Quantum anomalous Hall effects and various topological mechanisms in functionalized Sn monolayers

Y S Mu¹, Y Xue¹, T Zhou¹ and Z Q Yang¹,²,³

¹ State Key Laboratory of Surface Physics and Key Laboratory for Computational Physical Sciences (MOE) & Department of Physics, Fudan University, Shanghai 200433, People’s Republic of China
² Collaborative Innovation Center of Advanced Microstructures, Fudan University, Shanghai, 200433, People’s Republic of China

E-mail: zyang@fudan.edu.cn

Keywords: first-principles calculation, electronic structure, quantum anomalous Hall effect, Sn monolayer

Abstract

The topological behaviors of Sn monolayers partly passivated with H atoms are explored based on first-principles calculations. Obvious magnetism can be induced in the Sn monolayer due to the passivation. And the magnetism strength is found to be determined by the number difference of the H atoms bonding to the two sublattices of stanene. Quantum anomalous Hall (QAH) effects are found appearing easily in the systems with one of the sublattices fully passivated and the other not. The origin of the topological states can be ascribed to the coupling of the magnetism, the lattice symmetry, and the H-atom concentrations, which forms various mechanisms of the topological states. Particularly, band inversions are found playing completely different roles in forming the QAH effects for the different functionalized Sn monolayers.

1. Introduction

Quantum anomalous Hall (QAH) effects [1–3], owning one type of novel quantum topological states, are signaled by quantized charge Hall conductance. Despite the insulating bulk states, the chiral edge states can conduct the charge current without dissipation since the back scattering of electrons is totally held back in the system. The transport behaviors are also very robust against disorders and perturbations. Owing to these intriguing properties, the QAH effect has attracted considerable research interest recently and the concept of the topological states has deepened our understandings of condensed matter physics and material science. The QAH effect is generally identified and characterized by Chern numbers [4, 5] as shown below. The materials possessing the QAH effect can, thus, be called Chern insulators. Unlike quantum Hall states, QAH states can appear without the requirement of a strong magnetic field applied to the system. The internal magnetization is, however, essential to produce the QAH effect in a two-dimensional (2D) material. Thus, to achieve the effect, how to introduce long-range ferromagnetism in the 2D material systems needs to be considered first although the special band structures and strong spin-orbital coupling (SOC) interactions are also of significance to the effect.

Up to now, a series of theoretical predictions of QAH effects have been proposed in 2D material systems, including Hg₁₋ₓMnxTe quantum wells [6, 7], magnetized Bi₂Te₃ films etc [8], graphene [9–11], silicone [12–14], and other 2D thin films [15, 16]. Among them, only the magnetized Bi₂Te₃ films etc, concretely Cr-doped [17–20] or V-doped [21–23] (Bi, Sb)₂Te₃, have been reported hosting the QAH effect in experiments. The experimental observation conditions of the QAH effect are also very harsh, including very high quality of the crystals fabricated and an extremely low temperature (milli-Kelvin) [17–23], hindering seriously the development of the field. Recently, a theoretical study has shown that halogen-half-passivated stanane/germanene, with one sublattice of Sn/Ge fully saturated by halogen atoms and the other not, can exhibit a QAH effect with a pretty large energy band gap of 0.34/0.06 eV and high Curie temperature of 243/509 K [24]. The origin of the topological state was ascribed to band inversion of the Sn/Ge spin-down s-p bands [24]. In experiments, Sn ultrathin films with a buckled honeycomb lattice have been fabricated with molecular beam...
epitaxy techniques [25–27], making the experimental observation of the QAH effect in the 2D Sn films step forward. Thus, the systems, especially stanene, should be excellent candidates to be employed to observe QAH effects in experiments at a relatively high temperature. Some important problems, however, exist in the system and need to be solved in advanced.

For stanene, if the passivating halogen atoms are replaced with hydrogen atoms, our initial calculations indicate that the hydrogen-half-passivated Sn monolayer also presents the QAH effect. Oppositely, the hydrogen-full-passivated stanene was reported to be a trivial insulator due to the absence of band inversion [28]. How the topological phase transition happens with the decreasing of the H concentration is worthwhile to be studied. Additionally, the perfect half- or full-passivated Sn monolayers mentioned above are generally hard to be realized in experiments since the cases with more or less Sn atoms saturated may more easily appear in experiments. Under the same saturation concentration, different passivation patterns may also occur, which can lead to different topological electronic states. Therefore, it is full of theoretical and practical significances to explore the electronic states and topological behaviors for the imperfect passivated 2D systems.

In this work, based on density functional theory (DFT), we investigate the electronic states and topological properties of Sn monolayers partly passivated with H atoms. We find that the H concentration, the induced magnetism, and the lattice symmetry together determine the electronic structures and topological properties of the functionalized Sn monolayer systems. The induced magnetic strength of the system is associated with the number difference of passivated Sn atoms in the two sublattices. QAH effects are found appearing easily in the systems with one of the sublattices fully passivated and the other not. Various forming mechanisms are proposed to understand the QAH effects achieved. For the systems with a $C_{3v}$ lattice symmetry and strong magnetism, the nontrivial topology originates from the lifting of energy degeneracy due to the SOC. The band inversions appear in both of the systems with or without the $C_{3v}$ symmetries, whose roles are, however, completely different in forming the topological states.

2. Models and methods

A 2 × 2 stanene supercell, as shown in figure 1, is built to investigate the electronic and topological behaviors of the Sn monolayer partly saturated with H atoms. The two triangular sublattices in stanene are labeled as t (top) and b (bottom), respectively (see figures 1(b) and (d)). The numbers of the saturated Sn in the two sublattices are employed to distinguish the different saturated stanene systems. For example, the t3b1 means that three Sn atoms in the top sublattice are passivated by H atoms and one Sn atom in the bottom sublattice is passivated (see figures 1(a) and (b)). In this work, we primarily focus on the cases with half or more than half Sn atoms in the system saturated with H atoms. The systems investigated in this work are given in table 1. Note that t3b1 is equivalent to t1b3 because of the symmetry of the top and bottom sublattices. The behavior keeps for the other passivation schemes.

The geometry optimization and electronic structures are calculated by using a first-principles method based on the framework of DFT, as implemented in the Vienna ab initio simulation package [29] with projector augmented wave method [30]. The exchange correlation potential is described by using Perdew–Burke–Ernzerhof functional [31] within generalized gradient approximation [32]. Plane waves with a kinetic energy
belong to the same sublattice. For half-saturated stanene systems, i.e. with four H atoms in the 2×2 cutoff of 500 eV are adopted as basis set and all atoms are allowed to relax along any directions until the force on each atom is less than 0.01 eV Å⁻¹. The SOC interaction is calculated self-consistently by solving the generalized Kohn–Sham equations in the relativistic DFT [33]. To prevent interlayer interactions between the adjacent slabs, a 20 Å vacuum buffer space is applied between the neighboring layers. The 9 × 9 × 1 gamma central Monkhorst–Pack grids are set to integrate in the first Brillouin Zone.

### 3. Results and discussion

For half-saturated stanene systems, i.e. with four H atoms in the 2 × 2 supercell, if the saturated Sn atoms all belong to the same sublattice (namely t4b0 or t0b4), the case is named as ideal half-saturated systems. The ideal halogen-half-passivated Sn monolayers were explored previously [24] and a QAH effect was predicted in the systems. For an ideal half-passivated stanene with H atoms, our calculations predict a QAH effect in it, similar to those ideal iodine-half-passivated Sn monolayers. Thus, for the half-passivated Sn sheets, we mainly consider the cases with both of the Sn sublattices passivated with H atoms, such as t3b1. In table 1, the systems of the t2b2 and t3b3 are also not included due to the absence of the magnetism in both of the cases. Thus, there are totally five schemes for the Sn monolayers, where half or more than half Sn atoms are passivated, which are deeply explored in this work (table 1). Due to the relative locations of the passivated Sn atoms and translational symmetry of the lattice, three types of nonequivalent passivation patterns are found for both t3b1 and t3b2, as indicated by stars in table 1. For the left three schemes listed in table 1, there are only one nonequivalent passivation pattern.

The lattice constant of the pristine stanene (without the H atoms) is first optimized. The obtained value of 4.68 Å is consistent with the previous result of 4.65 Å [28]. The pristine stanene is a slightly buckled honeycomb lattice with in-plane sp² hybridization and out-of-plane pz dangling bonds. The latter forms the Dirac cone around the Fermi level (E_f) [34]. When the dangling bonds of one of the sublattice are all passivated by H or I atoms, very strong ferromagnetism is introduced in the system [24], one key condition to produce the QAH effect. The equilibrium lattice constants and the atomic positions for the systems listed in table 1 are all optimized. As an example, the lattice constant, buckled height between the two sublattices, and the average Sn–Sn bond length for t3b1 shown in figures 1(a) and (b) are 9.45 Å, 0.77 Å, and 2.86 Å, respectively. In table 1, only t4b1 and t4b3 own the C₃, lattice symmetry, which can result in very exotic topological mechanisms, to be discussed.

Since the long-range magnetism is essential to produce the QAH effect, we first explore the magnetism in the stanene partly passivated with the H atoms. The magnetization strength of each system studied is given in the third row of table 1. Very interestingly, we find that the magnetic momentum per supercell, induced by the H atoms, is exactly determined by the number difference of saturated Sn atoms in the top and bottom sublattices. For t3b1 and t3b2, the different passivation patterns all give the same magnetization strength. As shown in table 1, among the five studied systems, t4b1 has the strongest magnetism while t3b2 and t4b3 have the weakest magnetism. This trend can be ascribed to the counteracting effect of the dangling bonds from the top and bottom sublattices, which can also explain why the ideal half-passivated stanene (t4b0) has the largest magnetic momentum per supercell (4 μᵦ).

As mentioned above, the last three systems (t4b1, t4b2, and t4b3) in table 1 all have only one nonequivalent passivation, while t3b1 and t3b2 systems have three types of nonequivalent passivation patterns, due to the complex relative locations of the passivated Sn atoms in the top and bottom sublattices in t3b1 and t3b2. The electronic structures of these systems with the consideration of the possible nonequivalent passivation patterns are all calculated. The results show that although magnetism is induced in all the t3b1/t3b2 systems with the

| Scheme | t3b1⁺ | t3b2⁺ | t4b1 | t4b2 | t4b3 |
|--------|-------|-------|------|------|------|
| δ      | 4/8   | 5/8   | 5/8  | 6/8  | 7/8  |
| Cᵥ     | N     | N     | Y    | N    | Y    |
| M (μᵦ) | 2     | 1     | 3    | 2    | 1    |
| C      | −1    | 0     | −1   | −1   | −1   |
| Δ (meV) | 148/20 | 278/120 | 0/180 | 64/121 | 187/8 |

Table 1. Several properties of the investigated systems are given. The first line (δ) indicates the concentration of the H atoms added into the stanene. The ‘Y’ and ‘N’ in the second line give the lattices with and without the Cᵥ, symmetry, respectively. M and C denote the magnetic moment per supercell and the Chern number, respectively. The values in the last line (Δ) show the band gaps obtained without and with the consideration of the SOC. The stars in the second and third columns express more than one passivation patterns existing in the passivation schemes.
different passivation patterns, only 33%/67% of them own the QAH effect with Chern numbers of \(\pm 1\). Among the three types of t3b1 passivation patterns, only one has the topologically nontrivial band gap. Its total energy is, however, the highest, compared to those of the other two patterns. For t3b2, two passivation patterns own the topologically nontrivial band gaps, with the lowest and highest total energies, respectively. Therefore, the QAH effect is relatively easier to be observed experimentally in t3b2 than t3b1. Note that the Chern numbers \(C\) and the band gaps \(\Delta\) shown in table 1 for t3b1/t3b2 are only the results of the systems with the passivation patterns illustrated in figure 1. The last three systems (t4b1, t4b2, and t4b3) all possess the QAH effect, which will be discussed in detail. Thus, QAH effects appear easily in the systems with one of the sublattices fully passivated and the other not, which provides important guidance to the experimental observation of the QAH effect in the Sn monolayers passivated with H atoms.

We now focus on the electronic structures and topological behaviors of following four typical systems: t3b1, t4b1, t4b2, and t4b3. For t3b1, the passivation pattern displayed in figures 1(a) and (b) is chosen. The band structures of these systems without and with the SOC are displayed in figure 2. Obvious spin polarization is observed for each case without the consideration of the SOC. Except t4b1, all other systems (t3b1, t4b2, and t4b3) possess sizable band gaps at the \(E_F\) before the SOC is taken into account. In t4b1, the lowest conduction band and the highest valence band touch at the \(\Gamma\) point exactly at the \(E_F\). When the SOC is considered, a very large band gap of 180 meV is opened (figure 2(f)), while for the left three systems (t3b1, t4b2, and t4b3), the band gap becomes small if the original band gap is large and vice versa. For example, without the SOC, the band gap for t4b3 is the largest (187 meV). It becomes the smallest (8 meV) with the consideration of the SOC. Therefore, we can tentatively expect that the topological mechanisms for t4b1 and the other three systems in figure 2 must be different.

Figure 3 illustrates the orbital components for the four systems. Explicitly, the bands near the \(E_F\) are primarily contributed by Sn \(s\) and \(p_{xy}\) orbitals. For the Sn atoms passivated with H atoms, their \(p_z\) orbitals will interact with H \(s\) orbitals. Thus, bonding and antibonding states are formed by the two orbitals far away from the \(E_F\), at about \(-1.4\) and \(2.5\) eV, respectively. These behaviors lead to the breakdown of the linear Dirac bands around the \(E_F\) from the pristine stanene at the \(K\) point. Since in each case some Sn atoms are not passivated, nearly flat bands contributed chiefly by Sn \(p_z\) orbital are observed in figure 3 (the orange color curves). And the numbers of such flat bands for spin-up or spin-down components are precisely equal to the number difference of the passivated Sn atoms in the two sublattices, namely the value of the magnetic moment per supercell in the system. Besides, the spin-up and spin-down flat bands are located below and above the \(E_F\), respectively, indicating the magnetism of these Sn monolayers originates mainly from the dangling Sn \(p_z\) orbitals, consistent with above analysis.

For t4b1 and t4b3 without the SOC, degenerate bands composed of Sn \(p_x\) and \(p_y\) orbitals (green and blue hollow curves) appear near the \(E_F\) due to the \(C_{3v}\) lattice symmetry owned by the lattices. Concretely, in t4b1 (figure 3(b)), the spin-down unoccupied \(p_x\) band (green hollow curve) touch the spin-down occupied \(p_y\) band
(blue hollow curve) exactly at $E_F$. And in t4b3 (figure 3(d)), the spin-down $p_x$ and $p_y$ orbitals degenerate at the top of the valence bands. For t4b1, another exotic aspect is the spin-down Sn $s$ band (red hollow curve) located below the $E_F$, while for the left three systems in the upper panel of the figure 3, they are all located above the $E_F$. The schematic diagrams of band characteristics of these systems around the $E_F$ without the SOC are illustrated in figure 4 (the left panel for each case). The inverted band order of the spin-down $s$ orbital in t4b1 can be ascribed to the very strong exchange interactions induced in the Sn $s$ orbitals in this system, leading to the spin-down $p_x$ orbitals (green dotted curve) becoming unoccupied (figures 3(b) and 4(c)) due to the conservation of Sn electron numbers. When the SOC is considered, the degeneracy around the $E_F$ in t4b1 is lifted and one large band gap is opened. The trends for the other three systems are, however, different. For them, band inversions between the Sn spin-down $s$ and $p_x, p_y$ occur around the $E_F$ (figures 3(e), (g), and (h)), which are illustrated schematically in figures 4(b), (f), and (h). Since band inversions generally can induces topologically phase transitions [6], nontrivial topological states may appear in these three systems. Note that the Sn spin-down $s, p_x$, and $p_y$ bands
edge states are characterized by quantized charge Hall conductance, \( \sigma_y \Omega \), which is the momentum-space Berry curvatures summed over all occupied valence bands [4, 35, 36]:

\[
\Omega(k) = -\sum_n f_n \sum_{n'=n} \frac{2\text{Im} \langle \psi_{nk} | \sigma_y | \psi_{nk'} \rangle \langle \psi_{nk'} | \sigma_y | \psi_{nk} \rangle}{(E_{n'} - E_n)^2},
\]

where \( \sigma_y \) is a velocity operator and \( f_n = 1 \) for all occupied bands.

Figures 5(a)–(d) show the calculated Berry curvatures (red curves) along the high symmetry paths in the Brillouin zone. Nonzero values of the Berry curvatures imply the nontrivial topology. Especially, the peaks of Berry curvatures appear near the \( \Gamma \) point, inferring the nontrivial band gaps opened by SOC in these systems. Moreover, the peak values are inversely proportional to the size of the band gap, understood well by using the formula of \( \Omega(k) \). For example, in t3b1 and t4b3, very small band gaps are opened by SOC, as shown in table 1. Thus, very sharp Berry curvature peaks are observed in figures 5(a) and (d). The integrals of \( \Omega(k) \) over the whole first Brillouin zone for all the systems shown in figure 5 give a nonzero Chern number \( C = -1 \), manifesting all these systems have QAH effects and each of them owns only one nontrivial edge state.

By constructing maximally localized Wannier functions and surface Green’s functions of the corresponding semi-infinite systems, we calculate the edge states of these four systems shown in figure 3. Topologically nontrivial edge states, which connect the conduction and valence bands, can be easily recognized in figures 5(e)–(h). As expected from the Chern number \( C = -1 \) obtained, there is only one nontrivial edge state per edge for each of these systems considered. Some topologically trivial edge states, connecting two valence bands or two conduction bands, can also be seen in figures 5(e)–(h), owing to the existence of the Sn \( p_z \) dangling bonds in the systems as indicated by the flat bands in figure 3.

As discussed above, the band structures of t3b1, t4b2, and t4b3 possess SOC-induced band inversions as illustrated in figures 4(b), (f), and (h) while t4b1 just opens an energy gap when SOC is included (figure 4(d)). By orbital component analyses shown in figure 3, we find the band inversions all occur between Sn spin-down \( s \) and \( p_x/p_y \) orbitals for the former three systems (figures 4(b), (f), and (h)). Such nontrivial topology origin caused by the band inversion is expected to be similar to the mechanism proposed by Bernevig, Hughes, and Zhang [37], in which pseudospin of two relevant orbitals forms a skyrmion with unit topological charge in the momentum space.
For t4b1, the band inversion between Sn spin-down s and pₓ orbitals has already existed before the SOC is considered, similar to the trend in iodine-half-passivated stanene in [24]. The effect of SOC is merely to lift the degeneracy of the p orbitals at the E₀ and opens a topologically nontrivial band gap. Thus, the topological mechanism in t4b1 is completely different from those in other systems shown in figure 4 and also in magnetized Bi₂Te₃ films, where the band inversion plays an important role [8]. Due to the quadratic band dispersion near the Γ point, the QAH effect in t4b1 can be ascribed to the exotic two-meron structure of the pseudospin texture, as discussed in magnetized MoS₂ and Cu₃S systems [38, 39]. Thus, the topological origin is also similar to that of the Dirac type bands, as proposed in seminar researches by Haldane [40] or Kane and Mele [41], where a couple of merons with each contributing 1/2 topological charge are found at the K and K’ points in the momentum space. Therefore, the QAH effect obtained in t4b1 is very unique, caused by the strong magnetism as well as the C₃ᵥ symmetry owned by the lattice. Note that there is a band inversion of the Sn spin-down s orbital in t4b1, compared to those in other systems in figures 4(a), (c), and (g), which, however, does not directly lead to the nontrivially topological states in the system instead of the Sn pₓ orbital varying from the occupied state to the unoccupied state.

Besides the t4b1 system, the t4b3 case also possesses the C₃ᵥ rotation symmetry (table 1), guaranteeing the existence of the degenerate point of the Sn pₓ and pᵧ orbitals at the Γ point, without the consideration of the SOC (figure 4(g)). The band degeneracy in t4b3 occurs at the top of valence bands (figure 4(g)), different from the case in t4b1 (figure 4(c)), due to the absence of the band inversion of the Sn spin-down s orbital in t4b3. The SOC in t4b3 not only lifts the double degeneracy at the top of the valence bands, as in the case of t4b1, but also causes the band inversion of Sn spin-down s and pₓ orbitals around the E₀, as in t3b1 and t4b2 (figure 4(h)). It is interesting to explore intensively whether the band inversion in t4b3 plays the same role as those in t3b1 and t4b2.

To deeply explore the SOC effect on the topology in t4b3, we calculate the band structures of t4b3 with various SOC strengths. To compare directly, the corresponding bands of t3b1 are also calculated. Figures 6(a) and (b) give the bands of t3b1 and t4b3, respectively, with the SOC strengths of λ = 0.6 λ₀ and λ₀, where λ₀ indicates the real SOC strength of the corresponding system. With the increase of the λ from 0 to λ₀, the band gaps at the E₀ of the both systems undergo a closing and reopening transition. For t3b1, with λ = 0.6 λ₀, the band inversion does not happen yet. The system is topologically trivial, proved by the Chern number calculated (figure 6(a)). When the SOC is continued increasing, the band gap is closed and then reopened, accompanied by a band inversion. As shown in figure 6(a) for λ = λ₀, the system evolves into a topologically nontrivial state with C = −1. Thus, the band inversion in t3b1 is the most crucial factor to induce the topological state.

The role of the band inversion in t4b3, however, is different from that in the case of t3b1. In figure 6(b) with λ = 0.6 λ₀, the pᵧ degeneracy at the top of the valence bands has been lifted while the band inversion does not
appear yet. The energy gap opened between the first (the blue curve) and the second (the green curve) valence bands is found to be nontrivial with \( C = -1 \). The corresponding Berry curvature distribution is displayed in figure 6(c). The band gap around the \( E_F \) in the system is, however, still trivial with \( C = 0 \) (see the left panel of figure 6(b)). When \( \lambda = \lambda_0 \), the band inversion occurs and the band gap at the \( E_F \) becomes topologically nontrivial. The Berry curvature distribution of the valence bands without the topmost valence band for t4b3 with \( \lambda = \lambda_0 \) (figure 6(d)) also gives \( C = -1 \). Hence, the topology of the QAH effect obtained in t4b3 essentially comes from the lifting of the \( p_x \) degenerate bands by the SOC, not from the band inversion of Sn atoms and \( p_y \) orbitals. The role of the band inversion in t4b3 is merely to extend the topologically nontrivial energy region and making the band gap at the \( E_F \) also present the QAH effect, distinct from those in t3b1 and t4b2.

Therefore, various topological mechanisms are found in t3b1 (t4b2), t4b1, and t4b3, associated with the lattice symmetry, the induced magnetism strength, and the passivation concentration of the H atoms in the system. For t3b1 and t4b2, the band inversion, one classical topological mechanism, plays a key role in generating the topological state, similar to that of many other 2D topological systems [6, 8, 11, 13, 37]. The topological mechanism found in t4b1, however, is completely different from that of t3b1 and t4b2. The topology comes from the lifting of Sn \( p_x \) and \( p_y \) band degeneracy around the \( E_F \) due to the SOC interaction. The nontrivial band gap opened through this mechanism is usually very large (180 meV for t4b1). It is the atomic SOC rather than Rashba SOC that opens the band gap. This mechanism is very exotic and probably promotes quick developments of topological states in future applications. The topological mechanism of t4b3 may be regarded as a combination of those of t3b1 (t4b2) and t4b1 since it owns \( C_{2\varepsilon} \) symmetry and band inversion simultaneously. The role of the band inversion in t4b3, however, only extends the nontrivial energy region to the area around the \( E_F \), instead of producing the topology as in t3b1 (t4b2). With these three types topological mechanisms, the topology of stanene passivated partly with H atoms can be understood well, which can also be applied to comprehend the topologies of other systems or design new topological materials. Note that disordered arrangements of H or Sn atoms in the lattice may affect the band dispersion. If the disorder effect is not drastic, however, the topological behaviors predicted in the studied stanene systems should be kept.

In experiments, the Sn films are usually required to fabricate on an insulating substrate which is expected to keep the nontrivial features of the freestanding Sn films intact. For stanene studied, we find the hydrogen-terminated SiC (111) surface is a suitable substrate. As shown in figures 7(a) and (b), the t4b1 sample is deposited on the SiC (111) substrate modeled by a slab of three atomic layers of SiC, with the bottom layer fixed to mimic a semi-infinite solid. To eliminate the dangling bonds, both sides of the SiC slab are hydrogenated. The lattice mismatch between the stanene sample and the substrate is about 1.95%. The relaxed distance between the neighboring two \( H \) planes in the interface of the system is about 2.47 \( \AA \), indicating the van der Waals bonds formed between the sample and the substrate. The obtained band structures of t4b1 and t4b3 on the SiC (111) surfaces are displayed in figures 7(c)–(f), from which one can see that the Sn \( p_x \) orbitals (the flat bands) move down in energy due to the interactions from the substrate. The band trends around the \( E_F \) are, however, kept
well. For example, for t4b1 on the SiC substrate, the degenerate bands of Sn spin-down $p_x$ and $p_y$ orbitals at the $E_F$ is lifted after the SOC is included, similar to the case in t4b1 without substrates. The band gap opened in t4b1 with the substrate is also topological nontrivial. From the component analysis, the band inversion is also happened in t4b3 with the SiC substrate. Therefore, to observe experimentally the QAHL effect in the stanene studied, the SiC (111) slab is a suitable substrate.

4. Conclusion

We theoretically investigated electronic and topological properties of the Sn monolayers passivated with H atoms. We find 33% and 67% patterns of t3b1 and t3b2 as well as all t4b1, t4b2, and t4b3 functionalized Sn monolayers present the QAHL effect. Generally, the systems with one of the sublattices fully passivated and the other not are easy to present the topological states. Whether the lattice owns the $C_{3v}$ symmetry or not are easy to present the topological states. For the systems possessing the $C_{3v}$ symmetry (t4b1 and t4b3), the nontrivial topology essentially comes from the lifting of the $p_{xy}$ degenerate bands, due to the SOC. For the other systems without the protection of the $C_{3v}$ symmetry, the band inversions induced by the SOC are the topology origin. Especially, despite the band inversion also appearing in t4b3, its effect is completely different from the traditional one in the other systems (t3b1 and t4b2). The hydrogen-terminated SiC (111) surface is found to be a suitable substrate for the stanene to observe experimentally the QAHL effect.

Acknowledgments

This work was supported by National Natural Science Foundation of China under Grant Nos. 11574051 and 11874117. All the calculations were performed on the High Performance Computational Center (HPCC) of Department of Physics at Fudan University.

ORCID iDs

Z Q Yang @ https://orcid.org/0000-0002-4949-1555

References

[1] Weng H, Yu R, Hu X, Dai X and Fang Z 2015 Adv. Phys. 64 227
[2] Liu C-X, Zhang S-C and Qi X-L 2016 Annu. Rev. Condens. Matter Phys. 7 301
[3] Ren Y, Qiao Z and Niu Q 2016 Rep. Prog. Phys. 79 066501
[4] Thouless DJ, Kohmoto M, Nightingale MP and Den Nijs M 1982 Phys. Rev. Lett. 49 405
[5] Kohmoto M 1985 Ann. Phys. 160 343
[6] Liu C-X, Qi X-L, Dai X, Fang Z and Zhang S-C 2008 Phys. Rev. Lett. 101 146802
[7] Hsu H-C, Liu X and Liu C-X 2013 Phys. Rev. B 88 085315
[8] Yu R, Zhang W, Zhang H-J, Zhang S-C, Dai X and Fang Z 2010 Science 329 61
[9] Qiao Z, Yang S A, Feng W, Tse W-K, Ding J, Yao Y, Wang J and Niu Q 2010 Phys. Rev. B 82 161414
[10] Tse W-K, Qiao Z, Yao Y, MacDonald A and Niu Q 2011 Phys. Rev. B 83 155447
[11] Qiao Z, Ren W, Chen H, Bellaiche L, Zhang Z, MacDonald A and Niu Q 2014 Phys. Rev. Lett. 112 116404
[12] Zhang X-L, Liu L-F and Liu W-M 2013 Sci. Rep. 3 2908
[13] Zhang J, Zhao B and Yang Z 2013 Phys. Rev. B 88 165422
[14] Ezawa M 2012 Phys. Rev. Lett. 109 055502
[15] Wang Z, Liu Z and Liu F 2013 Phys. Rev. Lett. 110 196801
[16] Jiang H, Qiao Z, Liu H and Niu Q 2012 Phys. Rev. B 85 045445
[17] Chang C-Z et al 2013 Science 340 167
[18] Chechelski J, Yoshimi R, Tsukazaki A, Takahashi K, Kozuka Y, Falson J, Kawasaki M and Tokura Y 2014 Nat. Phys. 10 731
[19] Kou X et al 2014 Phys. Rev. Lett. 113 137201
[20] Kandala A, Richardson A, Kem pingser S, Liu C-X and Samarth N 2015 Nat. Commun. 6 7434
[21] Chang C-Z et al 2015 Nat. Mater. 14 473
[22] Chang C-Z, Zhao W, Kim D Y, Wei P, Jain I, Liu C, Chan M H and Moodera J S 2015 Phys. Rev. Lett. 115 057206
[23] Grauer S, Schreyeck S, Winnerlein M, Brunner K, Gould C and Molenkamp L 2015 Phys. Rev. B 92 201304
[24] Wu S-C, Shan G and Yan B 2014 Phys. Rev. Lett. 113 256601
[25] Osaka T, Om H, Yamamoto K and Ohtake A 1994 Phys. Rev. B 50 7567
[26] Zimmermann H, Keller R C, Meisen P and Seelmann-Eggebert M 1987 Surf. Sci. 377 904
[27] Zhu F-F, Chen W-J, Xu Y, Gao C-L, Guan D-D, Liu C-H, Qian-D, Zhang S-C and Jia J-F 2015 Nat. Mater. 14 1020–5
[28] Xu Y, Yan B, Zhang H-J, Wang J, Xu G, Tang P, Duan W and Zhang S-C 2013 Phys. Rev. Lett. 111 136804
[29] Kresse G and Furthmüller J 1996 Phys. Rev. B 54 11169
[30] Bloch P E 1994 Phys. Rev. B 50 17953
[31] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[32] Perdew J P, Chevary J A, Vosko S H, Jackson K A, Pederson M R, Singh D J and Fiolhais C 1992 Phys. Rev. B 46 6671
[33] Theurich G and Hill N A 2001 Phys. Rev. B 64 037106
[34] Xu Y, Tang P and Zhang S-C 2015 Phys. Rev. B 92 081112
[35] Chang M-C and Niu Q 1996 Phys. Rev. B 53 7010
[36] Yao Y, Kleinman L, MacDonald A, Sinova J, Jungwirth T, Wang D-S, Wang E and Niu Q 2004 Phys. Rev. Lett. 92 037204
[37] Bernevig B A, Hughes T L and Zhang S-C 2006 Science 314 1757
[38] Wei X, Zhao B, Zhang J, Xue Y, Li Y and Yang Z 2017 Phys. Rev. B 95 075419
[39] Xue Y, Zhao B, Zhu Y, Zhou T, Zhang J, Li N, Jiang H and Yang Z 2018 NPG Asia Mater. 10 467
[40] Haldane F D M 1988 Phys. Rev. Lett. 61 2015
[41] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 226801