Kinetic magnetoelectric effect in topological insulators

Ken Osumi1, Tiantian Zhang1,2 & Shuichi Murakami1,2

The kinetic magnetoelectric effect is an orbital analog of the Edelstein effect and offers an additional degree of freedom to control magnetization via the charge current. Here we theoretically propose a gigantic kinetic magnetoelectric effect in topological insulators and interpret the results in terms of topological surface currents. We construct a theory of the kinetic magnetoelectric effect for a surface Hamiltonian of a topological insulator, and show that it well describes the results by direct numerical calculation. This kinetic magnetoelectric effect depends on the details of the surface, meaning that it cannot be defined as a bulk quantity. We propose that Chern insulators and Z2 topological insulators can be a platform with a large kinetic magnetoelectric effect, compared to metals by 5–8 orders of magnitude, because the current flows only along the surface. We demonstrate the presence of said effect in a topological insulator, identifying Cu2ZnSnSe4 as a potential candidate.
In recent years, new responses leading to orbital magnetization have been proposed in systems without inversion symmetry. Among such proposals are kinetic magnetoelectric effect (KME)\textsuperscript{1-3,10,11,13-15,18}, also called orbital Edelstein effect, i.e., current-induced orbital magnetization, and the gyrotropic magnetic effect\textsuperscript{4-6}. These effects have similar response coefficients. In particular, KME is an orbital analog of the Edelstein effect\textsuperscript{19,21}. KME emerges even in systems without spin-orbit interactions.\textsuperscript{1,3} In particular, the KME emerges in crystals with a chiral structure\textsuperscript{1,3}, similar to the phenomenon in which the solenoid creates a magnetic field when a current flows. In a similar context, the recent finding of spin-selective electron transport through chiral molecules, the so-called chirality-induced spin selectivity (CISS) effect\textsuperscript{22-25}, suggests an alternative method of using organic materials as spin filters for spintronics applications.

In the KME, the electric field induces magnetization, which may look similar to the magnetoelectric (ME) effect\textsuperscript{27-35}. Nonetheless, in the spin Edelstein effect and KME, metallic systems are considered, and nonequilibrium electron distribution by the current leads to a change in an orbital magnetization due to the off-equilibrium electron distribution discussed above, the electric field also modifies the electronic states. In KME, where TRS is preserved within this order. On the other hand, in topological insulators without TRS, such as Chern insulators, this may also contribute to the orbital magnetization. This mechanism is similar to the conventional ME effect in insulators and has been discussed also in metals.\textsuperscript{36,37}

This calculation method is different from that in the previous study on metals,\textsuperscript{1,2,4} where bulk contribution in a system infinite along \(x\) and \(y\) directions are calculated.

Model calculation on a Chern insulator. As an example of a topological insulator, we consider an orbital magnetization in a Chern insulator with a chiral crystal structure. For this purpose, we introduce a three-dimensional tight-binding model of a layered Chern insulator, as shown in Fig. 1a, connected via right-handed interlayer chiral hoppings (Fig. 1b). Each layer forms a square lattice within the \(xy\)-plane, with a lattice constant \(a\), and they are stacked along the \(z\)-axis with a spacing \(c\) as shown in detail in the “Methods” section. The Brillouin zone and the band structure are shown in Fig. 1c–e. We set the Fermi energy in the energy gap.

We calculate KME in a one-dimensional quadrangular prism with \(xz\) and \(yz\) surfaces shown in Fig. 1f (see “Methods” section), with its results in Fig. 1g,h with the interlayer hopping \(t_{3} = 0.1t_{1}\) and \(t_{3} = 0.001t_{1}\), respectively, for several values of the system size, \(L_{x}\) and \(L_{y}\), representing the lengths of the crystal in the \(x\) and \(y\) directions. Thus, the KME is affected by boundaries and system size, and this size dependence remains even when the system size is much larger than the penetration depth of topological surface states. Therefore, KME cannot be defined as a bulk quantity. In contrast, the orbital magnetization in equilibrium is shown to be a bulk quantity in crystals\textsuperscript{38-40} in 2005, which is nontrivial, because the operator for the orbital magnetization involves the position $-e$ is the electron charge, \(\psi_{n,k}(x,y)\) and \(E_{n}\) is the \(n\)th occupied eigenstates and energy eigenvalues of \(H\) at the Bloch wave number \(k_{z}\), respectively, \(\beta(E)\) is the distribution function at the energy \(E\), \(S\) is the cross-section of the crystal along the \(xy\)-plane and \(N\) is the number of occupied states. We note that the position operator \(\mathbf{r}\) is unbounded and problematic if a system is infinite in some directions. Nonetheless, in the present case, the system is infinite only along the \(z\)-direction, while \((\mathbf{r} \times \mathbf{v})\) does not involve \(z\), which means Eq. (1) is well defined. The unit of the orbital magnetization is \([\text{A/m}]\) in the SI unit.

Then, within the Boltzmann approximation, the applied electric field \(E_{z}\) changes \(f(E)\) from \(\beta(E)\) into \(f(E) = \beta(E) + e\mathbf{E} \cdot \mathbf{v}\). in a linear order in \(E_{z}\), where \(\tau\) is the relaxation time assumed to be constant and \(\beta(E)\) is the Fermi distribution function $\beta(E) = (\exp(E-E_{F})+1)^{-1}$, $\beta=1/k_{B}T$, $k_{B}$ is the Boltzmann constant and $\mu$ is the chemical potential. Then the orbital magnetization is generated as

\[
M_{z}^{\text{KME}} = \frac{1}{2\pi} \int \frac{d\pi/\tau}{-\pi/\tau} \sum_{n} \int_{-\pi/\tau}^{\pi/\tau} \frac{f(E_{n}(k_{z}))}{E_{n}(k_{z})} \sum_{n} \int_{-\pi/\tau}^{\pi/\tau} \frac{f(E_{n}(k_{z}))}{E_{n}(k_{z})} \times (-\frac{\pi}{\tau}) \int d\mathbf{x} d\mathbf{y} \psi_{n,k_{z}}^{\dagger}(x,y)(\mathbf{r} \times \mathbf{v}) \psi_{n,k_{z}}(x,y),
\]

\[
(2)
\]

This is the KME. In Chern insulators, because the TRS is broken, an orbital magnetization is nonzero in equilibrium, and a current leads to a change in an orbital magnetization due to the KME. On the other hand, in 2D-TIs, an orbital magnetization vanishes in equilibrium, and the KME leads to the appearance of an orbital magnetization. We note that in addition to the off-equilibrium electron distribution discussed above, the electric field also modifies the electronic states. In 2D-TIs, where TRS is preserved, this modulation of the electronic states does not lead to the orbital magnetization in the linear order in \(E_{z}\) because the TRS is preserved within this order. On the other hand, in topological insulators without TRS, such as Chern insulators, this may also contribute to the orbital magnetization.
operator $\mathbf{r}$. Later, we give an interpretation on this characteristic size dependence.

**Surface theory of KME for a slab.** In topological insulators such as Chern insulators, only the topological surface states can carry a current. Here we calculate the KME using an effective Hamiltonian for the crystal surface. Thereby, we can capture the natures of KME through this surface theory. We consider slab systems, with their surfaces on $y=y_s(y_s>y_-)$. The slab is sufficiently long along with the $x$ and $z$ directions and we impose periodic boundary conditions in these directions. To induce the orbital magnetization $M_{z,\text{slab}}^{\text{KME}}$, we apply an electric field $E_z$ in the $z$-direction. Due to the interlayer chiral hoppings, the surface current acquires a nonzero $z$-component ($\mathbf{2}a$).

Let $E_\pm=E_-\{k_x,k_z\}=(E_\pm\{k_x,k_z+2\pi\})$ be the surface-state dispersion on the $y=y_-$ surface as shown in Fig. 2b,c. For simplicity, we assume $C_{2z}$ symmetry of the system. Then the surface state dispersion on the $y=y_+$ surface is given by $E_\mp=E_\pm\{-k_x,k_z\}=E_\pm\{-k_x,k_z\}$. Here, we assume that the surface states are sharply localized at $y=y_s$, namely, we ignore finite-size effects due to a finite penetration depth. Then, we rewrite Eq. (2) to

$$M_{z,\text{slab}}^{\text{KME}} = \frac{\hbar}{2\tau_0} \left[ \frac{\pi c}{\Delta} \frac{d}{dk_x} \frac{d}{dk_z} \right] \frac{\Delta E(k_x,k_z)}{dk_x} \left( \text{sgn} \left( \frac{\Delta E(k_x,k_z)}{dk_z} \right) \right) E_z(k_x,k_z) \right|_{E_z(k_x,k_z)=0},$$

(3)

(see Supplementary Note 1 for details). We note that the Fermi surface depends on the surface termination, and so does the KME. We also confirm the surface dependence from numerical calculations as shown in Fig. 2d–i. This formula applies to any topological insulators such as $Z_2$-TIs (see Supplementary Note 2).

**Surface theory of KME for a cylinder.** From this slab calculation, we calculate the KME for a cylinder geometry. We consider a current along the $z$-direction in a one-dimensional quadrangular prism with $xz$ and $yz$ surfaces (surfaces I–IV in Fig. 3a) through its surface Hamiltonian. Let $L_x$ and $L_y$ denote the system sizes.
Fig. 2 Chern insulator with a chiral structure and its kinetic magnetoelectric effect (KME) in slab systems. a Surface velocities (red arrow) of the topological surface states under an electric field $E$ (green arrow). b, c Band structure of the topological chiral surface states on the $y-y$ surface. Their (b) dispersion and (c) Fermi surface are shown. In b, the valence and conduction bands are represented by orange and blue boxes, and the topological surface states are drawn in purple in between the two bands. c is the Fermi surface, which is a section of b at the energy $E$ equal to the chemical potential $\mu$. d Slab models I and with chiral hopping on the surface. Only the section along the dispersion and ($\phi$) are amplitudes of the wavefunctions in the $x$- and $y$-directions, respectively.

Hamiltonians. For simplicity, we assume twofold rotation symmetry $C_{2z}$ of the system, which relates between I and III, and between II and IV. Then, only the surface I and II are independent. We write down the eigenvalues for these surfaces as

$$H^I \psi_{k,y}^I (x,z) = E^I_{k,y} \psi_{k,y}^I (x,z),$$

$$H^{II} \psi_{k,y}^{II} (y,z) = E^{II}_{k,y} \psi_{k,y}^{II} (y,z),$$

where $H^I$ and $H^{II}$ are the Hamiltonians for the surfaces I and II, respectively, and $\psi_{k,y}^I = u_{k,y}^I(k_x,k_z)e^{ik_x x}e^{ik_z z}$ and $\psi_{k,y}^{II} = u_{k,y}^{II}(k_x,k_z)e^{ik_x y}e^{ik_z z}$ are Bloch eigenstates on the surfaces I and II, respectively.

We can determine these eigenstates from four conditions, equality of the energy eigenvalues, current conservation at the corner (Fig. 3b), and periodic boundary condition on the crystal surface, and the normalization condition (see Supplementary Note 3).

Thus we obtain a formula for KME in a one-dimensional prism of a three-dimensional Chern insulator

$$M^{\text{KME}}_z = -\frac{e^2}{\hbar} \frac{1}{(2\pi)^2} \int_{-\pi/e}^{\pi/e} \int_{-\pi/e}^{\pi/e} \frac{L_x}{\gamma_x} + \frac{L_y}{\gamma_y} |E=\mu|.$$  

Fig. 3 One-dimensional prism of a Chern insulator. a Schematic figure of the one-dimensional prism of a Chern insulator, extended along z-axis, with its size $L_x \times L_y$ within the $xy$ plane. We call the four side surfaces I, II, III and IV. b The schematic figure for constant conservation at the corners around the one-dimensional prism in a. Here, $j^I_x$ and $j^{II}_x$ are current densities in the circumferential direction of the prism on the surfaces I and II, respectively, and we impose them to be equal. $v^I_x$ and $v^{II}_x$ are corresponding velocities of electrons, and $u^I_{k_x}$ and $u^{II}_{k_x}$ are amplitudes of the wavefunctions in the respective surfaces.

along the $x$ and $y$ directions, respectively. Because the KME is sensitive to differences in crystal surfaces, as shown in slab systems, we consider the individual surfaces separately.

In particular, in Chern insulators, we can calculate the energy eigenstates for the whole system from those for the surface.
When $v_x$ and $v_y$ are almost independent of $k_z$, we approximate Eq. (6):

$$M_{z}^{\text{KME}} = 2 \frac{L_e}{\sigma_{xx}} M_{z,\text{slab}}^{L_e} + \frac{L_t}{\sigma_{xx}} M_{z,\text{slab}}^{L_t},$$

where $M_{z,\text{slab}}^{L_e}$ and $M_{z,\text{slab}}^{L_t}$ represent the KME for a slab (Eq. (3)) with the surface I and that with the surface II, respectively. Thus, the KME of the one-dimensional system can be well approximated by Eq. (7) expressed in terms of that for the slabs along $xz$ and along $yz$ planes.

In general topological insulators, we can also derive KME in terms of a simple picture of a combined circuit, consisting of four surfaces I–IV with anisotropic transport coefficients. We obtain

$$M_{z}^{\text{KME}} = j_{\text{circ}} = \frac{L_e}{\sigma_{xx}} \sigma_{xyz}^I + \frac{L_t}{\sigma_{xx}} \sigma_{xyz}^II E_z,$$

where $j_{\text{circ}}$ is the circulating current density within the $xy$ plane around the prism per unit length along the $z$-direction. $\sigma_{xyz}^I$ is the electric conductivity tensor for the surfaces I and II (see Supplementary Note 4). On the other hand, we can also show $M_{z,\text{slab}}^{L_e} = \frac{1}{2} \sigma_{xx}^I E_z$, $M_{z,\text{slab}}^{L_t} = \frac{1}{2} \sigma_{xx}^II E_z$. In Chern insulators, by using $\sigma_{xx}^I \propto \langle v_x \rangle$ and $\sigma_{xy}^II \propto \langle v_y \rangle$, we arrive at Eq. (7). Thus, we can calculate the KME from the surface electrical conductivity from Eq. (8), which depends on the aspect ratio $L_e/L_t$.

We numerically confirm that the results of direct calculation by Eq. (2) and those for surface calculation by Eq. (7) agree well (Fig. 4a–c). When the interlayer hopping is large (Fig. 4c), they slightly deviate from each other. This is because we cannot ignore the $k_z$-dependence of $v_x$ and $v_y$ and they are out of the scope of the approximate expression (Eq. 7).

**Finite-size effect.** In our approximation theory, we assumed that the surface current is localized at the outermost sites and ignored a finite penetration depth. In fact, we can fit the data with various system sizes with a trial fitting function which includes a finite-size effect in Eq. (7) (see “Methods” section and Supplementary Note 5). From these results, the finite-size effect is of the order $1/L$ in the leading order, coming from the finite penetration depth. When the system size is much larger than the penetration depth, the result is well described by the surface theory as shown in Fig. 4d.

**Materials.** Topological insulators without inversion symmetry can be a good platform for obtaining large KME because the current flows on the surface. Therefore, the closed-loop created by the current is macroscopic and it efficiently induces orbital magnetization. In contrast, in the conventional KME in metals, a bulk current generates microscopic current loops in the bulk, which leads to a much smaller effect than a surface current in topological insulators. One can also regard this set of current loops as a macroscopic current loop along the surface, but the current, in this case, is of a microscopic amount, determined by the current per bulk unit cell. Therefore, the resulting effect in bulk metals is much smaller than the KME in topological insulators, where the current along the surface is of macroscopic size. Moreover, the surface states of topological materials are robust against perturbations caused by impurities.
Under the non-inversion-symmetry constraint, we cannot diagnose $Z_2$-TIs easily because the $Z_2$ topological invariant is expressed in terms of $k$-space integrals. Our idea here is to use $S_4$ symmetry to diagnose $Z_2$-TIs, where we only need to calculate wavefunctions at four momenta according to the symmetry-based indicator theories\textsuperscript{50–52}. After searching in the topological material database\textsuperscript{53}, we notice that Cu$_2$ZnSnSe$_4$ with 82 and CdGeAs$_2$ with 122 are two ideal candidates of $Z_2$-TIs with a direct gap for obtaining a large KME (see Supplementary Note 6 for details). In the following, we will use Cu$_2$ZnSnSe$_4$, which only has $S_4$ symmetry as shown in Fig. 5a, as an example to show the magnitude of the KME with different surfaces and different surfaces terminations.

Since the magnetoelectric tensor for the space group 82, defined by $M = aE$, is $a_{z2} = \begin{bmatrix} \alpha_{11} & \alpha_{12} & 0 \\ \alpha_{12} & -\alpha_{11} & 0 \\ 0 & 0 & 0 \end{bmatrix}$, we can obtain an orbital magnetization $M_{z}^{\text{KME}}$ by adding an external electric field $E$, through the surface currents both on the [001] surface and on the [010] surface thanks to the nonzero $\alpha_{11}$ (see Supplementary Note 7 for details). In our discussion of the KME effect, we set the current direction to be along $z$-axis. Therefore we will set the $1$-axis in the above magnetoelectric tensor to be the $z$-axis in our theory.

Figure 5b, c is the Brillouin zone and the band structure of Cu$_2$ZnSnSe$_4$ with a gap, through the first-principle calculations whose details are explained in “Methods” section. On the [001] surface, terminations with Cu-Sn layer (surface A) and with Se layer (surface B) have different surface energies and Fermi surfaces, as shown in Fig. 5d–g, which contribute to a magnetoelectric susceptibility of $\alpha_{11} = -1.804 \times 10^5 \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$ and $\alpha_{11} = -2.565 \times 10^5 \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$, respectively. On the A surface, there is a single surface Dirac cone at $\Gamma$ point, forming an electron-like Fermi surface. On the B surface, the Dirac cone at $\Gamma$ point forms an almost zero Fermi surface, but two surface Dirac cones at two $X$ momenta form two hole-like Fermi surfaces. Because the Fermi surfaces on the B surface are much larger than those on the A surface, the magnetoelectric susceptibility on the B surface is one order of magnitude larger than that on the A surface. Similar calculations on the [010] surface area in Supplementary Note 8, and the result is $\alpha_{11} = -2.324 \times 10^5 \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$ for surface C.

Let us compare the results with metallic materials in the bulk. For simplicity, we focus on the cases with the electric field $E$ and the resulting magnetization $M_{z}^{\text{KME}}$ along the $z$-direction. This kinetic magnetoelectric response is expressed as $M_{z}^{\text{KME}} = \alpha_{z} E_{z}$, and the conductivity is $j_{z} = \sigma_{z} E_{z}$. Thus the magnetization in response to the current is $M_{z}^{\text{KME}} = (\alpha_{z} / \sigma_{z}) j_{z}$. In the relaxation time approximation, both $\alpha_{zz}$ and $\sigma_{zz}$ are proportional to the relaxation time $\tau$. For simplicity we consider the system to be a cube with its size $L \times L \times L$. In the bulk metallic systems, the current is carried by the bulk states, and $\alpha_{zz} \propto L^{0}$, $\sigma_{zz} \propto L^{0}$. On the other hand, in topological systems, only the surface conducts the current, and the conductivity $\sigma_{zz}$ scales as $\sigma_{zz} \propto L^{-1}$. On the other hand, we have shown $\alpha_{zz} \propto L^{0}$, which means that $\alpha_{zz}$ is an intensive quantity. Thus, in topological insulators, the scaling of the KME as a response to the electric field is represented by the response coefficient $\alpha_{zz} \propto L^{0}$. Meanwhile, the response coefficient $\alpha_{zz}$ to the current is proportional to $L$. It means that as a response to the current, topological materials will generate a large amount of orbital magnetization as compared to metals.

We compare our results with KME in p-doped tellurium, which has a chiral crystal structure\textsuperscript{3}. For the acceptor concentration $N_{A} = 4 \cdot 10^{14} \text{cm}^{-3}$ at 50 K, the induced orbital magnetizations is $M_{z}^{\text{KME}} = 7.0 \cdot 10^{-2} \text{µB/atom} \sim 1.85 \times 10^{-2} \text{A/m}$ by a current density $j_{z} = 1000 \text{A/cm}^{2}$. Thus the response coefficient of the orbital magnetization $M_{z}^{\text{KME}}$ to the current density $j_{z}$ is $\alpha_{zz} = 1.85 \times 10^{-9} \text{m}$. If we approximate $\alpha_{zz} \sim \frac{\alpha_{zz}}{\frac{\sigma_{zz}}{\Omega}}$, with the electronic charge $e$ and mass $m$, we get $\alpha = 2.1 \times 10^{8} \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$. For other acceptor concentrations $N_{A} = 4 \cdot 10^{14} \text{cm}^{-3}$ and $N_{A} = 1 \cdot 10^{18} \text{cm}^{-3}$, one can similarly get $\alpha_{zz} = 2.1 \times 10^{8} \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$ and $\alpha_{zz} = 2.3 \times 10^{7} \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$. Thus, the size of $\alpha_{zz}$ for the topological insulator Cu$_2$ZnSnSe$_4$ is larger than that of Te by two to five orders of magnitude.

On the other hand, in topological insulators, the induced orbital magnetization as a response to the current becomes huge compared with metals. To show this, we consider a system with surfaces having anisotropic transport coefficients with sheet resistance $\sigma_{zz}$ and $\sigma_{zz}$, where $\square$ denotes a sheet conductance. Then we can define an angle $\theta$ by $\alpha_{zz} / \sigma_{zz} = \tan \theta$, where $\theta$ describes an angle between the electric field along the $z$-direction and the surface current density $j_{z}$. For example, for the [001] surface of Cu$_2$ZnSnSe$_4$, we get $\sigma_{zz}^{A} = 2 \alpha_{zz}^{A} = -3.6 \times 10^{5} \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$, $\sigma_{zz}^{A} = 7.3 \times 10^{5} \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$, $\sigma_{zz}^{B} = 2 \alpha_{zz}^{B} = -5.1 \times 10^{5} \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$, $\sigma_{zz}^{B} = 2 \alpha_{zz}^{B} = 2 \times 10^{5} \text{s}^{-1} \text{Ω}^{-1} \cdot \tau$, which yield $\tan \theta_{A} = -0.49$ and $\tan \theta_{B} = -0.26$ by identifying $x = 2$ and $z = 1$. Then the total
current along the $z$ direction is $4J_z$, while the circulating current is $j_{\text{circ}} = j_{\text{surf}}^x = j_{\text{surf}}^y \tan \theta$. Thus the magnetization response $M^{\text{KME}}_{\text{surf}}$ to the current density is $j_{\text{surf}}(=4J_z \tan \theta)$ is $M^{\text{KME}}_{\text{surf}} = j_{\text{circ}} / j_{\text{surf}}^x$ (L/4) = (L/4) $\tan \theta$, which is proportional to the system size. It is the response coefficient $a/\sigma$ shown in Table I. Thus for the macroscopic system size, the response $M^{\text{KME}}_{z,j_z}$ is also of the macroscopic size such as millimeters, and it is much order of magnitude larger than that in tellurium, where $M^{\text{KME}}_{z,j_z}$ is evaluated to be $M^{\text{KME}}_{z,j_z} = 1.85 \times 10^{-9}$ m.

This scaling to the system size shows a prominent difference in the KME in topological insulators from similar effects. In bulk metals studied in previous works, the KME is always independent of the system size $L$. In topological insulators, the current induces both the spin and the orbital magnetizations, and we propose that only the orbital magnetization shows a different scaling behavior. As a comparison, we calculate the spin magnetization induced by the electric field in Cu$_2$ZnSnSe$_4$, with calculation details and spin textures presented in Supplementary Note 9, and obtain $a_{\text{spin}} = 2.798 \times 10^{-2} m \cdot s^{-1} \Omega^{-1} \cdot \tau_{\Omega y}$, and $a_{\text{spin}} = -2.575 m \cdot s^{-1} \Omega^{-1} \cdot \tau_{\Omega y}$. Thus it inversely scales with the system size along the $y$-direction. Thus suppose the system size of 1 mm, they are of the order $10^8$ times smaller than in bulk metals. In Table I, we show scaling behaviors of the conductivity to the current density $\sigma$, their sum is calculated. In this paper, we found the response to the current in topological insulators is much larger than in bulk metals. In Table I, we show scaling behaviors of the conductivities for metals and TIs. The KME is shown as responses to an electric field, $\alpha$, and to a current, $a/\sigma$. In particular, in the response to a current, $a/\sigma$, it scales as $L^1$ only in the interatomic orbital magnetization, while other entities scale with $L^0$. This shows a particular feature of the interatomic orbital magnetization generated by a current proposed in the present paper.

In this paper, we put two $Z_2$ TIs as candidates for the topological KME. In addition to Chern insulators and $Z_2$ TIs, other classes of topological insulators such as various classes of topological crystalline insulators, and topological semimetals will also show the topological KME. In topological semimetals, topological surface states coexist with bulk metallic states, but the contribution from the former overwhelms that from the latter, and the topological KME is expected.

**Methods**

**Details of the first-principle calculations.** First-principle calculations of Cu$_2$ZnSnSe$_4$ are performed in the Vienna ab initio simulation package (VASP) with Perdew-Burke-Ernzerhof exchange-correlation. A Γ-centered Monkhorst-Pack grid with 10 $\times$ 10 $\times$ 2 k-points and 460.8 eV for the cut-off energy of the plane wave basis set is used for the self-consistent calculation. Surface states and Fermi surfaces calculations are performed by the tight-binding model obtained by the maximally localized Wannier functions.

**Details of the model Hamiltonian.** We consider a Chern insulating system with a chiral crystal structure. The model is composed of infinite layers of the two-dimensional Wilson-Dirac model. The lattice sites are expressed by $(i,j,b)$, with $i$, $j$, and $b$ being integers, specifying the $x$, $y$, and $z$-coordinates. At each lattice site, we consider two orbitals 1 and 2. Let $c_{ijl,\sigma}^\dagger$ denote the annihilation operator of the electron at the $(i,j,b)$-site with orbital $\sigma = (1,2)$, and we write $c_{ijl,\sigma} = (c_{ijl,\sigma^+}, c_{ijl,\sigma^-})^T$. The model Hamiltonian is $H = H_{\text{WD}}(m, t_1, t_2, b_1, b_2)$ + $H_{\text{interlayer}}(t_b, t_c)$, where $H_{\text{WD}}$ is an in-plane Wilson-Dirac Hamiltonian, and $H_{\text{interlayer}}$ is an interlayer Hamiltonian representing a structure similar to right-handed solenoids. The in-plane Wilson-Dirac Hamiltonian is

$$H_{\text{WD}} = m \sum_{ijl} c_{ijl,\sigma}^\dagger c_{ijl,\sigma} + H_{\text{c}} - \frac{b_1}{2} \sum_{ijl} c_{ijl,\sigma}^\dagger c_{ijl,\sigma} + H_{\text{c}} - \frac{b_2}{2} \sum_{ijl} c_{ijl,\sigma}^\dagger c_{ijl,\sigma} + H_{\text{c}} - 2c_{ijl,\sigma} c_{ijl,\sigma} c_{ijl,\sigma},$$

where $H_{\text{c}}$ stands for Hermitian conjugate of the preceding terms, $\dagger$ represents Hermitian conjugate, and $m, t_1, t_2, b_1$ and $b_2$ are real parameters. This Hamiltonian $H_{\text{WD}}$ can be rewritten in the momentum space as

$$H_{\text{WD}}(k) = t_b \sin k_x a_x + t_c \sin k_y a_y + (m - b_1(1 - \cos k_x a_x) - b_2(1 - \cos k_y a_y)) \sigma_x,$$

where $k$ is the Bloch wavevector. An isotropic two-dimensional Wilson-Dirac model with $b_1 \equiv b_1$, $b_2$, and $t_b = t_c$ exhibits the Chern insulating phase when $0 < m - b < 2 \pi$ and $0 < m - b < 4 \pi$. Next, we add interlayer hoppings, including a direct hopping $t_{\text{chiral}}$ along the $z$-axis and a chiral hopping $t_{\text{chiral}}$, where $t_{\text{chiral}}$ and $t_{\text{chiral}}$ are real parameters. To describe the chiral hopping $t_{\text{chiral}}$, the lattice sites in the square lattice in each layer into groups of four sites, $(2i - 1, 2j - 1)$, $(2i - 1, 2j - 1)$, $(2i, 2j - 1)$, and $(2i, 2j)$ where $i$ and $j$ are integers, and we introduce chiral hoppings between the groups on the neighboring layers. Then the total Hamiltonian for this model on a tetragonal lattice is given by

$$H = H_{\text{WD}} + H_{\text{interlayer}}.$$
where

\[ H_{\text{interlayer}} = \sum_{i,j} \left( \sum_{l} t_{ijl}^c \hat{c}_{i,l-1/2,j}^\dagger \hat{c}_{i,l+1/2,j} + H.c. \right) + t_{ij} \sum_{l} \left( \hat{c}_{i,l-1/2,j}^\dagger \phi_{i,l-1/2,j} + H.c. \right) + t_{ij} \sum_{l} \left( \hat{c}_{i,l+1/2,j}^\dagger \phi_{i+1/2,j} + H.c. \right) + t_{ij} \sum_{l} \left( \phi_{i,l-1/2,j}^\dagger \phi_{i,j} + H.c. \right) + t_{ij} \sum_{l} \left( \phi_{i,l+1/2,j}^\dagger \phi_{i,j+1/2} + H.c. \right) \]

(12)

These hoppings in \( H_{\text{interlayer}} \) form structures similar to right-handed solenoids. When \( H_{\text{interlayer}} \) is in the Chern insulator phase, even if \( H_{\text{interlayer}} \) is perturbed by \( H_{\text{interlayer}} \), the system remains in the Chern insulator with the Chern number within the xy plane equal to \(-1\) as long as \( t_{ij} \) and \( t_{ij} \) are small. In the main text, we are interested in the KME due to the topological surface states in the topological Chern insulating phase, in which the Fermi energy is in the energy gap.

**Fitting function for KME.** By taking into account the finite-size effect in Eq. (7), we give a fitting function. The finite penetration depth of the surface states will lead to \( O(1/L) \) correction to the KME, and that around the corner will lead to \( O(1/L^2) \) correction. Thus, the fitting function is

\[ M_{\text{KME}}^f = \frac{w_x L_x + w_y L_y}{w_x L_x + w_y L_y} \]

(13)

where \( w_i (i = 1, 2, \ldots, 7) \) are real constants.

**Data availability**

The datasets generated during and/or analyzed during this study are available from the corresponding authors upon reasonable request.

**Code availability**

The source code for the calculations performed in this work is available from the corresponding authors upon reasonable request.

Received: 18 January 2021; Accepted: 2 August 2021

Published online: 21 February 2021

**References**

1. Yoda, T., Yokoyama, T. & Murakami, S. Current-induced orbital and spin magnetizations in crystals with helical structure. *Sci. Rep.* 5, 12024 (2015).
2. Yoda, T., Yokoyama, T. & Murakami, S. Orbital Edelstein effect as a condensed-matter analog of solanoids. *Nano Lett.* 18, 916–920 (2018).
3. Furukawa, T., Shimokawa, Y., Kobayashi, K. & Itou, T. Observation of current-induced bulk magnetization in elemental tellurium. *Nat. Commun.* 8, 954 (2017).
4. Zhong, S., Moore, J. E. & Souza, I. Gyrotropic magnetic and the magnetic moment on the fermi surface. *Phys. Rev. Lett.* 116, 077201 (2016).
5. Tairkin, S. S., Puente, P. A. & Souza, I. Gyrotropic effects in triligonal tellurium studied from first principles. *Phys. Rev. B* 97, 035158 (2018).
6. Wang, Y.-Q., Morimoto, T. & Moore, J. E. Optical rotation in thin chiral/-twisted materials and the gyrotropic magnetic effect. *Phys. Rev. B* 101, 174419 (2020).
7. Moore, J. E. & Orenstein, J. Confinement-induced Berry phase and helicty-dependent photocurrents. *Phys. Rev. Lett.* 105, 026805 (2010).
8. Sodemann, I. & Fu, L. Quantum nonlinear Hall effect induced by Berry curvature dipole in time-reversal invariant materials. *Phys. Rev. Lett.* 115, 216806 (2015).
9. Ma, Q. et al. Observation of the nonlinear Hall effect under time-reversal-symmetric conditions. *Nature* 565, 337–342 (2018).
10. Shaliny, V. A., Sofronov, A. N., Vorob’ev, L. E. & Farbstein, I. Current-induced spin polarization of holes in tellurium. *Phys. Solid State* 54, 2362–2373 (2012).
11. Koretsune, T., Arita, R. & Aoki, H. Magneto-orbital effect without spin-orbit interactions in a noncentrosymmetric zeolite-templated carbon structure. *Phys. Rev. B* 86, 125207 (2012).
12. Furukawa, T., Watanabe, Y., Ogasawara, N., Kobayashi, K. & Itou, T. Current-induced magnetization caused by crystal chirality in nonmagnetic elemental tellurium. *Phys. Rev. Res.* 3, 023111 (2021).
13. Rou, J., Sahin, C., Ma, J. & Pesin, D. A. Kinetic orbital moments and nonlocal transport in disordered metals with nontrivial band geometry. *Phys. Rev. B* 96, 035120 (2017).
49. Takahashi, R. & Murakami, S. Gapless interface states between topological insulators with opposite Dirac velocities. Phys. Rev. Lett. 107, 166805 (2011).
50. Po, H. C., Vishwanath, A. & Watanabe, H. Symmetry-based indicators of band topology in the 230 space groups. Nat. Commun. 8, 1–9 (2017).
51. Song, Z., Zhang, T., Fang, Z. & Fang, C. Quantitative mappings between symmetry and topology in solids. Nat. Commun. 9, 1–7 (2018).
52. Khalaf, E., Po, H. C., Vishwanath, A. & Watanabe, H. Symmetry indicators and anomalous surface states of topological crystalline insulators. Phys. Rev. X 8, 031070 (2018).
53. Zhang, T. et al. Catalogue of topological electronic materials. Nature 566, 475–479 (2019).
54. Guen, L., Glaunsinger, W. S. & Wold, A. Physical properties of the quaternary chalcogenides CuI\textsuperscript{2}Bi\textsuperscript{II}Cl\textsuperscript{IV}X\textsubscript{4} \text{ (BII}= \text{Zn, Mn, Fe, Co; CIV}= \text{Si, Ge, Sn; X}= \text{S, Se}). Mater. Res. Bull. 14, 463–467 (1979).
55. Kresse, G. & Hafner, J. Ab initio molecular dynamics for liquid metals. Phys. Rev. B 47, 558–561 (1993).
56. Kresse, G. & Hafner, J. Ab initio molecular-dynamics simulation of the liquid-metal–amorphous-semiconductor transition in germanium. Phys. Rev. B 49, 14251–14269 (1994).
57. Kresse, G. & Furthmüller, J. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. Comput. Mater. Sci. 6, 15 – 50 (1996).
58. Mostofi, A. A. et al. Wannier90: a tool for obtaining maximally-localised Wannier functions. Comput. Phys. Commun. 178, 685–699 (2008).
59. Creutz, M. & Horváth, I. Surface states and chiral symmetry on the lattice. Phys Rev D 50, 2297–2308 (1994).
60. Yoshimura, Y., Imura, K.-I., Fukui, T. & Hatsugai, Y. Characterizing weak topological properties: Berry phase point of view. Phys. Rev. B 90, 155443 (2014).

Acknowledgements
This work was supported by the Japan Society for the Promotion of Science (JSPS) KAKENHI Grants No. JP18H03678, No. JP20H04633, and No. JP21K13865 and by Elements Strategy Initiative to Form Core Research Center (TIES), from MEXT Grant Number JP-MXP0112101001.

Author contributions
All authors contributed to the main contents of this work. K.O. performed the model calculation and formulated the theory for topological systems, through the discussions with T.Z. and S.M.T.Z. performed the ab initio calculation. S.M. conceived and supervised the project. All authors drafted the manuscript.

Competing interests
The authors declare no competing interests.

Additional information
Supplementary information The online version contains supplementary material available at https://doi.org/10.1038/s42005-021-00702-4.

Correspondence and requests for materials should be addressed to Shuichi Murakami.

Peer review information Communications Physics thanks the anonymous reviewers for their contribution to the peer review of this work. This article has been peer reviewed as part of Springer Nature’s Guided Open Access initiative.

Reprints and permission information is available at http://www.nature.com/reprints

Publisher’s note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made. The images or other third party material in this article are included in the article’s Creative Commons license, unless indicated otherwise in a credit line to the material. If material is not included in the article’s Creative Commons license and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this license, visit http://creativecommons.org/licenses/by/4.0/.

© The Author(s) 2021