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Computational study of edge configuration and the diameter effects on the electrical transport of graphdiyne nanotubes

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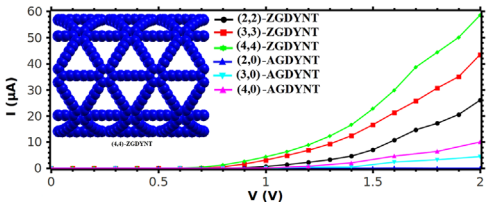
HIGHLIGHTS

- The structural and electronic properties of graphdiyne nanotubes studied via ab initio.
- .The effects of edge configuration and diameter on the electrical properties are determined.
- All the nanotubes exhibited semiconducting behavior with direct transition at Γ point.
- The zigzag nanotubes have smaller band gap and higher current comparing to the armchair.

GRAPHICAL ABSTRACT



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ABSTRACT

In this work, the structural and electronic properties of armchair and zigzag graphdiyne nanotubes (GDYNTs) have been investigated using the density functional theory (DFT). All the nanotubes under investigation exhibited semiconducting behavior. The edge configuration and diameter effects on the electrical transport of graphdiyne nanotubes are studied using non-equilibrium Green's function (NEGF) method. Our results showed that the currents in the zigzag graphdiyne nanotubes are remarkably higher comparing to the armchair nanotubes.

1. Introduction

During the past two decades, organic materials have been recognized as promising candidates to be used in fabricating new generation of electronic and optoelectronic devices. Among these materials, carbon-rich molecules have attracted much more attentions for using in nanotechnology and the related area. However, the new carbon structures are still under consideration [1–15].

Graphdiyne (GDY) which was first predicted by Haley et al. in 1997 belongs to the graphyne family [16]. Graphdiyne possesses both sp and sp^2-hybridized carbon atoms. The sp^2-hybridized carbon atoms create hexagonal rings, and are linked by diacetylenic linkages which consist of sp-hybridized carbon atoms [17–20]. Graphdiyne is predicted to be the most stable among the various diacetylenic non-natural carbon allotropes which have been studied so far [21,22].

Graphdiyne nanotubes were developed for the first time during 2003–2004, by rolling graphdiyne sheets to make seamless cylinders [23]. Ten years later, Li et al. reported the preparation of graphdiyne nanotube arrays through association of a template technique and catalyzed cross-coupling reaction [24]. Their results showed that GDYNT arrays have excellent field emission properties. GDYNTs were synthesized by this method exhibiting a reduced value of work function and showed to be more stable than carbon nanotubes.

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However, many properties of graphdiyne nanotubes are still remained unknown. To our knowledge, only recently, a single-layer sheet and (3, 3) nanotube of graphdiyne have been studied by Jalili et al., in 2015, theoretically [25]. Their results showed that the charge carrier mobility of the graphdiyne nanotube is higher than both graphdiyne sheet and the carbon nanotube.

In this work, first-principle calculations were employed to investigate the structural and electronic properties of armchair and zigzag graphdiyne nanotubes having different diameters. The effects of edge configuration and diameter on their electrical transport properties are also determined, which up to our knowledge have not already been studied.

2. Computational method

A single-walled carbon nanotube (CNT) is formed by rolling a graphene sheet to make a seamless cylinder. In the same way, GDYNT can be formed by rolling a graphdiyne sheet. As shown in Fig. 1, the nomenclature (n, m) can also be employed for GDYNTs, which (n, n) and (n, 0) represent zigzag and armchair GDYNTs, respectively [26]. These two types of graphdiyne nanotubes, with different diameters, are studied in the present work. The diameter of graphdiyne nanotube is given by $d=\frac{a}{\pi}\sqrt{n^2+nm+m^2}$, where a is the lattice constant of the graphdiyne sheet [27]. The following steps were performed to obtain the nanotube's coordinates:

1. Coordinates of the zigzag unit cell (x, y), which is shown by red lines in Fig. 1, were calculated manually. The results are given in Table 1. The coordinates of the armchair unit cell were obtained by the exchange of x and y.
2. By using the following formula, the unit cell of the sheet was converted to a cylinder:

$$x' = r\ \cos\left(\frac{x}{r}\right) y' = r\ \sin\left(\frac{x}{r}\right) z' = y \tag{1}$$

where r is the radius of the tube.

3. The other coordinates were obtained using

$$x' = r\ \cos\left(\theta' + \frac{x}{r}\right) y' = r\ \sin\left(\theta' + \frac{x}{r}\right) z' = y \tag{2}$$

where $\theta' = 2\pi/n$.

The geometry relaxation and electronic structure calculations

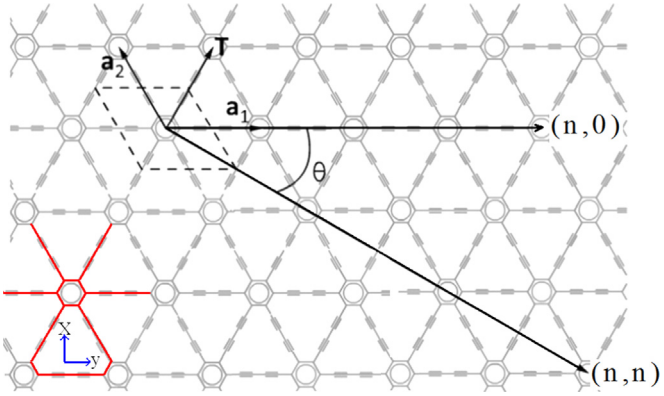

Fig. 1. Chiral and transition vectors for zigzag and armchair graphdiyne nanotubes. The rhombus drawn with dashed lines represents the unit cell. The unit cell of zigzag graphdiyne nanotube was shown by red lines at the bottom left. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1.
Coordinates of the unit cell of zigzag Graphdiyne nanotubes.

	x	y
1	0.7	1.415
2	0.7	2.815
3	0.7	4.045
4	0.7	5.375
5	0.7	6.605
6	0.7	8.005
7	1.938	0.7
8	3.15	1.4
9	4.216	2.015
10	5.367	2.68
11	6.433	3.295
12	7.646	3.995
13	7.646	5.425
14	6.433	6.125
15	5.367	6.74
16	4.216	7.405
17	3.15	8.02
18	1.938	8.72
19	15.82905	0.7
20	14.621	1.4
21	13.555	2.015
22	12.404	2.68
23	11.338	3.295
24	10.126	3.995
25	10.126	5.425
26	11.338	6.125
27	12.404	6.74
28	13.555	7.405
29	14.621	8.02
30	15.82905	8.72
31	8.884	0.745
32	8.884	1.975
33	8.884	3.375
34	8.884	6.045
35	8.884	7.445
36	8.884	8.675

were performed using linear combination of atomic orbitals (LCAO) as implemented in the SIESTA package [28]. The exchange-correlation functional of the electrons was described by the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE). A double-zeta polarized basis set (DZP) was adopted for all structures. An energy cutoff of 200 Ry was chosen and the vacuum layers were set 10 Angstrom in the non-periodic directions to prevent the interaction of adjacent tubes. The Brillouin zone k-point sampling was $1 \times 1 \times 5$ for all the nanotubes, based on the Monkhorst-Pack method. The nanotubes were relaxed until the residual forces on each atom were reached below 0.01 eV/Å. The temperature was set as 300 K for all calculations.

The transport properties of graphdiyne nanotubes were computed using standard DFT calculations combined with non-equilibrium Green's functional techniques, which were carried out in the TranMain code of OpenMX package [29]. For the NEGF formalism, the system was divided in three parts: the left electrode (L), the scattering region (CC) and the right electrode (R). It was assumed that the electrodes were coupled only with the scattering region, but not with each other. Conduction in 1D system could be viewed as a transmission problem. The electric current through the scattering region at a finite bias voltage (V) was evaluated using the Landauer -Buttiker formula:

$$I(V) = \frac{2e^2}{h} \int_{-\infty}^{+\infty} \left\{ T(E, V)\left[f\left(E,\mu_L\right) - f\left(E,\mu_R\right)\right]\right\} dE \tag{3}$$

where e is the electron charge, h is Planck's constant, f is the Fermi