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Structural and elastic properties characterization of Be and Mg doped boron nitride nanotubes using DFT calculations

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ABSTRACT

Through doping boron nitride nanotubes, their band gaps could be controlled which results in extending the range of their applications particularly in nanosensors. In this article, the structural and elastic properties of Be and Mg doped boron nitride nanotubes with various chiralities are studied based on *ab initio* density functional calculations. In order to perform the density functional theory (DFT) calculations, the exchange correlation of Perdew–Burke–Ernzerhof within the generalized gradient approximation (GGA) framework is employed. It is observed that doping Be and Mg atoms increases the equilibrium strain energy of boron nitride nanotubes. Furthermore, it is found that among all of the considered nanotubes, an increase in the value of Young's modulus of (4, 4) armchair boron nitride nanotube through doping Be atom instead of boron atom is so considerable.

1. Introduction

Boron nitride nanotubes (BNNTs) as the structural analogous of carbon nanotubes (CNTs) are important nanostructures with a wide range of applications. There are many studies on BNNTs and CNTs in the literature (e.g. [1–5]). BNNTs have interesting properties such as high thermal conductivity and impressive mechanical characteristics being more chemically stable than their carbon analogues [6–9].

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In recent years, several studies have been carried out to predict the mechanical properties of boron nitride nanotubes and their wide range of applications. For example, Chopra and Zettl [10] experimentally determined the elastic properties of an individual multi-walled boron nitride nanotube. Suryavanshi and Yu [11] measured the effective elastic modulus of boron nitride nanotubes using the electric-field-induced resonance method inside a transmission electron microscope. Peng et al. [12] studied the elastic properties and electronic structures of single-walled boron nitride nanotubes using the *ab initio* calculations. Verma et al. [13] calculated the elastic properties of boron nitride nanotubes using the Tersoff–Brenner potential. Zhi et al. [14] summarized the developed progresses in chemical functionalization and composite studies of boron nitride nanotubes. Zhukovskii et al. [15] performed *ab initio* simulations on the atomic and electronic structure of boron nitride nanotubes and nanoarches. Zhang et al. [16] reported the stability and electronic structures of boron nitride nanotubes by semiempirical quantum mechanical molecular dynamics simulations and *ab initio* calculations. Ju et al. [17] addressed the effect of uniaxial strain on the electronic properties of zigzag and armchair boron nitride nanotubes by density functional theory (DFT) calculation. Miller and Owens [18] used DFT to investigate the effect of altering the boron/nitrogen ratio and carbon doping on the electronic and magnetic structure of (7, 0) zigzag and (5, 5) armchair boron nitride nanotubes.

Because of considerable surface to volume ratio in nanostructured materials, they can be ideally situated for sensor applications [19,20]. An efficient way to make nanotubes possible to detect several gases is doping them with various foreign atoms [21–23]. Some investigations have been carried out to predict the characteristics of doped boron nitride nanotubes. Batista et al. [24] employed a first-principles formalism to investigate the structural and magnetic properties of iron oxide doped boron nitride nanotubes. Alencar et al. [25] studied the interaction of one iron atom with pristine zigzag boron nitride nanotubes with different diameters using DFT calculations. Zhukovskii et al. [26] calculated the electronic structure of an armchair boron nitride nanotube doped with periodically distributed various atoms. Roknabadi et al. [27] evaluated the band structure of the carbon doped zigzag boron nitride nanotubes using a simple tight-binding model. Peyghan and Noei [28] investigated doping of several alkali and alkaline earth metals into sidewall of an armchair ZnO nanotube employing DFT.

By controlling the level of doping, this chance is available to tune the bandgap of boron nitride nanotubes. As a result, additional theoretical investigations about doping of boron nitride nanotubes can be of great importance. Motivated by this consideration, in the current study, based on the density functional theory calculations, the structural and elastic properties of Be and Mg atoms doped boron nitride nanotubes with different chiralities are predicted. To this end, the Quantum-Espresso code is utilized using GGA.

2. Methodology

In the present study, the exchange correlation of Perdew–Burke–Ernzerhof (PBE) within the GGA framework is employed [29,30]. The Quantum-Espresso code [31] is put to use in order to obtain the elastic properties of Mg and Be doped BNNTs. Also, DFT calculations are carried out through choosing the smallest hexagonal unit cell, as the results have no dependency to the change of unit cell dimension. In addition, Brillouin zone integration is utilized with a Monkhorst–Pack [32] k-point mesh of $1 \times 1 \times 15$. The value of 80 Ry is assumed for the magnitude of cut-off energy of plane wave expansion.

In the present work, the elastic and structural characteristics of Be and Mg atoms doped (n, n) armchair and $(n, 0)$ zigzag boron nitride nanotubes are predicted corresponding to $n = 3, 4, 5$. The ways of doping are to replace the boron or nitrogen atoms with Be and Mg atoms.

3. Results and discussion

3.1. Structural properties

Fig. 1 represents the unit cells of a usual boron nitride nanotube without Be or Mg doped atom and after minimization of energy corresponding to various chiralities. Subsequently, in Fig. 2, the Be and