Organic Electronics 14 (2013) 3240–3248

Contents lists available at ScienceDirect

Organic Electronics

journal homepage: www.elsevier.com/locate/orgel

The design of spin filter junction in zigzag graphene nanoribbons with asymmetric edge hydrogenation

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ARTICLE INFO

Article history:
Received 21 July 2013
Received in revised form 4 September 2013
Accepted 28 September 2013
Available online 13 October 2013

Keywords:
Spin filtering effect
Graphene nanoribbons
Heterostructure
First-principles calculation

ABSTRACT

Using the non-equilibrium Green's function method combined with the density functional theory, we investigate the electronic transport properties of a heterostructure based on zigzag graphene, This heterostructure consists of H2–NZGNR–H and H–NZGNR–H. Results show that a perfect dual spin filtering effect can be realized with the parallel (P) and antiparallel (AP) magnetiesm configuration, and some magnetic domain walls (DW) at the interface between two component ribbons. The magnetic moments, DOS and PDOS, the transmission pathways and LDOS demonstrate that the edge of C–H2 bonds have important effects for magnetic and spin dependent transport properties compared to the edge of C–H bonds. Our results show that the H2–ZGNR–H/H–NZGNR–H heterostructure holds promise for magneto electronics devices which can keep steady properties when change the widths of the two component ribbons.

1. Introduction

Molecular nanostructures have been investigated actively in last few decades due to their promising potential for developing molecular devices [1–6]. Graphene, a two-dimensional (2D) network of sp^2 hybridized carbon atoms packed into hexagonal structure with a single-atom thickness, has attracted more and more attention due to its unique electronic transport properties and its profound potential for future device application [7–12]. Seeking for high performance graphene-based spintronics is a challenging work and has excited much research interest in recently years. In spintronics device, the spin-polarization of carriers will be partially kept when carriers have traveled across the conducting channel, as long as the channel length is shorter than the spin relaxation length. One remarkable property of graphene-based spintronics devices is that charge carriers have the spin relaxation times of 0.1–0.4 ns, and spin coherence lengths of 1.5–2.4 μm at room temperature [13,14]. At present, we are witnessing an intensive investigation on zigzag-edge graphene nanoribbons (ZGNRs) due to their potential applications in spintronics, including spin-polarized current rectification, spin filtering effects, giant magnetoresistance phenomenon, etc. Among them, four methods are of great importance in designing those desirable junctions, which are manipulating localized edge states of ZGNRs [15–17], matching the electrode band symmetry [18–20], tuning the electronic structure of the central molecule [21–25], and tuning the magnetic configuration of the two leads [14,26]. Generally speaking, the ground state of ZGNRs is antiferromagnetic (AFM) with zero total magnetic moment, no half-metallicity occurs unless edge modification [27], applying external electric field [15], doping other atoms [28] and topologic line defects [29], to break the spin degeneracy in ZGNRs. For example, more stable ferromagnetic (FM) states have been reported by the application of magnetic or electrical field in experiments [15,30]. But other some investigations showed that the nonmagnetism (NM) state would be the

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http://dx.doi.org/10.1016/j.orgel.2013.09.041

most stable compared with AFM or FM state at different temperature or under the condition of a ballistic current through the GNRs [31,32].

In order to stabilize the edges of the GNRs, the dangling bonds of the edge carbon atoms have to be passivated by various ways, including symmetric monohydrogenation (with one hydrogen atom saturating each dangling bond, referred as H–ZGNR–H, symmetric dehydrogenation (with two hydrogen atoms saturating each edge carbon atom, referred as H2–ZGNR–H2), and asymmetric hydrogenated ZGNR, referred as H2–ZGNR–H, which are C–H2 bonded at one edge while C–H bonded at the another. This H2–ZGNR–H scheme has been adopted in the design of graphene spin-current devices [33], and the ground state of such asymmetric hydrogenated ZGNR is ferromagnetic (FM) semiconductor. More importantly, the H2–ZGNR–H scheme is stable under room temperature with molecular dynamics simulations [34]. Recently, through studies on the chemical potential of hydrogen, researchers demonstrated that the composition of sp^2 and sp^3 types at the edges of the GNRs can be easily controlled, which indicates that the monohydrogen-terminated and dihydrogen-terminated grapheme nanoribbon heterojunction can be fabricated with experiment [35,36]. Kang et al. found that the DOS distribution of H_2–ZGNR–H has two peaks near E_F [28]. The valence states just below E_F belong to the up spin whereas the conduction states just above E_F correspond to the down spin. Furthermore, the ZGNR–H/ZGNR–H_2 heterojunction can be set as different magnetic configurations and 100% perfect spin filtering effect can be realized, but affected by the widths of the two component ribbons [37]. By tuning the magnetic field, the switch behaviors can also be achieved [20], which are originated from the matching or mismatching between the π or π^* states of the two ribbons under differently directional magnetic field. In fact, no attempt has been made so far to excavate the mechanism of this heterojunction at finite bias voltages.

In this work, we report a design of heterojunctions consisting of H2–ZGNR–H and H–ZGNR–H. Our results show that the perfect dual spin filter effect can be observed when those heterojunctions are designed as the parallel (P) or antiparallel (AP) magnetic configurations. Interestingly, it is not affected by the widths of the two component ribbons, which indicates a better prospect for device application.

2. Model and method

Following conventional custom, the width of ZGNRs can be characterized by the number of zigzag *C* chains, *N*, along the direction perpendicular to the nanoribbon axis, which is denoted as NZGNRs. Considering the geometrical symmetry, the NZGNRs are classified into two types, symmetric and asymmetric ZGNRs, corresponding to even and odd *N*, respectively. In this paper, we design four different heterojunctions with H2–ZGNR–H and H–ZGNR–H structures, namely, H2–5(6)ZGNR–H/H– 5(6) ZGNR–H, H2–5(6)ZGNR–H/H–6(5)ZGNR–H. For convenience, these four heterojunctions are denoted as M1, M2, M3, and M4, respectively, shown in Fig. 1a–d. A device is divided into three regions: left electrode, right electrode, and the central scattering region, marked by *L*, *R*, and *C*.

The first-principles transport calculations we present for a two-probe system are performed using the non-equilibrium Green's function method combined with the density functional theory (NEGF/DFT) as implemented in latest version of Atomistix ToolKit (ATK) [38–40]. We employ Troullier–Martins norm-conserving pseudo-potential to present the atom core and linear combinations of atom orbitals to expand the valence state of electrons. The local

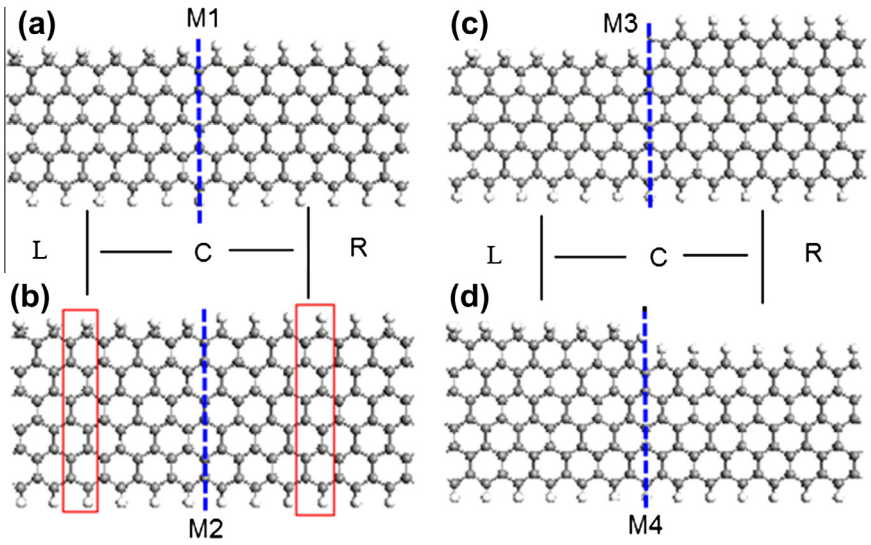

Fig. 1. The geometric structure (a) H2–5ZGNR–H/H–5ZGNR–H (M1), (b) H2–6ZGNR–H/H–6ZGNR–H (M2), (c) H2–5ZGNR–H/ H–6ZGNR–H (M3) and (d) H2–6ZGNR–H/ H–5ZGNR–H(M4), the blue dash lines is the boundary of heterojunctions, the red solid rectangle denotes the unit cell of ZGNRs. L, R, and C means the left and right electrodes, and the central scattering region. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)