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# Electronic properties of C-doped boron nitride nanotubes studied by first-principles calculations



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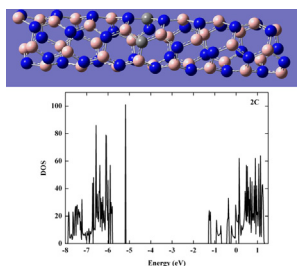
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## HIGHLIGHTS

- The tube diameter of (3,2) C-doped BNNTs is 0.37 nm, the length is 1.9 nm and atoms are seventy-six.
- We use one-dimensional periodic boundary condition in the geometrical structure optimization.
- In the G09, we use the HSE06/6-31G† basis set to calculate the bandgap.

## GRAPHICAL ABSTRACT

The geometry and electronic structure of C-doped BNNTs are investigated using the hybrid Heyd–Scuseria–Ernzerhof. The van Hove singularity (vHs) peaks split in density of states (DOS) The impurity states decrease the bandgap.



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## ABSTRACTS

The geometry and electronic structure of C-doped boron nitride nanotubes (BNNTs) of (3,2) are investigated systematically using the hybrid Heyd–Scuseria–Ernzerhof density functional theory (DFT) to obtain the geometry first. Then the band structure is calculated with the HSE06/6-31G† approach. We find that the geometry changes with the C-doping concentration. The van Hove singularity (vHs) peaks split in density of states (DOS) because of the doping. The impurity states appear in the bandgap region of the host BNNT. The bandgap decreases gradually toward the corresponding single-walled carbon nanotube value. In addition, first, second and third optical transitions decrease with the C-doping increase, changing the BNNTs' optical properties. The HSE06 is reliable for the band structure calculation of BNNT of (3,2) whose diameter is small but the lattice constant is large with a large number of atoms in the unit cell.

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## 1. Introduction

Single wall carbon nanotubes (SWCNTs) have attracted much attention due to their unique physical properties on nano-electronical device, indicators and strong fibers [1–3] since their discovery in 1991 by Iijima [4]. Recently, boron nitride nanotubes (BNNTs) have attracted heavy attention [5–15]. Like the SWCNTs, the boron and nitrogen atom in BNNTs have  $sp^2$  hybridization bonding

similar to the graphite, and BNNTs have single-walled and multi-walled structure. Except the structural similarities between BNNTs and SWCNTs, there are essential differences between them. Contrary to SWCNTs, BNNTs have a uniform electronic bandgap ( $\sim 5.5$  eV) that is independent of the tube diameter and chirality [16,17]; BNNTs are more chemically and thermally stable than SWCNTs, which open promising opportunities for their application in high temperature, high strength fibers, semiconductor, etc. Though people have studied the BNNTs' structure, electrical, and optical properties theoretically with different density functional methods, most of them use pure density functional, which are known to underestimate the bandgaps. Rubio [17] and Blasé [18] calculated the BNNTs theoretically using the

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semi-empirical tight-binding method (TB) and the local density approximation (LDA), respectively. They both found that the BNNTs' bandgap is fixed. Menon et al. [19] investigated the structure of boron nitride nanotubes using a generalized tight-binding molecular dynamics method. It was shown that dynamic relaxation results in a wave-like or 'rippled' surface in which the B atoms moved inward and the N atoms moved outward, reminiscent of the surface relaxation of the III–V semiconductors. Akdim et al. [20] compared the SWCNTs of (6,0)–(9,0) and the BNNTs of (6,0)–(9,0) using the DFT within generalized gradient approximation (GGA), they found that the up-shifts in the value of the radial breathing modes, due to interlude coupling, are small and systematic, about 2% in zigzag nanotubes, and varying from 2% to 7% in armchair tubes, for both materials. Kahaly and Waghmare [21] determined atomic and electronic structures of carbon-doped boron nitride nanotubes using first-principles pseudopotential-based density functional theory calculations. The geometrical structure and bandgap are both calculated with LDA. Zhao and Dai [22] calculated the electronic structures of several zigzag and armchair-carbon-doped boron nitride nanotubes with the B3LYP functional. The influence of different C-doping on the conductivity was also discussed. All their calculations were carried out at the 3-21G basis set level of the B3LYP functional. According to our previous experience [23], the HSE06/6-21G method should be more accurate for the geometrical calculation. The HSE06 [24] is the recommended version of Heyd–Scuseria–Ernzerhof hybrid functional.

In addition, there are admirable physical properties and chemical inertness on BNNTs because of their wide bandgaps. When BNNTs have an impurity, the local geometry will change around the impurity. Meanwhile, the impurity will introduce the additional

states in the band gap, consequently changing the electronic structure of BNNTs. Furthermore, the diameter of (3,2) BNNT is very small usually (about 0.4 nm), we are curious about whether the bandgap of the small diameter nanotubes are same as large diameter nanotubes. Since the carbon has one more electron than boron and one less electron than nitrogen atom, we choose the carbon as the impurity atom to improve the properties of BNNTs. The (3,2) SWCNTs has a small band gap (1.19 eV). We are interested how the band structure evolves from the (3,2) BNNT to the (3,2) SWCNTs, because of the doping concentration. Besides, the local environment effect will be relatively big, which will cause some inaccuracy for a pure DFT or tight-binding method. The pure density functional may not reflect the local environment of the small diameter nanotubes, while the hybrid functional can. Tight-binding method cannot reflect the curvature effect in small diameter nanotubes [17] when calculating the small diameter nanotubes for strong  $\sigma$ – $\pi$  hybridization. And for LDA, it always underestimates the bandgap, whereas the HSE06 improve distinctly in this respect.

We calculated the geometrical structure and bandgap of (3,2) C-doped BNNTs at the HSE06/6-21G level [25]. The HSE06 can predict the geometrical structure calculation accurately with much less resource compared with other hybrid functionals. The band-gap structure is calculated at the HSE06/6-31G† level. We find that the van Hove singularity (vHs) peaks split in density of states (DOS) because of the doping. The impurity states appear in the host bandgap region, while this distance between the two impurity states gradually decreases. The band gap of the doped BNNT decreases gradually at low impurity concentration, and it decreases dramatically at high impurity concentration. The geometry also changes with the doping concentration.

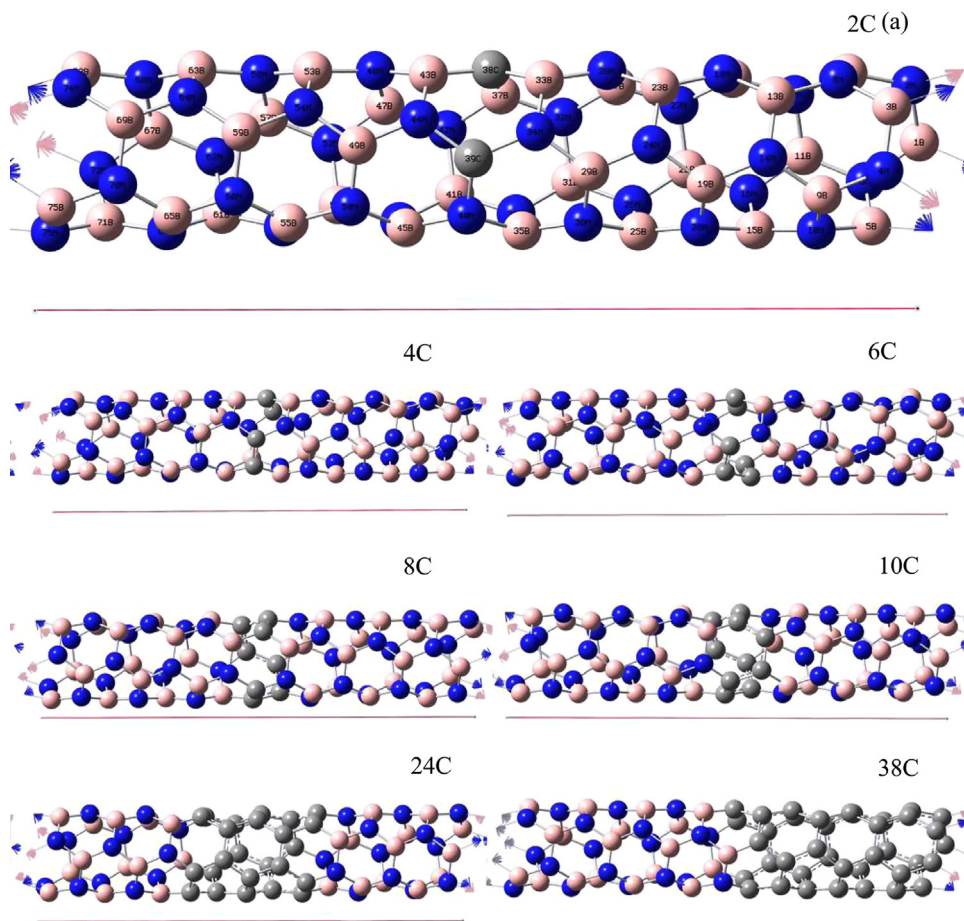


Fig. 1. The model of boron nitride nanotube (3,2) with two, four, six, eight, ten, twenty-four, thirty-eight carbon atoms doped.

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