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The spin-dependent transport and optoelectronic properties of the 6,6,12-graphyne-based magnetic tunnel junction devices

Maoyun Di[a], Zhi Yang[a,*], Jin Li[b,c], Huifang Bai[a], Luyao Hao[a], Li-Chun Xu[a], Ruiping Liu[a], Xuguang Liu[c,d]

[a] College of Physics and Optoelectronics, Taiyuan University of Technology, Taiyuan, 030024, China
[b] College of Chemistry and Chemical Engineering, Taiyuan University of Technology, Taiyuan, 030024, China
[c] Key Lab of Interface Science and Engineering in Advanced Materials, Ministry of Education, Taiyuan University of Technology, Taiyuan, 030024, China
[d] College of Materials Science and Engineering, Taiyuan University of Technology, Taiyuan, 030024, China

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ABSTRACT

Using density functional theory and nonequilibrium Green's function method, we investigated the spin-dependent transport and spin-polarized optoelectronic properties of the 6,6,12-graphyne-based magnetic tunnel junction (MTJ) devices. The results show that the MTJ devices have prominent dual spin-filtering effect and large tunneling magnetoresistance (TMR); the TMR values of the MTJ devices are as high as 10^5%. In addition, we found that the spin-polarized photocurrents of the MTJ devices are dependent on the polarization direction of light and the magnetization directions of the electrodes. Two spin-polarized photocurrents can be realized in the MTJ devices and, if the magnetization directions of the two electrodes are antiparallel, the two light-generated spins flow in opposite directions. These interesting phenomena indicate that the 6,6,12-graphyne-based MTJ devices could be used as optoelectronic or opto-spintronic devices.

1. Introduction

Spintronics has caught great attention due to the applications in different fields such as programmable logic elements and non-volatile information storage devices [1]. Among different spintronic devices, the most important one is the magnetic tunnel junction (MTJ). A typical MTJ is comprised of two ferromagnetic (FM) metal layers separated by a thin insulating (I) barrier layer, which can be formally expressed as FM/I/FM [2]. In the traditional MTJ devices, the magnetic metals are generally Fe, Co, Ni or related alloys, while the insulators are typically metal oxides such as Al_2O_3, MgO or Y_2O_3 [3–6]. The most important phenomenon in various MTJ devices is the so-called tunneling magnetoresistance (TMR) effect, i.e., the resistance or conductance of the MTJ is dependent on the magnetization directions of the two FM metals. The TMR value of a MTJ device is calculated from $TMR = (R^A - R^P)/R^P$, where R^P or R^A is the resistance when the magnetization directions of the two FM metal layers are parallel or antiparallel.

Outstanding TMR effect has been observed in different traditional MTJ devices. For example, a TMR value of 12% was observed in the $CoFe/Al_2O_3/Co$ MTJ [4]. Yuasa and the co-workers verified that, at room temperature, the TMR in the single crystal Fe/MgO/Fe MTJ can reach 220% [5]. Furthermore, the $Fe/PbTiO_3/Fe$ MTJ has been investigated and the results show that the TMR of the system is as high as 700% [6]. In order to obtain higher TMR value, recently much attention has been paid to the MTJ devices at molecular level [7–9], since in these microscopic systems quantum transport process is dominant. For instance, Dhungana et al. found that the terpyridine-based MTJ has a very large TMR value, 1470% [9].

Graphene, a novel two-dimensional (2D) carbon material, has motivated great interests recently, because of its unique physical and chemical properties, e.g. the Dirac cone in the energy band structure [10]. In addition to 2D graphene, one-dimensional (1D) graphene nanoribbons (GNRs) have been widely investigated as well [11]. According to the different arrangement of the edged C atoms, GNRs are typically classified into armchair graphene nanoribbons (AGNRs) and zigzag graphene nanoribbons (ZGNRs). Owing to the edge magnetism [12–14], ZGNRs are regarded as promising candidate materials for spintronic devices [15–20]. Previous study suggested that the ground state of ZGNRs is antiferromagnetic (AFM) with zero total magnetic moment, but ferromagnetic (FM) ZGNRs can also be achieved by various experimental methods [13,14].

Besides graphene, various 2D carbon materials have been carefully investigated so far; one typical example is the so-called graphyne [21–24]. Graphyne is a new carbon nanosheet composed of both sp and

* Corresponding author.
E-mail address: yangzhi@tyut.edu.cn (Z. Yang).

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sp^2 hybridized C atoms and, different from graphene, graphyne holds many allotropes, e.g. α-graphyne, β-graphyne and 6,6,12-graphyne [21]. A recent study indicated that α-graphyne, β-graphyne and 6,6,12-graphyne all have Dirac cones in the energy band structures but their symmetries are different [24]; the first two have hexagonal symmetries while the last one is rectangular. Graphyne has amazing electronic, optical and mechanical properties [25–30]. Especially, Chen et al. found that at room temperature the inherent carrier mobilities of the 6,6,12-graphyne can reach 5.41 × 10^5 and 4.29 × 10^5 cm^2/Vs for electrons and holes respectively, which are even larger than those of graphene [30]. The intriguing feature indicates that 6,6,12-graphyne could probably have excellent transport properties and can be employed to design spintronic devices. In fact, although α-graphyne and β-graphyne have been used to construct different spintronic devices [31–33], the related studies on 6,6,12-graphyne are still very limited so far.

Therefore, in this paper, using 6,6,12-graphyne we theoretically designed several different MTJ devices and discussed their spin-dependent transport and spin-polarized optoelectronic properties. The rest of the paper is arranged as follows. In section 2, the structures of the 6,6,12-graphyne-based MTJ devices are introduced and the computational details are discussed. In section 3, the spin-dependent transport properties of the devices under finite bias voltage are presented, and the spin-polarized optoelectronic properties of the systems are discussed in the section as well. Finally, we conclude this work in section 4.

2. Models and computational details

The designed two typical MTJ devices, M1 and M2, are shown in Fig. 1a; each device can be divided into three parts, namely, the left electrode, the central scattering region and the right electrode. Here, two identical FM ZGNRs are employed as left and right electrodes, while the central scattering region is a 6,6,12-graphyne nanodot (GYND). In the two devices, the connection ways between the ZGNRs and the GYND are different, forming two different ZGNR/GYND/ZGNR MTJ devices. For M1, the GYND is connected to the ZGNR electrodes through C—C bonds. Compared with M1, the GYND in M2 is rotated by π/2 and is then connected to the ZGNRs through the sp^2 hybridized C atoms. To stabilize the devices, all the edged C atoms are saturated with H atoms. Because the magnetization directions of the two FM electrodes could be parallel (P) or antiparallel (A), like other MTJ devices [15,34], M1 or M2 has the P and A spin configurations. Furthermore, in the structures of M1 and M2 there exists mirror symmetry perpendicular to the z axis, thus the two MTJ devices are symmetrical. In fact, various elaborate nanostructures, such as graphene/*h*-BN monolayer heterojunctions, graphene-based spin valves or organic single-molecule devices, have been constructed by using different experimental methods [35–37]; we believe the designed 6,6,12-graphyne-based MTJ devices could also be realized in the future experiments, and present theoretical study will promote the related experimental investigations on the graphyne-based technologies and devices.

The structures of M1 and M2 were optimized by using density functional theory (DFT) as implemented in *Atomistix ToolKit* (*ATK*) package [38]. The exchange-correlation functional was treated within the generalized gradient approximation (GGA) proposed by Perdew, Burke and Ernzerhof (PBE) [39], and the double-ζ plus polarization (DZP) basis sets were adopted in the calculation. After careful and extensive test, the 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 × 1 × 100 mesh points in *k*-space based on the Monkhorst-Pack scheme [40]. Since the transport direction is

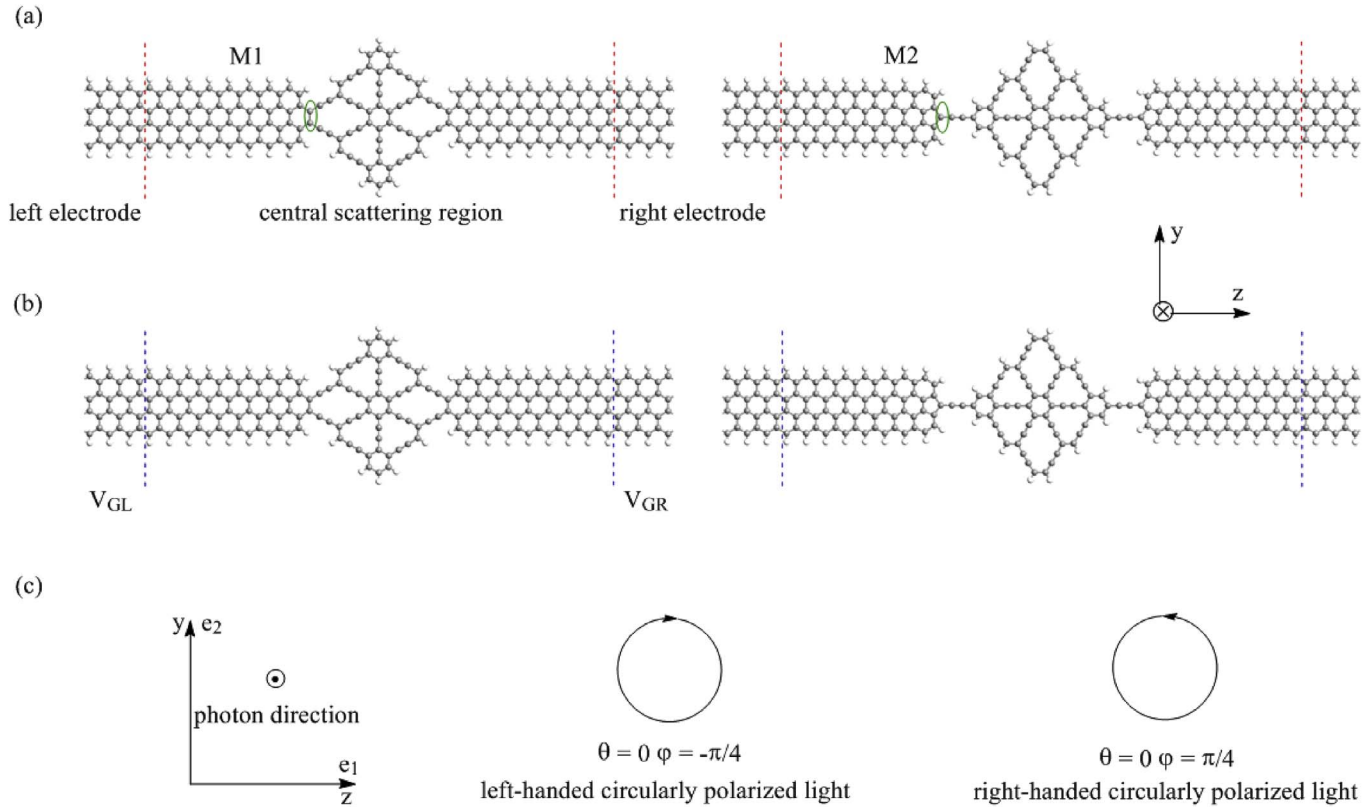

Fig. 1. (a) The designed two MTJ devices: M1 and M2. Each device is divided into three parts, namely, the left electrode, the central scattering region and the right electrode. The green circles indicate different connection ways between the GYND and the two ZGNRs. (b) The gate-voltage-controlled MTJ devices. Here V_{GL} and V_{GR} are the left and right local gate voltages respectively. (c) $\mathbf{e_1}$ and $\mathbf{e_2}$ are the unit vectors of the z and y axes and are used as basis vectors to characterize the polarization of the photon. The parameters θ and φ of the left-handed and right-handed circularly polarized light are presented. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)