Quantum Hall effect and semiconductor-to-semimetal transition in biased black phosphorus

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We study the quantum Hall effect of two-dimensional electron gas in black phosphorus in the presence of perpendicular electric and magnetic fields. In the absence of a bias voltage, the external magnetic field leads to a quantization of the energy spectrum into equidistant Landau levels, with different cyclotron frequencies for the electron and hole bands. The applied voltage reduces the band gap, and eventually a semiconductor-to-semimetal transition takes place. This nontrivial phase is characterized by the emergence of a pair of Dirac points in the spectrum. As a consequence, the Landau levels are no longer equidistant anymore but follow the characteristic integer quantum Hall effect regime of Dirac materials, with a 2n quantization of the Hall conductivity in the gapped phase (standard quantum Hall effect regime) and a 4(n + 1/2) quantization in the semimetallic phase, characteristic of Dirac systems with nontrivial topology.

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I. INTRODUCTION

Black phosphorus (BP) is a direct band gap semiconductor that has recently been exfoliated to obtain atomically thin samples [1–3]. Each BP layer forms a puckered surface due to sp3 hybridization, revealing a highly anisotropic electronic band structure [4,5], an ambipolar field effect, linear dichoism in optical absorption spectra [2,4,6–8], and anisotropic plasmons [9]. Encapsulation of BP with hexagonal boron nitride has led to high-carrier-mobility devices, with the observation of quantum magneto-oscillations [10–14] and the integer quantum Hall effect [15]. One of the most surprising characteristics of BP is its strong response to external electric and strain fields. As a consequence, the electronic and optical properties of this material can be efficiently tuned by applying external bias voltage [16–20] or by strain engineering [21–25]. In particular, it is possible to drive a semiconductor-to-semimetal transition, with the appearance of a Dirac-like dispersion [16–18,26].

In this paper we study the electronic spectrum of unbiased BP in the presence of a strong magnetic field. For this we use a tight-binding model which properly accounts for the band structure in a wide energy window of the spectrum [27,28]. The electronic density of states (DOS) is calculated from the solution of the time-dependent Schrödinger equation [27,28]. The electronic density of states (DOS) is calculated from the solution of the time-dependent Schrödinger equation [27,28]. The characteristic integer quantum Hall effect with \( \sigma_{xy} \propto 2n(\varepsilon^2 / h) \) is observed. We further calculated the Hall conductivity from the Kubo-Bastin formula in the context of the kernel polynomial method [36,37]. We find that unbiased BP presents a relativistic quantum Hall effect characteristic of Dirac materials, with \( \sigma_{xy}^{\text{RHE}} = 4(n + 1/2)(\varepsilon^2 / h) \) [38]. Although we perform the numerical calculations for the simplest case of bilayer BP, the physical results should hold for any multilayer sample exposed to external magnetic and electric fields.

II. ELECTRONIC BAND STRUCTURE AND LANDAU QUANTIZATION

BP is formed by stacking of phosphorene layers, coupled with a van der Waals interaction. Single-layer BP contains two atomic layers and two kinds of P-P bonds (in-plane and interplane) [4], as shown in Fig. 1. Our calculations are done using a GW-based tight-binding model that properly reproduces the conduction and valence bands in an energy range ~0.3 eV beyond the gap [27,28].

\[
\mathcal{H} = \sum_{i \neq j} t_{ij} c_i^\dagger c_j + \sum_{i \neq j} t_{p,ij} c_i^\dagger n_j,
\]

where \( c_i^\dagger \) (\( c_i \)) creates (annihilates) an electron at site \( i \), and 10 intralayer \( t_{ij} \) and 5 interlayer \( t_{p,ij} \) hopping terms are considered in the model. The values of the 10 intralayer hopping terms [shown in Fig. 1(a)] are \( t_1 = -1.486 \) eV, \( t_2 = 3.729 \) eV, \( t_3 = -0.252 \) eV, \( t_4 = -0.071 \) eV, \( t_5 = -0.019 \) eV, \( t_6 = -0.186 \) eV, \( t_7 = -0.063 \) eV, \( t_8 = 0.101 \) eV, \( t_9 = -0.042 \) eV, \( t_{10} = -0.073 \) eV, and the 5 interlayer hopping terms [Fig. 1(b)] are \( t_{p1} = 0.524 \) eV, \( t_{p2} = 0.180 \) eV, \( t_{p3} = -0.123 \) eV, \( t_{p4} = -0.168 \) eV, \( t_{p5} = 0.005 \) eV [28]. The effect of an electric field on the electronic dispersion is considered by introducing linearly a biased on-site potential difference

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FIG. 1. Lattice structure of single-layer (a) and bilayer (b) black phosphorus. Circles of different colors correspond to atoms located in different planes within a single puckered layer. The relevant hopping terms considered in Hamiltonian (1) are indicated: 10 in-plane hopping terms (a) and 5 interlayer terms (b).

between the outmost planes of two layers, without considering the screening effect. For example, in a single layer we include a different on-site potential $\pm \Delta/2$ in the top and bottom sublayers, respectively, whereas in a bilayer BP we include a sequence of on-site potentials in the four planes with the form $\Delta/2 + v_b \Delta$, $\Delta/2 - v_b \Delta$, $-\Delta/2 + v_b \Delta$, and $-\Delta/2 - v_b \Delta$, where $v_b = 0.202$ is a linear scaling factor accounting for the lattice position along the direction of the external electric field [28]. Figure 2 shows the band structure obtained from the tight-binding model, (1), for three representative cases, and their corresponding constant-energy contours (CECs) are shown in Fig. 3. As is well known [4] for unbiased BP ($\Delta = 0$) the band structure corresponds to an anisotropic direct band-gap semiconductor, with the gap placed at the $\Gamma$ point of the Brillouin zone.

It is interesting to consider the different effects of a perpendicular electric field in the band structure of single-layer versus multilayer BP. In Fig. 4 we show the evolution of the band gap at the $\Gamma$ point as a function of the biased potential, defined from the energy difference between the valence and the conduction band edges as obtained from the full tight-binding model, (1). We observe that, whereas the gap increases with $\Delta$ in single-layer BP, the gap in bilayer BP decreases with the applied bias, and eventually a semiconductor-to-semimetal transition takes place. A similar closing of the gap with the bias potential occurs for any multilayer sample. The opposite behavior between single-layer and multilayer BP can be understood analytically by using the tight-binding model, (1), with only the leading hopping terms, namely, $t_1$, $t_2$, and $t_{p1}$. In the absence of a perpendicular electric field, $\Delta = 0$, the gap

FIG. 2. Band structure of biased bilayer BP for three representative values of the applied voltage: unbiased ($\Delta = 0$), for which the system is gapped; $\Delta = \Delta_c$, for which the gap closes and there is a band crossing at the $\Gamma$ point; and $\Delta > \Delta_c$, corresponding to the semimetal phase with the creation of Dirac points in the $\Gamma$-$X$ direction of the Brillouin zone.

FIG. 3. Constant energy contours of biased bilayer BP for the three values of the applied voltage used in Fig. 2. For $\Delta > \Delta_c$, corresponding to the semimetal phase with the creation of Dirac points in the $\Gamma$-$X$ direction of the Brillouin zone.
FIG. 4. Evolution of the valence and conduction band edges at the Γ point as a function of the biased potential Δ, for single-layer and bilayer BP, as calculated from the full tight-binding model, (1). The dashed line in (b) indicates the chemical potential energy in the semimetal phase.

in single-layer BP is controlled by the difference between the in-plane hopping parameter $t_1$ and the interplane $t_2$,

$$E_{g1L}(\Delta = 0) \approx 4t_1 + 2t_2,$$

where it is important to note the different signs of the two terms, $t_1 \approx -1.5$ eV $< 0$ and $t_2 \approx 3.7$ eV $> 0$. For bilayer BP, the gap at $\Delta = 0$ is approximately given by

$$E_{g2L}(\Delta = 0) \approx 4t_1 + 2\sqrt{t_2^2 + 2t_1^2 + 2t_1^2 - 2|t_1|\sqrt{t_2^2 + t_1^2}}.$$  

Note that the interlayer hopping $t_{p1}$ in bilayer BP enters into the gap equation as an extra contribution to the interplane hopping term in single-layer BP, $t_2$. In the presence of a biased potential, and within the above approximation, the gap in single-layer BP can be expressed as

$$E_{g1L} \approx 4t_1 + 2\sqrt{t_2^2 + \left(\frac{\Delta}{2}\right)^2},$$

whereas for bilayer BP the gap is given by

$$E_{g2L} \approx 4t_1 + 2\sqrt{t_2^2 + \left(\frac{\Delta}{2}\right)^2 + f_{\text{inter}},}$$

where we have defined

$$f_{\text{inter}} = 2t_{p1}^2 + \Delta^2 - \sqrt{2t_2^2\left(4t_1^2 + \Delta^2\right) + \left(-2t_1^2 + \Delta^2\right)^2}.$$  

One can easily see that, for the hopping parameters of the model, there is no real solution for $\Delta$ that closes the gap in single-layer BP, which should fulfill $\Delta_{1L} \approx 2\sqrt{4t_1^2 - t_2^2}$. Therefore, this simple analytical analysis shows that application of a perpendicular electric field has the effect of opening the gap in single-layer BP, in agreement with the full tight-binding results shown in Fig. 4. Bilayer BP, on the other hand, has a real solution for the closing of the gap. The analytical expression is too long to be given here, but one can simply observe that the term $f_{\text{inter}}$, as defined in Eq. (6), is $<0$. This leads to a correction for the second contribution in the gap equation, (5), which can fully cancel the $4t_1$ term, driving a semiconductor-to-semimetal transition. From now on, we focus on the multilayer case, for which the aforementioned transition can take place in the presence of a bias potential. The topological nature of the transition has been addressed by Liu et al. [17] by combining DFT and group theory analysis [17]. Semiconducting unbiased BP has valence and conduction bands with different symmetric representations at the Γ point (point group $D_{2h}$); the conduction band has the representation $A_g(\Gamma_1)$, whereas the valence band has the representation $B_{2u}(\Gamma_8)$. One can define the inversion energy as $\Delta_{\text{inv}} = E_{\Gamma 1} - E_{\Gamma 8}$. When the bias voltage is high enough, the gap is 0 and $\Delta_{\text{inv}}$ becomes negative, indicating a band inversion. This band inversion is accompanied by a Dirac-like band crossing, as shown in Fig. 2. This band crossing is protected by fractional translation symmetry due to the different characters of the two bands. Therefore, the spectrum can be described at low energies by a $2 \times 2$ Dirac equation. The analysis of the wave function performed in Ref. [17] for multilayer samples reveals that the $\Gamma_1$ states are mainly localized in the top layer, whereas the spectral weight of the $\Gamma_8$ states is stronger in the bottom layer.

We insist that the approximation considered here does not take into account electrostatic screening due to the external electric field. This effect has been studied in Ref. [9], using a low-energy continuum model and within non-linear Thomas-Fermi theory. The potential difference across a BP sample obtained there suggests that BP presents an intermediate screening behavior between the strong-coupling limit of graphene, where the carriers concentrate close to the interface, and the weak-coupling regime with reduced screening properties that dominates the screening of other van der Waals semiconducting materials such as MoS2.

The presence of a magnetic field is accounted for by means of the Peierls substitution, which replaces the hopping term between two sites,

$$t_{ij} \rightarrow t_{ij} \exp \left[\frac{2\pi}{\Phi_0} e \int_{R} A \cdot dl\right].$$

where $\Phi_0 = \hbar c/\epsilon$ is the flux quantum and $A = (-B y, 0, 0)$ is the vector potential in the Landau gauge, $B$ being the strength of the magnetic field. The band structure can now be calculated by choosing a ribbon with 1 unit cell width and a height that exactly matches the period of the Peierls phase. After obtaining the Hamiltonian as a function of the momentum,

$$\mathcal{H}(\mathbf{k}) = \sum_{i \neq j} t_{ij} c_i^\dagger c_j e^{i \mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} + \sum_{i \neq j} t_{ij} c_i^\dagger c_j e^{i \mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)},$$

the energy eigenvalues corresponding to a momentum $\mathbf{k}$ can be found with exact diagonalization. Our results lead to a band structure composed of a set of LLs, as given in Fig. 5. The structure of the LL spectrum is discussed in detail later.

The DOS of the system is calculated by using an algorithm based on the evolution of the time-dependent Schrödinger equation. For this we use a random superposition of all basis states as the initial state $|\psi\rangle$

$$|\psi\rangle = \sum_i a_i |i\rangle,$$

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The DOS around such a band crossing is well beyond the transition. For low carrier densities, the Fermi surface suffers a semiconducting-to-semimetal transition, with a band crossing at the $\Gamma$ point [see Fig. 2(b)]. As shown in Fig. 6(b), the DOS around such a band crossing is $\propto \sqrt{\varepsilon}$, leading to a set of nonequidistant LLs at energies close to the band crossing energy, with dispersion $\varepsilon_n \propto \pm (n + 1/2)B^{1/2}$. As we move away from this band crossing, the LL spectrum has the same characteristics as in the previous case of unbiased BP, recovering the standard quantization of a 2DEG [Fig. 6(e)].

The most interesting situation occurs for higher bias voltages, well beyond the transition. For $\Delta = 2.2\,\text{eV} > \Delta_c$, the band dispersion presents two Dirac points, in the $\Gamma$-$X$ direction, and it is gapped in the $\Gamma$-$Y$ direction [see Figs. 2(c) and 3(c)]. As studied by Montambaux et al. within the framework of a universal Hamiltonian that describes the merging of Dirac points in the electronic spectrum of two-dimensional crystals [41,42], the topological character of the transition can be understood from the appearance of a Berry phase for $\Delta > \Delta_c$, which takes the values $\pm \pi$ around each Dirac point. If we reduce the bias voltage, we recover the trivial phase with the corresponding annihilation of the Berry phase for $\Delta < \Delta_c$. For low carrier densities, the Fermi surface consists of two pockets encircling the Dirac points along the $\Gamma$-$X$ direction [see Fig. 3(c)]. The DOS close to the Dirac points behaves as $[41] d_{\text{Dirac}}(\varepsilon) \propto |\varepsilon|/v_{F_x}v_{F_Y}$, where $v_{F_x(y)}$ is the Fermi velocity along the $x(y)$ direction within the Dirac cones. In a magnetic field, the LL spectrum is that of a semimetal with a relativistic quantization, $\varepsilon_n \propto \pm \sqrt{\varepsilon} B$ [see Fig. 6(f)]. The shift of $n + 1/2 \rightarrow n$ in the LL energy spectrum for $\Delta > \Delta_c$ is a consequence of the generation of $\pm \pi$ Berry phases around the Dirac points. If we increase the energy, we reach a highly nontrivial LL quantization because of the presence of a saddle point in the band structure, at which there is a transition from CECs encircling the Dirac points to CECs encircling the $\Gamma$ point. In the semiclassical limit, the cyclotron
orbits in reciprocal space follow the CECs. Therefore, at the saddle point there is a change in the topological Berry phase from \(\pm \pi\) for orbits encircling the Dirac points to 0 for orbits encircling the \(\Gamma\) point [43,44].

The two series of LLs shown in Fig. 6 is due to the different characters of the cyclotron frequencies, that or orbits at both sides of the saddle point, with different cyclotron frequencies, that merge at the saddle point. This transition resembles that of highly doped graphene at energies around the Van Hove singularity [45,46].

### III. HALL CONDUCTIVITY

The next step in our analysis, once we understand the LL spectrum of the biased system, is the calculation of the Hall conductivity \(\sigma_{xy}\). For this aim, we use an efficient numerical approach, recently developed by García et al. [36], that is based on a real-space implementation of the Kubo formalism where both diagonal and off-diagonal conductivities are treated on the same footing. In the limit \(\omega \to 0\) and for noninteracting electrons, the so-called Kubo-Bastin formula for the conductivity can be used to obtain the elements of the static conductivity tensor [35–37],

\[
\sigma_{\alpha\beta}(\mu, T) = \frac{i\hbar e^2}{A} \int_{-\infty}^{\infty} d\epsilon f(\epsilon) \text{Tr} \left( v_\alpha \delta(\epsilon - \mathcal{H}) v_\beta \frac{dG^+(\epsilon)}{d\epsilon} - v_\beta \frac{dG^-(\epsilon)}{d\epsilon} v_\alpha \delta(\epsilon - \mathcal{H}) \right),
\]

where \(\mu\) is the chemical potential, \(T\) is the temperature, \(A\) is the area of the sample, \(v_\alpha\) is the \(\alpha\) component of the velocity operator, \(G^\pm(\epsilon) = 1/({\epsilon - \mathcal{H} \pm i\eta})\) are the Green’s functions, and \(f(\epsilon)\) is the Fermi-Dirac distribution. Here the average is performed by using the same random initial state as in the calculation of DOS. By expanding the delta and the Green’s functions \(G^\pm(\epsilon)\) in terms of Chebyshev polynomials (using the so-called kernel polynomial method) [36], the conductivity tensor becomes

\[
\sigma_{\alpha\beta}(\mu, T) = \frac{4e^2}{\pi A} \frac{4}{\Delta E^2} \int_{-1}^{1} d\tilde{\epsilon} \int_{\epsilon_{\text{min}}}^{\epsilon_{\text{max}}} \frac{f(\tilde{\epsilon})}{(1 - \tilde{\epsilon}^2)^2} \sum_{m,n} \Gamma_{mn}(\tilde{\epsilon}) \mu_{mn}^{\alpha\beta}(\tilde{\mathcal{H}}),
\]

where \(\Delta E\) is the energy range of the spectrum, \(\tilde{\epsilon}\) is the rescaled energy within \([-1, 1]\), \(\Gamma_{mn}(\tilde{\epsilon})\) and \(\mu_{mn}^{\alpha\beta}(\tilde{\mathcal{H}})\) are functions of the energy and the Hamiltonian, respectively. More precisely,

\[
\Gamma_{mn}(\tilde{\epsilon}) = \frac{T_m(\tilde{\epsilon}) - i\delta_m \sqrt{1 - \tilde{\epsilon}^2} e^{im \arccos(\tilde{\epsilon})}}{(1 + \delta_m)(1 + \delta_0)},
\]

and

\[
\mu_{mn}^{\alpha\beta}(\tilde{\mathcal{H}}) = \frac{8e^2}{(1 + \delta_0)(1 + \delta_m)} \text{Tr}[v_\alpha v_\beta T_m(\tilde{\mathcal{H}}) v_\beta T_n(\tilde{\mathcal{H}})],
\]

is a scalar function of the rescaled energy, and

\[
\mu_{mn}^{\alpha\beta}(\tilde{\mathcal{H}}) = \frac{8e^2}{(1 + \delta_0)(1 + \delta_m)} \text{Tr}[v_\alpha v_\beta T_m(\tilde{\mathcal{H}}) v_\beta T_n(\tilde{\mathcal{H}})]
\]

is independent of the energy, where \(T_m(x)\) is the Chebyshev polynomial defined according to the recurrence relation \(T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)\) with \(T_0(x) = 1\) and \(T_1(x) = x\).

The Gibbs oscillations due to the truncation of the expansion in (12) are smoothed by using the Jackson kernel \(g_m\) [36,47].

Our results for \(\sigma_{xy}\) are shown in Fig. 7. For \(\Delta = 0\) the Hall conductivity consists of a series of plateaus with the well-known sequence \(\sigma_{xy} = 2ne^2/h\), characteristics of a standard 2DEG with a parabolic band dispersion (although the present case of BP is rather described by a paraboloidal band).

Our numerical calculations show the same quantization of the
Hall conductivity at the transition point $\Delta = \Delta_c$ [Fig. 7(c)]. This is due to the fact that, right at the transition, there is a single crossing of the bands at the time-reversal-invariant $\Gamma$ point of the Brillouin zone [41,42]. Most saliently, for $\Delta > \Delta_c$ [Fig. 7(c)] the Hall conductivity presents plateaus at $\sigma_{xy} = 4(n + 1/2)e^2/h$. This is due to the topological nature of the semimetallic phase, which is well captured by the numerical method. The plateau structure becomes blurred at high energies, which is an artifact due to the finite truncation order of the kernel polynomial approximation as well as the finite size of the sample [36]. These artifacts can be improved with a higher truncation order of the expansion and by considering a larger sample size. This would lead to an initial state, obtained from Eq. (9), that is a more accurate representation of the whole energy spectrum [29,39]. Furthermore, it has been shown that the convergence of the Hall conductivity in Eq. (12) is faster with larger magnetic fields [36]. Therefore, in order to catch several Landau levels within the emerged Dirac cones, the large magnetic field of $B = 130$ T is used in the calculations. Lower magnetic fields will give similar qualitative behaviors for the LL spectrum and for the Hall conductivity. In spite of the above choices in the simulation, the convergence of the results is still slow, especially if the band structure contains different topological features within a small energy range, such as in the case with $\Delta > \Delta_c$. We adopted a truncation order as large as $M = 15000$ for the kernel polynomial decomposition (the computational costs are proportional to $M^2$ and the maximum truncation order used in Ref. [36] is $M = 6144$), and the simulated systems consist of $2 \times 600 \times 600$ atomic sites. However, it is still not enough to overcome the blurred effects in the high-energy plateaus. Further calculations with a larger truncation order or sample size are beyond the computational resource that we can reach.

IV. DISCUSSION AND CONCLUSIONS

We note that the emergence of Dirac points in the spectrum of biased black phosphorus can be understood by thinking of the BP lattice as a honeycomb lattice (like the one in graphene) in which one of the three hopping terms between nearest-neighbor atoms can be different from the other two [41]. This is indeed the case in BP, in which two of the three nearest neighbors of one atom are on the same plane, whereas the third nearest neighbor is on a different plane. Moreover, the signs of these hopping terms are different, making BP a natural platform to realize Dirac point engineering near the $\Gamma$ point [42], either by tuning the external bias or by applying strain to the samples.

In summary, we have analyzed the electronic properties of biased black phosphorus in the presence of a perpendicular magnetic field. In the absence of an electric field, the external magnetic field leads to a quantization of the electron and hole bands into a set of equidistant Landau levels. This behavior is similar to the discretization of the energy dispersion in a 2DEG with a parabolic band. If we further apply a perpendicular electric field to the sample, we obtain a reduction of the band gap with the applied voltage. For a critical value of the voltage, the gap completely closes, and a pair of Dirac points appears in the $\Gamma$-X direction of the Brillouin zone. This semiconductor-to-semimetal transition is accompanied by a change in the topology of the system, due to the generation of $\pm \pi$ Berry phases around the Dirac points. We obtain a highly nontrivial LL spectrum in this phase, with the coexistence of relativistic LLs, with a $E_n \propto \sqrt{nB}$ quantization, with equidistant LLs at higher energies, following the standard $E_n \propto B(n + 1/2)$, characteristic of a 2DEG. The transition between these two regimes requires goingthrough a Van Hove singularity (saddle point) in the band dispersion, with the corresponding divergence in the DOS. Finally, we numerically compute the Hall conductivity of the system. The topological transition driven by the electric field is reflected in a different quantization of the Hall conductivity, which presents the characteristic $\sigma_{xy} \propto 2n$ behavior for low bias voltages (insufficient to close the gap) and a relativistic quantum Hall effect with $\sigma_{xy} \propto 4(n + 1/2)$ in the semimetallic phase, due to the generation of a pair of Dirac cones. Although we focus on the simplest case of bilayer BP, the results presented here apply to any multilayer BP sample, with the advantage that the gap decreases with the number of layers, and therefore the semiconducting-to-semimetal transition would be more easily reached for thicker samples. We note that the electric-field-induced semimetallic phase in BP is likely to present new broken-symmetry phases due to many-body effects, which are not included here. For example, it is known that bilayer graphene, whose low-energy spectrum reassembles that of biased semimetallic BP, suffers a nematic phase transition driven by Coulomb interactions [48]. Similar interaction-driven phase transitions might occur in BP and will be the object of future studies. The phenomena discussed

FIG. 7. Hall conductivity of pristine and biased BP for the biased potentials used in Fig. 6. The temperature is $T = 0.01$ K and the magnetic field is $B = 130$ T. The truncation order for the kernel polynomial in Eq. (12) is $M = 15000$. The calculated system contains $2 \times 600 \times 600$ atomic sites, and the results are averaged over five random realizations of initial states.
here could be observed by exposing a biased BP sample, chemically doped from in situ deposition of adatoms [16], to a strong quantizing magnetic field or by applying external strain (compression) to the samples [23]. These techniques have been shown to be appropriate routes to tune this material from a moderate-gap semiconductor to a band-inverted semimetal.

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