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Spin-polarized transport in multiterminal silicene nanodevices

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ABSTRACT

The spin-polarized transport properties of multiterminal silicene nanodevices are studied using the tight binding model and Landauer–Buttier approach. We propose a four-terminal †-shaped junction device and two types of three-terminal T-shaped junction devices, which are made of the crossing of a zigzag and an armchair silicene nanoribbon. If the electrons are injected into the metallic lead, the near-perfect spin polarization with 100% around the Fermi energy can be achieved easily at the other semiconducting leads. Thus the multiterminal silicene nanodevices can act as controllable spin filters.

Silicene, the counterpart of graphene for silicon, has been synthesized and attracts much attention [1–4] recently. The electronic structure of silicene is similar to that of graphene, and the valence and conduction band edges are located at the corners of the Brillouin zone around the K and K′ points. Distinct from graphene, silicene consists of two separate sublattices forming the low-bulked geometry owing to a large ionic radius of silicon atoms, which leads to a stronger intrinsic spin–orbit coupling (SOC) and a considerable bulk band gap at the Dirac point [5]. Thus silicene is considered to be a good candidate to realize the quantum spin Hall (QSH) state [6,7]. Interestingly, a tunable extrinsic Rashba SOC from the mirror symmetry breaking about the silicene plane destroys the QSH state [8,9] and establishes another striking topological effect—the quantum anomalous Hall effect (QAHE) [9–16]. The QAHE originates from the joint effects of SOC and local magnetization. By tuning the Rashba SOC strength, the valley-polarized QAHE state can be realized [17]. Therefore, silicene is regarded as a prospective material for application in spintronics and valleytronics devices.

More recently, the transport properties of the silicene nanoribbons (SNRs) attract much more attention [18–20]. Nearly perfect spin polarization can be realized by modulating both perpendicular electric and exchange fields [20]. The two open edges of SNRs can be usually passivated by hydrogen and/or other atoms [21,22]. The calculated results show that the near-perfect spin polarization can be realized in hydrogen passivated SNRs. In the present work, we carry out a numerical study of the spin transport properties of three- and four-terminal silicene devices. There exist a range of configurations for such devices. Only the basic junctions, which consist of zigzag and armchair SNRs intersecting, are considered, as shown in Fig. 1. We find that the multiterminal silicene nanodevices act as controllable multiterminal spin filters.

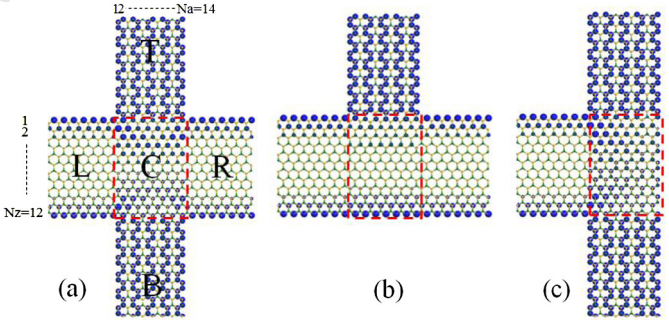

Fig. 1. (a) Geometry for †-shaped silicene nanodevice. Central region (boxed) is the conductor region, C, which is connected to four leads L, T, R and B. (b) and (c) are the Type I T-shaped junction device and Type II T-shaped junction device, respectively. The blue dot represents the local density of states. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 1(a) shows the four-terminal †-shaped silicene nanodevice, which can be treated as a central conductor region, C, connected to four leads, L (left), R (right), T (top) and B (bottom). The widths of L lead and T lead are represented by *Nz* and *Na*, respectively. Fig. 1(b) and (c) are the geometry for two types of T-shaped silicene junction devices.

The Hamiltonian of silicene is described by four-band tight-binding model that has been derived using ab initio calculations [23,24]. The symmetry analysis shows that the nearest-neighbor (NN) hopping terms has no contribution to the SOC, while the second-nearest-neighbor (SNN) hopping ones create SOC owing to

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Table 1
Material parameters used in the calculations (see Ref. [7]).

	Quantity (unit)		
	t (eV)	t_{so} (meV)	a (Å)
Magnitude	1.6	3.9	3.86

the buckled nature of silicene. The strength of the first and the second Rashba SOCs are about 10 μV and 0.7 meV, respectively. The intrinsic SOC is about 3.9 meV. The Rashba SOCs originating from the NN and SNN hopping terms are negligible compared to the intrinsic SOC. Thus Rashba SOCs can be omitted. In this case, only the intrinsic SOC is considered and the Hamiltonian can be written as [6,18,25]

$$\mathrm{H} = \sum_{i,\alpha} \varepsilon_i c^{\dagger}_{i\alpha} c_{i\alpha} - t \sum_{<i,j>\alpha} c^{\dagger}_{i\alpha} c_{i\alpha} + it_{so} \sum_{\ll i,j \gg \alpha} \nu_{ij} c^{\dagger}_{i\alpha} \sigma^{z}_{\alpha\beta} c_{i\beta} + M_z \sum_{i,\alpha} c^{\dagger}_{i\alpha} \sigma^{z} c_{i\alpha} + elE_z \sum_{i,\alpha} u_i c^{\dagger}_{i\alpha} c_{i\alpha} + \mathrm{H.C.} \quad (1)$$

where ε_i is the on-site energy and t is the hopping integral. $c^{\dagger}_{i\alpha}$ ($c_{i\alpha}$) is a creation (annihilation) operator with spin operator α. The sums in $<i,j>$ and $<<i,j>>$ are restricted to the NN and SNN atoms, respectively. $\nu_{ij} = +1$ or -1 if the SNN hoping term is anticlockwise or clockwise with respect to the positive z axis. M_z is the exchange field. E_z is the perpendicular electric field. l is the perpendicular distance between A and B atoms of silicene with $2l = 0.46$ Å. $u_i = \pm 1$ is the valley index (Table 1).

The spin transport properties of multiterminal device are calculated using the Landauer–Buttiker formalism [18,25], which can be written as

$$G^{\alpha}(E) = \frac{2e^2}{h} T^{\alpha}(E), \qquad \alpha = \uparrow, \downarrow . \quad (2)$$

Here $T^{\alpha}(E)$ is spin transmission coefficient between two leads. h is the Planck constant and e is the electron charge.

The spin transmission coefficient is calculated using the Green's function formalism. The spin transmission coefficient of electrons from lead p to lead q is expressed as

$$T^{\alpha}(E) = \mathrm{Tr}\left[\Gamma^{a}_{p} g^{a}_{C,C} \Gamma^{\alpha}_{q} \left(g^{a}_{C,C}\right)^{\dagger}\right], \quad (3)$$

where $g^{\alpha}_{C,C}$ is the retarded Green's function of the central conductor and $\Gamma^{\alpha}_{p,q}$ are the coupling matrices between the conductor and the leads. The coupling matrices are written as

$$\Gamma^{a}_{p} = i\left[\Sigma^{a}_{p} - \left(\Sigma^{a}_{p}\right)^{\dagger}\right], \quad (4)$$

where $\Sigma^{a}_{p} = (H^{a}_{Cp})^{\dagger} g^{r}_{p} H^{a}_{Cp}$, g^{r}_{p} is surface Green's function and H^{a}_{Cp} is the coupling Hamiltonian matrix between the conductor and the pth lead. The four-terminal silicene device has four leads, resulting in a conductor Green's function of the form [26],

$$g^{r}_{C,C} = \left[E^{+} I - H^{a}_{C} - \Sigma^{a}_{L} - \Sigma^{a}_{R} - \Sigma^{a}_{T} - \Sigma^{a}_{B}\right]^{-1}, \quad (5)$$

where H^{a}_{C} is Hamiltonian of the conductor. Then the density of states (DOS) of the devices is calculated by $\mathrm{DOS} = -\frac{1}{\pi}\,\mathrm{Im}[\mathrm{Tr}\, g^{r}_{C,C}]$.

In Fig. 1 (a), the repeating unit cell of semi-infinite left and top leads is labeled by dashed box. For both the zigzag and armchair semi-infinite leads, the number of atoms in a unit cell is given by $2Nz$ for the zigzag ribbon and $2Na$ for the armchair ribbon. A quick iterative algorithm is adopted to calculate surface Green's function of leads [25,26]. Assuming that the semi-infinite leads are comprised of pristine SNRs, in which only adjacent unit cell have interactions. Then the surface Green's function equation,

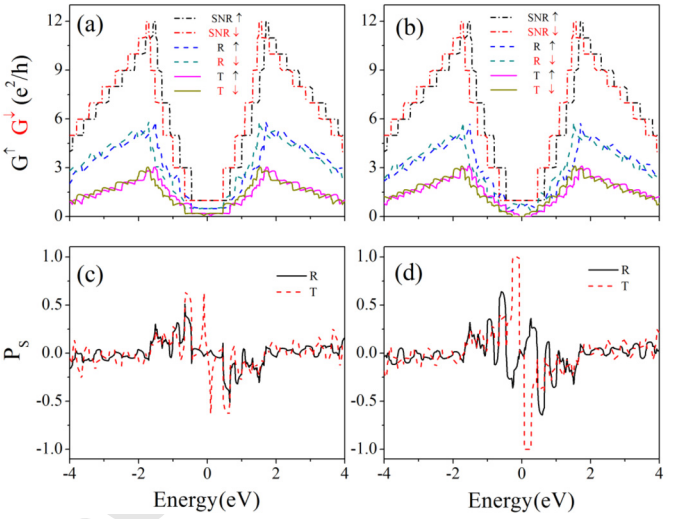

Fig. 2. Spin-resolved conductance for the †-shaped silicene nanodevice with (a) $Na = 14$, and with (b) $Na = 16$. (c) and (d) are the corresponding spin polarization of (a) and (b). The dashed dot line in Fig. 2(a) and (b) is the spin-resolved conductance for the zigzag SNR with $Nz = 12$. The dashed line is the spin-resolved conductance to lead R and solid line is the spin-resolved conductance to lead T (or B).

$$g^{r}_{p} = \left[(E + i\eta)\boldsymbol{I} - H_{0,0} - H^{\dagger}_{-1,0}\tilde{T}\right]^{-1}, \quad (6)$$

where E is energy, I is the unit matrix, and $i\eta$ is the infinitesimal imaginary. $H_{0,0} = H_{1,1}$ and $H_{-1,0} = H_{0,1}$. $H_{i,i}$ is the Hamiltonian of the unit cell of the semi-infinite leads. $H_{i,i+1}$ is coupling Hamiltonian of the nearest neighbor unit cell. $\tilde{T}$ are the transfer matrices, which can be calculated by an iterative procedure

$$\tilde{T} = t_0 + t_0\tilde{t}_1 + t_0\tilde{t}_1\tilde{t}_2 + \cdots + t_0 t_1 t_2 \cdots \tilde{t}_n, \quad (7)$$

where t_i and $\tilde{t}_i$ are defined by the recursion formulas

$$t_i = (I - t_{i-1}\tilde{t}_{i-1} - \tilde{t}_{i-1}t_{i-1})^{-1} t^2_{i-1}, \quad (8)$$

$$\tilde{t}_i = (I - t_{i-1}\tilde{t}_{i-1} - \tilde{t}_{i-1}t_{i-1})^{-1} \tilde{t}^2_{i-1}, \quad (9)$$

and

$$t_0 = \left(E^{+} I - H_{0,0}\right)^{-1} H^{\dagger}_{-1,0}, \quad (10)$$

$$\tilde{t}_0 = \left(E^{+} I - H_{0,0}\right)^{-1} H_{-1,0}. \quad (11)$$

The iterative process is implement until $t_n, \tilde{t}_n \le \delta$ with δ arbitrarily small value.

Three types of the multiterminal systems are discussed in this section: the †-shaped silicene nanodevice depicted in Fig. 1(a) and two T-shaped silicene devices depicted in Fig. 1(b) and (c). The zero temperature spin transport properties are explored using the Green's function formalism. To simplify our analysis, the zigzag nanoribbon (L lead) with $Nz = 12$ is chosen as the source lead. The parameters $t = 1.6$ eV, $t_{so} = 3.9$ meV and $M_z = 0.1$ eV are adopted in the present work.

In Fig. 2(a), the spin-resolved conductance $G^{\alpha}, \alpha = \uparrow, \downarrow$, is plotted for the †-shaped silicene device with $Nz = 12$ and $Na = 14$. The spin-up or -down electrons are injected into the system through L lead. For comparison, we plot the spin-resolved conductance through the perfect zigzag SNR (dashed dot line), showing a quantized behavior which can be controlled by the number of open channels using gate voltage. Because of the effect of exchange field, the band structure of SNRs is split into opposite spin states [18]. Therefore, the conductance profile $G^{\uparrow}$ shifts to high energy region, while the conductance profile $G^{\downarrow}$ shifts to low energy region, as shown in Fig. 2(a) and (b). In Fig. 2(a) and (b), the dashed