Fast Electrically Switchable Large Gap Quantum Spin Hall States in MGe$_2$Z$_4$

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Spin-polarized conducting edge currents counterpropagate in quantum spin Hall (QSH) insulators and are protected against disorder-driven localizations by the time-reversal symmetry. Using these spin-currents for device applications requires materials with a large bandgap and fast switchable QSH states. By means of in-depth first-principles calculations, this study demonstrates the large bandgap and fast switchable QSH state in a newly introduced 2D material family with 1T$'$-MGe$_2$Z$_4$ (M = Mo or W and Z = P or As). These Ge-based compounds show superior properties with respect to other members of the same family. For the WGe$_2$As$_4$ monolayer it can stabilize the 1T$'$-phase, while for the other members of the family, this study needs an appropriate strain. The dynamically stable 1T$'$-MGe$_2$Z$_4$ monolayers have a large energy gap up to 237 meV for WGe$_2$As$_4$. These materials undergo a phase transition from a QSH insulator to a trivial insulator with a Rashba-like spin splitting under the influence of an out-of-plane electric field, demonstrating a fast tunability of the bandgap and its band topology for the Ge-based compounds. Fast topological phase switching in a large gap 1T$'$-MGe$_2$Z$_4$ QSH insulators have potential applications in low-power devices, quantum computation, and quantum communication.

1. Introduction

The discovery of 2D materials has opened a new era in condensed matter and materials physics owing to their conceptual novelties and potential for a wide range of device applications.[1–7] The main importance of the quantum spin Hall (QSH) insulators is the 1D counter-propagating conducting helical edge modes protected by the time-reversal symmetry inside the 2D bulk. These helical modes make QSH insulators appealing for dissipationless, fast, and energy-efficient device applications.[8,9] The existence of QSH states has been theoretically predicted in diverse families of 2D materials and quantum well structures through bulk and edge state computations.[10–12] Their experimental verification has been reported in 2D quantum wells of HgTe/CdTe and InAs/GaSb by measuring the quantized spin Hall conductance.[13–16] On realizing the QSH state in single-phase materials, the thin films of WTe$_2$ have been extensively studied over the last few years.[17] The experimental signature of the QSH effect has been demonstrated recently in the monolayer films of the 1’T phase of WTe$_2$.[18–21] In van der Waals and 2D materials, many QSH candidates have been proposed and investigated.[22,23] However, for both quantum wells and 2D materials, the longest topological protection length is of the order of a few micrometers.[20,24] It has been proposed that different mechanisms may contribute to the shortening of the topological protection length, such as charge puddles,[25] spontaneous time-reversal symmetry breaking[26,27] and acceptor dopants.[28,29] However, some of these mechanisms are valid just for the quantum wells.[30] Considering also that the QSH phase in thin films and 2D materials can be tuned by the electric field, strain[31] and adatoms,[32] it is highly desirable to continue the search for new 2D materials with larger inverted bandgaps and superior transport properties to achieve the room temperature QSH phase and engineering device applications.[33,34]

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Recently, a new MoS$_2$N$_4$ class of 2D materials has been synthesized using a novel bottom-up technique.[33,35] These materials show remarkable properties such as stability under ambient conditions, a semiconducting behavior, high mobility, and correlation-driven quantum anomalous Hall states, among other
properties, which are superior to the well-known transition metal dichalcogenides (TMDs) class of materials. Theoretical predictions on Ising superconductivity have been proposed. The structural phases of these materials are further amenable to realize a semiconductor-to-metal transition by defects, and strain engineering as well as by applying electric field. The commonly investigated 2H phase of these materials is well characterized in connection to the formation of superlattices or Janus phases. More recently, we have shown that MoSi2N4 materials can form a 1T polystyptic structure that realizes robust QSH insulator states with excellent transport properties. Motivated by these studies, we here introduce the new members of this family of QSH insulators that are thermodynamically stable and realize fast electric-field switchable helical edge states with excellent spin transport and properties. Based on our in-depth first-principles calculations, we show that the 1T-phase of MGe2Z4 (M = Mo or W, Z = P or As) monolayers have large bandgaps up to 237 meV. To our knowledge, this topological bandgap is the highest reported in 1T′-phases and comparable with the gap of 260 meV measured in the high-temperature quantum spin Hall of a higher-order topological insulator. We also report a controlled transition from the topological state to the trivial state under an external electric field. Previous literature was limited to the 1H and 2H phases of the Ge-based compounds.

**2. Results and Discussion**

**2.1. Crystal Structure and Symmetries**

The crystal structure of the 2H-phase MGe2Z4 can be viewed as an MZ2 layer sandwiched in between two GeZ layers, where the M atoms are located at the center of the trigonal prism building-block with six Z neighbors and the MZ2 layer bonded vertically with the GeZ layers. This crystal structure has a hexagonal primitive cell with space group D\( _{3h} \) (P\( \bar{6}m \) No. 187). In the case of 1T′-phase MGe2Z4, the three atomic layers are stuck in such a way that the positions of the M atom is at the center of trigonal prism building block twisted by 60° and with six Z neighbors, which creates the octahedral building block of the M atoms with the six Z atoms in the MZ2 layer. The different M-M bond lengths of atomic chains in the MZ2 layer lower the symmetry of the space group to p\( \bar{2}m \) (No. 11) to form a rectangular primitive unit cell, as shown in Figure 1a,b. Interestingly, the 1T′ structure restores the inversion symmetry (I) in contrast to the 2H structure. The structural parameters are given in Table 1. Figure 1c shows the 2D Brillouin zone (BZ) of the 1T′-phase, the red dots represent band crossing points Σ in the bandstructure without SOC. The 1T′-phase of WGe2As4 is the ground state within HSE (see Supporting Information), while for the other Ge-based materials, a strain is necessary to stabilize the 1T′ phase as we have mentioned for the Si-based compounds. The absence of imaginary mode in the phonon band structure throughout the extended BZ in Figure 1d indicates the dynamical stability of the 1T′-phase of MoGe2P4. In addition, we have investigated the thermodynamic stability of the compounds by simulating compounds with AIMD at a temperature of 300 K. The thermodynamic stability of compounds is discussed in the Supporting Information (SI). Experimentally, the 1T′-phase of WTe2 was synthesized successfully in past works. However, compared to the structural stability of TMDs, we expect that the 1T′-phase of the MGe2Z4 compounds could be synthesized within certain thermal and mechanical conditions. Moreover, the topological phase
transition in MGe$_2$Z$_4$ family under the influence of an external electric field is illustrated schematically in Figure 1e.

2.2. Electronic Properties of MGe$_2$Z$_4$ Materials

In the main text, we will focus on the electronic band structure of 1T'-MoGe$_2$P$_4$ material, while in the Supporting Information, we report the details for the other compounds. Figure 2a shows the band structure of 1T'-MoGe$_2$P$_4$ using the vdW correction. The valence and conduction bands cross each other along the $\Gamma$-Y line, which indicates an inverted band ordering at the $\Gamma$ point. This band-crossing is protected because the two bands belong to different symmetry operation ($\Lambda_1$ and $\Lambda_2$) representations. Additionally, a camel-back like feature has been observed along the $\Gamma$-Y line, which is typical of the system with large SOC and broken inversion symmetry as HgTe-based systems.[54,55] When the SOC is included, the band crossing is lifted, and the system shows a bandgap $E_{g}^{\text{vdW}}$ of 33 meV with the valence band maxima (VCM) and the conduction band minima (CBM) located at $\pm(0, 0.102, 0)\AA^{-1}$ as shown in Figure 2b. We have analyzed the orbital character of the bands near the Fermi level, the bands are dominated by the p-orbitals of P atoms and d-orbitals of Mo atoms as in TMDs, the band inversion occurs between p of P and d of Mo at the $\Gamma$ point with an inverted gap ($\delta^{\text{vdW}}$) of 503 meV. We have checked the robustness of our results with the more accurate HSE functional as shown in Figure 2c without SOC and Figure 2d with SOC. The HSE band structures show similar results to that obtained within GGA with vdW correction. The bandgap ($E_{g}^{\text{HSE}}$) increases to 93.8 meV while the inverted gap ($\delta^{\text{HSE}}$) increases to 877 meV. Moreover, the 2D Wannier band structure also confirms the previous results (see Figure 2e,f) of a gapless Dirac semimetal phase in the absence of SOC and a QSH insulating phase in presence of SOC. The detailed data of the bandgap and the inverted bandgap of 1T'-MoGe$_2$Z$_4$ materials are reported in Table 1. The band structures of other materials are shown in the Supporting Information.

2.3. Topological Edge States

One of the most important signatures of QSH systems is the counter-propagating helical edge states. The electronic band structures with edge states projected on the (100) and (010) surface, are shown in Figure 3a,b, respectively. The topologically protected helical edge states connecting the conduction and valence band are observed on both edges. The band structures of both edges are qualitatively different, the Dirac cone is buried in the bulk of the (100) edge whereas the Dirac cone is in the bulk gap in the (010) edge. The significant electron-hole asymmetry that exists in the material is responsible for the surface-dependent edge band structure. The associated spin-projected edge band structures are shown in the bottom panels. The different spin channels are indicated with different colors i.e., spin-up in red and spin-down in blue, respectively. The 1T'-MoGe$_2$P$_4$ is a QSH
between 1.3 e and, we have calculated the Z2 invariant with the Wannier of the bandstructure. The SOC creates anticrossing gaps along Γ band, the distribution of the and spin Berry curvature distribution. We turn our discussion toward the spin Hall conductivity (SHC) formation. Other members of the family is described in the Supporting Information induced by an external out-of-plane electric field. Increases in the spin Hall conductivity is directly proportional to the integration of the SBC, it leads to a large SHC of the s_y as shown in Figure 4b, the value of SHC is quantized in the gap to a value of 1.0 e/h, while for the other compounds is between 1.3 e/h and 1.6 e/h (see Supporting Information). The ideal value of the quantized SHC is 2 e/h, however, deviations can occur due to the non-conservation of the z-component of the spin angular momentum, thanks to effects such as large spin-orbit, crystal field, and hybridization. We have bismuthene and jactingaite with an inverted band gap of 0.8 and 0.5 eV, respectively.[58,59] The critical electric force field for MoGe2P4 is lower than the values of bismuthene and jactingaite for which the critical electric force fields are 0.82 and 0.50 eVÅ⁻¹, respectively.[60,61] Even among the large gap QSH transition metal dichalcogenides, MoGe2P4 has the lowest value since the values of the critical force fields are 0.142 and 0.187 eVÅ⁻¹ for WTe2 and MoSi2P4, respectively.[50,62]

2.5. Electric Field Induced Topological Phase Transition

In this subsection, we show the appearance of a phase transition induced by an external out-of-plane electric field. Increases in the vertical electric field (E), the bandgap starts to reduce and reaches zero at a critical electric force field (qE_c = ±0.077) eVÅ⁻¹, further increases in the electric field reopens the trivial gap. The topological phase transition from non-trivial (Z_2 = 1) to trivial (Z_2 = 0) via the application of out-of-plane electric field E is demonstrated in Figure 5. A similar trend can be observed when the polarity of the electric field is reversed. The vertical electric field on 1T′-MoGe2Z4 compounds produces a charge imbalance between the GeZ sides, which changes the on-site potentials. Figure 6a shows the band structure in the absence of the electric field, the bands are double degenerate as the system preserves both time-reversal symmetry and inversion symmetry. On the other hand, when the electric field is applied, the degeneracy of the bands is lifted showing a strong Rashba spin-splitting around the bandgap due to the broken inversion symmetry (see Figure 6b,c)). We noticed that the bandgap decreases successively with the electric field and becomes zero at a critical electric force field qE_c=0.077 eVÅ⁻¹ as shown in Figure 6b. A further increase in the electric field opens up the band gap again as shown in Figure 6c, leading to the trivial insulating phase. This phenomenon is quite similar to the 1T′-phase of TMDs. Indeed, both the low energy Hamiltonian and the Rashba expression under an electric field have the same group symmetries of the 1T′-phase of TMDs. Furthermore, an analysis based on Z2 invariant and edge-state dispersion (see Figure 6) shows that the band closing drives a topological phase transition to a trivial state with Z2 = 0. This topological phase transition destroys the helical edge states by switching off the QSH state of the 1T′-MoGe2Z4. Such a tunability of the charge/spin conductance of the helical edge state can be used as electrical control of an ON/OFF switch that could lead to a QSH-based device. Our results predict that the switching from the QSH state to the trivial one can be achieved in the MoGe2P4 at a low electric field force of 0.077 eVÅ⁻¹. This low value of the critical electric field force allows a fast switching and we are going to compare it with the same quantity of other large gap QSH insulators. Among systems with large QSH gap, we have bismuthene and jactingaite with an inverted band gap of 0.8 and 0.5 eV, respectively.[58,59] The critical electric force field for MoGe2P4 is lower than the values of bismuthene and jactingaite for which the critical electric force fields are 0.82 and 0.50 eVÅ⁻¹, respectively.[60,61] Even among the large gap QSH transition metal dichalcogenides, MoGe2P4 has the lowest value since the values of the critical force fields are 0.142 and 0.187 eVÅ⁻¹ for WTe2 and MoSi2P4, respectively.[50,62]

Since the crystal symmetries of the 1T′-MoGe2Z4 materials are the same as the 1T′-WTe2, the devices conceived for the WTe2 can be proposed for the MoGe2Z4 materials too with the advantage of a larger inverted gap. One possible application is the realization of the topological transistor, where the interface with a wide gap insulator bearing a small lattice mismatch is needed to protect the helical edge channels from being gapped by the interlayer hybridization. Due to the difference in lattice constant with respect to WTe2, we propose h-BN and CoBr2 as suitable wide gap insulators, which bear comparable lattice constants.
Figure 4. a) Top panel. \( k \)-resolved spin Berry curvature (SBC) projected on the electronic band structure. It can be seen that SBC is maximum at the avoiding crossing at the Fermi level along the \( \Gamma - Y \) direction. \( \Omega^+ \) and \( \Omega^- \) represent the maximum and the minimum of the SBC, respectively. Bottom panel \( k \)-resolved spin Berry curvature in logarithmic scale (LBC). b) Intrinsic spin Hall conductivity in units of \( \frac{e^2}{h} \) for \( 1T' \)-MoGe\(_2\)P\(_4\) within the vdW functional. The Fermi level is set to zero.

Figure 5. Topological nature (\( Z_2 \)) and bandgap of \( 1T' \)-MoGe\(_2\)P\(_4\) as a function of the applied out-of-plane electric field. The critical electric fields \( qE_c = \pm 0.077 \text{ eVÅ}^{-1} \) are marked with vertical dashed lines.

Our results indicate that the \( 1T' \)-phase can be stabilized in the MgGe\(_2\)Z\(_4\) family, introducing the band inversion at \( \Gamma \) with consequent topological phases. Respect to other members of the family, these Ge-based compounds show superior properties as a better stability of the \( 1T' \)-phase and larger gaps. Indeed, the \( 1T' \)-phase of WGe\(_2\)As\(_2\) is stable with an inverted bandgap of 237 meV within HSE. Therefore, these Ge-based compounds have the largest inverted gap among the existing \( 1T' \)-phases of TMDs and MSi\(_2\)Z\(_4\) hosting QSH phases. The large spin Berry curvature around the spin-orbit induced anticrossing gap with an inverted bandgap leads to a quantized SHC. The MoGe\(_2\)P\(_4\) compound shows a perfect quantization of SHC in the bandgap with a value of 1.0\( \frac{e^2}{h} \). We have illustrated the electric field-driven topological phase transition i.e., QSH insulator to a trivial insulator phase with Rashba-like splitting. Our results suggest that fast switching from the QSH state to the trivial one can be achieved in the MoGe\(_2\)P\(_4\) at an electric force field of 0.077 eVÅ\(^{-1}\) that is lower with respect to the same property of other QSH systems with a large inverted bandgap. The faster switching with respect to the MoSi\(_2\)P\(_4\) compound is attributed to a weaker electronegativity of the Ge atoms on the external layers, therefore, the electric field acts on the Mo-states more efficiently. The appearance of both large inverted bandgap and fast electric switching from non-trivial to trivial phases in these Ge-based compounds could be very promising in designing room-temperature topological field-effect transistors.

4. Experimental Section

Electronic structure calculations were performed within the framework of density functional theory using the projector augmented wave method using the VASP package.\(^{[63]}\) The relativistic effects were considered self-consistently. A plane-wave energy cut-off of 500 eV was used. We used optPBE-vdW functional to consider exchange-correlation effects.\(^{[64]}\) Both the atomic positions and lattice parameters were optimized until the residual forces on each atom were less than 0.001 eVÅ\(^{-1}\) and the total energy was converged to \( 10^{-8} \text{ eV} \) with a Gaussian-smearing method. For a more accurate estimation of the band order and the bandgap, it employed HSE06 hybrid functional with 25% of the exact exchange. This study performed the calculations using a 6\( \times \)12\( \times \)1 \( \Gamma \) centered \( k \)-mesh with 72 \( k \)-points in the Brillouin zone. The dynamical stability had been checked within the density functional perturbation theory framework using PHONOPY\(^{[65]}\) code and the ab initio molecular dynamics simulations \(^{[66]}\) were performed using 2\( \times \)4\( \times \)1 supercell. It extracted the real space tight-binding Hamiltonian for calculated topological properties and electric field effect using the Wanniertools package.\(^{[67]}\) The Wannier functions were generated using M-d, Ge-s, and p, and Z-p orbitals within VASP2WANNIER.\(^{[68]}\) The electronic properties with the external electric field were computed using the recent version of wanniertools. The surface energy spectrum was obtained within the iterative Green’s function method.\(^{[69]}\)

This study obtain the SHC \( \sigma^z_{xy} \) using the Kubo formula.\(^{[70–74]}\)

\[
\sigma^z_{xy} = -\frac{e^2}{V N_k \hbar} \sum_k \Omega^z_{xy}(k)
\]

where,

\[
\Omega^z_{xy}(k) = \sum_{\alpha} f(E_{\alpha k}) \Omega^z_{\alpha \alpha}(k)
\]

\( Z = \text{P or As} \). Our results indicate that the \( 1T' \)-phase can be stabilized in the MgGe\(_2\)Z\(_4\) family, introducing the band inversion at \( \Gamma \) with consequent topological phases. Respect to other members of the family, these Ge-based compounds show superior properties as a better stability of the \( 1T' \)-phase and larger gaps. Indeed, the \( 1T' \)-phase of WGe\(_2\)As\(_2\) is stable with an inverted bandgap of 237 meV within HSE. Therefore, these Ge-based compounds have the largest inverted gap among the existing \( 1T' \)-phases of TMDs and MSi\(_2\)Z\(_4\) hosting QSH phases. The large spin Berry curvature around the spin-orbit induced anticrossing gap with an inverted bandgap leads to a quantized SHC. The MoGe\(_2\)P\(_4\) compound shows a perfect quantization of SHC in the bandgap with a value of 1.0\( \frac{e^2}{h} \). We have illustrated the electric field-driven topological phase transition i.e., QSH insulator to a trivial insulator phase with Rashba-like splitting. Our results suggest that fast switching from the QSH state to the trivial one can be achieved in the MoGe\(_2\)P\(_4\) at an electric force field of 0.077 eVÅ\(^{-1}\) that is lower with respect to the same property of other QSH systems with a large inverted bandgap. The faster switching with respect to the MoSi\(_2\)P\(_4\) compound is attributed to a weaker electronegativity of the Ge atoms on the external layers, therefore, the electric field acts on the Mo-states more efficiently. The appearance of both large inverted bandgap and fast electric switching from non-trivial to trivial phases in these Ge-based compounds could be very promising in designing room-temperature topological field-effect transistors.

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Figure 6. Electronic band structure band of the 1T'-MoGe₂P₄ monolayer at different values of the out-of-plane electric force field qE equal to a) 0, b) 0.077, and c) 0.16 eVÅ⁻¹. The corresponding helical edge states with spin polarization for the (010) edge are shown in the middle and bottom panels, respectively.

is the k-resolved spin Berry curvature and

\[ \Omega^{xy}_{n,k}(k) = \hbar^2 \sum_{m \neq n} -2Im \langle nk | j_z | mk \rangle \langle mk | \hat{v}_y | nk \rangle \]  

(3)

is the k- and band-resolved spin Berry curvature. In Equation from (1) to (3), \( N_k \) is the number of k-points in the BZ and \( \langle nk \rangle \) denotes the Bloch state with energy \( E_n \) and occupation \( f(E_n) \). The SHC \( \sigma^{xy}_{\tau} \) represents the spin-current along the x-direction generated by the electric field along the y-direction, and the spin current was polarized along the z-direction. This study had used a dense k-grid of 100 × 100 × 100 for the spin Berry curvature and SHC, therefore \( N_k = 100 \).

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

2D materials, DFT, quantum spin Hall insulators, topological field-effect transistors
[66] R. N. Barnett, U. Landman, *Phys. Rev. B* **1993**, 48, 2081.
[67] Q. Wu, S. Zhang, H.-F. Song, M. Troyer, A. A. Soluyanov, *Comput. Phys. Commun.* **2018**, 224, 405.
[68] A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt, N. Marzari, *Comput. Phys. Commun.* **2008**, 178, 685.
[69] M. P. L. Sancho, J. M. L. Sancho, J. M. L. Sancho, J. Rubio, *J. Phys. F: Met. Phys.* **1985**, 15, 851.
[70] Y. Sun, Y. Zhang, C. Felser, B. Yan, *Phys. Rev. Lett.* **2016**, 117, 146403.
[71] L. Matthes, S. Küfner, J. Furthmüller, F. Bechstedt, *Phys. Rev. B* **2016**, 94, 085410.
[72] R. Zhang, C.-Y. Huang, J. Kidd, R. S. Markiewicz, H. Lin, A. Bansil, B. Singh, *J. Sun, Phys. Rev. B* **2022**, 105, 165140.
[73] J. Zhou, J. Qiao, A. Bournel, W. Zhao, *Phys. Rev. B* **2019**, 99, 060408.
[74] J. Qiao, J. Zhou, Z. Yuan, W. Zhao, *Phys. Rev. B* **2018**, 98, 214402.