Systematic study on stanene bulk states and the edge states of its zigzag nanoribbon

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Abstract

Stanene, as a counterpart of graphene, but with much larger spin–orbit coupling (SOC) strength, has recently been synthesized experimentally. Based on first principle calculations and an effective model, we systematically study the electronic and topological properties of bulk stanene under vertical electric field and biaxial strain, which can be naturally introduced by substrates. We find that a topological nontrivial–trivial transition occurs under critical vertical electric field and an insulator–metal transition happens under critical biaxial strains. We also systematically study the edge state of zigzag nanoribbons. We find that the topological edge state has strong nonlinear dispersion that is different from the previous oversimplified tight-binding (TB) model. A much more practical TB model is built, which captures the strongly nonlinear dispersion of the edge states very well. We investigate four magnetic configurations of the zigzag ribbon edge states in detail and find that the emergence of magnetism for the edge atoms and the magnetization direction have a remarkable impact on the spin-current-carrying edge channels. Furthermore, a half-metallic state can be induced in stanene nanoribbons by applying a transverse electric field, and opposite spin channels can be chosen by reversing the electric field direction. Our results are instructive for future research and applications on stanene and other related buckled systems.

Introduction

Following the discovery of graphene and its marvelous properties over the last decade [1], its counterparts silicene [2–4], germanane and stanene have been sequentially predicted and grown. This is especially the case for germanene [5, 6] and stanene [7, 8], which have recently been grown on insulating substrates. It is known that graphene works as a precursor for two-dimensional (2D) topological insulators (TIs) [9] when considering the intrinsic spin–orbit coupling (SOC). However, it has a tiny bulk gap due to its light carbon element [10, 11], which makes it impractical for use as a TI in experiments. For silicene and germanane [12], as well as stanene [13], the effects of SOC greatly increase as the atomic number and degree of buckling increase, leading to 2D TIs with sizable band gaps and a measurable quantum spin Hall effect (QSHE) [12, 13]. In this way, lots of 2D TIs with large band gaps have been proposed [14–18], although most of them have been predicted by DFT calculations without real materials. However, a few predicted 2D TIs have been grown on metallic substrates, e.g. bi-layer bismuth [19, 20], silicene [21–23], etc. It is known that external electric fields are an effective way of tuning the electronic structure and topological properties in silicene [24] and germanane [25], due to their unique buckled structure, and the strain can modify the mechanical and electronic properties as well. With a very large SOC gap and buckled height, stanene will show more interesting properties under electric and strain effects. Several papers have investigated the effects of an electric field or strain on stanene separately [26–29]; however, a systematic study of the electric field and strain effects on its electronic and topological properties has not been done yet. On the other hand, the electronic properties of graphene [30, 31], silicene [24, 32, 33] and germanane [34, 35] nanoribbons with hydrogen-passivated edges have been extensively investigated. Since the
edge atoms of zigzag nanoribbons are inevitably magnetized [36], the impact of edge magnetism on the topological edge states in stanene has not been explored in detail through first principle calculations.

In this article, we systematically study the bulk band structures of stanene and its topological properties under a perpendicular electric field and biaxial strain. We find that perpendicular electric fields can drive topological phase transitions (TPTs), while strain can drive insulator–metal transitions (IMTs) in stanene. We also systematically study the influence of SOC, the finite size effect, edge magnetism and the transverse electric field effect on stanene zigzag nanoribbons. We find that the topological edge states with strongly nonlinear dispersion are significantly different from the linear edge states in the previous oversimplified TB models. We develop a better TB model that can perfectly reproduce the edge states with strongly nonlinear dispersion by taking into account the next-nearest-neighbor (NNN) hopping term, which is usually ignored. The emergence of edge magnetism and the orientation of the magnetization as well as the magnetic configurations can open and close the edge channels. Furthermore, it will be possible to induce a new stanene half-metal nanoribbon using a transverse electric field, resulting in promising application prospects in magnetic control and spintronics.

This article is organized as follows. The computation method is given in section 2. In section 3 we systematically study the bulk properties and the topological properties of stanene under various external fields, such as perpendicular electric fields and biaxial strain fields. We also place the stanene on an h-BN substrate as an example, to study the practical substrate effects and explore the synergy and competition between perpendicular electric fields and substrate effects. In section 4, we combine first principle calculations with a more practical TB model to study the edge states of stanene zigzag nanoribbons by considering SOC, edge magnetism and transverse electric fields comprehensively. After that, we will have a discussion and draw a conclusion.

Computation method

Our first principle calculations were carried out by the VASP (Vienna *ab initio* simulation package) with the generalized-gradient approximation (GGA) [37, 38] of Perdew, Burke and Ernzerh (PBE) [39] and the exchange correlation potential. All the structures were relaxed with a force on each atom of less than 0.01 eV Å⁻¹. The energy convergence criterion was less than 0.1 meV/atom. The cut-off energy was set to 450 eV for the calculations in order to guarantee converged computations. A vacuum layer of 15 Å was included along the z direction, and k-meshes of 15 × 15 × 1 and 1 × 15 × 1 were set for the unit cell and ribbons, respectively. SOC was included during the calculations, and the biaxial strain was implied by the change of lattice constant. The external vertical electric field was stimulated by an artificially implemented sawtooth potential in the VASP code.

Bulk states of stanene

Geometric and electronic structure of intrinsic stanene

The buckled honeycomb structure of stanene is shown in figures 1(a) and (b). The optimized lattice constant a = 4.68 Å is consistent with previous results [13, 14]. There are two nonequivalent stannum atoms in the unit cell with a buckling height difference of 0.86 Å in the out-of-plane direction. Each stannum atom bonds with the three nearest-neighbor atoms with a bond length of 2.83 Å. The band structures calculated without and with SOC are presented in figures 1(c) and (d). In the absence of SOC, the conduction band and valence band cross each other at the K/K' points, forming massless Dirac cones with a nearly linear dispersion, which is analogous to graphene. When including the nonignorable SOC for a heavy stannum atom, a gap of 74.2 meV is opened at the K/K' points, converting it from a semimetal to an insulator. Furthermore, at the Γ point, the SOC splits the four-fold degenerated valence bands into two spin-degenerated bands. The local band gap at the Γ point diminishes from 0.48 eV to 0.27 eV due to the SOC effect. It is known that stanene is a topological insulator with space inversion symmetry [13, 40], so we calculate the eigenvalue of the parity operation for Bloch wavefunctions at four time reversal invariant moment (TRIM) points [41], shown in figure 1(e), which gives $Z_2 = 1$, indicating nontrivial topological properties.

Biaxial strain effect

Strain is a powerful and clean way to tune the electronic properties of a 2D material due to its higher stretchability with respect to 3D materials [42]. On the other hand, strain usually inevitably exists in experiments when the 2D material is grown on substrates because of lattice mismatch [43]. Here we introduce both extensive and compressive biaxial strain on stanene and analyze the evolution of the electronic properties. The biaxial strain, defined as $\varepsilon = (a - a_0)/a_0$, ranging from −6%, −4%, −2%, 0%, 2%, 4%, 6% is applied, where the negative and positive values refer to compressive and extensive strain respectively. The dependence of total energy and stress on the external strain are shown in figure 2(a). The nearly parabolic and linear relations
indicate the mechanical stability of stanene within 6% deformation. The variation of geometric structures under strain is shown in figure 2(b), where we can see that the bond length and the buckled height of two neighboring atoms changes differently. The buckled height decreases monotonously, but the bond length increases with the increase of strain. The former varies greatly from $h_0 = 0.88$ to $h_0 = 1.28$ and the latter only changes from $d_0 = 1.05$ to $d_0 = 0.98$ by 6% (–6%) strain.

The band structures of these strained systems are calculated in figure 2(c). First we notice the band gap at the K(K') points changes very little under strain. This is because the band gap here is dominated by the intrinsic SOC effect, which is hardly affected by external strain. However, the valence band maximum (VBM) and the

| TRIM | VB | VB | VB | VB | CB | TOT |
|------|----|----|----|----|----|-----|
| $\Gamma$ | + | - | + | + | - | (-) |
| M | - | + | - | + | - | (+) |

Figure 1. The atomic and electronic structures as well as the topological invariant of stanene. (a) and (b) A schematic top and side view of the buckled honeycomb structure of stanene. (c) and (d) The band structure of stanene along high symmetry directions without and with SOC, respectively. Inset: the bands near K around the Fermi level. (e) The parity values for four pairs of occupied bands and one pair of conduction bands at the TRIMs; the last column shows the product of the parity values of all occupied bands.

Figure 2. The biaxial strain effect on the bulk properties of stanene. (a) The total energy change and stress versus the compressive and extensive strain. (b) The bond length $d$ and buckling height $h$ versus strain. (c) The evolution of the band structure with SOC for stanene under a biaxial strain $\varepsilon$ from –6% to 6%. The positive and negative value represent extensive and compressive strain, respectively.
conduction band minimum (CBM) at the $\Gamma$ point are modified remarkably by the strain. For strain-free stanene, the Fermi level just crosses the gaps at the K and $\Gamma$ points to make sure the system has a global band gap. With compressive strain applied, the VBM and CBM at the $\Gamma$ points will be lifted up, as shown in the bottom panel in figure 2(c). When the VBM at the $\Gamma$ points moves to a higher position than the CBM at the K points at a critical strain of about $$-2\%$$, it will transform into a metal with a Fermi level crossing the bottom of the conduction band at the K point and the top of the valence band at the $\Gamma$ point, as in the case of $\varepsilon = -4\%$, $-6\%$. Actually, it is a topological metallic state, because there is no local gap closing during the compressive process and the system should keep the same topology nature.

When extensive strain is implied, the VBM and CBM at the $\Gamma$ points decline, and the local gap simultaneously diminishes in the top panel of figure 2(c). Beyond a critical value (about $$1.5\%$$), IMT happens and the system will become a topological metal, as happens for compressive strain. With a further increase of extensive strain, the local gap at the $\Gamma$ points will close and reopen again, which indicates a topological transition from the topological metal to the normal metal. Furthermore, under $$6\%$$ extensive strain, we can see both the hole pocket at the K point and the electron pocket at $\Gamma$ have nearly linear dispersion, which make the stanene a self-doped 2D Dirac cone system. We notice that IMT happens for stanene within a relatively smaller strain compared with graphene\footnote{43} and silicene\footnote{44}.

Perpendicular electric field effect

The electronic structure can be effectively manipulated by an external electric field, especially in 2D systems. It has been reported that a transverse electric field can drive zigzag graphene nanoribbons to become half metals\footnote{31}. Recently, an out-of-plane electric field was used to drive few-layer black phosphorus to become a topological insulator\footnote{45}. Actually, using a perpendicular electric field to drive the topological transition in a buckled hexagonal lattice has also been proposed for the TB model\footnote{24} without considering the screening effect. As far as we know, first principle calculations for this issue have been done on silicene and germane in several articles\footnote{46, 47}. Recently, the effect that an electric field has on stanene was studied in order to understand its effect on the dielectric function and optical properties\footnote{48}, but detailed studies on its topological properties are rare\footnote{27, 49}. Here we study the electric field effect on stanene for two purposes. First, because of its structural similarity, the stanene may have a topological transition under an electric field. Second, in experiments, the substrate will naturally bring in an external potential, which may have interesting synergy and competition with a perpendicular external electric field. In figure 3, we plot the evolution of the band gap around the K points with a change of electric field value. We can see that the gap decreases linearly from an initial value of 74 meV to zero at two critical electric field strengths ($E_{c1,c2} = \pm 0.68$ V Å$^{-1}$) with a ratio of 0.11 eÅ, which is much smaller than 1 eÅ, indicating an obvious screening effect. When further increasing the electric field strength, the gap will reopen, making it a trivial insulator. The electric field in the opposite direction will present a similar band closing

**Figure 3.** The perpendicular electric field effect on the band structure and the topological properties of stanene. Top panel, band structures around the K points under different vertical electric fields. The bottom panel shows the dependence of the band gap at the K points on the vertical electric field. The blue and green regions refer to the BI (band insulator) and TI (topological insulator) region respectively. The black and red lines represent spin-up and spin-down states.
and reopening process, forming a \( W \)-type curve in the phase diagram. The corresponding band structure and spin texture around \( K(K') \) clearly shows this process. For example, at present \( E = 0.4 \text{ V \AA}^{-1} \), with the sublattice symmetry broken and the doubly degenerated CBM and VBM spin splitting, two spin-up (spin-down) bands approach, and two spin-down (spin-up) bands repel each other, which make \( K(K') \) spin-polarized. The band gap disappears at a critical value of \( E = 0.68 \text{ V \AA}^{-1} \) by making a well-defined spin-polarized Dirac cone system within the energy range –74 meV to 74 meV. Under a larger \( E = 1.0 \text{ V \AA}^{-1} \), the system is a trivial insulator as discussed before.

The physics around \( K(K') \) can be simply demonstrated by the low energy effective model \( [12, 24] \), which can be written as

\[
H_{\text{eff}} = v_f k_s \sigma_y + v_f k_t \tau_z \sigma_x + \lambda_{\text{so}} \tau_z \sigma_z + V \sigma_z,
\]

where \( \tau, s, \) and \( \sigma \) are the Pauli matrices representing the valley (K, K'), real spin and pseudo-spin (A, B sublattices) degrees of freedom respectively. \( v_f \) is the Fermi velocity and \( \lambda_{\text{so}} \) is the spin–orbital coupling constant. The on-site potential energy difference \( V \sim 1/2E \cdot h \) can be induced by a vertical electric field or substrates. The spectrum is easily obtained \( \varepsilon_k(\tau_z, s_z) = \pm \sqrt{(\tau_z s_z + V)^2 + v_f^2 k^2} \). At the K point, the band gap for two spin-up and two spin-down bands is \( \Delta_0 = 2|\lambda_{\text{so}} + V| \) and \( \Delta_0 = 2|\lambda_{\text{so}} - V| \), respectively. We can see the gap will close when the condition \( \lambda_{\text{so}} = \pm V \) is satisfied, which results in the \( W \)-type phase diagram. This topological transition can be detected by the Faraday magneto-optical effect.

**Substrate effect**

It is known that in practice, all 2D materials should be grown or sustained on proper substrates which will naturally deal with the lattice mismatch problem and substrate-host interaction problem. It has already been reported that even when the substrate belongs to the van der Waals type, it can also induce an external potential naturally deal with the lattice mismatch problem and substrate-host interaction problem. It has already been shown that in order to balance speed and efficiency, we simply keep the stanene lattice constant invariant. The results are almost unchanged when a larger supercell with a smaller mismatch is used.

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The electronic structure of stanene zigzag nanoribbons

The most famous feature of a 2D TI is the emergence of a helical edge state in the bulk band gap when considering their finite boundaries. The nanoribbons of graphene have been extensively studied in experiments and DFT calculations, but mostly without considering the SOC. Recently, the magnetism of the edge atoms and considering their finite size effect, which can decrease quickly to zeros with much wider nanoribbons. Among the bulk gap, we can clearly see that two degenerated edge states appear, which can be considered as Fermi arcs, like in the case of a Weyl semimetal [55]. In fact, the edge states have nearly parabolic dispersion in the region 

\[ \phi = \frac{2\pi}{3}, \frac{4\pi}{3} \], which may be steadily accessible experimentally, will trigger a topological phase transition from a TI to a BI, where the minus sign of \( \phi \) point within an energy range of 0.14 eV, which would be useful for spintronics devices.

The stanene zigzag nanoribbons

Stanene zigzag nanoribbons

Electronic structure of stanene zigzag nanoribbons

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displacement width of about 83 meV, which is comparable with the bulk SOC gap (74 meV), regardless of
the ribbon width. When turning on the SOC switch (red line), the bulk gap is opened, and for each edge the spin-
degenerated edge states are entirely split. Each spin-up and spin-down edge state connects the conduction band
and valence band providing dissipationless conducting channels and crossing each other at the \( \pi \) point, which is
protected by TRS (time reverse symmetry). This is the famous helical edge state of 2D TIs. Since our system has
a two symmetric zigzag boundaries, the edge states are thus degenerated with respect to the two boundaries.
However, it is worth noting that the shapes of the helical edge state of stanene in our DFT calculations are
also different from previous TB models, where two edge states cross the bulk band gap with perfect linear
dispersion. This is mainly due to oversimplified consideration of these TB models, such as directly overlooking
the NNN hopping term and the difference between the edge atoms and the internal atoms [56, 57]. We will
demonstrate these in detail in the following context.

**Edge magnetism configurations**

The zigzag ribbon of graphene has ferromagnetic order on each edge due to the Stoner instability of a flat edge
state, which results in insulating ground states with inter-edge magnetic coupling [58, 59]. Based on
first principle calculations, we study the interplay of possible edge magnetism and spin–orbital interaction on
the edge states. By considering the in/out-of-plane magnetization direction for each edge and ferro/antiferro
magnetic coupling between different edges, we obtained four types of magnetic configurations: out-of-plane
ferromagnetic (OP-FM), out-of-plane anti-ferromagnetic (OP-AFM), in-plane ferromagnetic (IP-FM) and in-
plane anti-ferromagnetic (IP-AFM), as shown in figures 6(a)–(d). For the \( N = 16 \) zigzag ribbon of stanene, all
four magnetic states have about 7–8 meV/edge atom lower energy than the nonmagnetic states, which clearly
indicates the existence of spontaneous magnetism. Although the OP-AFM configuration has the lowest energy,
the energy difference between the four magnetic configurations is less than about 1 meV. The magnetic moment
is about 0.14 \( \mu_B \) per edge atom.

The band structures for four magnetic configurations are shown in figures 6(e)–(h). The first important
result is that only the OP-FM state has conducting edge channels crossing the Fermi level, while the other three
cases have band gaps indicating insulating states. Thus we hope the transport properties of stanene ribbons will
be greatly affected by the magnetic ordering and magnetization direction.

Due to their helical nature, the spin texture of nonmagnetic edge states (figure 5(c)) in the left and right
boundaries is contrasting. In figure 6(e), for the OP-FM case, the positive local exchange field at each edge will lift
the spin-up edge states and push down the spin-down edge states. As a result, the original crossing (four-fold
degeneracy from two spins and two boundaries) at the \( \pi \) point (figure 5(c)) will split into two boundary-
contrast crossings. One (the other) crossing from the left (right) boundary will shift from the \( \pi \) point to \( K(K') \),

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2 Considering both SOC and magnetism, noncollinear calculations are performed in our DFT calculations. Here we set the initial local magnetic moment for each atom in the \( x, y \) and \( z \) directions respectively, like \( (M_x, M_y, M_z) \), with the unit \( \mu_B \). Specifically, the initial magnetic moments for the outermost Sn atom on the left and right boundaries are \((0, 0, 1)\) and \((0, 0, 1)\) for the OP-FM, \((0, 0, 1)\) and \((-1, 0, 0)\) for OP-AFM, \((1, 0, 0)\) and \((1, 0, 0)\) for IP-FM and \((1, 0, 0)\) and \((-1, 0, 0)\) for IP-AFM, respectively. The initial magnetic moments are set to \((0, 0, 0)\) for the other atoms.
highlighted inside the circles in figure 6(e). The two crossings near the Fermi level are formed by the edge states from the same boundary with opposite spin, which is protected by the conservation of $s_z$. Besides this, there are another two crossings above and below the Fermi level at the $\pi$ point, formed by the opposite edge state with the same spin, which is protected by the super weak inter-edge coupling (or strong localization of the edge states at the $\pi$ point). Although the exchange field breaks the TRS (time reversal symmetry), the SIS (space inversion symmetry) is still reserved. Thus the band is symmetric around the $\pi$ point.

For the OP-AFM state in figure 6(f), the positive exchange field at the right boundary will lift the spin-up and push down the spin-down edge states respectively, which will drive the crossing toward the $K'$ point, which is the same as the OP-FM case. However, the negative exchange field at the left boundary will lift the spin-down edge state and push down the spin-up edge state, which will still drive the crossing towards the $K'$ point. On the other hand, since the recombination symmetry of the SIS and TRS is reserved, all bands are still double–degenerate.

We notice that a band gap of 63 meV opens at the original crossing point (highlighted by a circle), making the system an insulator. We argue that this band gap is derived from the inter–edge interaction due to the finite size effect, and the gap will close when the ribbon width is large enough, as demonstrated in the following (figure 8(b)). As we know, both TRS and SIS are broken for the OP-AFM case, thus one can see the band structure is largely asymmetric around the $\pi$ point, especially around the $K$ and $K'$ points.

When considering the in-plane magnetization with FM and AFM configurations in figures 6(g) and (h), a dramatic change happens. The edge states of both systems are gapped regardless of the width of the ribbon (local band gaps within the circles are 112 meV for AFM and 71.2 meV for FM), indicating the insulating nature. By comparing figures 6(e) and (g), one finds the band gap (figure 6(g)) has little to do with the inter-edge coupling. In fact, it is dominated by the scattering between spin-up and spin-down states at the same edge. Because the in-plane exchange field can mix different spin states, which naturally allow the gap opening. Besides this, the band structures are symmetric with respect to the $\pi$ point due to the SIS. The joint $T$’$P$ symmetry and mirror symmetry operator $M_y$ result in a doubly degenerated and symmetric band structure, respectively, as shown in figure 6(h).

**Modified tight-binding model**

As mentioned before, there is a large difference in the edge state of the zigzag nanoribbon from our DFT calculations compared with the previous TB result. Here we build a much more practical TB model which can well fit the calculation results under various magnetic configurations. Also, based on the TB model, we further study the electronic structure of the large nanoribbon to eliminate the finite size effect and demonstrate the half-metallic properties in the following.

The generic TB Hamiltonian is written as follows [12, 24, 54]:

$$
H = \sum_{\langle ij \rangle, \alpha} h_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \sum_{\langle \langle ij \rangle \rangle, \alpha, \beta} i\Lambda_{\alpha\beta} c_{ij\alpha}^\dagger c_{i\beta}^\dagger c_{j\beta} + \sum_{i \in \{1, N\}, \alpha} M_i c_{i\alpha}^\dagger s_n c_{i\alpha} + \sum_{i, \alpha} V_i c_{i\alpha}^\dagger c_{i\alpha} + \sum_{\langle \langle ij \rangle \rangle, \alpha} t_2 c_{ij\alpha}^\dagger c_{j\alpha},
$$

(2)

where $c_{i\alpha}^\dagger$ creates an electron with spin polarization $\alpha$ at the $i$ site, and $\langle \langle ij \rangle \rangle / \langle \langle ji \rangle \rangle$ run over all the nearest- or next-nearest-neighbor hopping sites. The first term is the nearest-neighbor (NN) hopping term. The second term is the effective intrinsic SOC term. The first two terms determine the electronic and topological properties. The third term is the Zeeman term imposed only on the outermost atoms, which naturally exist for stanene zigzag ribbons. $s_n = \vec{s} \cdot \vec{n}$, where $\vec{n}$ is the magnetization direction. The fourth term is the onsite energy potential, which is different for internal atoms and edge atoms for the nanoribbon. The fifth term is the NNN hopping term, which is usually ignored by others. The hopping parameters $t_1, t_2$ and $\Lambda_{\alpha\beta}$ are obtained by fitting the TB band structure with the DFT results around the $K$ point near the Fermi level for bulk states. The $V_i$ and $t_2$ are modified for edge atoms and obtained by fitting the TB results with the DFT results for zigzag ribbons.

For the nonmagnetic case, the band structure of the TB model is shown in figure 7. In figure 7(a), we first compared the DFT result (red dotted line) with that of the oversimplified TB model [56] (black line), which only considers the first two terms in equation (2). A remarkable discrepancy is observed, which indicates that the oversimplified TB model cannot obtain the correct edge state. In figure 7(b), when we add up the NNN hopping terms and adjust the hopping strength and onsite energy for the edge atoms, the Rashba-like parabolic edge states are reproduced by our more practical TB model, which agrees with the DFT results very well. Because NNN hopping will naturally break the electron–hole symmetry and will thus bend the edge state, the different surroundings between the edge atom and internal atom will also inevitably affect the shape of the edge state. In order to clearly exhibit the edge states and eliminate the finite size effect, the band structures for a large $N = 128$ are calculated based on our TB model, as shown in figures 7(c) and (d). For a zigzag nanoribbon of the graphene series, it is worth noting that very recently the author in reference [60] developed a multi-orbital ($s$, $p_x$, $p_y$, $p_z$) TB model to describe the nonlinear edge states as well as the whole energy spectrum at the cost of more parameters.

Our modified one-orbital TB model with NNN coupling in this letter can be regarded as the downfolding case of
a multi-orbital TB model with NN coupling when the $p_z$ orbital is the dominating component, which well reproduces the DFT results with fewer parameters.

The four magnetic configurations are also stimulated by adding the Zeeman terms in equation (2) with $M = 0.14 \mu_B$. As demonstrated in figures 8(a)–(d), the band structures from TB match well with that of the DFT calculations. By comparing the results of $N = 128$ and $N = 16$, we can clearly see the band gap in figure 8(b) is indeed from the inter-edge coupling and disappears with a large size. The IP-FM and IP-AFM cases always remain as gapped insulating states regardless of the ribbon size. Besides this, we also test the band structure evolutions of the magnetization direction rotating from in-plane to out-of-plane in figure 9. We find that the crossing point of the edge state in the OP-AFM and OP-FM cases will be open as long as the magnetism direction deviates out-of-plane and the gap increases with the increase of the angle. This can be easily explained by the mixing of spin-up and spin-down states due to the appearance of the spin component of $s_z$ or $s_y$ in the Hamiltonian. The dependence of the electronic structure on the magnetization direction has a dramatic effect on its transport properties, such as giant magnetic resistance.

**Half-metallic stanene nanoribbons by applying a transverse electric field**

With joint T'P symmetry, the AFM ground state of the zigzag ribbons of the hexagonal lattice have spin degenerate edge states. By introducing an in-plane transverse electric field and thus breaking the T'P symmetry, the spin degeneracy is lifted and a half-metallic state will be obtained, which is of great importance for its applications in spintronics. Here, we simulate the transverse electric field effect on the stanene zigzag nanoribbons using both the DFT and TB model. For the TB model, the transverse electric field is realized by imposing a linearly varying electric potential $V_i$ in equation (2) for each atom from the left boundary to the right boundary. The band structures and spin texture are shown in figure 10. Taking the IP-AFM configuration for the $N = 16$ ribbon as an example, without an electric field, the band structure including the edge states are spin degenerate with the spin-up (down) from one (the other) edge as shown in figure 10(a). In figure 10(b), when a transverse electric field of 0.01 V Å$^{-1}$ is applied, we find it can effectively drive the system to be a half-metal by lifting up the spin-down state from one side (labeled with a blue arrow) and meanwhile pushing down the spin-down state from the other side (labeled with a red arrow), resulting in the left spin-down channel crossing the Fermi level. The dashed and solid lines represent the DFT and TB results respectively, and fit quite well with each other. When an inverse transverse electric field is applied, a half-metal system with a spin-up channel can be

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**Figure 7.** The band structures for the zigzag ribbons of stanene. The red dotted line represents the DFT result and the black solid line represents the TB results. The oversimplified TB model with only two parameters ($t_1 = 0.74$ eV, $\lambda_m = 0.0072$ eV) in equation (2) is used in (a) and (c) for $N = 16$ and $N = 128$, while our TB model with four terms in equation (2) is used in (b) and (d) for $N = 16$ and $N = 128$. These parameters are chosen as $t_1 = 0.74$ eV, $\lambda_m = 0.0072$ eV, $M = 0 \mu_B$, $t_2 = -0.06 \mu_B$, $V_1 = V_{\text{ex}} = 0.0072$ eV for the bulk (edge) atoms.
reached, as shown in figure 10(c). Thus the spin channel can be easily flipped by changing the sign of the electric field. For large ribbons such as $N = 128$ in figure 10(d), the TB result shows it is also possible to obtain a half-metal state using a proper electric field.

It is worth noting that the half-metallic graphene ribbon [31] is required to have a size effect to open a gap, so the width of the ribbon has an upper limit. However, the half-metallic stanene ribbons designed by us break this limit, because for the stanene ribbon here, the gap is opened by the much larger SOC rather than the size effect. In this respect, our designed half-metallic stanene ribbon is more readily experimentally confirmed and further applied.

**Discussion and conclusion**

We have systematically investigated the electronic and topological properties of the bulk state of stanene. Based on first principle calculations, we systematically studied the electric field and external strain effects on the electronic and topological properties of stanene. We find that both 1.5% compressive and 2% extensive strain...
can induce IMT. Furthermore, the vertical electric field can induce a topological nontrivial to trivial phase transition.

Combined with a more practical tight-binding model, we also systematically studied the topological edge states of zigzag nanoribbons of stanene, considering SOC and edge magnetism effects. First, we find that the helical edge states share a nonlinear dispersion relation, which can be well reproduced by adding the NNN hopping term and taking into account the difference between the edge and inner atoms in our TB model. Second, four different magnetic edge configurations are considered and it is found that only the OP-FM state has conducting edge channels crossing the Fermi level, while the other three cases have band gaps indicating insulating states. Thus, by changing the magnetization direction one can switch off/on the edge conducting channels of the zigzag nanoribbon. Third, we find that applying a transverse electric field can induce a half-metallic state with only one kind of spin channel in the stanene nanoribbons, and the other kind of spin channels can also be easily obtained by just reversing the transverse electric field. Thus our designed stanene half-metallic ribbon has promising prospects for use in magnetic control and spintronics. Finally, the above analysis methods and conclusions are very timely and can be steadily implemented with other 2D bulked honeycomb lattice materials such as germanene and silicene.

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Figure 10. The evolution of the band structures under transverse electric fields for a stanene nanoribbon with an IP-AFM configuration. The small arrows stand for opposite spin, the red (blue) color represents the opposite edge location of the edge states. (a) The band structure without an electric field for \( N = 16 \). (b), (c) The band structures from DFT (dashed lines) and TB (solid lines) with transverse electric fields for \( N = 16 \). The electric field is chosen as 0.01 V Å\(^{-1}\) and −0.01 V Å\(^{-1}\) in (b) and (c) in the DFT calculations, and the corresponding parameters in the TB model are 0.13/W V and −0.13/W V, where W is the width of the ribbons. (d) The TB model results in a larger size of \( N = 128 \) with a transverse electric field of 0.06/W V.
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