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Spin transport properties in silicene-based heterojunctions with different edge hydrogenation

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ABSTRACT

Using nonequilibrium Green's function in combination with the density functional theory, we investigate the spin-dependent transport properties of different edge hydrogenated zigzag silicene nanoribbon (ZSiNR) heterojunctions. The results show that H-6ZSiNR-H/H_0-6ZSiNR-H_0 (M1) and H-6ZSiNR-H/H_2-6ZSiNR-H_2 (M2) devices can exhibit spin filtering effect, negative differential resistance behavior, and rectifier effect when the two electrodes are aligned in spin antiparallel configuration. By analyzing the spin-resolved transmission spectra, the spatial resolved local density of states (LDOS), and the spatial resolved transmission eigenstates, as well as the band structure and symmetry of ZSiNR electrodes, we explained the mechanism for these intriguing properties.

1. Introduction

Graphene has attracted extensive attention in recent years due to its amazing properties and potential applications in nanodevices [1–4]. Zigzag graphene nanoribbons (ZGNRs) are particularly noteworthy owing to its potential applications in spintronics. Many interesting physical properties, such as current rectification, negative differential resistance, spin filtering, and giant magnetoresistance etc. have been found in ZGNR-based devices [5–10]. These interesting behaviors of graphene also motivate the further exploration of honeycomb structures with other group IV elements such as Silicene [11].

Silicene, a graphene-like monolayer honeycomb structure of silicon, has been successfully synthesized on Ag(111), ZrB_2(0001), and Ir(111) substrates [12–16]. Different from graphene, silicene is not planar, but has a buckled structure [11]. The height difference between two adjacent Si atoms is computed to be about 0.5 Å on account of the mixing of sp^2 and sp^3 hybridization rather than the complete sp^2 hybridization in graphene [17]. Recently, one-dimensional silicene nanoribbons (SiNRs) have been synthesized on an Ag(110) or Ag(001) surface in the experiments [18,19]. And silicene nanoribbons have an edge feature analogous to the graphene nanoribbons (GNRs) [17]. According to the basic edge configurations, there are also two types of SiNRs, namely zigzag-edged and armchair-edged silicene nanoribbons (referred as ZSiNRs and ASiNRs). The same as GNRs, the band gap of H-passivated ASiNRs exhibited metallic or semiconducting properties depending on the ribbon width, while ZSiNRs always exhibited metallic properties without being limited by the ribbon width, and the antiferromagnetic semiconducting state is most stable for ZSiNRs [11]. Given that ZGNRs show many outstanding transport properties [20–22], the transport properties of ZSiNRs is also a very interesting topic. And an obvious natural advantage of silicene over graphene is its better compatibility and expected integration with current silicon-based nanotechnologies.

For most of ZSiNR-based devices studied previously [23–27], the silicon atoms at the edges were terminated by one hydrogen atom (referred as H-ZSiNR-H). Moreover, the dangling bonds of the edge silicon atoms could also be passivated by other ways, such as symmetric dihydrogenation (H_2-ZSiNR-H_2, the H-rich environment can lead to H_2-saturated SiNRs), and asymmetric

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hydrogenated ZSiNRs which are Si—H_2 bonded at one edge while Si—H bonded at the other edge (H_2-ZSiNR-H). That is to say, the SiNRs with various edge hydrogenation can be derived from the chemical environment during the fabrication. This provides a possibility to construct the hydrogen-terminated heterojunctions in the experiment. If the silicon atoms at the edges were saturated in different ways, great changes in band structure, edge magnetism, edge states, and energy difference between the antiferromagnetic (AFM) and ferromagnetic (FM) configurations could be observed in the ZSiNRs. Yang et al. [28] have presented a systematic study of the electronic and magnetic properties not only for the hydrogenated ZSiNRs but also for the bare one (referred as H_0-ZSiNR-H_0). The studies show that the bare and symmetric ZSiNRs have the AFM ground state, while the asymmetric ZSiNRs show the FM ground state. And the magnetic moment in FM for the H-ZSiNR-H structure is the smallest ($0.5\mu_B$), while the bare ZSiNR has a maximum among the considered atomic structures. It is worth noting that the magnetic moment of the H_2-ZSiNR-H_2 is about $1.0\mu_B$. This can be explained by the Lieb's theorem [29]. That is to say, the electronic and magnetic properties of ZSiNRs can be tuned by the different forms of edge hydrogenation. However, as far as we know, the spin-dependent transport properties of ZSiNR heterojunctions with different forms of edge hydrogenation are less studied. In the present work, we report a design of heterojunctions consisting of H-ZSiNR-H, H_0-ZSiNR-H_0 and H_2-ZSiNR-H_2 which its ground states are all exhibited AFM coupling. Our calculations show that the heterojunctions can present perfect spin filter effect and negative differential resistance (NDR) behavior when the heterojunctions are sandwiched between two antiparallel (AP) aligned magnetic electrodes.

2. Simulation model and calculation method

The geometric structures of silicene-based heterojunctions are shown in Fig. 1. The ZSiNR heterojunctions can be formed using two component ribbons with different edge hydrogenation (including H-*n*ZSiNR-H, H_0-*n*ZSiNR-H_0 and H_2-*n*ZSiNR-H_2). The H-*n*ZSiNR-H (H_0 or H_2) indicate that the silicon atoms at both edges are terminated by one hydrogen atom (bare or two hydrogen atoms), and *n* is the number of silicon dimer lines across the ribbon width. In this paper, we design two different heterojunctions, namely, H-6ZSiNR-H/H_0-6ZSiNR-H_0 and H-6ZSiNR-H/H_2-6ZSiNR-H_2. For convenience, these two heterojunctions are denoted as M1 and M2, as shown in Fig. 1(a) and (b), respectively. The two-probe system is divided into three regions: left electrode, right electrode, and the central scattering region, marked by L, R, and C. Each electrode is described by a supercell with two repeated ZSiNR unit cells along transport direction, and the scattering region contains 9 unit cells.

The geometric optimization and spin-resolved transport properties are calculated by the first-principles software package Atomistix ToolKit (ATK), which is based on the spin-polarized density functional theory (DFT) combined with the non-equilibrium Green's function (NEGF) technique [30—33]. The spin-dependent generalized gradient approximation (GGA) is used for the exchange-correlation functional [34]. The double zeta polarization basis set (DZP) is used for all atoms in our constructed devices [35]. The cutoff energy is set to be 110 Ry and the mesh grid of the k space is $1 \times 1 \times 100$. The geometry optimization is performed using quasi-Newton method until the absolute value of force acting on each atom is < 0.02 eV/Å. Under a given bias V_{bias}, the spin-dependent current through the central scattering region is calculated by the Landauer-Büttiker formula [36]:

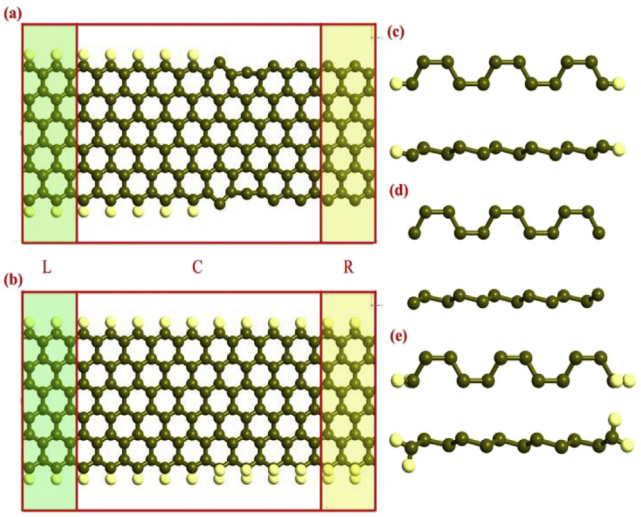

Fig. 1. (a) and (b) Two-probe systems of the M1 and M2 heterojunctions from top view. (c)–(e) Structures of per unit cell (H-ZSiNR-H, H_0-ZSiNR-H_0 and H_2-ZSiNR-H_2) from cross section view. The olive (yellow) spheres are the Si (H) atoms. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

$$I_\sigma(V_b) = \frac{e}{h}\int_{\mu_L}^{\mu_R} T_\sigma(E, V_b)[f_L(E-\mu_L) - f_R(E-\mu_R)]dE \quad (1)$$

where h and e are Planck's constant and the elementary charge. σ is a spin index where $\sigma = \uparrow$ (spin-up) and $\sigma = \downarrow$ (spin-down). $\mu_L = E_F - \frac{eV_b}{2}$ and $\mu_R = E_F + \frac{eV_b}{2}$ are the electrochemical potential of the left and right electrodes, respectively, where E_F the Fermi level is set to be zero in our calculations. The energy region $[\mu_L, \mu_R]$ contributing to the total current integral is called the bias window. T_σ is the spin-resolved transmission function defined as:

$$T_\sigma = T_r\left[\Gamma_{L\sigma} G^{R\sigma} \Gamma_{R\sigma} G^{A\sigma}\right] \quad (2)$$

where $G^{R\sigma}$ and $G^{A\sigma}$ are the retarded and advanced Green function. $\Gamma_{L\sigma}$ and $\Gamma_{R\sigma}$ are the coupling matrix resulting from the spin-dependent coupling of the central scattering region to the left and right electrodes.

3. Results and discussion

Generally, the magnetization of the left and right electrodes can be set to parallel (P) or antiparallel (AP) spin configurations by adjusting the applied magnetic field on two electrodes [37]. As shown in Fig. 2(a) and (b), we consider firstly the current as a function of applied bias (I–V) of M1 and M2 under the AP magnetism configuration, namely, the left and right electrodes with opposite spin directions (the left electrode is ↑-spin polarized and the right one is ↓-spin polarized). Fig. 2(c) and (d) shows the spin charge density distribution of M1 and M2 systems for AP spin configuration under zero bias, where the red and blue colors indicate the spin-up and down components, respectively. We can find that these spin-polarized states present strong edge effect, *i.e.*, they are mainly localized on the edge silicon atoms of ZSiNRs. The central part is also spin-polarized with a larger spin magnetism in M1 due to the different interfacial interactions between two component ribbons.

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