Zigzag nanoribbons of two-dimensional silicene-like crystals: magnetic, topological and thermoelectric properties

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Abstract
The effects of electron–electron and spin–orbit interactions on the ground-state magnetic configuration and on the corresponding thermoelectric and spin thermoelectric properties in zigzag nanoribbons of two-dimensional hexagonal crystals are analysed theoretically. The thermoelectric properties of quasi-stable magnetic states are also considered. Of particular interest is the influence of Coulomb and spin–orbit interactions on the topological edge states and on the transition between the topological insulator and conventional gap insulator states. It is shown that the interplay of both interactions also has a significant impact on the transport and thermoelectric characteristics of the nanoribbons. The spin–orbit interaction also determines the in-plane magnetic easy axis. The thermoelectric properties of nanoribbons with in-plane magnetic moments are compared to those of nanoribbons with edge magnetic moments oriented perpendicularly to their plane. Nanoribbons with ferromagnetic alignment of the edge moments are shown to reveal spin thermoelectricity in addition to the conventional one.

Keywords: silicene, magnetic order, thermoelectric effects

(Some figures may appear in colour only in the online journal)
interaction gives rise to a magnetic anisotropy, and when this coupling is sufficiently strong, an in-plane orientation of the edge moments is energetically more favourable [8]. Thus, the interplay of spin–orbit and Coulomb interactions is of fundamental importance for the edge magnetism.

The spin–orbit interaction in the materials under consideration also leads to topologically protected edge states in the spin–orbit gap [27], which are responsible for their topological properties [28, 29]. However, Coulomb interaction has a significant influence on these properties [30]. Thus, the interplay of spin–orbit and Coulomb interactions is important not only for the edge magnetism, but also for the topological state of these materials. Therefore, in this paper we consider the influence of Coulomb interaction and spin–orbit coupling on the transport properties of zigzag nanoribbons of two-dimensional buckled hexagonal crystals. We focus on the thermoelectric and spin thermoelectric properties of these materials in the ballistic transport regime, and on their dependence on the Coulomb and spin–orbit interactions. First, we calculate the energy of various magnetic configurations in zigzag nanoribbons, and find that the antiparallel configuration with in-plane magnetic moments is the ground state structure for large enough spin–orbit coupling [8]. For small spin–orbit coupling, the in-plane and perpendicular-to-plane configurations are roughly degenerate. Then, we calculate the electronic states with the main focus on the edge states responsible for topological properties. Having determined the magnetic state and also the electronic edge states, we calculate thermoelectric properties with the main focus on the role of topological edge states and transition from the topological to conventional insulator state.

Generally, the thermoelectric and especially the spin thermoelectric effects in systems of reduced dimensionality are currently of great interest [31–38], mainly due to the hope of finding an efficient way to convert dissipated heat into electrical energy. Indeed, thermoelectric properties of silicene-like nanoribbons have been studied theoretically in a couple of papers [39–43]. However, the role of Coulomb interaction and topological edge states in the gap has not been studied thoroughly enough yet. In a recent paper [44] we analysed the influence of topological states on the thermoelectric properties, with the main focus on the role of a staggered exchange field [5–7] and of an electric field perpendicular to the atomic plane. Only the regime of small spin–orbit coupling was considered there, with the edge magnetic moments oriented perpendicularly to the nanoribbon plane. Here, we consider in more detail the role of Coulomb interaction [30], and also the influence of strong spin–orbit coupling, when the edge magnetic moments are oriented in the nanoribbon plane [8]. In addition, we consider phase transitions between topological and conventional insulator states and the associated changes in the thermoelectric properties which occur with increasing spin–orbit coupling.

In section 2 we present the Hamiltonian used to describe the 2D materials under consideration, and also introduce briefly the method used to calculate the transmission function, and then all the thermoelectric and transport coefficients. In section 3 we present numerical results on the edge magnetism, topologically protected states, and thermoelectric properties of the corresponding zigzag nanoribbons. A summary and final conclusions are in section 4.

2. Theoretical description

2.1. Tight-binding Hamiltonian

The zigzag nanoribbons of hexagonal 2D crystals like silicene or germanene, which are analysed in this paper, consist of N zigzag atomic chains. The system can be described by the Hamiltonian of the following general form:

\[ H = H_{\text{tb}} + H_{\alpha \sigma} + H_{e-e}. \]

where the first term, \( H_{\text{tb}} \), is the tight-binding Hamiltonian, the term, \( H_{\alpha \sigma} \), represents the spin–orbit coupling, while the last term, \( H_{e-e} \), stands for the electron–electron Coulomb interaction.

The tight-binding Hamiltonian is assumed in the form

\[ H_{\text{tb}} = -t \sum_{\langle i,j \rangle} c^\dagger_{i\sigma} c_{j\sigma}, \]

where \( c^\dagger_{i\sigma} \) (\( c_{i\sigma} \)) is the creation (annihilation) operator for an electron with spin \( \sigma = \uparrow, \downarrow \) at the lattice point \( i \) (\( j \)). The spin quantisation axis is taken along the z-axis, which is normal to the nanoribbon plane. The tight-binding term is restricted here to electron hopping between nearest-neighbour sites, with the corresponding hopping parameter \( t \). For instance, \( t = 1.6 \) eV in silicene [5]. In the following we present energy in relative units, \( E_{\text{f}} \), so the results are also applicable to germanene and stanene.

The intrinsic spin–orbit interaction in equation (1) follows from electron hopping between next-nearest-neighbours in the hexagonal lattice, and can be written in the form [7],

\[ H_{\alpha \sigma} = i \lambda_{\alpha \sigma} \sum_{\langle i,j \rangle} \nu_{ij} (c^\dagger_{i\uparrow} c_{j\downarrow} - c^\dagger_{i\downarrow} c_{j\uparrow}), \]

where \( \lambda_{\alpha \sigma} \) is the spin–orbit interaction parameter, while \( \nu_{ij} = 1 \) (\( \nu_{ij} = -1 \)) when the hopping path from second-neighbour sites \( i \) to \( j \) in the hexagonal lattice is clockwise (anticlockwise) with respect to the positive z-axis.

The electron–electron interaction will be taken into account in the Hubbard form within the mean-field approximation (MFA). The form of the MFA Hubbard Hamiltonian depends on whether the spin quantisation axis is parallel to the local magnetisation orientation or not. We assume, similarly to Lado et al [8], that in a hypothetical state the magnetic moments are tilted from the normal orientation by an angle \( \alpha \), and will calculate the corresponding total energy. The ground state configuration will be thus the one with the lowest energy. Assuming the quantisation axis parallel to the local magnetic moments, the Hubbard term in the mean-field approximation can be written in the form

\[ H_{e-e} = U \sum_i (n^\sigma_{i\uparrow} n^\sigma_{i\uparrow} - n^\sigma_{i\uparrow} - n^\sigma_{i\downarrow} + n^\sigma_{i\downarrow}) \]

where \( n^\sigma_{i\uparrow} \) and \( n^\sigma_{i\downarrow} \) are the particle number operators for a site \( i \) and for electrons with spin \( \uparrow \) and \( \downarrow \) with respect to the spin quantisation axis tilted from the normal to the plane towards
a nanoribbon edge by an angle $\alpha$. In turn, $U$ is the on-site Coulomb repulsion parameter, $U > 0$. We also note that the Coulomb interaction of electrons at different lattice sites is omitted.

The MFA Hubbard Hamiltonian should be now written in the quantisation axis common for all terms of the Hamiltonian. This can be done by rotating the quantisation axis back to the orientation normal to the plane, which is achieved by the transformation [45]

$$c_{ia}^\dagger = \cos \left( \frac{\alpha}{2} \right) c_{ia} - \hat{s} \sin \left( \frac{\alpha}{2} \right) c_{i-\sigma}$$

(5)

where $\hat{s} = (\hat{a}^\dagger - 1)$ for $\sigma = \uparrow$ ($\sigma = \downarrow$).

The spin-dependent mean number of electrons, $\langle n_{0a}^\sigma \rangle$, at a site $i$, required to evaluate the Hubbard interaction term (4), is determined self-consistently from the band-structure of the corresponding nanoribbon,

$$\langle n_{0a}^\sigma \rangle = \sum_{\text{bands}} \frac{a}{2 \pi} \int_0^{2\pi/a} n_{0}^\sigma(k) f[E(k), \mu] \, dk,$$

(6)

where $f(E, \mu)$ is the Fermi–Dirac distribution function, with $\mu$ denoting the chemical potential, while $n_0^\sigma(k)$ is the spin-dependent electron density at site $i$ for a Bloch-wave of energy $E(k)$. The parameter $a$ denotes the length of the elementary cell of a zigzag nanoribbon. The chemical potential of a pristine nanoribbon is equal to the corresponding Fermi energy $E_F$. By doping with donor or acceptor impurities, or by applying an external gate voltage, one can shift up or down the Fermi level, and its position with respect to $E_F$ will be described by $\mu - E_F$. In the following $\uparrow$ and $\downarrow$ will denote spin projection on the quantisation axis parallel to the orientation of the magnetic moments.

To identify the edge-states, we evaluate the mean value of $\xi = 2(y - y_0)/w$, where the $y$-axis is on the nanoribbon plane and normal to the nanoribbon axis, $y_0$ is the $y$-coordinate of the nanoribbon centre, while $w$ is the width of the nanoribbon. For $\xi = -1$ ($\xi = 1$), the states are localised at the left-hand (right-hand) edge of the nanoribbon.

In general, the electronic properties of the nanoribbons depend on their width $w$ [46]. However, since the contribution of the edge states to the thermoelectric properties is only weakly dependent on $w$ [44], to show the main features of these properties at the topological transitions we have chosen a representative value of $w = 52 \, \text{Å}$ (corresponding to $N = 16$ dimers in the zigzag chain).

### 2.2. Electronic transmission and general formulas for thermoelectric coefficients

We consider a ballistic transport regime, when the corresponding mean free path is longer than the system’s length. The ballistic electronic transmission in quasi-one-dimensional structures is usually determined in terms of the Green’s function formalism and an expression derived by Caroli et al [47]. An alternative approach is based on matching wave functions in the scattering region to the Bloch modes of ideal bulk leads [48]. The total transmission, $T_{\text{tot}}(E)$, as a function of electron energy $E$ is then defined as the sum of transmissions for all incident Bloch waves for a given wave-number $k$, and is a piece-wise constant function equal to the number of energy bands for a given energy $E$. When we change energy, then each time the energy enters a new electron band, the transmission function increases step-wise by unity. If a particular band is relatively flat, then the corresponding contribution to the transmission function appears as a narrow peak.

The spin transmission, $T_{\text{spin}}$, is equal to the sum of the mean values of the Pauli operator $\hat{s}$. A more detailed description of the transmission calculation is presented in [44]. The total transmission, $T_{\text{tot}}$, and spin transmission, $T_{\text{spin}}$, are related to the spin-dependent transmission, $T_{\sigma}$ ($\sigma = \uparrow$, $\downarrow$), as $T_{\text{tot}} = T_{\uparrow} + T_{\downarrow}$ and $T_{\text{spin}} = T_{\uparrow} - T_{\downarrow}$, respectively.

Knowledge of the transmission function $T_{\sigma}(E)$ allows the calculation of all transport characteristics in the linear response regime, including also the thermoelectric properties. The spin resolved transport and thermoelectric coefficients can then be determined from the moments $L_{\text{mes}}$ of the electronic current series expansion around the Fermi level,

$$L_{\text{mes}} = -\frac{1}{\hbar} \int_{-\infty}^{\infty} T_{\sigma}(E) (\mu - E)^{\mu} \frac{\partial f(E, \mu)}{\partial E} \, dE.$$

(7)

For a piece-wise constant transmission function, the calculation of $L_{\text{mes}}$ can be reduced to the calculation of the so-called incomplete Fermi–Dirac integral [44],

$$F_{\mu}(x) = \frac{1}{m!} \int_{-\infty}^{\infty} \frac{z^{m} \, dz}{1 + e^{z}}, \quad \text{for} \, \, x \geq 0,$$

(8)

for which there exists an efficient numerical procedure [49].

The spin-dependent conductance $G_{\sigma}$ is proportional to the moment $L_{\text{mes}}, G_{\sigma} = e^2 L_{\text{mes}},$ where $e$ is the electron charge. The total conductance $G$ is then equal to $G_{\uparrow} + G_{\downarrow}$, and the spin conductance is described by $G_{\sigma} = G_{\uparrow} - G_{\downarrow}$. The heat conductance is defined at the vanishing charge current and can be written as $\kappa = (1/\hbar) \sum_{\sigma} (L_{2\sigma} - L_{\sigma}^2) L_{\text{mes}}$, where $T$ stands for temperature. In turn, the spin-dependent thermoelectric coefficient (thermopower) $S_{\sigma}$ can be expressed in the form

$$S_{\sigma} = -\frac{1}{|e| T} L_{1\sigma},$$

(9)

for $\sigma = \uparrow, \downarrow$. Then, one can define the conventional (charge) Seebeck coefficient (thermopower) as $S_c = \frac{1}{2} (S_{\uparrow} + S_{\downarrow})$ and also the corresponding spin Seebeck coefficient (spin thermopower) as $S_s = \frac{1}{2} (S_{\uparrow} - S_{\downarrow})$ [37]. When the spin thermopower is absent, one can write the conventional Seebeck coefficient $S$ ($S_{\sigma} \rightarrow S$) in the standard form $S = -(1/|e| T)(L_{1\uparrow} + L_{1\downarrow})/(L_{0\uparrow} + L_{0\downarrow}) = -(1/|e| T)(L_{1\uparrow}/L_{0\uparrow})$, with $L_{n} = L_{n\uparrow} + L_{n\downarrow}$ for $n = 0, 1, 2$. In turn, the electronic contribution $\kappa$ to the thermal conductance is given by $\kappa = (1/|e| T)(L_2 - L_1^2/L_0)$.

Finally, one can define the dimensionless figures of merit for the conventional and spin thermoelectric effects,

$$Z_c T = \frac{S_c^2 G T}{\kappa + \kappa_{ph}},$$

(10a)
\[ \kappa_{\text{ph}} = \frac{Z T S G T}{\kappa + \kappa_{\text{ph}}}, \]

where \( \kappa_{\text{ph}} \) is the phonon contribution to the heat conductance. In the absence of spin thermoelectricity, only the dimensionless figure of merit for the conventional thermoelectricity is relevant (\( ZT \rightarrow ZT_c \)), and

\[ Z T = \frac{S^2 |G| T}{\kappa + \kappa_{\text{ph}}}. \] (10b)

3. Numerical results

In this section we present some numerical results on the basic thermoelectric properties. Before this, however, we consider various stable and quasi-stable magnetic states of the nanoribbons. Then, we consider separately the antiferromagnetic (AFM) states, with magnetic moments at one edge being antiparallel to the magnetic moments at the other edge, and ferromagnetic (FM) states, with parallel alignment of all the edge moments.

3.1. Stability diagram

We performed numerical calculations of the total energy of nanoribbons with the edge magnetic moments tilted by an angle \( \alpha \) from the orientation normal to the nanoribbon plane, for \( \alpha \) ranging from \( \alpha = 0 \) to \( \alpha = \pi/2 \). The calculations were carried out for both FM and AFM magnetic configurations.

The numerical results clearly show that the states for \( \alpha = 0, \pi/2 \) are neither stable nor quasi-stable. The only stable or quasi-stable states are those for \( \alpha = 0 \) (moments normal to the plane) and \( \alpha = \pi/2 \) (moments in the nanoribbon plane). This applies to both FM and AFM configurations. From this analysis, we have constructed the stability diagram of the FM and AFM states. From this analysis, we have constructed the stability diagram of the FM and AFM states. From this analysis, we have constructed the stability diagram of the FM and AFM states. From this analysis, we have constructed the stability diagram of the FM and AFM states. From this analysis, we have constructed the stability diagram of the FM and AFM states. From this analysis, we have constructed the stability diagram of the FM and AFM states. From this analysis, we have constructed the stability diagram of the FM and AFM states.
obtained by Lado et al [8]. Both AFM⊥ and FM⊥ states correspond to energies higher than that of the AFM∥ state, and the energy difference strongly increases with the spin–orbit parameter. As one might expect, the AFM⊥ and AFM∥ states are practically degenerate in the limit of small values of λso. In turn, the energy of the FM⊥ state is considerably higher than the energy of the AFM⊥ state, and the difference increases roughly linearly with increasing U. Interestingly, the energy difference between the perpendicular phases AFM⊥ and FM⊥ for a given U decreases with increasing λso, so these two configurations become almost degenerate for strong spin–orbit coupling and moderate values of the Hubbard parameter U. Finally, in the limit of λso → 0, the states AFM∥ and AFM⊥ are fully degenerate for all relevant values of U (figure 2(a)), whereas the FM states are quasi-stable and correspond to higher values of energy.

Below we will analyse the transport and thermoelectric properties of the AFM∥ ground state as well as of the quasi-stable states AFM⊥, FM⊥ and FM∥. Although the quasi-stable states correspond to energies larger than the energy of the ground-state, they can be stabilised by some external forces. Ferromagnetic states FM⊥ and FM∥ can be stabilised, for instance, by an external magnetic field. Apart from this, these states as well as the AFM⊥ state can be stabilised by exchange coupling to adjacent magnetic contacts.

### 3.2. Phonon heat conductance

To calculate some of the thermoelectric parameters like thermoelectric efficiency (figure of merit), one needs to know not only the electronic contribution κ to the heat conductance, but also the corresponding phonon term κph. In a recent paper Yang et al [50] determined the phonon contribution to the heat conductance in narrow germanene and silicene nanoribbons, utilising the Landauer formula (ballistic transport approximation) and the phonon transmission functions calculated by an ab initio method. We checked that κph presented by Yang et al [50] scales linearly with the nanoribbon width, and then extrapolated κph up to zigzag nanoribbons containing N = 16 zigzag chains (32 atoms in the zigzag chain), which are considered in this paper. We obtained the following values for

![Figure 2](image_url)

**Figure 2.** Energy difference ∆E per unit cell for N = 16 zigzag nanoribbons, between the (a) AFM⊥, FM⊥, (b) FM∥ states and the AFM∥ ground state, presented as a function of the Hubbard parameter U for the indicated values of the spin–orbit parameter λso.
$N = 16$ and $T = 100$ K: $\kappa_{ph} = 0.92 \text{nW K}^{-1}$ for germanene, and $\kappa_{ph} = 1.09 \text{nW K}^{-1}$ for silicene. Thus, for the model calculations we take $\kappa_{ph} \approx 1 \text{nW K}^{-1}$ in equations (10) and (10a).

3.3. Antiferromagnetic phases

Now we analyse the ballistic transport and thermoelectric properties in the AFM configuration in more detail. The corresponding electronic states for the AFM $\perp$ (left panel) and AFM $\parallel$ (right panel) configurations are presented in figure 3 for three different values of the spin–orbit parameter. The corresponding transmission functions are presented in figure 4. The lowest value of $\lambda_{so}$ assumed in these figures is comparable to the spin–orbit parameter $\lambda_{so} = 3.9 \text{ meV}$ typical for silicene [51] (note the factor $3\sqrt{3}$ in the definition of spin–orbit coupling in this reference). However, larger values of the parameter $\lambda_{so}$ can appear in other related two-dimensional crystals, like germanane [52] ($\lambda_{so} = 43 \text{ meV}$) or stanene [52] ($\lambda_{so} = 29.9 \text{ meV}$). Moreover, the results for larger values of the spin–orbit parameter are very interesting from the point of view of the topological properties. Therefore, in numerical calculations of the band structure, transmission and thermoelectric coefficients we assume the following three values of $\lambda_{so}$: $\lambda_{so} = 0.02t = 32 \text{ meV}$ (strong spin–orbit coupling), $\lambda_{so} = 0.01t = 16 \text{ meV}$, and $\lambda_{so} = 0.001t = 1.6 \text{ meV}$ (weak spin–orbit coupling). In turn, for the electron–electron interaction we assume $U = 1.4 \text{ eV} = 0.875t$, typical for silicene.

To emphasise the behaviour of the edge states which are responsible for topological properties, we show in figures 3 and 4 only a small energy region near the Fermi level $E_F$ of the corresponding charge-neutral nanoribbon. Moreover, only the region of wavevectors $k$, in which the states are strongly localised near the left (L) or right (R) edges of the nanoribbons is presented there. As follows from these figures, the electronic spectra reveal an insulating gap for small values of $\lambda_{so}$, and this gap appears in both the AFM $\perp$ and AFM $\parallel$ phases. Moreover, the width of the gap is practically the same in both cases. Note that such a gap is absent in the limit of $U = 0$, when zero-energy topologically protected states appear [44]. Furthermore, the valence and conduction states localised at...
the left and right-hand edges are degenerate in both phases. These states are additionally spin degenerate.

Qualitatively different behaviour can be observed for larger values of $\lambda$. The edge states are then still degenerate, but in the AFM phase they cross the Fermi level, so the system acquires properties of a topological insulator, whereas the AFM/uni phase still exhibits properties of a conventional insulator. Thus, at a certain value of $\lambda$, there is a transition from the conventional to topological insulator in the AFM phase, while no such transition appears in the AFM/uni phase. Moreover, one may conceive that by applying an appropriate external magnetic field it would be possible to switch between the AFM and AFM/uni states, and thus also to change the character of the system from a conventional to a topological insulator, and vice versa. The opening of an energy gap near the Fermi level at the transition from the AFM⊥ state to the AFM/uni phase has a significant influence on the transport and thermoelectric properties of the system. The electrical conductance $G$ and the thermal conductance $\kappa$ due to electrons are practically equal to zero in the wide energy regions near the Fermi level $E_F$, which correspond to the energy gaps in the electronic spectrum. Then they strongly increase at the gap edges, see figure 5. This figure shows both $G$ and $\kappa$ as a function of the chemical potential, and for both the AFM/uni and AFM⊥ (insets) phases. Interestingly, both $G$ and $\kappa$ in the AFM/uni state remarkably depend on $\lambda_{so}$. This is rather obvious as the corresponding gap in the spectrum (see figures 3 and 4) significantly depends on the spin–orbit coupling parameter. On the contrary, owing to the transition to the topological insulator state in the AFM⊥ phase and the closure of the gap for large enough spin–orbit coupling, both $G$ and $\kappa$ are then constant and nonzero for chemical potentials in the region around $E_F$ (see the insets in figure 5).

Figure 4. Transmission function for the AFM⊥ (top panel) and AFM/uni (bottom panel) phases, calculated for the same parameters as in figure 3.
Due to the difference in the edge states, both the AFM\(\perp\) and AFM\parallel\(\perp\) phases also display remarkably different thermoelectric properties, especially the Seebeck coefficient (thermopower), see figure 6. Owing to the gap in the AFM\parallel\(\perp\) phase, see figure 4, the thermopower \(S\) considerably increases for chemical potentials in the vicinity of the Fermi level \(E_F\), achieving very high
Figure 7. Figures of merit $ZT$ for the AFM|| configuration, calculated as a function of the chemical potential for the indicated values of $\lambda_{so}$ and $T = 100 \, K$. The other parameters are as in figure 2. The inset shows the corresponding results for the AFM⊥ state.

Figure 8. Electronic structure for the FM⊥ (left panel) and FM|| (right panel) configurations, and for the indicated values of $\lambda_{so}$. The vertical lines denote the interval of wavevector $k$, where the edge parameter $\xi$ obeys the condition $|\xi| > 0.5$. The assumed parameters are: $U = 0.875t$ and $N = 16$. 
values at low temperatures. Since the gap remarkably depends on the spin–orbit coupling, the thermopower also significantly depends on $\lambda_{so}$. The situation in the AFM $\perp$ state is different. Now, the gap disappears for large values of $\lambda_{so}$, so the thermopower remains zero in a broad region of chemical potentials around $E_F$, see the inset in figure 6. Then smaller peaks appear due to the narrow peaks in transmission around $E \approx \pm 0.1t$, as shown in figure 4.

The presented results show that nanoribbons with relatively strong spin–orbit coupling and exhibiting AFM $\perp$ magnetic configuration may be attractive for applications for the conversion of thermal into electrical energy. The corresponding thermoelectric efficiency, described by the figure of merit $ZT$, is shown in figure 7. Unfortunately, $ZT < 1$, so the thermoelectric efficiency is below that anticipated for practical applications. However, one may conceive some ways of reducing the phonon heat conductance in order to increase $ZT$.

### 3.4. Ferromagnetic phases

Now we analyse the ferromagnetic arrangement of the edge moments and compare the results with those obtained for the corresponding antiferromagnetic phase, as presented and discussed above. Both the FM $\perp$ and FM $||$ configurations are quasi-stable states with the corresponding larger energy of the AFM $\perp$ ground state. The ferromagnetic configurations, however, can be stabilised externally by a magnetic field or due to proximity effects, as already mentioned above.

The calculated band structure near the Fermi level $E_F$ is presented in figure 8 for both the FM $\perp$ and FM $||$ phases, whereas the corresponding spin-dependent transmission functions are shown in figure 9. Note the spin degeneracy is now lifted. As in the AFM configurations, the electronic spectra of both the FM $\perp$ and FM $||$ phases are similar for small values of $\lambda_{so}$, but both phases are now in the topological insulator state. This situation changes for larger values of $\lambda_{so}$. According to figure 8, the FM $||$ phase remains in the topological insulator state, independent of the spin–orbit interaction strength assumed in this figure. However, significantly different qualitative behaviour is obtained for the FM $\perp$ phase. As the system is in the topological insulator phase for very small values of $\lambda_{so}$, its character changes for stronger spin–orbit interaction, and the system transforms into a conventional insulator with a relatively wide energy gap. It is interesting to note that the range of $k$-wavevectors, where the edge states appear in the FM $||$ phase (see the dotted vertical lines in figure 8), is much narrower than in the corresponding FM $\perp$ state, as well as in the previously discussed AFM phases.

The opening of an energy gap in the FM $||$ phase with increasing $\lambda_{so}$ and the absence of such a gap in the FM $\perp$ state.
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can be clearly seen in figure 9, where the spin-dependent transmission function is presented as a function of energy. It is worth noting that the transmission function corresponding to a particular spin orientation, up or down, is asymmetrical near the Fermi level, i.e., transmission in the spin-up channel exhibits a peak above $E_F$, while the appropriate peak in the spin-down channel appears below the Fermi energy. This practically applies to both the FM/uni and FM $\perp$ configurations.

The width of the energy gap in the FM/uni state increases with increasing $\lambda$. However, no gap appears in the FM $\perp$ phase. Thus, the situation is remarkably different from that in the AFM configurations discussed above.

In the ferromagnetic phases, the two spin channels contribute differently to electronic transport. If the spin relaxation time is long and therefore the spin mixing is negligible, the spin-up and spin-down channels can be treated as independent. One can then distinguish the contributions of individual spin channels to the electrical conductance (and also to the Seebeck coefficient). The spin-resolved electrical conductance for the case of strong spin–orbit coupling is presented in figure 10(a) as a function of chemical potential. The wide central region with the conductance close to zero in the FM/uni phase corresponds to the energy gap in the electronic spectrum. The conductance strongly increases for chemical potentials near the gap edges, where it also remarkably depends on the spin orientation. In turn, the conductance in the FM $\perp$ phase is finite and constant in a wide region of chemical potentials near the Fermi level $E_F$ (see the inset in figure 10(a)). The two peaks outside this region correspond to the enhanced transmission in narrow regions of chemical potential for the spin-up ($\mu > E_F$) and spin-down ($\mu < E_F$) channels, which appear near $E \approx \pm 0.1t$.

The thermal conductance due to electrons is shown in figure 10(b) for the medium and strong spin–orbit interactions. The conductance is suppressed in the regions of chemical potential corresponding to the gaps in the electronic spectrum (and in transmission functions). Accordingly, the gap in thermal conductance is wider for stronger spin–orbit coupling.
In turn, there is no gap in the FM\(\perp\) state, so the heat conductance remains finite and constant around the Fermi level, see the inset in figure 10(b). The peaks outside this region are due to enhanced transmission, as can be clearly seen in figure 9.

In addition to the conventional thermopower, one can now also define the spin thermopower. Both the charge \(S_c\) and spin \(S_s\) Seebeck coefficients are presented in figure 11 for two values of the parameter \(\lambda_{so}\). Due to the energy gap in the FM\(\parallel\) state, the conventional Seebeck coefficient \(S_c\) is considerably enhanced in the vicinity of the Fermi level. The enhancement strongly depends on \(\lambda_{so}\) and increases for higher values of the spin–orbit coupling. Similarly, the spin thermopower \(S_s\) also exhibits a very pronounced peak for a narrow region of chemical potential near \(E_F\), and then remains rather small for chemical potentials outside this region. The peak in \(S_s\) is very narrow, much narrower than the relevant energy gap. Furthermore, the height of the peak strongly depends on the spin–orbit parameter. Remarkably different behaviour was obtained for the FM\(\perp\) phase, which exhibits typical topological insulator features. Now the \(S_c\) and \(S_s\) Seebeck coefficients are vanishingly small for chemical potentials in the vicinity of the Fermi level, as shown in the insets in figure 11). The small peaks which appear for higher values of \(|\mu - E_F|\) follow from the narrow peaks in the corresponding transmission functions, see figure 9.

Let us now consider briefly the corresponding thermoelectric efficiency. The figures of merit for the conventional and spin thermoelectricity are shown in figures 12(a) and (b), respectively. Significant values of the figures of merit occur only in some of the regions of enhanced thermopower. Both \(Z_c T\) and \(Z_s T\), however, are relatively small, similar to the case of the AFM configurations. However, the spin figure of merit is especially small, even if the corresponding spin thermopower is relatively high. This is because the spin thermoelectric efficiency in the narrow region of chemical potential around \(E_F\), where the relatively high peak appears in the spin thermopower, is negligible (compare figures 11(b) and 12(b)). This suppression of \(Z_s T\) appears due to the vanishingly small spin conductance in this region of chemical potential (note, the transmission functions for both spin orientations are equal in this region, see figure 9).
4. Summary and conclusions

We have analysed the influence of Coulomb and spin–orbit interactions in nanoribbons of 2D buckled hexagonal crystals with zigzag edges on the edge magnetic moments and on the topological and thermoelectric properties. We have shown that the Coulomb interaction, taken in the form of the Hubbard term in the mean field approximation, leads to the formation of the edge magnetic moments, which for a sufficiently strong spin–orbit coupling are oriented on the nanoribbon plane in the ground state, and the moments at one edge are opposite to those at the other edge (AFM//uni2225 phase), in agreement with Lado et al [8]. For small spin–orbit coupling, this configuration is almost degenerate with the state in which magnetic moments are oriented perpendicular to the nanoribbon plane (AFM⊥uni2225 phase). States with a ferromagnetic arrangement of the moments (FM// and FM⊥ phases) are quasi-stable and correspond to higher energies. Such states can be stabilised externally, e.g. by a magnetic field and/or due to proximity to ferromagnetic contacts.

As the AFM|| phase remains in the gap insulator state when the spin–orbit coupling increases, the AFM⊥ phase then undergoes a transition from the conventional to the topological insulator, i.e. the energy gap in the corresponding edge states becomes closed. This gap closure has a significant influence on transport and thermoelectric properties. First of all, the gap is associated with a nonzero thermopower in the vicinity of the gap edges. When the gap becomes closed, the thermopower is suppressed.

The ferromagnetic quasi-stable states, FM|| and FM⊥, also behave differently with increasing $\lambda_{so}$. This behaviour qualitatively resembles that of the antiferromagnetic phases, but now the gap in the FM|| state, which opens with increasing $\lambda_{so}$, is spin dependent. Since the spin degeneracy is lifted in both ferromagnetic phases, a nonzero spin thermopower may be observed, in addition to the conventional one.

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