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RESEARCH ARTICLE

DFT comparison of structural and electronic properties of (5, 0) zig-zag GaAs nanotube and (5, 0) zig-zag GaSb nanotube

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ABSTRACT

Abstract. The structural, electronic and transport properties of the (5, 0) zig-zag GaAs nanotube and (5, 0) zig-zag GaSb nanotube have been studied by using Density Functional Theory (DFT) combined with Non-Equilibrium Green's Function (NEGF) formalism with TranSIESTA software. The electronic band structure (EBS), density of states (DOS), band gap (BG), current-voltage (I-V) characteristics and quantum conductance curves (dI/dV) of these two structures were studied under low-bias conditions. The obtained results demonstrate that these two structures exhibit semiconducting behavior, but the (5, 0) zig-zag GaSb nanotube has a smaller band gap and the highest value of the electron density of states, hence it is an important candidate in the field of infrared-radiation detectors, resonant tunnelling devices and laser diodes. Instead the (5, 0) zig-zag GaAs nanotube showed the amazing property of Negative Differential Resistance (NDR) that it has played a vital role in high frequency oscillators, reflection amplifiers, memories and switching devices.

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INTRODUCTION

Nanotubes have attracted increasing attention due to their great prospects in the fundamental physical sciences and modern nanotechnology [1]. Since the discovery of carbon nanotubes, many experiments and theoretical studies have focused on synthesizing nanometer-scale tubular forms of various materials and reviling their properties. III-V compound semiconductors are being used for development of novel electronic and optoelectronic device structures in the industry because of the advantages they offer such as direct band gap, better band gap tunability, versatile heterojunctions, increased carrier mobility and controllability of doping levels and types [2]. The composition of the constituent materials determines the physical characteristics of these semiconductors, which are being used in many optoelectronic and photonic devices, such as high electron mobility and heterostructure bipolar transistors[3], diode lasers[4], light emitting diodes[5, 6], and photo detectors [7]etc. GaAs as a most promising and popular III-V compound semiconductors has many distinctive properties, such as high electron mobility, high electron velocity and ultra-high frequency, which makes it ideal for optoelectronic, transistors, high-temperature diodes, high-power microwave sensors, low power and ultrahigh-speed device application [8-13]. GaSb is another III-V compound semiconductor that tuned out to be promising candidate for high-speed optoelectronic devices. GaSb has significant attention as channel materials for transistors because it has extremely high carrier mobility, electron mobility and low band gap also it was recently being used for advanced optoelectronic devices, laser diode, photodetector, resonant tunneling diodes, high-speed field effect transistors and high frequency and low threshold devices[14, 18].

In the present theoretical investigation the structural, electronic and transport properties of

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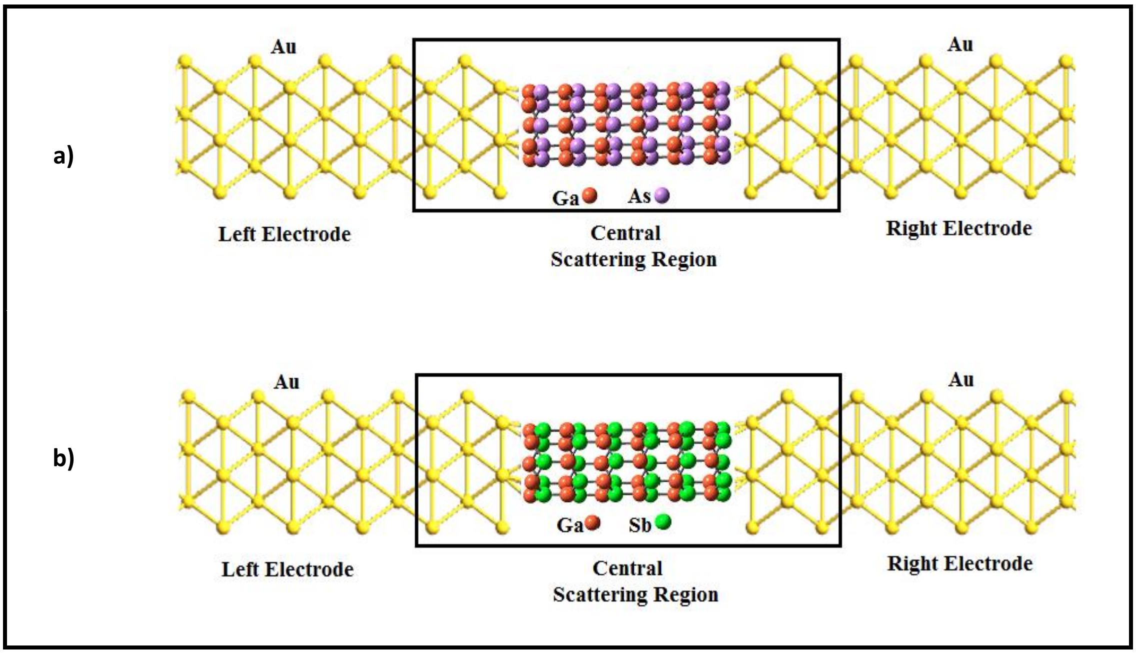

Fig. 1. Device structures of a) (5, 0) zig-zag GaAs nanotube and b) (5, 0) zig-zag GaSb nanotube as the scattering region.

(5, 0) zig-zag GaAs nanotube and (5, 0) zig-zag GaSb nanotube was compared by using Density Functional Theory (DFT) combined with Non-Equilibrium Green's Function (NEGF) formalism.

MATERIALS AND METHOD

In order to provide the device part of the two-probe system (contact–device–contact), we have taken a (5, 0) zig-zag GaAs nanotube and (5, 0) zig-zag GaSb nanotube with 60 atoms its central region (scattering region) for the charge transfer. The magnitude of the length and diameter of both tubes is 12 A° and 4 A° respectively. In the calculations the two probe system is divided into three parts: the left electrode (L), the right electrode(R) and the central scattering region. Therefore the left and right sides of the nanotube (scattering region) is connected to appropriate semi-infinite metal electrodes. These tubes were located on the bulk gold electrodes. Two gold (Au) (100) electrodes are used as a nanotube contact metal. 23% of the right and left electrodes were included in the scattering region in order to compensate the scattering losses at the joining ends of the central region and the electrodes. The zig-zag GaAs nanotube and (5, 0) zig-zag GaSb nanotube device setup is shown in Fig. 1.

The geometry of the two chosen structure was optimized and their structural and electronic properties were calculated by density functional theory and non-equilibrium Green's function (NEGF) formalisms using the TranSIESTA package [19]. All calculations have been performed within the local density approximation (LDA) framework using the exchange–correlation function of Perdew–Zunger (PZ) [20]. In addition, the standard norm-conserving Troullier–Martins pseudopotentials orbital [21] are used to the core–valance interactions. A numerical double-z polarized (DZP) basis set was used for all atoms in these structures. Relaxed geometries were obtained by minimization of the total energy using Hellmann–Feynman forces including Pulay-like corrections. A mesh cutoff 350 Ry was used for the computation of the electron densities and potentials. Then the proposed structures were optimized until all forces acting on the atoms become less than 0.01 eV/A°. For the accuracy of calculations, the electrode temperature was fixed at 300 K, and for the Brillouin zone integration, a 3 ´ 3 ´ 60 Monkhorst–Pack k-point grid was utilized. After that, the applied bias across two electrodes was varied in the range of 0–1 V (low bias) and the current passing through the central region of the system at a finite bias voltage can be obtained using the Landauer–Buttiker formalism [22], given by:

$$I = \frac{2e^2}{\hbar}\int T(E,V_b)\,dE \tag{1}$$

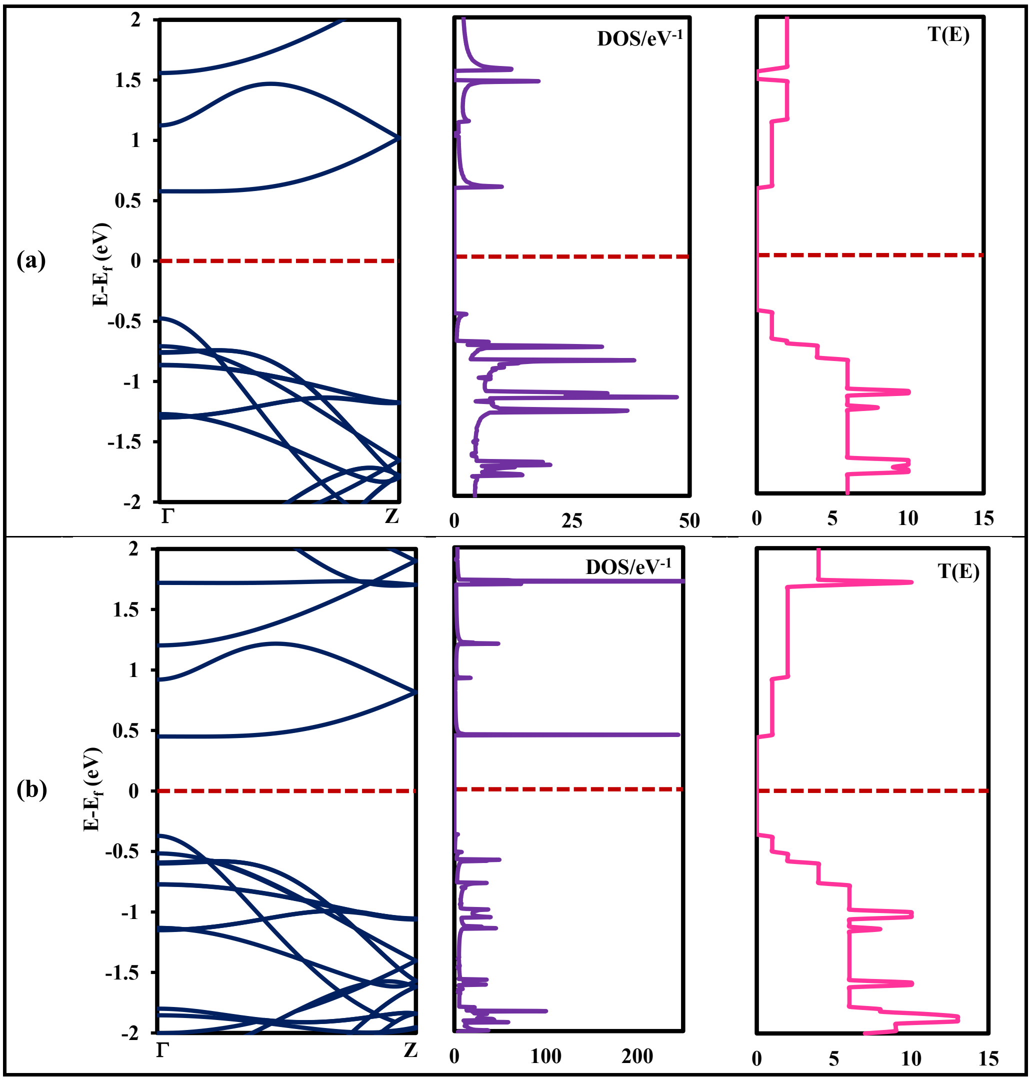

Fig. 2. Band structure, Density of States and zero bias transmission spectra of the a) (5, 0) zig-zag GaAs nanotube b) (5, 0) zig-zag GaSb nanotube.

Where $\frac{2e^2}{h}$ is the quantum unit of conductance and $T(E,V_b)$ is the total transmission probability for an incident at an energy E through the device under the applied bias voltages which itself can be calculated as $T(E,V_b)=\sum T_n(E,V_b)$ Here Vb is the applied bias voltage.

RESULTS AND DISCUSSION

In order to examine the conductance behavior, band structure calculations of two considered structures were done by performing the Brillouin zone integration within the Gamma (G) to Z point. Calculated electronic band structures, density of states and the transmission coefficient at zero bias are shown in Fig. 2. The Fermi level is set to zero in all plots.

The band structure diagram shows two these nanotubes are semiconducting. It can be clearly seen that the band gap for the (5, 0) zig-zag GaSb nanotube is smaller than the (5, 0) zigzag GaAs nanotube. The band gap of these tubes is 0.82 eV and 1.05 eV respectively. As well as according the DOS diagrams for both nanotubes, no peak has been found at their Fermi level, evidence of their semiconductor behavior, however dispersed peak can be seen in the conduction band and the valance band with one of them reaches the maxima. The DOS profile of the (5, 0) zig-zag GaSb

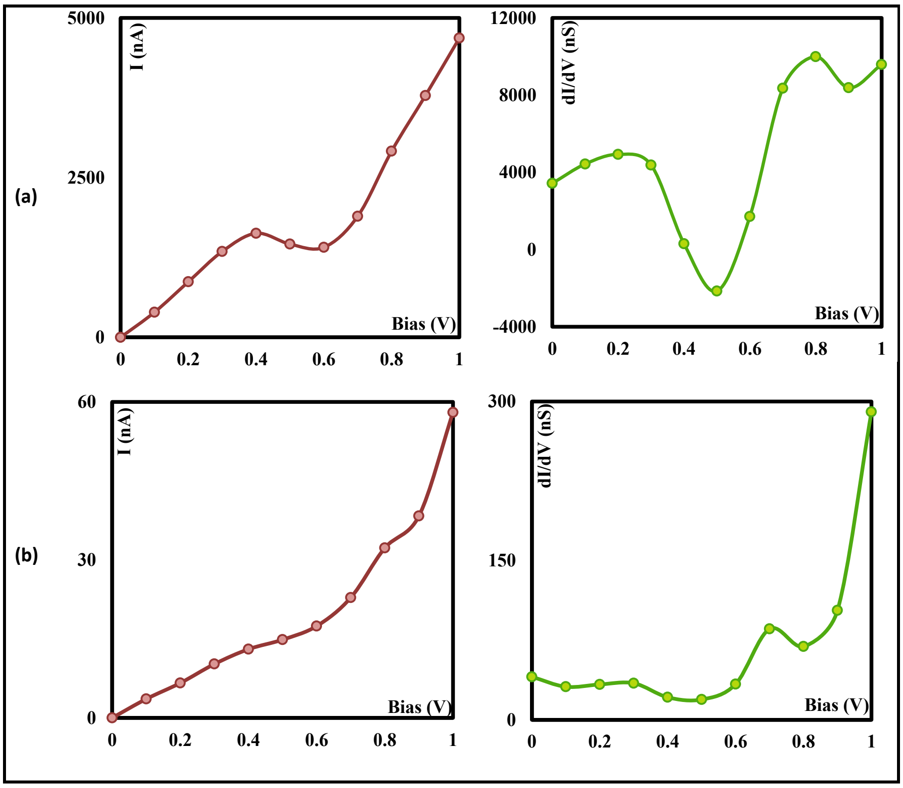

Fig. 3. Current-Voltage characteristics and dI/dV-V curves of a (5, 0) zig-zag GaAs nanotube (a) and (5, 0) zig-zag GaSb nanotube (b) contacting two metal Au electrodes.

nanotube is shown the higher value of the electron density than the (5,0) zig-zag GaAs nanotube. Also the transmission coefficient is directly related to the DOS of the nanotube. Transmission is normalized with respect to $G_0 = 2e^2/h$.An observing transmission gaps at Fermi level in transmission spectrum profiles of both structures confirm the semiconducting nature of these tubes which the transmission gap at (5,0) zig-zag Gasb nanotube smaller than the transmission gap at (5,0) zig-zag GaAs nanotube. The value of the transmission coefficient at (5,0) zig-zag Gasb nanotube reaches to $10G_0$ at 1.7 eV above the Fermi level whereas this value at (5,0) zig-zag Gasb nanotube no more than $2G_0$ in the vhole of above the Fermi level.

The transmission spectrum of the two investigated nanotubes were analyzed by plotting I-V and quantum conductance (dI/dV) curves with respect to different applied bias voltages in Fig. 3.

It can be seen in the (5, 0) zig-zag GaSb nanotube (b), with the increase in the applied voltage, the current flowing through this device increases steadily and reaches a maximum value, but in the (5, 0) zig-zag GaAs nanotube (a) for voltages 0.4 to 0.6 V, current flow decreases to a minimum value that this results in the onset of the NDR effect which is defined as a trade-off between voltage and current flow. NDR is a significant quantum transport phenomenon in electronic devices as it can potentially impact many key applications such as high frequency oscillators, reflection amplifiers, memories, multi-level logic devices and fast switches [23].

Also, it is clear that a (5, 0) zig- zag GaAs nanotube coupled two probe Au system is shown the maximum conductance over a wide range of applied bias voltages. In order to gain a clear description, it has been shown values of current and conductance of both the investigated devices at different voltages in Table I.

From the results, it is clear that the GaAs device shows enhanced quantum conductance with 9996.3872 (nS) at bias voltage of 0.8 V, furthermore as the applied bias is increased in this device, negative differential resistance is reported between 0.4-0.6 V. Probably the most peaks in dI/dV should be related to the increase in conduction states. Whereas GaSb device has shown the minimum

Table1. Values of current and conductance for two GaAs device and GaSb device at different bias voltages.

	Current (nA)		**Conductance (nS)**	
Applied Bias (V)	**(5,0) zig-zag GaAs nanotube**	**(5,0) zig-zag GaSb nanotube**	**(5,0) zig-zag GaAs nanotube**	**(5,0) zig-zag GaAs nanotube**
0	0	0	3429.9729	40.5535
0.1	393.1897	3.5870	4433.8229	31.1877
0.2	869.8774	6.6223	4931.0600	33.3657
0.3	1344.4728	10.2254	4380.4282	34.5020
0.4	1628.4435	13.0437	304.2087	31.266
0.5	1459.3707	14.8499	-2150.3271	19.1651
0.6	1409.0557	17.4302	1715.4656	33.6685
0.7	1895.0491	22.8336	8358.8167	85.6699
0.8	2913..9597	32.2781	9996.3872	69.0885
0.9	3786.0005	38.3396	8384.1774	103.1560
1	4684.7700	58.0108	9591.2129	290.2683

conductivity whole range of applied bias voltages.

The observed results suggest that the (5, 0) zig-zag GaSb nanotube may be an important candidate to design the nano-molecular diodes, tunneling field effect transistors and photodetector whereas the increase in conductance and the NDR feature shown by (5, 0) zig-zag GaAs nanotube, is important for the design of high speed optoelectronic devices, high frequency oscillators and switching devices.

CONCLUSIONS

In this work, DFT calculation was used to investigate and compare the structural, electronic and transport properties of (5, 0) zig-zag GaAs nanotube with (5, 0) zig-zag GaSb nanotube. To obtain information regarding the electronic efficiency of the both nanotube, we have to control several structural property such a density of states, band gap, band structure and I-V characteristic. Among two these structures the (5, 0) zig-zag GaSb nanotube, which indicated a small gap and higher DOS close to Fermi level was considered as the best electronic conductor in comparison to the other studied design structure. Two these devices exhibit a semiconducting character, with a direct band gap at the G point, which suggests that these nanotubes may have high potential for full-color display applications. Due to the larger band gap of (5, 0) zig-zag GaAs nanotube, it is also explored as a tunnel resistance device.

The higher conductance and the observed NDR feature I-V characteristic of a (5, 0) zig-zag GaAs nanotube reveal that this proposed structure is a useful semiconducting channel to design the novel high speed optoelectronic devices such as a oscillators, amplifiers and switching transistors. Whereas a (5, 0) zig-zag GaSb nanotube might also be promising candidates for advanced optoelectronics devices such as laser diodes, photodetector and tunnelling field effect transistors.

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CONFLICT OF INTEREST STATEMENT

All authors declare that no conflicts of interest exist for the publication of this manuscript.

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