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Tunable band gap, magnetoresistance and pseudo-magnetoresistance in silicene-based nanodevices

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ABSTRACT

Spin-dependent transport in two terminal zigzag silicene nanoribbon is investigated numerically in the presence of spin-orbit interactions, external spin splittings or exchange fields, and perpendicular electric field. We show by applying an exchange field, a tunable band gap emerges which depends on the exchange field vector angle with the plane of nanoribbon. Such behavior is interpreted using the low-energy Hamiltonian of the silicene which indicates qualitative agreement with results obtained from lattice model. Moreover, it is found that by decreasing the width of nanoribbon larger band gaps are achievable which can be promising for nanoelectronic applications. On the other hand, by imposing exchange fields inside the electrodes, the magnetoresistance of the junction is investigated. As a main result we observe that when the Rashba interaction becomes stronger the magnetoresistance decreases but it is not fully suppressed. Finally, in the presence of perpendicular electric fields applied to the electrodes, depending on their relative configuration, the so-called pseudomagnetoresistance is calculated. Our results indicates that the conductance of the silicene nanoribbon significantly differs between the parallel and anti-parallel configurations of electric fields in the electrodes.

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1. Introduction

By the isolation of graphene as a single atomic monolayer of carbon atoms in a stable crystallized form, the new field of two-dimensional (2D) materials established at 2004 and started to grow very fast [\[1\]](#page--1-0). Subsequently, a vast investigation on the fundamental properties and possible applications of 2D materials initiated [\[2\].](#page--1-0) Graphene as the prime mover of the group, is a material of a large amount of interest from both fundamental and technological point of views, due to its unique structural, mechanical and electronic properties $[3-5]$ $[3-5]$ $[3-5]$. However, the absence of an energy gap causes the main challenge for standard logic circuits applications of graphene since the required high on/off current ratio cannot be provided. So various groups suggested the electronic and logic applications of other 2D materials with complementary properties and particularly the controllable band gaps. Silicene, the silicon-based counterpart of graphene, has been synthesized in recent years $[6-11]$ $[6-11]$ $[6-11]$ and then it has received lots of attention from theoretical and experimental points of view $[12-14]$ $[12-14]$. Although it demonstrates many characteristics of graphene such as honeycomb lattice structure and relativistic Dirac dispersion, silicene reveals significant differences. First of all, because of the large atomic radius of silicon, the 2D lattice is buckled in silicene. In other

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words, unlike graphene with a true single atomic layer structure, silicene consists of two atomic layers (triangular sublattices) separated by a perpendicular distance $2k-0.46$ Å [\[13\]](#page--1-0). In addition, it shows a relatively large intrinsic spin-orbit interaction (SOI) which results in a gap of ~1.55 meV between the conduction and valence bands [\[13,14\].](#page--1-0) Very intriguingly, at the presence of a perpendicular electric field (E_z) this gap can be controlled and even a transition between trivial and topological insulating behaviors can be achieved $[15-18]$ $[15-18]$.

A natural advantage of silicene compared to graphene, is its better compatibility and integration with the existing silicon technology. In addition, it has long spin-diffusion time and spin coherence length at room temperature compared to graphene which suggests the usage of silicene for spintronic applications $[19-25]$ $[19-25]$ $[19-25]$. Since the pristine silicene is nonmagnetic, for the usage in spintronics, magnetic properties should be externally induced by methods including proximity with magnetic materials similar to the previously suggested proposals for inducing magnetism and spin polarization in graphene, MoS₂ and, etc. $[26-29]$ $[26-29]$ $[26-29]$. So, a finite exchange splitting can be achieved by growing silicene on top of a ferromagnetic insulator (e.g. EuO). Motivated by the advances in experimental works about the integration of the ferromagnetic insulator onto thin films, theoretical studies has been conducted in the case of silicene nanoribbons. An et al. have shown that local exchange field can produce spin-polarized current at the edges of zigzag silicene ribbon [\[30\]](#page--1-0). Subsequently, other works have investigated the valley and spin transport in ferromagnetic silicene junctions $[31-42]$ $[31-42]$. Very interestingly, fully polarized spin-valley conductances in ferromagnetic silicene nanoribbon has been predicted under certain circumstances [\[31,32,34,35,37,42\]](#page--1-0). Other investigations based on the ab-initio calculations have revealed that the silicene devices have giant magnetoresistance with a spin-filter efficiency which can be controlled via the electrical biases [\[43\]](#page--1-0).

In this paper, we investigate both spin and pseudospin-dependent transport through a zigzag silicene nanoribbon (ZSNR) in the presence of exchange field and perpendicular electric fields, respectively. We found from both lattice model and effective Hamiltonian when the exchange field applied to the central ZSNR, has an out of the plane component, a tunable band gap can be established. This gap can be varied substantially by the amplitude of the exchange field angle θ with respect to the z direction which is perpendicular to the silicene plane. Subsequently, we show the energy gap and transport properties of such device can be tuned by the exchange field vector (EFV) angle θ , exchange field strength, and the width of the ZSNR. When the exchange field is present at the two electrodes, a finite magnetoresistance (MR) can be observed which is large when the Rashba SOI is absent. Nevertheless, when the Rashba terms become large due to the spin precession the MR will be suppressed. Finally, we show a pseudomagnetoresistance effect for the devices based on ZSNR when perpendicular electric fields are applied the two electrodes. This behavior is revealed in the difference between transmission probabilities through the system when the electric fields at the two electrodes are parallel and anti-parallel, respectively. Such phenomenon is related to the pseudospin degree of freedom presented in silicene which can be controlled via a perpendicular electric field resulting in the staggered on-site energies for the neighboring silicene atoms.

2. Model and formalism

In this section, we will present the model and basic formulation which are used for the calculation of transport properties. We employ the well-known tight-binding model for silicene including extra terms such as the SOI as well as the spin splitting term. Then the recursive Green's function method will be used in order to obtain the conductance through different setups. The schematic of the considered setups and the one-dimensional unit cell which is used for band structure calculations are shown in Fig. 1.

Fig. 1. (a) The ZSNR connected to the two semi-infinite electrodes. One-dimensional sliced unit cells are indicated with dashed boxes. Unit cells denominated with 0 and N_x + 1 are interface of central region with left and right electrodes, respectively. Transparent layer in central region indicate the ferromagnetic insulator deposited on top of ZSNR with exchange field along arbitrary (θ, ϕ) directions. (b) The side view of ZSNR.

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