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Investigation of Electronic and Spintronic Properties in Co-Doped Graphene Nanodisks for Spin Filtering Applications

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Abstract:
Graphene nanodisks (GNDs) have attracted significant attention due to their unique electronic and magnetic properties, offering promising prospects for applications in nanoelectronics and spintronic devices. In this study, we investigate the density of states (DOS), spin currents, and spin polarization characteristics of pristine and Co-doped diamond-shaped and triangular GNDs using first-principles calculations. Our results reveal that Co doping induces spin splitting within the band gap of diamond-shaped GNDs, indicating spin-dependent phenomena. Additionally, fine spin splitting and metallic behavior are observed in the DOS of triangular GNDs. Through I-V curve analysis, we demonstrate that Co-doped diamond-shaped GNDs exhibit spin switch behavior and polarized spin currents, with a notable increase in peak current and polarization compared to pristine GNDs. The introduction of Co impurities enhances the spin filtering capabilities, making the device act as a spin filter in a wide voltage range. These findings provide valuable insights into the electronic and spintronic properties of Co-doped GNDs, offering possibilities for the development of efficient spintronic devices and spin filtering applications.

1. Introduction

Graphene nanoribbons (GNRs) and graphene nanodisks (GNDs) have garnered significant attention within the scientific community. In recent years, considerable research efforts have been directed towards exploring the distinctive electronic and magnetic properties exhibited by GNDs. This has led to the identification of their substantial potential for application in nanoelectronics and spintronic devices, thus stimulating further investigations and advancements in these fields[1-4]. Despite the inherent non-magnetic nature of carbon atoms, the presence of

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edge states in triangular nanodisks gives rise to notable ferromagnetic characteristics in these structures [5-7].

Presently, information processing is compartmentalized into three distinct functions, each implemented using materials from separate classes. Silicon transistors are employed for information processing, compound semiconductors like InAs, InP, and GaAs enable photon-based communication, and ferromagnetic metals are utilized for information storage. However, this categorization suffers from inefficiency and instability, particularly due to the limited availability of certain materials such as indium. Numerous investigations have demonstrated the potential of graphene, particularly graphene quantum dots, to serve as a viable alternative to existing information technologies, offering a promising avenue for future advancements in the field[8-10].

Magnetic materials play a pivotal role in various sectors of modern industry. The majority of magnetic materials employed today typically exhibit ferromagnetic behavior at ambient temperatures, with their electronic configurations characterized by half-filled f or d orbitals. Among these materials, carbon-based structures hold considerable significance due to their inherent stability, simplicity, versatility, and facile modifiability. These unique attributes facilitate more straightforward theoretical predictions of magnetization and enhance the likelihood of inducing spin-related phenomena. Consequently, carbon-based materials offer compelling prospects for advancing our understanding of magnetism and harnessing its applications in diverse technological domains[11]. The coexistence of π- and σ-bonding in graphene represents a distinct characteristic that endows it with exceptional properties. This unique feature enables the concurrent generation of localized spins and facilitates their coupling when manipulating these bonds into specific states, thereby facilitating the emergence of magnetic order. Moreover, graphene-based magnets hold significant promise for advanced applications in the realm of spintronics. The exceptional carrier mobility exhibited by graphene, coupled with its potential to seamlessly integrate spin and molecular electronics, presents a compelling avenue for future developments in this field.[12].

According to empirical evidence, triangular graphene nanodisks (GNDs) have demonstrated magnetic properties attributed to the presence of edge effects. These edge effects give rise to non-coupled electron states within the GND structure, leading to behavior reminiscent of ferromagnetic materials. [13]. In alternative scenarios, notable spin effects in diamond-shaped graphene nanodisks (DNDs) have not been extensively observed. However, it is possible to induce magnetic effects in DNDs by introducing impurities through the injection of specific dopants into the GND structure.

The application of Density Functional Theory (DFT) in investigating the electronic and physical properties of nanodisks has garnered considerable interest. Abdelati et al. conducted a study utilizing DFT to explore the optical properties of graphene quantum dots (GQDs). By employing DFT calculations, they were able to gain insights into the optical behavior and characteristics

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exhibited by GQDs. This approach offers a valuable methodology for elucidating the optical properties of nanodisks and provides a foundation for further investigations in this field. [14]. Li et al., employing Density Functional Theory (DFT), conducted a comprehensive investigation into the molecular spintronic properties of devices utilizing trigonal graphene nanodisks (GNDs). Through the application of DFT calculations, they explored the intricate interplay between spin-related phenomena and electronic transport in these devices. Their study shed light on the fundamental aspects of molecular spintronics in the context of trigonal GND-based systems. This research contributes to the growing understanding of spin-dependent processes and paves the way for the development of novel molecular spintronic devices based on trigonal GNDs. [15].

Recent studies have demonstrated that the introduction of nickel, cobalt, and iron impurities into nanodevices can effectively induce magnetic properties in boron nitride nanotubes (BNNTs). This finding highlights the potential for engineering magnetic behavior in BNNTs through controlled impurity doping. By carefully selecting and incorporating these transition metal impurities, researchers have observed the emergence of magnetic characteristics in BNNTs, opening up possibilities for the utilization of these materials in various magnetic and spintronic applications [16].

Considering the notable magnetic properties exhibited by triangular GNDs and the successful induction of magnetism in other materials through impurity doping, it is of interest to explore the utilization of cobalt as a dopant in graphene nanodisks. The inclusion of cobalt impurities in GND structures holds the potential to induce desirable magnetic properties and further enhance their applicability in spintronics and related fields.

Spin currents and spin polarization play pivotal roles in the field of spintronics, offering new avenues for advanced electronic devices. Unlike conventional charge currents, spin currents involve the flow of electron spins and hold the potential to carry valuable information beyond their charges. Spin polarization, on the other hand, measures the alignment of electron spins in a material or device. These properties open up exciting possibilities for spin-based information processing, including the development of spin filters that selectively transmit spins with a particular orientation.

In the context of our research, exploring spin currents and spin polarization allows us to contribute to the advancement of spintronic devices with improved performance and functionality. By investigating these key aspects, we can gain insights into the manipulation and control of spin states, leading to the design of efficient spintronic components. Furthermore, understanding spin-related phenomena enhances our understanding of fundamental spin physics and facilitates the development of next-generation technologies.

In this study, we delve into the characterization and analysis of spin currents and spin polarization in GND. By exploring the unique spin-related properties of our system, we aim to shed light on the underlying mechanisms and provide valuable insights for the design and optimization of spintronic devices.

2. Computational and Details

To calculate the current, we established a connection between the transition metal (TM)-doped nanodisk and two single-ring carbon nanoribbons, as depicted in Figure 1. The gate voltage was maintained at zero, while a bias voltage was applied to the electrodes.

To find electronic structures of the system we used density functional theory as implemented in the SIESTA package[17], based on norm-conserving pseudopotentials and pseudo atomic orbital basis sets with GGA-PBE as exchange-correlation functional, and the spin-polarized calculation was performed. We used 300 Ry as cutoff energy. Based on the Monkhorst-Pack model, we used 1×1×12 for gridding the space[18]. We used periodic boundary conditions to find electronic states of pristine and TM-doped GND.

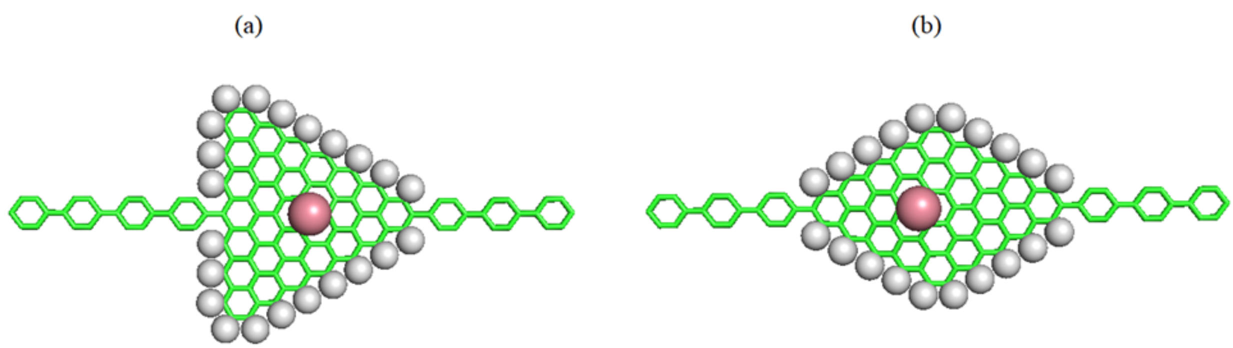

Fig.1 (a) TM doped triangular nanodisk and (b) TM doped diamond nanodisk attached to electrodes.

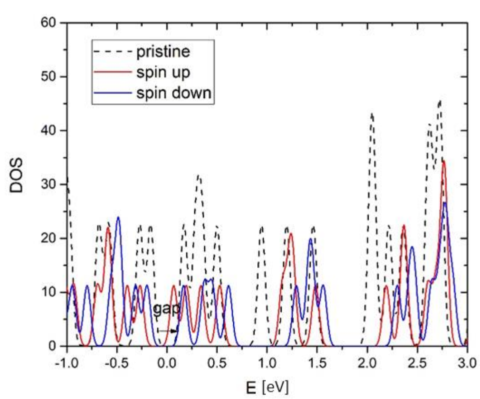

Fig.2 DOS of TM-doped diamond shape graphene nanodisk.

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3. Result and Discussion

The density of states (DOS) is a fundamental quantity that provides essential insights into the electronic properties of a system, including the presence of a band gap, the positioning of induced impurity levels, and the conductivity characteristics of materials [19-21]. In this study, we investigate the DOS of pristine and Co-doped diamond-shaped graphene nanodisks (GNDs) as depicted in Figure 2.

The pristine GND exhibits a well-defined band gap with a magnitude of approximately 0.2 eV, indicating its semiconducting nature. However, upon Co doping, a spin-up level emerges within the band gap, as clearly observed in the energy intervals of [1, 1.7] eV and [2, 2.7] eV, indicating the occurrence of spin splitting.

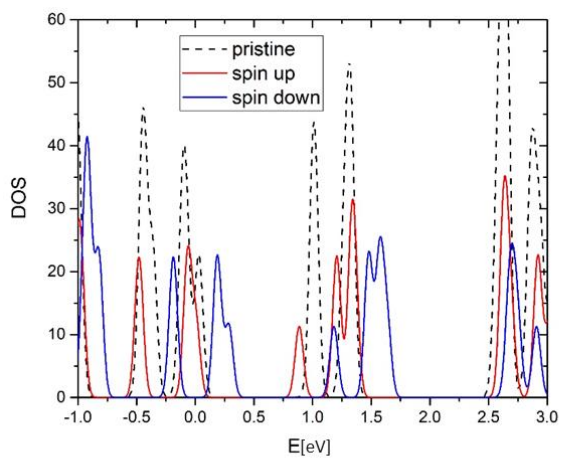

Fig.3 DOS of TM-doped diamond shape graphene nanodisk.

This observation suggests that the introduction of Co impurities introduces spin-dependent phenomena within these energy ranges. The emergence of spin-up levels within the band gap implies a modification of the electronic structure due to Co doping, potentially leading to spintronic functionality. To further elucidate the impact of Co doping on the electronic and spintronic properties of the diamond-shaped GNDs, we will conduct subsequent analyses to explore the presence of spin currents within these specific regions.

Moving forward, we examine the DOS of pristine and Co-doped triangular nanodisks, as illustrated in Figure 3. Notably, this structure does not exhibit a band gap upon initial examination. However, a fine spin splitting is observed in the energy range of [0, 0.4] eV. Furthermore, there is an absence of states within the range [1.8, 2.5] eV, followed by the appearance of additional fine spin-split levels. While this structure exhibits states at E=0, indicating metallic behavior, we will demonstrate that the obtained current values are not significant around V=0 volts.

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In Figure 4, we present the I-V curve of both pristine and Co-doped diamond-shaped GNDs. For this configuration, a monolayer graphene nanoribbon serves as the electrode, connected to the system via a single atom. Due to the inherent bandgap of the graphene nanoribbon electrode and the connection through a single atom, the threshold voltage is increased, resulting in a higher voltage required to initiate current flow. The current value exhibits a notable increase around 1.5 volts for this setup, suggesting a switch-like behavior.

At V=0.2, the device generates an 80% polarized spin current, although the current value itself is not significant at this voltage. When the voltage varies between 1.8 and 2.4 volts, the device exhibits a spin switch current, resulting in a change in polarization from +65% to +75%.

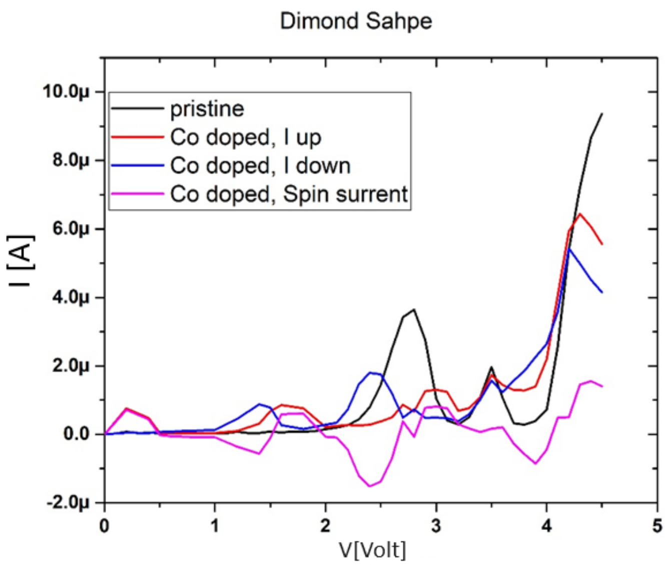

Fig.4 I-V curve of diamond shape nanodisk.

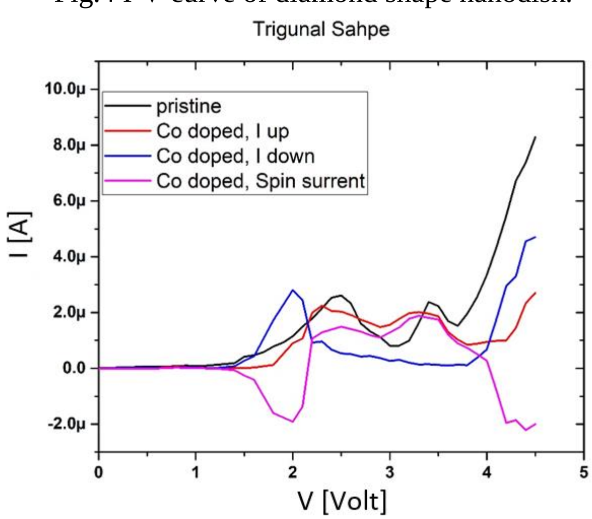

Fig. 5 I-V curve of triangular shape nanodisk.

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This behavior is depicted in Figure 5. Notably, there is a flat polarized spin current between 0.4 and 1.2 volts, with a polarization of -50%. Consequently, we anticipate that this device will generate a stable spin current for V=0.8 ± 0.4 volts and exhibit a spin switch behavior for V=2.1 ± 0.3 volts.

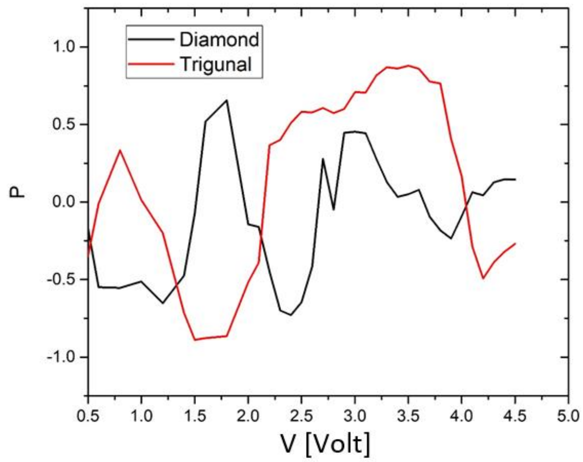

Fig.6 polarization of spin current

Figure 5 showcases the spin current characteristics for this device. In the case of the pristine nanodisk, the current value exponentially increases up to 2.4 volts before dampening. However, the effect of Co doping significantly enhances the peak value in the I-V curve and yields a 60% spin-polarized current at V=2.5 volts, which further increases to 87% at 3.5 volts. This implies that the device acts as a spin filter within a wide voltage range (1 volt) starting from 2.5 volts to 3.5 volts, after which it abruptly diminishes to zero. Figure 6 demonstrates the spin current polarization for Co-doped GNDs in diamond and triangular shapes.

In this device, a single-ring carbon nanoribbon is employed as the lead electrode. The band energy of such electrodes falls under the category of one-dimensional materials, and it is evident that their band energy is well-resolved. When the I-V curve of such a system is examined in conjunction with one-dimensional electrodes, negative conductance is observed. This behavior arises due to quantum interference effects and the geometry of the one-dimensional electrode.

These comprehensive analyses shed light on the intricate electronic and spintronic properties of the investigated systems, highlighting the influence of Co doping on the DOS, current characteristics, and spin polarization. The obtained results contribute to our understanding of these materials and pave the way for potential applications in spintronic devices and spin filtering."

4. Conclusion

In summary, this study provides a detailed examination of the density of states (DOS) and electronic properties of pristine and Co-doped diamond-shaped graphene nanodisks (GNDs). Our findings reveal that the pristine GND exhibits a semiconducting nature with a well-defined band gap of approximately 0.2 eV. The introduction of Co doping alters the electronic structure, resulting in the emergence of spin-up levels within the band gap and indicating potential for spintronic applications.

The analysis of triangular GNDs, while initially showing metallic behavior without a band gap, reveals fine spin splitting and additional spin-split levels, further emphasizing the complexity introduced by Co doping. The I-V characteristics demonstrate that the Co-doped devices exhibit enhanced current and significant spin polarization, particularly at higher voltages, suggesting effective spin filtering capabilities.

Overall, these results underscore the critical role of Co doping in modifying the electronic and spintronic properties of graphene nanodisks. The insights gained from this research not only deepen our understanding of these materials but also highlight their potential for future applications in advanced spintronic devices. Continued exploration into the effects of Co doping and other modifications will be essential for optimizing performance and expanding the utility of graphene-based materials in technology.

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