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Giant room-temperature spin caloritronics in spin-semiconducting graphene nanoribbons

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Spin caloritronics refers to generating spin current by thermal gradient. Here we report a theoretical study demonstrating giant spin caloritronic effects in a new class of materials, called spin semiconductors, which are characterized with a 'spin gap', the energy gap between spin-up and -down channels. Generally, spin Seebeck coefficient (S_s) is shown to increase linearly with the spin gap. Specifically, unprecedented large $S_s \sim 3.4$ mV/K and spin figure of merit, $Z_s T \sim 119$ were found in spin-semiconducting graphene nanoribbons (GNRs) with sawtooth (ST) zigzag edges, based on first-principles calculations. Such giant spin caloritronic effects are shown to originate from a large spin gap of ST GNRs, in addition to two other spin-independent features of large band gap and narrow band width which are commonly known for good thermoelectric materials. Our studies suggest that spin-semiconducting nanostructures, such as ST GNRs, are promising candidates for room-temperature spin caloritronics with high efficiency.

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With the continuing development of spintronics, there is a growing interest in materials that can inject and/or carry spin current as a new means to transfer information efficiently [1, 2]. It has been demonstrated that thermal energy can be used to generate spin current [3–6]. The conversion efficiency of such so-called spin caloritronic effect can be characterized by spin figure of merit as $Z_s T = G_s S_s^2 T / (\kappa_e + \kappa_{ph})$, where $G_s = G_\uparrow - G_\downarrow$ is spin conductance, $S_s = S_\uparrow - S_\downarrow$ is spin Seebeck coefficient, G_σ (S_σ) is the spin-dependent electric conductance (Seebeck coefficient) of spin- σ electrons, and κ_e (κ_{ph}) is electronic (lattice) thermal conductance [7–9]. Recently, a new class of material of spin semiconductors have been proposed [10]. A special property of spin semiconductors is that both spin channels are semiconducting and relatively energy-shifted, resulting in a finite spin gap, i.e. an energy gap between spin-up and -down channels around the Fermi level. In this Letter, using spin-semiconducting ST GNRs as model systems, we demonstrate that the spin-semiconductors provide a unique class of materials to exhibit exceptionally good spin thermoelectric (TE) properties, characterized by unprecedented giant S_s and $Z_s T$ values, mainly because the spin Seebeck coefficient is found to increase linearly with the increasing spin gap.

Beside this key *spin-dependent* property of large spin gap we discover here, there are other known *spin-independent* properties favored by conventional high- ZT materials which can be also beneficial for spin caloritronics materials. First, large band gap usually guarantees high specific heat of carriers, which is part of the reason that the best TE materials are mostly semiconducting [11]. Second, a narrow band around the Fermi energy leads to rapid variation of transmission function in the

energy window of interest and hence good TE performance, as shown in quantum dots [12, 13]. For these reasons, graphene nanoribbons (GNRs) with antidots [9] have been recently shown to exhibit large S_s and $Z_s T$ if they were assumed to be ferromagnetic instead of their paramagnetic ground state [14]. (We note that spin figure of merit in a nonmagnetic material is zero because of spin degeneracy. So, ferromagnetism is a mandatory condition for spin caloritronics effect, but it is not a tunable property for increasing spin figure of merit.) Surprisingly, however, we found that the maximum room-temperature S_s and $Z_s T$ of ST GNRs are 5 and 50 times larger than those of GNRs with antidots [15], respectively. This is because besides the common spin-independent features of large band gap and narrow band width, the ST GNRs with a ferromagnetic ground state have a special spin-dependent property of large spin gap not possessed by the GNRs with antidots which is a ferromagnetic metal without spin gap.

Specifically, our first-principles and tight-binding (TB) calculations show that the S_s of ST GNRs is generally of the order of mV/K and $Z_s T$ can be as high as over 100. For example, a ST GNR with a size of (4,4) [see size definition in Fig. 1(a)] can exhibit room-temperature S_s and $Z_s T$ as high as 3.4 mV/K and 119, respectively. The key to achieving such giant spin caloritronic effect is the special property possessed by the spin semiconductors, a finite spin gap, with S_s increasing linearly with the increasing spin gap. Also, S_s is nearly a constant when chemical potential is located inside the spin gap, indicating the robustness of high S_s against charge doping that shifts the Fermi energy, which can be a useful feature in real applications. S_s and G_s are decoupled when the

chemical potential is inside the spin gap, so it is highly possible for them to be tuned separately; energy states of different spins of ST GNRs near the Fermi energy can be separated in energy and spatially, which is advantageous for spin manipulation and detection. Additional benefit comes from thermal conduction in ST GNRs is naturally reduced by edge roughness and narrow ribbon width [16, 17], which restrict phonon conduction.

Our calculations for electronic structures are performed within density-functional theory in the Perdew-Burke-Ernzerhof generalized gradient approximation, as implemented in Vienna Ab-initio Simulation Package [18]. All structures are built with vacuum space larger than 10 Å and are fully relaxed until forces on atoms are less than 0.01 eV/Å using total energy minimization. Plane-wave cutoff of 600 eV and a Monkhorst-Pack k-point mesh of $11 \times 1 \times 1$ are used for geometry optimization and electronic structure calculations. Transmission function of individual spin channels $\mathcal{T}_\sigma(\varepsilon)$ are obtained by counting bands [19].

For thermal transport calculations, a supercell system is divided into three regions: left and right contacts, and central region, as shown in Fig. 1(b). After obtaining the force constants of the two-probe system using a second-generation reactive empirical bond order potential [20] within the general utility lattice program [21], phonon nonequilibrium Green's function method (NEGF) is applied to get phonon transmission $\Xi(\omega)$, where ω is the phonon frequency. Afterwards, we use Landauer-Büttiker formalism to get quasi-ballistic thermal conductance [16, 22]:

$$\kappa_{ph} = \frac{k_B^2 T}{h} \int_0^\infty dx \frac{x^2 e^x}{(e^x - 1)^2} \Xi\left(\frac{k_B T}{h} x\right), \quad (1)$$

where k_B is Boltzmann constant, h Planck constant, $\hbar = h/2\pi$, and T absolute temperature. In light of long spin relaxation length in graphene ($\sim 2 \mu\text{m}$), spin relaxation in ideal ST GNRs can be ignored [9, 23]. Then, with electronic transmission and thermal conductance at hands, we can calculate spin TE properties (i.e. S_s , G_s , and $Z_s T$) by virtue of the following quantities [24]:

$$G_\sigma = e^2 L_{0\sigma}, \quad (2)$$

$$S_\sigma = -\frac{1}{eT} \frac{L_{1\sigma}}{L_{0\sigma}}, \quad (3)$$

$$k_{e,\sigma} = \frac{1}{T} \left(L_{2\sigma} - \frac{L_{1\sigma}^2}{L_{0\sigma}} \right), \quad (4)$$

with e being the elementary charge, f the Fermi-Dirac distribution, $\sigma = \uparrow, \downarrow$, and

$$L_{n\sigma} \equiv \frac{1}{h} \int d\varepsilon (\varepsilon - \mu)^n (-f'_\varepsilon) |_{\mu, T} \mathcal{T}_\sigma(\varepsilon). \quad (5)$$

The reference electrochemical potential μ and temperature T are set as $\mu = \frac{1}{4}(\mu_{L\uparrow} + \mu_{L\downarrow} + \mu_{R\uparrow} + \mu_{R\downarrow})$ and $T = \frac{1}{2}(T_L + T_R)$.

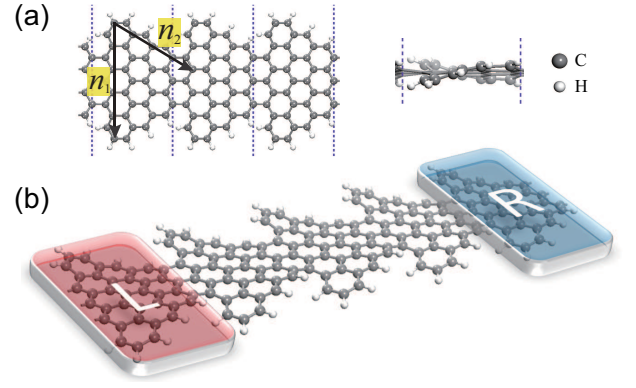


FIG. 1. (color online). (a) A top (left) and side view (right) of a (n_1, n_2) ST GNR, where $n_1 = 5$ and $n_2 = 4$ denote the size of the ST GNR. Carbon and hydrogen atoms are in grey (large) and white (small) colors, respectively. Violet dashed lines indicate division of unit cells. (b) A ST GNR is divided into left (L), right (R) thermal contacts, and center region for calculation of thermal transport.

First, we investigate the spin TE properties of a (5,4) ST GNR with hydrogen-saturated edges. Figure 1 (a) shows its optimized structure. This buckling configuration is energetically more stable than the previously studied planar structure [10] by 1.065 eV per unit cell, because the buckling reduces the steric repulsion between two neighboring H atoms at the inner corner of the ST edges. The optimized lattice constant is $a_0 = 8.587$ Å, which is slightly shorter than that of the planar structure. The ST edge is purposely designed to have an angle of 120° between any two zigzag edge orientations, so that its ground state is ferromagnetic [14], which has a lower energy than paramagnetic and anti-ferromagnetic state by 232 meV and 145 meV per unit cell, respectively.

ST GNRs have some common useful features in their distinctive electronic band structures, as illustrated in Fig. 2(a). There are four localized energy bands around the Fermi level: two occupied spin-up valence bands and two empty spin-down conduction bands, giving rise to a net magnetic moment of $2 \mu_B$ per unit cell. Similar to zigzag GNRs, these localized bands are edge states [10, 25]. Specific for spin-semiconducting ST GNRs, the spin-up and -down edge states are separated by a spin gap, which is 0.447 eV in a (5,4) ST GNR.

With the calculated band structure, spin-polarized transmission function can be obtained using band-counting method [19], as plotted in Fig. 2(b). Localized bands lead to narrow peaks in transmission, which is bad for electronic conductance, but good for obtaining large Seebeck coefficients [26, 27]. Away from the band gap, bands are dispersive and more extended in real space. Since spin-relaxation is absent, electrons see only one set of bands with the same spin. In this case, individual band gaps for a (5,4) ST GNR are $E_{g\uparrow} = 1.266$ eV and $E_{g\downarrow} = 1.378$ eV, respectively. Therefore, spin indepen-

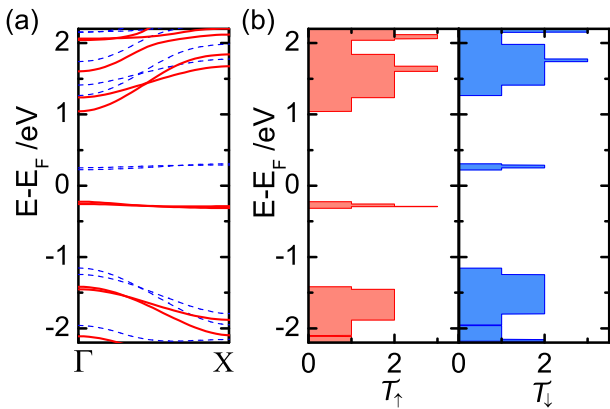


FIG. 2. (color online). (a) Spin-polarized band structure of ferromagnetic (5,4) ST GNR. Spin-up and -down bands are denoted by red solid and blue dashed lines, respectively. The Fermi energy is set to the middle of spin gap. (b) Transmission of spin-up (left panel) and -down (right panel) electrons.

dency in this system results in an about 3-fold increase in band gaps for individual spin channels.

The existence of spin gap indicates different specific heat of spin carriers, leading to different transmission for different spin channels. It can be readily shown that the spin Seebeck coefficient S_s scales linearly with the spin gap [28]. Therefore, the ST GNRs with a spin gap plus band localization are expected to have excellent spin TE properties. In Fig. 3(a), we plot room-temperature S_s . In the given energy range, both S_\uparrow and S_\downarrow have a maximum absolute value of around 2 mV/K. Notice that this value is even bigger than those of Bi₂Te₃ (bulk [29]: 70.5 μ V/K for n -type, 227 μ V/K for p -type; thin film [30]: 247 μ V/K), which is one of the best TE materials, by one order of magnitude. We note that $S_\uparrow = 0$ at $\mu = -0.272$ eV and 0.408 eV, which are denoted as A₁ and A₂ points in Fig. 3(a). At these points, thermal gradient induces only a spin down current and $Z_s T$ is as high as 95.4 at A₁ point [see Fig. 3(b)], which can be attributed to the flatness of S_s and little variation of thermal conduction (hence the coincidence of outlines of $Z_s T$ and G_s) and the fact that S_\uparrow has zero values at the symmetry center of conductance due to the odd-symmetric integration kernel in Eq. 3. Therefore, a 100% polarized spin current can be generated at $\mu = -0.272$ eV (A₁ point) using thermal gradient, with a process of $Z_s T = 95.4$. On the left/right hand side of A₁, S_\uparrow is negative/positive due to n -/ p -type-like transport [31, 32]. S_\uparrow gradually becomes negative on the right side far from the spin-up transmission peak. This can be attributed to the contribution of bulk conduction bands. Around the spin-up edge bands, S_\uparrow varies linearly, where the maximum absolute value is approximately proportional to the spin-up band gap [31].

S_\downarrow has a similar but antisymmetric trend with that of S_\uparrow . Correspondingly, S_\downarrow reaches zero at -0.468 eV and

0.265 eV, denoted as B₁ and B₂ points in Fig. 3(a), respectively. High $Z_s T$ can also be realized at B₂, where only accumulation of spin-down electrons will be induced by a thermal gradient. It is interesting to point out that $S_\uparrow = -S_\downarrow$ at the N point [$\mu \approx -0.002$ eV, see Fig. 3(a)], where the induced charge voltage is zero but spin voltage $V_s = S_s \Delta T \neq 0$ in an open circuit. Under this situation, a thermal gradient induces only a pure spin accumulation without charge accumulation. It is worth noting that the N point is the so-called neutral point, where contributions from holes and electrons cancel with other; it is supposed to be at $\mu = 0$ when the transmission functions are exactly symmetric [11, 33].

Further as shown in Fig. 3(b), S_s is rather flat inside the spin gap and across the localized bands. This can be inferred from Fig. 3(a), where S_\uparrow and S_\downarrow have an almost constant difference due to the inversely symmetric Seebeck coefficients between two spin channels and their linear dependence on chemical potential in between two transmission peaks. The flatness of S_s implies a decoupling of S_s and G_s , which can be useful for improving spin TE performance because overall $Z_s T$ can be enhanced by increasing S_s or G_s independently. Such decoupling is difficult for charge TE effect, because Seebeck coefficient S and electric conductance G generally have opposite trends against the carrier density [11]. Besides its flatness, S_s is positive around and between the two transmission peaks. This indicates that the sign of S_s has nothing to do with carrier types, noticeably different from S_σ . Also, it is shown that S_s has more contribution from spin-down electrons when $\mu < 0$ and vice versa. Experimentally, S_s is only -3.8 μ V/K for permalloy and -1.8 μ V/K for Cobalt [4, 34]. The maximum absolute value of S_s of a (5,4) ST GNR is about 3.0 mV/K, while the inside-band-gap value is 1.68 mV/K; both are two to three orders of magnitude larger than that of permalloy.

As shown in Fig. 3(b) thermal conductance changes little as the chemical potential varies, and is mostly contributed by phonons (over 80%). And it is worth noting that without electron-phonon interaction, lattice thermal conductance is independent of μ and electronic thermal conductance is almost zero off conductance peaks.

Giant S_s and $Z_s T$ are expected in most ST GNRs with the common features of spin gap and narrow bands. To confirm this, we now turn to calculations using the TB Hubbard Model [10, 35], so that ST GNRs of different sizes can be systematically studied. The Hamiltonian can be written as

$$H = t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i, \sigma} (\langle n_{i\sigma} \rangle - 1/2) n_{i\sigma}, \quad (6)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) a spin- σ electron at site i , $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ ($\langle n_{i\sigma} \rangle$) counts the number (average number) of spin- σ electrons at site i , t is the hopping energy between two nearest-neighbor carbon atoms, and

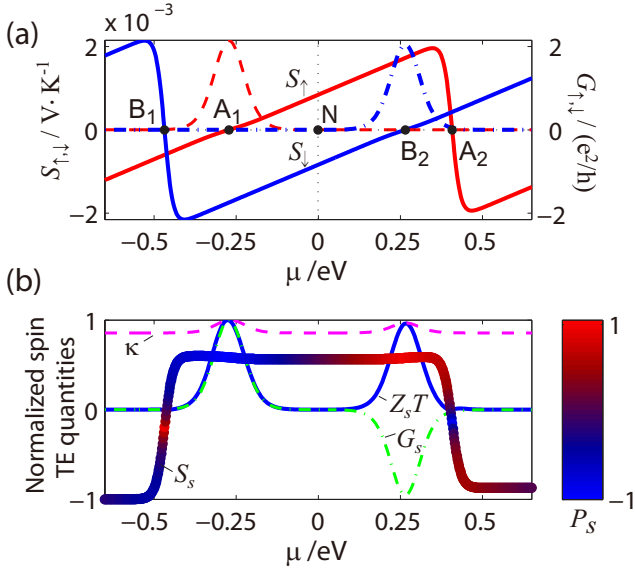


FIG. 3. (color online). Room-temperature spin TE properties. (a) Spin-up (red solid line) and -down (blue solid line) Seebeck coefficients. Spin-up (red dashed line) and -down (blue dash dotted line) conductances are also shown. (b) Normalized spin caloritronic properties as a function of chemical potential, with the zero potential set to the middle of spin gap. The normalization factors are $Z_s T = 95.6$, $S_s = 2.98$ mV/K, $G_s = 8.30 \times 10^{-5}$ Siemens, respectively, and $\kappa = 0.794$ nW/K. Colors of Seebeck coefficients in (b) change according to Seebeck polarization, $P_s = (|S_{\uparrow}| - |S_{\downarrow}|) / (|S_{\uparrow}| + |S_{\downarrow}|)$.

U is the on-site Coulomb repulsion. $\langle n_{i\sigma} \rangle$ is obtained self-consistently from

$$\langle n_{i\sigma} \rangle = \int_{-\infty}^{E_F} g_{i\sigma}(E) dE, \quad (7)$$

where $g_{i\sigma}$ is the local density of states. It is found that first-principles band structure of a buckling (5,4) ST GNR can be very well reproduced using $U = 3$ eV and $t = -2.6$ eV. Note that the U value here is different from Ref. [13] because of a buckled structure having less dispersive bands around Fermi energy.

Results calculated from the TB model are presented in Fig. 4. Fig. 4(a) shows that $S_s(\mu = 0)$ increases with n_2 monotonically for a given n_1 , and decreases with n_1 for a given n_2 . Among the total 56 configurations studied, 27 of them have a S_s value larger than 1 mV/K and all of them larger than 0.5 mV/K. The (4,4) ST GNR is found to have the largest in-gap S_s of 1.9 mV/K. Away from the band gap, S_s can be enhanced further [see Fig. 3(b)], and the maximum S_s is about 3.4 mV/K, which is further confirmed by *ab initio* calculations. However, S_s far away from the transmission peaks of localized bands corresponds to low $Z_s T$, while S_s near the peaks, almost equal to $S_s(\mu = 0)$, corresponds to high $Z_s T$. The TB model calculations clearly confirm the linear dependence of S_s on spin gap E_g , as illustrated in Fig. 4(b), which is

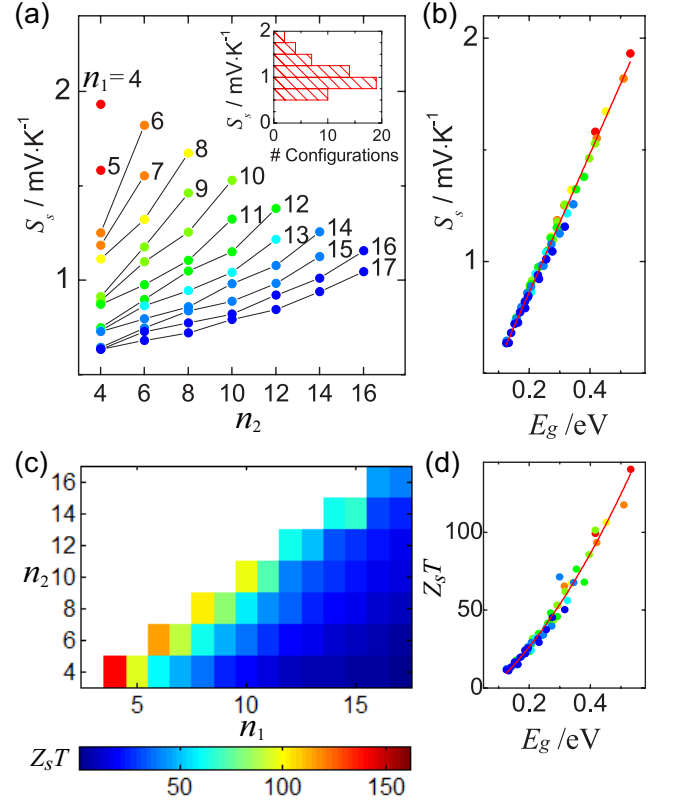


FIG. 4. (color online). Room-temperature S_s and $Z_s T$ of (n_1, n_2) ST GNRs, as calculated from the TB model. (a) $S_s(\mu = 0)$ of (n_1, n_2) ST GNR as a function of n_2 with $4 \leq n_1 \leq 17$. Data with the same n_1 are line-connected for clarity. Inset: Statistical distribution of S_s . (b) Room-temperature S_s (solid circles) plotted as a function of E_g . The red solid line is a linear fit to the data. (c) Maximum $Z_s T$ of (n_1, n_2) ST GNRs with $4 \leq n_1 \leq 17$ and $n_2 = 4, 6, \dots, 16$. (d) Maximum $Z_s T$ (circles) are plotted as a function of E_g . The red solid line is a quadratic fit to the data. Also note that for ST GNRs as shown in Fig. 1, we have $n_1 \geq n_2$ and n_2 to be even.

also consistent with the linear variation of S_s inside E_g as shown in Fig. 3(a).

ST GNRs with close n_1 and n_2 , which have a bigger sawtooth and narrower connection region, are found to have larger $Z_s T$, as shown in Fig. 4(c). Especially, the best value of $Z_s T$ is found in the (4,4) ST GNR, which is also confirmed to be 119 by *ab initio* calculations. When increasing n_1 without changing n_2 , $Z_s T$ decreases rapidly, which can be attributed to the monotonic decrease of band gaps and near-linear increase of thermal conductance due to the increase of the narrowest-part of ribbon width [17]. In contrast, increasing n_2 without changing n_1 , the structure becomes more sawtooth-like, and its $Z_s T$ increases fast. The lowest $Z_s T$ in Fig. 4(c) comes from (17,4) ST GNR, which is still as high as 4.5. Interestingly, $Z_s T$ has roughly a quadratic dependence on spin gap, as shown in Fig. 4(d), which is again consistent with the linear dependence of S_s on E_g .

In summary, we demonstrate that spin semiconductors can be excellent spin TE materials. Especially, giant spin caloritronic effects are expected in spin-semiconducting nanostructures due to additional benefits of narrow band width and reduced thermal conductance. The largest S_s (~ 3.4 mV/K) and $Z_s T$ (~ 119) values are found in the model systems of ST GNRs. It is further shown that S_s increases linearly with the spin gap. Also, S_s , being decoupled from G_s , is almost independent of chemical potential within the spin gap, so that the giant spin caloritronic effects are robust against doping in a device setting. Our studies show promise for thermal generation of 100% spin-polarized carriers at room temperature with high efficiency, paving the way for spin caloritronics towards real applications.

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