Computational study of Cr substituted single-walled GaN nanotubes

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Abstract. In present study, we have investigated electronic, optical and transport properties of Cr substituted SW GaNNT. We find that the (6, 0) nanotubes of GaN are stable and semiconducting with the band gap of 2.4 eV. Doping with Cr appears to reduce the band gap of GaN nanotubes. The V-I characteristics show typical tunnel diode behaviour for the device where the tunnelling current reaches a maximum value at the applied bias of 0.4 V and we observed a negative slope region when forward bias is applied. Because of this unusual behaviour, it can be used in number of special applications in electronic devices.

1. Introduction
In present scenario, interest in GaN based 1D structures are high in commercial and scientific level, because of the potential to apply in electronic devices[1]. Though 2D structure GaN materials were synthesized successfully for several years, research on (1D) GaN materials is limited due to the difficulties associated with their synthesis. But, pure BN nanotubes have been successfully produced by arc discharge[2,3], therefore, it opens the possibility of synthesis of other CN and GaN nanotube.

In this paper, electronic, optical and transport properties of GaN NT were carried out within the framework of density-functional theory (DFT) combined with NEGF, as implemented in the TranSiesta module within SIESTA-3.1 code[4]. We have also studied the issue of Cr doping on their electronic structure, morphological, optical and Transmission Coefficients of (6,0) GaNNTs will be talked about.

2. Computational detail
The transport properties were carried out utilizing the first-principles method implemented in the TranSiesta. The exchange–correlation energy are described by the RPBE[5] and generalized gradient approximation (GGA) implemented in calculations. TranSiesta provide the ability for the model open boundary conditions it is based on the NEGF i.e. is constructed using the DFT Hamiltonian obtained from a given electron density. The device setup for a (6,0) GaN NT was constituted by three parts: the left (L) and right (R) semi-infinite GaN leads (electrodes) and the scattering region. The size of the scattering regiontakes place enough to prevent the interaction between the left and right electrode and current through the scattering region was calculated using Landauer-Buttiker Formula [6].
3. Results and discussions
We begin with electronic structure calculations of pristine and doped (6, 0) GaN nanotube to determine their stability. The binding energy is calculated as follows:

\[ E_b = \frac{E_{tot} - (xE_{Ga} + yE_N + zE_{Cr})}{x+y+z}, \]

where \( E_{tot} \) is the total energy of GaN nanotube, \( E_{Ga}, E_N, E_{Cr} \) are energies of Ga, N and Cr atoms, respectively and \( x, y, \) and \( z \) are number of Ga, N and Cr atoms, respectively considered in the supercell. The formation energy \( E_{form} \) in terms of energies of constituents is calculated as follows:

\[ E_{form} = \frac{E_{doped\ GaNNT} - (E_{Prist\ GaNNT} + zE_{Cr})}{N}, \]

Table 1 lists the calculated binding energy (\( E_b \)) and formation energy (\( E_{form} \)) together with band gap of pristine and doped GaN nanotubes.

**Table 1.** The calculated structural and electronic properties of pristine and doped (6,0) GaN nanotubes.

| System       | Bond length (Å) | \( E_b \) (eV) | \( E_{form} \) (eV) | Bandgap (eV) |
|--------------|-----------------|----------------|---------------------|--------------|
| Pristine     | 1.84            | 6.51           | -                   | 2.41         |
| Doped - 8% Cr| 1.84            | 6.81           | 11.6                | metallic     |
| Doped - 17% Cr| 1.84          | 7.11           | 22.22               | metallic     |
| Doped - 25% Cr| 1.84          | 7.40           | 32.84               | metallic     |

**Figure 1.** Plot of Binding energy V/s Cr concentration for (6, 0) GaN nanotubes

Figure 1 shows that increase in the binding energy with the increase in the Cr concentration for (6, 0) GaN nanotubes, are related to the fact that the electronegativity of Cr (1.66) lies between Ga (1.81) and N (3.04), thereby facilitating formation of covalent bond in the doped lattice.

The calculated band structure and density of states of the pristine and chromium doped GaN nanotubes are shown in figure 2. The pristine GaN nanotube is found to be direct-gap material which is consistent with previous study [7]. Doping of nanotube with Cr induces an additional state in the band structure. Initially, the valence band maximum (VBM) shifts towards Fermi level as concentration of Cr increase in the lattice. Later, VBM shifts away from Fermi level, and the induced states starts shifting towards Fermi level yielding GaN nanotube to be metallic.

The reason for decrement of energy bandgap simply reflects the ionic bonding character of the doped lattice, i.e. s and p bands localized to Ga and N respectively are well separated. Due to doping of Cr atoms, more p states near the valence band edge and more s states near the conduction band edge appear to hybridize to metallicity of the system.
This is further confirmed by DOS showing that the lower part of the valance band is dominated by the N-4s states, and N-4p states near the Fermi level, while Ga-4s states reside just between them. On the other hand, Ga-4p states dominate in the conduction band of the tubular lattice. In the doped configuration, Cr associated additional peak near Fermi level leads to the metallic behaviour of GaN nanotube.

Next, we were calculate d the imaginary parts of dielectric function then, get real part of dielectric functions and other optical properties by using the Kramers-Kronigging relations, for incident light polarized parallel to the nanotube. TranSiesta. Figure 3 shows the absorption coefficient that is corresponding with imaginary dielectric curves of the configuration. Major peaks in the absorption coefficient of pristine GaN nanotubes are found at 1.75, 2.75, 6.25 and 9.6 eV, and are associated with transitions of electrons from different energy states of the valence band to the conduction band. The location of these peaks depend on the Cr concentration in the doped GaN nanotubes.

The electronic transport properties of the pristine and doped (6,0) GaN nanotubes for different Cr concentration are determined under equilibrium conditions in figure 4. The transmission probability reaches high when the electrons resonate with the covalent π orbital of the atomic [8]. It is also proves the transmission coefficient T(E) is zero at Fermi level confirming the semiconducting nature of the GaNNT. As the Cr concentration increases nature of transmission spectrum change and the transmission spectrum has a series of peaks and valleys. It is clear that the peaks and valleys of transmission spectrum and the density state curves have a similar trend.
Figure 4. Transmission spectrum (6,0) pristine and 8% Cr doped GaNNT.

Figure 5. V-I plot for pristine and Cr-doped (6,0) GaN nanotubes.

It is clear from figure 5, the current is almost zero in between 0.0 – 0.2 V, which means that the transmission probability $T(E)$ in the integral windows is zero. Next, in the bias voltage in the range 0.2 to 0.4 V, the current is increased with voltage. From 0.4 to 0.6V it gives ultimate result, as the voltage increases current decreases and valley occurs at 0.6 V. This region is very important because resistance is negative showing that pristine and doped GaN nanotubes. This is the ultimate behavior of (6,0) SWGaNNNT, due to which it can be used in number of special applications in electronic devices, it can act as a tunnel diode in the considered device architecture.

4. Conclusions
We conclude that, the pristine GaNNT are semiconductor having a direct band gap 2.41 eV and doping with Cr makes the tube to be metallic. This behavior is supported by density of states plots and transmission coefficient calculations. V-I curve exhibits ultimate behavior of GaN nanotubes. For the low bias region, resistance becomes negative leading to tunnel diode characteristics for pristine and doped GaN nanotubes. The calculated results thus suggest that GaN nanotubes may be used for full color displays in the nanoscale optoelectronic devices.

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References
[1] Sharma U S, Bisht P S and Verma U P 2009 J. Phys. Condens. Matter 21 025501
[2] Loiseau A, Pascard H, Willaime F, Demoncy N and Hug G 1996 Phys. Rev. Lett. 76 4737
[3] Suenaga K, Colliex C, Demoncy N, Loiseau A, Pascard H and Willaime F 1997 Science 278 653
[4] Ordejon P, Sanchez-Portal D, Garcia A, Artacho E, Junquera J and Soler J 2000 RIKEN Rev. 29 42
[5] Dreizler R M and Gross E K U 1990 Density Functional Theory (Berlin: Springer)
[6] Dutta S1995 Electronic Transport in Mesoscopic Systems ed Ahmed H, Pepper M and Broers A (Cambridge, England: Cambridge University Press)
[7] Srivastava A, Khan M I and Khare P S, 2014 The Scientific World Journal 2014 984591
[8] Moradian R, Azadi S and Farahani S V 2008 Phys. Lett. A 372 935