Electronic properties of α-graphyne nanoribbons under the electric field effect

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HIGHLIGHTS

- A tight binding study of α-graphyne nanoribbons is presented.
- We study the role of an external electric field on the electronic structure.
- The electric field tunes the electronic band gap.

GRAPHICAL ABSTRACT

We study the electronic structure of armchair and zigzag α-graphyne nanoribbon in the presence of an external electric field.
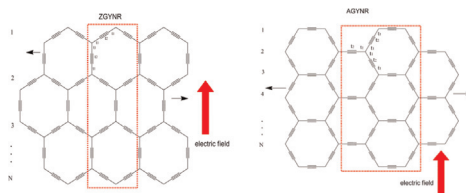
ABSTRACT

In this paper, we investigate the electronic structure of both armchair and zigzag α-graphyne nanoribbons. We use a simple tight binding model to study the variation of the electronic band gap in α-graphyne nanoribbon. The effects of ribbon width, transverse electric field and edge shape on the electronic structure have been studied. Our results show that in the absence of external electric field, zigzag α-graphyne nanoribbons are semimetal and the electronic band gap in armchair α-graphyne nanoribbon oscillates and decreases with ribbon's width. By applying an external electric field the band gap in the electronic structure of zigzag α-graphyne nanoribbon opens and oscillates with ribbon width and electric field magnitude. Also the band gap of armchair α-graphyne nanoribbon decreases in low electric field, but it has an oscillatory growth behavior for high strength of external electric field.

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1. Introduction

In the last few years, researchers have shown a keen interest in the two dimensional carbon nanostructures than graphene. At the first time Baughmanet et. al, introduced the family of graphyne and graphidyne structures [1]. It is well known that carbon atoms hybrid in diamond is sp^3 and concurrently sp^2 in graphene. But in graphyne and graphidyne it can be sp^2 or sp hybrids. Moreover graphyne includes some different structures such as α, β, γ,… that could be formed by replacing c(sp^2)-c(sp^2) with c(sp^2)-c(sp)-c(sp)-c(sp^2) linkages [2]. Until now some various structural, mechanical [3–5],

thermal and optical [4] properties of α-graphyne have been investigated for sheet [6–8], nanotube [9,10] and nanoribbon [11] geometries. Ab-initio and tight binding calculations have shown that the band structure of α-graphyne contains a Dirac point like graphene [6–8,11–17] and thus it could be an excellent competitor for graphene [18]. Although there is no report on graphyne synthesis, there are a few theoretical works that predict the electronic properties of graphyne. Graphyne nanoribbons (GYNR) like graphene nanoribbons (GNR) can be categorized in two different types based on their edge cutting shape called armchair and zigzag nanoribbons. Since the possibility of using two dimensional carbon nanostructures in nanoelectronic applications depends on their electronic properties [19–21], Different methods like applying external transverse electric fields [22] have been introduced to modulate their electronic properties.

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In this paper, in order to modulate the electronic properties of armchair and zigzag αGYNR the influence of transverse electric field and ribbon width on both armchair and zigzag αGYNRs band gap have been studied by using a single π-orbital tight binding model.

2. Method

The unit cell of armchair and zigzag GYNR are shown in Fig. 1. In addition ribbon's width is numbered and an external electric field is applied in the specified direction in this figure. A π-electronic tight binding model is employed in which only the p_z atomic orbitals are considered in the total Hamiltonian. In the real space the total Hamiltonian of structure can be written as $H = \Sigma_i \varepsilon_i \ C_i^\dagger C_i + \Sigma_{\langle i,j \rangle} t_{i,j} \ [C_i^\dagger C_j + C_j^\dagger C_i]$, where ε_i is the atomic on-site energy and t_{ij} is the hopping energy between nearest neighbors. The operator C_i^+ (C_i) creates (annihilates) a π electron at the i-th site of GYNR. Due to the infinite size of the ribbon in real space the above Hamiltonian should be transformed into the imaginary k-space. For the whole ribbon, we consider a periodic unit cell with lattice vector R in one dimension. After a Fourier transform to the k-space, the total Hamiltonian in the momentum space can be written as [23]

$$H = \sum_{i,k} \varepsilon_i C_{i,k}^\dagger C_{i,k} + \sum_{i,j,k,l} (t_{i,j} e^{ik(R+d_k-d_l)} C_{i,k}^\dagger C_{j,l} + t_{j,i} e^{ik(R+d_l-d_k)} C_{j,l}^\dagger C_{i,k}),$$

where the $C_{i,k}^\dagger (C_{i,k})$ is the creation (annihilation) operator in the k-space for the π electron of GYNR. The total Hamiltonian in the momentum space can be written as, $N \times N$ matrix that N is the number of π orbitals in the unit cell and depends on the width of ribbon. The diagonalization of the Hamiltonian matrix leads to eigenvalues for different k-point in the first Brillouin zone. By applying the external electric field shown in Fig. 1, an electric potential difference on the edges of nanoribbons affects different properties of the nanostructure. In the presence of external electric field, the on-site energy of each carbon atom is modified according to its relative position. In other words, an electric field changes the on-site energy of different atomic positions with the on-site electronic potential. Previous works indicate that there are two different kinds of hopping energy t_1 and t_2 due to the existence of single and triple bonds as well as different bond

length [12,24]. Here we assume that the external electric field has not influence on the hopping energy of carbon atoms.

3. Results and discussion

The band structure for armchair αGYNRs are calculated for $N=16$, 17 and 18 as shown in Fig. 2. The ribbons with $N=16$, 18 are semiconductor and $N=17$ is semimetal. In the absence of external transverse electric field, the band gap is in the Γ point of the brilluin zone. Fig. 3 shows the variation of armchair αGYNRs band gaps for different widths in the absence of an external electric field which indicates the oscillatory behavior for the band gap as a function of ribbon width as reported in the case of GNRs [25].

Fig. 3 is in a good agreement with the ab-initio results. The αGYNRs can be categorized in three different groups based on their width ($N=3p$, $3p+1$, $3p+2$). For $N=3p+2$ band gap will be approximately zero and for $N=3p$, $3p+1$ we fit the band gap to $E_g = a(w/w_0)^{-b} + c$ for specific values of a, b and $w_0 = 1$ Å. We add a constant c to the previous equation to obtain a better fit as is proposed in Ref. [11]. Table 1 contains different parameters of the fitting equation. For tuning the band gap, we applied an external electric field perpendicular to the ribbon width. The effect of electric field on armchair α-graphyne ribbons band gap is presented in Fig. 4.

By applying the external electric field, unlike the case $E=0$, for small ribbons $N \leq 14$ there is no specific order in variation of the band gap. But for wider ribbons, the band gap fluctuation depends on the ribbon width so that for ribbons with $N=$odd and $N=$even, the electronic band gap is unchanged and has separate constant values. Furthermore, for $N > 14$ and in the presence of the field, the band gap increases which is an interesting phenomenon for applications in nanoelectronics. Fig. 5 shows the band structure of zigzag α-graphyne nanoribbon (ZαGYNR) with $N=9$, 10 and 11 in the absence and presence of external electric field. If one includes the electron–electron interaction in the Hubbard term, the localized states in the Fermi level are split and a net spin density on the zigzag edge of nanostructure will be produced. Here, for more simplicity, we ignore the interaction between electrons and so we observe the zero band gap in zigzag αGYNRs. Also density functional theory confirms the finite band gap and localized magnetic moments on the zigzag edge of GYNRs ribbons [24].
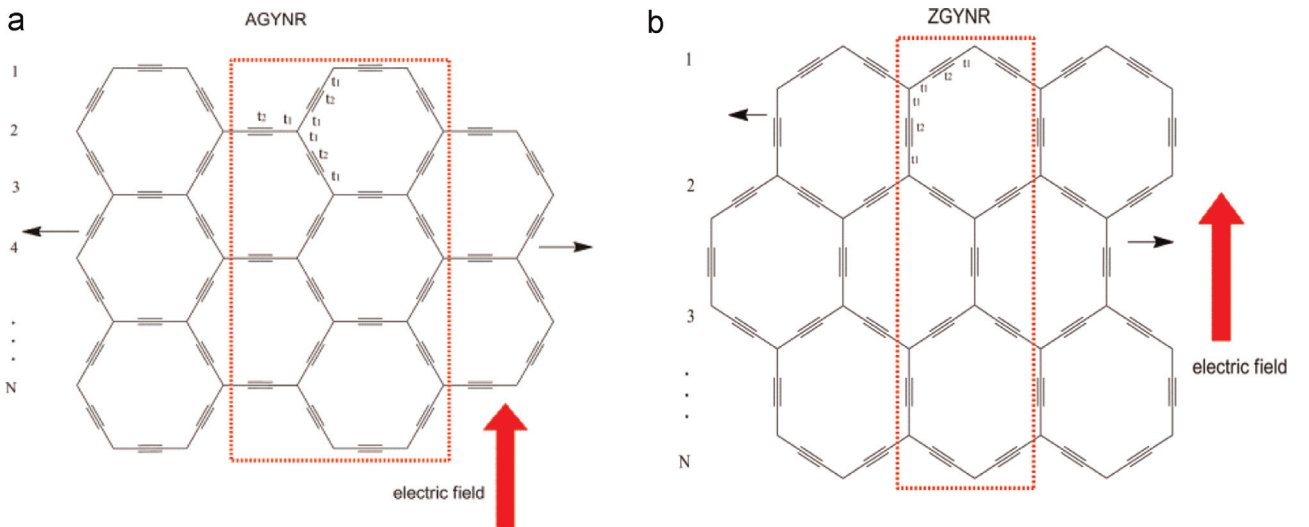

Fig. 1. (a) Armchair and (b) zigzag graphyne nanoribbone. Unit cells and external electric field are shown in the figure.

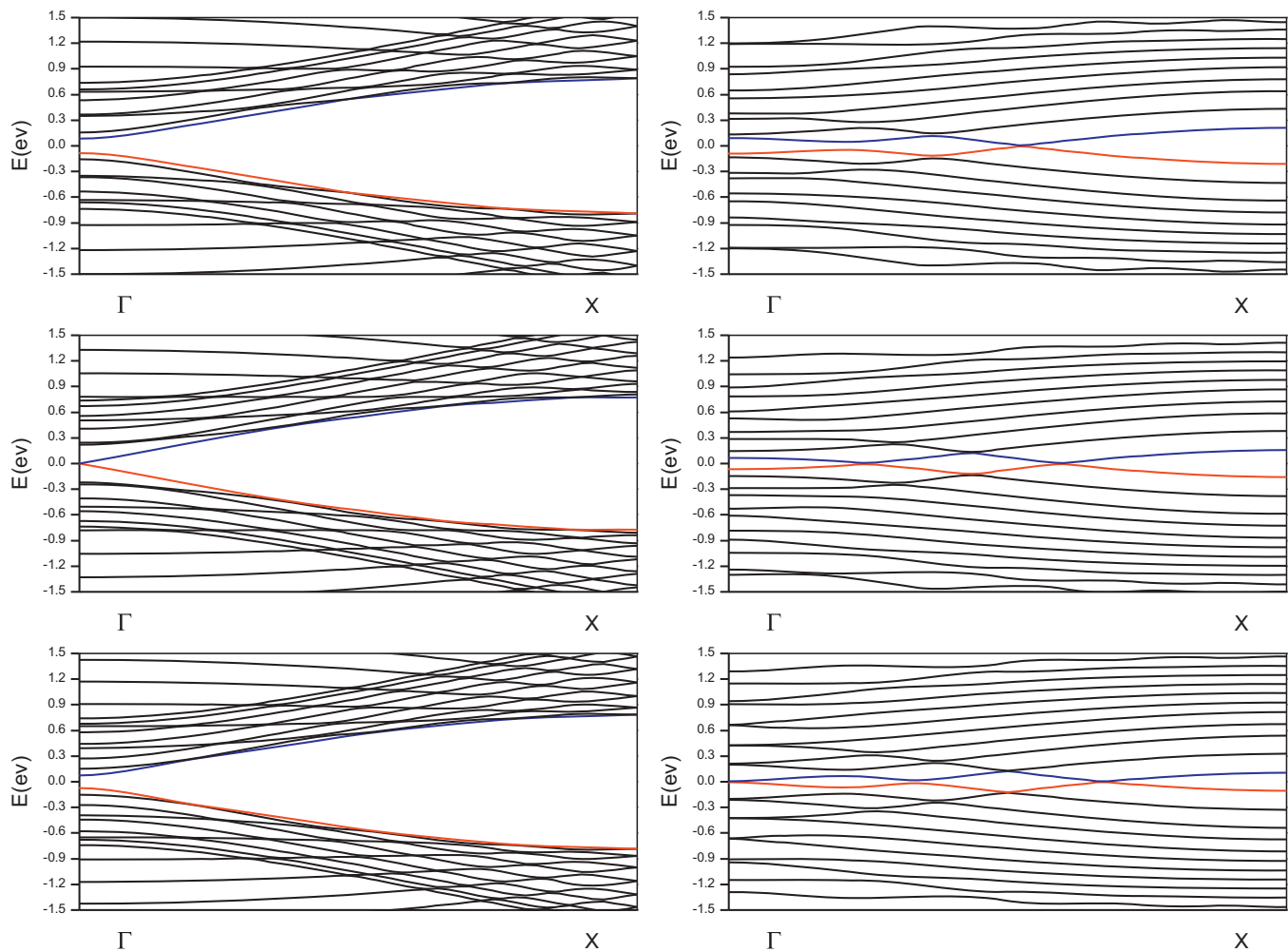**Fig. 2.** The band structure of $N=16$, 17 and 18 armchair αGYNRs in the absence (left) and presence (right) of an external electric field (0.03 eV/Å).
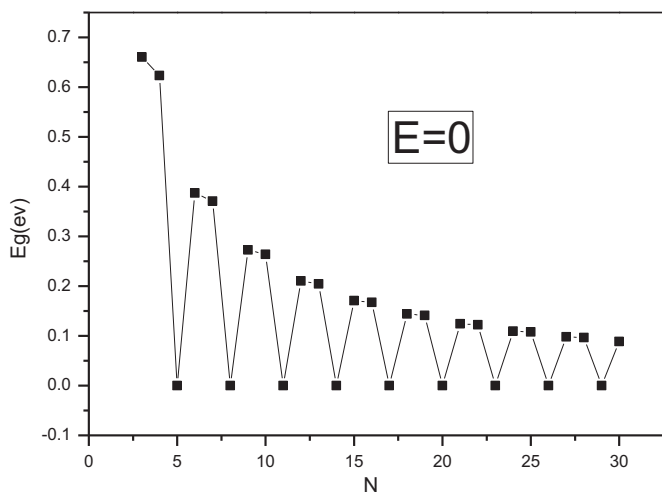

Fig. 3. Band gap of armchair αGYNR versus width in the absence of an electric field.

Table 1
Fitting parameters for band gap of armchair αGYNRs in the absence of a potential difference.

Parameter	$N=3p$	$N=3p+1$
a	2.03	3.4
b	0.47	0.68
c	-0.14	-0.05

band gap as a function of ribbon's width for different electric field strengths. The band gap oscillates with ribbon's width for different electric fields. For ribbons with $N \geq 13$ it is approximately constant for both $N=$odd and $N=$even numbers. Another salient outcome is that for ribbons with $N=$even, the band gap is less than $N=$odd ribbons. The effect of external electric field strength on the band gap of some ZαGYNRs with different widths is shown in Fig. 7. Generally armchair nanoribbons with different widths have an oscillatory behavior as a function of field strength. By increasing the ribbon width, the electric potential difference on the both sides of ribbon increases. As a result, by increasing the external electric field up to 0.03 eV/Å the band gap increases, and after the critical field, it decreases. This figure demonstrates that generally for wider ribbons the electronic band gap decreases and by applying an external electric field, the band gap has an oscillatory
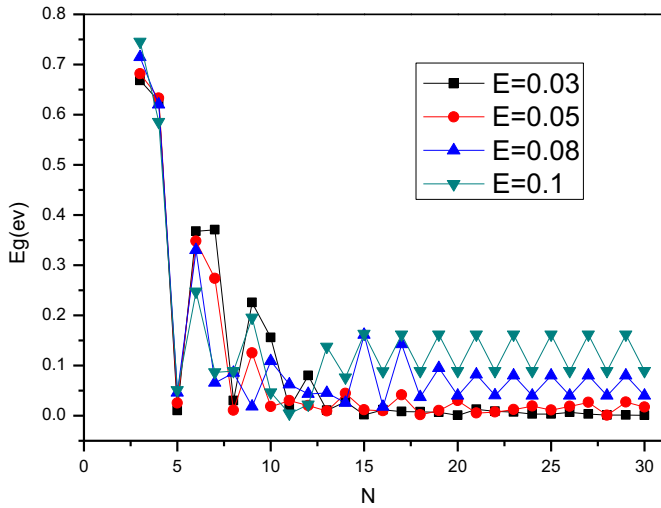
In the absence of an electric field the ZαGYNR is a semimetal and the electronic band gap is approximately zero. However, by applying the external electric field along the ribbon' width, the electronic band gap is opened. Fig. 6 illustrates the variation of

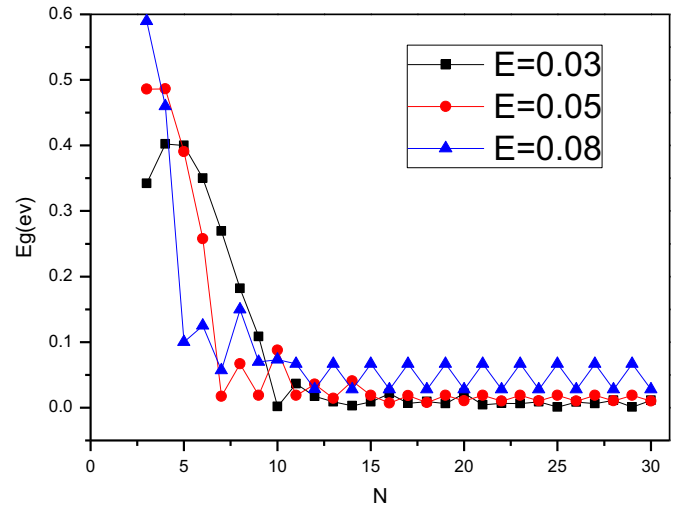**Fig. 4.** Armchair αGYNR band gap versus width and electric field magnitude.

Fig. 6. Zigzag αGYNR band gap versus width for different values of the electric field.

behavior. In the Fig. 8, the variation of the band gap in the presence of the external electric field for different ribbon widths is shown. Similar to ZαGYNR the results show that generally band gap decreases as the ribbon's width increases. Also for an external electric field between 0.02 and 0.05 eV/Å the electronic band gap is minimum.

4. Conclusion

In this paper, we studied the effects of electric field and ribbon's width on the AαGYNR and ZαGYNR band gap using a simple π-electronic tight binding model. For more simplicity, we neglected the effect of electric field on hopping energy. Our results
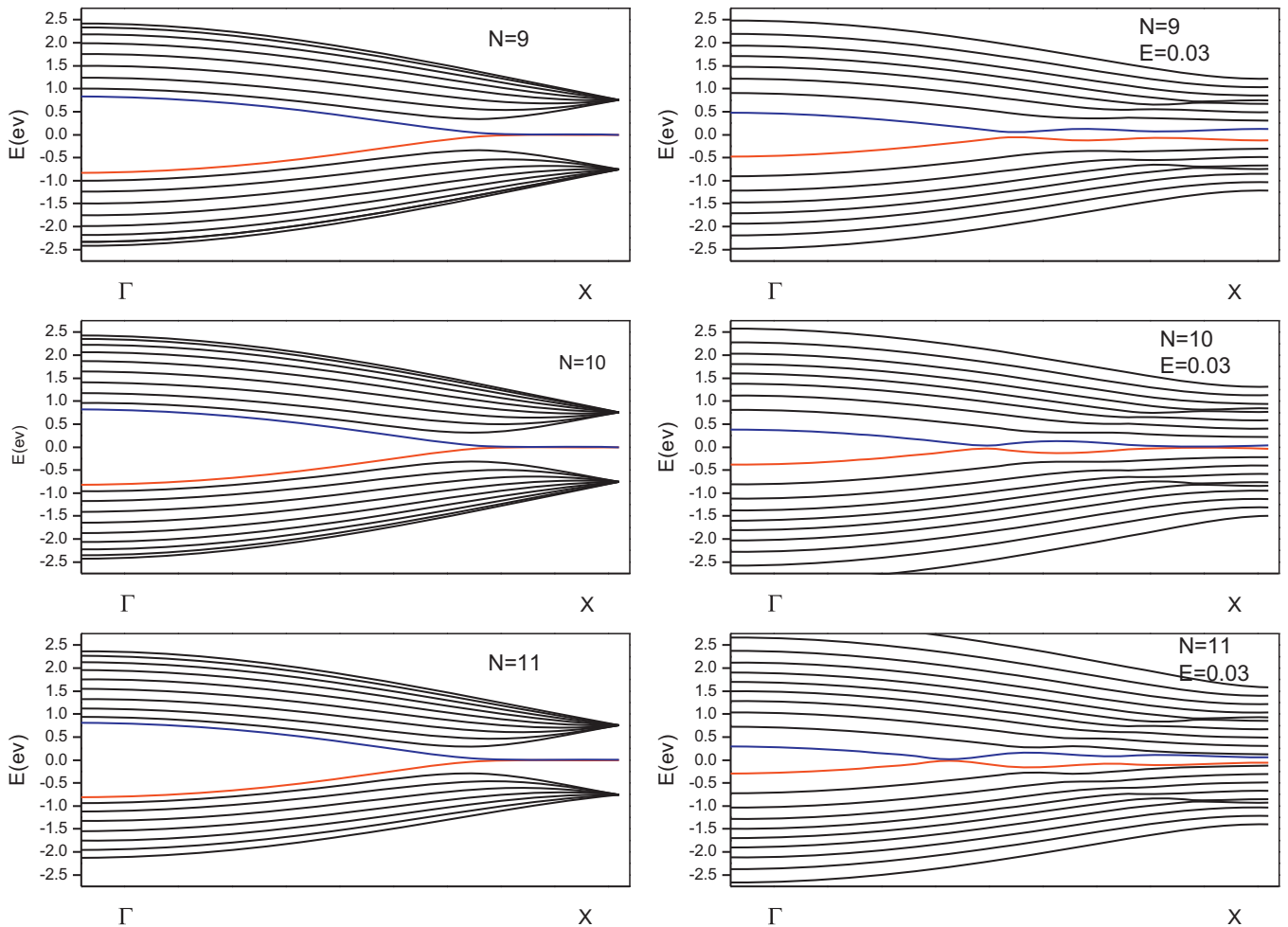

Fig. 5. Zigzag αGYNR band structure for $N=9$, 10 and 11 in the absence (left) and presence (right) of an external electric field.
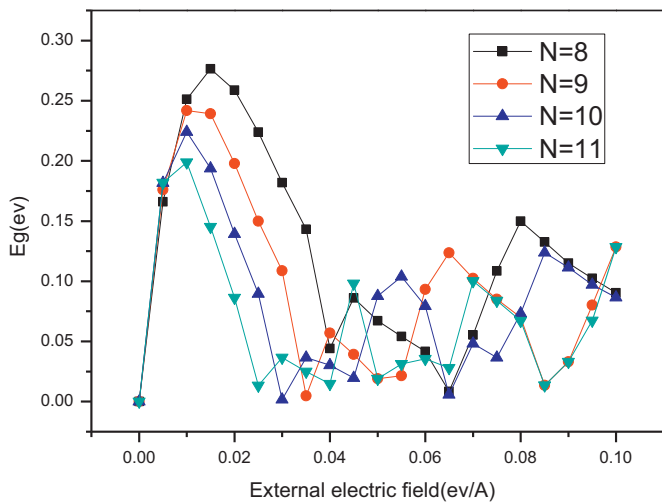
Fig. 7. Zigzag αGYNR band gap versus external electric field with different widths.
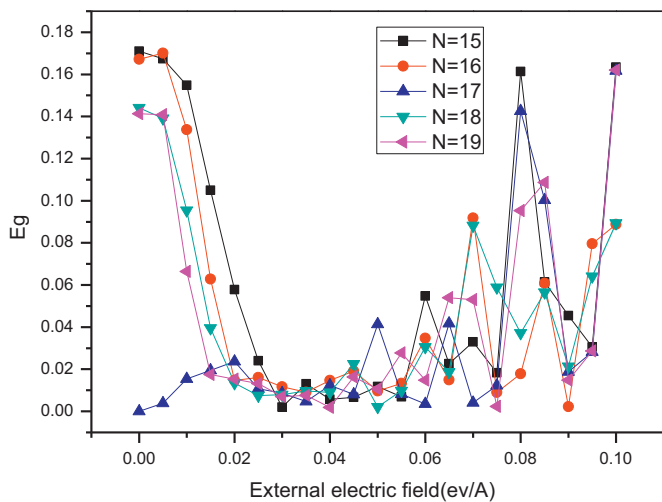

Fig. 8. Armchair αGYNR band gap versus external electric field with different widths.

show that in the absence of an electric field, AαGYNRs are semiconductor or semimetal but all of ZGYNRs are semimetal. Also, both the electric field and ribbon's width affect the value of band gaps. Moreover, we find that by applying the electric field, even by increasing the ribbon's width, the band gap remains constant. These results can open new possibilities in nanoelectronics.

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