H. Tarikhchi, et. al. International Journal of Engineering Research and Applications
www.ijera.com
ISSN: 2248-9622, Vol. 11, Issue 10, (Series-II) October 2021, pp. 21-27

RESEARCH ARTICLE OPEN ACCESS

Tuning Electronic Structures of double-walled boron nitride nanotubes using Ga atom encapsulated

H. Tarikhchi[1], A. Torabi[1] and A. Vatankhahan[2]
[1]*Physics Department, Khayyam University, Mashhad, Iran*
[2]*Physics Department, Shahrood University of Technology, Shahrood, Iran*

ABSTRACT
In this article, the electronic and stability features of double-walled Boron nitrideNano tubes (DWBNNTs) have been studied by density functional theory. The results show that all Nano tubes are semiconductors and have indirect band gaps which the amount of band gap for all these is greater than 2.9 eV. Also, we have investigated the effect a Ga atom encapsulated in DWNNT.Our calculations show that all of the considered Nano tubes have been turned into metal by encapsulation. In addition, the results indicate that encapsulating Ga atoms into DWBNNTs is a good way to make them more stable and modify their electronic properties.

Keywords: double-walled Boron nitrideNano tubes; Density functional theory (DFT); Stability**;**Encapsulating Ga atom intoNano tubes.

Date of Submission: 30-09-2021 Date of Acceptance: 13-10-2021

I. INTRODUCTION

Nanotechnology is a field of applied knowledge and technology that covers a wide range of topics. Its main subject is the inhibition of matter or devices smaller than one micrometer, usually about 1 to 100 nanometers, and the dimensions of matter are very influential in its properties, and the physical, chemical and biological properties of individual atoms and molecules are different from the mass properties of matter. Nanotechnology is the application of new properties of materials that the new physical effects are mainly affected by the dominance of quantum properties over classical properties. Nano tubes are one of the basic foundations of nanotechnology knowledge. Nano tubes have outstanding features such as high thermal conductivity compared to other compounds except for pure diamond, very high electrical conductivity, ability to carry a higher current than copper, very large magnetic moment, and the ability to emit and absorb light. Nano tubes have many applications in technology and industry, which have different types depending on the materials. One type of Nano tube is boron nitride Nano tubes (BNNTs). Boron nitride Nano tubes compared to carbon Nano tubes (CNTs) have attracted special attention in nanoelectronic and optoelectronic applications. For the first time in 1994, boron nitride Nano tubes were predicted through theoretical calculations [1, 2], and the successful synthesis of these Nano tubes was reported in 1995 [3].Boron nitride (BN) has great potential in nanotechnology. Boron nitride nanostructures are not only resistant to decomposition in a vacuum, air, and some liquids, but also do not decompose at temperatures above 900 ° C [4]. CarbonNano tubes oxidize in air at a temperature of 400 ° C [5]. Due to their high oxidation resistance, boron nitride Nano tubes are suitable for the production of composite materials.In this article, the electronic and stability properties of double-walled Boron nitrideNano tubes(DWBNNTs) are investigated using DFT calculations. The obtained calculation indicate that DWBNNTs are semiconductors with indirect band gaps. Also we have investigated the effect a Ga atom encapsulated in DWNNT on stability and electronic properties.

II. METHODS

We have used first-principles calculations based on density functional theory (DFT), as implemented in the SIESTA 4.1-b3 simulation package [8]. The vdw-DF2 functional of Berland and Hyldgaard (BH) [9] is used as the exchange-correlation functional.In this paper, the cutoff energy is equal to 500 Ry. For the Brillouin zone integrations, we have used a Monkhorst-Pack mesh with a gamma centered k-points grid of 1×1×9 for

gradient (CG) until the force between the atoms becomes smaller than 0.001 eV/Å.

as the inner Nano tube of the armchair-DWBNNTs. Out of it, we have placed different armchair-SWBNNT, varying its index n from 8 to 15.After the relaxation of the structures, we calculated the formation and binding energy. The results are indicated in Fig1.Any value below zero means that the DWBNNT is stable.A Nano tube becomes stable if the shape of the Nano tube is maintained after relaxation and has the formation and binding energy negatively and minimally.We can see that the DWBNNT composed by the (5,5) (10, 10) is the most stable DWBNNT studied.Fig2 shows some of the structures studied after relaxation. All Nano tubes retained their appearance.In the outer Nano tube with the large the diameter,the distance between the inner and outer Nano tube s is large, so there is no bonded between the two. Fig1 shows that as the dimensions of the outer Nano tube become larger, the formation and binding energyincrease until they reach a constant value. If the diameter of the Nano tube becomes so large that its curvature decreases, the Nano tube approaches the Nano sheet. Properties such as the formation andbinding energy of the Nano tubes in large diameters are similar toNano sheets. Thus, the formation and binding energy are approximately constant and are almost equal to the formation and binding energy of the Nano sheet.

structural optimization of all Nano tubes.Structural relaxation is performed by using the conjugate

III. RESULT

The structural and electronic characteristics of DWBNNTshave been investigated by a first-principles calculation.The stability of the structure of double-walled Nano tubes can be different, which is related to the different number of atoms of the inner tube with the outer tube and the bonding effect between the atoms of the outer and inner tube. We investigated the stability of double-walled Nano tube structures based on the parameters of formation energy, binding energy and appearance of the structure after relaxation. We have calculated the binding energy per atom,which is defined as[10]:

$$E_b = (E(BN) - aE(B) - bE(N))/(a+b)$$

Where $E(BN), E(B), E(N)$ are the total energy of the Nano tube, Batom and N atom, respectively.a and b arethe number of atoms B and N, respectively. Also,we have obtained the formation energy as following [11]:

$$E_{formation} = E[(m,m)@(n,n)] - E(m,m) - E(n,n)$$

Where $E[(m,m)@(n,n)], E(m,m), E(n,n)$ are the total energy of DWBNNTs, inner tube and outer tube, respectively.To evaluate the stability of double-walled Nano tubes, we selected single-walled Boron NitrideNano tubes(SWBNNT) (5, 5)

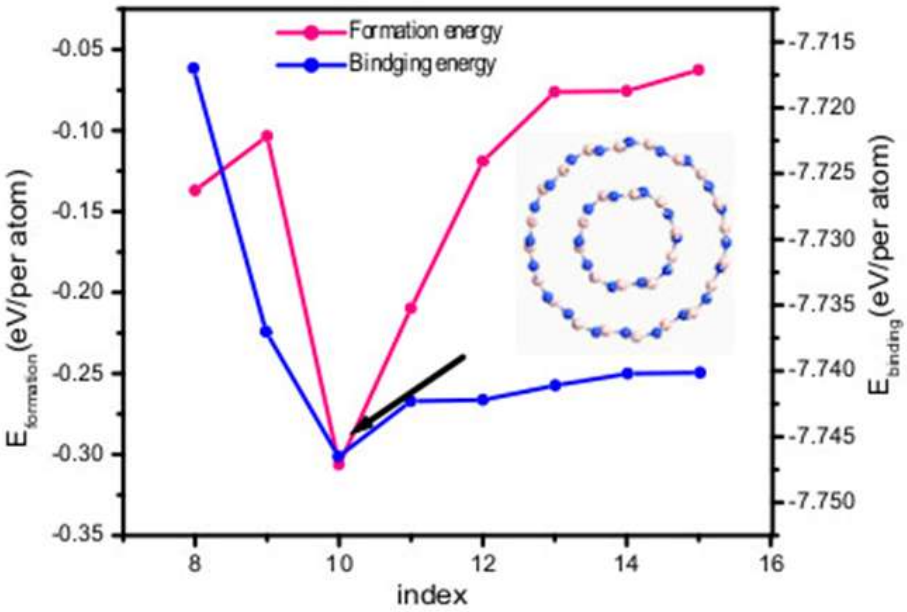

Fig.1.Binding energy (in blue color) and formation energy (in red color) for different DWBNNTs

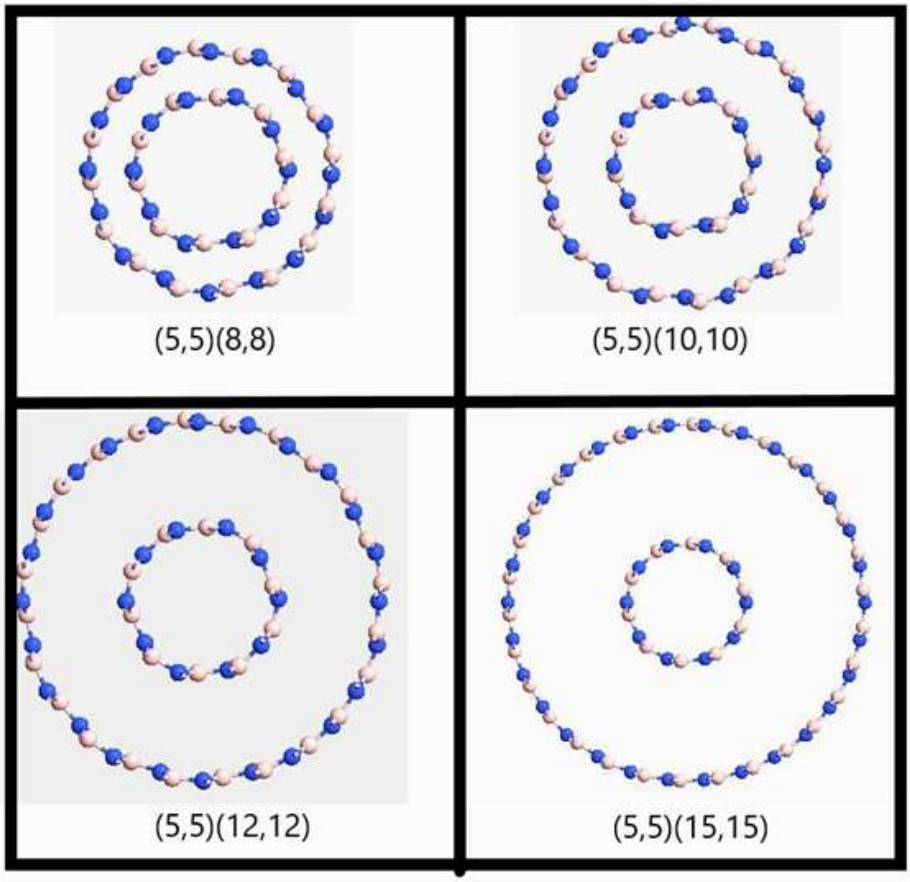

Fig.2. The top of optimized DWBNNT

the increase of the Nano tube diameter. The evidence shows that this increase is small in large diameters (Fig 4). Hybridization between the orbitals of the B and N atoms at the edges reduce the bandgap in the small-diameter Nano tube.In the large diameters of the Nano tube, the value of the bandgap is approximately equal to the value of the bandgap of the Nano sheet.The obtained results are in agreement with previous studies [12].

After identifying the most stable Nanotubes, we investigated their electronic properties. Fig3 shows the band structure of Nanotubes.The obtained calculation indicates that allNano tubesare semiconductors andhavean indirect band gaps. The amount of band gap for all Nano tubes is greater than 2.95 eV.The changes of band gap in terms of Nano tube diameter are shown in Fig. 4. The value of the band gap increases with

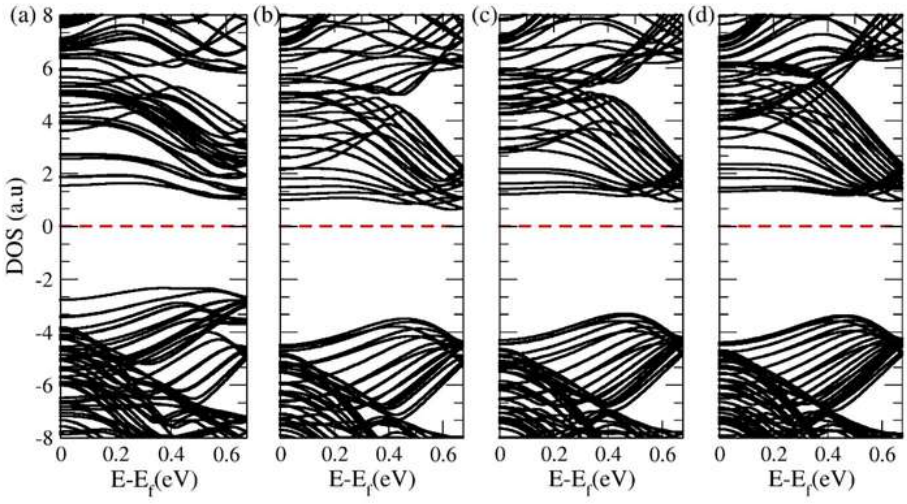

Fig.3. Band structure of DWBNNT (a) (5,5)(8,8) , (b)(5,5)(10,10), (c)(5,5)(12,12), (d)(5,5)(15,15).

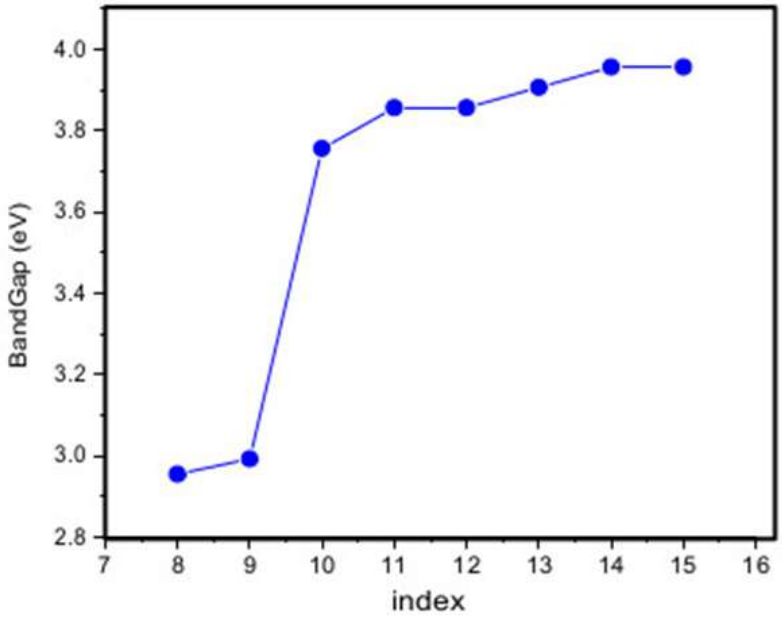

Fig.4. Band gaps of DWBNNT in term of chirality

tubesand Gaatom, respectively.Fig6 shows the formation energy before and after encapsulation. The results show that the formation energy of the Nano tube after placing Ga atom inside them decreases compared to the pure state. It can be indicated that encapsulating Ga atom into DWBNNT is a good way to increase stability. In this section, we investigate the electrical properties of Ga@DWBNNT. Fig7 shows the band structures Ga@(5,5)(12,12) and Ga@(5,5)(11,11). Our calculations show that the band gap of all studied Nano tubes has been removed by encapsulation. This occurrence could be due to the interaction between the Nano tube and the atom.

Stability and electrical properties of Ga@DWBNNT

First, we place a Ga atom at the center of the Nano tubes and then study their stability and electron properties. Fig 5 shows the structures of a Ga atom encapsulatedin DWBNNT (Ga@DWBNNT) after relaxation. All studied Nano tubes retained their appearance after Ga atom encapsulation. The formation energy is defined as [13]:

$E_{for} = \mathrm{E(Ga@DWBNT)} - \mathrm{E}(DWBNT) - \mathrm{E(Ga)}$

Where

$\mathrm{E(Ga@DWBNNT)}, \mathrm{E(DWBNNT)}$ and $\mathrm{E(Ga)}$ are the total energy of the Ga@DWBNNT, pure Nano

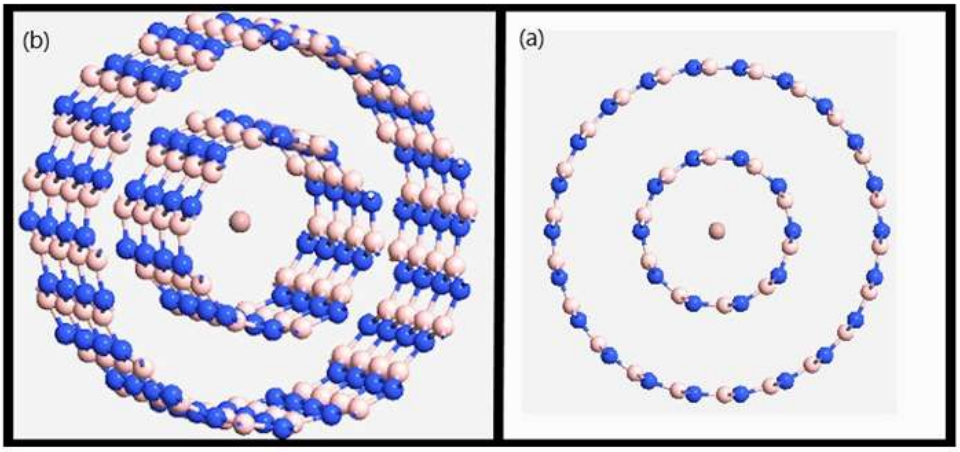

Fig.5. The top of optimized Ga@DWBNNT

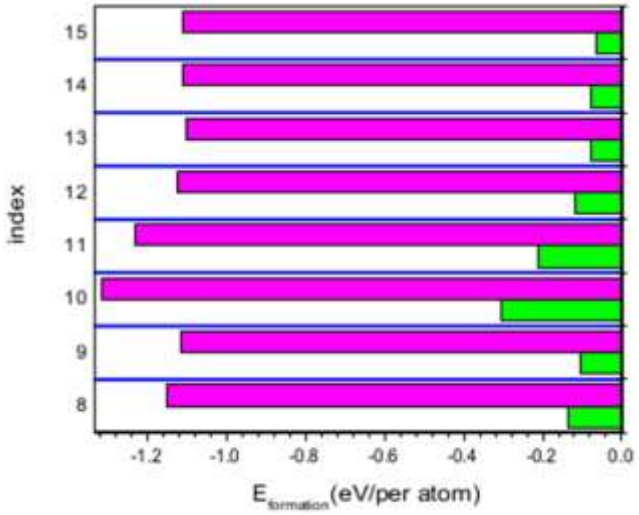

Fig.6. Formation energy Ga@DWBNNTs(in Magenta color) and formation energy pure-DWBNNTs (in green

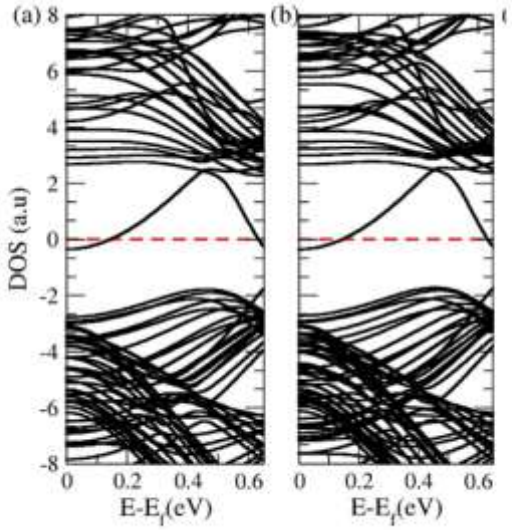

Fig.7. Band structure of Ga@DWBNNT (a) Ga@(5,5)(11,11), (b)

greater than 2.95ev.Also we have investigated the effect a Ga atom encapsulated in DWBNNT.Our calculations show that the bandgap of all studied Nano tubes has been removed by encapsulation. The results show that encapsulating Ga atom into DWBNNT is a good way to make them more stable and modification of electronic properties.To be able to tune the band gap is important in electronic devices, such as lasers and diodes. These results suggest these Nano tubes provide a wide range of applications.

IV. CONCLUSIONS

In this study, the stability and electronic properties of DWBNNT was investigated. We optimized the input parameters and the structure of the studied Nano tubes. By calculating the formation and the binding energy of systems, it is observed that the DWBNNT composed by the (5, 5) (10, 10) can be earned the highest stability. Theresults show that allNano tubesare semiconductors and have an indirect band gaps. The amount of band gap for all Nano tubes is

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Hadis Tarikhchi achieved the B. S. in physics from Payam Noor University in Quchan, Iran, in 2013 and the M. S. in solid-state physics from Khayyam University, Mashhad, Iran, in 2018.

Atefeh Torabi received the B.S degree in solid-state physics from the KhayyamUniversity,Mashhad, Iran in 2018.

AdelehVatankhahan received the M. S degree in physics from the Ferdowsi University of Mashhad, Iran, in 2005 and the Ph. D. degree in solid-state physics from shahroodut University, Iran, in 2021. Her current research interests include modulation of properties and structures of low-dimensional materials, Nano mechanics, spintronic devices simulation as well as the computational design of novel nanostructures