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The magnetoresistance effect and spin-polarized photocurrent of zigzag graphene-graphyne nanoribbon heterojunctions

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ABSTRACT

Using density functional theory and non-equilibrium Green's function method, we designed several zigzag graphene-graphyne nanoribbon heterojunction devices and investigated their spin-dependent transport and optoelectronic properties. Our results show that the heterojunctions have outstanding giant magnetoresistance (GMR) effect. The GMR value is as high as 10^6%. According to the symmetry and connection way, for the ferromagnetic states the heterojunctions may produce two spin currents and exhibit significant rectification behaviors. Furthermore, spin-polarized photocurrents can be generated by irradiating the devices with infrared, visible or ultraviolet light. More importantly, in these heterojunctions we found that the behavior of the spin-up (spin-down) photocurrent for the ferromagnetic state is similar to that of the spin-down (spin-up) photocurrent for the antiferromagnetic state. This novel effect provides an efficient way to control the spin transport in the systems.

1. Introduction

Graphene, a famous two-dimensional (2D) carbon material, is predicted to have a range of unique properties [1–7]. Recent studies have shown that not only the 2D graphene but also the one-dimensional (1D) graphene nanoribbons (GNRs) have extraordinary physical and chemical properties [8–21]. According to the arrangement of the edged carbon atoms, these nanoribbons could be divided into two typical categories, i.e., zigzag graphene nanoribbon (ZGNR) and armchair graphene nanoribbon (AGNR).

Experimentally, various GNRs have been successfully implemented by cutting graphene at the nanoscale [8–12]. Depending on the widths and edges, experimental results show that GNRs could exhibit metallic or semiconducting behaviors and have interesting magnetic properties [9–11]. Furthermore, these experimental observations have also been verified by different theoretical methods [13–21]. For example, although the ground state of ZGNRs is antiferromagnetic (AFM) with zero total magnetic moment, a lot of effective methods have been proposed to realize ferromagnetic (FM) state in ZGNRs [22–24].

Recently, it was shown that several graphene-like carbon allotropes can be stable and they widen the potential applications of carbon materials [25,26]. Of particular importance is the so-called graphyne, which is also a well-known 2D carbon material and is becoming a very interesting topic in carbon material research community. Graphyne holds four typical geometrical structures, namely α-graphyne, β-graphyne, γ-graphyne and (6, 6, 12)-graphyne [27]. These structures have different properties. For instance, γ-graphyne is a semiconductor while the other three systems are all metals [28,29].

Similar to GNR, 1D graphyne nanoribbon (GyNR), according to the edge shape, could be typically divided into zigzag graphyne nanoribbon (ZGyNR) and armchair graphyne nanoribbon (AGyNR). Previous study shows that one can design different heterojunctions using these nanoribbons [30]. Because ZGNR and ZGyNR have different properties, in present study we theoretically design several different ZGNR-ZGyNR heterojunction devices and investigate their spin-dependent transport properties. Since FM ZGNR is a metal while AFM ZGNR has semiconducting nature [23], in order to effectively construct metal-semiconductor or semiconductor-semiconductor heterojunction devices, here we chose γ-ZGyNR as the second part of the devices since the semiconducting nature of the γ-ZGyNR has been justified in our recent study [31]. Another

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important reason for choosing γ-ZGyNR is that among four graphynes, only one of the γ-graphynes, γ-graphdiyne, has been fabricated in experiment [32,33]. The experimental progress indicates that various typical γ-graphynes will hopefully be obtained in the near future.

The paper is organized as follows. In Section 2, the structures of ZGNR-ZGyNR heterojunctions are introduced and the computational details are discussed. In section 3, the spin-dependent transport properties of these heterojunctions under finite bias voltage are presented; the spin-polarized optoelectronic properties of the systems are investigated in the section as well. Finally, we conclude this work in Section 4.

2. Models and methods

The designed four ZGNR-ZGyNR heterojunction devices Mi (i = 1–4) are presented in Fig. 1a. Each device is divided into three parts, namely, the left electrode, the central scattering region, and the right electrode. The left and right electrodes of the four systems are the same, but the symmetries and the connection ways of ZGNR and ZGyNR are different.

The structures of all the devices were fully optimized by using density functional theory (DFT) as implemented in Atomistix ToolKit (ATK) package [34]. The exchange-correlation functional was treated within the generalized gradient approximation proposed by Perdew, Burke and Ernzerhof (PBE) [35], and the double-ζ plus polarization (DZP) basis sets were adopted in the calculation. The spin-dependent transport properties of the devices were then studied by combining of DFT and non-equilibrium Green's function (NEGF) method [36,37].

Careful and extensive convergence tests were performed. Finally, the kinetic cutoff energy was set to 200 Ry and, during the optimization, a criterion of 0.01 eV/Å for atomic force was employed. The Brillouin zone was sampled by $1 \times 1 \times 100$ mesh points in k-space. Since the transport is along z axis, in x and y directions large vacuum space was included in the supercell to avoid the interactions between the periodic images. For the four devices Mi (i = 1–4), the dimensions of the supercells used in the calculation are $20 \times 40 \times 52.91$, $20 \times 40 \times 51.65$, $20 \times 40 \times 52.95$ and $20 \times 50 \times 50.55$ Å^3, respectively.

The spin current I_σ as a function of bias voltage V_b can be calculated from Landauer-Büttiker formula [38]:

$$I_\sigma(V_b) = (e/h)\int T_\sigma(E,V_b)[f_L(E,V_b) - f_R(E,V_b)]dE \quad (1)$$

where σ = ↑ (spin up) and ↓ (spin down), e is the electron charge, h is the Planck's constant, $T_\sigma(E,V_b)$ is the bias-dependent transmission coefficient and $f_{L(R)}(E)$ is the Fermi-Dirac distribution of the left (right) electrode.

As mentioned before, ZGNRs have different magnetic states. For the ZGNR considered here, the calculated energy bands of the FM and AFM states are presented in Fig. 1b. It is obvious that the FM ZGNR is a metal while the AFM ZGNR is a semiconductor, and the spin-up and spin-down energy bands of the AFM state are degenerate. For ZGyNR, it is a nonmagnetic semiconductor (see Fig. 1c). Therefore, by changing the magnetic states of ZGNR, we can obtain metal-semiconductor or semiconductor-semiconductor heterojunction for a given device Mi. Since ZGyNR is a nonmagnetic semiconductor, in the rest of the paper we will use the magnetic state of ZGNR to represent that of the whole device. Note that in our models there is only one magnetic electrode, thus we will investigate various spin-dependent transport processes by changing the magnetic states of ZGNR; this is

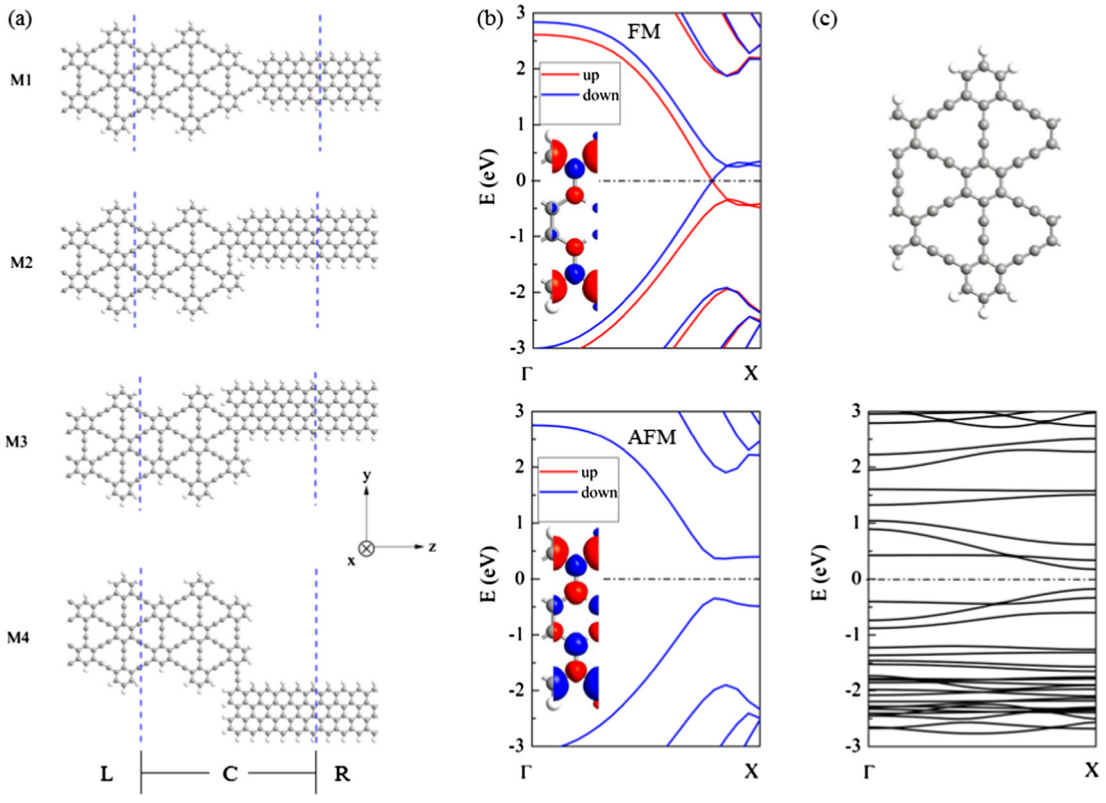

Fig. 1. (a) The designed four ZGNR-ZGyNR heterojunction devices Mi (i = 1–4). The gray and white spheres represent carbon and hydrogen respectively. Each device is divided into three parts: the left electrode (L), the central region (C) and the right electrode (R). (b) The energy bands of ZGNR for the FM and AFM states. The inset is the spin difference density and the values of red and blue isosurfaces are ±0.03 e/Å^3. (c) The unit cell and band structure of ZGyNR. The Fermi level is indicated by the dashed line.