin-polarized band structure; and (f) time evolution of Wannier charge centers (WCCs) at  $k_z = 0$  and  $k_z = 0.5$ . Black and purple lines denote spin-up and spin-down bands, respectively. The Fermi level is set to 0 eV (dashed line). Cr doping induces a semimetallic phase with strong exchange splitting and maintains topological order.



the band gap in Cr-doped GaBiCl<sub>2</sub> may also be attributed to Fermi level pinning. Chromium's partially filled 3d orbitals can introduce mid-gap states or defect-like electronic states that energetically align near the Fermi level. These states effectively shift the Fermi level into the conduction band, creating semi-metallic character despite the preservation of topological order. This mechanism has been previously observed in other TM-doped topological systems, such as Sn-doped Bi<sub>2</sub>Te<sub>2</sub>Se and Ag-doped Bi<sub>2</sub>Se<sub>3</sub>, where localized defect states interfere with global band gap formation.<sup>68,69</sup> Chromium doping results in a magnetic moment of 4.92 μ<sub>B</sub>, shown in Table 2, and induces strong spin polarization in the electronic structure, leading to the exchange splitting of the spin-up and spin-down bands near the Fermi level in Fig. 5(e). The conduction band dipping below the Fermi level leads to electron pockets, while the valence band contributes hole pockets, maintaining the topological nontrivial phase at the surfaces  $k_z = 0$  and  $k_z = 0.5$ , as shown in Fig. 5(f).

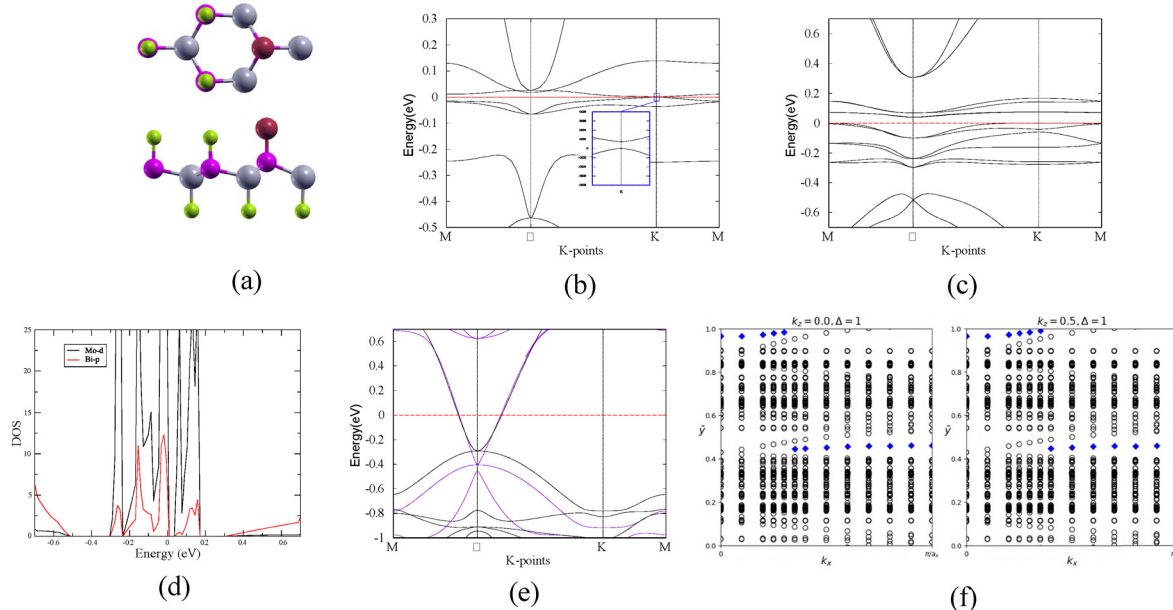
Although WCC evolution indicates a retained nontrivial topology, the absence of a global gap makes Cr-doped GaBiCl<sub>2</sub> a magnetic topological semimetal (MTSM). External tuning through strain, gating, or chemical substitution may reopen the gap, enabling a controllable MTSM–MTI transition. A precedent for such a transition is seen in (Mn<sub>1-x</sub>Sn<sub>x</sub>)Bi<sub>2</sub>Te<sub>4</sub>, where Sn doping initially collapses the band gap into a semi-metallic phase, but at higher concentrations, reopens it into a MTI.<sup>70</sup> By analogy, tuning parameters such as the chemical composition, strain, or layer thickness may stabilize an insulating phase in Cr-doped GaBiCl<sub>2</sub>. This makes the material a

strong candidate for further exploration in MTSM-to-MTI transition.

### 3.5. Mo-doped GaBiCl<sub>2</sub>

Fig. 6(a) shows the atomic structure of Mo-doped GaBiCl<sub>2</sub>, with a large buckling height in the local cell of the dopant shown in Table 1, signaling a rather strong bonding strength between Ga and Mo. In contrast to the Cr-doped case, Mo-doped GaBiCl<sub>2</sub> does develop a significant band gap. The band structure without SOC is shown in Fig. 6(b), showing a small gap of 0.001 eV opening at the  $k$  point. Upon introducing SOC, a direct band gap of 0.140 eV appears at the  $\Gamma$  point and, crucially, a global indirect band gap of 41.3 meV remains, as shown in Fig. 6(c). The 41.3 meV gap well exceeds the gap needed for room temperature, namely, 0.026 eV, and Mo-doped GaBiCl<sub>2</sub> is therefore anticipated to be a room-temperature magnetic topological insulator. This value is comparable to that of the most optimistic theoretical candidates such as Kagome-based systems and significantly larger than that of the gaps observed in prototypical MTIs such as Cr-doped (Bi,Sb)<sub>2</sub>Te<sub>3</sub> or MnBi<sub>2</sub>Te<sub>4</sub>, where exchange gaps are only a few meV.<sup>19,21,34–36,71</sup> The characteristic band inversion at the  $\Gamma$  point is preserved after Mo doping, indicative of topological nontrivial order.

Mo's success in preserving a band gap is likely due to the fact that Mo's 4d electrons, unlike other the 3d electrons of the other dopants used in this study, hybridize more weakly with Bi-p states around the Fermi level, as shown in Fig. 6(d), preventing impurity-induced gap closure.<sup>64</sup> It is noteworthy that the 2D material MoTe<sub>2</sub>F<sub>2</sub> has recently been predicted to



**Fig. 6** Mo-doped GaBiCl<sub>2</sub>'s (a) atomic structure, top view (top) and side view (bottom), with green, pink, grey, and red representing Cl, Ga, Bi, and Mo, respectively; (b) band structure without SOC; (c) band structure with SOC; (d) projected partial DOS on the dopant and the neighboring Bi atom; (e) spin-polarized band structure; and (f) time evolution of Wannier charge centers (WCCs) at  $k_z = 0$  and  $k_z = 0.5$ . Black and purple lines denote spin-up and spin-down bands, respectively. The Fermi level is set to 0 eV (dashed line). Mo doping preserves a large topologically nontrivial band gap while introducing strong magnetism and band splitting.



exhibit both a quadruple band crossing-induced high-performing QAHE and a large band gap.<sup>72</sup> Meanwhile, Mo-doping also successfully introduces ferromagnetism to the material with a strong magnetic moment, shown in Table 2, and evidence of strong band-splitting under spin-polarization, shown in Fig. 6(e). The emergence of a band gap alongside robust ferromagnetism confirms that time-reversal symmetry is broken in the system. Yet, this symmetry breaking does not disrupt its topology, as our  $\mathbb{Z}_2$  calculations reveal that the system retains its topologically non-trivial phase, characterized by  $\mathbb{Z}_2 = 1$ , at the surfaces with  $k_z = 0$  and  $k_z = 0.5$ , as shown in Fig. 6(f). Overall, Mo-doped GaBiCl<sub>2</sub> is a room-temperature MTI that is promising for spintronic applications and as a platform for realizing the QAHE at higher temperatures.

In this context, external tuning parameters such as strain, electric gating, and correlation strength provide promising routes to further enhance the topological phases. Recently, across diverse systems, these strategies have enabled either the stabilization of QAHE phases or the enlargement of topological gaps: stacking and strain modulation can generate altermagnetism with spin-split states even without net magnetization,<sup>73</sup> while strain- or correlation-driven tuning has enhanced the nontrivial band gap in LaPdO<sub>3</sub> and LaPtO<sub>3</sub> bilayers,<sup>74</sup> and group-IV monochalcogenides have exhibited multiple Hall effects controllable by strain and built-in fields, with reported gaps in the range of several tens of meV.<sup>75</sup> Recently, silicene on SiC was presented as a potential 2D candidate for realizing the QAHE with a reported band gap of 1.3 meV.<sup>76</sup> By comparison, Mo-doped GaBiCl<sub>2</sub> exhibits a robust gap of 41.3 meV, performing comparable to the recent leading 2D candidates, such as LaPtO<sub>3</sub> bilayers and VSiSnN<sub>4</sub>.<sup>73–76</sup> Interestingly, in LaPdO<sub>3</sub>, compressive in-plane strain increased the QAHE gap from 92 meV to 242 meV.<sup>74</sup> Given this precedent, Mo-doped GaBiCl<sub>2</sub> leaves open the possibility of further enlargement under external tuning, potentially positioning it alongside the most competitive candidates for high-temperature QAHE. For Cr-doped GaBiCl<sub>2</sub>, such strategies may provide a pathway to reopen the collapsed gap and drive the system from its present semimetallic state toward a true QAHE phase.

## 4. Conclusions

Through first-principles investigations, we have theoretically predicted the emergence of topologically nontrivial and ferromagnetic phases in Mo-doped and Cr-doped GaBiCl<sub>2</sub> monolayers. Pristine GaBiCl<sub>2</sub> is a topological insulator. Upon doping, spin-polarized calculations reveal that substituting a Cl atom with Cr or Mo introduces strong magnetism. Among them, Mo-doped GaBiCl<sub>2</sub> exhibits both a robust ferromagnetic ground state and a SOC-induced global room-temperature band gap of 41.3 meV, accompanied by band inversion and a nontrivial  $\mathbb{Z}_2$  invariant, firmly establishing it as a magnetic topological insulator and placing Mo-GaBiCl<sub>2</sub> among the most promising MTI candidates reported to date. Although Cr-doped GaBiCl<sub>2</sub> retains the nontrivial topology, it lacked an bulk gap, yielding a

magnetic topological semimetal state. Due to its proximity to an insulating phase, Cr-doped GaBiCl<sub>2</sub> is an intriguing platform for exploring transitions from an MTSM to an MTI *via* external tuning. The combination of an insulating gap and intrinsic ferromagnetism in Mo-doped GaBiCl<sub>2</sub> makes it a prime candidate for next-generation spintronic devices and a platform for further research and realizing the quantum anomalous Hall effect at elevated temperatures. Future research should assess the Curie temperature and stability of Mo-doped GaBiCl<sub>2</sub>, while exploring strain or chemical tuning to enlarge its gap and guide experimental realization toward practical spintronic and QAHE devices.

## Conflicts of interest

There are no conflicts to declare.

## Data availability

Data for this article, including input files, output files, raw data, and figures, are available at figshare at <https://doi.org/10.6084/m9.figshare.29924957.v1>, <https://doi.org/10.6084/m9.figshare.29924936>, <https://doi.org/10.6084/m9.figshare.29974192>, <https://doi.org/10.6084/m9.figshare.29974168> and <https://doi.org/10.6084/m9.figshare.29924933>.

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