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Pure Spin Current and Negative Differential Resistance in Born Nitride Nanoribbon Induced by Oxygen Doping

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Abstract

Boron nitrogen nanoribbon (BNNR) is semiconductor, doping is an important way to change the size of its bandgap. In this paper, oxygen doping armchair and zigzag BNNR (aBNNR and zBNNR) were studied by density functional and non - equilibrium Green 's function method. The substitution of nitrogen atoms by the oxygen atom in the BNNR introduces impurity state between the bandgap of the BNNRs. The impurity state is spin-splitting completely, and the system behaves ferromagnetic with 1μ B per supercell. The dispersive of impurity band introduced by Oxygen doping is very small, so it shows a strong localization. Considering the transport properties of oxygen-doped boron-nitrogen nanotubes, armchair type and zigzag type are different. For the aBNNR, pure spin current appears in the symmetrical range of positive and negative voltage, the peak of current is $32 \,\mu$ A, and the negative differential resistance is shown simultaneously. For the zBNNR, the positive and negative voltage interval is no longer symmetrical, the peak current is only 2.0 μ A. BNNR doped by oxygen have unique electronic structures and transport properties, so which provide more option for optoelectronic and spintronic devices.

Keywords

Boron Nitrogen Nanoribbon (BNNR), Doping, Negative Differential Resistance (NDR)

1. Introduction

In recent years, the research on the two-dimensional materials have made great progress, driven by fundamental physics as well as potential next generation device applications. Although graphene has been the frontrunner until now, single layer hexagonal boron nitride (h- BN) and whose hybrids with graphene has become hot research object [1-2].

Using micromechanical cleaving and chemically derived routes, single (or a few) layers of h-BN sheets have been prepared [3]. One-dimensional nanoribbons of h-BN have also been successfully synthesized. Due to novel electronic and properties, nanoribbons are of great interest. Unlike graphene, a h-BN sheet is a wide-gap insulator [4-6]. By cutting a monolayer of BN sheet along a straight line, the h-BN sheet will form two type of BN nanoribbons: aBNNR and zBNNR, the same with graphene nanoribbons. As known from previous first-principles calculations, the energy band gap of zBNNR decreases monotonically with the increase of ribbon width, while the gap oscillation observed for aBNNR. The ribbon width is the key effect on the band gap of BNNRs and application in electronic devices [7-12]. Thus, it is highly desirable to engineer the band gap of BNNRs. Many methods such as chemical decorated, hydrogen-terminated and by applying electric field, have been developed to tune the band gap of BNNRs [13-18].

Considering the potential application on modified BNNRs in opto-electronic and spintronic devices, the effect of various doping species on their electronic and magnetic properties are need further systematic studies. Recently, the electronic properties of oxygen doped BN nanotubes and the role of chirality on the magnetic properties of oxygen doped BN nanotubes have been clarified by DFT method [19]. In this paper, the electronic, magnetic and transport properties of oxygen doped BNNRs have been systematically studied by a method which combined with non-equilibrium Green's function (NQGF) and density functional theory (DFT). For oxygen doped BNNRs system, previous studies have shown oxygen atom prefer to substitute the N atom more than B atom because of more little formation-energy [19]. To explore the chirality and doping-site effect on the BNNRs, two types of BNNRs are chosen to be studied which shown in Figure 1. A-1, A-2, A-3, A-4 represent four different doping-sites for the substitution N atom by O atom in aBNNR are shown in Figure 1(a); In the Figure 1(b), Z-1, Z-2, Z-3, Z-4, Z-5, Z-6 stand for six different doping-sites in zBNNR. Those two types of oxygen doped BNNRs systems contain the same number of boron, nitride and oxygen atom, so it is conveniently to compare the difference of electronic, magnetic and transport properties between them.

2. Method of Calculation



Figure 1. Schematic of different doping-sites for substitution of N atom by O atom in BNNRs. (a) four different doping-sites for aBNNRs; (b) six different doping-sites for zBNNRs

Electronic and magnetic properties are calculated using the DFT-LSDA method which carry out using the SIESTA (Spanish Initiative for Electronics Simulations with Thousands of Atoms) package [20,21], which uses the numerical atomic orbitals as basis set and Troullier-Martin type norm-conserving pseudopotentials. Here, B, N and O atoms are described by 2s²2p¹, 2s²2p³ and 2s²2p⁴ valence electrons plus the corresponding pseudo-potential ion charges, respectively. Moreover, double ξ -plus-polarization basis set is used. Perdew-Burke-Ernzerhof (PBE) functional form of generalized gradient approximation (GGA) for the exchange-correlation approximation has been used. An energy cut-off 200 Ry is adopted to calculate some integrals in real-space grid. In addition, self-consistent calculations of the density matrix are performed with mixing rate of 0.02 and the convergence criterion of 10^{-4} . The conjugate gradient method is applied to do the geometrical relaxations. Moreover, spin-polarized description is applied to do the substitution calculation of transport properties of BNNRs substituted N atom by O atom.

The transport properties are calculated using the NEGF technique, based on DFT as implemented in TranSIESTA code within SIESTA package [20,]. It is computed the transport properties of nanoscale system as scattering region (or extended molecule) connected to two semi-infinite left and right electrodes using the TranSIESTA code. The transmission coefficient of an incident electron with energy E through the scattering region between two electrodes is obtained from the extended Green's functions of the device as

$$T(E) = Tr[\Gamma_L G^+ \Gamma_R G] \tag{1}$$

Here, broadening function describing the level broadening due to coupling of the scattering region with the electrodes is obtained from $\Gamma_{L(R)} = i[\Sigma_{L(R)}^+ - \Sigma_{L(R)}]$ is the self-energy of the left (right) electrode. Also, the Green's function of the scattering region is given by

$$G(E) = [ES - H - \Sigma_L - \Sigma_R]^{-1}$$
(2)

Where H and S are the Hamiltonian and the matrices of the scatting region, respectively. The current as a function of applied voltage, U_{a} can determined by integrating transmission function over a suitable voltage window.

$$I(U_{a}) = G_{0} \int_{E_{f}-eU_{a}}^{E_{f}+eU_{a}} T(E, U_{a}) dE$$
(3)

Here, $G_0 = 2e/h$ and E_f are the unit of the quantum conductance and the equilibrium Fermi energy respectively. The transmission coefficient as a function of the energy is obtained using a post-processing tool of TBTrans. Finally, after the calculations, the results were post-processed using the denchar and plrho utilities of SIESTA to calculate the electron charge density distribution and the electrostatic potential, respectively. All calculations have been done at temperature, namely below 10K.



Figure 2. The spin-resolved total densities of states (DOS) for four types of oxygen atom doped aBNNRs (left panel); The spin-resolved band structures for four types oxygen atom doped aBNNRs (right panel); Fermi energy is set as zero.



Figure 3. The spin resolved densities of states of the A-4 type of oxygen doping aBNNR. Black line for densities of states; Red line for projected densities of states of three born atoms nearest the doping site; Green line for projected densities of states of five nitrogen atoms next nearest the doping site; Blue line for the oxygen atom in the doping site; Fermi energy is set as zero energy.

3. Results and Discussion

3.1. Electronic Properties

As a start, O-doped armchair BNNRs (aBNNRs) are discussed. The electron structure of pure aBNNR calculated firstly, which is a semiconductor with 4.45 eV bandgap, which is in good agreement with the ab initio calculation by previous studies [15-18]. The four substitutional sites of the oxygen atom are labeled by A-1, A-2, A-3 and appear in the gap, the

in-gap state is fully spin splitting. The impurity states of spin splitting are mainly from the three boron atoms near A-4 as shown in Figure 1(a) and their structural optimization are all done. Though fully relaxation the local symmetry is broken under a little Jahn-Teller distortion, the oxygen is incorporated into the aBBNRs with negligible local deformation because of the closer electronegativity between oxygen and nitrogen element.

Figure 2 shows the electronical band-structures and the spin polarized density of states for the four types of oxygen doped aBNNRs. For all the doping types, the oxygen atom substituted nitrogen atom in aBNNRs introduced in-gap states near the fermi surface, although with little negligible local deformation. As we all know, that all the bands in pristine aBNNR are spin-degenerate. To study the doping effect on the electronic structures, both magnetic and non-magnetic states are investigated. The magnetic sates yield consistently lower energies than the nonmagnetic cases and differences in total energies are roughly 0.26, 0.29, 0.24 and 0.30 eV per cell for A-1 case, A-2 case, A-3 case and A-4. As can be seen from the Figure 2, near the fermi level, the doping induces almost flat bands in the whole first Brillouin zone and the impurity bands are fully splitting. The total magnetization of the aNBNR is $1\mu_{B}$ per impurity. The calculated total energy show that of the A-4 case is lowest. Here only the densities of states for A-4 case are discussed below. Figure 3 shows the doping induced state the heteroatom atom, while the contribution of adjacent five nitrogen atoms is smaller and the atomic oxygen atom is the least contributor.



Figure 4. The spin-resolved total densities of states (DOS) for six types of oxygen doping zBNNRs (left panel); The spin-resolved band structures for six types oxygen atom doped aBNNRs (right panel); Fermi energy is set as zero energy.

Next, the doping types of zBNNR are discussed. As shown in Figure 1(b), the number of atoms for zBNNR are the same as that of aBNNR; There are six types of oxygen atom substitution nitrogen atom, which are marked by Z-1, Z-2, Z-3, Z-4, Z-5, and Z-6. Through the calculation of the total energy of system, the total energy of Z-1system is lowest. For the convenience of comparison, the spin resolved band-structure and density of states are calculated. As shown in Figure 3, for all of six types of doping, the impurity states are introduced in the band gap, the spin splitting appears in the impurity states; The degree of spin splitting for Z-4 type and Z-5 type are smallest, while the spin is fully polarized for Z-1, Z-2, Z-3 and Z-6, the system behave semi-metal. As seen from the right side of Figure 4, the degree of spin splitting of the impurity band in the Z-4 type and Z-5 type are the smallest, and the dispersion of impurity band are the biggest, so the systems behave the weakest locality. For the Z-6 type, the impurity bands introduced by oxygen doping are almost flat, the locality.

In summary, the oxygen atom substitution of nitrogen in BNNR produce spin splitting impurity states. The dispersion of impurity states is small, shows strong locality. The doping system behave semi-metal.

3.2. Transport Properties

The electronic properties of oxygen doping BNNRs has been discussed in the previous section. Now, the transport properties of oxygen doping BNNRs will be studied. For convenience of discussion, Z-4 type is studied which is most stable in oxygen doping aBNNR, and for zBNNR the Z-1 type is studied. Figure 5(a) is a calculational model for oxygen doping BNNRs, left electrode and right electrode are represented by one supercell of oxygen doping BNNR, while the scatting region is represented by three supercells of oxygen doping BNNR.

The transport properties of oxygen doping aBNNR was studied firstly, which I-V curve was shown in Figure (b). There was no current in the voltage rang [-0.2V, 0.2V], while in the symmetrical voltage rang [0.2V, 0.65V] and [-0.65V, -0.2V], the system produce pure current of spin up, the value for current of spin down was zero. As shown in the Figure 5(b), the differential resistance is negative in the symmetrical voltage rang [0.2V, 0.65V] and [-0.65V, -0.2V]; As the electrode voltage increases, the value of pure spin current increases, at the voltage of 0.55V, the maximum value of pure spin current is $\pm 32\mu A$; Then with the voltage of electrode continuing to increase, the value of pure spin current decreases, at the voltage of 0.65V, the minimum value of pure spin current is 0μ A; In the other voltage range where the voltage is greater than 0.65V or lessen than -0.65V, the value of pure spin current is really small. The density of states and band-structure of A-4 type of oxygen doping aBNNR are shown in Figure 2, the impurity state appear in the bandgap, whose spin is completely splitting, and the dispersion of impurity band is small, behaves strong locality and whose dispersion is small, that is the reason of negative differential resistance appear in the certain voltage region.

Figure 5(c) is shown the I-V curve of oxygen doping zBNNR. There is pure spin current in the voltage region [-0.65V, 0.5V], but the value is small. Within the positive voltage region there are two regions which is [0.65V, 0.8V] and [0.8V, 1.1V] where the differential resistance is negative, the maximum value of pure spin current is 0.75μ A. When the voltage is negative the region is not symmetrical.



Figure 5. (a) Schematic for the calculation of transportation property of oxygen doping BNNRs, the three parts (left electrode, the central scatting region and right electrode) are all constructed by oxygen doping BNNRs; (b) The spin resolved I-V curve for A-4 type of oxygen-doping; (c) The spin resolved I-V curve for Z-1 type of oxygen-doping zBNNR.

In the region of [-1.2V, 0.65V] where the differential resistance is negative, the maximum value of pure spin current is 2.0 µAwhich is bigger than that of the positive voltage region. In the Figure 4 the density of state and band-structure of Z-1 type of oxygen doping zBNNR, there are two impurity states near the fermi energy obviously, which bring big effect on the transport properties of system, so the system behaves negative differential resistance in the certain voltage, the region for positive and negative voltage is not symmetrical.

In summary, the system of oxygen doping aBNNR and zBNNR produce the pure spin current in the certain voltage region, the value of pure spin current increase with the voltage increase; After the extreme value with voltage increase the value of spin current decrease. The characteristics of negative differential resistance appear in the system

4. Conclusion

In this paper, the oxygen-doped BNNR is studied by density function theory and non-equilibrium function method. The substitution of oxygen atoms by nitrogen atoms in the BNNRs produce the impurity states in the bandgap of BNNRs, the impurity states are fully spin splitting. The system is ferromagnetic with 1µB of magnetic moment per supercell. The dispersion of impurity states introduce by oxygen doping are small, so the impurity band show strong locality. Considering the transport properties of oxygen-doped boron-nitrogen nanotubes, armchair type and zigzag type are different. For the aBNNR, pure spin current appears in the symmetrical range of positive and negative voltage, the peak of current is 32 μ A, and the negative differential resistance is shown simultaneously. For the zBNNR, the positive and negative voltage interval is no longer symmetrical, the peak current is only 2.0 μ A; there are two negative differential resistance voltage range. BNNR doped by oxygen have unique electronic structures and transport properties, so which provide more option for optoelectronic and spintronic devices.

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