

Spin-Dependent Transport Properties of a Phenylene Rotor Bridging Carbon Chains Between Graphene Electrodes

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Abstract. We study the spin-dependent electron transport by using *ab initio* calculations for a molecular junction consisting of a phenylene capped by two carbon chains which is sandwiched between two zigzag-edged graphene nanoribbon (ZGNR) electrodes modulated by external magnetic fields or ferromagnets. It is shown that the spin-charge transport can be adjusted by the phenylene rotation angles in respect to ZGNR electrodes and spin orientation in electrodes. Specifically, we demonstrate that the proposed molecular device exhibits switching, (dual) spin-filtering, rectifying, negative differential resistance (NDR) effects. Interestingly, when the phenylene rotation angle is $\theta=60^\circ$, the maximum value of the peak-to-valley ratio of NDR is up to 26, the spin-resolved rectification ratio can reach up to 2.47×10^4 , and the spin filtering efficiency reaches up to 100%. The physical mechanisms of these effects are analyzed via the spin-resolved transmission spectrum associated with local density of states (LDOS) and molecular projected self-consistent Hamiltonian (MPSH) eigenvalues.

AMS subject classifications: 65Z05, 81V55, 92E10

Key words: ab initio calculations, spin-dependent transport, all-carbon molecular device.

1 Introduction

Since graphene [1] and graphene nanoribbons (GNRs) [2] have been fabricated, carbon-based electronics and spintronics have been attracting amount of interest. Graphene

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has advantage electronic properties [3] and can be cut into narrow graphene nanoribbons (GNRs) by self-assembly bottom-up methods [4]. In addition, graphene has been proposed in experimental and theoretical studies as carbon electrodes to form stable all-carbon-based molecular conduction junctions in high yield [5, 6]. The advantage of graphene electrodes is that it gives high thermal stability and chemical flexibility due to their π -conjugated skeletons. Particularly, it allows various possibilities to link diverse organic molecules as compared to metallic electrodes because the graphene of sp^2 -hybridized carbon atoms offer a natural compatibility with organic molecules. And the spin current can be injected into graphene sheets by ferromagnetic electrodes in spintronics devices [7–9]. Thus, these new low-dimensional carbon electrode-molecule junctions are most likely better suited for molecular electronics. Moreover, the zigzag GNRs (ZGNRs), due to its tunable band gap and intrinsic edge magnetism [10, 11], have been fabricated in molecular junction devices, and predicted many particular effects, such as electronic switching [5], negative differential resistance (NDR) [12], rectifying [13], dual spin-filtering [14, 15], and so on.

Recently, carbon atomic chains have been successfully carved out from graphene by a high energy electron beam in recent experiments [16–18]. and its transport properties were also measured experimentally [19]. The *ab initio* simulations have indicated [20–23] carbon chain bridging GNR electrodes may be used as a good spin-filter, spin-valve, bipolar spin diode or spin transistor. Moreover, an ideal carbon chain is characterized by σ -bonds (e.g. $s-p_x$ orbitals) along the axis, and two decoupled π -bonds (e.g. the perpendicular p_y and p_z orbitals) per atom, which lead to outstanding mechanical properties [24] and a specific metallic behavior. Therefore, carbon chains can be applied as ideal one-dimensional conductors for interconnecting ultimate nanodevices, and its transport behaviour is strongly influenced by the hybridization state of carbon atoms at the end of the chain [25].

Those experimental achievements brings up the possibility of having incorporated carbon chain into each side of the organic molecular backbone between graphene electrodes. This structural modification reduces the electrode-molecule coupling, as it has been demonstrated in diarylethene-reconnected molecular junctions [5], which determine the device performance. And it is the possibility for organic molecules to use a multitude of physical mechanisms for controlling electron transport. For example, it has been proposed to build nanodevices by changing molecular conformation [26–30]. Recently, the design of artificial molecular machines that can undergo reversible structural changes have received considerable attention [31, 32]. the molecules can spin with varying frequencies if enough free volume is present [33–36]. Inagaki have designed and synthesized a molecular gyrotop with the phenylene rotor. Recently, Commins and Garcia-Garibay developed a molecular gyroscope with a rotatable phenylene center block [37]. Such rotation demonstrates promise as a new class of mechanical switches, gyroscopes. However, there remain far fewer reports of organic molecule rotor sandwiched between plane ZGNR electrodes with a bridged carbon chain, in which the mechanistic rotation of organic molecular components has been exploited to manipulate electron transport. It is