Time-reversal symmetry broken quantum spin Hall phase in the van der Waals heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$

Xiaoliang Xiao$^1$, Fangyang Zhan$^1$, Weixiang Kong$^1$, Jing Fan$^2$, Rui Wang$^{1,3,4}$ and Xiaozhi Wu$^{1,3,*}$

$^1$ Institute for Structure and Function and Department of Physics, Chongqing University, Chongqing 401331, People’s Republic of China
$^2$ Center for Computational Science and Engineering, Southern University of Science and Technology, Shenzhen 518055, People’s Republic of China
$^3$ Chongqing Key Laboratory for Strongly Coupled Physics, Chongqing 401331, People’s Republic of China
$^4$ Center of Quantum Materials and devices, Chongqing University, Chongqing 401331, People’s Republic of China

* Author to whom any correspondence should be addressed.
E-mail: xiaozhiwu@cqu.edu.cn

Abstract
The topological phases with time-reversal symmetry (TRS) breaking have always attracted intense studies due to their potential applications to spintronics. The previous studies mainly focused on the exploration of quantum anomalous Hall effects, but another typical TRS-broken two-dimensional topological phase, i.e., the TRS-broken quantum spin Hall (QSH) effect, has rarely been proposed in realistic materials. Here, based on first-principles calculations and topology analysis, we show that the van der Waals heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$ can realize the robust TRS-broken QSH state. We utilize the topological edge states and spin Hall conductance, which can be measured in experiments directly, to confirm the appearance of TRS-broken QSH phase. Moreover, we uncover that the built-in electric field is essential to realize such topological state and an external electric field can effectively tune the nontrivial band gap. Our findings not only provide a reliable candidate to obtain the TRS-broken QSH phase with a high tunability but also can facilitate further applications to topological quantum transport.

1. Introduction
The investigation of the topological phase of matter has been a major subject in condensed matter physics as well as material science [1–4]. Among various topological phases, one of the most important members is the time-reversal invariant topological insulators (TIs) with a $\mathbb{Z}_2$ index, which were first predicted in two-dimensional (2D) graphene [5, 6] and HgTe quantum well [7], and experimentally confirmed soon in the latter [8]. The 2D TIs accompanied by the time-reversal symmetry (TRS) are also termed as the quantum spin Hall (QSH) insulators. The TRS is considered to be a prerequisite to the emergence of QSH states. Nevertheless, perturbations that break the TRS in realistic environments usually occur. In the absence of TRS, two typical spin-polarized insulating phases have been identified to host nontrivial band topology [9–11]. The one is the quantum anomalous Hall (QAH) insulator and the other is the TRS-broken QSH insulator. In the case of TRS-broken QSH insulator, the chiral gapless edge states are replaced by the helical gapped edge states where two spin channels are mixed. The previous investigation demonstrated that the competitions between the QAH and TRS-broken QSH phases were dependent on the interplay of Rashba spin–orbit coupling (SOC) and magnetic exchange energy [9]. Usually, the appearance of appropriate magnetic exchange fields and the strength of Rashba SOC in realistic materials is difficult. Hence, the material with the TRS-broken QSH state has been rarely reported in literature.

As mentioned above, a possible avenue for realizing the TRS-broken QSH phase is the design of a system that combines the magnetism and moderate strength of Rashba SOC. The introduction of magnetic doping [12, 13] or magnetic exchange fields [14, 15] can remove the TRS. Meanwhile, the systems with inversion...
symmetry breaking can induce built-in electric field and thereby realize the Rashba SOC [16]. Considering that the magnetic doping for realizing the TRS-broken QSH phase is difficult to control, we propose to use intrinsic magnetic materials to realize the TRS-broken QSH phase. Accordingly, building a van der Waals (vdW) heterostructure, which integrates intrinsic magnetism and topological features, is a reliable strategy. More importantly, the vdW heterostructures can spontaneously emerge the Rashba SOC from its structural asymmetry.

With improvements of the growth technology for 2D ferromagnetic (FM) semiconductors, some intrinsically magnetic vdW layered materials have been fabricated experimentally, such as magnetic TIs MnBi₂Te₄, CH₃, and Cr₂Ge₂Te₆ etc [17–21]. Moreover, several 2D vdW heterostructures with intrinsic magnetism are predicted to host band topology driven by magnetic proximity effects [22–25]. For instance, the QAH effects have been realized in Mn–Bi–Te superlattices MnBi₂Te₄/(Bi₂Te₃)ₙ (n = 0, 1, 2, 3, . . . ), graphene/Cr₂Ge₂Te₆, graphene/CrI₃, germanene/Cr₂Ge₂Te₆ [26–35]. Notice that the previous studies of magnetic vdW heterostructures mainly focus on the QAH phases. In contrast, there are a few TRS-broken QSH phases proposed in the FM order vdW heterostructures [36, 37]. Therefore, the design of promising vdW heterostructures with TRS-broken QSH phase is highly desired.

In this work, based on first-principles calculations and topology analysis, we demonstrate that the vdW heterostructure ZrTe₅/Cr₂Ge₂Te₆ can achieve the TRS-broken QSH state. ZrTe₅ is a well-known TRS-protected QSH insulator, which is a monolayer composed of Zr and Te atoms in a 2D square lattice with a zigzag chain geometry. Cr₂Ge₂Te₆ is the ideal basis for designing 2D vdW heterostructures with a FM order since its semiconducting feature does not intertwine with nontrivial bands near the Fermi level. By using first-principles calculations, we show the vdW heterostructure ZrTe₅/Cr₂Ge₂Te₆ with the out-of-plane FM order. We utilize the topological edge states (TESs) and spin Hall conductance (SHC), which can be measured in experiments directly, to confirm the TRS-broken QSH state. Moreover, we reveal that the nontrivial gap can be tunable through the introduction of external electric fields.

2. Methods

The calculations for electronic structures and topological properties of the vdW heterostructure ZrTe₅/Cr₂Ge₂Te₆ were performed using first-principles calculations based on the density functional theory (DFT) [38, 39], which were implemented in the Vienna ab initio simulation package [40, 41]. We used the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) formalism to describe the exchange–correlation functional [42]. The electron–ion interaction was treated by projector-augmented-wave potentials [43]. The kinetic energy cutoff of the plane-wave was set to be 400 eV, and the first Brillouin zone (BZ) was evaluated with a 9 × 9 × 1Γ-centered k mesh [44]. The structure were relaxed until the convergence threshold of maximum forces on each atom were be less than 0.01 eV Å⁻¹, and the criterion of total energy for convergence was set as 10⁻⁶ eV, which given rise to good convergence. For the 3D electrons of transition metals in the Cr₂Ge₂Te₆ layer, we employed the GGA + U scheme [45] and introduced an on-site Coulomb repulsive interaction of Cr-3D with a typical value of 1.0 eV [21, 34, 46]. The vacuum layer along the z direction was 20 Å thick to ensure decoupling between neighboring layers. The DFT-D3 method was used to correct the vdW interaction [47]. The effects of applying external electric fields normal to the vdW heterostructure ZrTe₅/Cr₂Ge₂Te₆ were directly included in DFT calculations. We constructed a tight-binding Hamiltonian based on maximally localized Wannier tools code [57].

The Kubo formula for SHC has the expression [52–54]

$$\sigma_{xy} = \frac{e}{(2\pi)^2} \int \Omega_{xy}(k)dk,$$

where \(\Omega_{xy}(k)\) is the \(k\)-resolved term, which is given by

$$\Omega_{xy}(k) = -\sum \int_{n} f_{nk} \Omega_{n,xy}(k),$$

where \(f_{nk}\) is the Fermi–Dirac distribution function and \(\Omega_{n,xy}(k)\) is the band-projected spin Berry curvature given as

$$\Omega_{n,xy}(k) = \sum_{m \neq n} 2 \text{Im} \left[ \frac{\langle u_{nk}| \hat{P}_{xy} | u_{mk} \rangle \langle u_{mk} | \hat{P}_{xy} | u_{nk} \rangle}{(\varepsilon_{nk} - \varepsilon_{mk})^2} \right],$$
Figure 1. (a) Top and (b), (c) side views of the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$ with the vdW-type interaction distance (vdW gap), which is composed by $p(3 \times 1)R90^\circ$ convention cells of single-layer ZrTe$_5$ and $p(2 \times \sqrt{3})$ unit cells of single-layer Cr$_2$Ge$_2$Te$_6$. (d) The variation of the free energy with 6 ps for the vdW heterostructure. AIMD simulation is carried with a unit cell of the vdW heterostructure under 300 K. The inset is the snapshot taken from the end of AIMD calculation and neither broken bonds nor structure reconstruction occur during the whole time interval.

where $\mathbf{j}_z = \frac{1}{2}\{s_z, \nu_y\}$ is the spin current operator, $\nu_y = \frac{1}{\hbar}\frac{\partial H(k)}{\partial k_y}$ is the velocity operator, $|u_{nk}\rangle$ is the wave function of energy $\varepsilon_{nk}$, and $\sigma_{xy}^s$ represents $xy$-plane SHC. According to the definitions of the Chern number ($C$) and spin Chern number ($C^s$), one has

$$C = C_\uparrow + C_\downarrow = \frac{1}{2}(C_\uparrow - C_\downarrow). \quad (4)$$

The SHC $\sigma_{xy}^s$ can be expressed as

$$\sigma_{xy}^s = \frac{e}{2\pi} C^s = \frac{e}{4\pi}(C_\uparrow - C_\downarrow), \quad (5)$$

where $C_\uparrow$ and $C_\downarrow$ are Chern numbers of the spin up and spin down channels.

### 3. Results and discussion

As inserted in figures 1(a)–(c), we show the top and side views of the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$, respectively, which is constructed by stacking the top ZrTe$_5$ monolayer and bottom Cr$_2$Ge$_2$Te$_6$ monolayer along the $z$ direction. The top ZrTe$_5$ monolayer is $p(3 \times 1)R90^\circ$ convention cells of single-layer ZrTe$_5$ and bottom Cr$_2$Ge$_2$Te$_6$ monolayer is $p(2 \times \sqrt{3})$ unit cells of single-layer Cr$_2$Ge$_2$Te$_6$. The optimized lattice constants are $|a| = 4.04$ Å and $|b| = 13.82$ Å for a convention cell of single-layer ZrTe$_5$, and $|a| = |b| = 6.93$ Å for a unit cell of single-layer Cr$_2$Ge$_2$Te$_6$, which agree well with previous publications [21, 34, 58, 59]. The lattice misfit between the $p(3 \times 1)R90^\circ$ ZrTe$_5$ and $p(2 \times \sqrt{3})$ Cr$_2$Ge$_2$Te$_6$ layers is less than 1%, so the influences on band structure are almost negligible. To obtain the equilibrium geometry structure of the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$, we optimize the compositive structure starting from the stacking configuration. The optimized equilibrium distance is 3.29 Å ($d_0 = 3.29$ Å) with the vdW-type interaction distance (vdW gap).
To study the energetic stability of the equilibrium geometry structure of the vdW heterostructure, the binding energy is calculated by using the following formula $E_b = (E_{\text{total}} - E_{\text{ZrTe}_5} - E_{\text{Cr}_2\text{Ge}_2\text{Te}_6})$, where $E_{\text{total}}$, $E_{\text{ZrTe}_5}$, and $E_{\text{Cr}_2\text{Ge}_2\text{Te}_6}$ represent the total energies of the isolated vdW heterostructure $\text{ZrTe}_5/\text{Cr}_2\text{Ge}_2\text{Te}_6$, isolated $\text{ZrTe}_5$ monolayer, and $\text{Cr}_2\text{Ge}_2\text{Te}_6$ monolayer, respectively. It is worth noting that the DFT + vdW functional method is only used for the total energy of the vdW heterostructure $\text{ZrTe}_5/\text{Cr}_2\text{Ge}_2\text{Te}_6$, while the total energies of $\text{ZrTe}_5$ and $\text{Cr}_2\text{Ge}_2\text{Te}_6$ monolayers are calculated via applying the DFT method. The calculated binding energy is $-1170.4$ meV. The negative value indicates that the vdW heterostructure is energetically stable. At the same time, we also use the density-functional-based $ab\ initio$ molecular dynamics (AIMD) simulations to evaluate the thermodynamical stability. We use the $1 \times 1 \times 1$ cell of the vdW heterostructure $\text{ZrTe}_5/\text{Cr}_2\text{Ge}_2\text{Te}_6$ to perform the AIMD simulations, including 8 Cr atoms, 8 Ge atoms, 6 Zr atoms and 56 Te atoms in total. There is no obvious structure deformation and broken bonds at 6 ps with $T = 300$ K, which also suggests that the vdW heterostructure is thermally stable (see details in figure 1(d)). Because the heterostructure is so large and the two of them can be synthesized experimentally, we don’t calculate phonon spectrum.

The electronic band structure of the pristine $p(3 \times 1)$ single-layer $\text{ZrTe}_5$ within SOC is shown in figure 2(a). Due to the two basic vectors $a$ and $b$ swapped, the bands at the high-symmetry points $X$ and $Y$ also have exchanged, it does not depend on whether there is SOC or not. Without SOC, the single-layer $\text{ZrTe}_5$ is a semimetal with one band crossing along the $\Gamma$–$Y$ direction, implying the existence of band inversion around $\Gamma$–$Y$ [58]. When the SOC effect is present, the band gap opens. Hence, the $\text{ZrTe}_5$ develops into an insulator with a large indirect band gap of $\sim104$ meV. It has been investigated that the $\text{ZrTe}_5$ is a nontrivial QSH insulator with the $\mathbb{Z}_2$ topological invariant [5, 6], which agrees well with the previous result [58]. The spin-polarized electronic band structure of the $p(2 \times \sqrt{3})$ $\text{Cr}_2\text{Ge}_2\text{Te}_6$ monolayer in the presence of SOC is depicted in figure 2(b). Our DFT calculations on the electronic properties indicate that the $p(2 \times \sqrt{3})$ $\text{Cr}_2\text{Ge}_2\text{Te}_6$ monolayer possesses a FM groundstate with a saturation magnetic moment of $\sim23.98$ $\mu_B$, which is consistent with previous studies ($\sim3$ $\mu_B$ per atom) [21, 34]. We can see that the...
Figure 2. (a) The electronic band structure of $p(3 \times 1)$ ZrTe$_5$ monolayer with SOC. (b) The electronic band structure of $p(2 \times \sqrt{3})$ Cr$_2$Ge$_2$Te$_6$ monolayer in the presence of SOC. (c) The spin-polarized electronic band structure of the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$ in the absence of SOC with electric field strength of $-0.1$ V Å$^{-1}$. The blue and red lines represent the majority and minority spin channels, respectively. (d) The orbital-resolved electronic band structures of the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$ with the out-of-plane magnetization along high-symmetry paths $Y$–$\Gamma$–$X$–$M$–$\Gamma$ in the presence SOC by applying electric field strength of $-0.1$ V Å$^{-1}$, blue and red weight with the respective contribution ZrTe$_5$ layer and Cr$_2$Ge$_2$Te$_6$ layer. The inset is the enlarged views with SOC at the $\Gamma$ point.

valence-band maximum (VBM) is located at the $\Gamma$ point and conduction-band minimum (CBM) is slightly away from the $\Gamma$ point, exhibiting an indirect gap of $\sim 216$ meV.

For the vdW heterostructure, the results show a unit cell of the vdW system has a saturation magnetic moment of $\sim 23.97$ $\mu_B$ for Cr$_2$Ge$_2$Te$_6$ layer, which is slightly smaller than the pristine $p(2 \times \sqrt{3})$ Cr$_2$Ge$_2$Te$_6$ monolayer of $\sim 23.98$ $\mu_B$. The Cr$_2$Ge$_2$Te$_6$ layer partially magnetizes the ZrTe$_5$ layer and the magnetic moment of each Te atom of the bottom Te in the ZrTe$_5$ layer is $\sim 0.001$ $\mu_B$. In figure 2(c), we can see the spin-polarized electronic band structure along high-symmetry paths $Y$–$\Gamma$–$X$–$M$–$\Gamma$. In the case without SOC, the system is a semimetal with the bands crossing along the $\Gamma$–$Y$ direction and near the Fermi level ($E_F$) are mostly contributed by the majority-spin channel.

With consideration of SOC, the coupling between the spin and orbital sectors leads to spontaneous magnetization. Hence, we have carried out total-energy calculations with different magnetic configurations, rotating the magnetization directions from out-of-plane to in-plane as well as in-plane magnetization with different directions. The magnetic anisotropy energy (MAE = 0.89 meV) is calculated by MAE = $E_{100} - E_{001}$. This result confirms that the easy axis is perpendicular to the 2D plane, which agrees well with the magnetic groundstate properties of Cr$_2$Ge$_2$Te$_6$ in experiments [21]. In figure 2(d), we illustrate the orbital-resolved electronic band structures along high-symmetry paths $Y$–$\Gamma$–$X$–$M$–$\Gamma$ with magnetization perpendicular to the 2D plane. The figures show that the vdW heterostructure converts into a insulator with a band gap of $\sim 45$ meV. It is worth noting that this band gap is smaller than that of ZrTe$_5$ or Cr$_2$Ge$_2$Te$_6$ monolayer. Since the VBM and CBM are completely contributed by the ZrTe$_5$ layer and Cr$_2$Ge$_2$Te$_6$ layer, respectively. To investigate the impact of Cr$_2$Ge$_2$Te$_6$ layer for ZrTe$_5$ layer, we plot the enlarged view of band structures around the $\Gamma$ point in the inset of figure 2(d). We can see that the FM order from the magnetic substrate Cr$_2$Ge$_2$Te$_6$ makes the bands of ZrTe$_5$ layer in the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$ lift the spin degeneracy. Moreover, it is found that the obvious Rashba SOC effect is present at the $M$ point (see figures 2(a) and (d)). This is due to the structural asymmetry of the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$.

In this case, the Cr$_2$Ge$_2$Te$_6$ layer only acts as the magnetic substrate material. This is similar to Mn$_4$Bi$_4$Te$_7$ system [27], Cr atoms only provide the intrinsic magnetism which can break the TRS. To determine whether such the system belongs to QAH or TRS-broken QSH insulator, we calculated local
density of states (LDOS) of a semi-infinite ribbon of the vdW heterostructure, as shown in figure 3(a). To understand the TESs more clearly, the schematic band structures are plotted in figure 3(b). It is visible that the TESs are gapped gap where two spin channels are mixed, which is different from a conventional QSH (or QAH) system with the helical (or chiral) gapless TESs. In addition, we calculated evolution of Wannier charge centers of the vdW system in the full closed plane of $k_z = 0$ using the Wilson loop method [60] and the anomalous Hall conductance $\sigma_{xy}$ [49], and the results confirm that $C = 0$ and $\sigma_{xy} = 0$. Hence, the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$ does not belong to the QAH insulator but the TRS-broken QSH insulator. The calculated $\sigma_{xy}$ is shown in figure 3(c), illustrated as the blue lines. This can clearly see that the value of $\sigma_{xy}$ is exactly quantized to $-\frac{2e^4}{4\pi}$ inside the nontrivial band gap, which is contributed from the spin Berry curvature $\Omega_{xy}^{\tau}(k)$ over the states below the Fermi level ($E_F$). These indicate that band topology of the FM vdW heterostructure is indeed described by the nonzero spin Chern numbers $C$. It is worth noting that the TRS-broken QSH insulator and the conventional QSH insulator with a $Z_2$ index belong the different topological classification.

In addition, due to the structural asymmetry and interlayer hybridization of the vdW heterostructure, we can see that the built-in electric field ($\Delta V$) is present between ZrTe$_5$ and Cr$_2$Ge$_2$Te$_6$ layers. In figure 3(d), the red (blue) line represents the electrostatic potential without (with) an external electric field $E$, whose strength is set to 0.1 V Å$^{-1}$. Here, the electric field $E$ with its positive direction along $z$ axis is normal to the atomic plane of ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$. It is found that a positive external electric field $E$ can effectively enhance the $\Delta V$ from 0.19 to 1.47 eV. As is well-known, the strength of Rashba SOC ($V_R$) is related to the gradient of $\Delta V$, it is quite vital for the FM vdW heterostructure to achieve the TRS-broken QSH phase. Thus the nontrivial band gap can be tuned by applying the external electric field $E$ (or changing interlayer distance $d$) (see figures 4(a) and (b)). We schematically illustrate the band gap as a function of $E$ or $\delta d = d - d_0$ in figure 4(c). It is found that the energies of ZrTe$_5$ layer is decreased monotonously with the $E$ increased and that are quite contrary for Cr$_2$Ge$_2$Te$_6$ layer. Overall, the increased monotonously electric field $E$ enlarges the nontrivial band gap. On the contrary to the external electric field $E$, changing interaction distance $d$ (vdW gap) has little effects on the nontrivial band gap and makes only bands of Cr$_2$Ge$_2$Te$_6$ layer split bigger (see figure 4(b)). As shown in figure 4(a), we can find that the band inversion at the $\Gamma$ point is still preserved when the electric field strength increases to 0.2 V Å$^{-1}$. In this case, the nontrivial band gap can be considerable up to $\sim$98.70 meV (see figure 4(c)). That is to say, applying external electric field $E$ (or changing interlayer distance $d$) in the physical regime does not change band topology of the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$.

In order to insightfully understand the physical phenomenon that the QSH state can exist in TRS-broken system, we begin with the theory of the spin Chern number. Generally speaking, the QSH phase is considered to be closely related to the TRS which provides a protection for the edge states and the $Z_2$ invariant [5, 6]. There is a doubt that whether the systems can have QSH-like phase or not when the TRS is broken. It is reported the QAH phase can be realized in graphene by introducing Rashba SOC and an exchange field [11]. Furthermore, Prodan redefines the spin Chern number in the thermodynamic limit
through band projection without using any boundary conditions [61], and Xing et al suggest that the competitions between the QAHE and TRS-broken QSH phases are dependent on the relation of Rashba SOC and magnetic exchange energy [9]. In other words, as long as the systems satisfy the finite magnetic exchange fields strength $g$, including intrinsic and external magnetic exchange energy, is below the critical value of magnetic exchange fields $g_c$ ($0 < g < g_c$) and Rashba SOC with coupling strength $V_R$ is less than intrinsic SOC with coupling strength $V_{SO}$ ($0 < V_R < V_{SO}$), the systems belong a topological class of the TRS-broken QSH phase. Usually, the appearance of appropriate magnetic exchange fields and the strength of Rashba SOC in realistic materials is difficult. However, in fact, the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$ satisfies exactly this condition, thus it should be the TRS-broken QSH phase. For the TRS-broken QSH state, although there is usually a weak scattering between forward and backward movers, as evidenced by the small energy gap in the edge states spectrum, leading to a low-dissipation spin transport, it still has a quantized conductance platform. This means that it is more slightly resistant to magnetic scattering than a conventional QSH system.

There are several methods to gain the realistic materials with the TRS-broken. However, the needful requirement is that the finite magnetic exchange filed induced by intrinsic magnetization is smaller than the critical magnetic field ($g < g_c$). Firstly, it can exist in a intrinsic magnetic topological system with $V_R < V_{SO}$. Secondly, we naturally take into consideration two magnetic materials to construct the vdW heterojunction. The vdW heterostructures can spontaneously emerge the Rashba SOC from its structural asymmetry. Thirdly, we can also search for one magnetic and another non-magnetic materials. For example, the magnetic TIs with the non-magnetic normal insulators (NIs) or the magnetic NIs with the non-magnetic TIs built the vdW system.

4. Conclusions

In conclusion, based on first-principles calculations and topology analysis, we theoretically demonstrate the emergence of the TRS-broken QSH state in the vdW heterostructure ZrTe$_5$/Cr$_2$Ge$_2$Te$_6$ characterized by the gapped TESs and quantized SHC $\sigma^x_{xy}$ with the nonzero spin Chern number $C^s = -1$. It is important that these can be measured in experiments directly to confirm the appearance of the TRS-broken QSH phase. Moreover, we uncover that the built-in electric field is essential to realize such topological state and an external electric field $E$ can effectively tune the nontrivial band gap. Our findings not only provide a reliable candidate to obtain the TRS-broken QSH phase with a high tunability but also can facilitate further applications to topological quantum transport. Besides, our results greatly enrich the physics and expand the domain of magnetic topological phase, which are expected to draw immediate experimental attention.

Acknowledgments

This work was supported in part by the Natural Science Foundation of China under Grant No. 12174040 and No. 12147102, and Chongqing Natural Science Foundation under Grant No. cstc2020jcyj-msxmX0118.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

ORCID iDs

Rui Wang https://orcid.org/0000-0002-5063-5691

References

[1] Haldane F D M 1988 Phys. Rev. Lett. 61 2015–8
[2] Thouless D J, Kohmoto M, Nightingale M P and den Nijs M 1982 Phys. Rev. Lett. 49 405–8
[3] Hasan M Z and Kane C L 2010 Rev. Mod. Phys. 82 3045–67
[4] Qi X L and Zhang S C 2011 Rev. Mod. Phys. 83 1057–110
[5] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 226801
[6] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 146602
[7] Bernevig B A, Hughes T L and Zhang S C 2006 Science 314 1757
[8] Wiedmann M K S, Brune C, Roth A, Buhmann H, Molenkamp L W, Qi X L and Zhang S C 2007 Science 318 766
[9] Yang Y, Xu Z, Sheng L, Wang B, Xing D Y and Sheng D N 2011 Phys. Rev. Lett. 107 066602
et al. 2020 Nat. Commun. 11 97
[19] Liu C et al. 2020 Sci. Adv. eaax9989
[20] Shi M Z, Lei B, Zhu C S, Ma D H, Cui J H, Sun Z L, Ying J J and Chen X H 2019 Phys. Rev. 041039
[21] Gong C et al. 2019 Sci. Adv. eaaw1874
[22] Vidal R C et al. 2019 Phys. Rev. 125327
[23] Mogi M et al. 2019 Phys. Rev. 021017
[24] Hou Y, Kim J and Wu R 2019 Phys. Rev. 17953–79
[25] Tow G, Yu H, Zhu Q, Wang Y, Xu X and Yao W 2016 Nat. Phys. 13 356
[26] Sun H et al. 2019 Phys. Rev. 096401
[27] Xiao S, Xiao X, Zhan F, Fan J, Wu X and Wang R 2020 Phys. Rev. 123 093029 XX i a o
[28] He K 2020 Nan. Mater. 20 5 90
[29] Wu J et al. 2019 Sci. Adv. eaaw5685
[30] Li H et al. 2019 Phys. Rev. 80 094039
[31] Wu J et al. 2019 Sci. Adv. eaaw9989
[32] Shi M Z, Lei B, Zhu C S, Ma D H, Cui J H, Sun Z L, Ying J J and Chen X H 2019 Phys. Rev. 100 155144
[33] Klímovskikh I I et al. 2020 npj Quantum Mater. 5 54
[34] Zhang J, Zhao B, Yao Y and Yang Z 2015 Phys. Rev. B 92 165418
[35] Zhang J, Zhao B, Zhou T, Xue Y, Ma C and Yang Z 2018 Phys. Rev. B 97 085401
[36] Zhao R, Zhan F, Zheng B, Wu X, Fan J and Wang R 2020 Phys. Rev. B 101 161108(R)
[37] Tong Q, Yu H, Zhu Q, Wang Y, Xu X and Yao W 2016 Nat. Phys. 13 356
[38] Sun H et al. 2019 Phys. Rev. 123 096401
[39] Xiao S, Xiao X, Zhan F, Fan J, Wu X and Wang R 2022 Phys. Rev. B 105 125126
[40] Heohenberg P and Kohn W 1964 Phys. Rev. 136 B864
[41] Kohn W and Sham L 1965 Phys. Rev. 140 A1133
[42] Kresse G and Furthmüller J 1996 Comput. Mater. Sci. 6 15
[43] Kresse G and Furthmüller J 1996 Phys. Rev. B 54 11169
[44] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[45] Blöchl P E 1994 Phys. Rev. B 50 17953–79
[46] Monkhorst H J and Pack J D 1976 Phys. Rev. B 13 5188–92
[47] Liechtenstein A I, Anisimov V I and Zaanen J 1995 Phys. Rev. B 52 R5467
[48] Gao Y, Wang X and Mi W 2021 Comput. Mater. Sci. 187 110085
[49] Grimme S, Antony J, Ehrlich S and Krieg H 2010 J. Chem. Phys. 132 154104
[50] Marzari N and Vanderbilt D 1997 Phys. Rev. B 56 12847
[51] Mostofi A A, Yates J R, Lee Y S, Souza I, Vanderbilt D and Marzari N 2008 Comput. Phys. Commun. 178 685
[52] Qiao J, Zhou J, Yuan Z and Zhao W 2018 Phys. Rev. B 98 214402
[53] Pizzi G et al. 2020 J. Phys.: Condens. Matter 32 165902
[54] Sinova J, Valenzuela S O, Wunderlich J, Back C and Jungwirth T 2015 Rev. Mod. Phys. 87 1213
[55] Yao Y, Kleinman L, MacDonald A H, Sinova J, Jungwirth T, sheng Wang D, Wang E and Niu Q 2004 Phys. Rev. Lett. 92 037204
[56] Yao Y and Fang Z 2005 Phys. Rev. Lett. 95 156601
[57] Sancho M P L, Sancho J M L and Rubio J 1984 J. Phys. F: Met. Phys. 14 1205
[58] Sancho M P L, Sancho J M L and Rubio J 1985 J. Phys. F: Met. Phys. 15 851
[59] Wu Q, Zhang S, Song H F, Troyer M and Soluyanov A A 2018 Comput. Phys. Commun. 224 405–16
[60] Weng H, Dai X and Fan Z 2014 Phys. Rev. X 4 011002
[61] Wu R et al. 2016 Phys. Rev. X 6 021017
[62] Yu R, Qi X L, Bernevig A, Fang Z and Dai X 2011 Phys. Rev. B 84 075119
[63] Prodan E 2009 Phys. Rev. B 80 125327