Thermoelectric transport properties of borophane

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Using the generalized Boltzmann equation, we have investigated the impact of impurity scattering on charge carrier transport in an anisotropic Dirac system. As a case study, we have studied the thermoelectric performance of borophane, a new monoelemental monolayer with a tilted and anisotropic Dirac cone, in the diffusive transport regime. Finding the exact solution to the linear-response Boltzmann equation, the electrical conductivity and thermoelectric properties of borophane in the presence of the short-range, long-range charged impurity and the electromagnetic impurities is studied. Contrary to the electron-hole asymmetry in borophane, its electron-hole conductivity is symmetric. We explain the effect of the chemical potential, on the thermoelectric properties of borophane. We demonstrate that, regardless of the type of impurities, the electric conductivity of borophane is highly anisotropic, while the Seebeck coefficient and figure of merit ($ZT$) are isotropic. The anisotropy ratio of the conductivities ($\sigma_{xx}/\sigma_{yy}$) for both long-range and short-range magnetic impurity are constant values of around 7.67 and 9.27, respectively. Along with ambipolar nature of borophane thermopower, we predict that borophane has a high figure of merit with the optimal values $ZT = 2.75$ at the low temperature and $ZT = 1$, and room temperature. More importantly, borophane attains its maximum value of the figure of merit at low chemical potentials, in the vicinity of the charge neutrality point. In comparison to phosphorene (a highly unique anisotropic 2D material) borophane with a high anisotropy ratio of about 10, is an unprecedented anisotropic material. This high anisotropy ratio together with the large figure of merit, suggest that borophane is promising for the thermoelectric applications and transport switching in the Dirac transport channels.

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I. INTRODUCTION

Boron, the left neighbor of carbon in the periodic table, has been expected to form various boron nanostructures, such as zero-dimensional all-boron fullerene-like cage cluster at $B_{40}$ [1–3], 1D boron nanowires, and nanotubes [4–7], double-ring tubular structures [8–10] and 3D superhard boron phases [11], at the past decade. Among these mono-elemental structures, graphene-like Two-dimensional (2D) structure of boron known as borophenes has attracted considerable attention both theoretically and experimentally recently, due to its exceptional properties and promising applications in nanoelectronics [12–15].

Theoretical investigations indicate that due to the electrons in Fermi surface arising from the hybridized states of the $\sigma$ and $\pi$ bond, 2D boron structure may be a pure single-element intrinsic superconducting material with the highest $T_c$ (higher than the liquid hydrogen temperature) on conditions without high pressure and external strain which can be modified by strains and dopings [16–18].

Several types of borophene is synthesized on Ag(111)[3, 19–21]. A similar striped phase, named as $\beta_{12}$ borophene, has an essentially flat structure that interacts weakly with the Ag(111) substrate. In particular, the existence of the Dirac cones with ultrahigh Fermi velocity, in $\beta_{12}$ borophene clearly proved using the angle-resolved photoemission spectroscopy (ARPES) experiment as well as by first-principles calculation [22].

This novel two-dimensional material was first proposed by Boustani, who using the systematic ab initio density functional method predicted that the quasi-planar 2D boron sheet could be constructed from a basic unit of puckered $B_7$ cluster [23, 24]. The first experimental evidence of the viability atomic-thin boron sheets was performed by Piazza et al. in the planar $B_{36}$ cluster with a central hexagonal hole [25].

As proposed by Tang and Ismail-Beigi, the mixed hexagonal-triangular 2D boron sheet ($\alpha$-borophene) was thought to be the more stable than one composed only of buckled triangular motifs [26–28]. Zeng’s group using the first-principle particle-swarm optimization global algorithm showed that another two flat monolayers as $\alpha$1-borophene and $\beta$1-borophene, are energetically most stable 2D boron structures among the state-of-the-art 2D structures of boron [29].

Recently, a new type of 2D boron polymorph, with an orthorhombic $8-Pmmm$ symmetry group, has been predicted to be more stable than the $\alpha$-borophene, exhibits anisotropic tilted Dirac conic [30]. A first-principles study reveals that borophene is the first known material with high-frequency plasmons in the visible spectrum [31]. Furthermore, in this borophene polymorph, the anisotropic plasmon mode remains undamped for higher energies along the mirror symmetry direction in which the anisotropic Friedel oscillation in borophene behaves like $r^{-3}$ in the large-$r$ limit [32].

An et al. by using the first-principles density functional theory plus the non-equilibrium Green’s func-

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tion approach, demonstrated that borophane displays a huge electrical anisotropy along with the mechanical anisotropy. Along the valley-parallel direction, the 2D borophane exhibits a metallic treatment with a linear current-voltage curve, in contrast to the perpendicular buckled direction, that shows off a semiconductor behavior [33].

However, theoretical calculations show that due to the imaginary frequencies in its phononic dispersion, the Free-standing 2D borophene is unstable against long-wavelength periodic vibration [34, 35], needing a substrate to be stabilized. A feasible method to dynamically stable borophene is the chemical fictionalization using surface hydrogenation. First-principles calculations of Xu et al. show that the fully hydrogenation of borophene, called borophane, is a viable method to stabilize borophene in the vacuum without a substrate [34]. It has been also predicted in this work that borophane has a remarkable Fermi velocity which is nearly four times higher than that of graphene.

Thermoelectric materials, based on a fundamental interplay between their electronic and thermal properties, have attracted much interest for energy efficient device applications. [36–41, 44–48]. The efficiency of the refrigeration or power generation devices is characterized by a dimensionless figure of merit $ZT$, which relates the Seebeck coefficient (thermopower) to the thermal conductivity. The small thermal conductivity and relatively high thermopower and electrical conductivity are required for high-efficiency thermoelectric materials. Even if the Seebeck coefficient becomes large, a heat current inevitably accompanies a temperature gradient and thus makes a tradeoff. The mainstream to prevail this issue is based on multiple quantum well [36, 37] and Bi$_2$Te$_3$ [38]. It is well understood that this efficiency improvement is due to the sharp-peaked electronic density of states (DOS) in low-dimensional materials [36, 49], which is the optimal way toward high thermoelectric efficiency [50]. A hallmark of the thermoelectric materials study came actually from the pioneering work [36], proposing that nanostructuring materials provide high thermoelectric efficiencies than bulk materials. This seminal work of the thermoelectric material could be an important starting point for today’s achievements. Due to the decreased thermal conductivity caused by phonon boundary scattering and consequently, improved power factors on quantum confinement in low dimensional systems, $ZT$ values become dramatically larger than the corresponding bulk materials. Large efforts in improving thermoelectric performance target energy filtering, which provides a way to increase the Seebeck coefficient by introducing a strongly energy-dependent scattering mechanism [50–53]. Recent advances in fabrication technologies have made exploring two-dimensional materials possible for thermoelectric applications [42–48].

Motivated by the great interest in search of thermoelectric Dirac material, the knowledge of thermoelectric efficiency of borophane is crucial for its application in potential thermal management devices. However, to our best knowledge, answers to these questions is still lacking. In this paper, we examine the electro-thermal transport in a fully hydrogenated borophene and in the 8-$Pmnn$ 2D boron allotrope.

In this paper, considering the electron–impurity, the thermoelectric effect in borophane away from the carrier neutrality point is studied by means of the Boltzmann transport equation. We first propose an accurate low-energy model Hamiltonian for borophane. Then, we investigate the electronic contribution to the thermoelectric transport of the monolayer of phosphorene. We consider a monolayer borophane in diffusive transport regime in the $x$–$y$ plane driven by a lattice temperature gradient $\nabla T$ and an electric field $\vec{E}$. The generalized Boltzmann transport equation is applied to obtain the conductivity, Seebeck coefficient and the figure of merit. Moreover, the diffusive transport coefficients are calculated by considering the various types of resistive scattering potential, (1) the short-range (SR) potential and (2) long-range (LR) Coulomb potential with a Thomas–Fermi screening as the source of scattering and (3) impurities containing short-range electric and ferromagnetically ordered magnetic potentials, called electromagnetic scatterers (SREM).

Our calculations show that although the electrical conductivity of borophane is highly anisotropic, the Seebeck coefficient and the corresponding figure of merit are nearly isotropic. The figure of merit, which is a measure of thermoelectric efficiency, reaches to $\sim 1.2$ at low temperatures, irrespective of the underlying scattering mechanisms. We also investigate the effect of the magnetic scatters on thermoelectric transport coefficients. These results propose that borophane could be a promising material for the thermoelectric applications.

The paper is organized as follows. In Sec. II, at first the model Hamiltonian and lattice structure of borophane is introduced and then the method which is used to calculate the conductivity and thermoelectric coefficients using the generalized Boltzmann method, is explained. In Sec. III, we present and describe our numerical results from the exact calculations for the conductivity and thermoelectric coefficients for borophane. Finally, we conclude and summarize our main results in Sec. IV.

II. MODEL HAMILTONIAN OF BOROPHENE

In the following we consider a monolayer of borophane at low temperature. The Bravais lattice constants of the conventional orthorhombic unit cell of the buckled crystal structures of borophene and borophane, are $a_x = 1.62$ Å, $a_y = 2.85$Å and $a_x = 1.92$ Å and $a_y = 2.81$ Å, respectively [25, 26, 34] and within a unit cell there are four atoms per unit cell. Notice that the buckling height of
Given by the Hamiltonian Eq. (1), the electronic band structure of borophane in the Γ-Y direction in the rectangular Brillouin zone. In the vicinity of two nonequivalent Dirac points $\mathbf{K}_D = (\pm 0.64, 0) \, \text{Å}^{-1}$ [32, 55, 56]

$$
H = \hbar v_x k_x \sigma_x + \hbar v_y k_y \sigma_y + \hbar v_t k_x \sigma_0.
$$

(1)

Here, $\sigma_x, \sigma_y$ are the Pauli matrices for the pseudospin representing the lattice degree of freedom while $\sigma_0$ is the $2 \times 2$ identity matrix. Typical values of the direction-dependent velocities, in unit of $(\times 10^6 \, \text{m/s})$, are $v_x = 19.58$, $v_y = 6.32$, and $v_t = 5.06$. The corresponding energy dispersion of the Hamiltonian Eq. (1), is analytically given by

$$
E^\tau (k) = \hbar v_t k_x + \tau \hbar \sqrt{v_x^2 k_x^2 + v_y^2 k_y^2},
$$

(2)

in which $\tau = 1(-1)$ denotes the conduction (valence) band in borophane. Isoenergy contour map of the electronic band structure of borophane in the $k$–space for $E(k_F) = -0.5$ to 0.5 eV is shown in Fig. 1(a). The contour lines are drawn at 0.05 eV intervals in both the electron (solid-navy) and hole (dashed-green) doped cases. The corresponding eigenfunctions for the Dirac electrons is given by the following equation

$$
\psi^\tau (\vec{k}) = \frac{1}{\sqrt{2A}} \begin{bmatrix} \tau e^{-i\xi} \\ 1 \end{bmatrix} e^{i\vec{k} \cdot \vec{r}},
$$

(3)

where $A$ is the system area and $\beta_k = t g^{-1} [v_y k_y / v_x k_x]$. Furthermore, by invoking the band energy dispersion given by Eq. (2), the $x$ and $y$ components of the velocity can be calculated as

$$
v_x^\tau = v_t + \tau \frac{v_x^2 k_x}{\sqrt{v_x^2 k_x^2 + v_y^2 k_y^2}},
$$

(4)

$$
v_y^\tau = \tau \frac{v_y^2 k_y}{\sqrt{v_x^2 k_x^2 + v_y^2 k_y^2}}.
$$

(5)

The density of states (DOS) can be obtained by solving the following equation

$$
D(\varepsilon) = \frac{1}{(2\pi)^2} \int_0^\infty k' \, dk' \delta (\varepsilon - \varepsilon_{k'})
$$

(6)

Performing this integral over energy, one finds the following expansion for the density of states:

$$
D(\varepsilon) = \frac{k^\tau}{v_t \cos(\phi) + \sqrt{v_x^2 \cos^2(\phi) + v_y^2 \sin^2(\phi)}}.
$$

(7)

Interestingly, similar to the low-energy DOS of graphene, DOS of borophane has the well-known linear form as shown in Fig. 1(b). In this figure, also the DOS of graphene (dashed-green) is plotted by setting $v_x = v_y = 1 \times 10^6 \, \text{m/s}$ and $v_t = 0$.

### A. Anisotropic transport framework

In this section, we present in the following our main formalism for the numerical evaluation of the transport coefficients in the diffusive regime, using the generalized semiclassical Boltzmann equation. In particular, we take into account three important cases of short-range impurities (e.g., defects or neutral adatoms) with Dirac delta potential, the long-range Coulomb impurities and finally the electromagnetic scatterers, containing short-range electric and ferromagnetically ordered magnetic potentials. Electrical conductance, thermal conductance, Seebeck coefficient, and thermoelectric figure of merit (ZT) of borophane in the presence of both the electric field and the temperature gradient will be studied. In order to calculate the transport coefficients, we use the following expression for the charge current $j$ and energy flux density

$$
\left[ \begin{array}{c} j^\tau \\ j^\phi \end{array} \right] = \int \frac{d^2 \vec{k}}{(2\pi)^2} \left[ \begin{array}{c} -e \\ \varepsilon(\vec{k}) - \mu \end{array} \right] v(\vec{k}) f(\vec{k}) \label{jh}
$$

(9)

where $v(\vec{k}) = v(\phi) (\cos \xi, \sin \xi)$ is the semiclassical velocity of the carriers which is related to the energy dispersion $\varepsilon(\vec{k})$ through $\varepsilon(\vec{k}) = (1/\hbar) \nabla \varepsilon(\vec{k})$. $f(\vec{k})$, is the nonequilibrium quantum distribution function, describes the evolution of the charge distribution in the presence of theromoelectric forces, must be computed from the Boltzmann equation. For this purpose, we take the Boltzmann equation up to a linear order in the presence of theromoelectric forces.

$$
\left( -e \vec{E} + \frac{e - \mu}{T} \nabla T \right) \cdot \vec{v}(\vec{k}) \left[ -\partial_\varepsilon f(\varepsilon(\vec{k})) \right] = \left( \frac{df}{dt} \right)_{\text{coll}}.
$$

(10)
In the following, we have implemented an approach for finding the exact solution to the linear-response Boltzmann equation for two dimensional anisotropic systems [42, 58–60]. Within the lowest order of the Born approximation, the scattering rates \(w(\mathbf{k}, \mathbf{k}')\) using the Fermi golden rule are given by

\[
w(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} n_{\text{imp}} |\langle \mathbf{k}' | \hat{V} | \mathbf{k} \rangle|^2 \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})
\]  

where \(n_{\text{imp}}\) is the background random-charged impurity density and \(\hat{V}_{\mathbf{k} \rightarrow \mathbf{k}'}\) is the Fourier transformation of the interaction potential between an electron and a single impurity. The short-ranged impurities are approximated with a zero-range hard-core potential \(\hat{V}_{\mathbf{k} \rightarrow \mathbf{k}'} = V_0\). On the other hand, the long-ranged electron-electron Coulomb potential, owing to the charged impurities is screened by other electrons of the system like the Thomas-Fermi approach.

By invoking the expression for \(f(\theta, \phi)\) into Eq. (9) for the charge and heat currents, the response matrix, which relates the resulting generalized currents to the driving forces, can be expressed in terms of some kinetic coefficients \(L^\alpha\) as the following [42],

\[
\left( \frac{1}{j^\alpha} \right) = \left( \begin{array}{cc} L^0 & -L^1/eT \\ L^1/e & -L^2/e^2T \end{array} \right) \left( \begin{array}{c} \vec{\xi} \\ -\vec{\nabla}T \end{array} \right) 
\]  

in which the two diagonal terms of this matrix are the electrical \(\sigma\) and thermal \(\kappa\) conductivities, and the two off-diagonal thermoelectric coefficients are the mixed coefficients relating electrical and thermal phenomena through the Onsager reciprocity relations. The thermoelectric power (or Seebeck coefficient) \(S = -\frac{1}{T} (L^0)^{-1} \cdot L^1\), describes the voltage generation due to the temperature gradient while Peltier coefficient \(\Pi = TS\) accounts for the heat current induction due to the charge current, respectively. The ability of a given material to efficiently produce thermoelectric power is related to its dimensionless figure of merit, described by a dimensionless quantity denoted by \(ZT = \frac{\sigma^2 T}{\kappa}\). By parameterizing \(\vec{\xi}\) and \(\vec{\kappa}\), as \(\vec{\xi} = \xi(\cos \theta, \sin \theta), \vec{\kappa} = k(\cos \phi, \sin \phi)\), respectively, all of the coefficients obey the relation

\[
L^\alpha(\theta, \theta') = \int d\varepsilon \left[ \frac{\partial f_0}{\partial \varepsilon} \right] (\varepsilon - \mu)^\alpha \sigma(\varepsilon; \theta, \theta')
\]  

in which, in the linear response theory, the generalized conductivity \(\sigma(\varepsilon; \theta, \theta')\) is defined as,

\[
\sigma(\varepsilon; \theta, \theta') = e^2 \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \delta (\varepsilon - \varepsilon(\mathbf{k})) v^2(\phi) \left[ a(\phi) \cos \theta + b(\phi) \sin \theta \right] \cos(\theta - \xi(\phi))
\]  

with \(\theta = \theta' = 0\) for \(\sigma_{xx}\) and \(\theta = \theta' = \pi/2\) for \(\sigma_{yy}\). We concentrate on low enough temperatures where only electrons contribute effectively in thermal transport and disregard phonon contribution.

Figure 1. (Color online) (a) Isoenergy contour map of the electronic band structure of borophane in the \(k\)-space for \(E(k_F) = -0.5\) to 0.5 eV. The contour lines are drawn at 0.05 eV intervals in both the electron (solid-navy) and hole (dashed-green) doped cases. (b) Density of states (DOS) calculated for monolayer borophane (solid-navy) and graphene (dashed-green).

where \(w(\mathbf{k}, \mathbf{k}')\) is the scattering rate from state \(\mathbf{k}\) to state \(\mathbf{k}'\) which needs to be specified according to the microscopic origin of the scattering mechanisms and \(f^0\) is the equilibrium distribution function.

The collision integral is given by

\[
\left( \frac{df}{dt} \right)_{\text{coll.}} = \int \frac{d^2 \mathbf{k}'}{(2\pi)^2} w(\mathbf{k}, \mathbf{k}') \left[ f(\mathbf{k}, \mathbf{\xi}, T) - f(\mathbf{k}', \mathbf{\xi}, T) \right]
\]  

(11)

Using the relaxation time approximation, the nonequilibrium distribution function cannot be exactly calculated that provides an inadequate explanation for the full aspects of the anisotropic features of the transport properties.
nistic parts of the impurity potential for the electromagnetic scatterer. Considering scattering off a δ-scatterer potential of \( \hat{V} \), the matrix elements of \( \hat{V} / V_0 \) in the basis (3) can be calculated as follows:

\[
| \langle \vec{k}' | \hat{V} / V_0 | \vec{k} \rangle | = \frac{1}{2} \left[ \alpha (1 + e^{i(\beta_{\kappa'} - \beta_k)}) + e^{i\beta_{\kappa'} + e^{-i\beta_k}} \right]
\]

\[
| \langle \vec{k}' | \hat{V} / V_0 | \vec{k} \rangle | = \frac{1}{2} \left[ \alpha + e^{-i\beta_k} (i + \alpha e^{i\beta_{\kappa'}}) - i \cos \beta_{\kappa'} + \sin \beta_k \right]
\]

\[
| \langle \vec{k}' | \hat{V} / V_0 | \vec{k} \rangle | = \frac{1}{2} \left[ (1 + \alpha) e^{i(\beta_{\kappa'} - \beta_k)} + \alpha - 1 \right]
\]

It is straightforward to show that the coefficients \( a(\phi), b(\phi) \) corresponding to the electromagnetic scatterers, in the conductivity formula (Eq.15), are obtained as:

\[
a(\phi) = \frac{2}{3\pi K} \cos \phi
\]

\[
b(\phi) = \frac{2}{\pi K} \sin \phi
\]

where \( K \) is a prefactor derived using the Fermi golden rule and given by

\[
K = w(\phi, \phi') |\langle \vec{k}' | \hat{V} / V_0 | \vec{k} \rangle|^{-2}.
\]

in which

\[
w(\phi, \phi') = \frac{1}{(2\pi)^2} \int_0^\infty k' dk' w(\vec{k}, \vec{k}')
\]

which leads to the solution of the Boltzmann equation 10 of the form

\[
f(\phi, \theta) = f_0 - ev\mathbf{E}(-\partial_\phi f_0) \frac{2}{\pi K} \left[ \frac{1}{3} \cos \theta \cos \phi + \sin \theta \sin \phi \right].
\]

for the non-equilibrium distribution function.

The difference in conductivities for current flowing parallel and perpendicular to the direction of the scatterer’s magnetic moments is described using the Anisotropic Magnetoresistance (AMR), defined as

\[
\text{AMR} = \frac{\sigma_{xx} - \sigma_{yy}}{\sigma_{xx} + \sigma_{yy}}.
\]

Interestingly, for each value of \( \alpha \), AMR is constant and is chemical potential independent for both \( n \) and \( p \) doped borophane. For example for \( \alpha = 0.5 \), AMR is about 0.805.

### III. NUMERICAL RESULTS AND DISCUSSION

In this section, we expand our theoretical analysis to a scattering by magnetic impurities seated on the surface of borophane. Magnetic scattering in dilute charged magnetic impurities, containing short-range electric and ferromagnetically ordered magnetic potentials whose magnetic moments are along the \( i \)-th direction, describes by the operator \( \hat{V} = V_0 (\alpha + \sigma_i) \) [61, 62], in which the dimensionless quantity \( \alpha \) is the ratio of the electric and magnetic moments along the direction of the scatterers.
We assume the scattering charge centers are at the SiO vector with the density of states of the system, \( \sigma = 2 \pi e^2 / (\varepsilon |\vec{k} - \vec{k}'| + q_{TF}) \) (21)

where \( q_{TF} = 2\pi e^2 D(E)/\varepsilon \) is the Thomas-Fermi screening vector with the density of states of the system, \( D(E) \). We assume the scattering charge centers are at the SiO₂- borophane interface, thus we use the dielectric constant of the this common substrate which is about \( \varepsilon = 2.45 \). Meanwhile, we note that we set \( T \sim 20 \) K in all calculated quantities.

In Fig. (2), the conductivity of borophane (in units of \( (\varepsilon^2/\hbar) \)) as a function of the chemical potential \( \mu \), is plotted in the presence of LR potential, along the \( x \), \( \sigma_{xx} \), and \( y \), \( \sigma_{yy} \), directions. The conductivity of graphene is also shown. As can be seen, a significant orientation dependent electrical conductivity is observed, where the conductivity in the armchair direction \( \sigma_{xx} \) is more than the zigzag conductivity \( \sigma_{yy} \). On the other hand, contrary to the electron-hole asymmetry in borophane, its electron-hole conductivity is nearly symmetric. We should mention that at very low temperatures the variation of thermal conductivity will be similar to the charge conductivity \( K \approx (\pi^2/3)k_B T \sigma \).

The electrical conductivity of borophane along the zigzag \( \sigma_{yy} \), and armchair \( \sigma_{xx} \), directions versus the chemical potential, in the presence of short-range electromagnetic scatterers is shown in the figure (3). In this figure \( \alpha = 0.5 \) and \( V_{\vec{k}-\vec{k}'} = V_0 = 1000 \) eVÅ² \( [64] \). The conductivity of the graphene is also shown. As can be seen, the overall energy dependence is the same as LR

impurity scattering. Importantly, the anisotropy ratio of the conductivity \( \sigma_{xx}/\sigma_{yy} \) for both long-range and short-range impurity has constant values of 7.67 and 9.27, respectively that are independent of chemical potential.

In comparison to phosphorene (a highly unique anisotropic 2D material) that the anisotropy ratio of the conductivities changes from 3 to 7 for electrons, in the presence of SR and LR potentials, respectively \( [42, 65, 66] \), borophane has an unprecedented conductivity anisotropy ratio.

As a more feasible quantity in the real experiments, the variation of the Seebeck coefficients \( S \), with chemical potential \( \mu \), in the presence of LR and SREM potentials is obtained, shown in Fig. (4). In convention, the sign of the Seebeck coefficient is the sign of the potential of the cold end with respect to the hot end of the temperature gradient. Thus a negative charge thermopower is obtained for when the Fermi energy lies in the conduction band because thermally activated electrons move along the temperature gradient which results in a charge accumulation gradient in the opposite direction due to the negative charge, however, thermally activated holes in the valence band lead to a positive thermopower. An important feature of the borophane thermopower is its isotropic behavior of three times lower in the SREM scatterers compared to the LR scatterers.

Moreover, the figure of merit \( ZT \) is depicted as a function of chemical potential \( \mu \), for both LR and SREM scatterers in Fig.5. Our findings reveal that, in contrast to highly anisotropic electrical and thermal conductivities, the Seebeck coefficient and its corresponding thermoelectric figures of merit are completely isotropic, consistent with the isotropic thermopower and figures of merit in
As a case study, we have investigated the thermoelectric performance of a monolayer borophane, with a tilted and classical Boltzmann approach for an anisotropic system. Impurity potentials is studied using the generalized semi-phane in the presence of short- and long-ranged charged impurity potentials, along the zigzag directions, respectively [68], we obtain numerically Eq. (14) for the electronic contribution. By using the room temperature contribution of the phonons in the thermal conductivity of borophane with (Kph ∼ 150 and ∼ 267 Wm⁻¹K⁻¹ along the armchair and zigzag directions, respectively [68]), we estimate the the figure of merit of borophane at room temperature. At high temperatures, the phonon becomes important but it only results in the overall decrease of the figures of merit, without affecting their qualitative behavior.

It can be seen that just like the low temperature figure of merit, the room temperature figure of merit is completely isotropic and compared with graphene, a high value ZT of about 1 can be achieved in a monolayer borophane at room temperature.

**IV. CONCLUSION**

In conclusion, the thermoelectric transport in borophane in the presence of short- and long-ranged charged impurity potentials is studied using the generalized semiclassical Boltzmann approach for an anisotropic system. As a case study, we have investigated the thermoelectric performance of a monolayer borophane, with a tilted and anisotropic Dirac cone in diffusive transport regime in the x–y plane driven by a lattice temperature gradient ∇T and an electric field E. Electron scattering from the impurities located at the surface of a monolayer borophane, is different for massless electrons. The charge conductivity, which is slightly different for n- and p-doped cases mostly owing to the unique dispersion of borophane, is found to be highly anisotropic, while the Seebeck coefficient and the corresponding figure of merit, without being affected either by type of scatterers or the presence/absence of coupling term, are nearly isotropic. Furthermore, it is shown that thermopower changes sign due to the conversion of electrons to holes and vice versa at the edge of the bands. Most strikingly, borophane could be a very promising material for thermoelectric studies and applications. Along with thermopower sign change, at the low temperature and room temperature, borophane is found to has large thermoelectric power factors of about 2.75 and 1, respectively.

Using the generalized Boltzmann equation, we have investigated the impact of impurity scattering on charge carrier transport in an anisotropic Dirac system. As a case study, we have investigated the thermoelectric performance of a monolayer borophane, with a tilted and anisotropic Dirac cone in diffusive transport regime in the x–y plane driven by a lattice temperature gradient ∇T and an electric field E. Finding the exact solution to the linear-response Boltzmann equation, the electrical conductivity and thermoelectric properties of a new ele-
mental monolayer (borophane) in the presence of short and long-range impurity, as well as the magnetic impurities, is studied. Contrary to the electron-hole asymmetry in borophane, its electron-hole conductivity is symmetric. We explain the effect of the chemical potential, that is characteristic of the linear energy-momentum relation, on the thermoelectric properties. We show that the electric conductivity of borophane is highly anisotropic, while the Seebeck coefficient and figure of merit are nearly isotropic. The anisotropy ratio of the conductivities ($\sigma_{xx}/\sigma_{yy}$) for both long-range and short-range magnetic impurity are constant values of around 7.67 and 9.27, respectively. Along with thermopower sign change, at the low temperature and room temperature, borophane is found to be a highly anisotropic material with large thermoelectric power factors of about 2.75 and 1, respectively.

In comparison to phosphorene (a highly unique anisotropic 2D material) that the anisotropy ratio of the conductivities changes from 3 to 7 for electrons, in the presence of SR and LR potentials, respectively [42, 65, 66], borophane with a high anisotropy ratio of about 10, is an unprecedented anisotropic material. This high anisotropy ratio together with the large figure of merit, suggest that borophane is promising for the thermoelectric applications and transport switching in the Dirac transport channels.

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