



# Giant magnetoresistance effect and spin filters in phthalocyanine-based molecular devices

Yan-Hong Zhou<sup>a</sup>, Jing Zeng<sup>a</sup>, Li-Ming Tang<sup>a</sup>, Ke-Qiu Chen<sup>a,\*</sup>, W.P. Hu<sup>b</sup>

<sup>a</sup> Department of Applied Physics, Hunan University and Key Lab for Micro-Nano Physics and Technology of Hunan Province, Changsha 410082, China

<sup>b</sup> Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Science, Beijing 100080, China

## ARTICLE INFO

### Article history:

Received 5 July 2013

Received in revised form 23 August 2013

Accepted 27 August 2013

Available online 8 September 2013

### Keywords:

Giant magnetoresistance

Spin filter

Phthalocyanine molecule

Density functional theory

## ABSTRACT

The spin transport properties of molecular devices constructed by hydrogen-phthalocyanine and transition metal (TM)-phthalocyanine molecule with zigzag graphene nanoribbon electrodes are investigated by the Keldysh nonequilibrium Green's function method in combination with the density functional theory. The results show that there exists giant magnetoresistance in both the hydrogen-phthalocyanine and the TM-phthalocyanine systems. The magnetoresistance ratio is much bigger than that found by Schmaus et al. [S. Schmaus, A. Bagrets, Y. Nahas, T. K. Yamada, A. Bork, M. Bowen, E. Beaurepaire, F. Evers, W. Wulfhekel, Nature Nanotechnology 6 (2011) 185–9] in single hydrogen-phthalocyanine-Co electrodes system. Moreover, it is found that the chromium-phthalocyanine molecular device is a good spin filtering device with nearly 100% spin filtering efficiency at a wide bias voltage region. The mechanisms are proposed for these phenomena.

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## 1. Introduction

The electron spin appeared in the device world two decades ago [1,2]. However, due to the technological revolution originated from the continual improvement in our understanding on how spins can be injected, manipulated and detected in the solid state, the spin state of a moving electron can be detected now, which underpins the entire magnetic data storage industry [3,4]. It is true that spin electronics have led to new generations of read heads in hard disk drives and random access memory, but further progress in downsizing spintronic devices is a challenge because reducing the device size will lead to high resistances and shot noise. Then a promising approach is to design single-molecule spintronic devices such as molecular rectifiers, switches and transistors [5–8]. Most of the development in this new technology, spintronics, is currently based on inorganic materials. In fact the organic molecules can provide desirable properties like flexibility,

inexpensive material and production methods, and compatibility with biological systems [9]. Indeed some works in this direction are underway. Organic electronics is finding its place as an important technology for production of various electronic devices like transistors and organic light emitting diodes [10,11]. Organic molecules have also been introduced into spin-valves, and spin dependent tunneling through organic molecules adsorbed on magnetic substrates has been demonstrated [12,13].

Among the many potential organic molecular candidates, hydrogen-phthalocyanine and transition metal (TM)-phthalocyanine form a promising and important family of compounds. Lots of experimental and theoretical investigations have been done to their electronic properties and electro-magnetic properties [14–17]. However, just a few researches on the electronic transport properties of phthalocyanine in electrode-molecule-electrode system have been reported [18–23]. Iacovita et al. investigated the spin transport across single cobalt-phthalocyanine molecules adsorbed on cobalt nanoislands and demonstrated that there was a spin-polarized electronic resonance over the center of the molecule [18]. In the year

\* Corresponding author.

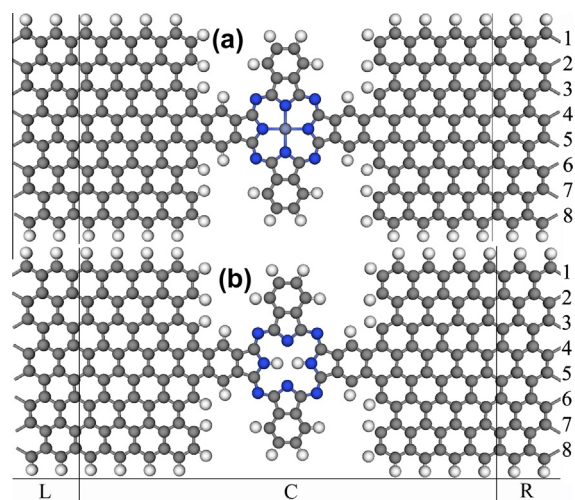
E-mail address: [keqiuchen@hnu.edu.cn](mailto:keqiuchen@hnu.edu.cn) (K.-Q. Chen).

2011, giant magnetoresistance was gained by Schmaus et al. in single hydrogen-phthalocyanine molecules coupled to two ferromagnetic Co electrodes [21]. And later in the year 2012, a little smaller magnetoresistance was shown in the heterojunctions of antiferromagnetic electrode/hydrogen-phthalocyanine molecules/ferromagnetic electrode [23]. Shen et al. studied spin transport properties of TM-phthalocyanines contacted with single-walled carbon nanotube electrodes and found that only manganese-phthalocyanine and iron-phthalocyanine molecules can act as nearly perfect spin filters [20]. Huang et al. got high spin filter efficiency in iron-phthalocyanine molecule sandwiched between two N-doped armchaired graphene nanoribbons [22]. These results indicate that there is great prospect for designing such molecule systems as the high-performance spintronic device.

Graphene, which was obtained experimentally in the year 2004, has been considered as a good candidate for spin-based quantum computing and spintronics for its long spin decoherence, relaxation time, and high electronic mobility [24]. For example, Wei et al. shows a strong gate-dependent rectifying behavior in a graphene nanoribbon/single-walled carbon nanotube junction [25]. The armchair-edged graphene nanoribbons are nonmagnetic semiconductors. However, the zigzag-edged graphene nanoribbons are magnetic that the ZGNR-based device can be designed as parallel [1,1] or antiparallel [1,−1] magnetic configurations [26]. What is more, dual spin filter effect was shown in a 8-zigzag graphene nanoribbon, but not in a 7-zigzag graphene nanoribbon [27]. Therefore, in the present work, we study the transport properties of the phthalocyanine based molecules coupled to two 8-zigzag-edged graphene nanoribbons electrodes. Giant magnetoresistance exists in all phthalocyanine two-probe configurations and chromium-phthalocyanine configurations own the best spin filter efficiency.

## 2. Simulation model and calculation method

The model structures for our theoretical study are illustrated in Fig. 1. An individual single molecule hydrogen-phthalocyanine shown in Fig. 1(b) or a TM-phthalocyanine (here taking chromium-phthalocyanine as an example) shown in Fig. 1(a) is sandwiched between two infinite 8-zigzag-graphene nanoribbon electrodes. The number 8 is the width of the zigzag-graphene nanoribbon as was defined by Fujita previously [28]. We have chosen a supercell with a large enough vacuum layer in the  $x$  and  $y$  directions so that the device has no interaction with its mirror images. The system is divided into three regions: the left electrode, the right electrode and the central region. The semi-infinite electrodes are described by a supercell with two repeated carbon unitcells due to their periodicity along the transport direction. The single molecule hydrogen phthalocyanine (Fig. 1(b)) or a TM chromium-phthalocyanine (Fig. 1(a)) together with four unit cells left and right electrodes is chosen as the central region, as indicated by two vertical lines. As the magnetic fields at two electrodes can point in the same or opposite direction, the zigzag-graphene nanoribbon electrodes can show the parallel



**Fig. 1.** Schematic view of the two probe systems: (a) zigzag-graphene nanoribbon/TM-phthalocyanine (here for example chromium-phthalocyanine)/zigzag-graphene nanoribbon device junction, (b) zigzag-graphene nanoribbon/hydrogen-phthalocyanine/zigzag-graphene nanoribbon device junction. The labels L, C, and R represent the left electrode, the central region, and the right electrode, respectively.

( $P$ ) or antiparallel ( $AP$ ) spin configuration. The geometric optimization and spin-resolved electron transport properties are calculated by a developed first-principles software package Atomistix ToolKit, which is based on the spin-polarized density-functional theory combined with non-equilibrium Greens functions [29–32]. In our calculations, the core electrons are described by norm-conserving pseudopotentials, and the local spin density approximation (LSDA) with the Perdew–Zunger exchange–correlation potential is employed. Moreover, a cutoff energy of 150 Ry and a Monkhorst–Pack  $k$ -mesh of (1,1,100) are chosen to achieve the balance between calculation efficiency and accuracy. A single-zeta polarized (SZP) basis set is adopted for electron wave function and the convergence criterion for Hamiltonian and the electron density are  $10^{-5}$ . The structures of every single phthalocyanine molecules are optimized firstly, and then are optimized in the environment of two-probes, respectively. All the structures are fully relaxed using quasi-Newton method until the force tolerance of 0.01 eV/Å is reached.

## 3. Results and discussions

### 3.1. A. Giant magnetoresistance

Giant magnetoresistance is found in the hydrogen phthalocyanine and in all TM-phthalocyanine systems. Here we just show the current and the magnetoresistance ratio as a function of bias for hydrogen-phthalocyanine, cobalt-phthalocyanine and chromium-phthalocyanine two-probe systems in Fig. 2. Figs. 2(a–c) are the  $I$ – $V$  curves for hydrogen-phthalocyanine, cobalt-phthalocyanine and chromium-phthalocyanine configurations, respectively, and (d–f) are the corresponding the magnetoresistance ratio as a function of applied bias. It can be found from

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