

Spin-dependent transport properties of an armchair boron-phosphide nanoribbon embedded between two graphene nanoribbon electrodes



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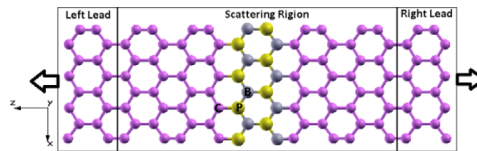
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HIGHLIGHTS

- The transport properties of a hybrid system in three different structures are calculated.
- We consider the effect of impurity in this system.
- This hybrid system is found to exhibit significant spin-filter efficiency.
- We observed the robust negative differential resistance in all examined structures.

GRAPHICAL ABSTRACT

Transport properties of a junction consisting of armchair hexagonal boron phosphide nanoribbon (ABPNR) contacted by two semi-infinite electrodes composed of armchair graphene nanoribbons (AGNRs) using non-equilibrium Green's function and ab initio calculations are investigated.



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ABSTRACT

Using non-equilibrium Green's function and ab initio calculations we investigate structural, electronic, and transport properties of a junction consisting of armchair hexagonal boron phosphide nanoribbon (ABPNR) contacted by two semi-infinite electrodes composed of armchair graphene nanoribbons (AGNRs). We consider three different configurations including the pristine AGNR-BP-GNR and substitutions for Iron atoms, namely on phosphorus and boron atoms at one edge of the BP nanoribbon. The spin current polarization in all these cases is extracted for each structure and bias. Such hybrid system is found to exhibit not only significant spin-filter efficiency (SFE) but also tunable negative differential resistance (NDR).

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1. Introduction

Graphene, a single layer of sp^2 hybridized carbon atoms, is one of the known allotropic forms of carbon. It consists of a single sheet of graphite made of carbon atoms in a honeycomb lattice [1,2]. Since the chemical synthesis of graphene sheets by Novosolov et al. [3] in 2004, intensive research efforts have been focused to examine the outstanding properties of this notable system, which has been considered as a hopeful candidate material for the next-generation nanodevices [4–6]. In addition, charge-carrier mobility of graphene is extremely large, enabling fast-speed atomically thin field-effect transistors (FETs) to be constructed [3,7–16]. Since graphene is a zero-band gap semiconductor, it

cannot be applied in semiconductor devices such as FETs. Therefore, considerable attempts have been made to opening a sizeable band gap for graphene and/or seeking other semiconducting graphene-like materials [3].

In addition to FET applications in some graphene devices, an important effect of electronic transport in these low-dimensional systems is the negative differential resistance (NDR) phenomenon [17–21] in current–voltage curve, which can be used in memory, frequency multipliers, fast switches, and most importantly, high-frequency oscillators up to the THz range [22,23]. In 2012, Yanqing Wu [24] discovered a new mechanism for NDR in three-terminal graphene devices based on a FET configuration. The NDR experimentally observed in graphene FETs of conventional design allows for fabrication of viable non-Boolean computational architectures with the gap-less graphene [25]. In contrast to graphene-based, graphene-like materials have been attracting much attention because of their unique advantages in low-dimensional scientific

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research and in nano-device structures [26–28]. Alejandro [29] characterized theoretically nanographene based on boron-phosphorus. He reported that comparative studies among boron-phosphorus nanographene (BPNG), carbon one (CNG), and boron-nitrogen (BNNG) also indicate that it is experimentally possible to obtain the BPNG.

First-principle theoretical calculations indicate that armchair boron-phosphide nanoribbons (ABPNRs) and armchair graphene nanoribbons (AGNRs) can crystallize, but their electronic properties should be different due to the different electronic structures of carbon, boron and phosphorus. Therefore, these nanoribbons might be used to fabricate hybrid nano-structures with stable coherent interfaces and multi-functionality. It is reported that high spin polarization can be achieved in GNR by doping of some transition metal (TM) atoms especially traditional ferromagnetic metals [30–38]. These ferromagnetic atoms (Iron, cobalt and nickel) are well known for peculiar magnetic properties and can be seen as a possible source of magnetism in GNR. These ferromagnetic impurities can tune the properties of GNR for spintronic applications. To our knowledge, information of the magnetic behavior of ferromagnetic atoms embedded in hybrid grapheme-like nanoribbons is not sufficient. Accordingly, it is of interest to investigate the electronic structures and the spin transport properties of considered device substitutionally doped with Iron atoms at different sites.

In this article, we investigate the spin dependent transport in a hybrid AGNR–BP–GNR structure. We consider three different configurations including the pristine AGNR–BP–GNR and substitutions for Iron atoms, namely on phosphorus and boron atoms at one edge of the BP nanoribbon. The spin current polarization in all these cases is extracted for each structure and bias, revealing the NDR, spin filter and spin current switching effects. In this way we point out the applicability of BPC hybrid materials in novel nanoscale spintronic devices.

2. Computational method

In this study, we report first-principle calculations based on a density functional theory (DFT) method [39] to determine the structural, electronic, and transport properties of the planar hybrid armchair C–BP–C nanoribbon devices. Optimized geometries and total-energy calculations are computed by using the DFT code SIESTA [40] with the Perdew–Burke–Ernzerhof (PBE) [41] form of the generalized gradient approximation (GGA) for exchange and correlation. The transport calculations of two-probe systems are performed by using the TRANSIESTA code [42] which is based on the combination of DFT with the nonequilibrium Green's function (NEGF) formalism.

The wave functions of the valence electrons are expanded by a linear combination of atomic orbitals (LCAO). To describe the

interactions of the valence and core electrons we used norm conserved pseudopotentials, as proposed by Troullier–Martins [43]. The valence electronic orbitals of systems were described using a single- ζ basis set plus a polarization function (SZP). A sample of $1 \times 1 \times 10$ k-points chosen according to the Monkhorst–Pack method was used to describe the Brillouin zone [44] and the mesh cutoff energy is chosen as 300 Ry. A vacuum layer larger than 10 Å is used to avoid interaction between adjacent ribbons. The ribbons are periodic along the z direction.

In Fig. 1, we show a schematic view of the system before relaxation. The considered nanoribbon is flat in the zx -plane, with 8-armchair chains along the z -direction (the transport direction). The system was divided in three parts, a left-hand (L) and a right-hand (R) side current/voltage electrodes and a central scattering region (CC) which composed of a few unit cells of the electrodes and one unit cell of an armchair hexagonal boron phosphide nanoribbon. The central scattering region is defined such that it includes the portion of the physical electrodes where all the screening effects take place. We also assume that the electrodes only couple with the central scattering region, but not with each other. The structure optimizations of the central scattering region were first carried out until the forces on all atoms are less than 0.02 eV/Å.

The total Hamiltonian of the system include contributions from both central scattering regions and leads to

$$H = \begin{pmatrix} H_{LL} & H_{LC} & 0 \\ H_{LC}^\dagger & H_{CC} & H_{CR} \\ 0 & H_{CR}^\dagger & H_{RR} \end{pmatrix} \quad (1)$$

and constructing the Green's function equation with H yields;

$$\begin{pmatrix} ES_{LL} - H_{LL} & ES_{LC} - H_{LC} & 0 \\ (ES_{LC} - H_{LC})^\dagger & ES_{CC} - H_{CC} & ES_{CR} - H_{CR} \\ 0 & (ES_{CR} - H_{CR})^\dagger & ES_{RR} - H_{RR} \end{pmatrix} \begin{pmatrix} G_{LL} & G_{LC} & G_{LR} \\ G_{CL} & G_{CC} & G_{CR} \\ G_{RL} & G_{RC} & G_{RR} \end{pmatrix} = \begin{pmatrix} I_{LL} & 0 & 0 \\ 0 & I_{CC} & 0 \\ 0 & 0 & I_{RR} \end{pmatrix} \quad (2)$$

where S and I are overlap and unitary matrices, respectively. One needs to solve the above equation to obtain Green's function of the scattering region

$$G_{CC} = \{ES_{CC} - (H_{CC} + \sum_L + \sum_R)\}^{-1} \quad (3)$$

Self energies of the left and right leads are defined by

$$\sum_L = (ES_{LC} - H_{LC})^\dagger G_{LL} (ES_{LC} - H_{LC}) \quad (4)$$

$$\sum_R = (ES_{CR} - H_{CR})^\dagger G_{RR} (ES_{CR} - H_{CR}) \quad (5)$$

The self-energies contain the information regarding which states are available in the leads at a given energy. Electrons can

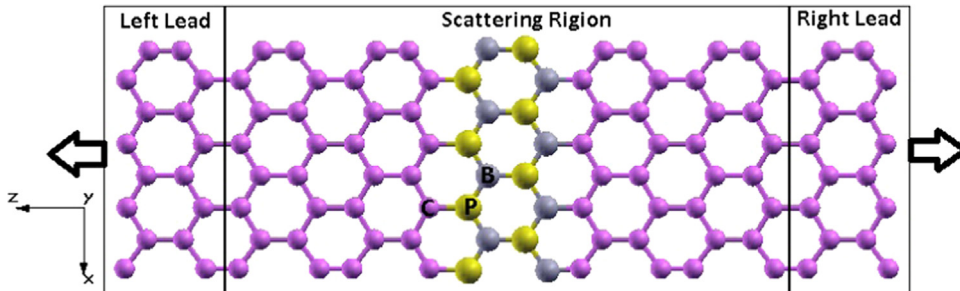


Fig. 1. Schematic illustration of the system before relaxation. This system is flat in the z - x plane, with 8-armchair chains along the z -direction. Armchair hexagonal boron phosphide nanoribbons contacted with two semi-infinite armchair graphene nanoribbon electrodes. The device was divided in three parts, a left-hand and a right-hand side electrodes and a central scattering region which composed of a few unit cells of the electrodes and one unit cell of an armchair hexagonal boron phosphide nanoribbon.

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