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Spin filtering and rectifying effects in the zinc methyl phenalenyl molecule between graphene nanoribbon leads

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ABSTRACT

The molecule zinc methyl phenalenyl (ZMP), which is a neutral planar phenalenyl-based molecule, has been successfully synthesized experimentally, and large magnetic anisotropy was demonstrated when it is grown on the ferromagnetic metal surface [K. V. Raman et al. Nature, 2013, **493**, 509]. Here, by using nonequilibrium Green's functions combined with the density functional theory, we investigate the electronic transport properties in the ZMP molecule coupled to graphene nanoribbon (GNR) leads. When the ZMP molecule is linked to zigzag GNR (ZGNR) electrodes, perfect spin-filtering effect and large spin-rectifying effect are found. And when the ZMP molecule is coupled to armchair GNR (AGNR) electrodes, rectifying effect is obtained and the rectifying directions can be manipulated by substituting the hydrogen atoms at the edge of ZMP molecule with atoms oxygen or nitrogen. The above interesting properties can be used for the next generation nanoscale device. Analyses are proposed for these phenomena.

1. Introduction

With the development of electronic science, the traditional silicon-based devices face the challenge of further miniaturization. And the molecular devices will become the ideal candidate for replacing the traditional silicon-based devices [1–3]. In recent years, scientists have studied many different types of molecular devices both in theory and in experiment, and have synthesized many new suitable molecular materials for molecular devices, such as phthalocyanine [4], perylene tetracarboxylic diimide [5], graphene [6] and so on. In 1974, Aviram and Ratner put forward the first molecular theory model and the concept of molecular rectifier [7]. Soon, the United States professor, Moodera et al. proposed the concept of spin-filtering firstly [8]. After that, the exposures of molecular nanostructures are very popular due to their promising potential for developing molecular devices [9–13]. As we all know, we can design molecular devices to realize useful functions of electronic devices based on silicon material, such as negative differential resistance (NDR) [2,14], rectifier [15,16], spin-filter [17,18], spin-valve [19,20], giant magnetoresistance device [21,22], etc.

Recently, graphene has attracted more and more attention since it was discovered experimentally in 2004 [6]. Graphene is found to have many unique electronic transport properties, which is a good candidate for future nano-device [23–27]. GNR has two typical types, armchair-edged GNR and zigzag-edged GNR [28], according to different edge shapes. The AGNR doesn't show the magnet, but the ZGNR has three magnetic states, ferromagnetic (FM) state, antiferromagnetic (AFM) state and non-magnetic (NM) state. And the AFM state is the ground state [29]. Moreover, the ZGNR has long spin diffusion length, spin relaxation time and electron spin coherence time [29,30]. Also, the magnetic direction of the ZGNR can be controlled by adding the external magnetic field [31,32]. Given the differences in performance between the ZGNR and the AGNR, we can use different edged GNRs as electrodes to design nanodevices for the purpose of different transport properties [15,33,34]. For molecular device, however, the most important thing is to found the suitable small organic molecule. Recently, Raman et al. has synthesized a new neutral planar phenalenyl-based molecule (ZMP, $C_{14}H_{10}O_2Zn$), which has no net spin [35]. However, when these molecules are grown on a ferromagnetic metal surface, the system shows a large magnetic anisotropy and spin-filter properties [36]. The results showed that this nonmagnetic molecule had a great effect on spin transportation.

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In present paper, we systematically investigated the electron transport properties of the ZMP molecule linked to two ZGNR electrodes or two AGNR electrodes, respectively. In magnetization configurations, when the ZGNR electrodes are set as it's ground state (AFM state), the electron transport properties of spin up and spin down are almost consistent, but, when the ZGNR electrodes are set as ferromagnetic (FM) state, the transport channel of spin up is open while the spin down one is closed at Fermi level, which leads to the 100% spin filtering ratio. Moreover, we calculate other two types of magnetic directions of the ZGNR electrode [1,0], and [1,−1], which can be realized by adding the external magnetic field. Interestingly, the dual spin-filtering and great spin-rectifying effects appeared in [1,−1]. Further, when taking the AGNR as electrodes to construct nonmagnetic configuration, rectifier phenomenon is obtained and the rectifying directions will be changed by using different atoms to modify the hydrogenated edge of ZMP molecule [15,37,38].

2. Model and method

The models we study are shown in Fig. 1. All the devices are divided into three parts: left electrode, scattering region and right electrode. Firstly, we consider the magnetic system: a new neutral planar ZMP molecule is linked to the 4-ZGNR electrodes through a five-membered carbon ring (Fig. 1a), which is a stable connection according to previous study [18]. The carbon atoms at the zigzag edges own magnets. Here, we consider four types of magnetic systems. The first one is that the magnets of left and right ZGNR electrodes are set as its ground state (AFM), which is called M_{11}. The second one is that set as FM state (M_{12}). The third one and the fourth one are that set as [1,0] and [1,−1], respectively, which are called M_{13} and M_{14}. The magnetic direction [1,0] stands for one electrode is magnetized while the other is nonmagnetic and the anti-parallel magnetic direction [1,−1] stands for the left and right ZGNR electrodes having opposite magnetic directions. What's more, we show the nonmagnetic device that the ZMP molecule is connected to the 11-AGNR electrodes in Fig. 1b. The molecule can attach onto AGNR electrodes with atom precision by sharping zigzag edge in GNR which has been obtained experimentally [39]. The left part of the ZMP molecule is a trigonal graphene and the edge carbon atoms of the molecule ZMP can be passivated by H atoms, O atoms, or N atoms [15,34]. The above three different passivation configurations are referred as M_{21}, M_{22} and M_{23}, respectively.

The structure relaxations and transport properties calculations for all of the above models are carried out within the framework of density-functional theory (DFT) method as implemented in the atomistix toolkit (ATK) [40,41]. These geometries are optimized until all residual forces on each atom are smaller than 0.02 *eV/Á*. The local density approximation is adopted for the exchange-correlation functional, and the basis set for zinc and oxygen atoms is double zetas plus polarization (DZP) and that for other atoms is single zetas plus (SZP). We employ troullier−martins norm−conserving pseudo-potentials to represent the atom core and linear combinations of atomic orbitals to expand the valence states of electrons. The k-point sampling is $1 \times 1 \times 100$ in the x, y, z direction and here *z* is the transport direction, we also set 150 *Ry* as the cutoff energy and select 10^{-5} *eV* as the convergence criterion for the total energy, the electron temperature is set to 300 *K* in the transport calculation. Here, the only purpose of setting the temperature to 300 K is to accelerate the convergence in our calculations. This is a general technique in all DFT calculations. In the calculations, the order of energy levels may frequently change around the Fermi level in the converging process, which may lead

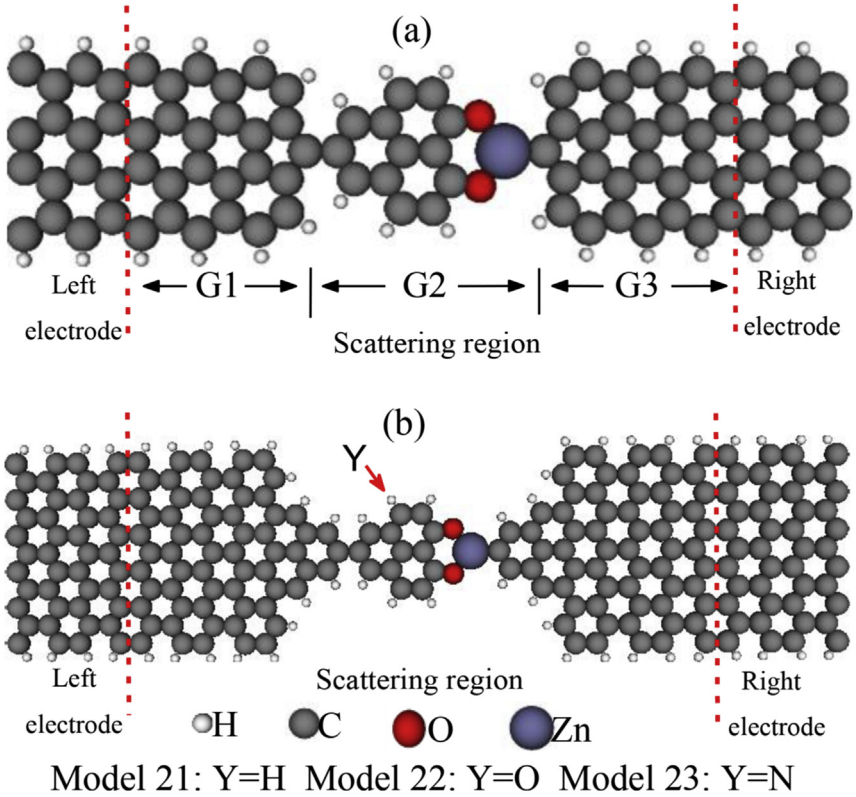

Fig. 1. The device models of a ZMP molecule sandwiched to (a) ZGNR leads and (b) AGNR electrodes respectively. The Y denotes the passivation atoms of the edge carbon atoms of the ZMP molecule and Y can be H, O or N atoms, respectively.