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Electronic and Transport Properties of Boron Nitride Nanodevice

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Abstract: Boron Nitride Nanotubes are valued due to their physical and chemical properties**.** They can be found their possible applications in the field of design and developing of optoelectronic devices of new generation. In this paper the transport and electronic properties of both clear Boron Nitride and Boron Nitride Nanotube with embedded carbon atoms have been calculated in the framework of Density Functional Theory (DFT). Results show that nanodevice with embedded carbon atoms has wider transmission spectrum than clear one. It has been computed transmission eigenvalues for both nanodevices. Nanodevice with impurity has higher transmission eigenvalues than clear one.

Keywords: Boron Nitride Nanotube, Transmission spectrum, Eigenvalue, Eigenstate

1. Introduction

Structurally boron nitride nanotubes (BNNT) are similar to carbon nanotubes (CNT). But they significantly differ in their mechanical properties. As BNNTs consist of B and N atoms their chemical and physical properties are different from CNTs. The charge distribution is asymmetric in B-N bonds in contrast to CNTs. Some of the electron charge on B is transferred to N and because of it the bonds have some ionic properties which bring about a gap between valence and conductance bands. Therefore, BNNTs are wide gap semiconductors [1]. The significant difference in structure and stability has been founded with small tube size [2-3]. In the current paper the transport properties of both clear BNNT device and BNNT with embedded carbon atoms has been investigated in the framework of Density Functional Theory method using linear combination of atomic orbitals (LCAO) basis sets combined with the non-equilibrium Green's function (NEGF) calculation method. Simulations and calculations of nanodevice have been done with Quantum ATK software tool.

2. Investigation method and tool

As mentioned above all calculations has been done with Quantum ATK software tool in the framework of DFT method using LCAO basis sets combined with the NEGF calculation method. Schematic view of boron nitride $(6,0)$ nanotube presented in Figure 1. The system consists of right and left electrodes and central region which is always called scattering region because charge carriers moving between the two electrodes are scattered by the environment of

central region. The electrode extensions are replicas of the corresponding electrodes and here element types and ionic positions are matched with the electrodes. These extensions provide a smooth transition between the potential of the central region and electrodes. Left electrode has low potential and right electrode has higher V_{bias} voltage. The electrons flow from left to right, corresponding to an electrical current from the right to the left. Within the NEGF formalism, the current that passes through the central region at a finite bias voltage can be computed using the Landauer–Büttiker formula [4-6]

$$I(V) = \frac{2e}{h}\int_{\mu L}^{\mu R} dE\left[f_L(E - V_b) - f_R(E - V_b)\right]T(E, V_b),$$

where μL and μR are the electrochemical potentials of the left and right electrodes, and $T(E, V_b)$ is the transmission coefficient at energy E and bias voltage V_b. There is presented $BN(6,0)$ nanotube with embedded carbon atoms in Figure 2. Temperature of electrodes in both structures has been $300K$.

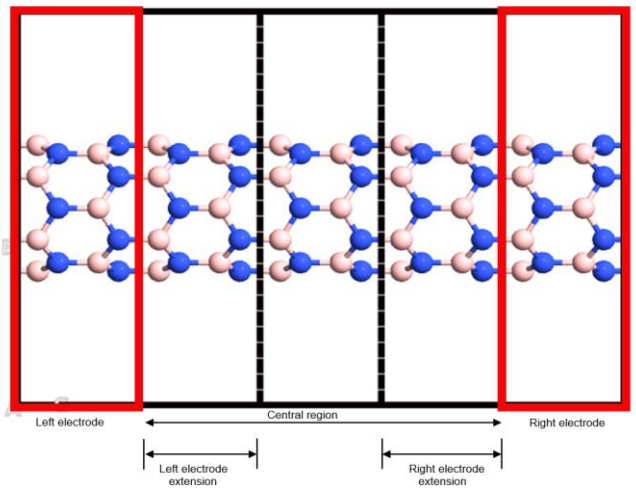

Figure 1. Schematic view of BNNT nanodevice

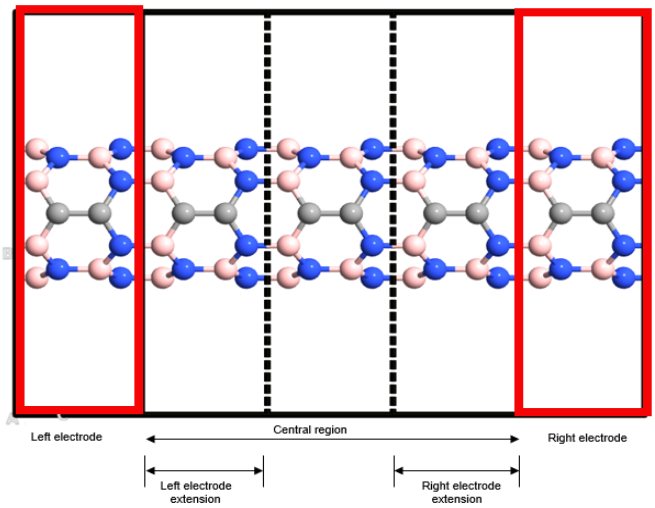

Figure 2. Schematic view of BNNT nanodevice with embedded carbon atoms

3. Results and discussions

It is firstly discussed the transport properties of nanodevices. Transmission spectrum has been calculated for both clear BNNT device and with embadded carbon atoms. Figure 3 shows comparision of transmission spectra with $0V$ bias. And it's obvious that nanodevice with embadded carbon atoms (blue) has big transmission spectrum than clear one. Green plot is the transmision of clear BNNT and it almost has constant value in $(-1.5-1)eV$ energy levels. But transmission's drastic change is observed in nanotube with embadded carbon atoms. Which means that multiple intrinsic transmission chanels exist in those energy levels. Howewer, for some energy levels transmission of clear nanodevice more than with impurity.

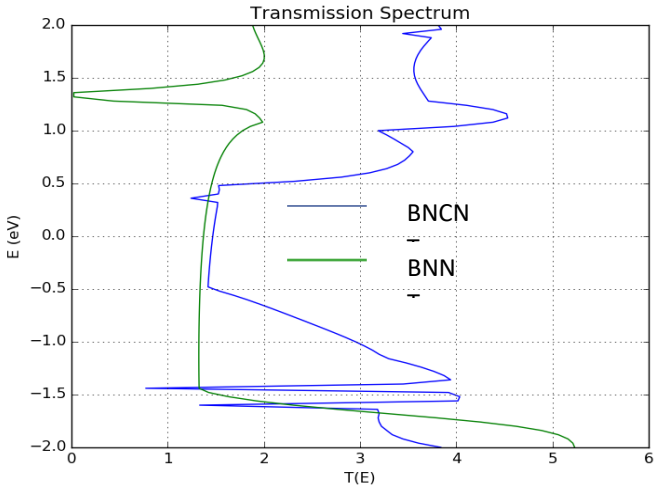

Figure 3. Comparision of transmission spectrum of BNNT clear nanodevice (green) and BNNT nanodevice with embadded carbon atoms (blue)

In order to understand electronic transport properties the transmission eignstates have been calculated. The eignvalues of both devices are presented in Table 1. Figure 4 shows eigenstates for both devices in $2V$ bias voltage. The eigenstates have large amplitude in the left part of central region. Here eigenstates are sum of incoming and a reflected sates. In the right side the probability of transmission is higher than in the left side.

Table 1 Eigenvalues of BNNT and BNCNT with $2V$ bias voltage.

BNNT device	BNCNT device
0.7634	0.6943
0.0159	0.1656
0.0008	0.0064
0.0008	0.0024
0.0004	0.0005
0.0004	0.0003
------	0.0001

Figure 4(a) presents eigenstate of BNNT corresponding to the eigenvalue 0.7634, (b) is the eigenstate of BNNT with embedded carbon atoms corresponding to the eigenvalue 0.6943. It is obvious that those eigenstates which have higher transmission eigenvalue also has larger amplitude on the right side, so they are transmitted to the right side. Figure 4(c) corresponds to 0.0159 eigenvalue of BNNT, in the right side amplitude is equal to zero so there is not transmission. Figure 4(d) presents eigenstate of BNCNT corresponding to the 0.1656 eigenvalue. Here transmission probability is small.

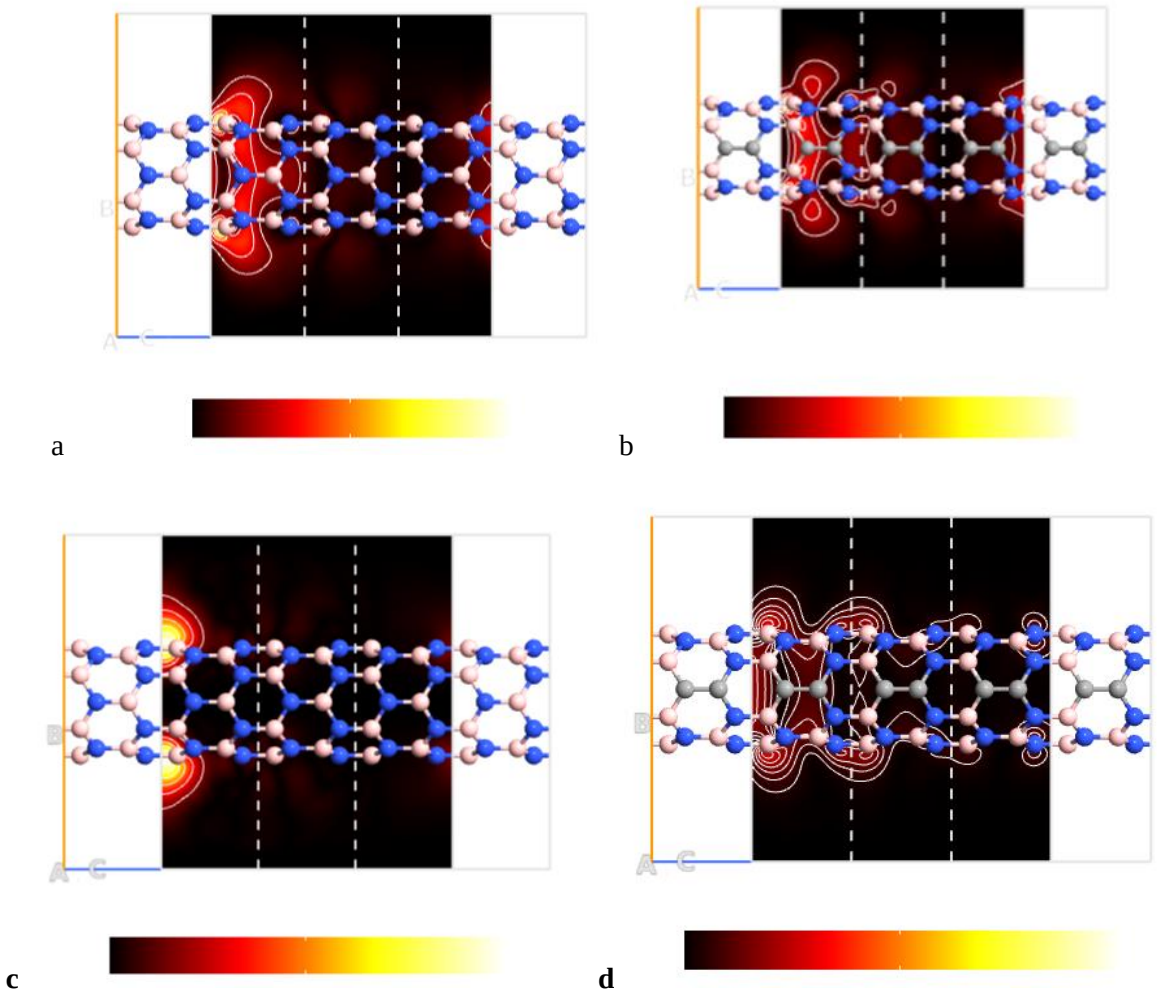

Figure 4. Eigenstates with 2V bias a) clear BNNT device with 0.7634 eigenvalue b) BNNT device with embedded carbon atoms with 0.6943 eigenvalue c) clear BNNT device with 0.0159 eigenvalue d) BNNT device with embedded carbon atoms with 0.1656 eigenvalue

4. Conclusion

In summary, DFT LCAO basis sets combined with the NEGF calculation method has been used to compute transmission spectrum with $0V$ bias voltage of both BNNT and BNCNT

devices. It has been found that nanodevice with embedded carbon atoms has wider transmission spectrum than clear one. Howewer, for some energy levels transmission of clear nanodevice more than with impurity. Transmission eigenstates with $2V$ bias also have been calculated. Results show that BNCNT has higher eigenvalues and larger amplitude in the right side of nanodevice, so probability of transmission is higher than that in BNNTs.

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