Enhancement of thermoelectric performance of a nanoribbon made of $\alpha - T_3$ lattice

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Received 27 June 2019, revised 29 July 2019
Accepted for publication 16 August 2019
Published 6 September 2019

Abstract

We present electronic and transport properties of a zigzag nanoribbon made of $\alpha - T_3$ lattice. Our particular focus is on the effects of the continuous evolution of the edge modes (from flat to dispersive) on the thermoelectric transport properties. Unlike the case of graphene nanoribbon, the zigzag nanoribbon of $\alpha - T_3$ lattice can host a pair of dispersive edge modes at the two valleys for specific width of the ribbon. Moreover, gap opening can also occur at the two valleys depending on the width. The slope of the dispersive edge modes and the energy gap strongly depend on the relative strength of two kinds of hoping parameters present in the system. We compute corresponding transport coefficients such as conductance, thermopower, thermal conductance and the thermoelectric figure of merits by using the tight-binding Green function formalism, in order to explore the roles of the dispersive edge modes. It is found that the thermopower and thermoelectric figure of merits can be enhanced significantly by suitably controlling the edge modes. The figure of merits can be enhanced by thirty times under suitable parameter regime in comparison to the case of graphene. Finally, we reveal that the presence of line defect, close to the edge, can cause a significant impact on the edge modes as well as on electrical conductance and thermopower.

Keywords: thermoelectric, nanoribbon, two dimensional system

(Some figures may appear in colour only in the online journal)

1. Introduction

The discovery of graphene [1, 2] has boosted the search of graphene-like two-dimensional Dirac materials because of their peculiar band structure and possible technological applications. The electronic properties of Dirac materials are described by the linear band dispersion in low energy regime. The $T_3$ or dice lattice [3] is the graphene-like 2D material with an additional atom at the centre of hexagon. One of the unique feature of such material is that its quasi particles exhibit higher pseudo spin $S = 1$ states [3] unlike 1/2 in graphene. Apart from it, the additional atom in the $T_3$ lattice causes dispersionless flat band at each valley in addition to the Dirac cones [3]. In recent times, much attention have been paid on such Dirac–Weyl materials with higher spin states, $S = 1, 3/2, 2$, etc [4–7], in order to reveal the roles of the additional atom.

The $T_3$ lattice (pseudo spin $S = 1$) can be smoothly interpolated to the graphene (pseudo spin $S = 1/2$) by using the $\alpha - T_3$ model. Here, $\alpha$ is related to the strength of the hopping between the central atom to its nearest neighbors and ranges from ‘0’ (graphene) to ‘1’ (dice lattice or $T_3$) lattice. It has recently been shown in Hg$_{1-x}$Cd$_x$Te that this material can be mapped to $\alpha - T_3$ model [4] with $\alpha = 1/\sqrt{3}$ under the suitable doping concentration. The continuous evolution from graphene to dice lattice by using $\alpha - T_3$ model has been extensively exploited in unusual Hall conductivity [8, 9], Weiss oscillation [10], Klein tunneling [11, 12], optical [4, 13–16] properties, irradiation effects [17], topological properties [18]
and wave packet dynamics [19]. However, most of the study of transport properties in the $\alpha - T_3$ lattice are limited to the bulk in spite of the fact that electronic band structure as well as the transport phenomena are very sensitive to the edge geometry of honeycomb lattice [2, 16].

The thermoelectric properties of material [20] have been always under active consideration among research community for its ability to probe the electronic system and potential technological applications [21, 22]. The thermal gradient across the two ends of an electronic system can drive charge carriers from hotter to cooler end and can generate a voltage gradient across these two ends-known as thermopower (S) per unit temperature gradient. Apart from the thermal transport in the bulk of 2D hexagonal lattice [23–27], several works have demonstrated that thermoelectric performance can be further improved by considering nanoribbon of graphene [28, 29] or black phosphorus [30, 31].

In this work, we first address the energy band dispersion of the nanoribbon of such material by using tight binding method. Here, we particularly focus on zigzag edge only as it hosts a pair of edge modes. We observe that unlike the case of graphene, the zigzag nanoribbon of $\alpha - T_3$ exhibits gapless dispersive edge modes (chiral edge modes) for width of $N = 3q + 1$ ($q$ is the positive integer). On the other hand, the edge modes are gapped for the width $N \neq 3q + 1$. This is in contrast to the case of a zigzag ribbon of graphene [2] where edge modes are dispersionless, gapless and not chiral. Subsequently we use tight-binding Green function approach to obtain the conductance, thermopower and thermoelectric figure of merits of such ribbon. We found that thermopower and figure of merits can be enhanced significantly by controlling the features of edge modes by means of $\alpha$. Finally, we discuss the effects of line defects on edge modes and transport properties.

The paper is organized as follows: in section 2, we discuss the tight-binding Hamiltonian and energy band dispersion for zigzag nanoribbon. A brief review of the tight-binding Green function formalism for the evaluation of transport coefficients are presented in section 3. In section 4 we present our numerical results and discussions. Finally, we summarize our results and conclude in section 5.

2. Tight binding Hamiltonian and energy dispersion

In this section, we first present a brief description of the lattice geometry of the $\alpha - T_3$ lattice. This lattice mimics the geometry of graphene monolayer with an additional atom at the centre of the hexagon. A typical sketch of its hexagon is shown in the figure 1. It has two different hoping parameters. The hoping parameter between A and B sublattices is denoted $t'$ whereas $\alpha t$ is between the sublattice C and B. The tight-binding Hamiltonian of this lattice, without any spin-orbit coupling is given by

$$H_0 = \sum_{<ij>} t_{ij} c_i^\dagger c_j + \sum_{<ij>} t'_{ij} c_i^\dagger c_j + \text{h.c.},$$

where the summation index $i, j$ and $l$ run over $A, B$ and $C$ sublattices. The relevant hoping parameters are $t_{ij} = t$ and $t_{ij} = \alpha t$. The creation (annihilation) operators at $i$th site are denoted by $c_i^\dagger$ ($c_i$).

However, we briefly comment here that the Hamiltonian in the continuum model inside the bulk without any boundary can be written in three sublattice space as [7]

$$H_0 = \begin{bmatrix} 0 & g_p \cos \phi & 0 \\ g_p^* \cos \phi & 0 & g_p \sin \phi \\ 0 & g_p^* \sin \phi & 0 \end{bmatrix}. \quad (2)$$

Here, $g_p = v_F (\xi p_x - ip_y)$ where $\xi = \pm$ denotes the two valleys $K$ and $K'$, respectively. $p = (p_x, p_y)$ is the 2D momentum vector and $v_F$ is the Fermi velocity. Note that, the angle $\phi$ is related to the $\alpha$ as $\phi = \tan^{-1} \alpha$. The energy dispersion of the above Hamiltonian is linear as $E_{k,\lambda} = \lambda h v_F k$, with $\lambda = \pm$ correspond to band index, with an additional dispersionless branch as shown in figure 2. It is also worthwhile to mention that the central atom does not play any role in the conic bands except the appearance of dispersionless flat band. However, in presence of magnetic field the C atoms (and hence $\alpha$) can lift valley degeneracy in the Landau levels [8, 9] as well as can give rise to the unusual Hall conductivity. This is in contrast to the graphene where the Landau levels at two valleys are identical (degenerate).

In the present study, we particularly focus on such lattice with finite width (nanoribbon), which has not been considered previously in the context of transport. The nanoribbon is considered to be infinitely extended along the $x$-direction with a finite width along the $y$-direction. The nanoribbon can be thought as a linear chain made of iterative unit cells as shown by the rectangular shaped orange shadowed region in figure 3. The width of the nanoribbon is given by $N$-the number of atoms per unit cell. To study the transport properties, we consider a two terminal device which consists of three regions as shown in the figure 3. The central region is made of zigzag ribbon which is attached to the left and right identical leads. The locations of all the unit cells forming the left and right leads are at $-\infty, -1, 0$ and $M, M + 1, \ldots, \infty$, respectively. Whereas the central regions are composed of the unit

![Figure 1. Schematic of the hexagon of $\alpha - T_3$ lattice. Three different colors are used to denote three sub-lattices, i.e. A (red), B (green) and C (blue). The two different hoping terms $t$ and $\alpha t$ are denoted by blue and magenta lines, respectively.](image-url)
cells at 1, 2, 3...M. By implementing Bloch’s theorem, total Hamiltonian of the device can be written as

\[ H_{k} = H_{00} + H_{-10}e^{-ikx}a + H_{01}e^{ikx}a, \]  

(3)

where \( H_{00} \) is the on-site energy matrix of the unit cell at site 0. On the other hand, \( H_{01} \) or \( H_{-10} \) denotes the coupling matrix between the left and right adjacent unit cells. Here, \( a \) is the unit cell separation. The numbering of atoms in each unit cell is shown in figure 4, in order to construct the Hamiltonian matrix. The momentum (\( k_x \)) along the x-direction is conserved as the ribbon is translationally invariant along this direction.

We solve numerically the above equation to obtain the energy dispersion of the nanoribbon and plotted in figure 5. We observe that edge modes (sky blue line) can be gapless dispersive or gapped depending on the width. The gapless chiral edge modes appear for the width \( N = 3q + 1 \), otherwise gapped. The hoping parameter between \( B \) and \( C \) sublattices are taken corresponding to \( \alpha = 0.4 \) in both cases. The figures 5(a) and (d) show gapless chiral edge modes for the widths \( N = 40 \) and 43 which satisfy the condition of width \( N = 3q + 1 \) and of course both edges are composed of \( A \) and \( B \) sublattices only. On the other hand, figures 5(b) and (c) exhibit a pair of gapped edge modes for widths \( N = 41 \) and 42 (i.e. when width \( N \neq 3q + 1 \)). Note that the crossing of the edge modes for gapless dispersion is the outcome of the additional hoping parameter due to the presence of \( C \) sublattices in addition to the usual three nearest neighbor sublattices.

Now we examine how the variation of \( \alpha \) affects the features of chiral and gapped edge modes. First, we plot the energy dispersion for different values of \( \alpha \) in figure 6. The figure 6(a) is plotted for \( \alpha = 0 \) and it enforces edge modes to collapse on the dispersionless flat band. Note that the width \( N = 40 \) is corresponding to the case of non-identical edges for \( \alpha = 0 \) i.e. one edge is zigzag and another one is Klein-edge shape as named in [32]. In such case a gap can be seen between flat band and other transverse modes which is also in agreement with the results based on the Harper equation in [16] and analytical work in [33]. With the increase of \( \alpha \), edge modes emerges and exhibit dispersive feature (see figure 6(b)) and the slope of which increases further with \( \alpha = 1.0 \) as shown in figure 6(c). This slope actually gives rise to the non-zero group velocity and hence induces significant contribution to the transport properties.
To recover the spectrum of zigzag nanoribbon of graphene, we must make sure that both edges are composed of A and B sublattices which corresponds to the case of $\alpha = 0$ and width $N = 41$. The figure 7(a) is plotted for these parameters, which shows the dispersionless edge modes as in graphene nanoribbon except the presence of the flat band. Note that the flat band corresponds to the presence of C sublattices. We plot the same for $\alpha = 0.5$ in figure 7(b) which shows that a gap opening occurs between the edge mode and the zero energy flat band. This gap opening increases slowly with the further increase of $\alpha$ as shown in figure 7(c).

Note that we are not considering the case of armchair edged ribbon as it does not give any new feature to the band dispersions in comparison to the armchair edged graphene [2, 33].

### 3. Basic formalism of TB Green function approach

In this section, we discuss the formalism to calculate different transport coefficients under thermal/potential gradient. Let a temperature gradient of $\nabla T$ is applied between the left and right lead, which induces a voltage gradient $\nabla V$. Following the most conventional approach at low temperature regime, the electrical current density $J$ and the thermal current density $J_q$ can be written by following Onsager relation [34, 35]

$$J^q = Q^{11} E + Q^{12} (-\nabla T),$$

where $E$ is the electric field and $Q^{ij}$ ($i,j = 1, 2$) are the phenomenological transport coefficients which can be expressed in terms of an integral $L(\nu)$.

$$Q^{11} = L_0, \quad Q^{21} = TQ^{12} = -\frac{L_1}{e},$$

$$Q^{22} = \frac{L_2}{e^2 T}.$$  

(6)

where $\nu = 0, 1, 2$ and $f(E) = [1 + \exp(E - \mu)/k_B T]^{-1}$ is the Fermi–Dirac distribution function with $\mu$ being the chemical potential. Here, $T(E)$ is the energy-dependent transmission amplitude. Thermopower can be defined under open circuit condition $(J = 0)$ as [36–41]

$$S = \frac{Q^{12}}{Q^{11}} = -\frac{1}{eT} \frac{L_1}{L_0}.$$  

(7)

On the other hand, the electronic contribution to the thermal conductance [40, 41] can be written as

$$\kappa_e = \frac{1}{N} [L_2 - L_1 (L_0)^{-1} L_1].$$  

(8)

The thermoelectric performance of a material is quantified by a parameter known as thermoelectric figure of merits and it is given by [40, 41]

$$\frac{ZT}{\kappa_e} = \frac{S^2 G_T T}{\kappa_e} = \frac{L_1^2}{L_0 L_2 - L_1^2}.$$  

(9)
Here, $G_T = (e^2/h)\mathcal{L}_0$ is the energy dependent electrical conductance following Landauer–Buttiker formula at non-zero temperature. Here, in the expression of ZT, thermal conductance is taken to be electronic contribution only. The phonon/lattice contribution can be suppressed under very low or very high temperature. One of the key ingredients in all the above equations is the energy dependent transmission probability $T(E)$. In order to obtain $T(E)$ for a nanoribbon of this lattice, we shall use the well known tight-binding Green function approach. We first give a brief review of this formalism which was developed by Sancho [42] to study the transfer matrices and spectral density of states at the surface of a semi infinite crystal made of stacked layers. This approach can be used in the hexagonal lattice too, where each supercell acts as independent layer. The method has been already used in several hexagonal lattices like graphene [43], silicene [44], MoS$_2$ [45], phosphorene [46] etc. It is also worthwhile to mention at this stage that electron–electron Coulomb interaction can play significant role in nanoribbon geometry which requires many-body Green function GW approximation approach [47] or DFT method [48] and will not be considered here.

Our device is composed of three regions, the central region, the left lead and right lead as shown in figure 3. As the left and right leads are identical, we can write $\mathcal{H}_{MM} = \mathcal{H}_{00}$ and $\mathcal{H}_{M+1} = \mathcal{H}_{-10}$. By implementing transfer matrix approach, the surface Green function can be written as

$$G_{00}^L(E) = [(E + i\eta)I - \mathcal{H}_{00} - \mathcal{H}_{-10}^\dagger\Lambda]^{-1},$$

and

$$G_{00}^R(E) = [(E + i\eta)I - \mathcal{H}_{00} - \mathcal{H}_{10}^\dagger\bar{\Lambda}]^{-1},$$

where $I$ is identity matrix. The notations $\Lambda$ and $\bar{\Lambda}$ in above two equations can be evaluated as

$$\Lambda = c_0 + c_0c_1 + \bar{c}_0\bar{c}_1c_2 + .... + \bar{c}_0\bar{c}_1\bar{c}_2...c_l$$

and

$$\bar{\Lambda} = \bar{c}_0 + c_0\bar{c}_1 + c_0c_1\bar{c}_2 + .... + c_0c_1c_2...\bar{c}_l,$$

where $c_0$ and $\bar{c}_0$ are defined as

$$c_0 = [(E + i\eta)I - \mathcal{H}_{00}]^{-1}\mathcal{H}_{10}^\dagger,$$

and

$$\bar{c}_0 = [(E + i\eta)I - \mathcal{H}_{00}]^{-1}\mathcal{H}_{-10}.$$  

The summation in equations (12) and (13) has to be taken until $c_1$ and $\bar{c}_1$ reach to zero. The main advantage of this technique is that $2^l$ unit cells can be captured by just performing $l$ iteration. Now we calculate surface Green function $G_{22}$ by using the following recursion formula

$$G_{mn}^R = [(E + i\eta)I - \mathcal{H}_{mm} - \mathcal{H}_{m+1}^\dagger\mathcal{G}_{m+1}^R\mathcal{H}_{m+1}]^{-1}. $$

The effects of the left and right leads can be finally incorporated into the total Green function via self energy as

$$G_{11} = [(E + i\eta)I - \mathcal{H}_{11} - \Sigma_L - \Sigma_R]^{-1},$$

with

$$\Sigma_L = \mathcal{H}_{01}^\dagger\mathcal{G}_{00}\mathcal{H}_{01},$$

and

$$\Sigma_R = \mathcal{H}_{12}^\dagger\mathcal{G}_{22}\mathcal{H}_{12}. $$

Now we can define broadening matrix as

$$\Gamma_{L(R)} = i(\Sigma_{L(R)} - \Sigma_{L(R)}^\dagger),$$

which gives the transmission probability

$$T(E) = \text{Tr}[\Gamma_LG_{11}\Gamma_R(G_{11})^\dagger].$$

Finally, using the Landauer–Buttiker formula, we obtain the electrical conductance as

$$G = \frac{e^2}{h} T(E)$$

at zero temperature which subsequently leads to the temperature dependent conductance in terms of $\mathcal{L}_\nu$ as follows:
Figure 9. Conductance for (a) $\alpha = 0.2$ and (b) $\alpha = 0.6$. The width is $N = 41$ in both cases.

$$G_T = \frac{e^2}{h} \mathcal{L}_0.$$  \hfill (25)

4. Numerical results and discussion

In this section, we present all transport coefficients numerically. First, we evaluate the conductance by using equation (24) and plot it with respect to the energy dispersion for $\alpha = 0.2$ in figure 8(a). Here, we keep the width $N = 3q + 1$ with $q$ being the positive integer, in order to capture the gapless chiral edge modes. The conductance appears to be quantized as $2e^2/h$ (r being the positive integer) with the ‘2’ factor attributes to the two valleys. The integer ‘r’ accounts the number of transverse modes (black line) including the edge modes. With the increase of chemical potential, transverse modes start to penetrate through the chemical potential one by one, leading to the increase of conductance. Each transverse modes contributes conductance by 2 units. However, an unusual behavior is also seen in the region $0.4 \leq E/t \leq 0.4$ where edge modes (sky blue line) reside. Note that the pair of edge modes gives rise to the quantized conductance of $2e^2/h$ unit before stepping down by one unit. This happen at a region where edge modes and 1st transverse modes interfere each other. A central peak in the conductance emerges corresponding to the dispersionless flat band. Similar peak resembles the divergence in dc bulk conductivity of such lattice under clean limit due to interband scattering [49], at the band touching point between the flat band and the conic band. We find almost similar feature for $\alpha = 0.6$, as shown in figure 9(b), except edge modes contribute for a wide range of energy.

Now we explore how the conductance gets affected by changing $\alpha$ for the gapped dispersion. To keep the band dispersion gapped, we take the width of the ribbon $N \neq 3q + 1$ (41 and 43). The conductance is plotted against the gapped energy dispersion as a function of chemical potential in figure 9. It is already shown in figure 7 that the band gap increases slowly with the increase of $\alpha$. This fact has a direct impact on the conductance, as shown in figure 9, in terms of widening the zero conductance region with the increase of $\alpha$. This is a direct signature of the gap opening in transport measurement in a zigzag edge nanoribbon of such material provided the width has to be other than $N = 3q + 1$. Note that the degenerate flat bands also induce a central peak in the conductance spectra, however its height varies with the strength of $\alpha$. Another noticeable point here is that although the conductance steps down by unity in case of $\alpha = 0.2$ at $E/t = \pm 0.2$, it disappears for $\alpha = 0.6$. The origin of it can be attributed to the peculiar feature of the edge modes in the region $1.2 < \frac{k_F a}{\hbar c} < 2.5$ in both cases.

Now we plot thermopower by using equation (7) in figure 10. We consider both cases i.e. gapless and gapped dispersion by choosing the width $N = 40$ and $N = 41$.

The thermopower for the width $N = 40$ is plotted in figure 10(a) which shows that non-zero $\alpha$ has no much significant impact except the shifting of the thermopower peaks. However, a significant enhancement of thermopower can be found for gapped dispersion as can be seen in figure 10(b). It is worthwhile to mention that the thermopower can be further linked to the conductance via the standard Mott’s relation

$$S \sim -\left[ \frac{d}{dE} \ln G_T(E) \right]_{E=\mu} = -\left[ \frac{1}{G_T(E)} \frac{d}{dE} G_T(E) \right]_{E=\mu} \hfill (26)$$

which indicates that thermopower should be maximum around the slope of conductance spectrum, which can be confirmed from the plot figure 11. At the same time, the amplitude of thermopower decreases with $G_T(E)$ as they are inversely related. On the other hand, it is noted from figure 10(b) that thermopower increases with the strength of $\alpha$. Note that for gapped edge modes ($N = 41$), the thermopower is enhanced with the increase of $\alpha$, where as such enhancement does not occur with $\alpha$ for gapless edge modes ($N = 40$). The reason can be attributed to how $\alpha$ affects the product of the slope of conductance spectrum and it’s inverse. The enhancement of thermopower with the $\alpha$ reveals that this product is much sensitive to the $\alpha$ for gapped edge modes in comparison to the gapless edge modes. The corresponding thermal conductance are also evaluated by using equation (8) and plotted in
Figure 10. Thermopower as a function of chemical potential for (a) $N = 40$ and (b) $N = 41$. The temperature is taken at $T = 0.02\frac{\hbar}{k_B}$.

Figure 11. Thermopower (upper panel) and conductance(lower panel) versus chemical potential. Thermopower for $N = 41$ is scaled down by a factor 1/4.

Figure 12. Thermal conductance versus chemical potential for (a) $N = 40$ and (b) $N = 41$. The temperature is taken at $T = 0.02\frac{\hbar}{k_B}$.

Figure 13. Thermoelectric figure of merits ($ZT$) versus the chemical potential (a) $N = 40$ and (b) $N = 41$ at $T = 0.02\frac{\hbar}{k_B}$.

Finally, we look whether the dice lattice (or $T_3$) can of a way to improve the thermoelectric figure of merits of such hexagonal lattice. In order to address this concern, the thermoelectric figure of merit is plotted as a function of $\alpha$ for two different widths in figure 13. It shows that the maximum value of the thermoelectric figure of merit remains unaltered with the variation of $\alpha$ except a shift of the peaks for gapless edge modes (width $N = 40$). However, on the other hand the figure of merits for $N = 41$ is plotted in figure 13(a) (gapped dispersion) which shows that figure of merits gets almost thirty times larger than than $N = 40$ figure 13(b) (gapless dispersion). We can conclude that the zigzag ribbon of a $T_3$/dice lattice with gapped dispersion can be a better choice for thermoelectric material.

Line defects and its consequences:

The line defects in honeycomb lattice are formed or created out of the absence of one or more sublattices in each unit cell [50, 51]. The presence of vacancy/line defects is one of the most common issue which arises during experimental realization of such lattice. It has been previously observed that such line defects yield some important consequences on the band structure as well as in transport phenomena, such as opening the gap in graphene [52], valley polarization [53] etc.

In this section, we examine the effects of the line defects, formed out of the absence of C/A sublattices in each unit cell at different distances from the edge. The effects of line defects/vacancy out of the absence of A or B sublattices were investigated previously in graphene [43, 52] or silicene [44]. In order to incorporate the line defect in tight-binding calculation, we set on-site energy to infinity at the missing site which prevents hoping between vacancy to nearest sites. The band dispersion of zigzag nanoribbon in presence of line defects are numerically presented in figure 14. The figure 14(a) is plotted for line defects created out of the absence of C atoms (C atoms) at $N_i = 3$ where ‘i’ is the sublattice number index with $1 \leq i \leq N$. It shows that the line defect causes drastic changes to the feature of the edge modes by enforcing them to touch at the middle of the two Dirac points. This feature can be expected to have significance consequences on the transport properties.

On other hand if the line defect is situated away from the zigzag edge i.e. for distance $N_i = 6, 9, 12$, the effects

\[ N = 40 \]
The origin can be traced to the band dispersion in figure 14(a). A peculiar behavior occurs for contribute two units of conductance in the low energy regime. On the other hand, in absence of line defects, it is the two valleys which the conductance is the appearance of conductance by $\frac{3}{2}\hbar$ steps down and steps up by $2\hbar$ instead of $2\hbar$. The width of the ribbon is $N = 40$ and $\alpha = 0.4$ for all cases.

In order to probe the consequences of the effects of line defects on transport properties, we also plot conductance in presence if line defects. Four cases are considered here. Line defects are inserted by removing $C$ sublattices at the $i$th position i.e. (a) $N_i = 3$ (b) $N_i = 6$ (c) $N_i = 9$ and (d) $N_i = 12$. The width of the ribbon is $N = 40$ and $\alpha = 0.4$ for all cases.

As it is already shown in figures 14(b)–(d) that line defects, situated away from the edge has very less consequences and hence it can easily be anticipated that such defects would not have any significant impacts on electric or thermoelectric transport properties.

5. Summary and conclusions

In this work, we explore the roles of zigzag edge geometry of $\alpha - T_3$ lattice on the band dispersion, conductance, thermopower and thermoelectric figure of merits under the continuous evolution of from graphene to dice lattice (by means of tuning $\alpha$). We notice that the feature of edge modes are very much sensitive to the width of the nanoribbon. The energy dispersion can be gapped or gapless depending on the width of the ribbon. The edge modes are not dispersionless flat as found in graphene, rather it can be gapless dispersive at the two valleys for specific width $N = 3q + 1$. Additionally, the slope of the gapless chiral edge modes increases with the increase of $\alpha$. On the other hand, the gap opening occurs between the pair of edge modes for the width of $N \neq 3q + 1$ and the energy gap increases with the evolution towards dice lattice. Subsequently, we use tight-binding Green function approach to analyses the roles of edge modes and $\alpha$ on electrical and thermoelectric transport coefficients of the zigzag nanoribbon based device, attached to the left and right lead. We found that possibility of reshaping the edge modes, by means of width and $\alpha$, can be exploited to improve the thermoelectric performances of such materials. It is found that the thermopower and thermoelectric figure of merits can be enhanced significantly by means of $\alpha$. The thermal conductance remains less sensitive to the $\alpha$ in comparison to thermopower whereas the figure of merits exhibits a sharp enhancement. Finally, we have studied the consequences of line defects out of the absence of $C$ sublattices. We have found that such line defect
has too weak impact on the band structure as well as on transport properties as long as the defects resides away from the edge. However, there is a drastic changes in the nature of the edge modes and corresponding transport signature if the line defects reside very near to the edge.

Acknowledgments

The authors thank the Deanship of Scientific Research in King Faisal University (Saudi Arabia) for funding the facilities required for this research as part of the Research Grants Program Nasher: 186124).

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