Supporting Information

Anisotropic carrier mobility of distorted Dirac cones: theory and application

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1. Rigorously analytic solution of the relaxation time and the residual error due to expansion.

Inserting Eq. (14) into Eq. (15), it yields the integral form of the relaxation time $\tau_{\mathbf{k}}$ as

$$\begin{aligned}
\frac{1}{\tau_{\mathbf{k}}} &= \int\left(1-\frac{\boldsymbol{\upsilon}_{\mathbf{k}}\cdot\boldsymbol{\upsilon}_{\mathbf{k}'}}{|\boldsymbol{\upsilon}_{\mathbf{k}}|^2}\right)\frac{2\pi k_B T}{C_{11}\hbar}\frac{1}{(2\pi)^2}\left[S_1\cos\frac{\theta_{\mathbf{k}'}-\theta_{\mathbf{k}}}{2}-E_\beta\cos\left(\frac{3(\theta_{\mathbf{k}'}+\theta_{\mathbf{k}})}{2}-\theta_0\right)\right]^2\delta(\varepsilon_{\mathbf{k}'}-\varepsilon_{\mathbf{k}})\mathrm{d}^2\mathbf{k}' \\
&= \frac{k_B T\varepsilon_{\mathbf{k}}}{2\pi C_{11}\hbar}\int\left(1-\frac{\upsilon_F^2\cos(\theta_{\mathbf{k}'}-\theta_{\mathbf{k}})+\upsilon_t^2+\upsilon_t\upsilon_F(\sin\theta_{\mathbf{k}}+\sin\theta_{\mathbf{k}'})}{\upsilon_F^2+2\upsilon_t\upsilon_F\sin\theta_{\mathbf{k}}+\upsilon_t^2}\right)\frac{\left[S_1^2\cos^2\frac{\theta_{\mathbf{k}'}-\theta_{\mathbf{k}}}{2}+E_\beta^2\cos^2\left(\frac{3}{2}(\theta_{\mathbf{k}'}+\theta_{\mathbf{k}})-\alpha\right)\right]}{(\hbar\upsilon_F+\hbar\upsilon_t\sin\theta_{\mathbf{k}'})^2}d\theta_{\mathbf{k}'} \\
&= \frac{k_B Tk}{2\pi C_{11}\hbar^2\upsilon_F}\int\left(1-\frac{\cos(\theta_{\mathbf{k}'}-\theta_{\mathbf{k}})+\alpha_t^2+\alpha_t(\sin\theta_{\mathbf{k}}+\sin\theta_{\mathbf{k}'})}{1+2\alpha_t\sin\theta_{\mathbf{k}}+\alpha_t^2}\right)\frac{(1+\alpha_t\sin\theta_{\mathbf{k}})\left[S_1^2\cos^2\frac{\theta_{\mathbf{k}'}-\theta_{\mathbf{k}}}{2}+E_\beta^2\cos^2\left(\frac{3}{2}(\theta_{\mathbf{k}'}+\theta_{\mathbf{k}})-\alpha\right)\right]}{(1+\alpha_t\sin\theta_{\mathbf{k}'})^2}d\theta_{\mathbf{k}'} \\
&= \frac{k_B Tk}{2\pi C_{11}\hbar^2\upsilon_F}\times A
\end{aligned}$$

,(S1)

where the integral item A is solved to be

$$
\begin{aligned}
A = 2\,\mathrm{Re}\{ &(1+\alpha_t \sin\theta_{\mathbf{k}})\Big(\frac{E_\beta^2 \alpha_t^{\,3}[2Lg(-\sqrt{-1+\alpha_t^{\,2}}) - Lg(-1+\alpha_t^{\,2})]}{4\alpha_t^{\,3}(-1+\alpha_t^{\,2})^{3/2}} \\
&+ \frac{E_\beta^2[16(1-\alpha_t^{\,2})^{3/2}\pi - 2(8-12\alpha_t^{\,2}+3\alpha_t^{\,4})Lg(-\sqrt{-1+\alpha_t^{\,2}}) + (8-12\alpha_t^{\,2}+3\alpha_t^{\,4})\,\mathrm{Lg}(-1+\alpha_t^{\,2})]\sin(2\theta_0 - 3\theta_{\mathbf{k}})}{4\alpha_t^{\,3}(-1+\alpha_t^{\,2})^{3/2}} \\
&+ \frac{S_1^2\sqrt{\dfrac{1}{1-\alpha_t^{\,2}}}\,\pi(-1+\alpha_t \sin\theta_{\mathbf{k}})}{2(-1+\alpha_t^{\,2})} + \frac{S_1^2 \cos\theta_{\mathbf{k}}^{\,2}[2\sqrt{-1+\alpha_t^{\,2}}\,\pi + 2Lg(-\sqrt{-1+\alpha_t^{\,2}}) - Lg(-1+\alpha_t^{\,2})]}{4\alpha_t^{\,2}\sqrt{-1+\alpha_t^{\,2}}\,(\cos\theta_{\mathbf{k}}^{\,2} + (\alpha_t + \sin\theta_{\mathbf{k}})^2)} \\
&+ \frac{3E_\beta^2 \cos(2\theta_0 - 3\theta_{\mathbf{k}})\cos\theta_{\mathbf{k}}[(2(-4+\alpha_t^{\,2})\sqrt{-1+\alpha_t}\,\pi + (-8+6\alpha_t^{\,2})Lg(-\sqrt{-1+\alpha_t^{\,2}}) + (4-3\alpha_t^{\,2})Lg(-1+\alpha_t^{\,2})]}{4\alpha_t^{\,2}\sqrt{-1+\alpha_t^{\,2}}\,(\cos\theta_{\mathbf{k}}^{\,2} + (\alpha_t + \sin\theta_{\mathbf{k}})^2)} \\
&- \frac{E_\beta^2(\alpha_t + \sin\theta_{\mathbf{k}})[\alpha_t^{\,5}(-2\,\mathrm{Lg}(-\sqrt{-1+\alpha_t^{\,2}}) + \mathrm{Lg}(-1+\alpha_t^{\,2})) + \alpha_t^{\,3}(2\,\mathrm{Lg}(-\sqrt{-1+\alpha_t^{\,2}}) - \mathrm{Lg}(-1+\alpha_t^{\,2}))]}{4\alpha_t^{\,2}\sqrt{-1+\alpha_t^{\,2}}\,(\cos\theta_{\mathbf{k}}^{\,2} + (\alpha_t + \sin\theta_{\mathbf{k}})^2)} \\
&+ \frac{E_\beta^2(\alpha_t + \sin\theta_{\mathbf{k}})[2\sqrt{-1+\alpha_t^{\,2}}\,(12-13\alpha_t^{\,2}+\alpha_t^{\,4})\pi + 2(12-19\alpha_t^{\,2}+6\alpha_t^{\,4})\,\mathrm{Lg}(-\sqrt{-1+\alpha_t^{\,2}}) + (-12+19\alpha_t^{\,2}-6\alpha_t^{\,4})\,\mathrm{Lg}(-1+\alpha_t^{\,2})]\sin(2\theta_0 - 3\theta_{\mathbf{k}})}{4\alpha_t^{\,2}\sqrt{-1+\alpha_t^{\,2}}\,(\cos\theta_{\mathbf{k}}^{\,2} + (\alpha_t + \sin\theta_{\mathbf{k}})^2)} \\
&- \frac{E_\beta^2(\alpha_t + \sin\theta_{\mathbf{k}})[16(-1+\alpha_t^{\,2})^{3/2}\pi - 2(8-12\alpha_t^{\,2}+3\alpha_t^{\,4})Lg(-\sqrt{-1+\alpha_t^{\,2}}) + (8-12\alpha_t^{\,2}+3\alpha_t^{\,4})Lg(-1+\alpha_t^{\,2})]\sin(2\theta_0 - 3\theta_{\mathbf{k}})}{4\alpha_t^{\,2}\sqrt{-1+\alpha_t^{\,2}}\,(\cos\theta^2 + (\alpha_t + \sin\theta)^2)} \\
&+ \frac{S_1^2\alpha_t(\alpha_t \sin\theta_{\mathbf{k}})(-1+\alpha_t \sin\theta_{\mathbf{k}})(2Lg(-\sqrt{-1+\alpha_t^{\,2}}) - Lg(-1+\alpha_t^{\,2}))}{4(-1+\alpha_t^{\,2})^{3/2}(\cos\theta_{\mathbf{k}}^{\,2} + (\alpha_t + \sin\theta_{\mathbf{k}})^2)} + \frac{2\alpha_t^{\,3}S_1^2(\alpha_t + \sin\theta_{\mathbf{k}})[2Lg(-\sqrt{-1+\alpha_t^{\,2}}) - Lg(-1+\alpha_t^{\,2})]}{8\alpha_t^{\,2}(-1+\alpha_t^{\,2})^{3/2}(\cos\theta_{\mathbf{k}}^{\,2} + (\alpha_t + \sin\theta_{\mathbf{k}})^2)} \\
&- \frac{2\sin\theta_{\mathbf{k}} S_1^2(\alpha_t + \sin\theta_{\mathbf{k}})[2(-1+\alpha_t^{\,2})^{3/2}\pi + (-2+4\alpha_t^{\,2})Lg(-\sqrt{-1+\alpha_t^{\,2}}) + (1-2\alpha_t^{\,2})\,\mathrm{Lg}(-1+\alpha_t^{\,2})]}{8\alpha_t^{\,2}(-1+\alpha_t^{\,2})^{3/2}(\cos\theta_{\mathbf{k}}^{\,2} + (\alpha_t + \sin\theta_{\mathbf{k}})^2)}\Big)\}
\end{aligned}
$$

.(S2)

This rigorous analytic result is complicated. By expanding the result to the second-order terms of the tilting factor α_t, an approximate result with a much simpler expression is obtained as Eq. (17). A comparison between the rigorous and approximate expressions is provided in Fig. S1 based on the parameters of 8B-*Pmmn* Borophene. It demonstrates that the difference (residual error) is small. More importantly, the approximate expression overestimates at some $\theta_{\mathbf{k}}$ while underestimates at others, so the discrepancy would be even reduced when an integral on $\theta_{\mathbf{k}}$ is conducted to give the carrier mobility [see Fig. 5(b)].

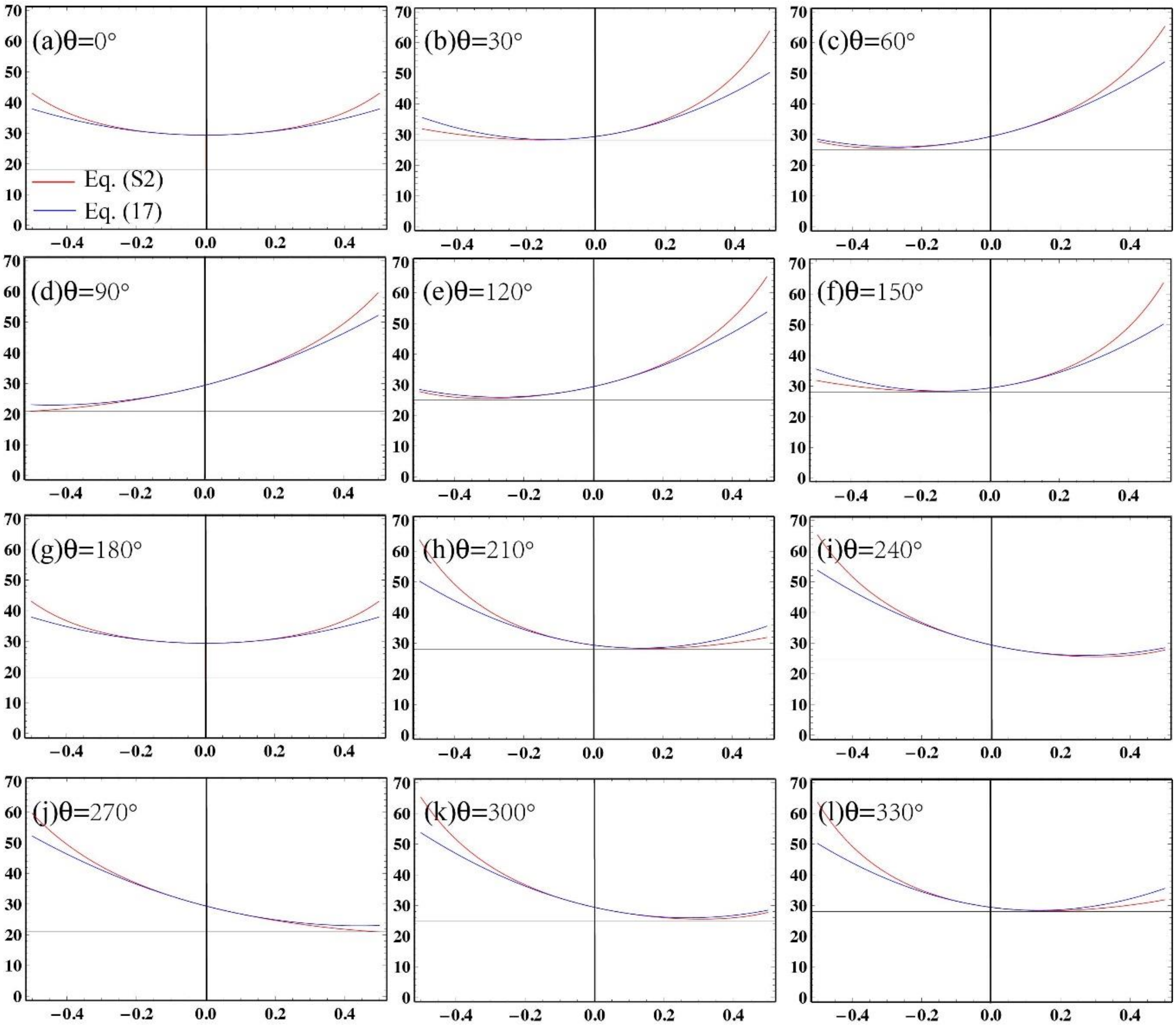

Figure S1. The integral A in the expression of $\tau_{\mathbf{k}}$ as a function of α_t under various $\theta_{\mathbf{k}}$. Red lines are rigorous analytic result of Eq. (S2), while blue lines are the approximate result of expanding to the second-order terms of α_t as given in Eq. (17). $S_1 = 0.43$ and $E_\beta = 3.04$ were adopted to mimic 8B-*Pmmn* according to Eq. (33) and Table 1. Based on the movement direction of Dirac point under strain, $\theta_0 = \pi / 2$.

2. Detailed deduction on the carrier mobility of tilted elliptic cone.

With the effective Hamiltonian Eq. (24) for tilted elliptic Dirac cones and the transformation Eq. (28), the eigenfunction can be written as

$$\psi_{\mathbf{k}} = \frac{1}{\sqrt{2}}\begin{pmatrix} \pm\exp\left(-i\theta_{\tilde{\mathbf{k}}}\right) \\ 1 \end{pmatrix}, \tag{S3}$$

where $\theta_{\tilde{\mathbf{k}}}$ is the angle of $\tilde{\mathbf{k}}$. The corresponding carrier velocity is

$$\boldsymbol{\upsilon}_{\mathbf{k}} = \left(\upsilon_{\mathrm{F}x}\cos\theta_{\tilde{\mathbf{k}}}, \upsilon_{\mathrm{F}y}\sin\theta_{\tilde{\mathbf{k}}} \pm \upsilon_{\mathrm{t}}\right) \ . \tag{S4}$$

Following a similar way to the case of tilted cone, the relaxation time is deduced to be

$$\frac{1}{\tau_{\mathbf{k}}} = \frac{k_B T \varepsilon_{\mathbf{k}}}{2\pi C_{11}\hbar}\int \frac{\left(1-\frac{\upsilon_{\mathrm{F}x}{}^2\cos\theta_{\tilde{\mathbf{k}}}\cos\theta_{\tilde{\mathbf{k}}'}+\upsilon_{\mathrm{F}y}{}^2\sin\theta_{\tilde{\mathbf{k}}}\sin\theta_{\tilde{\mathbf{k}}'}+\upsilon_t{}^2+\upsilon_t\upsilon_{\mathrm{F}y}\left(\sin\theta_{\tilde{\mathbf{k}}}+\sin\theta_{\tilde{\mathbf{k}}'}\right)}{(\upsilon_{\mathrm{F}x}\cos\theta_{\tilde{\mathbf{k}}})^2+(\upsilon_{\mathrm{F}y}\sin\theta_{\tilde{\mathbf{k}}}+\upsilon_t)^2}\right)\left[S_1{}^2\cos^2\frac{\theta_{\tilde{\mathbf{k}}'}-\theta_{\tilde{\mathbf{k}}}}{2}+E_\beta{}^2\cos^2\left(\frac{3}{2}\left(\theta_{\tilde{\mathbf{k}}'}+\theta_{\tilde{\mathbf{k}}}\right)-\theta_0\right)\right]}{\hbar^2\upsilon_{\mathrm{F}x}\upsilon_{\mathrm{F}y}(1+\alpha_t\sin\theta_{\tilde{\mathbf{k}}'})^2}d\theta_{\tilde{\mathbf{k}}'}$$

,(S5)

where $\varepsilon_{\mathbf{k}} = \hbar\sqrt{\left(\upsilon_{\mathrm{F}x}k_x\right)^2+\left(\upsilon_{\mathrm{F}y}k_y\right)^2}(1+\alpha_t\sin\theta_{\mathbf{k}})$. Denote c=$\frac{\upsilon_{\mathrm{F}x}{}^2}{\upsilon_{\mathrm{F}y}{}^2}$, then Eq. (S5) becomes

$$\frac{1}{\tau_{\mathbf{k}}} = \frac{k_B T k}{2\pi C_{11}\hbar^2\upsilon_{\mathrm{F}x}\upsilon_{\mathrm{F}y}}\int \frac{\left(1-\frac{c\cos\theta_{\tilde{\mathbf{k}}}\cos\theta_{\tilde{\mathbf{k}}'}+\sin\theta_{\tilde{\mathbf{k}}}\sin\theta_{\tilde{\mathbf{k}}'}+\alpha_t{}^2+\alpha_t\left(\sin\theta_{\tilde{\mathbf{k}}}+\sin\theta_{\tilde{\mathbf{k}}'}\right)}{(c\cos\theta_{\tilde{\mathbf{k}}})^2+(\sin\theta_{\tilde{\mathbf{k}}}+\alpha_t)^2}\right)(1+\alpha_t\sin\theta_{\tilde{\mathbf{k}}})\left[S_1{}^2\cos^2\frac{\theta_{\tilde{\mathbf{k}}'}-\theta_{\tilde{\mathbf{k}}}}{2}+E_\beta{}^2\cos^2\left(\frac{3}{2}\left(\theta_{\tilde{\mathbf{k}}'}+\theta_{\tilde{\mathbf{k}}}\right)-\theta_0\right)\right]}{(1+\alpha_t\sin\theta_{\tilde{\mathbf{k}}'})^2}d\theta_{\tilde{\mathbf{k}}'}$$

.(S6)

The integral can be expanded to the second-order of the tilting factor ($\alpha_{\mathrm{t}} \equiv \frac{\upsilon_{\mathrm{t}}}{\upsilon_{\mathrm{Fy}}}$) to get an analytic form:

$$\frac{1}{\tau_{\mathbf{k}}} = \frac{k_B T k}{4C_{11}\hbar^2\upsilon_{\mathrm{F}x}\upsilon_{\mathrm{F}y}}\times B \qquad .(S7)$$

with denotation

$$
\begin{aligned}
B &= [S_1^2 + 2E_\beta^2] + \alpha_t \times [2E_\beta^2 + S_1^2(-1 + \frac{2}{1+c+(-1+c)\cos 2\theta}))\sin\theta] \\
&+ \frac{1}{8}\alpha_t^2[-\frac{16(S_1{}^2 + 2E_\beta{}^2)(-1+c+(1+c)\cos 2\theta)}{(1+c+(-1+c)\cos 2\theta)^2} \\
&+ 2\frac{4E_\beta{}^2(5+3c) + S_1{}^2(5+7c) + 3E_\beta{}^2(1+c)\cos(2(\theta_0 - 2\theta)) - 3S_1{}^2\cos 2\theta}{1+c+(-1+c)\cos 2\theta} \\
&+ 2\frac{(9S_1{}^2 c + 4E_\beta{}^2(-5+3c))\cos 2\theta + 2S_1{}^2(-1+c)\cos 4\theta}{1+c+(-1+c)\cos 2\theta} \\
&+ \frac{2E_\beta{}^2(-7+3c) + S_1{}^2(-5+9c) + 4(2E_\beta{}^2(2+c) + S_1{}^2(1+2c))\cos 2\theta - (S_1{}^2 - 2E_\beta{}^2)(-1+c)\cos 4\theta}{(c\cos\theta^2 + \sin\theta^2)^2}]
\end{aligned}
\tag{.S8}
$$

where $\theta_{\tilde{\mathbf{k}}}$ is abbreviated into θ for simplicity. The zero-order term of the integral is $\frac{\pi}{2}(S_1^2 + 2E_\beta^2)$, being consistent with the result of the untilted case.[1] If c=1, then the above results return to that for the tilted cones in Eq. (17).

We now deduce the mobility formula of tilted elliptic cones. Insert Eq. (S9) into the mobility equation

$$
\mu = \frac{\sigma}{ne} = \frac{e\int \tau_{\mathbf{k}} \frac{\partial n_{\mathrm{F}}}{\partial \varepsilon} \upsilon_{\mathbf{k}} \upsilon_{\mathbf{k}} \mathrm{d}^2\mathbf{k}}{\int n_{\mathrm{F}} \mathrm{d}^2\mathbf{k}}, \tag{S9}
$$

we have

$$
\begin{aligned}
\mu_{x,\mathrm{NP}} &= \frac{\sigma_{xx}}{ne} = \frac{\mu_{x,\mathrm{NP}}^{(0)}}{\pi}\left[S_1{}^2 + 2E_\beta{}^2\right]\left(1-\alpha_t{}^2\right)^{\frac{3}{2}} \int \frac{\cos^2\theta}{B} \frac{d\theta}{1+\alpha_t \sin\theta} \\
\mu_{y,\mathrm{NP}} &= \frac{\sigma_{yy}}{ne} = \frac{\mu_{y,\mathrm{NP}}^{(0)}}{\pi}\left(1-\alpha_t{}^2\right)^{\frac{3}{2}}\left[S_1{}^2 + 2E_\beta{}^2\right] \int \frac{\left(\sin^2\theta + 2\alpha_t \sin\theta + \alpha_t{}^2\right)}{B} \frac{d\theta}{1+\alpha_t \sin\theta}
\end{aligned}
\tag{S10}
$$

at the neutrality point (NP), where $\mu_{x,\mathrm{NP}}^{(0)}$ and $\mu_{y,\mathrm{NP}}^{(0)}$ are given in Eq. (31). We now need to solve

$$
C = \frac{\left[S_1{}^2 + 2E_\beta{}^2\right]}{\pi} \int \frac{\cos^2\theta}{B} \frac{d\theta}{1+\alpha_t \sin\theta}, \tag{S11}
$$

and

$$D=\frac{\left[S_1^{\ 2}+2E_\beta^{\ 2}\right]}{\pi}\int\frac{\left(\sin^2\theta+2\alpha_t\sin\theta+\alpha_t^{\ 2}\right)}{B}\frac{d\theta}{1+\alpha_t\sin\theta}\,. \tag{S12}$$

The zero-order term of α_t in (S11, S12) is C_0=1 and D_0=1. The odd-term is zero due to the symmetry. The second-order term of α_t is

$$C_2=\frac{\left[\begin{array}{l}-6E_\beta^4(1+c)^3-S_1^4(-1+c)(16-\frac{20}{\sqrt{\frac{1}{c}}}-2\sqrt{\frac{1}{c}}+3c+3c^2)\\ +S_1^2E_\beta^2(15+\frac{4}{(\frac{1}{c})^{3/2}}-\frac{4}{\sqrt{\frac{1}{c}}}-39c+37c^2-13c^3)-3E_\beta^2(S_1^2+2E_\beta^2)c(6-\frac{4}{\sqrt{\frac{1}{c}}}-4\sqrt{\frac{1}{c}}+\frac{1}{c}+3c)\cos(2\theta_0)\end{array}\right]}{2(S_1^2+2E_\beta^2)^2(-1+c)^3}$$

.(S13)

and

$$D_2=\frac{c\left[\begin{array}{l}-\frac{10E_\beta^4(-1+c)^3}{c}-\frac{S_1^4(-1+c)(-19c-4c^2+\frac{6+\sqrt{\frac{1}{c}}+16c}{\sqrt{\frac{1}{c}}})}{c}\\ +S_1^2E_\beta^2(-35-\frac{4}{(\frac{1}{c})^{3/2}}+\frac{4}{\sqrt{\frac{1}{c}}}+\frac{11}{c}+33c-9c^2)-3E_\beta^2(S_1^2+2E_\beta^2)c(6-\frac{4}{\sqrt{\frac{1}{c}}}-4\sqrt{\frac{1}{c}}+\frac{1}{c}+c)\cos(2\theta_0)\end{array}\right]}{2(S_1^2+2E_\beta^2)^2(-1+c)^3}$$

,(S14)

In tilted circular cones with c=1, C_2 and D_2 becomes

$$\left[-\frac{19S_1^4+54S_1^2E_\beta^2+24E_\beta^4}{8\left(S_1^2+2E_\beta^2\right)^2}\right]\text{ and }\left[-\frac{5S_1^4+42S_1^2E_\beta^2+40E_\beta^4}{8\left(S_1^2+2E_\beta^2\right)^2}\right]. \tag{S15}$$

The above results Eqs. (S13, S14) are only a little different with the formula of tilted circular cones Eq. (S15). We introduce notation $\bar{\upsilon}=\sqrt{\upsilon_x\upsilon_y}$ and substitute the value of 8B-*Pmmn*, then the difference between Eqs. (S13, S14) and Eq. (S15) was evaluated as a function of c in Fig. S2. Results of 8B-*Pmmn* and 2BH-*Pmmn* based on their realistic c are also listed in Table S1. We can see that the difference is small, verifying that the improvement of the accuracy is limited if we use a complicated form of Eqs. (S13, S14) instead of the approximated Eq. (S15).

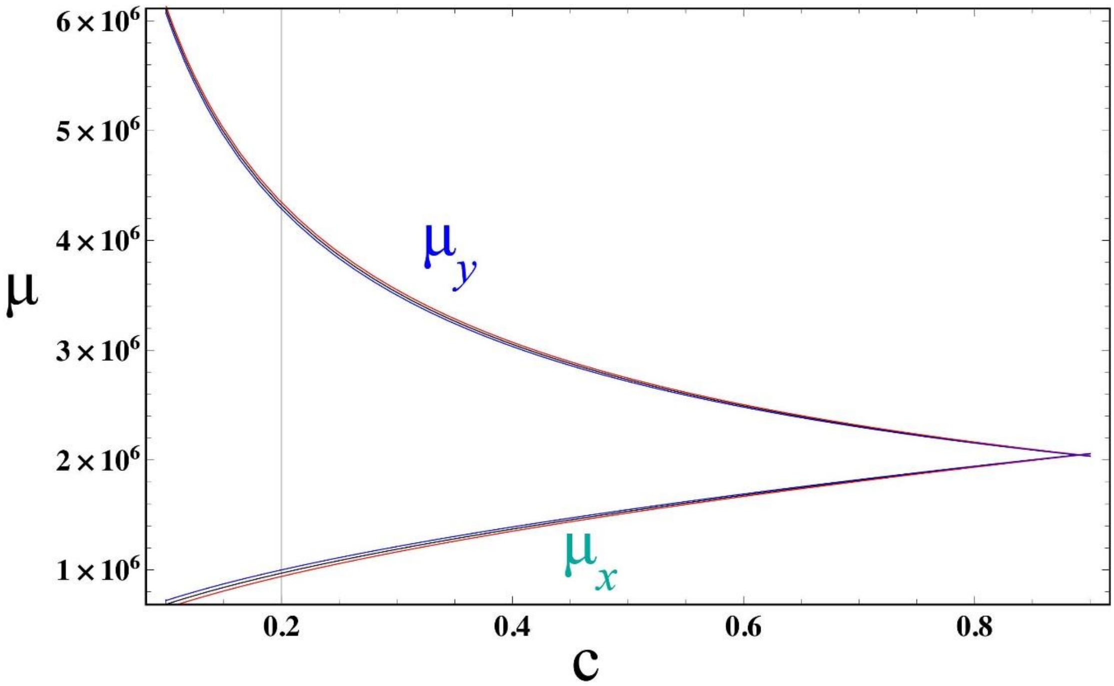

Figure S2. Comparison between Eqs. (S13, S14) and Eq. (S15). $\bar{\upsilon} = 6.47\times10^5$ m/s , S_1 = 0.43 and E_β = 3.04 were adopted to mimic 8B-*Pmmn* according to Eq. (33) and Table 1. Black lines are the results using Eq. (S15), red and blue lines represent the results making $\cos\theta_0 = \pm1$ respectively by using Eqs. (S13, S14).

Table S1. Results of carrier mobilities of 8B-*Pmmn* and 2BH-*Pmmn* calculated with two methods.

System	8B-*Pmmn*	2BH-*Pmmn*
$\mu_{\mathrm{NP},x/y}$ (10^5cm^2/V/s)[a]	14.8, 28.4	4.48, 13.4
$\mu_{\mathrm{NP},x/y}$ (10^5cm^2/V/s)[b]	14.6, 28.6	4.45, 13.4
$\mu_{\mathrm{doped},x/y}$ (10^5cm^2/V/s)[a]	7.72, 14.9	0.78, 2.34
$\mu_{\mathrm{doped},x/y}$ (10^5cm^2/V/s)[b]	7.63, 14.9	0.77, 2.34

[a] calculated with Eq. (S15) as its second-item.

[b] calculated with Eqs. (S13, S14) as the second-item.

3. Movement of Dirac cones under shear strains for 8B-*Pmmn* and 2BH-*Pmmn*.

After applying shear strains, we could do the 3D-fit near the original unstrained Dirac point and obtain the position of new Dirac cones. The results are summarized in Fig. S3. We could find that the Dirac point all moves perpendicular to the Γ-X line under shear strains in both two systems (8B-*Pmmn* and 2BH-*Pmmn*), verifying our analysis. They are protected by the symmetry.

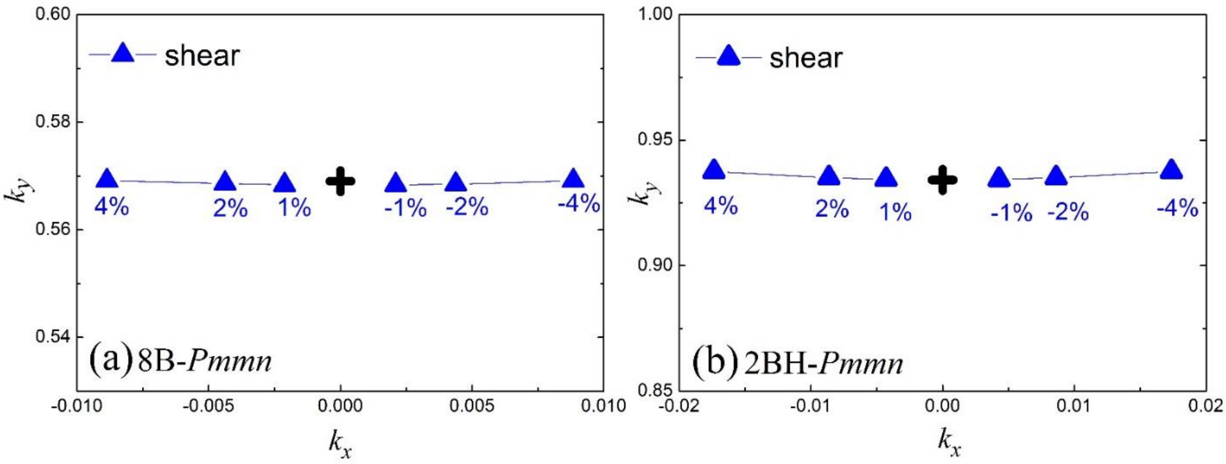

Figure S3. Movements of Dirac point under shear strains in (a) 8B-*Pmmn* and (b) 2BH-*Pmmn*. Dirac point is trajectoryed in the (k_x, k_y) plane. $\varepsilon=\pm0.01$, 0.02, 0.04 was used. The position of unstrained Dirac point is marked with symbol "+" in figure.

References:

[1] Z. Li, J. Wang, and Z. Liu 2014 *J. Chem. Phys.* **141** 144107