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Ab Initio study of stability and electronic structure of InN nanotubes

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ABSTRACT
In this article, the electronic and stability features of indium nitride (InN) nanotubes have been studied by density functional theory. The results show that the stability of nanotubes increases with increasing diameter. The band structure calculations indicate that the nanotubes have indirect gaps. Also, the band gap of InN nanotubes increases with increasing diameter and it can be modify by changing the diameter of nanotube. InN nanotubes have different applications due to small bandages and indirect gaps such as solar cells and light-emitting devices.
KEYWORDS: Single-walled InN nanotubes; Density functional theory (DFT); Stability

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bandgap. Indium nitride (InN) is an essential member of group III-nitrides. Because it has the lowest electron effective mass [5] and smallest band gap [6] between other groups III-nitride. These features indicate that InN can be used in high-speed electronic devices and light-emitting devices**.** It is beneficial to theoretical investigation on the electronic and stability features of InNNTs, which will be necessary for its synthesis and future applications. In this article, the electronic and stability properties of InN nanotubes are investigated using DFT calculations. The obtained calculation indicate that InN nanotubes are semiconductors with small direct band gaps.

I. INTRODUCTION

In recent years, nanowires and nanotubes have had many applications in nanoelectronics and nano-optics. Investigations on the features of various nanometer-scale synthesis and their structures are ongoing [1]. Many studies have been done in group III-nitrides due to their potential applications. In recent years, some group III-nitride nanotubes have been synthesized, such as single-walled BN nanotubes [2]. The electronic and stability features of BN, AlN and GaN nanotubes (NTs) have been studied by density functional theory (DFT) [3–4]. The results indicate that these nanotubes are all in metastable states and semiconductors with a direct and an indirect

II. METHODS

We have used first-principles calculations based on density functional theory (DFT), as implemented in the SIESTA 4.1-b3 simulation package [7]. The vdw-DF2 functional of Berland and Hyldgaard (BH) [8] 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 structural optimization of all nanotubes. Structural relaxation is performed by using the conjugate gradient (CG) until the force between the atoms becomes smaller than 0.001 eV/Å.

III. RESULT

The structural and electronic characteristics of armchair InNNTs have been investigated by a first-principles calculation. First, we have optimized the structure of studied armchair InNNTs with a diameter range of 8 to 28 Å. The single-walled InNNTs, which are investigated in this study, include 12 armchair NTs: (5,5), (6,6), (7,7), (8,8), (9,9), (10,10), (11,11), (12,12), (13,13), (14,14), (15,15),(16,16). Fig. 1 indicate the structure of this group of nanotubes after optimization. You can see that all the systems are stable in terms of maintaining the cylindrical shape. To evaluate the

a and b are the number of atoms In and N, respectively. The number of atoms in nanotube (n), the diameter of the nanotube (R), the binding energy per atom (E_b), and the amount of bandgap (Eg) is given in Table 1.

stability of the structures, we have calculated the binding energy per atom defined as [9]:

$$E_b = (aE(In) + bE(N) - E(InN))/(a+b)$$

where $E(InN), E(In), E(N)$ are the total energy of the nanotube, In atom and N atom, respectively.

Fig. 1. The top of side views of optimized InNNTs **a** (5,5), **b** (8,8), **c** (9,9), **d** (16,16).

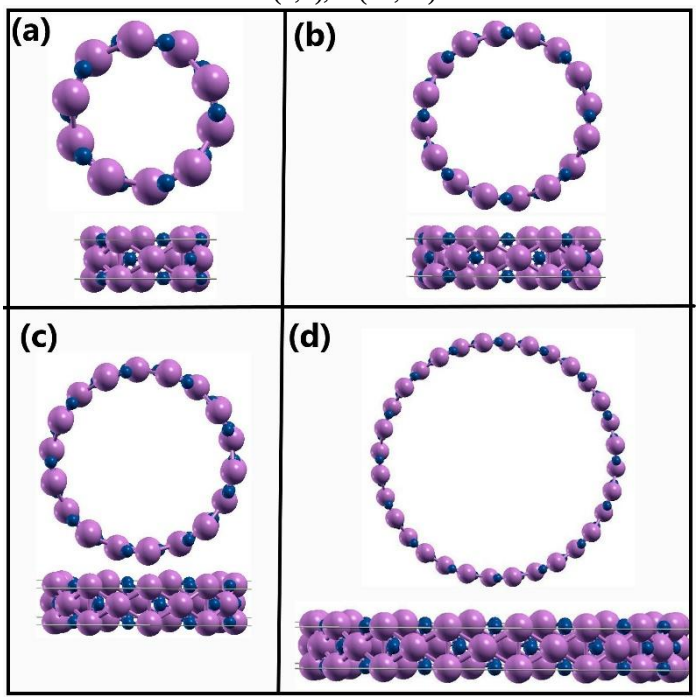

Table 1. The number of atoms in nanotube (n), the nanotube diameter (R), the binding energy per atom (E_b), the bandgaps(Eg) for armchair InNNTs.

nanotube	n_{tot}	R(Å)	E_b (eV)	E_g (eV)	
(5,5)	20	8.855	7.7114	0.77	indirect
(6,6)	24	10.985	7.7265	0.79	indirect
(7,7)	28	12.312	7.7357	0.82	indirect
(8,8)	32	13.98	7.7419	0.83	indirect
(9,9)	36	15.78	7.7461	0.89	indirect
(10,10)	40	17.47	7.7493	0.89	indirect
(11,11)	44	19.26	7.7515	0.91	indirect
(12,12)	48	20.97	7.7533	0.92	indirect
(13,13)	52	22.75	7.7543	0.93	indirect
(14,14)	56	24.5	7.7555	0.95	indirect
(15,15)	60	26.24	7.7563	0.95	indirect
(16,16)	64	27.99	7.7571	0.95	indirect

Fig. 2 shows that the binding energy changes with increasing chiral for nanotubes. As shown in Fig. 2, the binding energy increases until it reaches an almost constant value. The interaction between the atoms at the edges of the ring decreases with the increase of the nanotube's diameter, so the binding energy and stability increase. The higher the binding energy for each atom, the greater the stability. Therefore, among the nanotubes studied, the armchair InNNTs (16,16) with a diameter of 27,993 have the highest stability.

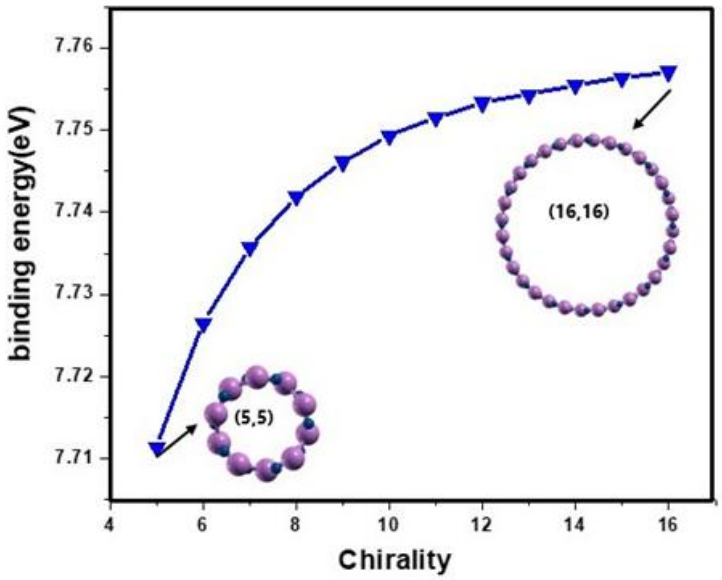

Fig 2. Binding energy of InN nanotube in term of chirality

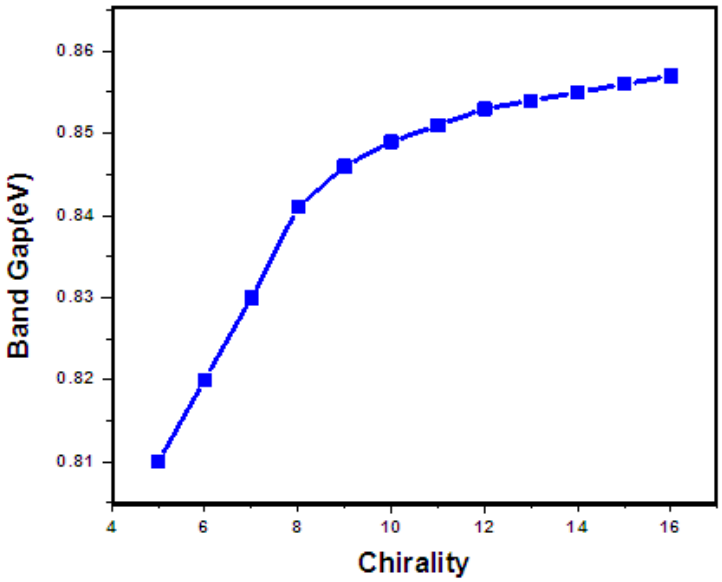

Fig3. Band gaps of InN nanotube in term of chirality

changes of band gap in terms of nanotube diameter are shown in Fig. 3. The results obtained for InN nanotubes are in agreement with previous studies [2].

In this step, we investigated the electronic properties of InN nanotubes. The obtained calculation indicates that all of these nanotubes are semiconductors and have an indirect band gap. The study of the electronic properties of structures shows that all nanotubes are semiconductors with direct band gaps and their band gaps have an increasing trend with increasing diameter of nanotubes, which slows down the process of change in higher diameters. To be able to tune the band gap is important in optoelectronic devices, such as lasers

IV. CONCLUSIONS

In this study, the stability of nanotubes was investigated. We optimized the input parameters and the structure of the studied nanotubes. By calculating the binding energy of systems, it is observed that the armchair nanotubes (16, 16) with a diameter of 27,993 have the highest stability. The

provide a wide range of applications.

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.

and diodes. These results suggest these nanotubes

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