Band gaps in jagged and straight graphene nanoribbons tunable by an external electric field

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Abstract
Band gap control by an external field is useful in various optical, infrared and THz applications. However, widely tunable band gaps are still not practical due to a variety of reasons. Using the orthogonal tight-binding method for $\pi$-electrons, we have investigated the effect of the external electric field on a subclass of monolayer chevron-type graphene nanoribbons that can be referred to as jagged graphene nanoribbons. A classification of these ribbons was proposed and band gaps for applied fields up to the SiO$_2$ breakdown strength (1 V nm$^{-1}$) were calculated. According to the tight-binding model, band gap opening (or closing) takes place for some types of jagged graphene nanoribbons in the external electric field that lies on the plane of the structure and perpendicular to its longitudinal axis. Tunability of the band gap up to 0.6 eV is attainable for narrow ribbons. In the case of jagged ribbons with armchair edges larger jags forming a chevron pattern of the ribbon enhance the controllability of the band gap. For jagged ribbons with zigzag and armchair edges regions of linear and quadratic dependence of the band gap on the external electric field can be found that are useful in devices with controllable modulation of the band gap.

Keywords: graphene nanoribbons, superlattices, electronic properties
(Some figures may appear in colour only in the online journal)

1. Introduction
Since it was obtained in a freestanding form graphene [1] has been attracting the attention of the scientific community both as an interesting object for fundamental study (due to its massless Dirac fermions [2]) and as a base for future technological advances due to its chemical stability, mechanical strength [3], and high electrical and thermal [4, 5] conductivities. Numerous graphene applications [6] include field effect transistors [7] and their interconnects [8, 9], sensors [10, 11], hydrogen storage [12], terahertz emitters [13, 14], transparent electrodes etc. Many of these applications would benefit from a full control over the band gap. For instance, great effort has been made to develop novel tunable sources and detectors of THz radiation [15]. Speaking of electronic applications, one must confess that there is a problem of contact resistance [16] that can be easily overcome in all carbon electronic devices [17], but this again requires a complete control over the band gaps of the nanostructures. Additionally, all carbon electronics can be easily recycled and used in a closed-loop production cycle. Therefore, it is desirable to control the band gap both by structural modification and external fields.

A number of techniques have been proposed for band gap engineering in graphene: patterning of graphene [18, 19], straining of graphene [20–24], lateral confinement of charge carried in one dimension in a graphene nanoribbon (GNR), vertical inversion symmetry breaking in bilayer graphene [25, 26], or trilayer graphene [27]. All of them have some advantages and disadvantages, for instance, patterning allows a...
higher current compared to a GNR, while symmetry breaking by an external electric field provides tunability of the band gap, giving rise to tunable devices, which is not the case for patterning or carrier confinement.

The universal approach to band gap control was also attempted in a combination of strategies. Recently, after extensive theoretical study [28, 29], simultaneous lateral attempt in a combination of strategies. Recently, after extensive theoretical study [28, 29], simultaneous lateral attempt in a combination of strategies. Recently, after extensive theoretical study [28, 29], simultaneous lateral attempt in a combination of strategies. Recently, after extensive theoretical study [28, 29], simultaneous lateral attempt in a combination of strategies. Recently, after extensive theoretical study [28, 29], simultaneous lateral attempt in a combination of strategies. Recently, after extensive theoretical study [28, 29], simultaneous lateral attempt in a combination of strategies. Recently, after extensive theoretical study [28, 29], simultaneous lateral attempt in a combination of strategies. 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respectively. L and L, respectively. L, L, and W are chief vectors, \( \ell_1, \ell_2 \) and \( w \) are elementary vectors, \( a_1 \) and \( a_2 \) are primitive translations of the graphene lattice, \( T \) is the JGNR translation vector, and \( \ell_1, \ell_2 \) are the centers of the JGNR inversion symmetry.

Table 1. The coordinates of JGNR elementary vectors \( \ell_1, \ell_2 \) and \( w \) on the basis of primitive translations of a graphene lattice \( a_1 \) and \( a_2 \).

|         | Z60 | Z120 | A60 | A120 |
|---------|-----|------|-----|------|
| \( \ell_1 \) | (1, 0) | (1, -1) | (2, -1) | (2, -1) |
| \( \ell_2 \) | (0, 1) | (0, 1) | (1, 1) | (-1, 2) |
| \( w \)   | (1, 1) | (1, 0) | (1, 0) | (1, 1) |

The coordinates of JGNR elementary vectors \( \ell_1, \ell_2 \) and \( w \) are primitive translations of the graphene lattice \( a_1 \) and \( a_2 \).

Figure 1. JGNRs characteristic vectors for zigzag \((a)\) and armchair \((b)\) ribbon orientations on a graphene sheet represented by ribbons Z60\((3, 3; 2)\) and A60\((2, 2; 3)\), respectively. Lines 2–2 and 1–1 (insets) show all possible zigzag \((Z)\) and armchair \((A)\) directions, respectively. \( L_1, L_2 \) and \( W \) are chief vectors, \( \ell_1, \ell_2 \) and \( w \) are elementary vectors, \( a_1 \) and \( a_2 \) are primitive translations of the graphene lattice, \( T \) is the JGNR translation vector, and \( \ell_1, \ell_2 \) are the centers of the JGNR inversion symmetry.

The width of the GNR that one cut some parts from to produce jagged edges, can be expressed as follows:

\[
W_{\text{eff}} = \frac{T \times P_{1(2)} \times T}{T^2},
\]

where \( P_{1(2)} = L_{1(2)} + W \). This definition is independent of the choice of vector \( L_1 \) or \( L_2 \) and is useful for a result comparison to clarify the role of jags in the electronic properties of a JGNR. Other characteristics closely related to the width are the widths of the JGNR arm ribbons which have the form of:

\[
W_{1(2)} = \frac{L_{1(2)} \times W \times L_{1(2)}^T}{L_{1(2)}^T}. \quad (6)
\]

For the present paper, as the width vector was chosen to be the bisector of the apex angle, these two quantities defined by equation (6) are equivalent. Finally, one can think about some JGNRs as a host ribbon with triangle fragments attached on both sides (see figure 4); therefore, for quite a wide JGNR one can introduce a host ribbon width:

\[
W_h = 2W - W_{\text{eff}}. \quad (7)
\]

Equating the right-hand side of equation (7) to zero, one can easily obtain the criterion for the host ribbon presence in the structure for each type of JGNR: Z60 \( \ell \geq 2w \), Z120 \( \ell \geq 2w \), A60 \( \ell > 2w/3 \), A120 \( \ell > 2w \). This simple mapping of a JGNR onto ordinary straight GNRs is only possible in a symmetric case when \( \ell_1 = \ell_2 \). As for an asymmetric case, it is more complicated because the effective, the host, and the straight ribbons become specific JGNRs with low values of indexes. Additionally, this mapping would be of no practical use for ribbons from the same class that can be compared straightforwardly.
3. Method

The electronic structure of the presented JGNRs was investigated within the orthogonal tight-binding model for $\pi$-electrons. Electronic bands were obtained as eigenvalues for the matrix Hamiltonian $H$ with elements of the following form:

$$H_{nn'} = \sum_{i,j,q} t_{ni} \exp(ikr_{nij}) \delta_{r_{nij},r_{nq}}$$  \hspace{1cm} (8)

where $r_{nij}$ is a vector pointing the $j$-th position of the $i$-th order nearest neighbour from the $n$-th atom position in the unit cell of the structure, $r_{nq}$ is a radius-vector pointing the position of the $n$-th atom in the $q$-th unit cell. Within the tight-binding model, the so-called hopping integral $t_{ni}$ for the $n$-th atom in the unit cell of the structure is expressed as:

$$t_{ni} = \langle \phi_n | \hat{H} | \phi_{ni} \rangle,$$  \hspace{1cm} (9)

where $\hat{H}$ is a system Hamiltonian, $\phi_n$ is an atomic orbital of the $n$-th atom, and $i$ can be referred to as the neighbour order. In the presence of an external field the Hamiltonian takes the form:

$$\hat{H} = \hat{H}_0 + \hat{U},$$  \hspace{1cm} (10)

where $\hat{H}_0$ is the Hamiltonian of the system without an external field, and $\hat{U} = -eE \hat{r}$ is the potential energy operator for a
homogeneous electric field. Taking this into account one has $t_{n\ib} = t_{n\ib} + \delta t_{n\ib}$, with $\delta t_{n\ib} = \langle \phi_n(U|\phi_{n\ib}) \rangle$. Note that the external electric field is much less than the atomic one, i.e.

$$eE \ll \frac{t_{n\ib,0}}{a_0},$$

where $t_{n\ib,0} \approx 3$ eV, $a_0 = 1.42$ Å. This allows one to neglect any change in the atomic orbitals $\phi_0, \phi_{n+1}$ due to the field. It is also worth mentioning that we do not expect a large field enhancement at the sharp ends of the jags as their sizes in the structures under consideration are about 5 nm, which is quite small, and they are arranged periodically in an infinite line so that their influence on each other averages and reduces the resulting field.

As we are interested in the pure effect of the jagged edges and its influence on the electronic properties of JGNRs, we eliminate the possible differences of hopping integrals at various sites within the unit cell so that $t_{n\ib} = t_i$; $t_{n\ib,0} = t_{i,0}$; $\delta t_{n\ib} = \delta t_i$. In fact, the model of ideal geometry was implemented, which is close to the real geometry of the structures under consideration are about 5 nm, which is quite small, and they are arranged periodically in an infinite line so that their influence on each other averages and reduces the resulting field.

It is worth noting that on one hand the hopping integral values at the edge can differ from those in the GNR interior so that it could cause band gap opening in an armchair GNR [47]. On the other hand, the same band gap opening can be explained by accounting for higher order hopping integrals [48]. A more accurate model taking into account both effects was reported later [49]. Interestingly, a more precise model accounting for edge distortions showed that this effect leads to a small correction only for armchair ribbons of 3$n$ series. However, it is very unlikely that this small correction to the band gap does affect its tunability. Therefore, admitting an error for the band gap of no more than 10%, the nearest neighbours up to the third order were taken into account and model parameters were chosen as proposed in the paper [48]: $t_{0,0} = 0$ eV, $t_{1,0} = -3.2$ eV, $t_{2,0} = 0$ eV $t_{3,0} = -0.3$ eV.

In the present paper we neglect the screening effect and assume that an applied field directly influences each lattice site. This seems reasonable for strong electric fields. However, for weak fields one should keep in mind that the values presented should be interpreted as a value of an effective field. The applied electric field contributes mainly to the site energy $t_i$. In fact, there are additional terms for higher order hopping integrals $\delta t_{1,\infty}$. To assess them one can approximate carbon $\pi$-orbitals by the $p_z$ wave functions of the hydrogen-like atom [50]:

$$\phi_n(|r - r_n|, \theta) = \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_B} \right)^{5/2} \exp \left( -\frac{Z|r - r_n|}{2a_B} \right) \times |r - r_n| \cos \theta,$$

where $Z = 6$ (for carbon), $a_B$ is the Bohr radius, and $\theta$ is the polar angle measured from the $z$-direction (in a spherical coordinate system) and calculates the ratios $\delta t_i/t_{i,0}$. Obviously, the value obtained for $i = 0$ is of greater significance than any other. That is why we adopted $\delta t_{1,\infty} \approx 0$, $\delta t_0 = -E_F$ eV.

The band gap dependence on an applied electric field was investigated for electric strength magnitudes up to 0.1 V Å$^{-1}$ = 1 V nm$^{-1}$. This value is 10 times less than the typical strength used in field emission calculations [51, 52], but corresponds to the breakdown strength of the electric field in SiO$_2$ [53]. Even though this seems to be quite a high magnitude of field, it must be noted that it still meets the requirement of equation (11). It is often chosen as a natural upper limit by others [26, 29, 33] for the electric field applied normally to the plane of the structure. Thus, our choice makes for an easier comparison of the two field arrangements. It is worth noting that the break down values are very sensitive to the material used. For instance, in the experimental work [30] it was possible to increase the value by more than twice by using a combination of SiO$_2$ with HfO$_2$, so that the resulting value was $\sim 0.033$ V Å$^{-1}$, which is only 3 times lower than that mentioned above.

Figure 4. JGNR Z60 (1, 5, 6) mapping onto straight GNRs, where $W$, JGNR and the straight ribbon width; $W_{\text{eff}}$, the effective ribbon width; $W_h$, the host ribbon width; $W_i$, the arm ribbon width.
4. Results

Let us now consider typical JGNR band structures and their changes in an external electric field. Throughout this paper all the ribbons are assumed to be lying on the $xy$-plane and the $y$-axis is collinear with the ribbon translation vector so that the transverse electric field strength has only one non-zero component $\varepsilon_x$. In figure 5, one can see that the most profound changes take place for JGNR Z60 and A120. In the first case, one is dealing with a band gap opening, while in the second case—with a band gap closing. Surprisingly, there are no observable changes for the band gaps of JGNR Z120 and A60. However, some alterations in the Z120 and A60 band structures can be noticed. For the sake of clarity of the discussion, let us take the following convention: all the bands are numbered by indexes $J$ so that the first conduction band corresponds to $J = 1$ and the first valence to $J = -1$ and so on. Then it can be pointed out that a profound splitting takes place at the edge of the Z120 Brillouin zone for bands $J = \pm 1$ and $J = \pm 2$, respectively. A similar splitting, but of less magnitude and shifted towards the center of the Brillouin zone, is observed for the A60 bands $J = \pm 2$ and $J = \pm 3$, correspondingly. With respect to the A60 ribbon one must confess that the least variations occur for bands $J = \pm 1$ compared to the equivalent bands of the other ribbons presented. This means that the effective mass of the charge carriers changes only slightly due to the presence of a transverse electric field. In the case of the Z120 ribbons the change in the effective mass for low doping concentrations should also be negligible. However, more significant changes take place for ribbons Z60 and A120. In both cases profound band bending can be observed for the magnitude of the electric field $\varepsilon_x = 0.05 \text{ V Å}^{-1}$. In general, it can be seen that the influence of the field is stronger at the edge of the Brillouin zone, as has already been shown in the nanotube and nanohelix superlattice properties analysis, which is very relevant to a JGNR in the external electric field as it creates for the JGNR’s electron a periodic electrostatic potential similar to that discussed in papers [54–56].

Next we consider the band gap dependence on the magnitude of the transverse electric field in more detail. Let us proceed with the JGNR Z60. For figure 6 we took a slightly wider ribbon Z60 ($3, 3; 9$) to show that for a high value of the electric field strength of about $0.06 \text{ V Å}^{-1}$ band gap closing can be observed. The next feature that can be noticed in figure 6 is the dispersionless bands, whose the positions clearly correlate with the magnitude of the external field. These bands arise from the zigzag edge states reported in the paper [57]. However, as a JGNR is a superlattice with a longer translation period, its band structure, if one does not take into account interactions leading to band anticrossing, is a folded structure of a straight GNR with zigzag edges (ZGNR). As one can see, due to this folding these bands are absolutely dispersionless throughout the whole Brillouin zone compared to a ZGNR, where the edge bands are dispersionless only throughout $1/3$ of the Brillouin zone. Changing the superlattice period of translation $T$ by means of jag arms $L_1, L_2$ (see equation (3)) one can control a number of foldings, or in other words a number of dispersionless bands. Without the external electric field almost all of them are degenerate, but with a switched-on field their splitting is observed. These bands must result in sharp peaks in the density of states, whose positions in turn must be field dependent as well. However, as one can see from figure 6 for a high magnitude of electric strength of about $0.06 \text{ V Å}^{-1}$ they drown among the multitude of other bands. But for the narrower Z60 ribbons the density of states arising from all the other bands except the edge ones around the Fermi level is low in quite a wide region from $-1$ to $1$ eV, as shown in figure 7. This means that the peaks should act in this region as energy levels as we showed for the JGNR Z60 with $w = 6$ in figure 7. Taking into account all the abovementioned results, we predict that for a JGNR Z60 with $w = 4, \ldots, 8$ in an external transverse electric field, a series of electromagnetic

![Figure 5](image_url)

*Figure 5.* The effect of a transverse electric field $\varepsilon_x$ on the band structure of four types of JGNR, where $E_F$—the Fermi energy. $k$ is expressed in the units of $1/T$ everywhere.
emission and absorption lines will be observed, and the number of lines will be consistent with $T$. We tested that this result remains true for asymmetric JGNRs Z60 characterized by indexes $\ell_1 \neq \ell_2$ and for JGNRs Z60 of a slightly different structure; see appendix.

Considering in figure 8 the band gap closing for JGNR A120, one must notice that this closing takes place owing to the splitting of bands $J = \pm 1$, $\pm 2$ at the edge of the Brillouin zone. This splitting leads to the band gap shift in $k$-space from $k = 0$ for $\varepsilon_x = 0 \, \text{V} \, \text{Å}^{-1}$ to the region $k > \pi/2$ for $\varepsilon_x = 0.06 \, \text{V} \, \text{Å}^{-1}$. Although there are some bands with low dispersion near energies $\pm 1$ eV their positions are not affected by the applied electric field. On the contrary, an almost flatness of the bands $J = \pm 1$ can be achieved for $\varepsilon_x = 0.06 \, \text{V} \, \text{Å}^{-1}$ in $k$-space from $k = \pi/2$ to $k = \pi$. This is very useful because it must increase the probability of interband transitions with a frequency corresponding exactly to the band gap due to the higher density of states on both its sides. It is very interesting to see how the dependence of the band gap on the transverse electric field is affected by symmetric JGNR parameters $w$ and $\ell_1 = \ell_2$. These results are presented for JGNRs Z60 and A120 in figure 9. As can be seen from figure 9(a) the maximum value of the band gap opening ($\sim 0.6$ eV) is higher for the narrower ribbon with $w = 7$, but it is attainable for a stronger transverse electric field ($0.04 \, \text{V} \, \text{Å}^{-1}$) compared to Z60 (3, 3; 8) and (3, 3; 9); moreover, for the specified ribbon the band gap cannot be closed within the restricted range $<0.1 \, \text{V} \, \text{Å}^{-1}$ as for ribbon Z60 (3, 3; 9). For a low strength field $<0.02 \, \text{V} \, \text{Å}^{-1}$ the band gap opening for a narrower Z60 is slightly less than for wider ones, but this results in a more significant divergence for a greater difference of width indexes. The influence of the jag arm index on the band gap opening of the ribbon Z60 as shown in figure 9(b) is opposite to that just mentioned. For higher indexes the maximum value increases and drifts to greater values of $\varepsilon_x$, while the band gap closing at $\varepsilon_x = 0.1 \, \text{V} \, \text{Å}^{-1}$ is not affected by them. In low strength fields the difference in band gap opening is almost negligible. According to figure 9(c) the band gap closing

**Figure 6.** The band structure evolution for an increasing magnitude of transverse electric field for JGNRs Z60 (3, 3; 9) (left) and the atomic structure of the ribbon (right).

**Figure 7.** The splitting of dispersionless bands in the transverse electric field for JGNRs Z60 (3, 3; 6), (5, 5; 6), (7, 7; 6). DOS—normalized density of states.
Figure 8. The band structure evolution for an increasing magnitude of transverse electric field for JGNRs A120 \( \langle 3, 3; 6 \rangle \) (left) and the atomic structure of the ribbon (right).

does not take place immediately, and JGNRs A120 \( \langle 3, 3; 6 \rangle \) are quite resistant to low electric fields with \( \varepsilon_x < 0.02 \text{ V Å}^{-1} \). However, this resistance decreases if the width index increases, which leads to lower values of the electric strength required to close the band gap completely: \( \varepsilon_x = 0.055 \text{ V Å}^{-1} \) for A120 \( \langle 3, 3; 8 \rangle \) and \( \varepsilon_x = 0.08 \text{ V Å}^{-1} \) for A120 \( \langle 3, 3; 6 \rangle \). Another fascinating feature of the ribbons is the peak in the band gap dependence on the electric field strength observed for A120.
(3, 3; 7) at $\epsilon_x = 0.85 \text{ V \AA}^{-1}$. This peak position shifts to lower magnitudes of $\epsilon_x$ as the width index $w$ increases, while its height seems to remain unaffected. This is quite strange if we take into account that there is an obvious decrease in the initial values of the band gap, e.g. for $\epsilon_x = 0 \text{ V \AA}^{-1}$, for greater indexes $w$. Compared to this case the data presented in figure 9(d) are very different. While the decrease in the initial values of the band gap for incremented jag arm indexes $\ell_1$ and $\ell_2$ is less than in figure 9(c), for increasing $w$ the resistance to the band gap closing is of the same measure, e.g. achieved at $\epsilon_x = 0.053 \text{ V \AA}^{-1}$ for A120 (7, 7; 6). This value is compared to the value for A120 (3, 3; 8); however in the case of A120 (7, 7; 6) one closes a wider band gap. In figure 9(d) a peak similar to that in figure 9(c) in dependence of $E_g$ on $\epsilon_x$ is manifested. Its position shifts to a lower $\epsilon_x$ for a greater $\ell_1$, $\ell_2$ and it resembles the behaviour of the peak in figure 9(c), but its height decreases if the jag arms indexes $\ell_1, \ell_2$ both increase.

It is obvious that the dependences $E_g(\epsilon_x)$ for the Z60 and A120 JGNRs presented in figure 9 cannot be described by simple functions; however, they can be approximated by polynomials that are truncated Taylor series. One can quite easily specify the regions where two or three terms of Taylor expansion are necessary for a reasonable approximation. These regions correspond to linear and quadratic dependencies $E_g(\epsilon_x)$ and good knowledge about them is of great importance for possible applications in linear and non-linear devices; therefore, we calculated the parameters characterizing the rate of the band gap opening/closing and presented them in table 2.

Moreover, table 2 enables a comparison between the two types of ribbons, which is difficult to do by means of plotting. Although it might seem strange to compare different patterns we want to notice that an A120 ribbon placed in a sufficiently strong electric field so that the point of complete band gap closing, for instance $\epsilon_x = 0.08 \text{ V \AA}^{-1}$ for A120 (3, 3; 6), is achieved can work in the same regime as a Z60 ribbon—metal–dielectric transition for a decreasing field. As can be clearly seen in table 2 the absolute value of $\beta$ is larger for all the Z60 ribbons than for the A120 ribbons presented in table 2, which means their band gaps can be controlled more efficiently.

Having studied the dependence of $E_g$ on $\epsilon_x$ for the JGNRs Z60 and A120, we proceed with a comparison of the found patterns with similar ones for simple GNRs with zigzag and armchair edges, which will be referred to as ZGNR(n) and AGNR(n), respectively, where $n$ is the number of carbon atom pairs in the unit cell of the structure. The mapping mentioned at the end of section 2 is very useful for doing this. Using the mapping based on equations (5)–(7) the results presented in figures 10(a)–(d) were obtained. For the sake of completeness ribbons Z60 and A120 with and without host ribbons were considered. The presence of the host ribbon in a JGNR is our criterion for large values of jag arm indexes $\ell_1, \ell_2$ with respect to width index $w$. As can be seen from figure 10(a) the dependence of $E_g$ on $\epsilon_x$ for Z60 (3, 3; 9) lies between the curves for the straight and the effective ribbons. There is no likeness with the arm ribbon that allows one to obtain a high value for $E_g$ of about 0.8 eV but requires close to SiO2 breakdown electric strength magnitude. Comparing the curves for the host and Z60 ribbons, one can see that the former lies below the latter for low values of $\epsilon_x \sim 0.025 \text{ V \AA}^{-1}$ and above for greater values of $\epsilon_x$. In general, the curve for Z60 is to a great extent similar to the curves for effective, straight and host ribbons, especially in the region of low values of $\epsilon_x < 0.02 \text{ V \AA}^{-1}$. However, figure 10(b) provides quite different results. The curve describing $E_g$ versus $\epsilon_x$ dependence for Z60 (12; 12; 6) almost coincides with the curve for the arm ribbon ZGNR(6) for $\epsilon_x < 0.02 \text{ V \AA}^{-1}$ and considerably deviates from it at a higher $\epsilon_x$. It does not approach the curves for the effective ZGNR(24) or straight ZGNR(12). The case of the JGNR A120 (3, 3; 6) as shown in figure 10(c) significantly differs from that one of the JGNR Z60, because A120 ribbons have armchair edges while they are mapped onto ZGNRs. However, in spite of the fact that the arm ribbon for A120 ribbons has the same type of edges, one notices a crucial difference between them. Firstly, it is impossible to control the band gap of AGNR(18), which is the arm one for the A120 (3, 3; 6), by means of a transverse electric field. And secondly, the value of the band gap is greater for a jagged ribbon. In figure 10(d) one can see the effect of deeper jaggs which leads to the absence of the host ribbon in A120 (8, 8; 4). This JGNR is slightly narrower than that presented in figure 10(c), but its band gap is closed nearly at the same magnitude of $\epsilon_x \sim 0.08 \text{ V \AA}^{-1}$ as for A120 (3, 3; 6). It is a straightforward result of the jag arm elongation that shifts this point of closing back to lower values of $\epsilon_x$ after its shift to higher ones due to the decrementation of width index $w$. It is also useful to compare the curves for the A120 ribbons in figures 10(c) and (d) in the region

| JGNR   | $\epsilon_x$, eV | $\beta$, eV $\cdot \text{Å}^{-1}$ | $\alpha$, eV | $E_g$, eV $\cdot \text{Å}^{-1}$ | $\epsilon_{\min}$, V $\cdot \text{Å}^{-1}$ | $\epsilon_{\max}$, V $\cdot \text{Å}^{-1}$ |
|--------|------------------|-------------------------------|-------------|-----------------------------|-------------------------------|-----------------------------|
| Z60    | 0                | 23.3                          | 0.010       | 29.8                       | -361.4                        | 0.010                       |
| Z60    | 0                | 25.9                          | 0.010       | 33.7                       | -526.3                        | 0.010                       |
| Z60    | 0                | 29.6                          | 0.007       | 35.7                       | -680.7                        | 0.007                       |
| Z60    | 0                | 28.4                          | 0.007       | 29.2                       | -425.5                        | 0.007                       |
| Z60    | 0                | 27.0                          | 0.007       | 27.7                       | -365.0                        | 0.007                       |
| A120   | 0                | -412.5                        | 0.035       | 0.6                        | 177.8                         | 0.010                       |
| A120   | 0                | -12.5                         | 0.025       | 0.5                        | -264.4                        | 0.025                       |
| A120   | 0                | -15.7                         | 0.035       | 0.6                        | -349.5                        | 0.010                       |
| A120   | 0                | -14.8                         | 0.020       | 0.5                        | -616.2                        | 0.020                       |
close to zero magnitude of the electric field. One sees that while the initial value of the band gap is greater for A120 (8, 8; 4), \( E_g \sim 0.8 \text{ eV} \) compared to \( E_g \sim 0.65 \text{ eV} \), the closing point is almost the same. Moreover, the drop in the band gap of A120 (8, 8; 4) in the region of \( \varepsilon_x < 0.02 \text{ V Å}^{-1} \) is greater than for A120 (3, 3; 6), which means the band gap of the former can be more readily controlled. In all other respects figures 10(c) and (d) demonstrates very similar curve behaviour, where the observable distinctions can be attributed only to the quantitative differences of the jagged ribbon parameters and, consequently the straight, effective, and arm ribbons ones. For instance, the curve for the arm ribbon in figure 10(d) is also field independent while corresponding to a higher value of the band gap of about 0.6 eV compared to 0.4 eV in figure 10(c). Finally, we report on the effect of asymmetry \( \ell_1 \neq \ell_2 \) on both JGNRs Z60 and A120. Having analyzed the results for the JGNRs and ordinary straight GNRs, it is easy to comprehend the data shown in figures 11(a) and (b). The increment of just one index \( \ell_2 \) results in \( E_g \) versus \( \varepsilon_x \) curve evolution to the form inherent for the arm ZGNR and AGNR, respectively. To be more persuasive, we suggest the reader looks again at the curves for ZGNR(14) and AGNR(18) in figures 10(a) and (c), correspondingly. After that the results in figure 11 are easy to understand. As in the case of figure 9 for the ribbons in figure 11 we specified the linear and quadratic regions of \( E_g(\varepsilon_x) \) and calculated the parameters (see table 3). In contrast to the data in table 2, the absolute values of \( \beta \) for different ribbons in table 3 are very close and imply an approximately equal efficiency in the band gap control.

5. Conclusions

To summarize, in this paper we have studied a subclass of chevron-type GNRs—jagged graphene nanoribbons (JGNRs). It was shown that it is possible to control the band gap of two types of JGNRs, namely Z60 and A120, by an external transverse electric field, e.g. applied on the plane of the ribbon normally to its longitudinal axis. The band gap opening is possible for Z60 ribbons, while the band gap closing is characteristic for A120 ribbons. In both cases the value of the band gap opening/closing is greater for narrower ribbons and requires stronger electric fields. As there is a natural limit for electric strength values due to the breakdown phenomenon, there must be an optimal value of ribbon width providing the highest possible value of the band gap. We argue that for \( \varepsilon_{x, \text{max}} = 0.1 \text{ V Å}^{-1} \), e.g. SiO\textsubscript{2} as a substrate, the optimal width is about \( w \sim 6 \). For these values of width Z60 ribbons in a transverse electric field behave like a quantum dot system and series of emission and absorption lines must be observed if they are not forbidden by optical selection rules. Some enhancement in the controllability of the band gap in the transverse electric field is achievable for A120 ribbons as for the longer jag arms the lower field is required to close the band gap, while this is not the case for the Z60 ones. Also we must mention the second peak for A120 JGNRs, which seems to be unique for this type of structure as it was not mentioned for ordinary straight GNRs in the paper [31]. Finally, we notice that the value of the band gap opening for the Z60 is about 0.6 eV and so high that even taking into account possible error in the band gap evaluation (≈10%) and assuming the

![Figure 10. The comparison of the JGNRs Z60 (a), (b) and A120 (c), (d) with various straight GNRs, where (n) denotes the number of atom pairs in the unit cell of the structure.](image-url)
same field screening ($\sim 25\%$ for $\varepsilon_s = 0.05 \text{ V Å}^{-1}$) as for bilayer graphene one can assess the band gap opening as no less than $\sim 0.4$ eV, which is about two times larger than for bilayer graphene in a normal electric field [26]. The value is also large compared to that for carbon nanotubes, and can be implemented for the fabrication of all metallic transistors first proposed for nanotubes in the paper [58]. Following this work, it even seems reasonable to combine normal and transverse geometry to control the conductivity of the channel and carrier concentration separately. Actually, the separate control of the band gap and the Fermi energy paves the way to a new type of device that could build a bridge between optics and electronics. Speaking again of A120, one must stress also the quite wide range of band gap variation of about 0.6 eV. This property makes the A120 ribbons good as a theoretical model but unfortunately it is very likely that these configurations are difficult to realize experimentally. Therefore, we decided to provide additional results to prove that the found effect is not due to the peculiar structural configuration associated with one carbon atom missing in hexagons on the border between two jags, but is rather due to the ribbon chevron-type pattern and zigzag edge. A structure with one carbon atom removed from the jag apex and placed at the opposite edge to complete one carbon atom missing in hexagons on the border between two jags, but is rather due to the ribbon chevron-type pattern and zigzag edge. A structure with one carbon atom removed from the jag apex and placed at the opposite edge to complete the ribbon chevron-type pattern and zigzag edge. We became aware of recent results confirming spin ordering on the zigzag edges at room temperature [62]. This effect can reduce the range of tunability for Z60 ribbons and needs a separate detailed investigation.

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Appendix: Realistic Z60 structure

Ribbons of the Z60 type are good as a theoretical model but unfortunately it is very likely that these configurations are difficult to realize experimentally. Therefore, we decided to provide additional results to prove that the found effect is not due to the peculiar structural configuration associated with one carbon atom missing in hexagons on the border between two jags, but is rather due to the ribbon chevron-type pattern and zigzag edge. A structure with one carbon atom removed from the jag apex and placed at the opposite edge to complete hexagons seems to be more stable. This structure can be
Figure 12. The splitting of dispersionless bands in the transverse electric field for JGNRs Z60r.

referred to as Z60r, where ‘r’ stands for ‘realistic’. As one can see in figure 12, the band gap opening and dispersionless band splitting in the external transverse electric field can also be found in structures of a more energetically favourable configuration.

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