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Gate-induced half-metallicity in semihydrogenated silicene

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HIGHLIGHTS

- Semihydrogenation can induce half-metallicity in silicene.
- The transport properties of semihydrogenated silicene were studied by *ab initio* quantum transport theory.
- A high on/off current ratio of 10^6 was obtained in the single-gated semihydrogenated silicene device.
- A spin-polarized current was observed in the studied device, and the spin-filter efficiency can reach 100% at a voltage of 1.9 V.

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ABSTRACT

The first-principles calculations indicate that the semihydrogenated silicene (H@Silicene) is a ferromagnetic semiconductor. By the *ab initio* quantum transport theory, we study for the first time the transport properties of H@Silicene with pristine silicene as electrodes. A high on/off current ratio of 10^6 is obtained in the single-gated H@Silicene device. More importantly, a spin-polarized current can be generated. The spin-filter efficiency increases with the gate voltage and reaches 100% at a voltage of 1.9 V. Our results suggest that a gate voltage can induce half-metallicity in H@Silicene. Therefore, a new avenue is opened for H@Silicene in application of spintronics.

1. Introduction

In the last few years, graphene has drawn much interests from scientists and engineers as this two-dimensional structure shows exclusive properties like high carrier mobility [1] and potential applications in nanoelectronics [2,3], such as field-effect transistors (FETs) [4], negative differential resistance (NDR) [5], magnetic tunnel junctions [6,7], and gas sensors [8]. As the silicon analog of graphene [9], silicene is also predicted to be a zero-gap semiconductor, with a Dirac cone near the Fermi level [10]. Experimentally, silicene has been successfully grown on Ag substrate [11–16], zirconium diboride thin film [17], and Ir substrate [18] recently. Different from graphene, silicene is probably compatible with current Si-based technology. Besides, Si has a longer spin-diffusion time and spin coherence length [19–21]. Therefore, silicene is expected to be used for future spintronic applications. In spintronics, half-metallic materials, with a metallic nature for one spin and insulating or semiconducting for the other spin, are highly desired because they provide 100% spin polarized current [22–25]. Besides, half-metals are better spin injection sources than ferromagnetic (FM) metals due to the conductivity mismatch between FM metals and semiconductors [26].

Very recently, semihydrogenated silicene and germanene (H@Silicene and H@Germanene) attracted researchers' attention as they show FM semiconducting characters [10,27]. To the best of our knowledge, the transport properties of H@Silicene remain open. In this paper, we first study the structure and electronic properties of H@Silicene. An indirect band gap of 0.93 eV is opened in silicene after semihydrogenation. Then, a single-gated H@Silicene FET is simulated by using the *ab initio* quantum transport theory, and a transport gap of 1.10 eV is found in this device, in agreement with the band calculation. This device has a very high on/off current ratio (10^6). Moreover, a perfect spin-polarized

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current is observed by applying an appropriate gate voltage, suggesting that half-metallicity can be induced by gate voltage in H@Silicene.

2. Methods

The structural optimizations and electronic structure calculations based on the spin-polarized density functional theory (DFT) were performed in the CASTEP package [28]. Ultrasoft pseudopotential was applied and plane waves up to energy cut off 400 eV were used in the calculation. The Brillouin-zone integration was conducted by the Monkhorst–Pack special k-point scheme [29] with $24\times24\times1$ grid meshes. For geometrical optimization, the system was allowed to fully relax until the maximum force converged to lower than 0.01 eV/Å. Vacuum space of 20 Å normal to silicene plane was used to avoid interactions between two layers. Both the atomic positions and lattice constant were relaxed without any symmetry constraints.

The transport calculations were performed by using the ATK 12.2 package [30,31]. The single-zeta polarized (SZP) basis set was used, and the mesh cut-off was chosen as 100 Ry. The temperature was set to 300 K. The Monkhorst–Park k-points mesh [29] of the electrodes and central region was set to $1\times100\times100$ and $1\times100\times1$, respectively. The current was calculated with the Landauer–Bűttiker formula [32]:

$$I(V_g,\ V_{bias})=\frac{2e}{h}\int_{-\infty}^{\infty}\{T(E,\ V_g,\ V_{bias})[f_L(E-\mu_L)-f_R(E-\mu_R)]\}dE \quad (1)$$

where $T(E, V_g, V_{bias})$ is the transmission probability at a given gate voltage V_g and bias voltage V_{bias}, $f_{L/R}$ is the Fermi–Dirac distribution function for the left (L)/right (R) electrode, and μ_L/μ_R the electrochemical potential of the L/R electrode. The generalized gradient approximation (GGA) of the Perdew–Burke–Ernzerhor (PBE) [33] form for the exchange correlation functional was used throughout this paper.

3. Results and discussion

First, we optimize the geometric structures of H@Silicene in their nonmagnetic state. As shown in Fig. 1, the initial lattice vectors of the unit cell are given with $a_1=a_2=a=3.899$ Å. The structure is slightly buckled with a buckled height of $\Delta Z=0.685$ Å.

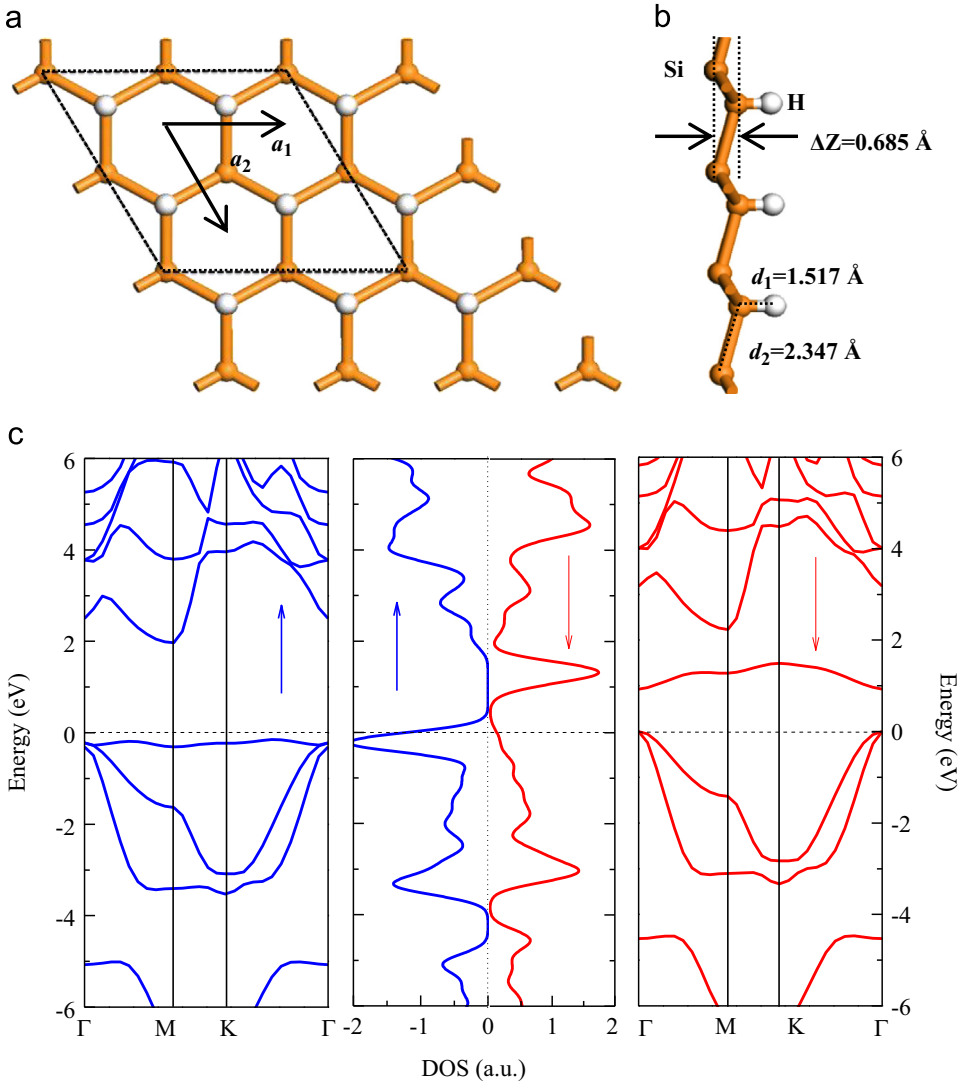

Fig. 1. The optimized geometric atomic configurations and the structural parameters of H@Silicene. (a) Top view with the rhombus marked in black shows the supercell. The Bravais lattice vectors of unit cell are given with $a_1=a_2=a=3.899$ Å. (b) The side view. The average bond length d_1 (Å) between Si and H atoms, d_2 (Å) between Si and Si atoms, and buckled height ΔZ (Å) between Si and Si layers. The yellow and white balls stand for Si and H atoms, respectively. (c) Band structures and density of states of H@Silicene. The arrow denotes the spin-polarized direction. The top of the valence band is set to zero. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)