Strongly localized states and giant optical absorption induced by multiple flat-bands in AA-stacked multilayer armchair graphene nanoribbons

Xiongwen Chen\(^1,2,^{*}\), Qian Wang\(^1,2\), Ping Wu\(^1\) and Guanghui Zhou\(^2\)

\(^1\) Department of Physics, Huaihua University, Huaihua 418008, People’s Republic of China
\(^2\) Key Laboratory for Low-Dimensional Structures and Quantum Manipulation, Synergetic Innovation Center for Quantum Effects and Applications, Hunan Normal University, Changsha 410081, People’s Republic of China

\(^{*}\) Author to whom any correspondence should be addressed.
E-mail: chenxiongwen@hhtc.edu.cn

Keywords: multilayer armchair graphene nanoribbons, multiple flat bands, selective localization rule, giant optical absorption, electric-field manipulation

Abstract

We propose an AA-stacked multilayer graphene nanoribbon with two symmetrical armchair edges as a multiple flat-band (FB) material. Using the tight-binding Hamiltonian and Green’s function method, we find that the FBs are complete and merged into many dispersive bands. The FBs cause multiple strongly localized states (SLSs) at the sites of the odd lines in every sublayer and a giant optical absorption (GOA) at energy point \(2t\), where \(t\) is the electronic intralayer hopping energy between two nearest-neighbor sites. By driving an electric field perpendicular to the ribbon plane, the bandgaps of the FBs are tunable. Accordingly, the positions of the SLSs in the energy regime can be shifted. However, the position of the GOA is robust against such field, but its strength exhibits a collapse behavior with a fixed quantization step. On the contrary, by driving an electric field parallel to the ribbon plane, the completeness of FBs is destroyed. Resultantly, the SLSs and GOA are suppressed and even quenched. Therefore, such ribbons may be excellent candidates for the design of the controllable information-transmission and optical-electric nanodevices.

1. Introduction

The flat band (FB) system [1–3], possessing dispersionless subband in its band structure, has attracted an increasing interest recently. One is partly because this system is a possible platform to understand the fundamental physics of the topological insulator [4, 5], the fractional quantum Hall effect [6–8], and the superconducting transition [9–11]. Other is partly because this system has some significant applications in the nanotechnology, for example, the manipulation of the FB can induce a metal–insulator transition [12] and an insulator–metal transition [13]. Therefore, there are many efforts to obtain the FB systems by translationally constructing the invariant lattice systems such as Lieb lattice [14–16], Kagome lattice [17, 18], hexagonal structure [19, 20], and their composite structures [21, 22], etc.

It is well known that the monolayer graphene (GR) is a natural hexagonal structure [23]. And its one-dimensional counterparts, e.g. the armchair-edged ribbons (AGNRs) and the zigzag-edged ones (ZGNRs), are the basic elements in the graphene-based nanodevice [24–26]. All pristine ZGNRs are the FB systems which have been extensively studied [27–30]. In fact, the pristine AGNRs with two symmetrical edges in atomic configuration, i.e. containing an odd number of the carbon dimer atom lines crossing the ribbon width, are also the FB systems. And two complete FBs at energies \(E = \pm t\) (\(t\) is the hopping energy between two nearest-neighbor sites) always exist in such AGNRs [28, 31]. However, to our knowledge, the attentions toward them have been insufficient except the investigation on the ferromagnetism induced by the FBs [31]. It is partly owing to that it is difficult to manipulate an FB and remain its completeness by introducing an external electric field based on the structure of a single plane. Moreover, the properties of...
the electronic transports are not changed obviously even if the FBs are destroyed because they are merged into the dispersive bands.

Recently, the AA-stacked graphite [32], i.e. the bilayer and the multilayer graphene samples are fabricated experimentally [33, 34]. In such samples, only atoms at the equivalent sites of two nearest-neighbor sublayers generate adjacent to each other with a weak coupling. Therefore, it is easy to cut them into one-dimensional armchair- and zigzag-edged nanoribbons. The electronic properties of the bilayer nanoribbons have some investigations [35–38]. It was found that some good properties in the monolayer nanoribbons still partly remain in the bilayer ones such as three categories of the semiconducting and metallic conduction according to the widths of the armchair ribbons [36, 37].

Motivated on this evidence, here, we propose an AA-stacked multilayer armchair-edged graphene nanoribbon (AAMLAGNR) with two symmetrical edges as a multiple FB material.

In this paper, we theoretically investigate the band structure of the pristine AAMLAGNRs, by directly solving the tight-binding Hamiltonian. We show that the AAMLAGNRs with two symmetrical edges are the multiple FB systems, in which the complete FBs are merged into the dispersive bands. The FBs cause use of strong localized states (SLSs) only at the sites of the lines with odd order numbers, counting from one edge to the other edge. And these states can be obtained by calculating the local density of states (LDOS) at the corresponding sites based on the Green’s function approach. Additionally, the FBs also produce a giant optical absorption (GOA) at energy \( \hbar \omega = 2t (h = 1) \), which is displayed by a prominent sharp peak in the optical absorption spectrum \( A(\omega) \). Moreover, the SLSs and the GOA are tunable by applying an electric field perpendicular or parallel to its sublayers, which is easily achievable in nowadays nanotechnological experiments.

2. Hamiltonian and method

The sketch of a pristine \((M, N)\)-AAMLAGNR is depicted in figure 1, where it contains \( M \) sublayers in thickness (figure 1(a)) and each sublayer has \( N \) carbon dimer lines in width (figure 1(b)). When \( N \) is odd, its two armchair edges are symmetrical in atomic configuration, otherwise they are antisymmetrical. In layer \( m \), an unit cell \( \alpha \) (the rectangle in figure 1(b)) contains 2\( N \) carbon atoms. We describe the atom sites in the cell as \( (m, n, \alpha, \beta) \), where \( \beta = A, B \) denote the sites of atom \( A \) and \( B \) in dimer line \( n \), respectively. Using the tight-binding model in the molecular orbital representation [39, 40], the Hamiltonian can be written as

\[
H = H_1 + H_2 + H_3
\]

with

\[
H_1 = -t \sum_{m=1}^{M} \sum_{n=1}^{N} \sum_{\alpha} \sum_{m} \langle m, n, \alpha, A | m, n, \alpha - 1, B \rangle + \langle m, n, \alpha, A \rangle \times \langle m, n - 1, \alpha, B \rangle + \langle m, n, \alpha, A \rangle \langle m, n + 1, \alpha, B \rangle + \text{H.c.},
\]

\[
H_2 = -\gamma \sum_{m=1}^{M} \sum_{n=1}^{N} \sum_{\alpha} \sum_{\beta} \langle m, n, \alpha, \beta \rangle (m - 1, n, \alpha, \beta) + \langle m, n, \alpha, \beta \rangle (m + 1, n, \alpha, \beta) + \text{H.c.},
\]

and

\[
H_3 = \sum_{m=1}^{M} \sum_{n=1}^{N} \sum_{\alpha} \sum_{\beta} U_m |m, n, \alpha, \beta \rangle \langle m, n, \alpha, \beta \rangle + \sum_{m=1}^{M} \sum_{n=1}^{N} \sum_{\alpha} \sum_{\beta} U_m |m, n, \alpha, \beta \rangle \langle m, n, \alpha, \beta | + \text{H.c.}.
\]

Here, the state vector \(|m, n, \alpha, A(B)\rangle\) denotes the molecular orbital of carbon atom \((m, n, \alpha, A(B))\). \(H_1\) and \(H_2\) describe the nearest intralayer hopping with strength \( t \) and the interlayer hopping with strength \( \gamma \), respectively. \(H_3\) describes the field-staggered on-site potentials \( U_m \) and \( U_n \), which are induced by the perpendicular electric field \((E_y \text{ in figure 1(a)})\) and the parallel electric field \((E_x \text{ in figure 1(b)})\) to its sublayers, respectively. In our paper, the intrinsic interactions between electrons in the GRs, such as the weak spin–orbit interaction, are neglected just like most studies. Of course, the interactions between electrons can cause interesting properties [41, 42]. For example, a small local Coulomb interaction can generate a large intervalley gap at the assistance of the FB in the dice model [42]. We believe that some manipulations of the FB in the monolayer GRs, such as local Coulomb interactions induced by dopants [31], also are good ways to adjust our results which we will consider in the future investigations.
where parameters $L_x$ and $z$ boundary conditions to the thickness of ribbon in the $a$ direction (see figure 1(b)). The total wavefunction can be expressed as

$$|\Psi\rangle = \frac{1}{\sqrt{L_x}} \sum_{m=1}^{M} \sum_{n=1}^{N} e^{i \beta k_x} \psi_{\alpha}(k_x, m, n)|m, n, \alpha, \beta\rangle,$$

where parameters $L_x$ and $k_x$ denote the total number of unit cells of the ribbon and the electron momentum along the $x$ direction, respectively. $R_{\alpha, \beta}$ is the $x$-position of a site in unit cell $\alpha$, and $\psi_{\alpha}(k_x, m, n)$ is the coefficient function of the wavefunction at site $(m, n, \alpha, \beta)$. Substituting equations (1) and (2) into the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$, we obtain

$$\begin{align*}
(E - U_m - U_n) \psi_{\alpha}(k_x, m, n) &= -t \left[ e^{-i \delta x} \psi_{\beta}(k_x, m, n) + e^{i \delta x} \psi_{\beta}(k_x, m, n - 1) + e^{i 2 \delta x} \psi_{\beta}(k_x, m, n + 1) \right] \\
&- \gamma \left[ (|\psi_{\beta}(k_x, m + 1, n) + \psi_{\beta}(k_x, m - 1, n)|) \right] 
\end{align*}$$

and

$$\begin{align*}
(E - U_m - U_n) \psi_{\beta}(k_x, m, n) &= -t \left[ e^{i \delta x} \psi_{\alpha}(k_x, m, n) + e^{-i \delta x} \psi_{\alpha}(k_x, m, n - 1) + e^{-i 2 \delta x} \psi_{\alpha}(k_x, m, n + 1) \right] \\
&- \gamma \left[ (|\psi_{\alpha}(k_x, m + 1, n) + \psi_{\alpha}(k_x, m - 1, n)|) \right], 
\end{align*}$$

where $a$ is the intralayer lattice constant between two nearest carbon atoms. Applying the hard-wall boundary conditions to the thickness of ribbon in the $z$ direction (see figure 1(a)) as

$$\psi_{\beta}(k_x, M + 1, n) = \psi_{\beta}(k_x, 0, n) = 0$$

and to the width of ribbon in the $y$ direction (see figure 1(b)) as

$$\psi_{\beta}(k_x, m, N + 1) = \psi_{\beta}(k_x, m, 0) = 0.$$

Taking equations (5) and (6) into equations (3) and (4), we can numerically obtain the band structure $E(k_x)$ for the $(M, N)$-AAMLNR with definite $M$ and $N$.

In this work, we also need to obtain the LDOS at arbitrary site in the $(M, N)$-AAMLNR, in which contains the information of the SLSs originating from the FBs. In the tight-binding model, the Green’s function at site $(m, n, \alpha, \beta)$ in cell $\alpha$ can be written as

$$g_{(m, n, \alpha, \beta)}(\omega, k_x) = \frac{1}{2L_x} \frac{\psi_{\beta}(k_x, m, n)\psi_{\alpha}(k_x, m, n)}{\omega - E(k_x) + i\delta},$$
Figure 2. Band gap $\Delta E$ for pristine AAMLGNRs with various widths (a) and thickness (b) without external electric field, respectively.

where $\delta$ is a positive infinitesimal real quantity. Thus the LDOS at site $(m, n, \alpha, \beta)$ in the ribbon can be expressed as

$$\text{LDOS}(\omega) = -\frac{2}{\pi} \int_{-\pi/3a}^{\pi/3a} g_{(m,n,\beta)}(\omega, k_x) dk_x. \quad (8)$$

Although the electronic transport is insensitive to the FBs, the electronic hopping can realize between the states of two FBs. When an appropriate electric field is applied to a $(M, N)$-AAMLGNR, electrons are excited from the occupied valence band $E_v(k_x)$ to the unoccupied conduction band $E_c(k_x)$. The vertical optical transitions with the same wavevector ($\Delta k_x = 0$) occur, which can be described by the optical absorption spectrum with the $x$-polarized photons. According to the Kubo formula, the spectrum is expressed by [43, 44]

$$A(\omega) = C \sum_{\alpha, \beta} \int_{-\pi/3a}^{\pi/3a} \left[ f(E_v) - f(E_c) \right] |\langle \Psi_c(k_x) | p_x | \Psi_v(k_x) \rangle|^2 \delta |E_v(k_x) - E_c(k_x) - \omega|^2 + \delta^2 dk_x, \quad (9)$$

where $C$ is a constant determined by the system parameters, $p_x$ is the $x$-component of the momentum operator, $f(E_v)$ is the Fermi–Dirac distribution function in conduction/valence band. At zero temperature, $f(E_v) = 1$ and $f(E_c) = 0$ are taken when the on-site potential $U_{\text{on}}(m, n)$ is chosen symmetrically around the Fermi level ($E_F = 0$). By drawing $A(\omega)$, one can see a GOA peak at a fixed energy point $2\tau$ in all AAMLGNRs with two symmetrical edges.

3. Results and discussion

In this section, we present the numerical examples of the band structure ($E(k_x)$), the SLSs, and the optical absorption spectrum ($A(\omega)$) for a few-layer $(M, N)$-AAMLGNR without and with external electric field, respectively. In our calculations, the nearest-neighbor intralayer hopping $t = 2.57$ eV and the interlayer hopping $\gamma = 0.36$ eV are taken according to the first-principles calculation [45]. The total units of ribbon $L_x = 5001$ and the positive infinitesimal real quantity $\delta = 0.001$ are fixed in the LDOS($\omega$) in equation (8) and the $A(\omega)$ in equation (9).

3.1. SLSs and optical absorption without external electric field

We firstly give the bandgap $\Delta E$ of AAMLGNRs as the function of width ($\sim N$) and thickness ($\sim M$) in figure 2. We find that the ‘$3p$’ conducting rule in the AGNRs [27, 28] only applies to the AAMLGNRs with $p = 1$. As shown in figure 2(a), the $(M, 3)$-AAMLGNR with $N = 3p$ and the $(M, 4)$-AAMLGNR with $N = 3p + 1$ are semiconducting. Naturally, the $(M, 5)$-AAMLGNR with $N = 3p + 2$ is metallic. However, when $p = 2$ is taken, the $(4, 6)$-AAMLGNR with $N = 3p$ and the $(4, 7)$-AAMLGNR with $N = 3p + 1$ are semiconducting while the $(6, 6)$- and $(6, 7)$-AAMLGNRs are metallic. Here, the ‘$3p$’ rule is destroyed. More clearly, when $p \geq 3$ is satisfied, all the $(M, N)$-AAMLGNRs are metallic with gaps $\Delta E = 0$. This is different from the AA-stacked bilayer nanoribbons [36, 37], and is also very different from the AB- and ABC-stacked multilayer nanoribbons [46]. Additionally, the $(M, 3)$- and $(M, 4)$-AAMLGNRs have always large bandgap $\Delta E (\geq 0.2t)$ as shown in figure 2(b). Moreover, the bandgap $\Delta E$ is nearly insensitive to the thickness when $M > 20$ is taken. These results are owing to that the band structure of the $(M, N)$-AAMLGNR is composed of the band structures of $M$-layered $N$-AGNRs. A weak interlayer coupling $\gamma$ between nearest sublayers can cause the subband structures of sublayers to dislocate each other in the AA-stacked types [36, 37]. But it is insufficient to shut off the bandgaps of the $(M, 3)$- and
(M, 4)-AAMLGNRs because the pristine 3- and 4-AGNRs have very large bandgaps $\Delta E > 0.5t$ [28]. Therefore, the (M, 3)- and (M, 4)-AAMLGNRs are stable semiconducting channels which have potential applications as current switch in the molecular devices [47, 48]. Moreover, they can also be produced experimentally in nowadays nanotechnology since a rigid monatomic linear chain of carbon atoms has been successfully carved out from graphene by employing energetic electron irradiation inside a transmission electron microscope [49].

Figure 3 shows the band structure $E(k_x)$ for a set of the pristine AAMLGNRs without external electric field. It is easily seen that all ribbons are metallic since $p = 3$ is taken. However, obviously, only the (5, 11)- and (6, 11)-AAMLGNRs have additional 10- and 12-FBs [the (red) solid lines in figures 3(c) and (d)], respectively, which are merged into many dispersive bands. This property originates from the fact that a $(N, M)$-AAMLGNR is composed of $M$-layered $N$-AGNRs. When $N$ is odd, the two FBs with energies $E = t$ and $-t$ always exist in the band structures of such AGNRs [28, 31]. Accordingly, it is natural to having $2M$-FBs in the $(M, N)$-AAMLGNRs with $N =$ odd number. Moreover, the existence of interlayer coupling with strength $\gamma$ causes the conduction (valence) FBs to discrete symmetrically around $E = t (−t)$. These FBs can induce multiple SLSs at the sites of the odd lines in the AAMLGNRs, which will be marked by the sharp peaks in LDOS($\omega$) discussed as follow.

In figure 4, we display the calculated LDOS($\omega$) at different carbon sites in the (5, 11)-and (6, 11)-AAMLGNRs, respectively. Similar to the monolayer AGNRs [31], a site-selective localization rule exists in these systems. For the (5, 11)-AAMLGNR, we can see that the sharp and high peaks of LDOS appear at the sites of the odd carbon dimer lines (see figure 4(a) for layer 1, (b) for layer 2, and (c) for layer 3). Such peaks are the signs of the SLSs induced by the FBs. Note that the SLSs can change into the compact localized states (CLSs) [50, 51] by gapping the FBs away from the dispersive energy spectrum [52]. The CLSs are ideal candidates for the transmission of information [53]. In contrast, the SLSs vanish at the sites of the even lines (see figure 4(d) for layer 1, (e) for layer 2, and (f) for layer 3). In this case, there are only lower oscillation LDOS peaks due to the Van Hove singularity in quasi-1D systems. This above rule is also applicable to the (6, 11)-AAMLGNR (see figures 4(g)–(i)). Moreover, there also is an FB-selective occupancy rule in the AAMLGNRs with $M =$ odd number. The numbers of the SLSs are unequal at the sites of any sublayer in the (6, 11)-AAMLGNR (figures 4(g) and (i)). In order to understand the two rules, we use Onipko’s approach [54] to obtain the analytical expression of the electronic band structure in the pristine AAMLGNR without external electric field. Hence we have

$$E(k_x) = \pm t \sqrt{1 \pm 4 \cos \left( \frac{\pi j_1}{N + 1} \right) \cos \left( \frac{k_x a}{2} \right) + 4 \cos^2 \left( \frac{\pi j_1}{N + 1} \right) - 2 \gamma \cos \left( \frac{\pi j_2}{M + 1} \right)}, \quad (10)$$

Figure 3. Band structure $E(k_x)$ for pristine AAMLGNRs without external electric field: (a) and (b) for the (5, 10)- and (6, 10)-AAMLGNRs, (c) and (d) for the (5, 11)- and (6, 11)-AAMLGNRs. 

5
Figure 4. Local density of states LDOS(ω) for pristine AAMLGNRs without external electric field: (a)–(f) for the sites in (5,11)-AAMLGNR and (g)–(i) for the sites in (6,11)-AAMLGNR. The notation (m, n, A(B)) represents the A(B) atom sites in layer m and line n.

where \( j_1 = 1, 2, 3, \ldots \), \([N/2]\) and \( j_2 = 1, 2, 3, \ldots, M \) are integers. Here \([N/2]\) means the maximum integer of \( N/2 \), for example, the widths \( N = 10 \) and 11 correspond to the maximum integer \([N/2]=5\) and 6, respectively. The coefficients of the wavefunction component at the sites of the odd lines (\( n = 1, 3, 5, \ldots \)) can be written as

\[
\psi_{A(B)}(k_x, m, n) = C_{A(B)} \sin \left( \frac{2\pi j_1}{N + 1} \left( \left\lfloor \frac{n}{2} \right\rfloor - \frac{1}{2} \right) \right) \sin \left( \frac{\pi m j_2}{M + 1} \right),
\]

and those at the sites of the even lines (\( n = 2, 4, 6, \ldots \)) can be written as

\[
\psi_{A(B)}(k_x, m, n) = D_{A(B)} \sin \left( \frac{2\pi j_1}{N + 1} \left\lfloor \frac{n}{2} \right\rfloor \right) \sin \left( \frac{\pi m j_2}{M + 1} \right),
\]

where the parameters \( C_{A(B)} \) and \( D_{A(B)} \) are structure functions determined by the position of the site and the normalization condition over an unit cell in the AAMLGNR. For the (5,11)-AAMLGNR, when the integer \( j_1 = 6 \) is taken, the FB energies \( E_{FB} = \pm t - 2\gamma \cos(\pi j_2/6) \) with \( j_2 = 1, 2, 3, 4, 5 \) can be derived from equation (10), thus 10-FBs exist in the figure 3(d). Moreover, their corresponding 10-SLSs all appear at sites of the odd lines in layer 1 (see figure 4(a)) since the wavefunction components \( \psi_{A(B)}(k_x, 1, n) \neq 0 \) are satisfied according to equation (11). However, when \( j_2 = 3 \) and \( m = 2 \) are taken, \( E_{FB} = \pm t \) and \( \psi_{A(B)}(k_x, 2, n) = 0 \) are obtained. Accordingly, the SLSs at \( E = \pm t \) disappear in layer 2 (figure 4(b)). Equivalently, the SLSs at \( E = \pm 0.86t \) and \( \pm 1.14t \) disappear in layer 3 (figure 4(c)), which can be deduced from equations (10) and (11) when \( j_2 = 2 \) and \( m = 3, j_2 = 4 \) and \( m = 3 \) are taken, respectively. According to equation (12), it is easily to be found the wavefunction components \( \psi_{A(B)}(k_x, m, n) = 0 \) at \( E_{FB} = \pm t - 2\gamma \cos(\pi j_2/7) \) in equation (10).
Figure 5. Optical absorption spectrum $A(\omega)$ and FB structure $E(k_x)$ without external electric field: (a) for $A(\omega)$ and (b) for $E(k_x)$ in the $(5,11)$-AAMLGNR. Additionally, (c) and (d) exhibit $A(\omega)$ at fixed $\omega = 2t$ with the varying layers $M$ in the $(M,11)$-AAMLGNRs and the varying width $N$ in the $(5,N)$-AAMLGNRs, respectively.

Figure 6. Band structure $E(k_x)$ and local density of states LDOS($\omega$) in $(5,11)$-AAMLGNR under a perpendicular electric field: the top panel for total potential $U = t$, the down panel for total potential $U = 2t$.

Figure 5 shows the optical absorption spectrum $A(\omega)$ and FB structure $E(k_x)$ in the $(M,N)$-AAMLGNRs without external electric field. In figure 5(a), a GOA peak abruptly appears at $\hbar\omega = 2t$ ($\hbar = 1$) (blue solid line), comparing to other peaks (black dash line in figure 5(a1)). This property stems from the electronic excitation from the occupied valence band to the unoccupied conduction band in
Figure 7. Flat-band structure $E(k_x)$ and optical absorption spectrum $A(\omega)$ in (5, 11)-AAMLGNR under a fixed total potential $U$ of perpendicular electric field: (a) and (b) for $U = t$, (c) and (d) for $U = 2t$.

Figure 8. Optical absorption peak of $A(\omega)$ at $\omega = 2t$ in (M, 11)-AAMLGNRs as a function of total potential $U$ under a perpendicular electric field.

an FB-pair with gap $\Delta E = 2t$. As shown in figure 5(b), there are 5-paired FBs with gap $\Delta E = 2t$ in the (5, 11)-AAMLGNRs. Such FB-pair is mainly induced by electrons in a same sublayer of the AAMLGNRs, according to equation (10). Therefore, the superposition effects of the electronic excitations, induced by the FB-pair of the different sublayers, produce the giant absorption peak at $\hbar \omega = 2t$. It is also acceptable that the giant peak increases linearly as the layers $M$ in the (M, 11)-AAMLGNRs (see figure 5(c)) while it is insensitive to the width $N$ in the (5, N)-AAMLGNRs with $N =$ odd number (see figure 5(d)). Accordingly, it is possible to obtain the layer-number of the AAMLAGNR with two symmetrical armchair edges by probing the GOA at $\hbar \omega = 2t$.

3.2. Perpendicular electric-field manipulation on SLSs and optical absorption

Nextly, we turn to a perpendicular electric field manipulation on the above discussed FBs, SLSs, and optical absorption spectrum $A(\omega)$ in the pristine AAMLGNRs. When an uniform electric field with strength $E_z$ is perpendicularly applied to the AAMLGNRs as shown in figure 1(a), all sites in layer $m$ obtain a same potential $U_m = U_1 + (m - 1)(U_M - U_1)/(M - 1)$. Here, potentials $U_M$ and $U_1$ are for the sites of layers $M$ and 1, respectively. To fix the Fermi level $E_F = 0$, we take $U_1 = -U_M$. We choose the total potential $U = 2U_M$ to describe the electric field since the field strength $E_z = U/[(M - 1)de]$ is defined, where $d$ and $e$ are the interlayer distance and electron charge, respectively.

Figure 6 shows the band structure $E(k_x)$ and the LDOS$(\omega)$ under a perpendicular electric field in the (5, 11)-AAMLGNR. Comparing to figure 6(a) with $U = t$ and figure 6(b) with $U = 2t$, an enhancing electric field can widen the bandgaps $\Delta E$ between two nearest conduction (valence) FBs. Therefore, the lowest conduction (highest valence) FB very closes to the Fermi level when $U = 2t$ is taken (figure 6(b)). At
this case, the completeness of FBs remain unchanged. Accordingly, a perpendicular electric field can shift the positions of the SLSs (see the sharp peaks of the LDOS in figures 6(c) and (d)). However, the field manipulation on the strength of the SLSs is complicated. As the total potential $U$ increases, comparing to figures 6(c) and (d), some SLSs become strong, others become weak. Therefore, such electric field can destroy the FB-selective occupancy rule in figure 4. But, the site-selective localization rule in figure 4 is robust against the perpendicular electric field (see from figures 6(c)–(f)).

Figure 7 displays the FB structure $E(k_x)$ and the optical absorption spectrum $A(\omega)$ under a perpendicular electric field in the (5, 11)-AAMLAGNR. Despite the fact that the electric field can shift the FBs, there is still 5-paired FBs with bandgap $\Delta E = 2t$ (figure 7(a)) when the total potential $U = 1t$ is taken. Therefore, the strength of giant absorption $A(\omega)$ at $\omega = 2t$ (figure 7(b)) almost remains unchanged, comparing to the zero-field case in figure 5(a). However, when the potential $U = 2t$ is taken, the FB-pairs with bandgap $\Delta E = 2t$ reduces to 3-pairs (figure 5(c)). As a result, the peak of $A(\omega)$ at $\omega = 2t$ decreases in figure 5(d) by a comparison with figure 5(c). This is reasonable since the other 2-paired FBs with bandgap $\Delta E_1 = 2t$ are located above and down the Fermi level $E_F = 0$, respectively. Electronic excitation in two occupied valence FBs is forbidden. Apparently, such excitation also does not occur in two unoccupied conduction FBs. Motivated on this, we can produce a quantized optical absorption spectrum by driving a perpendicular electric field as shown in figure 8.

Figure 8 displays the optical absorption spectrum $A(\omega)$ at $\omega = 2t$ as the function of the total potential $U$ in the (M, 11)-AAMLAGNRs. One can see that a conspicuous set of quantized steps exists in this system. For instance, in the (10, 11)-AAMLAGNR, the potential $U$ varies away 0, the spectrum $A(\omega)$ at $\omega = 2t$ (figure 8(a)) abruptly jumps down from 10.4 to 8.4, where $A(\omega)$ at $\omega = 8.4$ is the absorption peak of the (8, 11)-AAMLAGNR at the zero case (figure 8(a)). Continually, steps $A(\omega)$ at $\omega = 6.3$ of the (6, 11)-AAMLAGNR and $A(\omega)$ at $\omega = 4.2$ of the (4, 11)-AAMLAGNR (figure 8(b)) appear one by one. Similarly, the peak $A(\omega)$ of the (9, 11)-AAMLAGNR at the zero electric field can degenerate into that of the (7, 11)-AAMLAGNR, of the (5, 11)-AAMLAGNR, and of the (3, 11)-AAMLAGNR. Accordingly, it is possible that the giant absorption peaks of the (10, 11)- and (9, 11)-AAMLAGNRs collapse to the cases of bilayer and monolayer AGNRs, respectively.
3.3. Parallel electric-field manipulation on SLSs and optical absorption

Lastly, we discuss a parallel electric field manipulation on the above discussed FBs, SLSs, and optical absorption spectrum \( A(\omega) \) in the pristine AAMLGNRs. When an uniform electric field with strength \( E_p \) is applied and parallel to the layer-planes (figure 1(b)), different potentials \( U_n = U_1 + (n-1)(U_N - U_1)/(N-1) \) are given to the sites of different lines \( n \) in every sublayer, where potentials \( U_N \) and \( U_1 \) are for lines \( N \) and 1, respectively. To fix the Fermi level \( E_F = 0 \), we take \( U_1 = -U_N \). Additionally, we choose the total potential \( U = 2U_N \) to describe the electric field since the field strength \( E_p = 2\sqrt{U}/[3(N-1)\alpha] \) is defined.

Figure 9 exhibits the results of above manipulations in the (5, 11)-AAMLGNR. The parallel electric field gives the different potentials \( U_n \) to the sites of the different line \( n \) in the same sublayer \( m \), but the same on-site potential distribution exists in the different sublayers. Therefore, we can see that the completeness of FBs are destroyed more and more severely with the increase of the total potential \( U \) (see figures 9(a) and (b)), but the FB positions remain unchanged by a comparison with the case of the zero electric field (figure 3(c)). Correspondingly, the positions of SLSs are also very stable. Their peaks become lower as the potential \( U \) increases (see figures 9(c) and (d)). Specifically, when the potential \( U = 1t \) is taken, the SLSs are indistinguishable because they have hidden into other electron states (figure 9(d)). Therefore, the parallel electric field can suppress the SLSs and hide them, which may be useful in the secure transmission of information by hiding data [55]. Here, the sharp peak of the giant optical absorption \( A(\omega) \) at \( \omega = 2t \) also is strongly suppressed by the parallel electric field, comparing figure 9(e) with \( U = 0.5t \) to figure 5(a) with \( U = 0 \). As expected, when a strong electric field with \( U = 1t \) is taken, such peak disappears nearly (figure 9(f)). Therefore, the strength of the giant optical absorption is tunable by driving a parallel electric field, but its position is robust against such field.

4. Summary

In this paper, we have theoretically studied the band structure, the local density of states and the optical-absorption spectrum in the pristine \((M, N)\)-AAMLGNRs by using the tight-binding model. The ‘3p’ conducting rule of the AGNRs only applies to the AAMLGNRs with \( p = 1 \). It is said that the \((M, 3)\)- and \((M, 4)\)-AAMLGNRs are semiconducting, and the \((M, 5)\)-AAMLGNR is metallic. Moreover, their bandgaps are very large and insensitive to the thickness \( M \), which should be useful as a narrow semiconducting channel in the molecular devices. When the integer \( p > 2 \) is taken, all AAMLGNRs are metallic. Interestingly, 2M-FBs exist in the \((M, N)\)-AAMLGNRs with two symmetrical edges, i.e. \( N \) is an odd number. Moreover, they are complete. A site-selective localization rule exists in this system. Namely, these complete FBs induce the SLSs at the sites of the odd lines in every sublayer, which can be exhibited by the sharp peaks of the LDOSs at the corresponding sites. An FB-selective occupancy rule also exists in this system. Namely, in the \((M, N)\)-AAMLGNRs with \( M = \) odd number, electrons in different sublayers occupy different FBs, which has been revealed by the different number of the sharp peaks in the SLSs. A giant optical absorption abruptly appears and holds at the energy point \( h\omega = 2t \) (\( h = 1 \)), which’s strength is determined mainly by the number of the layers of AAMLGNRs.

Additionally, the completeness of the FBs are robust against the perpendicular electric field but their positions can be shifted. The FB-selective occupancy rule in the zero field is destroyed. Some SLSs become increasingly strong while others become decreasingly weak as the total potential \( U \) increases. The giant optical absorption at \( \omega = 2t \) is relatively stable under a suitable electric field. However, by adjusting the potential \( U \), the giant optical absorption of the \((M, N)\)-AAMLGNR can collapse to the zero-field cases of the \((M-2, N)\)-AAMLGNR, \((M-4, N)\)-AAMLGNR, . . . , in turn. Resultantly, a quantized steps of absorption spectrum is observed in this system. On the contrary, by applying a parallel electric field, the positions of the FBs remain unchanged while their completeness is destroyed. The SLSs and the giant optical absorption become increasingly weak. The position of the giant absorption at \( \omega = 2t \) is also robust against such electric fields. The SLSs can change into the CLSs by gapping the FBs away from the dispersive energy spectrum. Therefore, such AAMLGNRs may be ideal candidates for the transmission of information. These systems may also be excellent candidates for the design of the controllable optical-electric FB-devices since the giant optical absorption exists and is tunable. It needs to be pointed out that the SLSs and GOA do not appear in the antisymmetrical AAMLGNRs with even dimer lines in width since there are no FB in their band structures.

It is worth mentioning that to enhance the stability of the graphene nanoribbons, the carbon atoms at the two edges are often passivated by other atoms such as the hydrogen- and oxygen-passivations [56]. For the \( H \)-passivated case, an \textit{ab initio} calculation shows that the bond lengths at the edges, parallel to dimer lines, are shortened by 3.3\%–3.5\% for the 12-, 13-, and 14-AGNRs as compared to those in the middle of the ribbon [57]. A 3.5\% decrease would cause the nearest-neighbor hopping energy at the edges \( t_1 = 1.12t \)}
Our calculations find that the multiple FBs, SLSs, and GOA also exist in the \(H\)-passivated AAMLAGNRs with two symmetrical edges (no show here). The edge passivations change their positions and values, but not inherently.

Acknowledgments

The authors are thankful for the National Natural Science Foundation of China under Grant Nos. (11347009, 11804092 and 12174100), the Hunan Provincial Natural Science Foundation under Grant No. 14JJ2130.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

ORCID iDs

Guanghui Zhou @ https://orcid.org/0000-0002-1536-3440

References

[1] Lieb E H 1989 Two theorems on the Hubbard model Phys. Rev. Lett. 62 1201–4
[2] Mielke A 1991 Ferromagnetic ground states for the Hubbard model on line graphs J. Phys. A: Math. Gen. 24 L73–7
[3] Tasaki H 1992 Ferromagnetism in the Hubbard models with degenerate single-electron ground states Phys. Rev. Lett. 69 1608–11
[4] Weeks C and Franz M 2010 Topological insulators on the Lieb and perovskite lattices Phys. Rev. B 82 085310
[5] Volokh G E 2011 Flat band in the core of topological defects: bulk-vortex correspondence in topological superfluids with Fermi points JETP Lett. 93 66–9
[6] Tang E, Mei J-W and Wen X-G 2011 High-temperature fractional quantum Hall states Phys. Rev. Lett. 106 236802
[7] Sun K, Gu Z, Katsura H and Sarma S D 2011 Nearly flatbands with nontrivial topology Phys. Rev. Lett. 106 236803
[8] Neupert T, Santos L, Chamoun C and Mudry C 2011 Fractional quantum Hall states at zero magnetic field Phys. Rev. Lett. 106 236804
[9] Tang E and Fu L 2014 Strain-induced partially flat band, helical snake states and interface superconductivity in topological crystalline insulators Nat. Phys. 10 964–9
[10] Iglovikov V I, Hidbert F, Gr"enmaud B, Batrouni G G and Scalettar R T 2014 Superconducting transitions in flat-band systems Phys. Rev. B 90 094506
[11] Balents L, Dean C R, Efetov D K and Young A F 2020 Superconductivity and strong correlations in moiré flat bands Nat. Phys. 16 725
[12] Kimura T, Tamura H, Shiraishi K and Takayanagi H 2002 Magnetic-field effects on a two-dimensional Kagomé lattice of quantum dots Phys. Rev. B 65 081307
[13] Goda M, Nishino S and Matsuda H 2006 Inverse Anderson transition caused by flatbands Phys. Rev. Lett. 96 126401
[14] Nitta M, Ostahie B and Aldo A 2013 Spectral and transport properties of the two-dimensional Lieb lattice Phys. Rev. B 87 125428
[15] Vicenzi R A, Cantillano C, Morales-Inostroza L, Real B, Mejía-Cortés C, Weimann S, Sazeait I and Molina M I 2015 Observation of localized states in Lieb photonic lattices Phys. Rev. Lett. 114 245403
[16] Mukherjee S, Spracklen A, Choudhury D, Goldman N, Öhberg P, Andersson E and Thomson R R 2015 Observation of a localized flat-band state in a photonic Lieb lattice Phys. Rev. Lett. 114 245404
[17] Masumoto N, Kim N Y, Byrnes T, Kusudo K, Löffler A, Höfling S, Forchel A and Yamamoto Y 2012 Exciton-polariton condensates with flat bands in a two-dimensional Kagome lattice New J. Phys. 14 065002
[18] Zong Y, Xia S, Tang L, Song D, Hu Y, Pei Y, Su J, Li Y and Chen Z 2016 Observation of localized flat-band states in Kagome photonic lattices Opt. Express 24 8877–85
[19] Nidiso N, Goda M and Kusakabe K 2003 Flat bands of a tight-binding electronic system with hexagonal structure J. Phys. Soc. Japan 72 2015–23
[20] Wu S, Bergman D, Balents L and Sarm D S 2007 Flat bands and Wigner crystallization in the honeycomb optical lattice Phys. Rev. Lett. 99 070401
[21] Misumi T and Aoki H 2017 New class of flat-band models on tetragonal and hexagonal lattices: gapped versus crossing flat bands Phys. Rev. B 96 155137
[22] Barreteau C, Ducastelle F and Mallah T 2017 A bird’s eye view on the flat and conic band world of the honeycomb and Kagome lattices towards an understanding of 2D metal-organic frameworks electronic structure J. Phys.: Condens. Matter. 29 465302
[23] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 Electric field effect in atomically thin carbon films Science 306 666–9
[24] Liang G, Neophytou N, Lundstrom M S and Nikonov D E 2007 Ballistic graphene nanoribbon metal-oxide-semiconductor field-effect transistors: a full real-space quantum transport simulation J. Appl. Phys. 102 054307
[25] Li X, Wang X, Zhang L, Lee S and Dai H 2008 Chemically derived, ultrasmooth graphene nanoribbon semiconductors Science 319 1229–32
[26] Wang X, Ouyang Y, Li X, Wang H, Guo J and Dai H 2008 Room-temperature all-semiconducting sub-10 nm graphene nanoribbons field-effect transistors Phys. Rev. Lett. 100 206803
[27] Miyamoto Y, Nakada K and Fujita M 1999 First-principles study of edge states of H-terminated graphitic ribbons Phys. Rev. B 59 9858–61
[28] Nakada K, Fujita M, Dresselhaus G and Dresselhaus M S 1996 Edge state in graphene ribbons: nanometer size effect and edge shape dependence Phys. Rev. B 54 17954–61
[29] Karamitaheri H, Neophytou N, Pourfath M, Faez R and Kosina H 2012 Engineering enhanced thermolectric properties in zigzag graphene nanoribbons J. Appl. Phys. 111 054501
[30] Lee K W and Lee C E 2017 Dissipationless spin-valley current in zigzag-edge graphene ribbons with a net magnetization Phys. Rev. B 95 195132
[31] Lin H H, Hikihara T, Jeng H T, Huang B L, Mou C Y and Hu X 2009 Ferromagnetism in armchair graphene nanoribbons Phys. Rev. B 79 035405
[32] Lee J K, Lee S C, Ahn J P, Kim S C, Wilson J I B and John P 2008 The growth of AA graphite on (111) diamond J. Chem. Phys. 129 234709
[33] Liu Z, Suenaga K, Harris P J F and Iijima S 2009 Open and closed edges of graphene layers Phys. Rev. Lett. 102 015501
[34] Borysiuk J, Sołys J and Piechota J 2011 Stacking sequence dependence of graphene layers on SiC (0001) experimental and theoretical investigation J. Appl. Phys. 109 093523
[35] Zhong X, Pande R and Karna S P 2012 Stacking dependent electronic structure and transport in bilayer graphene nanoribbons Carbon 50 784–90
[36] Mohammadi Y and Nia B A 2015 Electronic properties of graphene nanoribbons with AA-stacking order Solid State Commun. 201 76–81
[37] Chen X, Shi Z, Xiang S, Song K and Zhou G 2017 Finite-size effects on electronic structure and local properties in passivated AA-stacked bilayer armchair-edge graphene nanoribbons J. Phys.: Condens. Matter. 29 085301
[38] Morell E S, Vergara R, Pacheco M, Wilson J I B and Chico L 2014 Electronic properties of twisted bilayer nanoribbons Phys. Rev. B 89 205403
[39] Wakabayashi K, Sasaki K, Nakanishi T and Enoki T 2010 Electronic states of graphene nanoribbons and analytical solutions Sci. Technol. Adv. Mater. 11 054504
[40] Guassi M R, Diniz G S, Sandler N and Qu F 2015 Zero-field and time-reversal-symmetry-broken topological phase transitions in graphene Phys. Rev. B 92 075426
[41] Mandal S and Herbut I F 2021 p-wave superconductivity and the axiplanar phase of triple-point fermions Phys. Rev. B 104 L180507
[42] Gorbar E V, Gusynin V P and Oriekhov D O 2021 Gap generation and flat band catalysis in dice model with local interaction Phys. Rev. B 103 155135
[43] Chang C P, Huang Y C, Lu C L, Ho J H, Li T S and Lin M F 2006 Electronic and optical properties of a nanographite ribbon in an electric field Carbon 44 508–15
[44] Hsu H and Reichl L E 2007 Selection rule for the optical absorption of graphene nanoribbons Phys. Rev. B 76 045418
[45] Charlier J C, Michenaud J P and Gonze X 1992 First-principles study of the electronic properties of simple hexagonal graphite Phys. Rev. B 46 4531–9
[46] Sahu B, Min H and Banerjee S K 2010 Effects of edge magnetism and external electric field on energy gaps in multilayer graphene nanoribbons Phys. Rev. B 82 115426
[47] Yan Q, Huang B, Yu J, Zheng F, Zang J, Wu J, Gu B-L, Liu F and Duan W 2007 Intrinsic current—voltage characteristics of graphene nanoribbon transistors and effect of edge doping Nano Lett. 7 1469–73
[48] Nozaki D, Sevinçli H, Li W, Gutiérrez R and Cuniberti G 2010 Engineering the figure of merit and thermopower in single-molecule devices connected to semiconducting electrodes Phys. Rev. B 81 235406
[49] Jin C, Lan H, Peng L, Suenaga K and Iijima S 2009 Deriving carbon atomic chains from graphene Phys. Rev. Lett. 102 205501
[50] Röntgen M, Morfonios C V, Brouzos I, Diakonos F K and Schmelcher P 2019 Quantum network transfer and storage with compact localized states induced by local symmetries Phys. Rev. Lett. 123 080504
[51] Maimaiti W, Hlach S and Andreanov A 2019 Universal d = 1 flat band generator from compact localized states Phys. Rev. B 99 125129
[52] Ramachandran D, Danieli C and Flach S 2018 Fano resonances in flat band networks (arXiv:1801.03210 [cond-mat])
[53] Vicenço R A, Cantillano C, Morales-Inostroza L, Real B, Mejia-Cortés C, Weimann S, Szameit A and Molina M I 2015 Observation of localized states in Lieb photonic lattices Phys. Rev. Lett. 114 245403
[54] Onipko A 2008 Spectrum of π electrons in graphene as an alternant macromolecule and its specific features in quantum conductance Phys. Rev. B 78 245412
[55] Ariz D 2001 Digital steganography: hiding data within data IEEE Internet Comput. 5 75–80
[56] Peng X and Velasquez S 2011 Strain modulated band gap of edge passivated armchair graphene nanoribbons Appl. Phys. Lett. 98 023112
[57] Son Y-W, Cohen M I and Louie S G 2006 Energy gaps in graphene nanoribbons Phys. Rev. Lett. 97 216803
[58] Porezag D, Frauenheim T, Köhler T, Seifert G and Kaschner R 1995 Construction of tight-binding-like potentials on the basis of density-functional theory: application to carbon Phys. Rev. B 51 12947–57