Organic Electronics xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Organic Electronics

journal homepage: www.elsevier.com/locate/orgel

Armchair α-graphyne nanoribbons as negative differential resistance devices: Induced by nitrogen doping

Amin Mohammadi[a], Esmaeil Zaminpayma[b,*]

[a] Department of Electrical, Biomedical, and Mechatronics Engineering, Qazvin Branch, Islamic Azad University, Iran
[b] Department of Physics, Qazvin Branch, Islamic Azad University, Qazvin, Iran

ARTICLE INFO

Keywords:
Armchair α-graphyne nanoribbon
Nitrogen
Doping
Electronic transport properties
Negative differential resistance

ABSTRACT

Using non-equilibrium Green's functions (NEGF) in combination with tight-binding (TB) model, the electronic transport properties of pristine and nitrogen (N) doped armchair α-graphyne nanoribbons (A-α-GYNRs) are studied under finite bias. Initially, we have calculated the total energy in order to find the most stable place for N atom. Then we have investigated the effect of width (W) and length (L) of the ribbon and also the position (edge and center of the ribbon) and concentration of doping on the electronic transport properties. Our results reveal that, doping changes the semiconducting behavior of $3n$ and $3n+1$ A-α-GYNRs to semi metallic. Moreover, it is observed that the electronic transport properties are more affected by central doping rather than the edge doping. Interestingly, both edge and central doped ribbons show negative differential resistance (NDR) in all widths. Our results show that doping concentration and the NDR are inversely proportional to each other. We have also found that, as the length of the central region of the device gets longer, the NDR reaches up to 159. Transmission spectrum, bandstructure of the electrodes, Bloch wave functions and density of states (DOS) are analyzed subsequently to more elucidate the electronic transport properties. Our findings could be used to develop the nano-scale NDR devices.

1. Introduction

Two-dimensional (2D) carbon based nano-materials have attracted tremendous attention due to their remarkable electronic properties. Carbon atoms can form different hybridized states (sp, sp^2 and sp^3) and thus an inexhaustible reservoir of high-performance synthetic carbon allotropes (nanotubes, graphene, graphdiyne, etc.) were prepared or predicted theoretically [1–4].

Graphyne (GY) which has the same symmetry as graphene is predicted by Baughman et al. [5]. GY is a family of carbon allotropes which consists both sp and sp^2 hybridizations, modified by inserting a carbon triple bond (–C≡C–) into the C–C bonds of graphene [6]. Although, in the case of graphyne just some finite-size flake building blocks have been synthesized [7] and single sheet of graphyne has still not been available, in 2010 graphdiyne (which is a graphyne substructure) was successfully synthesized on copper substrate and a semiconducting behavior was reported [8]. This experimental progress shows that GY will hopefully be obtained in future. The presence of acetylene linkages introduces a rich variety of properties for GY, including extreme hardness, high thermal resistance, good chemical stability, large surface area, high electrical conductivity, etc [9–14]. According to sp and sp^2 hybridization proportions and their arrangement in the lattice structure, α-graphyne, β-graphyne and γ-graphyne are formed [15]. α-graphyne and β-graphyne exhibit Dirac cone band structures, however, the γ-graphyne is predicted to be semiconducting with a direct band gap at the M point [16]. Due to its graphene like structure and symmetry, we have chosen α-graphyne for further studies.

Alike graphene, cutting α-graphyne into quasi 1D nanoribbons (α-GYNRs), is a way to adjust its band gap (B_g) [17]. According to their edge pattern, α-GYNRs divide into two main categories: 1) A-α-GYNRs and 2) zigzag (Z-α-GYNRs) [18]. All of A-αGYNRs are nonmagnetic, and B_g oscillates with a period of three when the ribbon width increases, while the Z-α-GYNRs are zero gap and have a stable antiferromagnetic configuration [19,20].

Introducing impurities is another way to adjust the electronic properties of carbon nano materials. Although experimental and theoretical studies have been conducted on doped α-GYNRs, but they mostly focus on doped Z-α-GYNRs and little information about doped A-α-GYNRs has been reported [19–24]. Mingjun Li et al. [19]. have studied Z-α-GYNRs passivated with 3d transition-metal atoms at one of the ribbon edge. They found half-metallic behavior in response to the Fe-, Co- and Ni-doping at the edge of Z-α-GYNRs and also a large spin

* Corresponding author. Tel.: +982833665275.
E-mail addresses: zaminpayma@qiau.ac.ir, esi.zamin@gmail.com (E. Zaminpayma).

https://doi.org/10.1016/j.orgel.2018.06.012
Received 24 March 2018; Received in revised form 16 May 2018; Accepted 9 June 2018

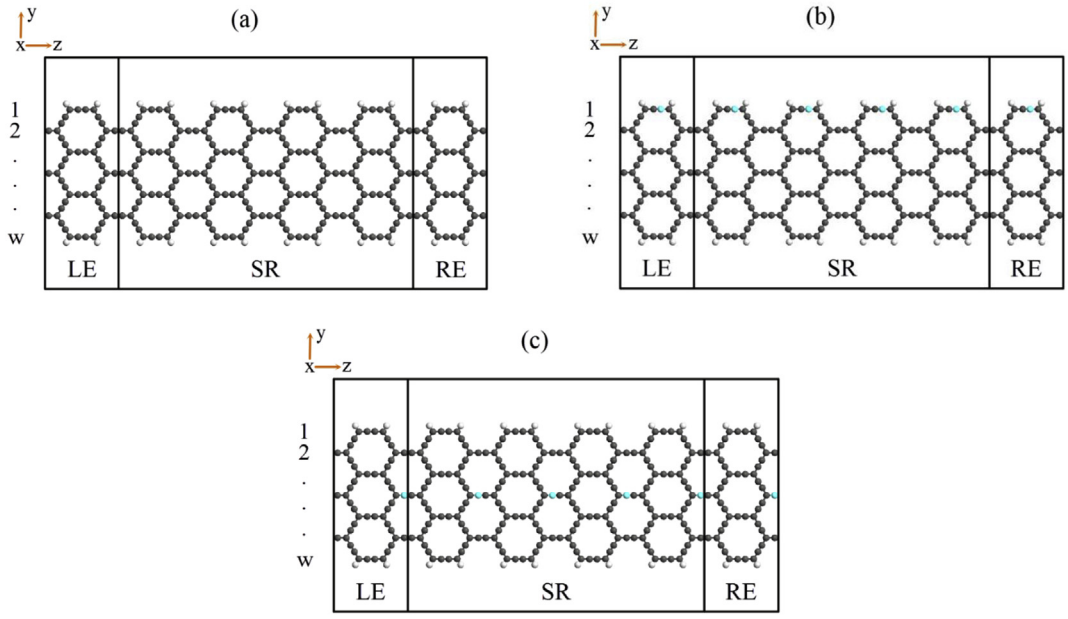

Fig. 1. The optimized structure of devices based on A-α-GYNR. (a) Pristine (P) model, (b) Edge doped (E) model, (c) central doped model. In (a–c) $L = 4$ UC while W changes from 6 to 8. The doping atoms are nitrogen and the concentration of doping is about 1.92%. The vacuum pad along x and y directions are 25 and 65 Å, respectively.

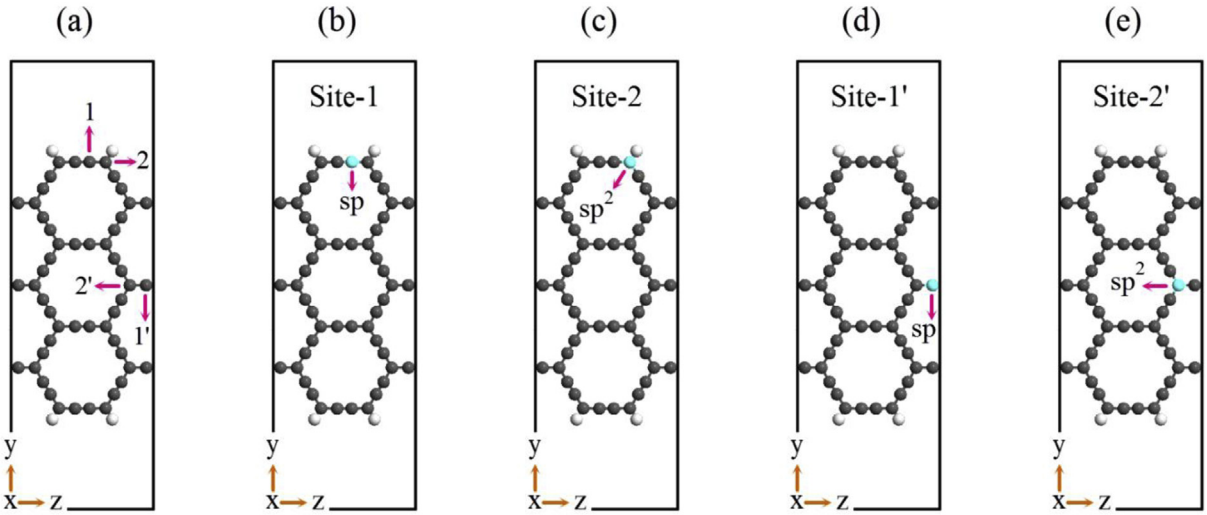

Fig. 2. Schematic representation of (a) doping sites in a unit cell, (b, c) edge doped and (d, f) center doped A-α-GYNR unit cell. The most stable place for nitrogen atom is site-1 (*sp*) at the edge, and site-1′ (*sp*) in the center of the ribbon.

Table 1
Total energy of A-α-GYNR UCs with central or edge N doping at site −1, −2, −1′ and -2′.

N position	Total Energy (eV)			
	Edge		Center	
W	Site-1 (sp)	Site-2 (sp^2)	Site-1′ (sp)	Site-2′ (sp^2)
6	−2090.399	−2089.456	−2090.285	−2088.808
7	−2459.940	−2458.989	−2459.888	−2458.404
8	−2829.471	−2828.518	−2829.408	−2827.923

polarization on currents. Dan Zhang et al. [21]. have investigated the stability and spin-resolved electronic transport properties of Z-α-GYNRs with symmetric and asymmetric edge fluorinations. They have shown that edge fluorination can enhance the stability of Z-α-GYNRs. Ming-Xing Zhai et al. [22] have observed that magnetoresistance can be manipulated in a wide range by the dopants on the edges of Z-α-GYNRs. Sunkyung Kim et al. [6]. have seen that the structural, electronic, and magnetic properties of graphyne were changed according to the dopant