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Giant magnetoresistance and spin-filtering effects in zigzag graphene and hexagonal boron nitride based heterojunction

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ABSTRACT

The spin-dependent electronic transport properties of heterojunction constructed by bare zigzag graphene nanoribbon and hexagonal boron nitride nanoribbon are investigated by the non-equilibrium Green's function method in combination with the density functional theory. The results show that the giant magnetoresistance effect can be realized in the heterojunction, and the magnetoresistance ratio can reach to 10^6. Moreover, it is found that the heterojunction is a good spin-filtering device with nearly 100% spin filtering efficiency at a wide bias voltage region in both ferromagnetic and antiferromagnetic magnetic configurations.

1. Introduction

Graphene, a two-dimensional C atom with hexagonal crystal symmetry, has tremendous interest in potential applications in nano-electronics [1–7]. Meanwhile, researchers began to focus on other emerging two-dimensional (2D) materials, such as, hexagonal boron nitride (*h*-BN) [8], molybdenum disulphide (MoS_2) [9], and silicon/germanium 2D sheets [10]. Electrons in these 2D materials also behave like massless and massive Dirac fermions [11], and display unique transport properties [12,13]. However, compared to this explosive research of individual 2D materials, the hybrid nanostructures composed of different types of 2D materials could provide us a new route to engineering the band gap and spin-relevant properties of nano-materials [14], which is becoming an essential part in electronics. The lateral heterostructure based on graphene and *h*-BN has attracted much attention since graphene is a gapless semi-metal whereas an atomically thin layer of *h*-BN is a dielectric with a wide bandgap of 5.9 eV [15]. If the precise two-dimensional domains of graphene and *h*-BN can be seamlessly stitched together, hybrid atomic layers with interesting electronic applications could be created [16–18]. By growing graphene in lithographically patterned *h*-BN atomic layers, Liu et al. succeed in building in-plane graphene/*h*-BN atomic layer with controlled domain shapes at larger sizes (millimeter range) [19]. Gao et al. have successfully grown a perfect single-layer *h*-BN-graphene (BNC) patchwork on a selected Rh(111) substrate and convinced that at the in-plane linking interface, graphene and *h*-BN can be linked perfectly at an atomic scale [20]. At the same time, the significant advances of theoretical simulations on the hybridized in-plane heterostructures of graphene and *h*-BN have also been performed on the computer [21].

Due to sensitivity of the electronic properties to the details of the edge shapes of graphene [22] and *h*-BN, a few of works focused on the hybrid atomic layers of graphene nanoribbons (GNRs) and *h*-BN nanoribbons (BNNRs) [23–27]. Seol et al. [28] studied the electronic properties of armchair graphene nanoribbons (AGNRs) confined by *h*-BN nanoribbons (BNNRs) and found the AGNRs confined by BNNRs exhibit a considerable bandgap. Chen et al. [29] investigated a hybridized structure constructed by a zigzag boron nitride nanoribbon (ZBNNR) and a zigzag graphene nanoribbon (ZGNR) and found the band gap of the hybridized structure can be tuned from insulator to metal by changing the unit number of ZGNR. However, up to now, very few attempts have been made to excavate the mechanism of ZBNNR/ZGNR heterojunction at finite bias voltage. Moreover, the edge modulations, such as dehydro-

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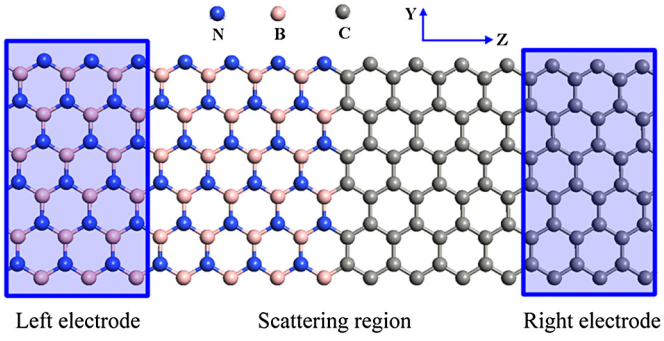

Fig. 1. (Color online.) Two-probe system of 6-ZBNNR/6-ZGNR heterojunction. Pink, blue, and gray balls represent B, N, and C atoms, respectively. The blue arrow correspond to X and Z axis.

genation, can affect the electronic structures of ZGNR and ZBNNR [30–35]. And on the other hand, bare ZGNR (ZBNNR) has also been demonstrated to exist and stable [36,37]. Thus, in this work, we propose a configuration of heterojunction based on the bare ZGNR and ZBNNR, and the spin-dependent transport properties have been studied. Our results show that the ZGNR/ZBNNR heterojunction is a perfect spin-filtering device with nearly 100% spin-filtering efficiency. And giant magnetoresistance effect can also be realized in this heterojunction.

2. Computational method and details

We consider a heterojunction based on 6-ZBNNR and 6-ZGNR structures, namely, 6-ZBNNR/6-ZGNR, as shown in Fig. 1, where the prefix "6" represents the C(B–N) number of zigzag chains in the sublattice being across ZGNR (ZBNNR) along the lateral direction. We created a two-probe system that is divided into three regions: the left electrode, the right electrode and the scattering region. Left (right) electrode is described by a supercell with three repeated B–N (C) unit cells along transport direction, and the scattering region is ZBNNR of 4 unit cells combine with ZGNR of 4 unit cells length. As the ferromagnetic (FM) and antiferromagnetic (AF) configurations can be stabilized over the other magnetic configurations by applying an external magnetic field for bare ZGNRs and ZBNNRs [37,38], both FM and AF initial configurations of the atoms between the two edges are considered.

We perform first-principles calculations based on the fully self-consistent non-equilibrium Green's functions and the density functional theory by applying an *ab initio* software package, ATOMISTIX TOOLKIT (ATK) [39,40]. With the help of the non-equilibrium Green's function (NEGF) method and the Landauer–Büttiker formula, the spin-dependent current I_σ through the scattering region is calculated from the formula [41]

$$I_\sigma = \frac{e}{h}\int_{\mu_l(V_b)}^{\mu_r(V_b)} T_\sigma(E, V_b)dE \tag{1}$$

where the σ is a spin index, represents spin-up ($\uparrow$) and spin-down ($\downarrow$). $\mu_{l/r}(V_b)$ is the electrochemical potentials of the left (l)/right (r) electrode. When external bias V_b is applied, the chemical potential of the left and right electrode will be shifted rigidly relative to each other, namely, $\mu_l(V_b) = \mu_l(0) - eV_b/2$, $\mu_r(V_b) = \mu_r(0) + eV_b/2$. For every spin state, the electron transmission coefficient $T_\sigma(E, V_b)$ can be written as

$$T_\sigma(E, V_b) = T_r\left[\Gamma_l G^R \Gamma_r G^A\right] \tag{2}$$

where $G^{R(A)}$ are the retarded and advanced Green's functions of the scattering region and $\Gamma_{l/r}$ are coupling matrices to the left/right electrodes.

The spin-polarized local density approximation (SLDA) is used to describe the exchange-correlation energy and single $\xi+$ polarization basis set was used for the geometrical optimization and the electronic transport calculation. The calculation for electrode part is performed under periodical boundary conditions, the k-point grid being $1 \times 1 \times 100$, the cutoff energy of all atoms being 150 Ry. The supercell is large enough to ensure that the vacuum space is at least 15 Å to avoid the interaction between periodic images. All structures were relaxed until atomic forces were below 0.05 eV/Å.

3. Results and discussions

To calculate spin-dependent transport properties, in Fig. 2, we firstly show the current and the corresponding magnetoresistance ratio as a function of bias for 6-ZBNNR/6-ZGNR two-probe system

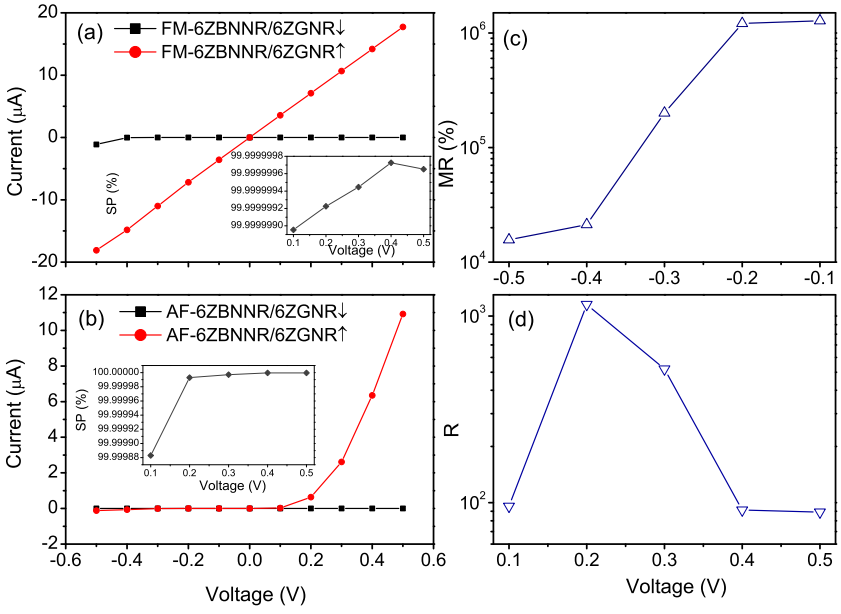

Fig. 2. (Color online.) (a)–(b) Spin-dependent I–V curves for the FM and AF configurations, respectively; (c) the magnetoresistance ratio (MR); (d) rectifying ratio (R) of spin-up current changes with the applied bias at AF configuration. The insets of (a) and (b) denote the spin polarization (SP) at FM and AF configurations, respectively.