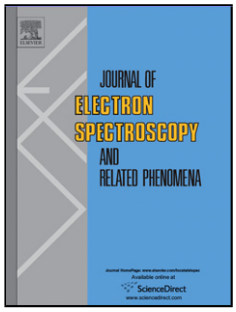

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Analysis the electronic properties of the zigzag and armchair single wall boron nitride nanotubes with single Li impurity in the various sites

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Highlights:

- -We invesitagted the electronic properties of the ASWBNNTs and ZSWBNNTs.
- These properties of all tubes also studied with single Li impurity in various sites.
- With Li impurity in N site, the band gap is reduced, and all tubes became p-type.
- Single Li in B site,the behaviors of all tubes altered to metallic behaviors.
- Total, Kinetic, and Electrostatic energies are dependent on the diameter of tube.

ABSTRACT:

We utilized the first-principle density functional theory (DFT) calculation to investigate the structural and electronic properties of various diameters for zigzag and armchair single wall boron nitride nanotubes (ZSWBNNTs and ASWBNNTs) with and without single Li impurity in the various sites. Using DFT method, which employed in the Quantum espresso package, to calculate the electronic band structure, band gap, density of states (DOS), total, kinetic, and electrostatic energies. In the pristine case, there are large electronic band gaps, which make all SWBNNTs have insulator behaviors. Also, total, kinetic energies are reduced with increasing the diameter of the tube, but the opposite behavior with the electrostatic energy. By substituting one B atom with single Li impurity, the electronic band gap is reduced. This impurity also changed the shape and reduced the value of the DOS, which confirmed all the obtained results in this report. Similarly, the values of all the above energies are decreased, which make the structure unstable and more reactive. The significant result in this work is that addition of only one lithium atom in the unit cell of SWBNNTs can take the Fermi level down so significantly and result in insulating to semiconducting phase transition. When we replaced one N atom with one Li impurity, all these energies are dependent on the diameter, so the values of energies are reduced with this impurity. The behaviors of these SWBNNTs are altered to P-type. This impurity is converted these SWBNNTs from an insulator to a semimetal state with zero electronic band gap and changing the shape and value of the DOS, which is very important in various applications.

Keywords: DFT; Electronic band gap; Total energy; DOS; BNNTs.

1. Introduction

Theoretically, boron nitride nanotubes (BNNTs) are proposed in 1994 [1], and it is synthesized by the arc discharge method in 1995 [2]. BNNTs can be formed by rolling up a graphene sheet (2-D hexagonal BN atoms) to the cylinder form. BNNTs have the same geometry of the carbon nanotubes (CNTs), which is designated by a chiral vector. Based on the number of layers, there