Proceedings of the European Conference Physics of Magnetism, Poznań 2017

Effect of Magnetic Zigzag Edges in Graphene-like Nanoribbons on the Thermoelectric Power Factor

S. Krompiewski[a,*] and G. Cuniberti[b,c,d]

[a]Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznań, Poland
[b]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany
[c]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany
[d]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

This study shows that magnetic edge states of graphene-like nanoribbons enhance effectively the thermoelectric performance. This is due to the antiparallel alignment of magnetic moments on opposite zigzag edges and the confinement effect, which jointly lead to the appearance of a gap in the electronic energy spectrum. Consequently, the Seebeck coefficient as well as the thermoelectric power factor get strongly enhanced (with respect to other alignment cases) at room temperature and energies not far away from the charge neutrality point. Moreover the corresponding figure of merit (ZT) is also improved as a result of the reduced electronic thermal conductance.

DOI: 10.12693/APhysPolA.133.535
PACS/topics: 73.63.Kv,72.25.-b,73.50.Lw

1. Introduction

The present studies are focused on the search for new materials for modern electronics. In view of the quickly progressing miniaturization process, these materials have to be scalable, i.e. they must maintain their physical properties even if they are extremely small (of the order of 1nm) when the principles of quantum mechanics start being in force. It is important to make use of not only the electron charge but its spin, too, so as to enhance technological capabilities. Then spintronics as well as spin caloritronics (in the context of thermal transport) come into play. Here, of main interest are silicene, germanen and stanene (2D-Sn) – the structures akin to graphene but with some buckling and significant intrinsic spin-orbit coupling. Although graphene gives great hope for future electronics [1, 2], its thermal conductivity is very high and hence its figure of merit is quite low.

2. Methodology

The model which has been proved to provide a good description of graphene-like nanostructures reads as follows (see [3,4] and references therein)

$$H_0 = -\sum_{\langle i,j\rangle,\sigma} t_{i,j} c^+_{i\sigma} c_{j\sigma} + H(\theta) + H_{ISOI} + H_V, \quad (1)$$

where the hopping parameter is the energy unit, $t = 1$, and the second term takes into account intraatomic Coulomb interactions for both in-plane and out-of-plane magnetic moment alignments ($\theta = \pi/2$ and 0, respectively). Specifically, in terms of the creation and annihilation operators (c, c$^+$):

$$H(\theta) = U\sum_i [\delta_{\theta,0}(\langle n_{i\downarrow}\rangle n_{i\uparrow} + \langle n_{i\uparrow}\rangle n_{i\downarrow} - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle) - \delta_{\theta,\pi/2}(\langle S^+_i\rangle S^-_i + \langle S^-_i\rangle S^+_i - \langle S^+_i\rangle\langle S^-_i\rangle)], \quad (2)$$

with U=t and

$$n_{i\sigma} = c^+_{i\sigma} c_{i\sigma}, S^+_i = c^+_{i\uparrow} c_{i\downarrow}, S^-_i = c^+_{i\downarrow} c_{i\uparrow}, \sigma = \uparrow, \downarrow . \quad (3)$$

The last two terms describe the effect of the intrinsic spin-orbit interaction (ISOI) and an external electrical gate voltage (V) applied perpendicularly to the nanostructure.

$$H_{ISOI} + H_V = it_{SO} \sum_{\langle\langle i,j\rangle\rangle} \nu_{i,j}(c^+_{i\uparrow} c_{j\uparrow} - c^+_{i\downarrow} c_{j\downarrow}) + V\sum_{i,\sigma} \mu_i c^+_{i\sigma} c_{i\sigma}. \quad (4)$$

Above $\nu_{i,j} = \pm 1$ depending on whether the route from i to its next-nearest neighbour j is clockwise or counterclockwise, whereas μ_i =1 for one of the two sublattices and –1 for the other one.

In order to find electrical conductance (G), Seebeck coefficient (S), electronic thermal conductance (κ_{el}), thermoelectric power factor (TPF) and the figure of merit (ZT), the following standard relations are used (in terms of the transmission T$_{el}$):

$$G = (2e^2/h) I_0\ [1/\Omega], S = -k_B/|e|\,(I_1/I_0)[V/K],$$
$$\kappa_{el} = (2Tk_B^2/h)(I_2 - I_1^2/I_0)[W/K],$$
$$TPF = S^2 G[pW/K^2], \quad ZT = S^2 GT/\kappa_{el},$$
$$I_j = -\int_{-\infty}^{\infty} \left(\frac{E-\mu}{k_B T}\right)^j T_{el}(E) \frac{\partial f(E-\mu)}{\partial E}\,\mathrm{d}E. \quad (5)$$

The adopted definition of ZT takes into account no phonon thermal conductance, what is acceptable in the case of extremely narrow graphene-like nanoribbons considered here (about 1 nm wide), and strong quantum confinement effects [5-7]. With this limitation, however,

*corresponding author; e-mail: stefan@ifmpan.poznan.pl

the obtained values for ZT should be regarded as upper estimates.

3. Discussion of the results

It has been shown earlier [3, 4, 8] and confirmed experimentally [9,10] that graphene-like nanoribbons and nanoflakes get spontaneous magnetization at zigzag edges (even at room temperature). It has also been shown that usually the in-plane magnetic configuration is energetically more favourable than the out-of-plane one. So in the following the main interest will be in the former.

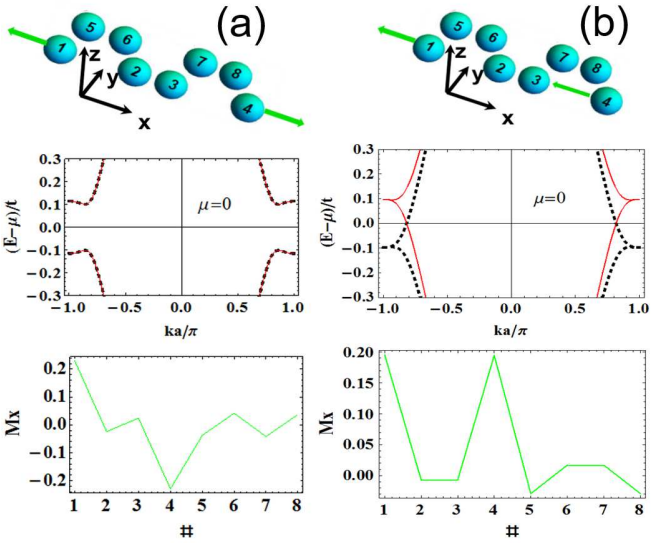

Fig. 1. Energy bands and the magnetization profile (for the periodicity units shown at the top) in the case of stanene in the AP configuration (a) and the P configuration (b) for $V = 0$.

In Fig. 1(a) energy bands are shown for energies close to the charge neutrality point (CNP, $\mu = 0$) together with magnetic moments within the periodicity unit of the nanoribbons (infinite in the y direction). It is readily seen that significant magnetic moments occur at the zigzag edges in the antiparallel (AP) configuration. For comparison the less energetically stable parallel (P) configuration is also shown in Fig. 1(b). Noteworthy in this case energy bands are spin-polarized and there is no energy gap. Figure 2, in turn, shows that both the TPF as well as the Seebeck coefficient reveal pronounced extrema close to the CNP in the AP configuration, but are negligible in the P configuration. So, akin to graphene nanoribbons, like silicene, germanene and stanene with AP magnetic edges can be attractive as potential high performance thermoelectric materials.

If perpendicular gate voltage is applied, the bands in the AP configuration get spin-polarized, too. Consequently, the heat and charge transport characteristics also change as shown in Figs. 3 and 4. In general, the presence of the gate voltage reduces thermoelectric performance (see Fig. 4c), but its effect is interesting for

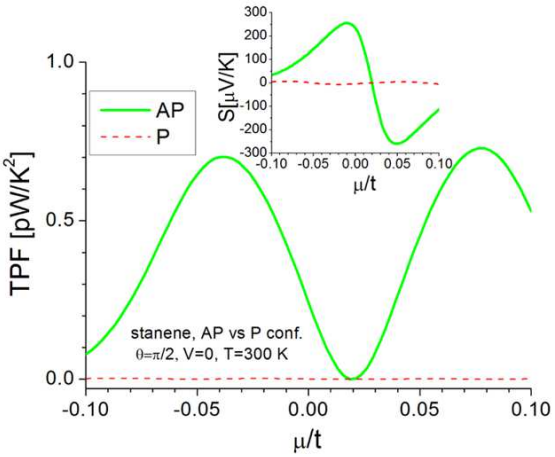

Fig. 2. Room temperature thermoelectric power factor and the S factor for stanene. In the case of the P configuration (dashed lines) both the quantities are negligible in comparison with their AP counterparts.

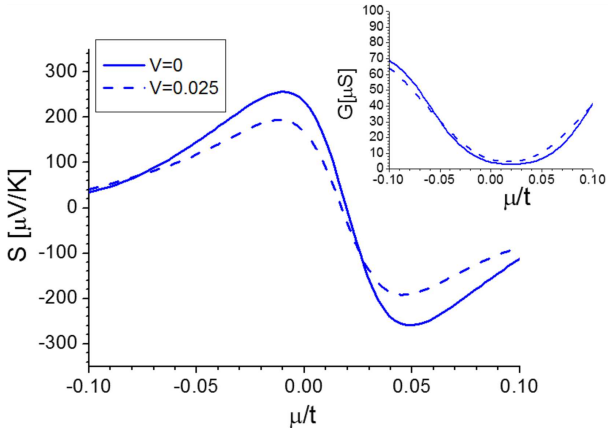

Fig. 3. Modification of the Seebeck coefficient and the electrical conductance G of stanene for indicated values of the perpendicular gate voltage.

spintronic application due to the large spin-polarization of the conductance (Fig. 4a,b).

Having got electrical and electronic thermal conductivities it is interesting to look at the Wiedemann-Franz law in the present context. This is shown in Fig.5, for silicene. Incidentally, the corresponding figures for germanene and stanene are qualitatively the same (the parameterization used here is that of Ref. [11]). It is readily seen that, regardless of the AP magnetic configuration, the Lorenz number strongly exceeds the textbook value ($L = \pi^2 k_B^2/(3e^2) = 2.45 \times 10^{-8}$ W ΩK^{-2}) in the close vicinity of the CNP. It is so due to the fact that in these circumstances the electronic thermal conductance gets less strongly reduced than the electrical conductance.

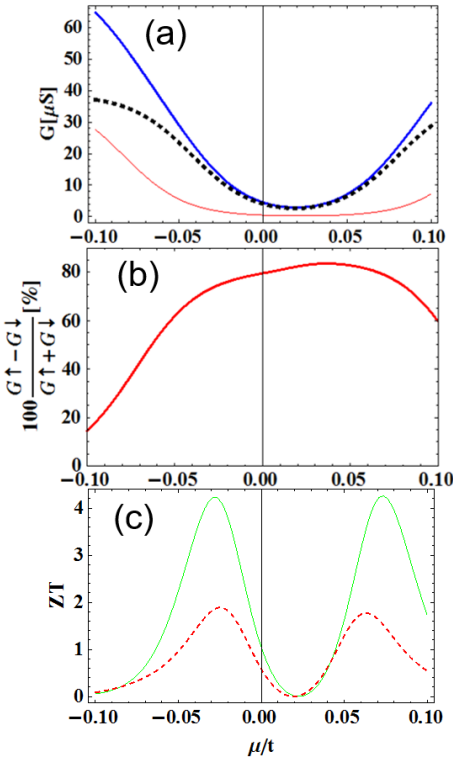

Fig. 4. Germanene for $V/t = 0.025$: (a) total conductance (upper curve) and spin-projected conductnces; (b) relative spin-polarization of the conductance; (c) figure of merit, the upper curve refers to the case of $V = 0$.

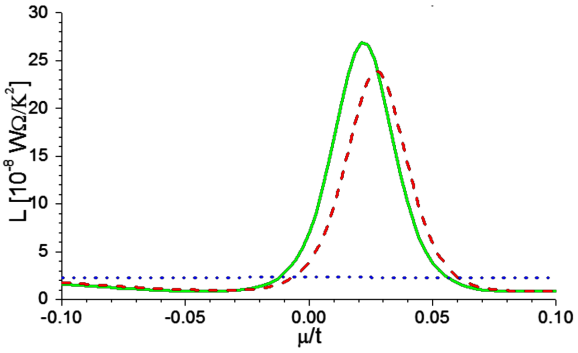

Fig. 5. Lorenz number for silicene at $V = 0$ for the AP configuration and in-plane (solid line) as well as out-of-plane (dashed line) configurations. The dotted line corresponding to the nonmagnetic case ($U = 0$) is nearly identical with that for the textbook Lorenz number.

4. Conclusions

These studies have been focused on the combined effect of key physical mechanisms, i.e. Coulomb correlations, intrinsic spin-orbit interactions and a perpendicular electric field – on spintronic and caloritronic properties of graphene-like nanoribbons. It has been shown that due to the edge magnetism both the Seebeck coefficient as well as the thermoelectric power factor are strongly enhanced. On the one hand the perpendicular voltage reduces edge magnetic moments and worsens thermoelectrical properties. On the other hand it generates significant spin polarization of the electrical conductance. Of interest is also a clear violation of the Wiedemann-Franz law near the charge neutrality point.

Acknowledgments

This work was supported by the Polish National Science Centre from funds awarded through the decision No. DEC-2013/10/M/ST3/00488.

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