Photogalvanic Effect in Weyl Semimetals from First Principles

Yang Zhang,1, 2 Hiroaki Ishizuka,3 Jeroen van den Brink,2 Claudia Felser,1 Binghai Yan,4 and Naoto Nagaosa5, 3

1Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany
2Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany
3Department of Applied Physics and Quantum Phase Electronics Center (QPEC), University of Tokyo, Tokyo 113-8656, Japan
4Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 7610001, Israel
5RIKEN Center for Emergent Matter Science (CEMS), Wako, 351-0198, Japan

Using first-principles calculations, we investigate the photogalvanic effect in the Weyl semimetal material TaAs. We find colossal photocurrents caused by the Weyl points in the band structure in a wide range of laser frequency. Our calculations reveal that the photocurrent is predominantly contributed by the three-band transition from the occupied Weyl band to the empty Weyl band via an intermediate band away from the Weyl cone, for excitations both by linearly and circularly polarized lights. Therefore, it is essential to sum over all three-band transitions by considering a full set of Bloch bands (both Weyl bands and trivial bands) in the first-principles band structure while it does not suffice to only consider the two-band direct transition within a Weyl cone. The calculated photoconductivities are well consistent with recent experiment measurements. Our work provides the first first-principles calculation on nonlinear optical phenomena of Weyl semimetals and serves as a deep understanding of the photogalvanic effects in complex materials.

Introduction. Weyl fermions correspond to the massless solutions of Dirac equation [1] and have been observed in solids as quasiparticles recently [2–5]. Related materials are called Weyl semimetals (WSM) [7–13]. A WSM gives rise to linearly band-crossing points called Weyl points (WPs) in the momentum space. WPs are monopoles of the Berry curvature [14, 15] with finite chirality and are related to the chiral anomaly in the context of high-energy physics [16–19] and unique surface Fermi arcs [2].

The monopole-type Berry curvature of WSMs can lead to appealing nonlinear optical effects that are intimately related to the Berry phase in the band structure [20–24]. Under strong light irradiation, a noncentrosymmetric material exhibits photocurrents as nonlinear functions of the electric field of the light and also generates higher harmonic frequencies, referred to as the photogalvanic effects. The photogalvanic effect rectifies light to dc currents and often play a crucial role in optical devices and solar cells beyond the p-n junction platform [25–27]. Under linearly polarized light, the induced photocurrent is usually called shift current that originates in the charge center shift between the valence and conduction bands in the optical excitation. Under the circularly polarized light, the photocurrent generation is referred to as the circular photogalvanic effect (CPGE). It can be expressed in the formalism of Berry curvature and Berry connection [22–24], revealing a topological nature. Therefore, WSMs have recently been theoretically investigated for such nonlinear optical phenomena [28–44]. In these works, two-band or four-band effective models are commonly adopted to reveal the relation between the photocurrent and the Weyl bands. For example, the tilt of Weyl cones is proposed to play an essential role to generate a net CPGE current by considering the two-band transition from the occupied Weyl band to the empty Weyl band [39]. However, the first-principles investigation on the photogalvanic effects of WSMs, which accounts for the realistic material band structures, is still missing.

Recent experiments [45–50] have reported giant photocurrents effects and the second-harmonic generation (SHG) in the TaAs-family WSMs exhibiting in orders of magnitude larger responses than conventional nonlinear materials. However, some experiments are seemingly controversial to each other. Reference [48] reported a photocurrent caused by the circularly polarized light, but claimed that a negligible photocurrent was caused by the linearly polarized light through the shift current mechanism. In contrast, Ref. [48] reported a colossal shift current with linearly polarized light in the same compound. Therefore, accurate estimations of photocurrents are necessary and timely to identify quantitative contributions from CPGE and shift current for a specific material. In addition, nonlinear optical phenomena are highly sensitive to the bulk Fermi surface topology but are insensitive to surface states. Hence, they can serve a direct pathway to probe the topology inside the bulk.

In this letter, we perform first-principles studies on the CPGE and shift current effect in WSMs. With the second-order Kubo formulism, we calculate the photocurrent conductivity in the inversion-asymmetric WSM TaAs via a multiband approach. Our results agree quantitatively with recent experiments. The shift current displays a close relation with the existence of WPs. Especially in the long-wavelength region, the shift current is predominantly contributed by virtual transitions from the occupied Weyl to the empty Weyl band through a third trivial band, referred to as the three-band transition, as illustrated in Fig. 1b. For CPGE, the three-band virtual transitions make the dominant contributions and distribute relatively uniformed in the momentum space.

arXiv:1803.00562v4 [cond-mat.str-el] 22 May 2018
In contrast, the two-band real transitions contribute much less photocurrent, which is mainly caused by the Weyl cone regions. Given the significance of the three-band transitions, it is necessary to sum over all intermediate states by considering a full set of Bloch states. Then the first-principles method is naturally the best way to compute the nonlinear response. For the same photon energy used in experiment, we find that the CPGE photocurrent is nearly two orders of magnitude greater than the shift current and clarify the possible reason why the shift current was not detected in a previous experiment that reported the CPGE [46].

To calculate the photocurrent also the steady-state short-circuit photocurrent under the linearly polarized light. To calculate the photocurrent also the steady-state short-circuit photocurrent under the linearly polarized light. It indicates that the shift vector directly connects the response photocurrent with a charge center shift between valance and conduc- tion bands, and is not suited to deal with scattering processes with finite relaxation time. of valence and conduction bands, but is quite numerically unstable for metallic systems with a low-frequency driving field, due to the energy delta function and gauge fix of Berry connection of valence and conduction bands, and is not suited to deal with scattering processes with finite relaxation time. In a two-band approximation, the shift current response \( \sigma_{ab}^{\text{N}}(a = x, y, z) \) is zero as the velocity numerator \( N \) is real (here \( l = m, N = \langle \hat{l} \hat{k} | \hat{v}_a | \hat{l} \hat{k} \rangle = \langle \hat{l} \hat{k} | \hat{v}_b | m \hat{k} \rangle = \langle m \hat{k} | \hat{v}_c | n \hat{k} \rangle > \). \( \hat{T} \) reverses the velocity and brings an additional minus sign to the imaginary part of \( N \) by the complex conjugation. Thus, in materials with time reversal symmetry, the real part of the numerator is odd to \( \hat{k} \) and therefore vanishes in the integral, and hence, only the imaginary part of the numerator has to be taken into account for calculations on non-magnetic WSMs. Since there is no current from \( l = n \) or \( m = n \), we can separate the contribution into two parts with respect to band number \( l \) and \( m \). The three-band processes \( (n \rightarrow m \rightarrow l) \) are given by \( l \neq m \), and the two-band processes are given by \( l = m \) (two-band transition). By applying the point group symmetry operations to the numerator \( N \), the third rank conductivity tensor shape can be determined, as can be the tensor form of the anomalous Hall conductivity and spin Hall conductivity [54, 55].

To see the relations between photocurrent response and the detailed band structure, we analyze the energy denominator by decomposing it into real and imaginary parts:

\[
D_1 = \frac{1}{E_n - E_m - i\delta} = \frac{P}{E_n - E_m - i\delta} + i\pi\delta(E_n - E_m),
\]

\[
D_2 = \frac{1}{E_n - E_l + i\delta} = \frac{P}{E_n - E_l + i\delta} + i\pi\delta(E_n - E_l + i\delta),
\]

Since the product of the three velocity matrices is purely imaginary, \( \text{Im}(D_1D_2) \sim \pi\pi\delta_{E_n - E_l} \) gives the shift current response when \( \phi_{ab} \) is real. Only the momentum vector with band gap equal to photon energy \( \langle E_n - E_l \rangle = \hbar\Omega \) contributes to the response under the linearly polarized light. It indicates that the shift current distribute mainly in some selective small areas in the momentum space. When the incident photon energy is sufficiently small, the response current only comes from the gap between two Weyl bands due to the energy selection rule. In the \( \delta = h/\tau \rightarrow 0 \) limit (long relaxation time limit, which is valid for semiconductors and insulators), the summation over band \( m \) can be performed analytically via the first-order perturbation correction of Bloch-wave function [52]. In the end, we obtain the shift vector formula for the shift current density [22,52]. The shift vector directly connects the response photocurrent with a charge center shift between valance and conduc- tion bands, but is quite numerically unstable for metallic systems with a low-frequency driving field, due to the energy delta function and gauge fix of Berry connection of valence and conduction bands, and is not suited to deal with scattering processes with finite relaxation time. In a two-band approximation, the shift current response \( \sigma_{ab}^{\text{N}}(a = x, y, z) \) is zero as the velocity numerator \( N \) is real (here \( l = m, N = \langle \hat{l} \hat{k} | \hat{v}_a | \hat{l} \hat{k} \rangle = \langle \hat{l} \hat{k} | \hat{v}_b | m \hat{k} \rangle = \langle m \hat{k} | \hat{v}_c | n \hat{k} \rangle > \). \( \hat{T} \) reverses the velocity and brings an additional minus sign to the imaginary part of \( N \) by the complex conjugation. Thus, in materials with time reversal symmetry, the real part of the numerator is odd to \( \hat{k} \) and therefore vanishes in the integral, and hence, only the imaginary part of the numerator has to be taken into account for calculations on non-magnetic WSMs. Since there is no current from \( l = n \) or \( m = n \), we can separate the contribution into two parts with respect to band number \( l \) and \( m \). The three-band processes \( (n \rightarrow m \rightarrow l) \) are given by \( l \neq m \), and the two-band processes are given by \( l = m \) (two-band transition). By applying the point group symmetry operations to the numerator \( N \), the third rank conductivity tensor shape can be determined, as can be the tensor form of the anomalous Hall conductivity and spin Hall conductivity [54, 55].

\[
\sigma_{ab}^{\text{N}} = \frac{|e|^3}{8\pi \omega^2} \text{Re} \left\{ \phi_{ab} \sum_{\Omega=\pm \omega} \sum_{l,m,n} \int_{BZ} d^3k (f_1 - f_n) \right\}
\]

\[
\frac{n\hat{k}|\hat{v}_a|\hat{l}\hat{k} > \langle \hat{l}\hat{k}|\hat{v}_b|m\hat{k} > \langle m\hat{k}|\hat{v}_c|n\hat{k} >}{(E_n - E_m - i\delta)(E_n - E_l + i\delta)} \right\}
\]

The conductivity \( (\sigma_{ab}^{\text{N}}; a, b, c = x, y, z) \) is a third rank tensor and represents the photocurrent \( J^c \) generated by an electrical field \( \vec{E} \) via \( J^c = \sigma_{ab}^{\text{N}}E_aE_b \). Here \( \hat{v}_a = \frac{\vec{P}_a}{m_a}, \)

\( E_n = E_n(\hat{k}) \), and \( m_0, \delta = \hbar/\tau, \tau \) stand for, respectively, free electron mass, broadening parameter, and the quasiparticle lifetime. \( \phi_{ab} \) is the phase difference between driving field \( \hat{E}_a \) and \( \hat{E}_b \), i.e. \( \phi_{yz} = i \) for left-circular polarized light propagating in \( x \) direction with light-polarization vector \((0, 1, i)\). It is clear that the real part of the integral in Eq. 1 describes the shift current response under linearly polarized light and the imaginary part of the integral gives the helicity dependent CPGE. Next, we analyze the response tensor under time reversal symmetry (\( T \)) and the point group symmetry. For simple, we define \( N \equiv \langle n\hat{k}|\hat{v}_a|\hat{l}\hat{k} > \langle \hat{l}\hat{k}|\hat{v}_b|m\hat{k} > \langle m\hat{k}|\hat{v}_c|n\hat{k} > \). \( \hat{T} \) reverses the velocity and brings an additional minus sign to the imaginary part of \( N \) by the complex conjugation. Thus, in materials with time reversal symmetry, the real part of the numerator is odd to \( \hat{k} \) and therefore vanishes in the integral, and hence, only the imaginary part of the numerator has to be taken into account for calculations on non-magnetic WSMs. Since there is no current from \( l = n \) or \( m = n \), we can separate the contribution into two parts with respect to band number \( l \) and \( m \). The three-band processes \( (n \rightarrow m \rightarrow l) \) are given by \( l \neq m \), and the two-band processes are given by \( l = m \) (two-band transition). By applying the point group symmetry operations to the numerator \( N \), the third rank conductivity tensor shape can be determined, as can be the tensor form of the anomalous Hall conductivity and spin Hall conductivity [54, 55].

\[
\sigma_{ab}^{\text{N}}(a = x, y, z) \text{ is zero as the velocity numerator } N \text{ is real (here } l = m, N = \langle \hat{l}\hat{k}|\hat{v}_a|\hat{l}\hat{k} > \langle \hat{l}\hat{k}|\hat{v}_b|m\hat{k} > \langle m\hat{k}|\hat{v}_c|n\hat{k} > \rangle, \text{ in which the velocity } \nu_a \equiv \langle \hat{l}\hat{k}|\hat{v}_a|\hat{l}\hat{k} > \text{ is odd to } \hat{k} \text{ due to the time reversal symmetry. Therefore, to calculate the shift current in real materials properly, one needs to use a multiband approach beyond the two-band approximation. For circularly polarized light with helicity dependent term } \phi_{ab} = i, \text{ the dispersive part } \text{Re}(D_1D_2) \sim (2)
(\varepsilon_n - \varepsilon_n^0) / (\varepsilon_n - \varepsilon_1 + \delta) \) (note relaxation time plays a minor role in CPGE) contributes to the response photocurrent. The absence of \( \delta \)-function in \( \text{Re}(D_1D_2) \) indicates that there is no specific energy selection rule in the transition. Thus, in contrast to the concentrated distribution of the shift current, the CPGE distribution can be rather smeared out in momentum space. It also indicates that different transition pathways (real and virtual) contribute relatively equally to the photocurrent, assuming comparable numerators \( N \). Given the large number of three-band virtual transitions, the virtual process might overwhelm the two-band direct process to induce the photocurrent.

To calculate the second-order photoconductivity in realistic compounds, we obtain the density-functional theory (DFT) Bloch wave functions from the Full-Potential Local-Orbital program (FPLO) [56] within the generalized gradient approximation (GGA) [57]. By projecting the Bloch wave functions onto Wannier functions, we obtain a tight-binding Hamiltonian with 32 bands, prepared with more realistic momentum dependent relaxation time; lead to almost the same results compared with more realistic momentum dependent relaxation time. Another possible effect on the conductivity comes from the change in the electron distribution. However, since most of the experiments are carried out at low temperature \( (k_BT = 4.3 \text{ meV} \ (T = 50\text{K}), \text{which is comparable to} \delta \) and much smaller than the frequency of light), we expect the temperature change in the Fermi-Dirac distribution function does not modify the conductivity significantly.

Figure 3 show the chemical potential dependence of shift current and CPGE, calculated with different relaxation time. As shown in Fig. 3 both terms show only small dependence to the relaxation time. For shift current \( \sigma_{zz}^c \), the response current is maximized when Fermi level is adjusted around the Weyl nodes energy, and change only by 20% even if the relaxation time is changed by a factor of 100. For the CPGE \( \sigma_{zz}^c \) curve, the response current is almost unchanged at the charge neutrality point, and does not show strong dependence on the Weyl nodes energy level.

For the photon energy dependence of CPGE, the \( 1/(\hbar \omega)^2 \) behaviour is observed in the region where our approach is valid. Since the energy denominator \( \text{Re}(D_1D_2) \) is the dispersive part of the second order optical response, the complex integral is nearly unchanged in low-frequency regime, leading to a \( 1/(\hbar \omega)^2 \) dependence due to the prefactor of Eq. 4.

Effect of disorders and fluctuations. Next, we discuss the effect of temperature and impurity scattering to the photocurrent generation. In our calculation, the effect of disorder and fluctuations are taken into account by the constant relaxation time \( \tau \), which is not considered in the shift vector formalism [22, 23]. Since the distribution of shift current in momentum space is quite concentrated around Weyl nodes, the constant relaxation time would lead to almost the same results compared with more realistic momentum dependent relaxation time.

Two- and three-band processes. For given valence band \( n \) and conduction band \( l \), the CPGE and shift current should sum over the real transition \( (n \rightarrow l, l = m \text{ in Eq. 1}) \) and also the virtual transitions \( (n \rightarrow m \rightarrow l) \text{ in Eq. 1} \) for all third bands \( m \). To understand the impor-
tance of virtual transitions, here we separate the two- and three-band process contributions for the response at incident photon energy $\hbar\omega = 120$ meV, to investigate which one is more essential in the photocurrent generation.

As shown in Fig. 4(a), the three-band part of CPGE $\sigma_{yy}$ is 1825 $\mu$A/V², while the two-band part is only 75 $\mu$A/V² at the charge neutrality point. We obtain the $J_y = 1.2 \times 10^{-4}$ A with only two-band transitions in our method, which matches well with the theoretical calculated result $1.015 \times 10^{-4}$ A in Ref.[46] via an effective two-band model.

Similarly, for the entire range of Fermi level we calculated, a large contribution to the photocurrent comes from the three-band processes. The distribution of three-band contribution for $\sigma_{yy}$ is quite dispersed in momentum space, in contrast to the of the two-band part concentrating around WPs. In total magnitude, the two-band process is ten times smaller than the three-band process. Taking a closer look into the small area around $W_1$ WPs, the two-band part solely comes from $E_x(\vec{k}) - E_c(\vec{k}) = 120$ meV, which is the direct transition between two Weyl bands; while the three-band contribution stay almost uniformly in the momentum space, implying that virtual transitions have a larger contribution than the real transitions.

It should be stressed that the shift current $\sigma_{zz}$ is purely a three-band process, as we have analyzed according to Eq. 1 and have also confirmed in numerical calculations. Therefore, it is necessary to include a third band for the evaluation of the photocurrent $\vec{J}$ parallel to electric field $\vec{E}$. In the momentum space distribution of shift current $\sigma_{zz}$, the nonzero part is concentrated around the WPs, which shows the absorptive nature of shift current. Thus, we can conclude that shift current in Weyl system comes from the interplay of Weyl nodes and third trivial bands when the incident photon energy is at the same scale of the energy of Weyl nodes.

**Discussion.** We have systematically studied the photocurrent response both for linearly and circularly polarized lights in type-I WSM TaAs, and show that shift current spectrum has a strong dependence with Weyl points energy, while CPGE shows a $1/\omega^2$ behaviour in mid infrared regime, when the incident photon energy is larger than the smearing energy. Comparing our calculated results with a recent photocurrent experiments, we observe that the CPGE experiment of TaAs [46] measured $\sigma_{zy}$ (CPGE) with incident photon energy $\hbar\omega = 120$ meV. Our calculated $\sigma_{zy}$ is 1900 $\mu$A/V², gives a photocurrent $J_y = 2.1 \times 10^{-3}$ A under the experimental laser power. Taking into account a scaling factor $10^{-4}$ determined in experiment [46] and other unspecified decay channels, our results agrees well with the experimental value of $40 \times 10^{-9}$ A. The calculated shift current $J_y$ is $8 \times 10^{-5}$ A in this setup (4% of the photocurrent from circularly polarized light), which may possibly explain why shift current was neglected in Ref. [46] that focused on the CPGE.

Recently the shift current was experimentally studied in TaAs [48] and $\sigma_{zz}$, $\sigma_{zy}$ and $\sigma_{zy}$ were measured at photon energy $\hbar\omega = 117$ meV, which is at least an order of magnitude larger than previously measured materials (e.g. $\sigma_{zz}$ (shift)) = 0.013 $\mu$A/V² in BaTiO₃ with visible light [22, 58]). Our calculated $\sigma_{zz}$ (shift) is 79 $\mu$A/V², in good agreement with the experimental result $\sigma_{zz}$ = 26 $\mu$A/V².

Apart from the above fixed photon energy experiments, it would be interesting to investigate the frequency dependent photocurrent both for circularly and linearly polarized light, to verify the $1/\omega^2$ dependence of CPGE and the peak of shift current for $\hbar\omega$ being around twice of the WP ($W_1$) energy.

In addition, the calculated SH susceptibility $\chi_{zz}$ and the ratio of $\chi_{zz}^r/\chi_{zz}^i$ are 6200 pm/V and 0.3 respectively, which are quite close to the measured value 7200 pm/V and 0.031 at low temperature [43, 59].

In summary, we have developed a first-principles multiband approach to determine the photocurrent response from linearly and circularly polarized lights. We have...
established that the virtual transitions from Weyl bands to trivial bands play an essential role in the photocurrent generation process. In general, our method is also useful to study the nonlinear optical responses in ordinary metallic and insulating materials.

[1] H. Weyl, Zeitschrift für Physik A Hadrons and Nuclei 56, 330 (1929).
[2] H. Weng, C. Fang, Z. Fang, B. A. Bernevig, and X. Dai, Phys. Rev. X 5, 011029 (2015).
[3] S.-M. Huang, S.-Y. Xu, I. Belopolski, C.-C. Lee, G. Chang, B. Wang, N. Alidoust, G. Bian, M. Neupane, C. Zhang, S. Jia, A. Bansil, H. Lin, and M. Z. Hasan, Nat. Commun. 6, 8373 (2015).
[4] B. Q. Lv, H. M. Weng, B. B. Fu, X. P. Wang, H. Miao, J. Ma, P. Richard, X. C. Huang, L. X. Zhao, G. F. Chen, Z. Fang, X. Dai, T. Qian, and H. Ding, Phys. Rev. X 5, 031013 (2015).
[5] S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Y. Zhujun, C.-C. Lee, H. Shing-Ming, H. Zheng, J. Ma, D. S. Sanchez, B. Wang, A. Bansil, F. Chou, P. P. Shibayev, H. Lin, S. Jia, and M. Z. Hasan, Science 349, 613 (2015).
[6] L. X. Yang, Z. K. Liu, Y. Sun, H. Peng, H. F. Yang, T. Zhang, B. Zhou, Y. Zhang, Y. F. Guo, M. Rahn, D. Prabhakaran, Z. Hussain, S. K. Mo, C. Felser, B. Yan, and Y. L. Chen, Nat. Phys. 11, 728 (2015).
[7] X. G. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011).
[8] G. E. Volovik, The Universe in A Helium Droplet (Clarendon Press, Oxford, 2003).
[9] S. Murakami, New Journal of Physics 9, 356 (2007).
[10] A. A. Burkov, M. D. Hook, and L. Balents, Phys. Rev. B 84, 235126 (2011).
[11] P. Hosur and X. L. Qi, C. R. Physique 14, 857 (2013).
[12] B. Yan and C. Felser, Annual Review of Condensed Matter Physics 8, 337 (2017).
[13] N. P. Armitage, E. J. Mele, and A. Vishwanath, arxiv (2017), [1705.01111].
[14] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, Reviews of Modern Physics 82, 1539 (2010).
[15] D. Xiao, M.-C. Chang, and Q. Niu, Rev. Mod. Phys. 82, 1950 (2010).
[16] H. B. Nielsen and M. Ninomiya, Nucl. Phys. B 185, 20 (1981).
[17] H. B. Nielsen and M. Ninomiya, Phys. Lett. B 130, 389 (1983).
[18] J. Xiong, C. Fang, Z. Fang, B. A. Bernevig, and X. Dai, Phys. Rev. X 5, 011029 (2015).
[19] J. Gooth, A. C. Niemann, T. Meng, A. G. Grushin, K. Landsteiner, B. Gotsmann, F. Menges, M. Schmidt, C. Shekhar, V. Su, R. Huhne, B. Rellinghaus, C. Felser, B. Yan, and K. Nielsch, Nature 547, 324 (2017).
[20] J. E. Moore and J. Orenstein, Phys. Rev. Lett. 105, 026805 (2010).
[21] E. Deyo, L. E. Golub, E. L. Ivchenko, and B. Spivak, arxiv (2009), [0904.1917].
[22] S. M. Young and A. M. Rappe, Physical review letters 109, 116601 (2012).
[23] J. E. Sipe and A. I. Shkrebttii, Phys. Rev. B 61, 5337 (2000).
[24] T. Morimoto and N. Nagaosa, Science advances 2, e1501524 (2016), note that the two-band model of the shift current in this paper does not contradict with the conclusion in the present paper. Their two-band model effectively takes into account the multi-band effect through the momentum dependence of the inter-band matrix elements of the current, while we take the pure p/m0 as the current operator.
[25] T. Choi, S. Lee, Y. J. Choi, V. Kiryukhin, and S.-W. Cheong, Science 324, 63 (2009).
[26] S. Y. Yang, J. Seidel, S. J. Byrnes, P. Shafer, C. H. Yang, M. D. Rossell, P. Yu, Y. H. Chu, J. F. Scott, J. W. Ager III, L. W. Martin, and R. Ramesh, Nature Nanotechnology 5, 143 (2010).
[27] I. Grinberg, D. V. West, M. Torres, G. Gou, D. M. Stein, L. Wu, G. Chen, E. M. Gallo, A. R. Akbashev, P. K. Davies, J. E. Spanier, and A. M. Rappe, Nature 503, 509 (2013).
[28] M. M. Vazifeh and M. Franz, Phys. Rev. Lett. 111, 027201 (2013).
[29] P. Goswami, G. Sharma, and S. Tewari, Phys. Rev. B 92, 161110 (2015).
[30] M. Kargarian, M. Randeria, and N. Trivedi, Sci. Rep. 5, 12683 (2015).
[31] H. Ishizuka, T. Hayata, M. Ueda, and N. Nagaosa, Physical Review Letters 117, 216601 (2016).
[32] H. Ishizuka, T. Hayata, M. Ueda, and N. Nagaosa, Physical Review B 95, 245211 (2017).
[33] P. Hosur, Phys. Rev. B 83, 035309 (2011).
[34] I. Sodemann and L. Fu, Physical review letters 115, 216806 (2015).
[35] C.-K. Chan, P. A. Lee, K. S. Burch, J. H. Han, and Y. Ran, Physical review letters 116, 016805 (2016).
[36] T. Morimoto, S. Zhong, J. Orenstein, and J. E. Moore, Physical Review B 94, 245121 (2016).
[37] K. Taguchi, T. Imaeda, M. Sato, and Y. Tanaka, Physical Review B 93, 201202(R) (2016).
[38] F. de Juan, A. G. Grushin, T. Morimoto, and J. E. Moore, Nature communications 8, 15995 (2017).
[39] C.-K. Chan, N. H. Lindner, G. Refael, and P. A. Lee, Physical Review B 95, 041104 (2017).
[40] E. J. König, H. Y. Xie, D. A. Pesin, and A. Levchenko, Phys. Rev. B 96, 075123 (2017).
[41] H. Rostami and M. Polini, arXiv , arXiv:1705.09915 (2017).
[42] L. E. Golub, E. L. Ivchenko, and B. Z. Spivak, Jett Lett. 105, 782 (2017).
[43] Y. Zhang, Y. Sun, and B. Yan, Physical Review B 97, 041101 (2018).
[44] X. Yang, K. Burch, and Y. Ran, arxiv , arxiv:1712.09363 (2017), [1712.09363].
[45] L. Wu, S. Patankar, T. Morimoto, N. L. Nair, E. Thewalt, A. Little, J. G. Analytis, J. E. Moore, and J. Orenstein, Nature Physics 13, 350 (2017).
[46] Q. Ma, S.-Y. Xu, C.-K. Chan, C.-L. Zhang, G. Chang, Y. Lin, W. Xie, T. Palacios, H. Lin, S. Jia, et al., Nature Physics (2017).
[47] K. Sun, S.-S. Sun, L.-L. Wei, C. Guo, H.-F. Tian, G.-F. Chen, H.-X. Yang, and J.-Q. Li, Chinese Physics Letters 34, 117203 (2017).
[48] G. B. Osterhoudt, L. K. Diebel, X. Yang, J. Stano, X. Huang, B. Shen, N. Ni, P. Moll, Y. Ran, and K. S.
Burch, arXiv preprint arXiv:1712.04951 (2017).

[49] S. Lim, C. R. Rajamathi, V. Stüß, C. Felser, and A. Kapitulnik, arXiv preprint arXiv:1802.02838 (2018).

[50] Z. Ji, G. Liu, Z. Addison, W. Liu, P. Yu, H. Gao, Z. Liu, A. M. Rappe, C. L. Kane, E. J. Mele, et al., arXiv preprint arXiv:1802.04387 (2018).

[51] W. Kraut and R. von Baltz, Physical Review B 19, 1548 (1979).

[52] R. von Baltz and W. Kraut, Physical Review B 23, 5590 (1981).

[53] N. Kristoffel and A. Gulbis, Zeitschrift für Physik B Condensed Matter 39, 143 (1980).

[54] J. Železný, H. Gao, A. Manchon, F. Freimuth, Y. Mokrousov, J. Zemen, J. Mašek, J. Sinova, and T. Jungwirth, Physical Review B 95, 014403 (2017).

[55] Y. Zhang, Y. Sun, H. Yang, J. Železný, S. P. P. Parkin, C. Felser, and B. Yan, Physical Review B 95, 075128 (2017).

[56] K. Koepernik and H. Eschrig, Physical Review B 59, 1743 (1999).

[57] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).

[58] A. Zenkevich, Y. Matveyev, K. Maksimova, R. Gaynutdinov, A. Tolstikhina, and V. Fridkin, Physical Review B 90, 161409 (2014).

[59] The method to compute the SHG can be found in the Supplemental Material.