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# Effect of boron and nitrogen doping on electro-optical properties of armchair and zigzag graphyne nanoribbons

M. Jafari [a,*], M. Asadpour [a], N. Ashtari Majelan [b], M. Faghihnasiri [c]

[a] Department of Physics, K.N. Toosi University of Technology, Tehran, Iran
[b] Islamic Azad University, Karaj Branch, Iran
[c] Departments of Physics, University of Guilan, Rasht, Iran

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ABSTRACT

In this paper, electrical and optical properties of zigzag and armchair graphyne nanoribbon (GNR) doped with nitrogen and boron were studied in two different atom hybridization. All the calculations were based on density functional theory (DFT). The results showed that both structures (armchair and zigzag) had a band gap of about 1 (eV); therefore, they were semiconductor. As expected, by doping impurity on these structures in eight new states of GNR, the band gap was reduced. Effects of n-type and p-type impurity on nanostructures were investigated and it was found that position of impurity had a main role in electronic and optical properties, particularly in optical absorption and reflection coefficients, energy loss function and dielectric function. Moreover, formation energy of the structures that were doped by impure atoms was also calculated. The results showed that, in zigzag and armchair GNRs, the lowest formation energy was related to doping of boron in SP2 hybridization.



## 1. Introduction

Carbon nanostructures exhibit various electrical and optical properties and some of them have been studied thus far. One of these structures is graphdyne, which is a graphene-like structure with triple carbon–carbon bond around carbon rings [1,2]. Graphyne has one triple carbon–carbon bond between two nearest-neighbor carbon rings [3–6].

Baughman et al. proposed graphyne structures [1]. In the mentioned study, this structure was predicted to have crystalline state formation energy of 12.4 kcal/mol carbon that seemed to be much lower than any carbon phase containing acetylenic groups as a major structural component [1]. Although graphyne has similar mechanical properties to graphite, it is predicted to be a large band gap semiconductor (Eg = 1.2 eV) than a metal or semimetal [1–7].

Graphyne is the name of the lowest-energy member of a family of carbon phases, which consists of planar molecular sheets that contain only SP and SP2 carbon atoms. The presence of acetylenic groups in these structures introduces a rich variety of optical and electronic properties which are completely different from those of ordinary carbon nanotubes [7].

Nanoribbons are two-dimensional sheets with wide applications owing to their various widths and edges [8]. GNRs are useful for gas absorption and impurity doping to fabricate n-doping or p-doping semiconductors. Edge of these structures is saturated with hydrogen atoms.

Synthesis of graphyne structures such as graphyne sheets and nano tubes is done by chemical vapor deposition [2,9–17].

Li et al. [17] successfully prepared a new carbon allotrope-graphdiyne film (GDF) on the surface of copper via a cross-coupling reaction using hexaethynyl benzene. This film demonstrated excellent semiconducting properties.

Graphene as a two-dimensional (2D) carbon material is a single atom-thick flat sheet. It consists of carbon atoms which are arranged in a honeycomb lattice. Owing to unusual electronic and magnetic properties, graphene is considered a revolutionary material for various devices for future generations of high-speed electronics, radio frequency logic devices, thermally and electrically conductive reinforced composites, sensors, transparent electrodes and so on [18].

## 2. Method and calculation specifications

All the calculations were based on density functional theory (DFT) and performed using plane wave and quantum espresso code [19]. The simulation was carried out with a unit cell including 96 atoms (16 hydrogen and 80 carbon) for both zigzag and armchair nanoribbons. The structures were optimized by local density approximation (LDA). This approximation has been used in [8,18,20,21]. The brillouin zone was formed by $1 \times 10 \times 1$ k point for nscf and $1 \times 5 \times 1$ k point for scf calculation. Vacuum of about

* Corresponding author. Tel.: +98 2122853308; fax: +98 2122853650.
*E-mail address:* jafari@kntu.ac.ir (M. Jafari).

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**Table 1**
The optimized bond length.

| Label (Å) | Zigzag | Armchair | Zig-B-sp | Zig-B-sp2 | Zig-N-sp | Zig-N-sp2 | Arm-B-sp | Arm-B-sp2 | Arm-N-sp | Arm-N-sp2 |
|---|---|---|---|---|---|---|---|---|---|---|
| A | 1.42 | 1.42 | 1.45 | 1.43 | 1.45 | 1.44 | 1.43 | 1.55 | 1.44 | 1.43 |
| B | 1.42 | 1.42 | 1.45 | 1.43 | 1.45 | 1.44 | 1.43 | 1.54 | 1.43 | 1.43 |
| C | 1.41 | 1.41 | 1.37 | 1.40 | 1.39 | 1.41 | 1.50 | 1.50 | 1.35 | 1.35 |
| D | 1.21 | 1.21 | 1.34 | 1.23 | 1.19 | 1.21 | 1.35 | 1.23 | 1.18 | 1.22 |
| E | 1.41 | 1.41 | 1.50 | 1.50 | 1.36 | 1.35 | 1.37 | 1.40 | 1.38 | 1.41 |
| F | 1.42 | 1.42 | 1.42 | 1.53 | 1.44 | 1.43 | 1.45 | 1.43 | 1.45 | 1.43 |
| G | 1.42 | 1.42 | 1.43 | 1.54 | 1.44 | 1.43 | 1.45 | 1.43 | 1.45 | 1.43 |

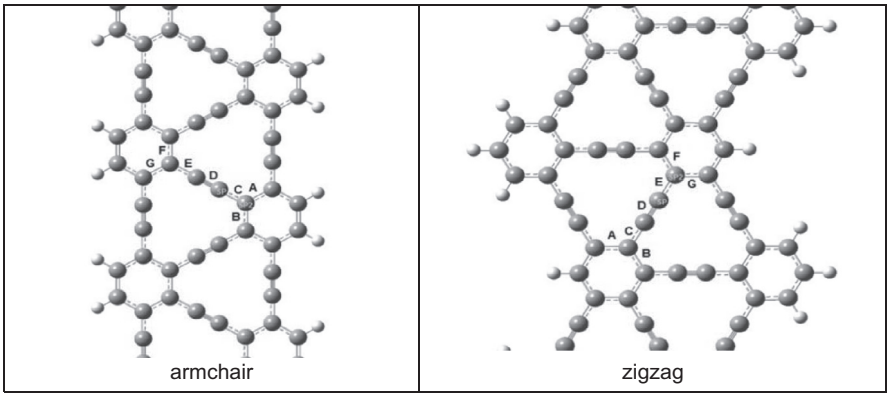


**Fig. 1.** Label of bonds of zigzag and armchair structures.

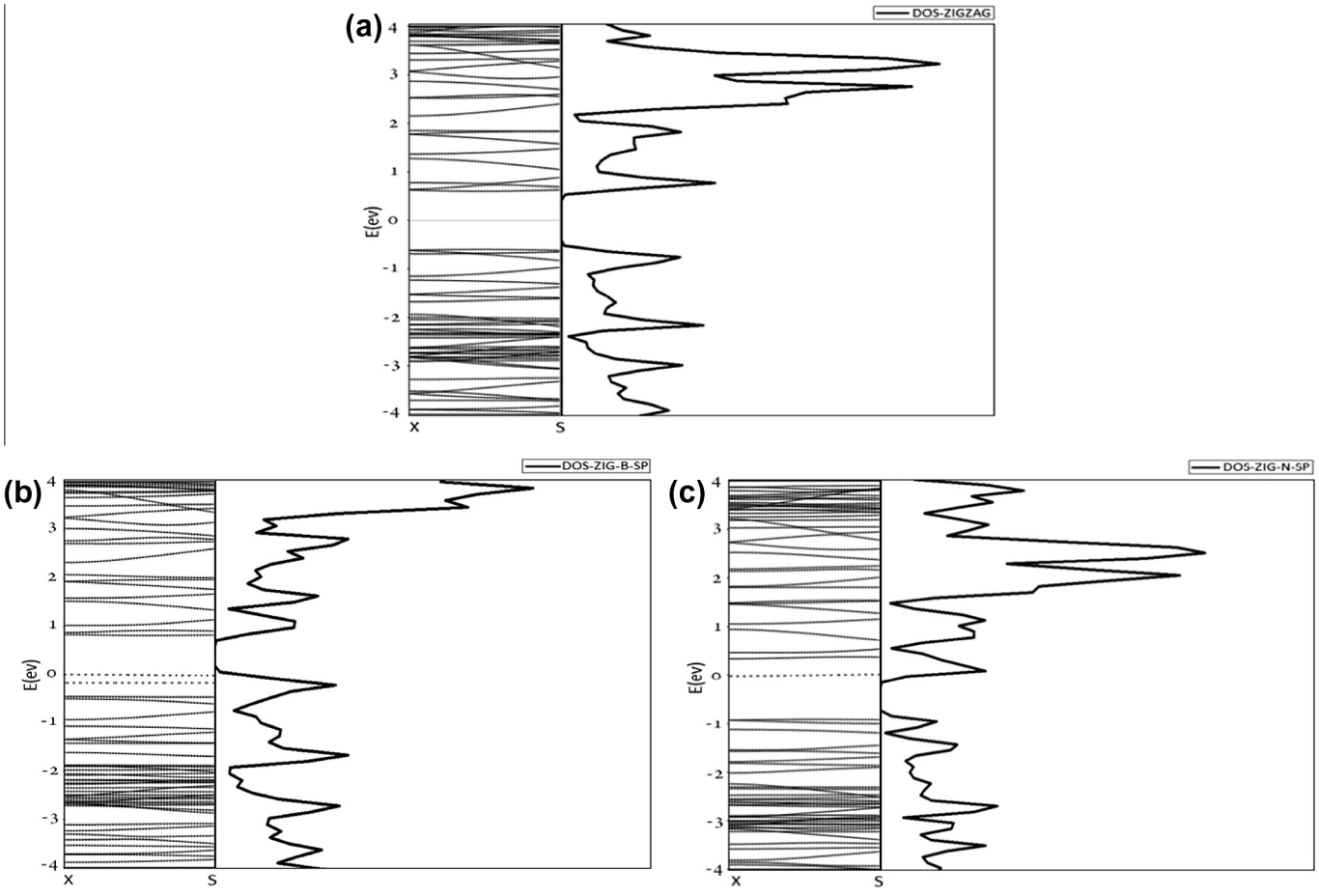


**Fig. 2.** Density of states and band structure of zigzag GNRs: (a) zigzag, (b) boron doping in sp position, and (c) nitrogen doping in sp position.