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Modified (n, 0) BN nanotubes (n = 3–10) by acetic acids: DFT studies

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ABSTRACT

Covalent additions of one acetic acid molecular group to the tips of eight (n, 0) boron nitride nanotubes (n = 3–10) have been investigated by density functional theory (DFT) calculations. The results indicated that the properties of pristine and modified models detect almost similar effects by widening the nanotubes. The values of dipole moments and energy gaps have been increased for wider nanotubes. Comparing to the pristine models, the values of dipole moments and energy gaps show different properties for the models of two types of modifications. The values of binding energies have not been significantly changed for wider nanotubes. The atomic scale properties have been also investigated by computations of quadrupole coupling constants, in which the most significant effects of modifications have been observed for the atoms close to the modified regions. And finally, the properties for carbon atoms of methyl groups and oxygen atoms of carbonyl groups of the acetic acid molecular groups have been notably changed among the investigated modified BNNTs.

1. Introduction

After the pioneering discovery of carbon nanotubes (CNTs), tubular structures of counterparts of boron (B) and nitrogen (N) atoms have been observed as boron nitride nanotubes (BNNTs) by either computations or experiments [1–3]. In contrast with the CNTs, which are hydrophobic materials, the polarity was raised in BNNTs due to different electronegativities of B and N atoms [4,5].

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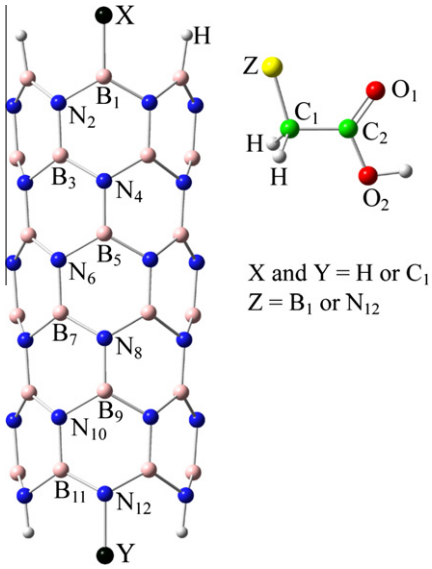

Fig. 1. *X* and *Y* are substituted by H atoms in the original BNNTs. *X* and *Y* are substituted by C_1 and H atoms in the B_C model. *X* and *Y* are substituted by the H and C1 atoms in the N_C model.

Furthermore, the electronic properties of BNNTs are independent of structural factors such as tubular diameters and chiralities whereas the characteristics of CNTs are mainly dependent on the mentioned factors [6,7]. Since the BNNTs are constructed by heteroatoms, the tips of zigzag nanotubes are completely different, in which B-tip and N-tip have been recognized at the tubular ends. Earlier works have indicated that modifications of nanotubes could candidate them for several newer applications based on the types of modifications [8–10]. Up to now, modifications of nanotubes by various biological and synthetic molecules or functional groups have been reported by either computations or experiments [11–14]. The processes of chemical and physical additions of substances to the targeted nanotubes have been also examined to investigate the properties of multi components products [15]. Previous works have indicated that the carboxylated nanotubes could show highlighted properties in comparison with the pristine nanotubes [16].

In this work, we have investigated properties of eight (n, 0) zigzag BNNTs (n = 3–10) in three forms of pristine, B_C, and N_C models (Fig. 1). The B-tip of BNNT is functionalized by an acetic acid molecular group in the B_C model whereas the same functionalization has been taken place for the N-tip of BNNT to make the N_C model. Density functional theory (DFT) calculations have been done to obtain the optimized structures and the corresponding properties. The major goal of this work is determining the effects of acetic acid modifications on the properties of BNNTs. The zigzag BNNTs have been considered to achieve our purposes within this work because they have two independent atomic tips.

2. Computational details

DFT calculations have been performed employing the B3LYP exchange-correlation functional and the 6-31G* standard basis set as implemented in the Gaussian 98 program [17]. The reliabilities of employed level of calculations for the structures of nanotube have been approved by earlier works [16,18]. The models of this work are eight structures of (n, 0) zigzag BNNTs (n = 3–10) in the pristine, B_C, and N_C forms. The pristine models only include the B and N atoms, in which their tips are saturated by the hydrogen atoms to avoid the dangling effects [19,20]. In the B_C and N_C models, one hydrogen atom has been removed from the B-tip and N-tip respectively to make possible the covalent modification of nanotube by the acetic acid group ($-CH_2COOH$) (Fig. 1). It is noted that one hydrogen atom has