

Quantum Anomalous Hall Effect and Spin-filter Design Under the Control of Light and Exchange Field

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Abstract. We advance the theory that achieving quantum Hall effect in silicone can be possible. We investigate that a bulk band gap can be reopened by regulating optical and exchange field. Through tuning these external fields, perfectly nearly 100% spin-filter can be achieved with interesting spin separated edge state and be verified by calculating the spin polarizability. This finding provides a platform for designing high efficiency spin-filter.

1. Introduction

Currently, for the solid-state electronic devices, whether classic or quantum, transmission information is realized by using charge as a carrier, which exists a conversion rate because of heat dissipation. The development of spintronics and valleytronics breaks this limitation and gives a new way to realize information transmission [1–3]. We can use the characteristics of spin and valley to carry the information, and this can reduce the conversion cost of the charge information encoding. It improves the transmission efficiency, which is of epoch-making significance for the electronic devices. In crystal, electrons are propagated in the form of waves, which can be described by different quantum numbers, such as momentum and spin. At present, transport related to spin and valley in the materials has been discussed theoretically and experimentally, e.g. graphene, diamond and molybdenum disulfide.

Graphene as a novel material with unique properties has attracted wide attention [4–8]. The energy structure of graphene shows a linear dispersion close to the Dirac point [9] and some singular qualities, for instance Klein tunneling effect and quantum spin Hall (QSH) effect [10–13]. The effect of spin-orbit coupling (SOC) in graphene [14–18] leads to a topological phase with robust edge states under the system chaos and defects, which can be applied in the nanoelectronic devices. Compared with graphene, silicene has a buckled structure besides the similar hexagonal lattice structure, which provides the possibility and convenience for the regulation of topological properties under the external field [19]. In addition, the large intrinsic spin orbit coupling effect of silicene makes it easier than graphene to observe QSH at the room temperature, which is great significance for the application of spintronic devices.

In the article, we found that by tuning the optical field, the electric field and the exchange field, we can to achieve a nontrivial topological phase: the spin-polarized quantum anomalous Hall (QAH) phase. Although a great deal of work has been researched for topological nature of materials, there are still some unavoidable defects such as the field uncontrollable and impurities easy to introduce. We introduced a circular polarized light (CPL) with strong anti-jamming and controllability [20–22] to control the topological characteristics of silicene. By the regulating all of the above external fields, we can achieve nearly 100% of the spin-polarized filtered in silicene. This work can provide a particular significance theoretical basis for the application of spintronics device in silicene.

2. Tight-binding Model

The tight-binding Hamiltonian is as shown as [23, 24]:



$$\begin{aligned}
H = & -t \sum_{\langle i,j \rangle \alpha} c_{i\alpha}^\dagger c_{j\alpha} + it_{R1} (E_z) \sum_{\langle i,j \rangle \alpha\beta} c_{i\alpha}^\dagger (\mathbf{s} \times \hat{\mathbf{d}}_{ij})_{\alpha\beta}^z c_{j\beta} \\
& -l \sum_{i\alpha} \mu_{ij} E_z c_{i\alpha}^\dagger c_{i\alpha} + it_p \sum_{\langle\langle i,j \rangle\rangle \alpha\beta} v_{ij} c_{i\alpha}^\dagger s_{\alpha\beta}^0 c_{j\beta} \\
& + M \sum_{i\alpha\beta} c_{i\alpha}^\dagger s_{\alpha\beta}^z c_{i\beta}
\end{aligned} \quad (1)$$

Here, $c_{i\alpha}$ ($c_{i\alpha}^\dagger$) means that an electron is generated (annihilated) with the spin α at site i . $\langle \dots \rangle$ ($\langle\langle \dots \rangle\rangle$) means that summation go through all the nearest- (next-nearest-) neighboring sites, where $\mathbf{s}$ is the Pauli matrices who are used to express spin degree of freedom. (i) The first term describes the nearest neighbor hopping term of the lattice. (ii) The second is the extrinsic Rashba SOC term with coupling strength t_{R1} . $\hat{\mathbf{d}}_{ij}$ stand for the unit vector pointing from site j to i . (iii) The third term is the action of stagger potential under the influence of the external electric field, here $l=0.33\text{\AA}$, and $\mu_{ij}=+(-)1$ indicates that the lattice connection is AA (BB). (iv) The fourth term represents the effect of light which is induced by a non-resonant CPL, where $v_{ij}=+(-)1$ means a hopping along the (anti)clockwise direction from site j to the nearest-neighbor site i . (v) The last term is the exchange field perpendicular to the plane on lattice sites. As we all known, the CPL [21,25] and the exchange field [27] can destroy the time reversal symmetry, respectively, which have be verified in past work, but it is interesting that there will be some curious phenomenon in our work under both of the two field.

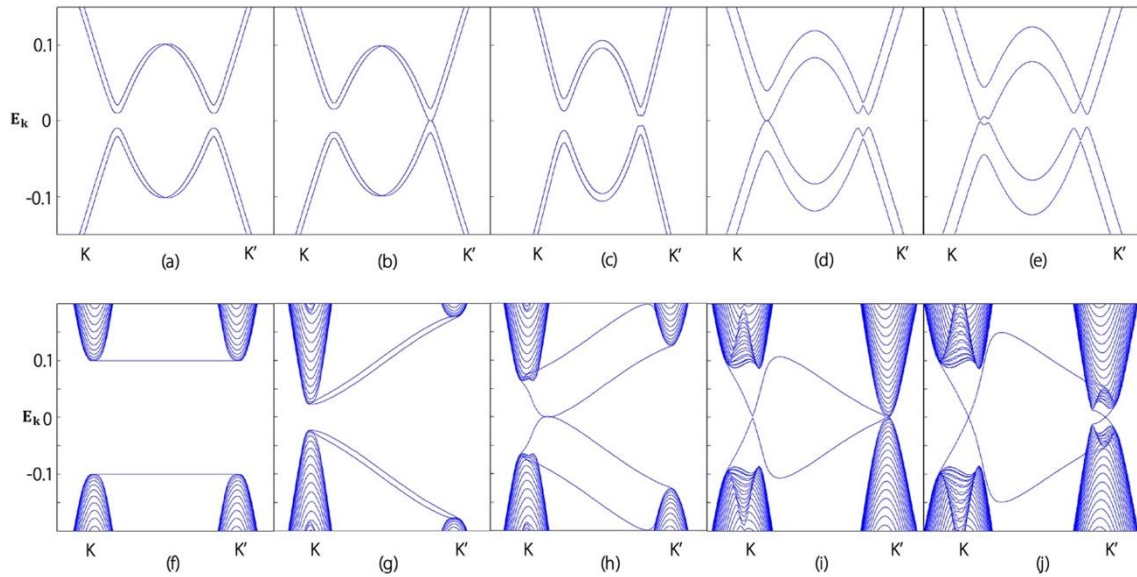


FIG. 1 (color online). Improvement of energy structures of the bulk [(a)–(e)] and zigzag-terminated [(f)–(j)] silicene along the $k_y = 0$ direction. The parameters of CPL field t_p and exchanged field M take in turn: (a) $t_p/t=0$, $M/t=0$; (b): $t_p/t=0.077$, $M/t=0$; (c): $t_p/t=0.077$, $M/t=0.052$; (d): $t_p/t=0.077$, $M/t=0.18$; (e): $t_p/t=0.077$, $M/t=0.23$. The parameters of (f)–(j) are corresponding to (a)–(j). In the picture we can find easily that a process of gap reopen appear at the K/K' points in the bulk energy spectrum when we controlled M at fixed t_p . Other parameters as follows: $t_{R1}/t=0.06$, $lE_z/t=0.1$.

With the Hamiltonian of Eq.1, we can have a 4×4 matrix H_k , we can solve H_k by diagonalizing it to obtain the bulk band structure of silicene. Fig.1 shows the improvement of the energy structure of silicene with non-resonant CPL and exchange fields. Panel Fig.1 (a) plots the energy structure of original silicene in k space. Due to the wrinkled structure, the bulk is a trivial insulator state with a Dirac point of double degeneration. When only the CPL is applied, Fig.1 (b) shows that the gap is

closed at the K' point which has a linear dispersion but is unchanged at the K point which has a parabolic dispersion at $t_p/t=0.077$. When both the CPL and the exchange field exist, as the Fig.1(c), shows that the bulk gap reopened in K' with perpendicular exchange field and CPL: $M/t=0.052$ and $t_p/t=0.077$. When we increase M/t to 0.18 and 0.23 as shown in Fig.1(d), (e), what we has found bulk energy gap in valley K is closed and then reopened, while the gap in the valley K' is still opened, which provides theoretical support for our topological phase transition. In addition, the changes of nanoribbons are shown in (f)~(j) corresponding to (a)~(e), which exhibit the transformation of topological phase. In this process, we have perfectly realized the topological regulation in silicene. In this case, a phase transition is achieved from trivial insulator to QAH effect insulator in silicene.

For the sake of the better studying of the topological properties of the material, we further analyze the energy spectrum of the silicene nanoribbon. The energy spectrum [Fig.2 (a)] (equal to Fig.1 (j)) is considerably amusing. Therefore, we analysis varies characters of its. From Fig.2 (a), there are four edge state near the fermi surface. Obviously, that points (A) and (C) are in the same direction yet points (B) and (D) are in the opposite directions. Our model is completely different from the helical edge state caused by the QSH effect (opposite direction of spin with the opposite propagation direction at each edge), which has two channels with opposite direction of spin along the same propagation direction at each edge. In evidence, that is a typical QAH effect insulator.

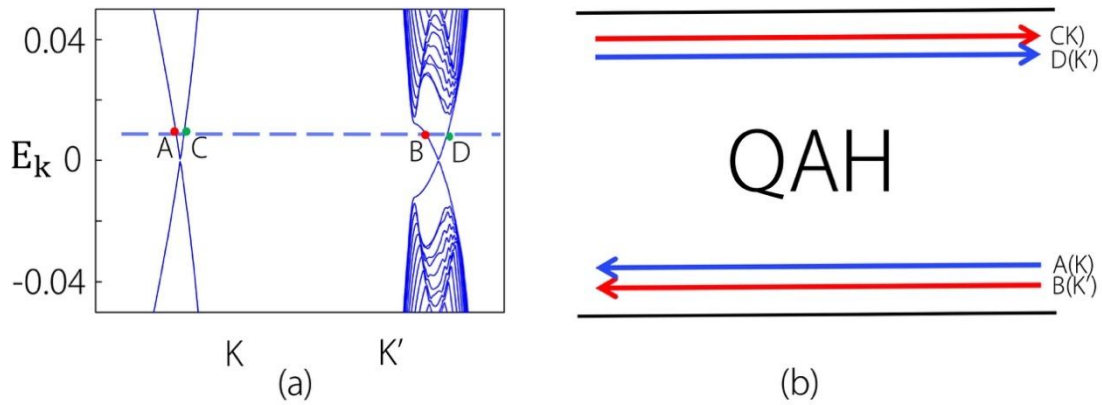


FIG. 2 (color online). (a) shows the zig-zag edge state of the silicene ribbon. Where $t_{R1}/t=0.06$, $IE_z/t=0.1$ and $t_p/t=0.077$, $IE_z/t=0.1$, $M/t=0.23$. The Fermi level $E=0.02$ through 4 different edge states A, B, C, and D. (b) sketch map displays the spatial distribution of the edge channels in the ribbon. The different colors denote the different valley's edge state. Under this condition, we find a quantum anomalous Hall effect with chiral symmetry.

The Chern number as mentioned above can be calculated from the Berry curvature, which is an integer topological invariant of all the electron-occupying wave functions below the Fermi energy. As long as the band gap near Fermi level does not turn off, the value of Chern number will never change by the disorderly interference. The specific formula [28, 29] is as follows:

$$C = \frac{1}{2\pi} \sum_n \int_{BZ} d^2k \Omega_n \quad (2)$$

The Brillouin zone is the integral interval here, and at the same time, all the occupied valence bands are covered in the sum interval. The berry curvature of the n th band in momentum expressed by $\Omega_n(k)$ is calculated as: [28, 30, 31]

$$\Omega_n(k) = - \sum_{n' \neq n} \frac{2 \operatorname{Im} \langle \Psi_{nk} | v_x | \Psi_{n'k} \rangle \langle \Psi_{n'k} | v_y | \Psi_{nk} \rangle}{(\epsilon_{n'k} - \epsilon_{nk})^2} \quad (3)$$

In the formula above, $v_{x(y)}$ is the Fermi velocity and Ψ_{nk} is the Bloch-eigenstate with the intrinsic energy ε_{nk} . The absolute value of C equals to the number of gapless chiral edge state along any edge of the nanoribbon, which corresponds to the value of standard two leads transport conductance calculated. To calculate the conductivity of the model in a standard two leads transport structure, we use the Landauer-Büttiker formula [32]:

$$T = \frac{e^2}{h} \text{Tr} [T_L G^r T_R G^a] \quad (4)$$

The $G^{r(a)}$ is the retarded (advanced) Green's function. $T_{L/R}$ indicates the coupling line width function of the left/right lead and the middle scattering region, which can be achieved by the formula $T = i(\sum_p^r - \sum_p^a)$, Here $\sum_p^{r/a}$ represents the Pth (P=L, R) semi-infinite lead retarded self-energy and advanced self-energy respectively, which can be calculated by recursive numerical methods [33].

3. Fully Spin-polarized Filter

We have analyzed the changes of the corresponding transport and energy spectral by the numerical calculation under the control of CPL and M_z in the material. In order to realize the spin-polarized in a two leads structure with zig-zag edge, we take the method of Green function and Tight-binding. Here $M/t=0.052$ and $t_p/t=\pm 0.077$, we find that there is a spin-separated edge state as shown in Fig.3(b) corresponding to nanoribbon energy spectral Fig.3(c). In the vicinity of the Fermi level, there is only

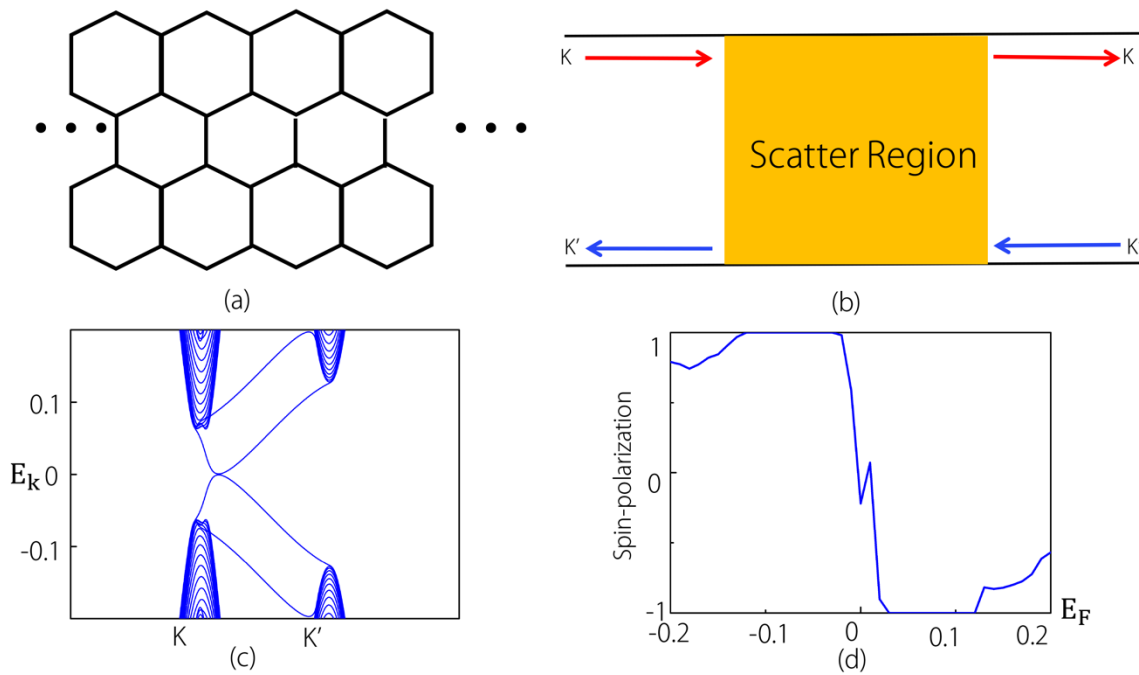


FIG. 3 (color online). (a) shows the evolution of the two leads model with zig-zag edge. (b) is a standard two leads structure transport model, where the charges are injected from the left. In contrast, the output can be seen from the right. (c) is the energy spectrum at $M/t = 0.052$ (reference from Fig1.(c)). In this condition, the silicene topological insulator with only one pair of edge state. (d) displays the rate of spin-polarized of the structure.

one channel on the upper edge with a propagating along the right (red line shown in Fig.3(b)), while the lower edge also has only one channel with a left propagating (blue line shown in Fig.3(b)).

Obviously, the conductance of two leads structure is $G = 1$ (in units) which has been verified with the calculation methods proposed before.

The aim is to come true the control of spin-filter at above design. Under this premise, the method of spin polarizability calculation can be obtained and the non-equilibrium Green function. The calculation formula of conductance is shown as[34] :

$$G = \frac{e^2}{h} \sum_{\mu\nu} |t_{\mu\nu}|^2 \equiv \frac{e^2}{h} (T_{\uparrow} + T_{\downarrow}) \quad (5)$$

In order to calculate the spin polarizability, we define a function shown as $T_{\uparrow(\downarrow)} = \sum_{m \in \uparrow(\downarrow)} \sum_n |t_{mn}|^2$, where the parameters m and n represent the input and output leads, respectively. The scattering matrix t_{mn} can be calculated from the Green function [35-37]. Therefore, the spin polarizability can be expressed as $P = \frac{T_{\uparrow} - T_{\downarrow}}{T_{\uparrow} + T_{\downarrow}}$. When $0 < P \leq 1$ ($-1 \leq P < 0$), the transmitted current behaves polarized with spin-up (spin-down) electrons.

By calculating the spin polarizability using the above method with respect to Fig.3 (b), we find that the spin polarizability at the output lead reach 100%, which can be a perfect candidate to achieve spin transport. The result of calculation shown in Fig.3 (d), it is clearly that the fully spin-up fermions appear below the Fermi level, yet for the spin-down fermions mainly display over the Fermi level (the picture take $t_p/t = 0.077$). When we take $t_p/t = -0.077$, the phenomenon is just the opposite. In another word, we actualized tunable spin-filter and realized perfectly nearly 100% spin-polarized transport.

4. Conclusion

In summary, the interesting topological phase transition can be actualized by controlling CPL and exchange field in silicene, as well as spin-filter can be regulated owing to the destroyed of space and time reversal symmetry. Underlying the formation of the topological phase transformation by some enjoyable adjustment, we designed spin-filter with high polarizability, which can be adjusted by external field. We derived unusual transmission properties through the tunable interaction among electric-, optical- and magnetic-fields in silicene. Based on the uniqueness of the work discussed above and its potential for future spintronic applications, we expect that a spin-controllable filter will be available in silicene through some regulation of external fields.

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