Maximum Thermoelectric Power Factor and Optimal Carrier Concentration of Bilayer Graphene at Various Temperatures

Hikaru Horii,a Manaho Matsubara,b,c Kenji Sasaoka,c Takahiro Yamamotob,c,†

aDepartment of Electrical Engineering, Faculty of Engineering, Tokyo University of Science, Nijuku 6-3-1, Tokyo 125-8585, Japan
bDepartment of Physics, Faculty of Science, Tokyo University of Science, Kagurazaka 1-3, Tokyo 162-8601, Japan
cResearch Institute for Science and Technology, Tokyo University of Science, Kagurazaka 1-3, Tokyo 162-8601, Japan
†Corresponding author: takahiro@rs.tus.ac.jp

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The thermoelectric response of bilayer graphene over a wide temperature range (0 < T ≤ 400 K) was theoretically investigated using linear response theory combined with a Green’s function technique. We found that the power factor \( P_F \) for a fixed chemical potential \( \mu \) exhibits a maximum at a certain \( T \). On the other hand, we found that the \( P_F \) for a fixed \( T \) exhibits a maximum (\( P_{F_{\text{max}}} \)) at an optimal \( \mu \) [or optimal carrier concentration (\( n_{\text{opt}} \)]). In addition, we clarified the \( T \) dependence of \( n_{\text{opt}} \) and \( P_{F_{\text{max}}} \) and explained the existence of \( n_{\text{opt}} \) in terms of the thermal excitation of electrons between the valence and conduction bands, which cannot be predicted by the conventional Mott formula.

Keywords Thermoelectric effect; Seebeck coefficient; Power factor; Bilayer graphene; Linear response theory

I. INTRODUCTION

Recently, thermoelectric (TE) conversion has been attracting attention as a key technology for harvesting low-temperature (< 150°C) waste heat. Bismuth telluride-based materials are widely used as high-performance TE materials in the low-\( T \) region [1–3]. However, they have disadvantages such as heaviness, high toxicity, and mechanical weakness. As potential candidates to overcome these disadvantages, several organic materials (e.g., polyphenylene vinylene [4] and poly(3,4-ethylenedioxythiophene)-based materials [5, 6]) and nanocarbon materials (e.g., carbon nanotubes [7–17] and graphene [18–25]) have been actively researched over the past two decades.

In particular, bilayer graphene (BLG), which consists of two-layered graphene, is a new type of nanocarbon TE material whose TE performance can be controlled by applying an electric field normal to the BLG surface. In our previous study [24], we theoretically showed that the TE power factor \( (P_F) \) for BLG can be enhanced by the applied electric field. We also determined the optimal chemical potential \( \mu_{\text{opt}} \) that gives the maximum power factor (\( P_{F_{\text{max}}} \)) for different electric fields at 300 K [24]. For example, the room-temperature \( P_{F_{\text{max}}} \) for BLG reaches approximately 7 mW K\(^{-2}\) m\(^{-1}\) in the absence of an applied electric field, and this theoretical prediction is in excellent agreement with the results of a recent TE experiment of BLG using electric double-layer transistors with ionic liquids [25]. However, the temperature dependences of \( P_{F_{\text{max}}} \) and \( \mu_{\text{opt}} \) (or corresponding carrier concentration) for BLG have not yet been elucidated even though they are important for designing BLG-based TE devices for operation at various environmental temperatures.

In the present study, we theoretically investigate the TE power factor for BLG over a wide temperature range (0 < \( T \) ≤ 400 K) using linear response theory [26, 27] combined with a Green’s function technique.
II. THEORY

A. Electronic states of bilayer graphene

The lattice structure of AB (Bernal)-stacked BLG [28] is shown in Figure 1. Because four carbon atoms are included in the unit cell, the Hamiltonian for this system can be described by a $4 \times 4$ $\pi$-orbital tight-binding Hamiltonian. However, to describe the low-energy physics in the temperature range $0 < T \leq 400$ K, the Hamiltonian can be reduced to a $2 \times 2$ effective Hamiltonian given by [24, 29–31]

$$H(k) = -\frac{\hbar^2}{2m_1} \begin{pmatrix} 0 & (k_x - i k_y)^2 \hfill \\
(k_x + i k_y)^2 & 0 \hfill \end{pmatrix}, \quad (1)$$

where $m_1$ ($\equiv t_1/2v^2$) is the effective mass for BLG, $v$ ($\equiv \sqrt{3a_0/2\hbar} \approx 10^6$ m s$^{-1}$) is the group velocity for the monolayer graphene, $a$ ($=|a_1| = |a_2| = 0.246$ nm) is the lattice constant, $\hbar$ is the Dirac constant, $t_0$ ($=3.033$ eV) is the intralayer hopping integral between 1(2)A and 1(2)B, and $t_1$ ($=0.390$ eV) is the interlayer hopping integral between 1A and 2B [32]. The interlayer hopping integrals between 1B and 2A and between 1A(B) and 2A(B) are neglected because these effects are negligibly small in the low-energy region [33, 34]. Here, $k = (k_x, k_y)$ is the wavenumber vector measured from the K point. By diagonalizing the $2 \times 2$ Hamiltonian in Eq. (1), we obtain the parabolic energy dispersions $\varepsilon_{\pm}(k)$ as

$$\varepsilon_{\pm}(k) = \pm \frac{\hbar^2 k^2}{2m_1}. \quad (2)$$

Here, the origin of energy ($\varepsilon = 0$) is chosen as the charge-neutral point (CNP) for the BLG and $k$ is defined as $k \equiv \sqrt{k_x^2 + k_y^2}$.

Next, to account for the effects of disorder on the BLG, we introduce a retarded/advanced Green’s function given by

$$G^{R/A}(\varepsilon, k) = [\varepsilon - \Sigma^{R/A}(\varepsilon, k) - H(k)]^{-1}, \quad (3)$$

where $I$ is a $2 \times 2$ identity matrix and $\Sigma^{R/A}(\varepsilon, k)$ is the retarded/advanced self-energy due to the disorder potential. Similar to the theoretical procedure described in our previous study [24], the $k$ dependence of $\Sigma^{R/A}(\varepsilon, k)$ is neglected; that is,

$$\Sigma^{R/A}(\varepsilon, k) \rightarrow \Sigma^{R/A}(\varepsilon) = \mp i \frac{\hbar}{2\varepsilon} I. \quad (4)$$

Here, $\tau(\varepsilon)$ is the relaxation time, which depends on $\varepsilon$ but not on $k$. The $\varepsilon$ dependence of $\tau(\varepsilon)$ is given by

$$\tau(\varepsilon) = \tau_c + \frac{A}{|\varepsilon|^r}, \quad (5)$$

where $\tau_c$, $A$, and $r$ ($0 < r \leq 1$) are fitting parameters. In the reproduction of the experimental TE results for BLG in Ref. 25, three parameters are determined as $\tau_c = 60$ fs, $A = 1.42$ eV fs, and $r = 1.00$, respectively. Similar behavior of $\tau(\varepsilon)$ has been experimentally confirmed elsewhere [35].

Using $\tau(\infty) = \tau_c = 60$ fs and the group velocity $v_g \approx 10^6$ m s$^{-1}$ in the high-$|\varepsilon|$ region, the mean free path $l_m$ is estimated as $\approx 100$ nm, which is consistent with the averaged grain size in the polycrystalline graphene reported in Ref. 36. On the other hand, $l_m$ due to phonons is longer than that due to the grain boundaries in the region of $T \leq 300$ K except for the extremely low-carrier-concentration case [37]. Therefore, we assume that the electron scattering characterized by $\tau(\varepsilon)$ in Eq. (5) is mainly originated from the elastic scattering at the grain boundaries and the electron–phonon interaction can be neglected in this study. Under this assumption, the Green’s functions can be straightforwardly rewritten as

$$G^{R/A}(\varepsilon, k) = -\left(\frac{2m_1}{\hbar^2}\right)^2 \frac{1}{(k^2 + z^{R/A}(\varepsilon))(k^2 - z^{R/A}(\varepsilon))} \times \begin{pmatrix} \varepsilon \pm i\hbar \hfill \\
\frac{\varepsilon}{2\tau(\varepsilon)} \hfill \\
-\frac{\hbar^2(k_x + ik_y)^2}{2m_1} \hfill \\
\frac{\varepsilon}{2\tau(\varepsilon)} \hfill \end{pmatrix}, \quad (6)$$

where $z^{R/A}(\varepsilon)$ are defined as

$$z^{R/A}(\varepsilon) = \frac{2m_1}{\hbar^2} \sqrt{\left(\frac{\varepsilon}{2\tau(\varepsilon)}\right)^2}. \quad (7)$$

Here, the imaginary part of the square root in Eq. (7) is chosen to be positive. Using the retarded Green’s function in Eq. (6), we can calculate the density of states (DOS) $\rho(\varepsilon)$ per unit area of the BLG as

$$\rho(\varepsilon) = -g_S g_V \frac{1}{\pi \Omega} \text{Tr} \left( \sum_k \text{Im} G^{R}(\varepsilon, k) \right) = g_S g_V \frac{m_1}{2\pi \hbar^2}, \quad (8)$$
which is independent of $\varepsilon$. Here, $\Omega$ is the system area and $g_S = 2$ and $g_V = 2$ are the spin and valley degrees of freedom, respectively. Interestingly, the DOS for BLG with disorder in Eq. (8) coincides with that without disorder obtained from the dispersions in Eq. (2). Using the DOS in Eq. (8), we express the net carrier concentration by

$$\Delta n(\mu, T) = n_e(\mu, T) - n_h(\mu, T).$$

Here, $n_e(\mu, T)$ and $n_h(\mu, T)$ are the electron and hole concentrations, defined as

$$n_e(\mu, T) = g_S g_V \frac{m_1}{2\pi \hbar^2} \int_0^\infty d\varepsilon f(\varepsilon - \mu, T)$$

and

$$n_h(\mu, T) = g_S g_V \frac{m_1}{2\pi \hbar^2} \int_0^\infty d\varepsilon [1 - f(\varepsilon - \mu, T)],$$

where $f(\varepsilon - \mu, T) = [1 + \exp((\varepsilon - \mu)/(k_B T))]^{-1}$ is the Fermi-Dirac distribution function, $k_B$ is the Boltzmann constant, and $\mu$ is the chemical potential.

### B. Thermoelectric effects in bilayer graphene

In linear response theory, the Seebeck coefficient $S$ is defined as the electric field induced by a finite temperature gradient under the condition of no electrical current density, which leads to

$$S(\mu, T) = \frac{1}{T} \frac{L_{12}(\mu, T)}{L_{11}(\mu, T)}.$$  \hspace{1cm} (12)

Similarly to $S$ in Eq. (12), the power factor $PF(\equiv L_{11} S^2)$ is also expressed in terms of $L_{11}$ and $L_{12}$ as

$$PF(\mu, T) = \frac{1}{T^2} \frac{L_{12}^2(\mu, T)}{L_{11}(\mu, T)^2}. \hspace{1cm} (13)$$

Thus, we can easily obtain $S$ and $PF$ after we obtain $L_{11}$ and $L_{12}$. Here, Onsager’s coefficients $L_{11}$ and $L_{12}$ are called the electrical conductivity and the thermoelectrical conductivity, respectively. For the present system (i.e., BLG with a disorder potential), $L_{11}$ and $L_{12}$ can be expressed as Sommerfeld-Bethe relations ($15$–$17, 24, 38, 39$):

$$L_{11}(\mu, T) = \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{\partial f(\varepsilon - \mu, T)}{\partial \varepsilon} \right) \alpha(\varepsilon), \hspace{1cm} (14)$$

and

$$L_{12}(\mu, T) = -\frac{1}{e} \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{\partial f(\varepsilon - \mu, T)}{\partial \varepsilon} \right) (\varepsilon - \mu) \alpha(\varepsilon). \hspace{1cm} (15)$$

Here, $e$ is the elementary charge and $\alpha(\varepsilon)$ is the spectral conductivity (i.e., the electrical conductivity at $T = 0$). Using the retarded/advanced Green’s function in Eq. (6) and the velocity matrix $v_x(k)$ ($= \hbar^2 \partial H(k)/\partial k_x$) in the $x$-direction along the temperature gradient of the BLG,

$$v_x(k) = -\frac{\hbar}{m_1} \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix},$$  \hspace{1cm} (16)

the spectral conductivity can be calculated as

$$\alpha(\varepsilon) = g_S g_V \frac{\hbar^2}{2\pi \hbar} \sum_k \text{Re} \text{Tr}[v_x(k) G_A(\varepsilon, k) v_x(k) G_R(\varepsilon, k)],$$

$$= g_S g_V \frac{\hbar^2}{2\pi \hbar} \left( 1 + \left| \frac{\varepsilon}{\hbar/2\tau(\varepsilon)} \right| \right) \left( \frac{\varepsilon}{\hbar/2\tau(\varepsilon)} \right) \text{arctan} \left( \frac{2\hbar \tau(\varepsilon)}{\varepsilon} \right),$$ \hspace{1cm} (17)

Here, $V$ is the system volume and $t = 7$ Å is the thickness of the BLG.

### III. RESULTS AND DISCUSSION

**A. Spectral conductivity**

As already mentioned in Sec. II.A, we chose $A = 1.42$ fs eV, $\tau_c = 60$ fs, and $\tau = 1.00$ in Eq. (5), which reproduce the experimental results at $T = 300$ K in Ref. 25. Figure 2 shows $\alpha(\varepsilon)$ for $T(\varepsilon) = 60$ fs $+ 1.42|\varepsilon|$ (black solid curve) with constant $\tau (= 60$ fs) (black dashed curve). In the limit of $|\varepsilon| \rightarrow A/\tau_c$, the solid curve approaches the dashed curve; by contrast, in the present region of $|\varepsilon|/\tau_c \lesssim 0.8$ ($\tau_c |\varepsilon| \lesssim 18.7$ fs eV) shown in Figure 2, the influence of $\alpha(\varepsilon)$ is not negligible. In the weak-disorder region of $|\varepsilon|/\gamma(\varepsilon) = 2(\tau_c |\varepsilon| + A)/\hbar \gg 1$, which means that $|\varepsilon|$ is much larger than the characteristic energy

\[
\gamma(\varepsilon) = \sqrt{(h/2\tau(\varepsilon))},
\]

\[
\alpha(\varepsilon) = \frac{60}{60} + 1.42|\varepsilon| \quad \text{(black solid curve)}
\]

\[
\tau = 60 \quad \text{fs}
\]

\[
\gamma(\varepsilon) = \frac{h}{2\tau(\varepsilon)}
\]

\[
\text{Approximation in Eq. (18)}
\]

\[
\text{Figure 2: Spectral conductivity $\alpha(\varepsilon)$ of BLG for $\tau(\varepsilon) = 60$ fs $+ 1.42|\varepsilon|$ (black solid curve) and $\tau = 60$ fs (black dashed curve). Here, the origin of energy ($\varepsilon = 0$) is set to be the CNP for BLG. The horizontal axis above represents $\varepsilon$ scaled by the characteristic energy $\gamma(\varepsilon) = h/2\tau(\varepsilon)$ originating from $\tau(\varepsilon)$. $\alpha(\varepsilon)$ for $\tau(\varepsilon) = 60$ fs $+ 1.42|\varepsilon|$ approximated as in Eq. (18) is also displayed as a red dotted line.}
\]
\(\gamma(\varepsilon) \equiv h/2\tau(\varepsilon)\) originating from \(\tau(\varepsilon)\), \(\alpha(\varepsilon)\) in Eq. (17) is approximated as
\[
\alpha(\varepsilon) \approx g_S g_v \frac{e^2}{2m_0^2}\left(|\varepsilon| + \frac{A}{\tau_c}\right) . \tag{18}
\]

Note that, in the present case of \(A = 1.42\) fs eV, the whole \(\varepsilon\) region can be regarded as the weak-disorder region of \(|\varepsilon|/\gamma(\varepsilon) \gg 1\), where \(\alpha(\varepsilon)\) can be well approximated by Eq. (18), as shown by the red dotted line in Figure 2.

### B. Electrical conductivity and thermoelectric conductivities

Using \(\alpha(\varepsilon)\) in Figure 2, the electrical conductivity \(L_{11}\) and the thermoelectric conductivity \(L_{12}\) can be obtained from Eqs. (14) and (15), respectively. In the present study, we use three values of \(\mu/t_1 = -0.1, -0.3, -0.5\) as the chemical potentials that satisfy the low-\(\mu\) condition \(|\mu|/t_1 \ll 1\). Figure 3(a) shows the \(T\) dependence of \(L_{11}(\mu, T)\) scaled by \(\alpha(\mu)\) for BLG with \(\mu/t_1 = -0.1\) (black curve), \(-0.3\) (blue curve), and \(-0.5\) (red curve). As evident in Figure 3(a), \(L_{11}\) for the three \(\mu\) values is almost constant with respect to \(\alpha(\mu)\) in the extremely low-\(T\) region. In this region, the contribution of electrons thermally excited from the valence to the conduction band is negligibly small, \(L_{11}\) can be expressed by a Sommerfeld expansion of Eq. (14). As described in Sec. III.A, \(\alpha(\varepsilon)\) is approximately proportional to \(|\varepsilon|\) and \(\alpha(\mu)\approx 0\); thus, \(L_{11}\) in the extremely low-\(T\) region is well expressed by
\[
L_{11}(\mu, T) \approx \alpha(\mu) \approx g_S g_v \frac{e^2}{2\pi h^2}\left(|\mu| + \frac{A}{\tau_c}\right). \tag{19}
\]

As \(T\) increases, \(L_{11}\) increases from \(\alpha(\mu)\) at a different temperature for each \(\mu\) value. To explain the increase in \(L_{11}\), we display \(L_{11}(\mu, T)/\alpha(\mu)\) as a function of \(k_B T/|\mu|\) in the inset of Figure 3(a). \(L_{11}(\mu, T)/\alpha(\mu)\) for the three \(\mu\) values increases from unity at \(k_B T/|\mu| \sim 0.1\), where the conduction electrons start to contribute to \(L_{11}\).

Figure 3(b) shows the \(T\) dependence of \(L_{12}(\mu, T)\) for BLG for \(\mu/t_1 = -0.1\) (black solid curve), \(-0.3\) (blue solid curve), and \(-0.5\) (red solid curve). \(L_{12}\) for the three \(\mu\) values increases monotonically with increasing \(T\). In the extremely low-\(T\) region, \(L_{12}\) is similar for all \(\mu\) values and exhibits \(T^2\) behavior, which can be understood by the Sommerfeld expansion of Eq. (15) as
\[
L_{12}(\mu, T) \approx -\frac{\pi^2}{3e} \alpha(\mu) (k_B T)^2 \approx \frac{g_S g_v \pi \tau_c}{6 h^2} (k_B T)^2 , \tag{20}
\]
where the minus (plus) sign corresponds to the case of \(\mu > 0\) \((\mu < 0)\). Notably, Eq. (20) is independent of \(\mu\), as shown by the dashed line in Figure 3(b). As \(T\) increases, \(L_{12}\) deviates downward from the \(T^2\) behavior at \(k_B T/|\mu| \sim 0.1\) because of cancellation of the contributions from conduction electrons and valence holes.

### C. Seebeck coefficient and power factor

Substituting the \(L_{11}\) data in Figure 3(a) and the \(L_{12}\) data in Figure 3(b) into Eqs. (12) and (13), we obtained the Seebeck coefficient \(S\) and the power factor \(P_F\). Figure 4(a) represents the \(T\) dependence of \(S\) for BLG for \(\mu/t_1 = -0.1\) (black solid curve), \(-0.3\) (blue solid curve), and \(-0.5\) (red solid curve). In the low-\(T\) region, \(S\) increases linearly with increasing \(T\) irrespective of \(\mu\). Such behavior can be expressed by the well-known Mott formula [40] as
\[
S(\mu, T) \approx -\frac{\pi^2 k_B}{3e} \frac{k_B T}{\mu \pm A/\tau_c} , \tag{21}
\]
which can be derived by substituting Eqs. (19) and (20) into Eq. (12). Here, the plus (minus) sign is for the case of \(\mu > 0\) \((\mu < 0)\). As shown in Figure 4(a), \(S\) for the three \(\mu\) values deviates downward from the prediction of Mott formula in Eq. (21), which is shown by the dashed lines at \(k_B T/|\mu| \sim 0.1\), corresponding to the temperatures where \(L_{11}\) in Figure 3(a) and \(L_{12}\) in Figure 3(b) deviate from Eqs. (19) and (20), respectively. As \(T\) increases, \(S\) for \(\mu/t_1 = -0.1\) eventually begins to decrease at \(T \approx 260\) K. That is, \(S\) exhibits a \(T^2\) behavior at low-\(T\) region, which can be expressed by the well-known Mott formula [40] as
\[
S(\mu, T) \approx -\frac{\pi^2 k_B}{3e} \frac{k_B T}{\mu \pm A/\tau_c} , \tag{21}
\]
which can be derived by substituting Eqs. (19) and (20) into Eq. (12). Here, the plus (minus) sign is for the case of \(\mu > 0\) \((\mu < 0)\). As shown in Figure 4(a), \(S\) for the three \(\mu\) values deviates downward from the prediction of Mott formula in Eq. (21), which is shown by the dashed lines at \(k_B T/|\mu| \sim 0.1\), corresponding to the temperatures where \(L_{11}\) in Figure 3(a) and \(L_{12}\) in Figure 3(b) deviate from Eqs. (19) and (20), respectively. As \(T\) increases, \(S\) for \(\mu/t_1 = -0.1\) eventually begins to decrease at \(T \approx 260\) K. That is, \(S\) exhibits a \(T^2\) behavior at low-\(T\) region, which can be expressed by the well-known Mott formula [40] as
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S(\mu, T) \approx -\frac{\pi^2 k_B}{3e} \frac{k_B T}{\mu \pm A/\tau_c} , \tag{21}
\]
exhibits a peak, which is not observed for $L_{11}$ and $L_{12}$, at $T \approx 260$ K for $\mu/t_1 = -0.1$, $T \approx 730$ K for $\mu/t_1 = -0.3$, and $T \approx 1120$ K for $\mu/t_1 = -0.5$, where $S \approx 56.0$, $\sim 73.2$, and $\sim 77.0$ $\mu$V K$^{-1}$, respectively. We emphasize that the appearance of the peak in $S$ cannot be predicted by the conventional Mott formula.

Figure 4(b) displays the $T$ dependence of the PF for BLG for $\mu/t_1 = -0.1$ (black solid curve), $-0.3$ (blue solid curve), and $-0.5$ (red solid curve). The extremely low-$T$ PF exhibits a peak, which is not observed for BLG for $\mu/t_1 = -0.1$. Similarly to $S$, the peaks in $PF$ are observed at $T \approx 330$, $\sim 900$, and $\sim 1240$ K for $\mu/t_1 = -0.1$, $-0.3$, and $-0.5$, where $PF \approx 4.6$, $\sim 17.8$, and $\sim 29.4$ mW K$^{-2}$ m$^{-1}$, respectively. Among the three $\mu$ cases, $PF(-0.1t_1,T) > PF(-0.3t_1,T) > PF(-0.5t_1,T)$ for $T = 150$ K and $PF(-0.3t_1,T) > PF(-0.5t_1,T) > PF(-0.1t_1,T)$ for $T = 350$ K because of the decrease in $PF$ for $\mu/t_1 = -0.1$.

From another perspective, $PF$ exhibits a maximum value ($\equiv PF_{\text{max}}$) for the optimal chemical potential ($\equiv \mu_{\text{opt}}$) at fixed $T$. Figure 5(a) shows the $\mu$ dependence of the $PF$ for BLG for $T = 150$ K (black curve), 250 K (blue curve), and 350 K (red curve). As can be seen, $PF_{\text{max}}$ depends on $T$ and appears at $\mu_{\text{opt}}/t_1 \sim -0.12$, $-0.19$, and $-0.25$ for $T = 150$, 250, and 350 K, respectively, as indicated by the arrows. Next, we show $\mu_{\text{opt}}$ [or the optimal carrier concentration $n_{\text{opt}}$ (\equiv $\Delta n_{\text{or}}$)] and $PF_{\text{max}}$ as functions of $T$. Figure 5(b) shows the $T$ dependence of $\mu_{\text{opt}}$ and the corresponding $n_{\text{opt}}$ for the BLG. $PF_{\text{max}}$ is shown in the inset as a function of $T$. It is evident that $PF_{\text{max}}$ and $n_{\text{opt}}$ monotonically increase with increasing $T$ and eventually reach $\sim 11$ mW K$^{-2}$ m$^{-1}$ and $\sim 3.3 \times 10^{12}$ cm$^{-2}$ at $T = 400$ K, respectively. Therefore, to maximize the $PF$ for BLG in the region $0 < T \leq 400$ K, carrier doping should be performed to the concentration of $\sim 3.3 \times 10^{12}$ cm$^{-2}$.

IV. CONCLUSION

We investigated the TE properties of BLG over a wide $T$ range ($0 < T \leq 400$ K) on the basis of linear response theory combined with a Green’s function technique. $S$ and $PF$ for fixed $\mu$ show a peak at certain $T$ values because of

![Figure 4](image-url)

**Figure 4:** Temperature dependences of (a) Seebeck coefficient $S$ and (b) power factor $PF$ for BLG for $\tau(\varepsilon) = 60 \varepsilon + 1.42|\varepsilon|$ and $\mu/t_1 = -0.1$ (black solid curve), $-0.3$ (blue solid curve), and $-0.5$ (red solid curve). The horizontal axis above represents the thermal energy $k_B T/t_1$. Equations (21) and (22) are respectively displayed by the dashed lines in (a) and the dashed curves in (b) for each $\mu$ value.

![Figure 5](image-url)

**Figure 5:** (a) Chemical potential dependence of power factor $PF$ of BLG for $\tau(\varepsilon) = 60 \varepsilon + 1.42|\varepsilon|$ and $T = 150$ K (black curve), 250 K (blue curve), and 350 K (red curve). The arrows indicate the positions where the $PF$ has a maximum value ($PF_{\text{max}}$) for each $T$. (b) Temperature dependence of optimal chemical potential $\mu_{\text{opt}}$ giving $PF_{\text{max}}$. The right vertical axis represents the corresponding optimal carrier concentration $n_{\text{opt}}$. The horizontal axis above represents the thermal energy $k_B T/t_1$. $PF_{\text{max}}$ is displayed as a function of $T$ in the inset.
thermal excitation of electrons between the valence and conduction bands, which cannot be predicted by the conventional Mott formula. Moreover, the \( P_{\text{F}} \) values for a fixed \( T \) have maximum values \( \left(P_{\text{F}}\right)_{\text{max}} \) at the optimal chemical potentials \( \mu_{\text{opt}} \), and we determined \( \mu_{\text{opt}} \) and the corresponding carrier concentration \( n_{\text{opt}} \) as functions of \( T \). As \( T \) increases, \( n_{\text{opt}} \) monotonically increases, eventually reaching \(~3.3 \times 10^{12} \text{ cm}^{-2} \) at \( T = 400 \text{ K} \), where \( P_{\text{F}}\) max is \(~11 \text{ mW K}^{-2} \text{ m}^{-1} \). On the basis of these findings, we expect that the \( P_{\text{F}} \) for BLG is optimized by optimal carrier doping using electric double-layer transistors with ionic liquids, as reported in Ref. 25.

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