

## Current-induced spin and orbital polarization in the ferroelectric Rashba semiconductor GeTe

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The Edelstein effect is a promising mechanism for generating spin and orbital polarization from charge currents in systems without inversion symmetry. In ferroelectric materials, such as germanium telluride (GeTe), the combination of bulk Rashba splitting and voltage-controlled ferroelectric polarization provides a pathway for electrical control of the sign of the charge-spin conversion. In this work, we investigate current-induced spin and orbital magnetization in bulk GeTe using Wannier-based tight-binding models derived from *ab initio* calculations and semiclassical Boltzmann theory. Employing the modern theory of orbital magnetization, we demonstrate that the orbital Edelstein effect entirely dominates its spin counterpart. This difference is visualized through the spin and orbital textures at the Fermi surfaces, where the orbital moment surpasses the spin moment by one order of magnitude. Moreover, the orbital Edelstein effect remains largely unaffected in the absence of spin-orbit coupling, highlighting its distinct physical origin compared to the spin Edelstein effect.

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## I. INTRODUCTION

The pursuit of electric control of magnetic properties has led to intense exploration of materials exhibiting Rashba-like spin splitting in their electronic structures. Rashba spin-orbit coupling, originally discussed for three-dimensional wurtzite crystals [1,2] and later for two-dimensional systems with broken inversion symmetry [3–5], can also occur in the bulk of ferroelectric semiconductors, called ferroelectric Rashba semiconductors [6,7]. Among them, germanium telluride (GeTe) is a paradigm material example. The switchable ferroelectric polarization allows electric control of the Rashba-like band splitting, and hence also the charge-spin conversion [6,8–11].

One of the most promising phenomena providing charge-spin conversion is the spin Edelstein effect (SEE) [12,13], also known as the inverse spin galvanic effect, or current-induced spin polarization. An applied external electric field generates a homogeneous spin polarization in systems without inversion symmetry due to spin-orbit coupling (SOC). This effect

has been studied in many materials with various sources of broken inversion symmetry, such as Rashba systems [13–17], topological insulators [14,18–20], Weyl semimetals [21,22], chiral materials [23–25], oxide interfaces [26–29], helical materials [30], *p*-wave magnets [31,32], transition metal dichalcogenides [33–35], ferroelectric semiconductors [36], and superconductors [37].

A second contribution to the Edelstein effect, the orbital Edelstein effect (OEE), arises from the orbital angular momentum of the electrons [38–40], resulting in a current-induced nonequilibrium orbital magnetization in systems with broken inversion symmetry. Unlike the SEE, the OEE does not require the presence of SOC, as has been shown for various magnetic and nonmagnetic materials and their interfaces [41–45].

Calculating the orbital angular momentum in extended bulk crystals comes with the challenge of defining the position operator of translationally invariant systems. To circumvent this problem, the modern theory of orbital magnetization (MTOM) has been introduced, using localized Wannier functions and wave packets from Bloch states, respectively. In contrast to the atom-centered approximation (ACA), within which the orbital angular momentum is evaluated in finite spheres around the atomic positions, the MTOM also includes nonlocal, itinerant contributions to orbital magnetism [38]. However, applying the MTOM to metals and semimetals, local and itinerant contributions cannot be clearly separated, since they are not individually gauge invariant, only their sum, the total orbital magnetization, is gauge invariant. The MTOM

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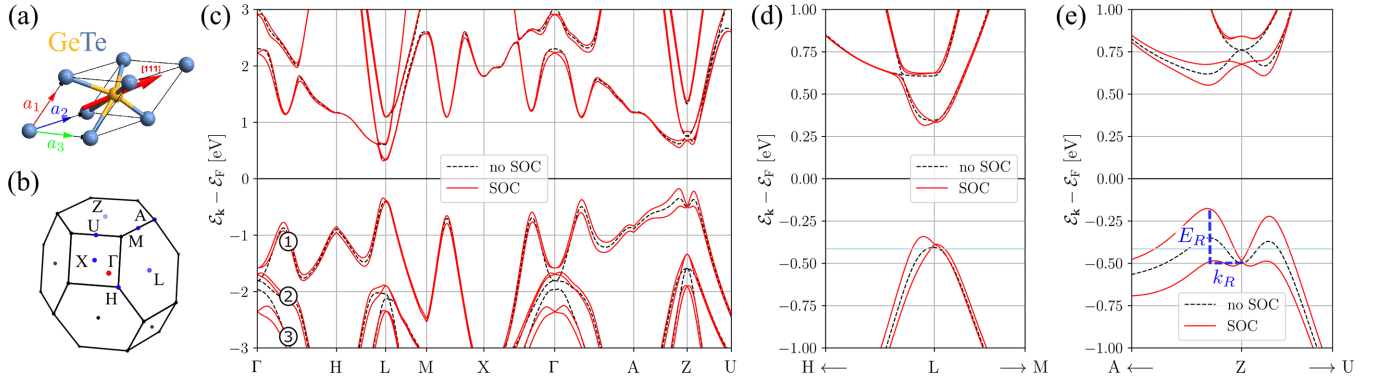


FIG. 1. Electronic structure of  $\alpha$ -GeTe. (a) Crystal structure of GeTe with the primitive lattice vectors, and a relative displacement of the central Ge atom along the [111] direction, indicated by the red arrow. (b) First Brillouin zone with labeled high-symmetry points of the distorted rhombohedral structure. (c) Band structure from the Wannier tight-binding model with (solid lines) and without (dashed lines) spin-orbit coupling, along the high-symmetry path. Zoom-in energy around (d) the  $L$  and (e)  $Z$  points, including the effective Rashba energy splitting  $E_R$  and momentum splitting  $k_R$ . In panel (c), the valence bands are grouped in three pairs ①, ②, ③ for further analysis.

has been implemented in several density functional theory (DFT) codes [46–48] and tight-binding models [41,42].

Previous experimental studies on GeTe have mostly focused on spin textures of the surface states and bulk states [49–51] of GeTe, and on charge-spin conversion via the inverse spin Hall effect and the inverse SEE [8,10]. Spin textures [6] of GeTe and the resulting SEE [36] and spin Hall effect [10] have been investigated theoretically. In Ref. [52], orbital textures of GeTe are calculated in selected regions of the Brillouin zone, using the ACA, and a giant orbital Rashba splitting is identified. However, in addition to these existing studies, we analyze the orbital textures and the OEE in GeTe using the MTOM and demonstrate that the orbital contribution significantly dominates the total Edelstein effect.

In this work, we calculate both charge-spin and charge-orbital conversion via the SEE and OEE, respectively, in bulk GeTe by employing DFT, a Wannier tight-binding model, the MTOM, and semiclassical transport theory. The paper is organized as follows: In Sec. II, we provide an overview of the computational methods and the theory of the SEE and OEE. In Sec. III, we discuss the electronic structure with an estimation of the Rashba parameter. In Sec. IV, we present the spin and orbital textures and Edelstein effects in GeTe.

## II. METHODOLOGY

Density functional theory calculations were performed using the Vienna *Ab initio* Simulation Package (VASP) [53–56] with Perdew-Burke-Ernzerhof functional [57] and DFT-D3 correction of Grimme *et al.* [58] with Becke-Johnson damping [59]. The Brillouin zone of bulk GeTe is sampled by a  $12 \times 12 \times 12$   $\Gamma$ -centered  $k$ -mesh. A plane-wave basis set is used with a cutoff energy of 520 eV. The convergence for the electronic density is set to  $10^{-7}$  eV. The atomic structure is relaxed with the threshold forces of  $1 \text{ meV } \text{\AA}^{-1}$ .

The Wannier tight-binding models were constructed using the WANNIER90 package [47,60,61], including the spin operator [62,63] for a 16-orbital basis (Ge,Te-s,p orbitals) within a  $9 \times 9 \times 9$  real-space supercell. The orbital angular momentum was interpolated in  $k$ -space using the WANNIER-BERRI package [48].

The magnetic moment per unit cell  $\mathbf{m}$ , induced by an external electric field  $\mathbf{E}$ , is calculated within the linear-response regime,

$$\mathbf{m} = (\chi^s + \chi^l)\mathbf{E}. \quad (1)$$

The spin and orbital Edelstein susceptibility tensors,  $\chi^s$  and  $\chi^l$ , are calculated using the semiclassical Boltzmann approach, assuming zero temperature, as

$$\chi_{ij}^O = \frac{g_O V_0 e \mu_B}{V_s \hbar} \sum_{\mathbf{k}} \langle \mathcal{O} \rangle_{\mathbf{k}}^i \Lambda_{\mathbf{k}}^j \delta(\mathcal{E}_{\mathbf{k}} - \mathcal{E}_F), \quad (2)$$

with  $\langle \mathcal{O} \rangle_{\mathbf{k}}^i$  the  $i$ th component of the expectation value of the spin and orbital angular momentum operators, respectively. Here,  $g_{s(l)}$  indicates the spin(orbital) Landé  $g$  factor,  $V_0$  ( $V_s$ ) is the volume of the unit cell (of the system), and  $\mu_B$ ,  $\hbar$ ,  $\mathbf{k}$ ,  $\mathcal{E}_{\mathbf{k}}$ , and  $\mathcal{E}_F$  represent the Bohr magneton, the reduced Planck constant, the crystal momentum, the energy of the state  $\mathbf{k}$ , and the Fermi energy, respectively. Here and in the following,  $\mathbf{k}$  is a multi-index, including the band index as well as the crystal momentum. Within the constant relaxation time approximation, the mean free path is calculated as  $\Lambda_{\mathbf{k}} = \tau_0 \mathbf{v}_{\mathbf{k}}$ , with  $\tau_0$  the relaxation time and  $\mathbf{v}_{\mathbf{k}} = \frac{1}{\hbar} \frac{\partial \mathcal{E}_{\mathbf{k}}}{\partial \mathbf{k}}$  the group velocity. Using this approximation, the Edelstein susceptibility tensors given by Eq. (2) scale linearly with  $\tau_0$ . The Dirac delta function  $\delta$  in Eq. (2) indicates that only states at the Fermi surfaces contribute to the nonequilibrium magnetic moment, i.e., states with band energy  $\mathcal{E}_{\mathbf{k}}$  equal to the Fermi energy  $\mathcal{E}_F$ . The intrinsic contributions to the charge-spin and charge-orbital conversions vanish due to time-reversal symmetry. Details of the Boltzmann approach and the operators are presented in Appendixes A and B.

## III. ELECTRONIC STRUCTURE

Figures 1(a)–1(c) show the crystal structure of bulk  $\alpha$ -GeTe, the first Brillouin zone, and the band structure with and without SOC calculated from the Wannier tight-binding model based on the DFT results. For the rest of this paper, the reference energy is set to the Fermi energy computed from DFT. The upper valence band energies at  $\Gamma$ ,  $L$ , and  $Z$

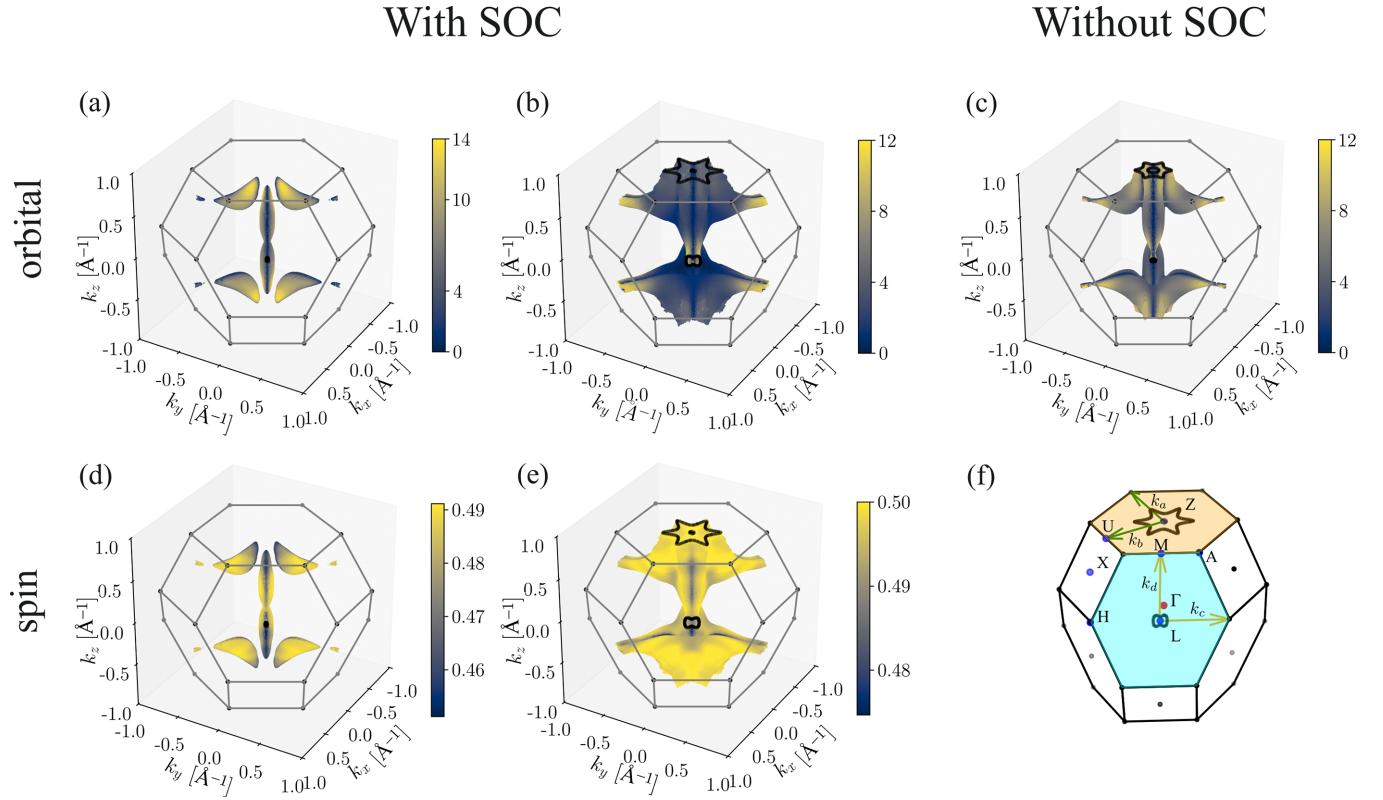


FIG. 2. Isoenergy surfaces of the valence band(s) at  $\mathcal{E} = -0.41$  eV with respect to  $\mathcal{E}_F$ . (a) Lower and (b) upper bands of the topmost valence band pair ①, with SOC. (c) Valence band without SOC. (a)–(c) Color shows the absolute value of the OAM in units of  $\hbar$ . (d), (e) Same as panels (a) and (b) but with color showing the absolute value of the spin momentum in units of  $\hbar$ . (f) Brillouin zone with highlighted Z (orange) and L (light blue) planes and relative coordinates  $k_a, k_b, k_c, k_d$ .

are  $-1.57$ ,  $-0.39$ ,  $-0.49$  eV, respectively. The relative displacement of the Ge versus Te ions along the  $[111]$  direction breaks inversion symmetry and leads to a ferroelectric polarization along the  $[111]$  direction. Due to this bulk inversion asymmetry, the eight hexagonal faces of the Brillouin zone can be separated into two groups. The first group, with the two faces perpendicular to the  $[111]$  direction, has the Z point at their centers, while the second group, the remaining six faces, has the L points at their centers. For simplicity, we refer to the faces orthogonal to the  $[111]$  and  $[100]$  directions as plane Z and plane L, respectively, where plane Z (L) contains the Z (L) point, as shown in Fig. 1(b). It is important to note that the global valence band maximum and the conduction band minimum are not captured by the high-symmetry path in Fig. 1(c).

The displacement of the Ge atom along the  $[111]$  direction, breaking bulk inversion symmetry and the resulting ferroelectric polarization, leads to Rashba-like splittings around Z and L, some of which are close to the Fermi energy, as shown in detail in Figs. 1(d) and 1(e). The spin splitting, however, is present only with SOC. Rashba-like splittings also occur around  $\Gamma$ , located deeper below the Fermi energy.

Figures 2(a)–2(e) show the isoenergy surfaces for GeTe with and without SOC at  $\mathcal{E} = -0.41$  eV, clearly illustrating the distinction between the two sets of hexagonal faces in the Brillouin zone. As expected from the band structure in Figs. 1(c)–1(e), the isoenergy surfaces in Figs. 2(b) and 2(e) show Rashba-like splitting around the Z and L points. In the

Z plane, the isoenergy line has a starlike shape, resulting from the  $C_{3v}$  symmetry in this plane. Similar isoenergy lines have been observed for surface states of topological insulators [64] and Rashba systems [65] with  $C_{3v}$  symmetry.

Based on the energy and momentum splitting in Fig. 1(e) and the isoenergy lines in Figs. 3(a) and 3(c), the electronic structure of the two topmost valence bands in plane Z can be approximated by an effective Rashba model with warping, as usually occurring in systems with  $C_{3v}$  symmetry [64],  $H_R = \frac{\hbar^2}{2m_{\text{eff}}}k^2 + \alpha_R(k_a\sigma_y - k_b\sigma_x) + \frac{\lambda}{2}(k_+^3 + k_-^3)\sigma_z$ , where  $k_{\pm} = k_a \pm k_b$ . Here,  $\alpha_R$  is the effective Rashba parameter,  $\lambda$  is the warping parameter, and  $k_a$  and  $k_b$  are in the Z plane, as indicated in Fig. 2(f). This warping term is a cubic  $k$  contribution to the Rashba effect and occurs due to the  $C_{3v}$  symmetry around Z [66], which is reduced compared to the isotropic Rashba model. However, even in the absence of SOC, the isoenergy lines exhibit warping, which can be interpreted as a signature of a cubic contribution to the orbital Rashba effect.

Focusing on the isoenergy lines around the Z point and neglecting the cubic terms, we use an isotropic Rashba model to estimate characteristic parameters of the valence band in the  $\bar{Z}\bar{A}$  ( $\bar{Z}U$ ) direction as shown in Fig. 1(e): the Rashba energy splitting  $E_R = 0.310$  eV (0.264 eV), momentum splitting  $k_R = 0.123 \text{ \AA}^{-1}$  (0.098  $\text{\AA}^{-1}$ ), effective mass  $m_{\text{eff}} = -0.187 m_e$  ( $-0.139 m_e$ ) with  $m_e$  the electron's mass, and a huge Rashba parameter  $\alpha_R = 5.02 \text{ eV \AA}$  (5.37 eV  $\text{\AA}$ ). These results are in agreement with previous calculations in Refs. [6,7,49,51].

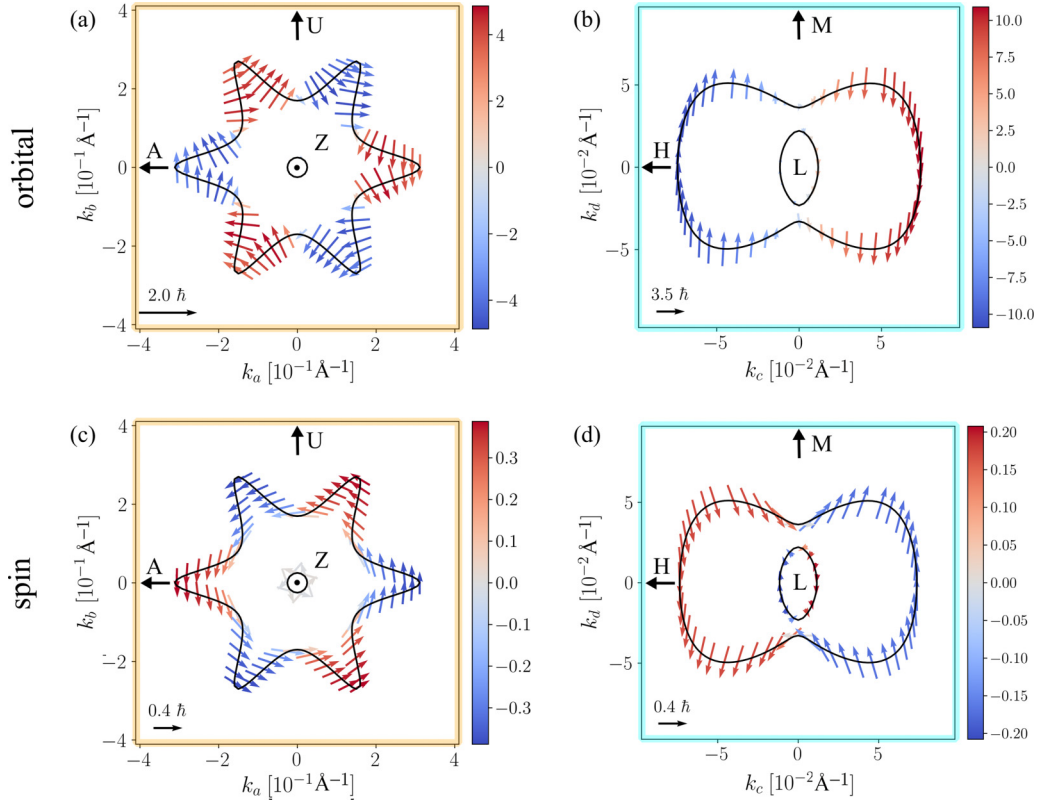


FIG. 3. Isoenergy lines at planes Z and L for  $\mathcal{E} = -0.41$  eV from the Fermi energy, with the orbital [panels (a) and (b)] and spin [panels (c) and (d)] textures. The lines correspond to the isoenergy  $k$  points at the surface of the Brillouin zone, which contain the Z [panels (a) and (c)] and L [panels (b) and (d)] points, highlighted in Fig. 2(f). The color corresponds to the out-of-plane spin and orbital component in units of  $\hbar$ , and the arrows indicate the in-plane spin and orbital components in the respective planes. Note that panels (a), (c) and (b), (d) use different  $k$  scales for better visualization of the isoenergy lines at planes Z and L.

#### IV. SPIN AND ORBITAL TEXTURES AND EDELSTEIN EFFECTS

Figures 2(a)–2(e) show the absolute value of the orbital and spin angular momentum, where spin expectation values are almost constant on the isoenergy surfaces in Figs. 2(d) and 2(e). However, from Figs. 2(a)–2(c), it is clear that the orbital texture presents hotspots at  $L$  faces. Our DFT calculations reveal that the states have mainly  $p$  character. Within the ACA, the expectation value of the OAM would be up to  $1\hbar$ . Hence, the large values of the OAM around  $L$  within the MTOM must originate from additional itinerant contributions, which are not included in the ACA. Around  $L$ , the two top conduction bands are very close in energy, leading to pronounced contributions to the (MTOM) orbital angular momentum: As indicated by Eq. (B2), the OAM can become very large when two bands are close in energy. However, the majority of electronic states exhibit orbital angular momenta around  $2\hbar$  to  $4\hbar$ , indicating that contributions to the OAM beyond the ACA are also relevant here. Similarly large values of the OAM have been predicted for gapped bilayer graphene [67].

Figure 3 displays the isoenergy lines on planes Z and L with the expectation values of orbital and spin angular momentum. The coordinate system for each plane is illustrated in Fig. 2(f), where in plane Z,  $-k_a$  and  $k_b$  are along  $\overline{ZA}$  and  $\overline{ZU}$ , respectively, and analogously  $-k_c$  and  $k_d$  are along  $\overline{LH}$  and  $\overline{LM}$  in plane L, respectively. Here, the displacement between

Ge and Te, combined with SOC, leads to Rashba-like spin splitting of the top valence bands. A comparison of the orbital and spin textures around the Z point in Figs. 3(a) and 3(c) reveals that in the Z plane, the orbital and spin textures exhibit opposite orientation, with the expectation values of orbital angular momentum being up to 10 times larger than the spin expectation values, mainly due to contributions to the OAM beyond the ACA. Figure 3(c) shows good agreement with previous results reported for GeTe [6,7,36], both in the shape of the isoenergy lines and in the spin texture. The spin texture in Fig. 3(c) is Rashba-like with approximately perpendicular spin-momentum locking of the in-plane components, with the amplitude almost constant along the isoenergy line. This Rashba-like structure results from the polar displacement of Ge and Te atoms along the  $[111]$  direction, which breaks bulk inversion symmetry. On the other hand, the orbital texture in Fig. 3(a) is weakly unlocked [68] with relevant variations in the length of the orbital momenta. These variations are most noticeable along the  $\overline{ZU}$  direction, where the orbital momentum is minimum. These anisotropies of the OAM reflect the crystal symmetries of bulk GeTe, which are reduced compared to the highly oversimplified pure Rashba model. Note that  $\mathcal{E} = -0.41$  eV is above the band degeneracy point and hence both isoenergy lines exhibit approximately the same orientation of spin expectation values, as expected within the Rashba model.

Similarly, the orbital and spin textures along the isoenergy lines around the  $L$  point, shown in Figs. 3(b) and 3(d), exhibit mainly opposite orientation and a larger orbital than spin momentum. However, in the  $L$  plane, the magnitudes of spin and orbital momenta differ by more than one order of magnitude, caused by pronounced nonlocal contributions to the OAM around  $L$ , where the two top valence bands are energetically close. Remarkably, moving along the isoenergy lines, the in-plane spin texture in Fig. 3(d) rotates in the opposite direction to that in Fig. 3(c), clearly deviating from a pure Rashba-like spin texture. On the other hand, the in-plane orbital momenta in Fig. 3(b) are mainly aligned along one direction and decay rapidly around the  $\overline{LM}$  direction. Whereas the orbital momenta of both bands share the same sense of rotation, the spin momenta of the two bands point in opposite directions. Note that  $\mathcal{E} = -0.41$  eV is here below the band degeneracy point.

In the  $L$  plane, the spin splitting is not purely Rashba-like. Unlike the  $Z$  plane, the  $L$  plane is not oriented perpendicular to the polarization direction  $[111]$  of the bulk crystal, but perpendicular to  $[001]$ . Therefore, the spin texture around  $L$  is classified as Rashba-Dresselhaus spin texture in Ref. [36].

Using Eq. (2), we compute the spin and orbital susceptibility tensors,  $\chi_{ij}^s$  and  $\chi_{ij}^l$ . We simulate a modified Fermi energy  $\mathcal{E}_F^*$ , focusing on a region below the DFT-calculated Fermi energy  $\mathcal{E}_F$  since a  $p$ -type doping is observed experimentally in GeTe [10,49,72], possibly caused by a Te-rich stoichiometry [11,73]. Due to the  $C_{3v}$  symmetry around the  $[111]$  direction that defines the  $\hat{z}$  direction, the only nonzero components are  $\chi_{xy}^{s/l} = -\chi_{yx}^{s/l}$ , where  $\hat{x}$  and  $\hat{y}$  are defined by  $[1\bar{1}0]$  and  $[11\bar{2}]$ , respectively [28,45]. Figure 4 shows the spin and orbital susceptibilities for energies below the real Fermi energy, as well as the band structure with the  $y$  components of spin and orbital expectation values. As expected from the relation between the textures around the  $Z$  point, the spin and orbital susceptibilities have opposite signs in the energy range below the valence band maximum; however, the orbital tensor is approximately one order of magnitude larger than the spin, which mainly results from the strongly enhanced orbital expectation values around the  $L$  point, as shown in Figs. 3(b) and 3(d). As shown in Appendix C, the global maximum of the valence band is not located along the high-symmetry path and hence not shown in the band structure in Figs. 1(c), 4(b), and 4(d). Nevertheless, these states contribute to the SEE and OEE, and therefore, the spin and orbital Edelstein susceptibilities are nonzero already above the local maxima around  $Z$ , which are visible in the presented band structure.

Figure 4(c) shows further the contribution of each band pair to the spin Edelstein susceptibility. Similar to the two-dimensional Rashba model, usually both bands of a spin-split pair contribute with opposite sign to the spin Edelstein effect, and hence their contributions partially compensate, leading to a reduced total Edelstein response. Sign changes of the total spin Edelstein susceptibility arise from the multiband character of the band structure, which is far more intricate than the two-dimensional effective Rashba model. Hence, the exact energies at which the SEE reverses sign are not directly tied to specific features of the band structure but arise from the multiband character. Comparing Fig. 4(c) with the spin expectation values and the band structure shown in Fig. 4(d),

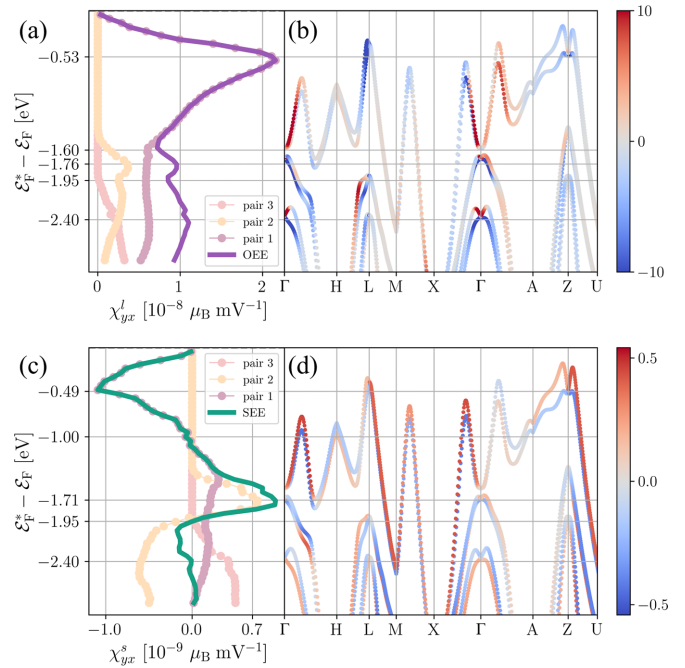


FIG. 4. Orbital and spin Edelstein susceptibility. (a) Band-resolved orbital Edelstein susceptibility in GeTe calculated with the Wannier tight-binding model. (b) Band structure with  $y$  component of the orbital expectation values in units of  $\hbar$ . (c), (d) Same as panels (a) and (b), but for the spin degree of freedom. Calculations were performed for  $V_0 = 56.8 \text{ \AA}^3$ ,  $g_s = 2$ ,  $g_l = 1$ , and  $\tau_0 = 10$  fs, which is the typical order of magnitude reported for GeTe [69–71].

it becomes obvious that the extrema of the SEE can be related to the pronounced Rashba-like splittings at the  $Z$  and  $\Gamma$  points, occurring at approximately  $-0.5$  and  $-1.7$  eV, respectively. Remarkably, modifying the Fermi energy  $\mathcal{E}_F^*$  would allow to switch the orientation of the current-induced spin polarization (SEE), without switching the ferroelectric polarization. However, the energy range studied here extends beyond energy shifts typically achieved experimentally (order of magnitude: 0.1 eV), for example, by doping and gating [10,70]. Nevertheless, studying the Edelstein effect over a broad energy range provides valuable insights into general relations between electronic structure, spin and orbital textures, and characteristics of the SEE and OEE, such as sign changes and maxima.

In contrast to the SEE, the OEE does not exhibit any sign changes within the studied energy range, as shown in Fig. 4(a). In a broad energy range, both bands of a pair contribute with the same sign to the orbital Edelstein effect, leading to an enhanced total OEE. The orbital Edelstein susceptibility is maximum slightly below the band crossing at the  $Z$  point. This maximum, hence, does not result from compensations from the inner band as for the SEE, but rather from the interplay of density of states and energy-dependent orbital textures: Moving from the valence band maximum below in energy, the density of states increases. On the other hand, moving away from the band crossing, the average orbital angular momentum at the isoenergy surface decreases due to larger energy splitting of the bands. The observed maximum of the OEE around  $-0.53$  eV, slightly below the band crossings at  $L$  and  $Z$ , is hence a result of these competing energy

dependencies. A detailed discussion of the energy evolution of the isoenergy surfaces, density of states, and orbital texture around the maximum of the OEE is shown in Appendix D. We observe that the other extrema of the OEE are also not tied to the band crossings, but rather occur slightly below, suggesting a similarly intricate dependence on the orbital texture of the isoenergy surface.

Previous works have shown that switching the ferroelectric polarization along the [111] direction, either by changing the termination [8,11] or by an applied electric field [74], allows inverting the Rashba effect, leading to a reversal of the spin texture and, consequently, the direction of charge-spin conversion [6,7]. This behavior arises naturally for our bulk system because inverting the ferroelectric polarization is equivalent to maintaining the polarization and inverting the coordinate system. Therefore, it is clear that switching the ferroelectric polarization in our system leads to a reversal of the spin and orbital textures, and hence the charge-spin and charge-orbital conversion.

Our results for the SEE are consistent with previous observations of spin-charge conversion through spin pumping experiments [8,10], and in particular, the connection between the sign change of the conversion signal [10] under electrically controllable ferroelectric switching [74]. In Ref. [10], the experimentally observed spin-charge conversion has been found to mainly originate from the inverse spin Hall effect. On the other hand, in Ref. [8], both inverse SEE and inverse spin Hall effect are considered as the origin of the spin-charge conversion. Although no quantitative numbers for the spin-charge conversion efficiencies are given, our theoretical results are in agreement with the experimentally observed sign of spin-charge conversion. However, in Ref. [8], the observed spin-charge conversion could originate from surface as well as bulk states, whereas we consider only the bulk contribution to the SEE. The spin texture around both studied symmetry points  $Z$  and  $L$ , as well as the SEE in Fig. 4(c), is in qualitative agreement with the theoretical results in Ref. [36]. Other ferroelectric materials have been shown to present similar charge-spin conversion efficiencies, such as  $\text{In}_2\text{Se}_3$  [36],  $\text{WTe}_2$  [75], and  $\text{SnTe}$  [76]. Additionally, we find a remarkably large OEE that dominates the direct Edelstein effect in GeTe across a wide energy range, which has not yet been reported either theoretically or experimentally. Therefore, GeTe is not only a very promising material for spintronics and ferroelectric applications but also for orbitronics.

In the absence of SOC, the spin Edelstein response naturally vanishes, but an orbital response is expected to exist regardless of the SOC [77]. In Fig. 5(a), we compare the orbital Edelstein susceptibilities with and without SOC. The OEE remains largely unchanged with few deviations due to the modified band structure. The approximately constant maxima strongly suggest that the OEE originates mostly from the bulk inversion asymmetry of the crystal structure. Figure 5(b) shows the orbital texture in plane  $Z$  without SOC. In agreement with the orbital Rashba effect reported in Ref. [52], this texture is qualitatively similar to the orbital texture around  $Z$  with SOC, shown in Fig. 3(a), but the out-of-plane component is strongly increased. In Fig. 5(c), the orbital texture in the  $L$  plane is shown, which resembles the orbital texture with SOC. Differences in the size of the isoenergy surfaces and

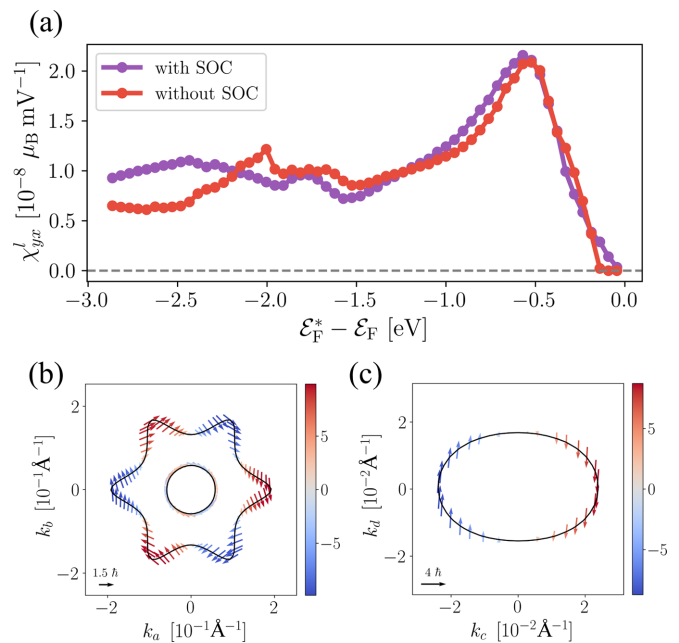


FIG. 5. (a) Comparison of the OEE with and without SOC. Isoenergy line and orbital texture of GeTe without SOC on (b) plane  $Z$  and (c) plane  $L$ , at  $\varepsilon = -0.41$  eV. The arrows represent the orientation of the in-plane components, and the color shows the value of the out-of-plane component in units of  $\hbar$ . Note the different  $k$  scales in panels (b) and (c) for better visualization of the isoenergy lines.

the density of state result from the modified band structure, leading to slightly different transport properties like the orbital Edelstein susceptibility, as shown in Fig. 5(a).

## V. CONCLUSION

In this work, we have investigated the current-induced spin and orbital magnetization in the bulk ferroelectric Rashba semiconductor GeTe, revealing that the orbital Edelstein effect is approximately one order of magnitude larger than its spin counterpart. The interplay between spin-orbit coupling and the ferroelectric polarization along the [111] direction in GeTe leads to an anisotropic Rashba-like deformation of the Fermi surface, its projection to the  $Z$  plane resembling the starlike shape from a warping Rashba model, whereas the Fermi surface projection to the  $L$  plane resembles an anisotropic Rashba-Dresselhaus model. Remarkably, the spin Edelstein effect presents clear sign changes within an energy window of approximately 2 eV below the valence band maximum. These sign changes are not linked to ferroelectric switching. Furthermore, we demonstrate that the OEE persists even in the absence of SOC with minimal differences for the top valence bands.

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### DATA AVAILABILITY

The data that support the findings of this article are openly available [78]; embargo periods may apply.

### APPENDIX A: SEMICLASSICAL BOLTZMANN TRANSPORT THEORY

The magnetic moment per unit cell from the spin and orbital angular momentum is given by

$$\mathbf{m} = -\frac{\mu_B}{\hbar} \frac{V_0}{V_s} \sum_{nk} f_{nk} (g_s \mathbf{s}_{nk} + g_l \mathbf{l}_{nk}), \quad (\text{A1})$$

within the semiclassical Boltzmann transport theory. The prefactors in Eq. (A1) are explained in Sec. II. The distribution function  $f_{nk}$  can be separated into two parts: the equilibrium part  $f_{nk}^0$ , in this case the Fermi-Dirac distribution, and the nonequilibrium part  $g_{nk}$ . It is easily concluded by symmetry analysis that in nonmagnetic materials, the equilibrium contribution would yield no magnetic moment.

For a stationary and spatially homogeneous system, the Boltzmann equation is reduced to

$$\dot{\mathbf{k}} \frac{\partial f_{nk}}{\partial \mathbf{k}} = \left( \frac{\partial f_{nk}}{\partial t} \right)_{\text{scatt}}. \quad (\text{A2})$$

We can further simplify the above equation if we apply the semiclassical equation of motion in the presence of an electric field,  $\dot{\mathbf{k}} = -\frac{e}{\hbar} \mathbf{E}$ , neglecting scattering-in contributions, and using the linear ansatz for the nonequilibrium part of the distribution function,  $g_{nk} = \frac{\partial f_{nk}^0}{\partial \mathcal{E}} e \mathbf{\Lambda}_{nk} \cdot \mathbf{E}$ , with  $\mathbf{\Lambda}_{nk}$  the mean-free path, so then the Boltzmann equation is linearized and we can solve it for  $\mathbf{\Lambda}_{nk}$  as

$$\mathbf{\Lambda}_{nk} = \tau_{nk} \mathbf{v}_{nk}, \quad (\text{A3})$$

with  $\tau_{nk}$  the momentum relaxation time given by the microscopic transition probability rate  $P_{n'k' \leftarrow nk}$  as

$$\frac{1}{\tau_{nk}} = \sum_{n'k'} P_{(n'k') \leftarrow (nk)}. \quad (\text{A4})$$

For the purpose of this paper, we consider a constant relation time  $\tau_{nk} = \tau_0$  [15,39].

### APPENDIX B: SPIN AND ORBITAL ANGULAR MOMENTUM OPERATORS

The spin operator from the *ab initio* calculations is expressed in the real-space Wannier tight-binding basis  $\hat{S}_R$  [47,60,61] and subsequently used to obtain the interpolated spin expectation values in the reciprocal space  $\hat{S}_k^{(H)}$ . Our treatment [62,63] agrees well with the results obtained using the WANNIERBERRI package [48]. The orbital angular momentum

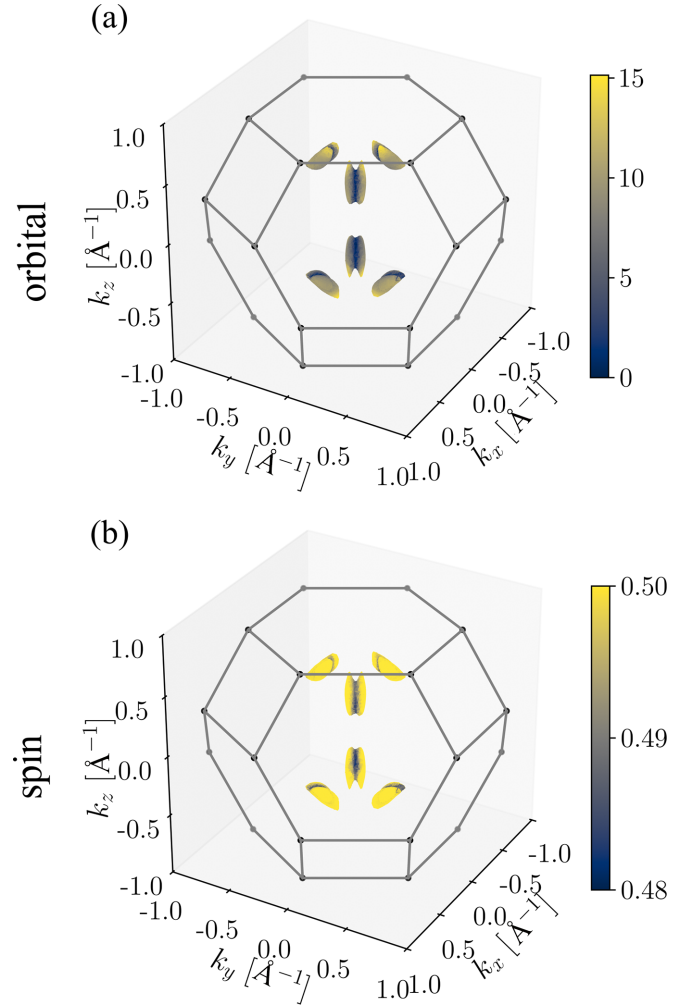


FIG. 6. Isoenergy surface of the topmost band at  $\mathcal{E} = -0.09$  eV, close to the global maxima. Color shows the absolute value of (a) the orbital and (b) spin angular momentum, in units of  $\hbar$ .

is computed from the MTOM [38] expression

$$l_{\gamma,nk} = \frac{-e}{2\mu_B g_l} \epsilon_{\alpha\beta\gamma} \text{Im} \langle \partial_\alpha u_{nk} | \hat{H} - \mathcal{E}_{nk} | \partial_\beta u_{nk} \rangle, \quad (\text{B1})$$

with  $|u_{nk}\rangle$  the lattice-periodic part of the Bloch state,  $\hat{H}$  the Hamiltonian of the system, and  $\alpha, \beta, \gamma$  Cartesian indices. This expression can be transformed to

$$l_{\gamma,nk} = \frac{e}{2\mu_B g_l} \epsilon_{\alpha\beta\gamma} \times \text{Im} \sum_{m \neq n} \frac{\langle u_{nk} | \partial_\alpha \hat{H} | u_{mk} \rangle \langle u_{mk} | \partial_\beta \hat{H} | u_{nk} \rangle}{\mathcal{E}_{nk} - \mathcal{E}_{mk}}. \quad (\text{B2})$$

Equation (B1) is directly obtained from the WANNIERBERRI package [48].

### APPENDIX C: VALENCE BAND MAXIMUM

As mentioned above, the global maximum of the valence band at  $\mathcal{E} = -0.05$  eV is very close to the Fermi energy [51,79], but not along the high-symmetry path of the band

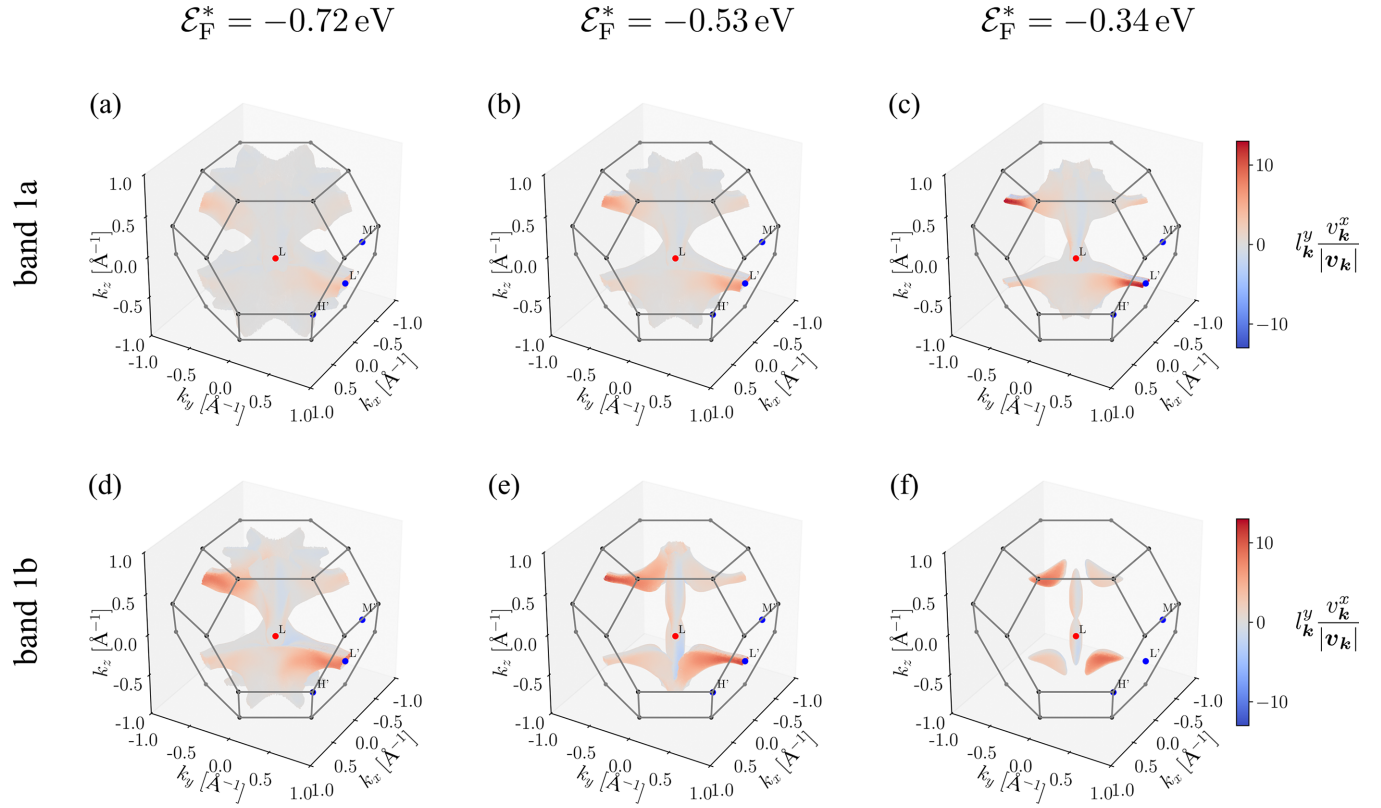


FIG. 7. Isoenergy surfaces of the top valence band (top row) and the second (bottom row) valence band at various energies around the global maximum of the OEE;  $-0.72$  eV [panels (a) and (d)],  $-0.53$  eV [maximum OEE, panels (b) and (e)],  $-0.34$  eV [panels (c) and (f)]. The color scale represents the contribution of each state to the OEE susceptibility tensor  $\chi_{yx}^1$  (in arbitrary units): Each state at the respective Fermi surface contributes  $\propto l_y^y v_{kx}/|v_k|$ . Around the band crossing ( $\mathcal{E} = -0.37$  eV), pronounced hotspots of this integrand occur, in particular, in the topmost band.

structure shown in Fig. 1. Figure 6 shows the isoenergy surface at  $\mathcal{E} - \mathcal{E}_F = -0.09$  eV, with the absolute values of the

orbital and spin angular momentum. Hence, the SEE and OEE are nonzero in this energy range, as shown in Fig. 4.

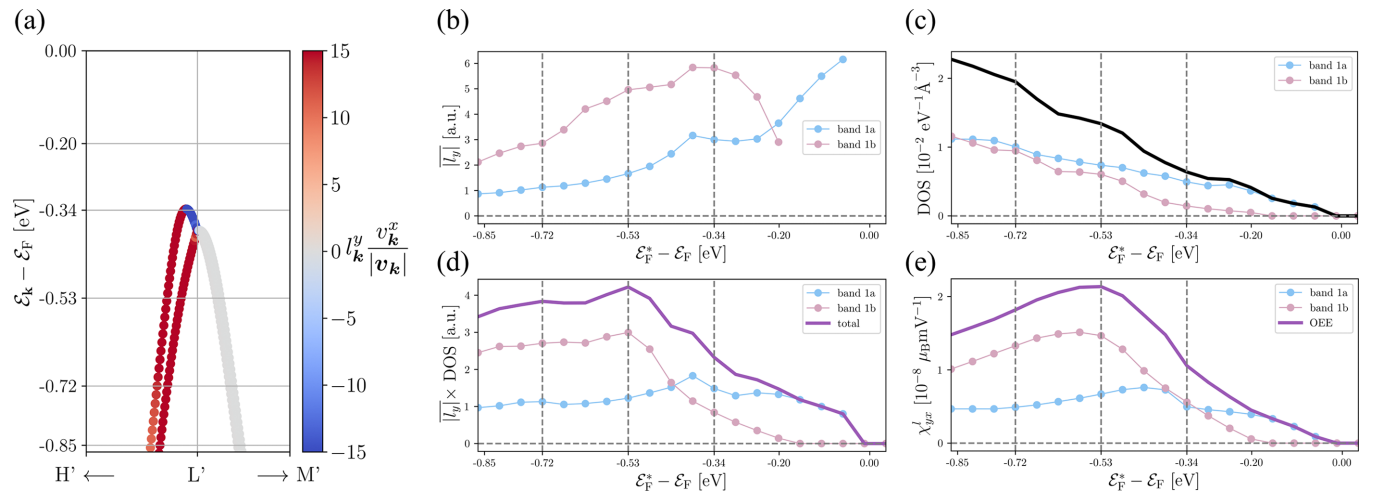


FIG. 8. (a) Band structure around the symmetry points indicated by blue dots in Fig. 7, with the contribution of each state to the OEE susceptibility tensor  $\chi_{yx}^1$  (in arbitrary units). Energy dependence of (b) the averaged y component of the orbital angular momentum along y, (c) the density of states, (d) the product of panels (b) and (c), and (e) the OEE susceptibility  $\chi_{yx}^1$ . Blue and red curves indicate the contributions of the top (1a) and second (1b) bands, respectively.

#### APPENDIX D: EXPLORATION OF THE GLOBAL MAXIMUM OF OEE

The global maximum of the OEE occurs at  $\mathcal{E} = -0.53$  eV and does not coincide with any particular point of the band structure, as shown in Fig. 4(a). The origin of this maximum can be understood by a detailed analysis of the summands of the OEE in Eq. (2). Figure 7 shows the evolution of the isoenergy surfaces around this maximum and the contribution of each individual state to the OEE tensor  $\chi_{yx}^1$ . Moving from low to high energies toward valence band crossing at  $L$  (around  $\mathcal{E} = -0.39$  eV), pronounced hotspots of this contribution occur around  $L'$ . On the other hand, the Fermi surface area

and the density of states generally decrease toward the band edge.

Figure 8(b) shows the average  $y$  component of the orbital angular momentum for the two topmost valence bands. It reaches its maximum at (band 1a) and slightly below (band 1b) the respective band edge. In contrast, the density of states, shown in Fig. 8(c), decreases toward the band edges. Figure 8(d) shows the product of the averaged OAM and the density of states of each band, which is a rough approximation for the OEE susceptibility shown in Fig. 8(e). The competing energy dependence of OAM and density of states leads to the maximum of the OEE around  $-0.53$  eV, clearly below the band crossing.

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