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Spin-filtering and rectifying effects for Al-doped zigzag-edged silicene nanoribbons with asymmetric edge hydrogenation

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ABSTRACT

Spin transport features of the Al-doping zigzag-edged silicene nanoribbons (ZSiNRs) are investigated by using the nonequilibrium Green's function method and the spin-polarized density functional theory, where ZSiNRs are Si—H_2 bonded at one edge while Si—H bonded at the other to form an asymmetric edge hydrogenation. It is found that a perfect spin filtering effect (100%) in such ZSiNRs can be achieved in the calculated bias region. The rectifying performance of spin-polarized currents with a ratio larger than 10^5 can be achieved by changing the position of the doping atoms. Moreover, the negative differential resistance (NDR) effect is also observed in the spin-polarized current. Our calculation suggests Al-doping ZSiNRs with the asymmetric edge hydrogenation hold promise for multifunctional spintronic devices.

1. Introduction

Since the discovery of graphene, one has witnessed an increasing interest in other two-dimensional honeycomb structures. One of such materials is silicene — a two dimensional hexagonal lattice of silicon (Si) atoms. The similarity between graphene and silicene arises from the fact that C and Si belong to the same group in the periodic table of elements. Due to the similarity of the lattice structure, the band structure of silicene resembles that of graphene. Namely, silicone are zero-gap semimetallic, and their charge carriers are also massless fermions because their π and π^* bands are linear around the Fermi level (E_f) [1–3]. However, as an important element for semiconducting and high-tech device, Si also possesses some unique properties which carbon does not have [4]. In recent years, quasi-one-dimensional Si nanostructures have been studied theoretically and experimentally [5–7], including Si nanowires (SiNWs) and Si nanotubes (SiNTs). First-principles calculations have predicted that the most stable structure of silicene monolayer prefers a low-buckled (LB) structure [8,9], unlike planar graphene monolayers. Similar to graphene nanoribbons (GNRs), silicene nanoribbons can also be classified into two types: zigzag-edged silicene nanoribbons (ZSiNRs) and armchair-edged silicene nanoribbons (ASiNRs) [10,11]. In particular, intensive investigations have been focused on ZSiNRs due to unique edge magnetism and transport properties [12–14]. H-passivated ZSiNRs at the ground state exhibit a ferromagnetically (FM) ordered state at each edge individually due to the unsaturated p electron existing for each edge Si atom but antiferromagnetic (AFM) coupling between opposite edges, leading to a spin-polarized semiconducting behavior with zero net spin, which limits their applications in spintronic devices. Therefore, the edge states can significantly affect the electronic and magnetic properties [15], for example, ZSiNRs with asymmetric sp^2-sp^3 edges could cause diverse magnetic properties, which has attracted the research interest of many researchers recently [15,16]. Moreover, different edge types and hydrogenations can induce more peculiar magnetic states into Si nanoribbons [17]. Theoretical studies have demonstrated that ZSiNRs with asymmetric edge hydrogenation are more stable than symmetric single H saturation [12], showing an interesting bipolar magnetic semiconducting behavior, which can be changed to half-metals by doping and strain.

In a previous publication by Lalmi et al., the synthesis of 2D silicene on Ag(111) was claimed based on STM observations [18]. While, the Si—Si distance determined by Lalmi et al. is about 0.19 nm, a value far too small compared to the expected value between 0.22 and 0.24 nm and the DFT calculations [19]. Then, G Le Lay et al. emphasize that the STM image presented by Lalmi et al. does not show a silicene sheet but refers to the clean Ag(111)

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substrate [20]. At present, silicene has been fabricated experimentally by means of depositing silicon on Ag (111) or I (111) surfaces by controlling the coverage and temperature [21–23], and the honeycomb structures of silicene are very similar to those for graphene or hexagonal boron-nitride [24,25], and in agreement with all related expectations for silicene. Since silicon plays a crucial role in the present-day electronics, integration of silicene into nanoelectronics seems to be more promising than that of graphene, and this possibility opens new perspectives for this novel material [26,27]. Therefore, exploring the promising properties of silicene nanoribbons for applications of nanodevice is currently of great interest. Another attractive property of silicon-based spintronics devices is their possible compatibility with the contemporary semiconductor industry.

In this work, based on the ZSiNR with asymmetric sp^2-sp^3 edges, we investigate its Al-doping effects and find that it can be tuned to a half-metal, and a perfect spin filtering effect (100%) can be achieved at FM state. Interestingly, the rectification properties in such a electronics device are indeed enhanced substantially with a rectification ratio up to 10^5 at a certain suitable doping site.

2. Model and method

Following conventional custom, the ribbon widths of ZSiNRs can be characterized by the number of zigzag Si chains, N, along the nanoribbon axis, which is denoted as NZSiNR. In this paper, we choose 6ZSiNR as a representative. The structure of H_2-6ZSiNR-H is shown in Fig. 1(a), where the Si atoms at one edge of the ZSiNR are passivated by two H atoms (Si–H_2 edge), while the Si atoms at the opposite edge are passivated by one H atom (Si–H edge). We investigate the band structure for Al-doping models, mainly focusing on the doping-position effects of the H_2–6ZSiNR–H with the distance from the Al atom to the ribbon edges. For the pristine supercell with three repeated unit cells, as shown in Fig. 1(a), the Si atoms from top to down in the cell are labeled as Pi (i = 1–6), representing six different.

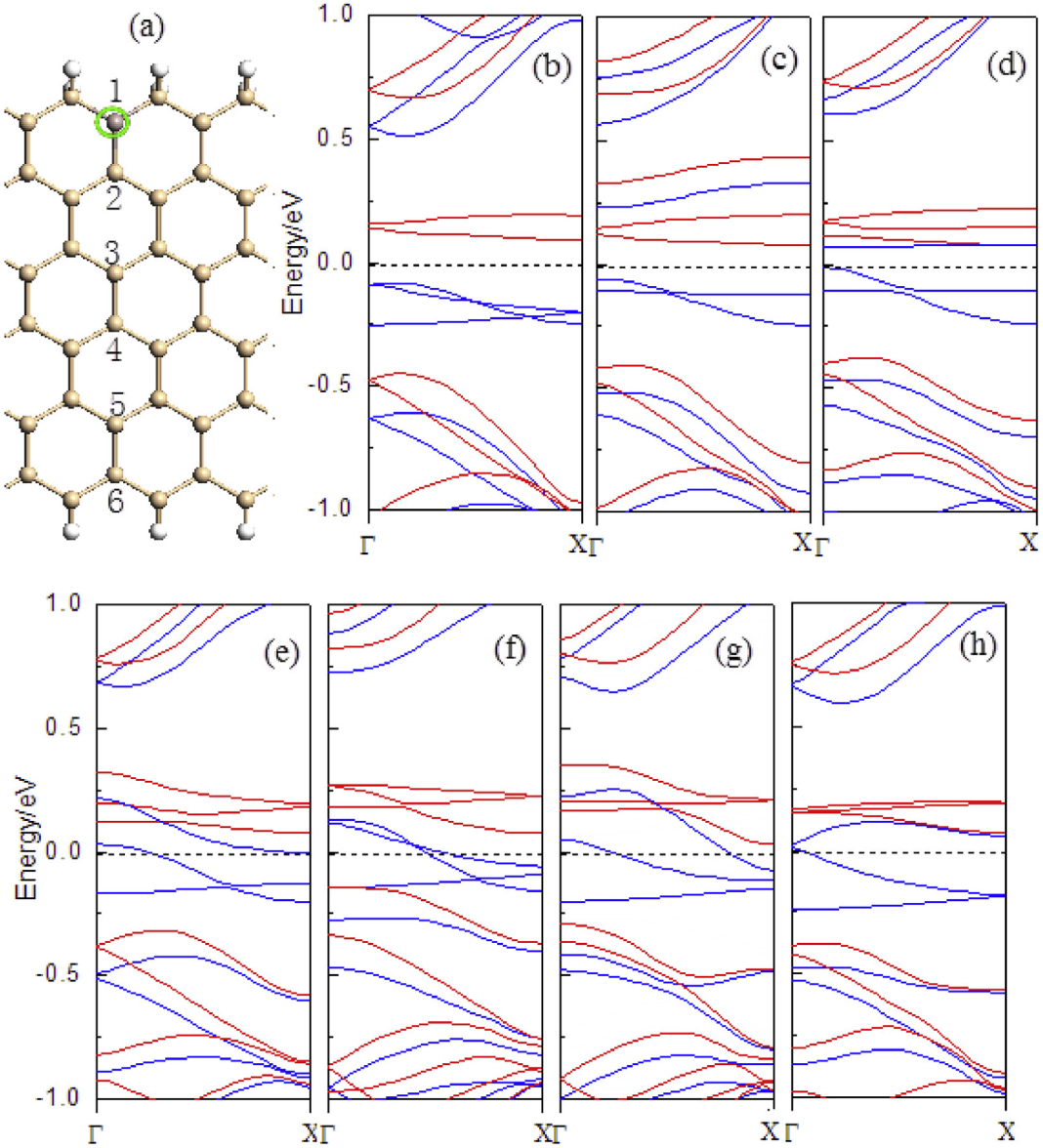

Fig. 1. (a) Supercell of H_2-6ZSiNR-H is doped with Al atom, the band structure at the FM state for H_2-6ZSiNR-H without Al- doping (b) and with Al-doping at Pi (i = 1–6) (c)~(h). The Fermi level is set to zero throughout the paper, the blue and red line stand for the α-spin and β-spin, respectively.