

X-ray magnetic circular dichroism of altermagnet α -Fe₂O₃ based on multiplet ligand-field theory using Wannier orbitals

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Hematite α -Fe₂O₃ is a *g*-wave altermagnetic material which has an easy-axis phase and easy-plane weak ferromagnetic phase below and above the Morin transition temperature, respectively. The presence of these phases renders it a good candidate to study the characteristic spin splitting in altermagnets under the impacts of the relativistic effect and finite temperature. In this regard, we calculate the band structure of α -Fe₂O₃ based on density functional theory (DFT) which also considers the Hubbard *U* correction and spin-orbit coupling (SOC) effects. Additionally, charge self-consistent DFT plus dynamical mean-field theory (DMFT) calculations are performed at finite temperatures. We find that the altermagnetic spin splitting in α -Fe₂O₃ is preserved by taking either SOC or the temperature effect into account. Furthermore, we present a numerical simulation of the x-ray magnetic circular dichroism (XMCD) of the *L*_{2,3} edge of Fe using a combination of DFT and multiplet ligand-field theory. In terms of the different Néel vectors present in α -Fe₂O₃, we calculate the x-ray absorption spectroscopy of the *L*_{2,3} edge of Fe in the form of a conductivity tensor and analyze the XMCD response from the perspective of symmetry. A characteristic XMCD line shape is expected when the Néel vector is along the [010] direction (magnetic point group 2'/*m*') and the light propagation vector is perpendicular to the Néel vector, which can be further distinguished from the XMCD response originating from weak ferromagnetism with the light propagation vector parallel to the Néel vector.

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I. INTRODUCTION

Recently, altermagnets have attracted a great deal of attention due to their intriguing properties, including the anomalous Hall effect [1–4], linear magneto-optical effects [5–8], and other phenomena, such as spin Hall effects [9,10]. The altermagnets are characterized by macroscopic time-reversal symmetry breaking, giving rise to finite nonrelativistic momentum-dependent spin splitting. As a matter of fact, the macroscopic time-reversal symmetry breaking in some special types of antiferromagnets was proposed by Dzyaloshinskii in the 1950s [11], highlighting their capability of hosting weak ferromagnetism, piezomagnetism [12], and magnetoelectricity [13]. This aspect was revisited alongside Turov's phenomenological classification of these unconventional antiferromagnets as either “centrosymmetric” or “centroantisymmetric” [14], and it was argued that a deeper analogy exists between certain classes of centrosymmetric antiferromagnets with broken time-reversal symmetry and ferromagnets. Namely, such antiferromagnets can be described using only a single magnetic site in the unit cell [15]. On the other hand, this analogy raises a problem in distinguishing the effects originating from altermagnetic and weak ferromagnetic contributions.

The x-ray magnetic circular dichroism (XMCD) technique demonstrates an advantage in this respect in that the valence spin-orbit coupling (SOC) plays only a limited role in determining the spectral features of XMCD in certain altermagnets, such as α -MnTe [6,16]. Instead, the XMCD response is primarily dictated by symmetry considerations associated with the Néel vector. As proposed in Ref. [16], in the free valence spin approximation, the Hall vector is nonzero for some structures (e.g., rutile) but vanishes for others (e.g., NiAs), where symmetry lowering through core-valence exchange or valence SOC is required to enable XMCD. In previous studies, XMCD in α -MnTe, [6] rutile RuO₂ [7], MnF₂ [17], and NiF₂ [18] was discussed in terms of symmetry. For α -MnTe, both theoretical and experimental studies have confirmed a characteristic XMCD line shape when the compensated moments align perpendicular to the light propagation vector, which is unconventional for XMCD measurements, as the light propagation vector typically lies parallel to the magnetic moments [6]. Later, based on group theory, Kuneš [16] derived a general relationship between the Hall vector and the orientation of the Néel vector in altermagnets under the free valence spin (FVS) approximation. It was found that XMCD may be present within the FVS approximation, may emerge only when the multipolar core-valence exchange terms and valence SOC are included, or may be fully forbidden, depending on the system symmetry.

Out of the many possible altermagnets which can be straightforwardly identified by spin group theory [19], hematite α -Fe₂O₃ is of particular interest; it experiences the Morin transition at $T_M \approx 250$ K [20], below which it demonstrates an easy-axis phase, while at high temperature it

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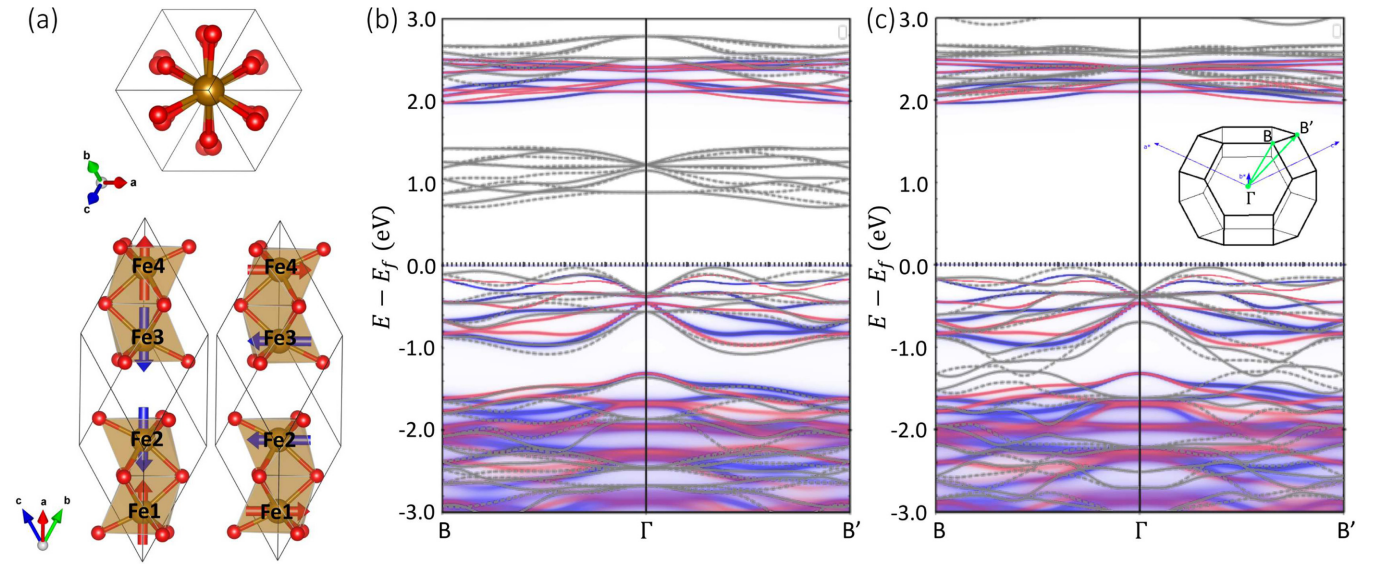


FIG. 1. (a) Top view (top panel) and view along the [001] direction (in Cartesian coordinates; bottom panel) of the primitive cell of α -Fe₂O₃. The directions of the magnetic moment below (bottom left) and above (bottom right) the Morin transition are illustrated, corresponding to Néel vectors along the [001] and [010] directions, respectively. (b) Band structure calculated using the DFT + DMFT method at 116 K (red and blue contours represent spin-up and spin-down channels, respectively) and the DFT method (gray lines, with the solid and dashed line representing spin-up and spin-down channels, respectively). (c) The same DFT + DMFT calculated band structure as in (b), but compared to the DFT + U results. The inset marks the selected k path in the Brillouin zone.

hosts an easy-plane phase with a weak ferromagnetic moment arising from the Dzyaloshinskii-Moriya interaction [11,21]. In addition, the high-temperature weak ferromagnetic phase is stable up to the Néel temperature $T_N \approx 955$ K [20]. Recently, α -Fe₂O₃ was also identified as a g -wave altermagnet [22] which shows spin (chirality) splitting in the electronic (magnon) band structure [23,24]. These magnetic properties make hematite a promising candidate for spintronic applications [25–27].

The Morin transition of α -Fe₂O₃ makes it well suited for studying the symmetry dependence of the XMCD response and for differentiating altermagnetism from weak ferromagnetism. In this work, we carry out *ab initio* calculations to investigate the electronic structure and XMCD of α -Fe₂O₃; the former is obtained using the self-consistent density functional theory plus dynamical mean-field theory (DFT + DMFT) approach, and the latter is obtained by constructing and solving the multiplet ligand-field model [28], as summarized in Sec. II B. We find that the nonrelativistic spin splitting is quite robust against electron-electron interaction at finite temperature. Detailed symmetry analysis is conducted for XMCD, and the different features of XMCD originating from altermagnetism and weak ferromagnetism are demonstrated.

II. METHODOLOGY

A. Band structure

The band structure of α -Fe₂O₃ was calculated using DFT + DMFT in a charge self-consistent manner [29,30], in which nominal double counting was adopted [30]. The continuous-time quantum Monte Carlo method was utilized to solve the quantum impurity problem [31] with 600 million Monte Carlo steps. The charge density of the system at each

self-consistent loop was converged to an accuracy of 10^{-5} . The Coulomb interaction U and Hund's coupling J were set to 7.0 and 0.8 eV, respectively, with the Coulomb repulsion described by the density-density form. For comparison, the band structures were also calculated using the primitive cell of α -Fe₂O₃ based on DFT and DFT + U approaches, as implemented in the Vienna *ab initio* Simulation Package (VASP) [32]. An energy cutoff of 520 eV and a k mesh of $10 \times 10 \times 10$ were adopted, with the energy convergence criterion being 10^{-8} eV. In terms of the DFT + U calculation, the method introduced by Dudarev *et al.* [33] was used with $U = 3.5$ eV. We will show later that this value of U gives a band gap similar to that obtained with the DFT + DMFT calculations.

B. XMCD

The XMCD spectra of α -Fe₂O₃ were obtained using DFT combined with multiplet ligand-field theory (DFT + MLFT) [28]. After self-consistent DFT calculations using the full-potential local-orbital (FPLO) package [34,35] with a k mesh of $30 \times 30 \times 30$, the symmetry-conserving maximally projected Wannier functions [36] were constructed for Fe 3d and O 2p orbitals. The constructed Wannier functions well represent the band structure obtained directly from DFT (see Appendix A, Fig. 6). It should be noted that for the Fe1 site [see Fig. 1(a)], the local axes in Cartesian coordinates a' ([100]), b' ([010]), and c' ([001]) are adopted for Wannier function construction. Following the symmetry relation, e.g., for the Fe2 site, which is related to the Fe1 site by a C_{2y} rotation followed by a half translation along the crystallographic c axis (hexagonal setting) of the conventional α -Fe₂O₃ cell, the local axes of the Fe2 site are $-a'$, b' , and $-c'$. The Fe3 and Fe4 sites are connected to the Fe2 and Fe1 sites, respectively, through the

inversion relation. Correspondingly, the local axes of Fe3 and Fe4 are kept the same as those of Fe2 and Fe1, respectively.

The tight-binding model representing the DFT Hamiltonian was set up considering a cluster with a radius of around 2.2 Å. The Slater integrals were computed from DFT radial wave functions and are listed in Table II in Appendix A. Additionally, in the MLFT calculations, the double-counting term was carefully corrected as demonstrated in Ref. [28]. In this regard, we constructed an atomic Hamiltonian which also addresses the ligand-metal charge transfer effect,

$$H_{\text{CTM}} = H_U^{dd} + H_U^{pd} + H_{l,s}^d + H_{l,s}^p + H_o^d + H_o^p + H_o^L + H_{\text{hyb}}^{dL} + H_{\text{ex}}, \quad (1)$$

where H_U^{dd} and H_U^{pd} denote the Coulomb interactions between the 3d electrons of Fe and the Fe 2p and 3d electrons, respectively. $H_{l,s}^d$ and $H_{l,s}^p$ represent the SOC term for the Fe 3d and 2p orbitals. The on-site Hamiltonians corresponding to Fe 3d and 2p and ligand orbitals are denoted by H_o^d , H_o^p , and H_o^L , respectively. H_{hyb}^{dL} defines the hybridization interaction between Fe 3d and the ligand orbitals, and H_{ex} is the Weiss magnetic field acting on Fe, which represents the magnetic order of the Fe atom.

For symmetry analysis, Eq. (1) is rewritten as

$$H_{\text{CTM}} = H_{\text{at}}^0 + H_{\text{at}}^1, \quad (2)$$

where H_{at}^1 defines only valence SOC and multipole core-valence (CV) exchange interactions terms,

$$H_{\text{at}}^1 = \sum_{i,j,k,l} W_{ijkl} \mathbf{d}_{i\sigma}^\dagger \mathbf{p}_{j\sigma'}^\dagger \mathbf{d}_{k\sigma'} \mathbf{p}_{l\sigma} + \sum_{m,m'} h_{m\sigma,m'\sigma'}^{(3d)} \mathbf{d}_{m\sigma}^\dagger \mathbf{d}_{m'\sigma'}. \quad (3)$$

The tensor W_{ijkl} contains the nonspherical part of the 2p – 3d Coulomb interaction, including the anisotropic direct term F_{pd}^2 and the exchange terms G_{pd}^1 and G_{pd}^3 . The remaining terms constitute H_{at}^0 ,

$$\begin{aligned} H_{\text{at}}^0 = & \sum_{i,j,k,l} U_{ijkl} \mathbf{d}_{i\sigma}^\dagger \mathbf{d}_{j\sigma'}^\dagger \mathbf{d}_{k\sigma} \mathbf{d}_{l\sigma} + U_{pd} \mathbf{n}_p \mathbf{n}_d \\ & + \sum_{m,m',\sigma,\sigma'} h_{m\sigma,m'\sigma'}^{(2p)} \mathbf{p}_{m\sigma}^\dagger \mathbf{p}_{m'\sigma'} + \sum_{m,m',\sigma} h_{mm'}^{(\text{CF})} \mathbf{d}_{m\sigma}^\dagger \mathbf{d}_{m'\sigma} \\ & + \sum_L \sum_{m,m',\sigma} h_{L,mm'}^{(\text{CF})} \mathbf{L}_{m\sigma}^\dagger \mathbf{L}_{m'\sigma} \\ & + \left(\sum_{m,m',\sigma} V_{mm'}^{(dL)} \mathbf{d}_{m\sigma}^\dagger \mathbf{L}_{m'\sigma} + \text{H.c.} \right) \\ & + \left(\sum_L \sum_{m,m',\sigma} V_{mm'}^{L,L+1} \mathbf{L}_{m\sigma}^\dagger \mathbf{L}_{m'\sigma} + \text{H.c.} \right) \\ & + b \sum_{m,\sigma} \mathbf{d}_{m\sigma}^\dagger \mathbf{d}_{m-\sigma}. \end{aligned} \quad (4)$$

In the calculation of XMCD, to account for in-plane weak ferromagnetism, the Weiss fields along the Néel vector and perpendicular to it were set to 0.1 and 10^{-4} eV, respectively. This setup yields spin moments of approximately $4.71 \mu_B$ and $0.004 \mu_B$ along the Néel vector and perpendicular to it,

respectively. In an experimental setup, applying external magnetic field, e.g., along the [100] direction, results in a Néel vector and weak ferromagnetic moment along the [010] and [100] directions, respectively. Note that when the Néel vector is oriented along the [001] direction, weak ferromagnetism is forbidden by symmetry and thus does not arise, as will be discussed in Sec. III B 1.

The spectroscopy was then calculated in accordance with Fermi's golden rule using the equation

$$G_{\pm}(\omega) = \langle \psi | T_{\pm}^\dagger \frac{1}{(\omega + i\Gamma/2 + E_i - H_{\text{CTM}})} T_{\pm} | \psi \rangle. \quad (5)$$

The difference between the responses brought by right (T_+) and left (T_-) circularly polarized light gives rise to the XMCD signal. Additionally, the Green's function that defines the calculated Fe $L_{2,3}$ conductivity tensor is given by Eq. (A6) in Appendix A. It should be noted that the element-specific XMCD of the crystal consists of contributions from all atoms. Unlike conventional collinear antiferromagnets, altermagnets can exhibit XMCD because their magnetic symmetry permits an axial vector response despite zero net magnetization [6].

III. RESULTS AND DISCUSSION

A. Altermagnetic splitting in electronic band structure

Hematite $\alpha\text{-Fe}_2\text{O}_3$ has space group $R\bar{3}c$ (No. 167) in the Hermann-Mauguin notation, which is centrosymmetric and has a rhombohedral primitive cell [see Fig. 1(a)]. The lattice parameters used in this work are $a = 5.19$ Å and $c = 13.77$ Å. The chiral splitting of magnons caused by altermagnetic ordering was predicted using Heisenberg exchange parameters evaluated by first-principles calculations [37]. Later a four-sublattice spin-wave theory was developed by Hoyer *et al.* considering the two different magnetic configurations undergoing the Morin transition and showed that SOC does not obscure the altermagnetic features [24]. As shown in Fig. 1(b), the altermagnetic splitting in the band structure can be captured by the DFT + DMFT calculation at around 116 K. A band gap of approximately 2.1 eV is derived, which aligns well with the reported values from experiment [38]. The bare DFT calculation underestimates the band gap, but the band characters, e.g., the valence bands below E_f , align reasonably well with the DFT + DMFT results. On the other hand, adding the Hubbard U correction results in a larger gap opening, giving rise to a band gap comparable to that derived from the DFT + DMFT results [see Fig. 1(c)]. However, the valence band features, e.g., the location of the valence band maximum and the band splittings, are also largely altered, which can be attributed to the many-body interactions considered in DMFT calculations.

The band structure demonstrated in Fig. 1 does not include the SOC effect. In order to examine whether the altermagnetic splitting remains intact, we further performed DFT + U + SOC calculations for the two magnetic configurations with Néel vectors $\hat{L}$ directed along the [001] and [010] directions. As can be seen from Fig. 7 in Appendix B, the inclusion of SOC has a negligible effect on the band structure, and the altermagnetic splitting exists for both $\hat{L} = [001]$

TABLE I. Sign variation of the components of $\mathbf{l}_3$ and $\mathbf{m}$ during transformation of group $\tilde{D}_{3d}^6$ in α -Fe₂O₃. The plus sign indicates that the element is included in the magnetic group, while the minus sign indicates the element must be multiplied by time inversion; elements with a 0 are not included in the magnetic group.

Vector component	E	Element of Symmetry								
		$2C_3 \pm 3C_2$	$U_2^1 2_y$	$U_2^2 2_{\perp}^{(2)}$	$U_2^3 2_{\perp}^{(3)}$	$\tilde{I}\tilde{I}$	$\tilde{\sigma}_d^1 c_y$	$\tilde{\sigma}_d^2 c_{\perp}^{(2)}$	$\tilde{\sigma}_d^3 c_{\perp}^{(3)}$	$2\tilde{S}_6 \pm \tilde{3}$
l_{3x}	+	0	+	0	0	+	+	0	0	0
l_{3y}	+	0	-	0	0	+	-	0	0	0
l_{3z}	+	+	+	+	+	+	+	+	+	+
m_x	+	0	-	0	0	+	-	0	0	0
m_y	+	0	+	0	0	+	+	0	0	0
m_z	+	+	-	-	-	+	-	-	-	+

and $\hat{L} = [010]$. In addition, we investigated the robustness of the altermagnetic splitting with respect to temperature. For $T = 116$ K, the local magnetic moment of Fe obtained from the DFT + DMFT calculation is around $4.42 \mu_B$, which agrees well with the neutron diffraction measurement ($\sim 4.16 \mu_B$) [39]. As demonstrated in Fig. 8 in Appendix B, at a higher temperature of about 1450 K, the altermagnetic splitting can still be observed, especially for those bands that are close to the Fermi level, while the bands below become more strongly smeared. It should be noted that it is known that the density-density form of the Coulomb interaction overestimates the magnetic transition temperature [40]. Therefore, the obtained local magnetic moment of Fe at $T = 1450$ K is only slightly reduced to $4.22 \mu_B$.

B. Altermagnetism and weak ferromagnetism

1. Symmetry analysis

Following the definition used by Dzyaloshinskii *et al.* [11,41] α -Fe₂O₃ belongs to the crystallographic space group $D_{3d}^6 = R\bar{3}c$. The representatives of the cosets $D_{3d}^6/\mathcal{T}$ then form the group $\tilde{D}_{3d}^6$, which has the following elements:

$$E, 2C_3, 3U_2, \tilde{I}, 3\tilde{\sigma}_d, 2\tilde{S}_6, \{1, \pm 3_z, 3(2_{\perp}), \tilde{I}, 3(c = \tilde{m}), \pm \tilde{3}_z\}. \quad (6)$$

Here, the $\tilde{\cdot}$ symbol means that a translation along the z axis through half the period of the crystal accompanies the corresponding symmetry operation. We follow the definition in Ref. [41] by denoting the magnetic moments located at the points of the Fe ion positions by μ_{α} , with $\alpha = 1, 2, 3, 4$, and the following linear combinations of μ_{α} form the irreducible representations of $\tilde{D}_{3d}^6$:

$$\begin{aligned} \mathbf{l}_1 &= \mu_1 + \mu_2 - \mu_3 - \mu_4, \\ \mathbf{l}_2 &= \mu_1 - \mu_2 + \mu_3 - \mu_4, \\ \mathbf{l}_3 &= \mu_1 - \mu_2 - \mu_3 + \mu_4, \\ \mathbf{m} &= \mu_1 + \mu_2 + \mu_3 + \mu_4, \end{aligned} \quad (7)$$

where $\mathbf{l}_3$ represents the magnetic configuration, as shown in Fig. 1(a). In the following analysis, we focus on vectors $\mathbf{l}_3$ and $\mathbf{m}$. Table 1.5.3.2 of Ref. [41] lists the sign variation of the components of magnetic vectors during transformations of group $\tilde{D}_{3d}^6$. Here, Table I gives a recap, with the slight modification of symmetry operation element 2_x being altered

to 2_y , following the definition of the basis vectors of α -Fe₂O₃ in FPLO.

In Table I, the plus sign indicates that the element is included in the magnetic group, while the minus sign indicates the element must be multiplied by time inversion. The elements that yield a 0 are not included in the magnetic group. Accordingly, when the magnetic moments are directed along the x , y , and z directions with vector $\mathbf{l}_3$ (with the corresponding magnetic structures denoted by A_{3x} , A_{3y} , and A_{3z}), the corresponding magnetic point groups are $2/m$, $2'/m'$, and $\bar{3}m$, respectively. For the ferromagnetic vector $\mathbf{m}$, the magnetic point groups are $2'/m'$, $2/m$, and $\bar{3}m'$ for the magnetic moments directed along x , y , and z , respectively (with corresponding magnetic structures denoted by F_x , F_y , and F_z). That is, the antiferromagnetic structure A_{3x} (A_{3y}) and ferromagnetic structure F_y (F_x) have the same magnetic point group. From a symmetry standpoint, the crystal structure permits the coexistence of antiferromagnetic and ferromagnetic components, thereby accounting for the weak ferromagnetism observed in α -Fe₂O₃ above the Morin transition temperature, where the magnetic moments lie within the basal plane.

Inspired by the XMCD distinction between altermagnetism and weak ferromagnetism reported in α -MnTe [6], we apply a similar analysis to α -Fe₂O₃, additionally focusing on the spectroscopic variation below and above the Morin transition temperature. Below the Morin transition temperature, the Néel vector is along the z direction ($\hat{L} \parallel [001]$) with magnetic point group $\bar{3}m$. Following the symmetry-adapted form of tensor properties for $\bar{3}m$, the table of tensor components has the following form:

$$\begin{bmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix}. \quad (8)$$

The mirror planes containing the z axis forbid any off-diagonal (Hall-type) components in the conductivity tensor. As demonstrated in Fig. 2(a), the off-diagonal terms of the x-ray absorption spectroscopy (XAS) conductivity tensor are zero, and the diagonal components exhibit $\sigma_{xx} = \sigma_{yy} \neq \sigma_{zz}$. We emphasize that the spectra reported in this work are normalized to the contributions from the four Fe atoms in the primitive cell, which is allowed by the local nature of the core-level excitations [42]. The symmetry analysis for magnetic point group $\bar{3}m$ indicates that no XMCD signal exists when the Néel vector is along the $[001]$ direction. However, the

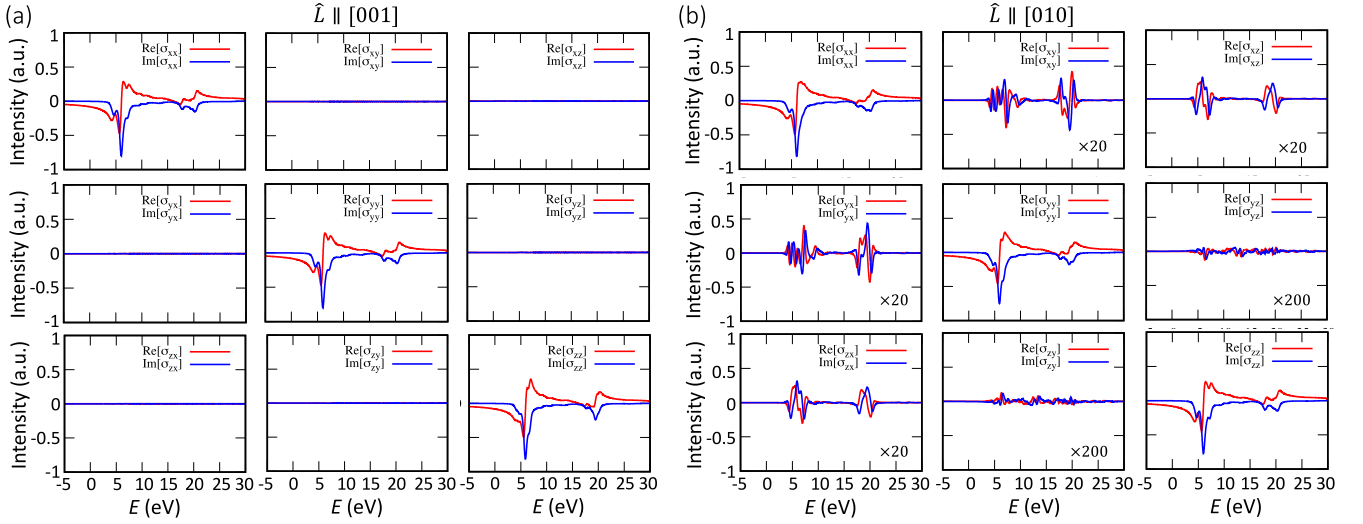


FIG. 2. X-ray absorption spectroscopy of the Fe $L_{2,3}$ edge in the form of a conductivity tensor for Néel vectors (a) $\hat{L} \parallel [001]$ and (b) $\hat{L} \parallel [010]$. The red and blue curves represent the real and imaginary parts, respectively.

x-ray linearized dichroism (XLD) persists because of the intrinsic uniaxial anisotropy, as indicated by Eq. (8) (see Fig. 3). Additionally, Fig. 3(b) shows the calculated XAS when $\hat{L} \parallel [001]$ with x-ray polarization perpendicular and parallel to the $[001]$ direction, in good agreement with experimental measurements [43].

Above the Morin transition temperature, the Néel vector switches its direction towards $[010]$, with the magnetic point group belonging to $2'/m'$. The corresponding symmetry-adapted tensor has the form

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ -\sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & -\sigma_{yz} & \sigma_{zz} \end{bmatrix}. \quad (9)$$

The calculated tensor form of XAS for $\hat{L} \parallel [010]$, as shown in Fig. 2(b), coincides well with the form described by Eq. (9). There are six independent components: σ_{xx} , σ_{yy} , σ_{zz} , σ_{xy} , σ_{xz} , and σ_{yz} . The conductivity tensor contains the antisymmetric part, i.e., $\sigma_{yx} = -\sigma_{xy}$ and $\sigma_{zy} = -\sigma_{yz}$. This indicates that for $\hat{L} \parallel [010]$, when the x-ray propagation vector $\hat{k}$ is along the z or x direction, the XMCD response should be expected. In addition, the XLD signal is also present, and the spin reorientation across the Morin transition causes a sign reversal of the dichroic signal [see Fig. 3(a)], as also observed experimentally in Refs. [43,44].

2. XMCD

As indicated by the symmetry analysis in Sec. III B 1 and as demonstrated in Figs. 4(a) and 4(b), with $\hat{L} \parallel [010]$, XMCD responses are present for the x-ray propagation vectors $\hat{k}$ along the $[001]$ and $[100]$ directions. However, the XMCD response is rather weak for $\hat{k} \parallel [100]$. Note that in these two cases, the x-ray propagation vector is perpendicular to the direction of the spin moment, which is not a common application for XMCD measurements in ferromagnets. Subsequently, with the setup $\hat{L} \parallel [010]$ and $\hat{k} \parallel [001]$, the atom-resolved XMCD spectra are shown in Fig. 4(c). For clarity we show only the contributions from the Fe1 and Fe2 atoms because as an inversion pair of Fe1 and Fe2, Fe4 and Fe3 have the same crystal

fields as Fe1 and Fe2, respectively. Therefore, the XMCD spectra from Fe1 and Fe4 (Fe2 and Fe3) are identical.

The top panel of Fig. 4(c) shows that for $\hat{k} \parallel [001]$ with $\hat{L} \parallel [010]$, Fe1 and Fe2 contribute equally to the XMCD. In contrast, when $\hat{k}$ is aligned in the same direction as $\hat{L} \parallel [010]$, the XMCD components contributed by antiparallel spin moments of Fe1 and Fe2 should cancel out [see Fig. 4(d)]. Moreover, due to the presence of spin canting, in practice, for $\hat{L} \parallel [010]$, weak ferromagnetic moment exists along the $[100]$ direction. In other words, the XMCD spectroscopy displayed in Fig. 4(b) should be a combination of altermagnetism and ferromagnetism. To further validate this argument, we examine the case of $\hat{k} \parallel [100]$ in greater detail. In specific, XMCD simulations were performed with the weak ferromagnetic component removed to separate the contributions from altermagnetism and weak ferromagnetism. As shown in Fig. 10 in Appendix C, the XMCD response persists via the removal of the weak ferromagnetic contribution. The difference between the two XMCD spectra, with and without the weak ferromagnetic component, thus yields the XMCD response arising solely from weak ferromagnetism, whose line shape resembles that of Fe1 shown in Fig. 4(d). Furthermore, for α -Fe₂O₃ the XMCD response is strongly dependent on the direction of $\hat{L}$. For instance, as demonstrated in Fig. 2(a) and Fig. 11 in Appendix C, for $\hat{L} \parallel [001]$ and $\hat{L} \parallel [100]$, which correspond to magnetic point group $\bar{3}m$ and $2/m$ respectively, the XMCD signals are either totally forbidden by symmetry or negligible.

We also emphasize that the conductivity tensor, e.g., the one shown in Eq. (9), represents a bulk property. Taking the antisymmetric component σ_{xy} in Eq. (9) as an example, we further decompose σ_{xy} into site-resolved contributions. Interestingly, we find that the site-resolved σ_{xy}^i (with i denoting the site index) contains both symmetry [$S_{xy}^i = \frac{1}{2}(\sigma_{xy}^i + \sigma_{yx}^i)$] and antisymmetry [$A_{xy}^i = \frac{1}{2}(\sigma_{xy}^i - \sigma_{yx}^i)$] contributions. That is, although the bulk symmetry suppresses the symmetry part of σ_{xy} , locally, it is allowed and finite. Since Fe2 is connected to Fe1 by the $C_{2y}t_{1/2}$ symmetry operation, $S_{xy}^1 = -S_{xy}^2$, and $A_{xy}^1 = A_{xy}^2$. This statement is also valid for σ_{yz} . In terms of σ_{xz} ,

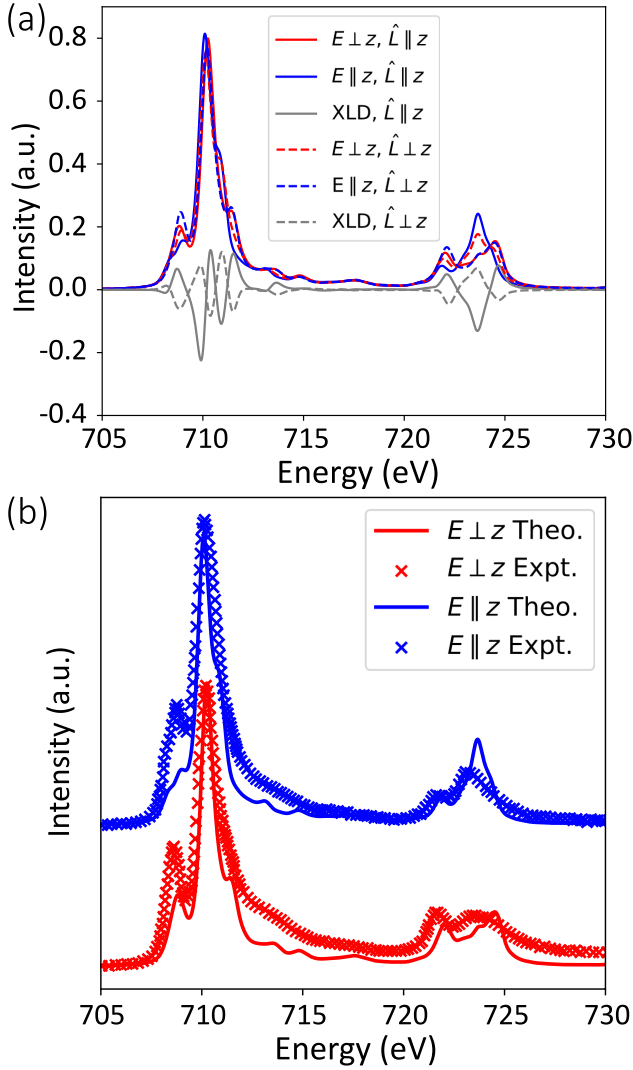


FIG. 3. (a) Fe 2p XAS of $\alpha\text{-Fe}_2\text{O}_3$ for Néel vector $\hat{L}$ along z with x-ray polarization perpendicular and parallel to $\hat{L}$. (b) X-ray linearized dichroism for $\hat{L}$ perpendicular and parallel to z .

which shows symmetric behavior ($S_{xz}^1 = S_{xz}^2$), its site-resolved antisymmetric component A_{xz}^i has a quite large magnitude although A_{xz}^1 and A_{xz}^2 cancel out when being summed up for the bulk system (see Fig. 12 in Appendix D). Consequently, a small symmetry-breaking perturbation can instantly release those locally present but globally canceled contributions.

3. Discussion

We performed a more detailed analysis of the obtained single-site XMCD spectrum for $\hat{L} \perp \hat{k}$ to inspect the origin of the XMCD response. Hariki *et al.* showed that for altermagnetic $\alpha\text{-MnTe}$ the valence SOC has a negligible effect on its XMCD, whereas the XMCD response disappears when a combination of core SOC and multipole CV exchange interactions are absent [6]. Nevertheless, this observation is system dependent based on the specific symmetry in the crystal [16]. For instance, in altermagnetic MnF_2 , the XMCD is still present even if the core SOC and CV terms are excluded [17].

In the present work, we provide a symmetry analysis of the Hamiltonian in Eq. (1) for $\alpha\text{-Fe}_2\text{O}_3$ following the argument in Ref. [6].

First, we show in Fig. 5 the single-site XMCD of Fe1 in $\alpha\text{-Fe}_2\text{O}_3$ with $\hat{k} \perp \hat{L}$ ($\hat{k} \parallel [001]$, $\hat{L} \parallel [010]$). If we manually eliminate the valence SOC term in H_{CTM} , the XMCD response is only slightly modified. In contrast, if the core-valence Coulomb interaction terms beyond monopole are removed, the remaining XMCD signal becomes very tiny. Finally, when both valence SOC and CV terms are removed, the XMCD response almost disappears.

This observation can be properly rationalized from the perspective of symmetry. As expressed in Eq. (5), the spectrum object can be equivalently written as

$$F_{\pm}(\omega) = \sum_f |\langle f | T_{\pm} | i \rangle|^2 \delta[\omega - (E_f - E_i)], \quad (10)$$

with the transition operator for obtaining XMCD defined by

$$T_{\pm} \equiv \sum_{\sigma} T_{\pm}^{\sigma} = \sum_{m,\sigma} \Gamma_{\pm m} d_{m\pm 1\sigma}^{\dagger} p_{m\sigma} + \text{H.c.}, \quad (11)$$

describing the absorption of circularly polarized light propagating along the z axis ($\hat{k} \parallel [001]$). Here, $d_{m\pm 1\sigma}^{\dagger}$ ($p_{m\sigma}$) create an electron (a hole) in the valence (core) orbital with angular momentum projection $m \pm 1$ (m) and spin projection σ . The square of the matrix element in Eq. (11) is then

$$|\langle T_{\pm} \rangle|^2 = \sum_{\sigma} |\langle T_{\pm}^{\sigma} \rangle|^2 + \sum_{\sigma} \langle T_{\pm}^{\sigma} \rangle \overline{\langle T_{\pm}^{-\sigma} \rangle}. \quad (12)$$

It has been shown for $\alpha\text{-MnTe}$ that the symmetry operation C_3 commutes with the Hamiltonian that omits the valence SOC and CV terms. In this case, the second term in Eq. (12) drops out, considering the C_3 transformation acts only on the valence orbital indices and both core spin and orbital indices [6]. Together with the vanishing cross terms in Eq. (12), the antiunitary symmetry $\mathcal{T}' \equiv \mathcal{T} C_2^{S,3d}$ (time reversal combined with rotation of the valence spin around an axis perpendicular to the ordered moments) leads to $F_+(\omega) = F_-(\omega)$ and hence zero XMCD in $\alpha\text{-MnTe}$ [6].

Similar to $\alpha\text{-MnTe}$, the $\alpha\text{-Fe}_2\text{O}_3$ crystal demonstrates C_{3z} symmetry (see Table I). Accordingly, in the angular momentum basis, the matrix elements of the crystal-field Hamiltonian $h_{mm'}^{(\text{CF})}$, which do not fulfill the relation $m - m' = 3k$, should be zero. The $h_{mm'}^{(\text{CF})}$ extracted from the FPLO calculation indeed verifies this symmetry relation [see Eq. (D1)]. Similarly, the crystal-field Hamiltonians for the ligands that are the same size as the $3d$ orbital $h_{L,mm'}^{(\text{CF})}$, as well as their hybridization terms, all follow the same symmetry since, in the applied MLFT, the Hamiltonian corresponding to the selected cluster is rotated using a unitary transformation so that the consequent representation defines a one-dimensional chain of interactions. In other words, the site ($3d$ orbital of Fe) under consideration interacts only with one ligand orbital directly, which in turn interacts with another ligand [45]. In addition, there is a term that is not explicitly visible in Eq. (4) but considered in DFT + MLFT calculations, i.e., the correction for the screening effect, which is applied by deducting the on-site energies of the Fe $2p$ and $3d$ and ligand orbitals obtained

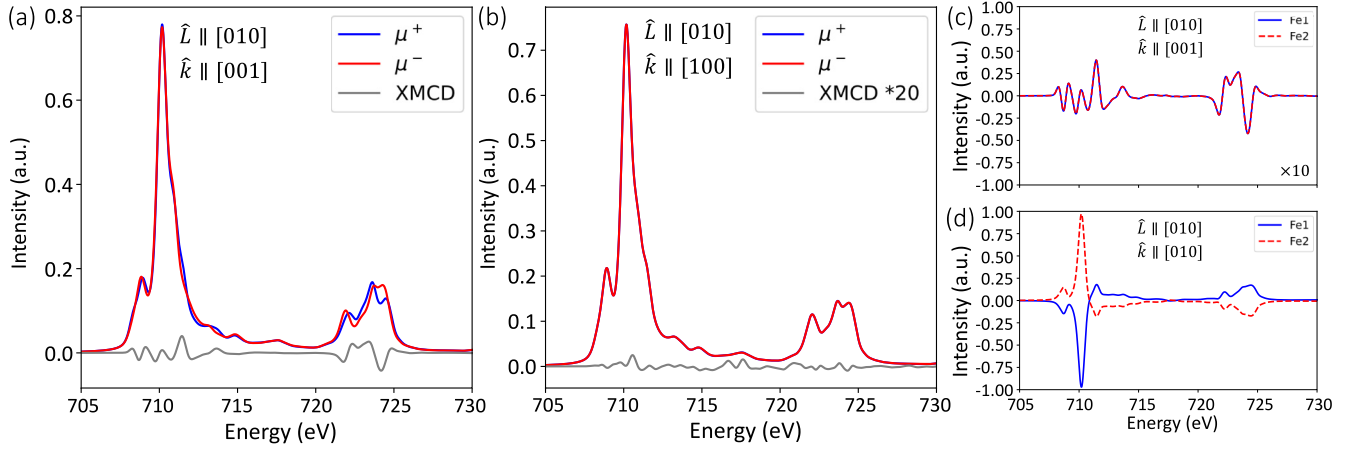


FIG. 4. Fe 2p XMCD spectra for $\hat{L} \parallel [010]$ when the x-ray propagation vector $\hat{k}$ is along the (a) [001] and (b) [100] directions. Separate contributions from Fe1 and Fe2 to XMCD with (c) $\hat{L} \parallel [010]$ and $\hat{k} \parallel [001]$ and (d) $\hat{L} \parallel [010]$ and $\hat{k} \parallel [010]$.

following the convention used in the work of Bocquet *et al.* [46].

We now consider the C_{3z} transformation in which only the orbital indices are transformed for the valence states, while both orbital and spin indices are transformed for the core states, following Ref. [6]. The commute relation between C_{3z}

transformation and H_{at}^0 is mostly recovered, as indicated by the vanishing XMCD intensity (pink line) in Fig. 5(a). However, it is not fully recovered because, with the DFT + MLFT method employed in this work, the rotated cluster Hamiltonian with the form of one-dimensional chain interactions gives not only ligand orbitals with the same size and symmetry as the 3d orbital but also ligand orbitals the size of the s orbital.

Next, we validate the theoretical results by comparing them with experiment. In the case of α -MnTe [6], the shapes of the calculated and measured XMCD spectra agree rather well, while the measured XMCD intensity is about 1 order of magnitude smaller than the calculated result. This reduction is attributed to the presence of magnetic domains with Néel vectors pointing along multiple easy-axis directions. A similar consideration applies to α -Fe₂O₃. Notably, we find that the calculated XMCD already agrees well with recent experimental measurements [47] in both line shape and intensity, even without the explicit inclusion of thermal effects since the XMCD response in altermagnetic α -Fe₂O₃ is symmetry allowed only above the Morin transition temperature. To further assess possible thermal effects, we performed XMCD simulations at $T = 250$ K by incorporating thermally populated excited states via Boltzmann weighting (see Appendix B, Fig. 9). At this temperature, the XMCD magnitude is largely reduced, indicating that in practice, the excited states should provide a marginal correction to the XMCD response.

IV. CONCLUSIONS

In conclusion, despite the different band features demonstrated by the DFT, DFT + U , and DFT + DMFT approaches, the characteristic spin splitting in altermagnetic α -Fe₂O₃ persists. Additionally, the spin splitting near the Fermi level is still very apparent and becomes only slightly smeared at high temperatures, as indicated by the finite-temperature DFT + DMFT calculations. Moreover, the spin splitting was found to be insensitive to the spin orientation with SOC included. Below the Morin transition temperature, the Néel vector is along the [001] direction, and the crystal belongs to the $\bar{3}m$ magnetic point group. For this configuration, only diagonal

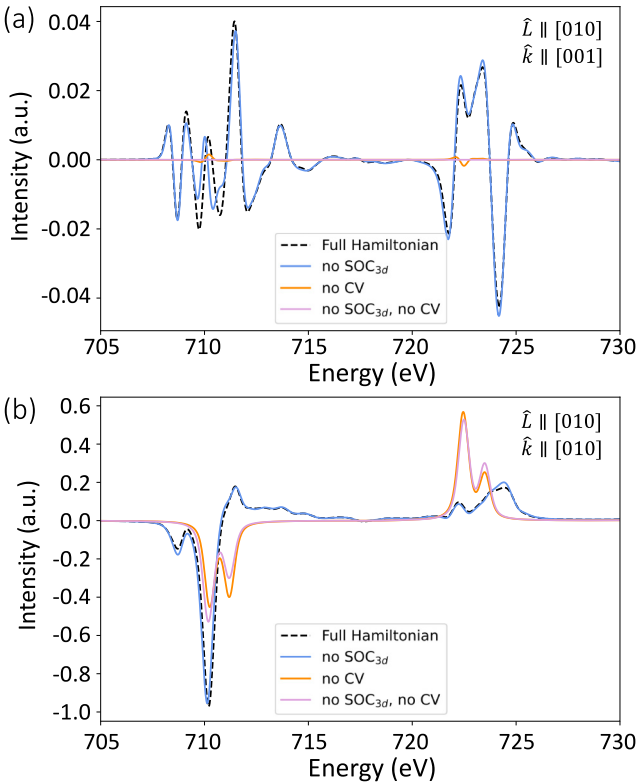


FIG. 5. The single-site Fe1 2p XMCD spectra for $\hat{L} \parallel [010]$ with the x-ray propagation vector (a) $\hat{k} \parallel [001]$ and (b) $\hat{k} \parallel [010]$. In each panel, the calculated XMCD spectra are also shown for three reduced cases: with the SOC of the 3d valence states switched off, with the core-valence (CV) interactions restricted to the monopole term only, and with both contributions simultaneously removed.

terms of the conductivity tensors are allowed: $\sigma_{xx} = \sigma_{yy} \neq \sigma_{zz}$. In this regard, XLD is present, and the calculated XLD agrees well with the experimental measurements. On the other hand, the XMCD response is allowed only above the Morin transition temperature when the Néel vector is along the [010] direction, which corresponds to magnetic point group $2'/m'$. Interestingly, we found that the site-resolved contributions to the off-diagonal terms in the conductivity tensor for the $\hat{L} = [010]$ configuration involve both symmetric and anti-symmetric components, although the specific tensor form is restricted by the magnetic point group as a whole. This observation indicates that a small symmetry-breaking perturbation is able to instantly release those locally present but globally canceled terms, which is an intriguing property that can be exploited via, e.g., doping.

We would like to emphasize that the *ab initio* DFT + MLFT approach adopted in this work is an effective and reliable tool to simulate XMCD spectroscopy. Nevertheless, when performing a symmetry analysis, one should pay extra attention to the hybridization terms between the valence orbitals of the transition metal (TM) and its ligands. Specifically, the hybridization terms within the considered TM-centered clusters might include ligands that do not possess the same symmetry as the TM site after unitary transformation. Through symmetry analysis, we demonstrated that the valence spin-orbit coupling plays a negligible role in the XMCD response of α -Fe₂O₃, establishing XMCD as a promising probe of altermagnetism that does not rely on relativistic effects and therefore avoids ambiguities related to weak ferromagnetism. Furthermore, the distinct XMCD spectral line shapes for light propagation vectors parallel and perpendicular to the Néel vector provide a clear means to disentangle altermagnetic contributions from weak ferromagnetic ones. While the inclusion of temperature effects in the XMCD simulations is expected to reduce the overall signal intensity, our results nevertheless offer clear guidance on experimental conditions under which the altermagnetism-induced XMCD response can be identified.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: COMPUTATIONAL DETAILS

1. Conductivity tensor

Under dipole approximation, the interaction term between light and an electron is given by $\varepsilon \cdot \hat{r}$, with ε being the polarization of the light and $\hat{r}$ being a unit vector. In quantum the operator $\hat{r}$ can be expanded using renormalized spherical harmonics C_k^m :

$$\varepsilon \cdot \hat{r} = (\varepsilon_x + i\varepsilon_y)C_1^{-1} + \varepsilon_z C_1^0 + (-\varepsilon_x + i\varepsilon_y)C_1^1. \quad (\text{A1})$$

Accordingly, the transition operators for light polarized along the x , y , and z directions can be defined as

$$T_x = \frac{\sqrt{2}}{2}(C_1^{-1} - C_1^1), \quad (\text{A2})$$

$$T_y = \frac{\sqrt{2}}{2}i(C_1^{-1} + C_1^1), \quad (\text{A3})$$

$$T_z = C_1^0. \quad (\text{A4})$$

Equivalently, one can write Eq. (A1) as

$$\varepsilon \cdot \hat{r} = \sum_{\alpha=x,y,z} \varepsilon_\alpha T_\alpha. \quad (\text{A5})$$

With the definition in Eq. (A5), the calculated spectrum can be written as a rank-2 tensor:

$$G_{\alpha\beta}(\omega) = \sum_{\alpha,\beta} \varepsilon_\alpha^* \varepsilon_\beta \langle \psi | T_\alpha^\dagger \frac{1}{\omega + i\Gamma/2 + E_i - H_{CTM}} T_\beta | \psi \rangle. \quad (\text{A6})$$

2. Electronic structures derived from Wannier orbitals

As shown in Fig. 6, the Wannierization process in FPLO was performed with an energy window of $[-8, 3]$ eV, in which the Fe 3d and O 2p orbitals are included for constructing the Wannier functions. The obtained band structure from Wannier functions agrees well with that directly calculated with DFT, thus validating the accuracy of using Wannier functions to further construct the tight-binding model. In addition, the specific values of the atomic Slater integral which are derived from the radial functions generated by FPLO are listed in Table II.

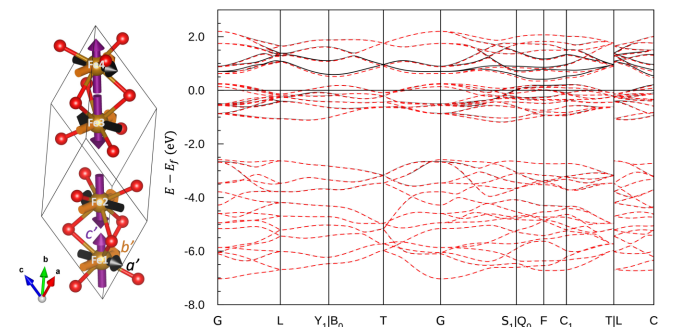


FIG. 6. Band structures of α -Fe₂O₃ calculated using FPLO with DFT (black solid line) and Wannier functions (red dash lines). Here, a' , b' , and c' define the local coordination axes (in Cartesian coordinates) of Fe atoms.

TABLE II. The atomic Slater integral values derived from DFT radial functions.

	F_2^{dd}	F_4^{dd}	F_2^{pd}	G_1^{pd}	G_3^{pd}
Value (eV)	10.42	6.44	5.96	4.35	2.47

APPENDIX B: SOC AND TEMPERATURE EFFECTS

The band structures of α -Fe₂O₃ with Néel vectors along the [001] and [010] directions are calculated using vasp in the regime of DFT + U + SOC (Fig. 7). By projecting the spin angular momentum to the corresponding quantization axis, we find that the characteristic spin splitting in altermagnetic α -Fe₂O₃ persists with the inclusion of SOC or with different spin orientations in the presence of SOC.

The band structure obtained using the DFT + DMFT method at the higher temperature $T = 1450$ K is shown in Fig. 8 and was discussed in Sec. III A. Figure 9 demonstrates that if the temperature effect is included in MLFT simulation by taking excited states into account, the XMCD response intensity is diminished.

APPENDIX C: XMCD: ALTERMAGNETISM AND WEAK FERROMAGNETISM

Figure 10 demonstrates the contributions from altermagnetism and weak ferromagnetism separately. It explicitly shows that in α -Fe₂O₃ the altermagnetic effect introduces finite XMCD responses after excluding the weak ferromagnetism. Figure 11 displays the XAS of Fe $L_{2,3}$ edge in the form of conductivity tensor for Néel vector $\hat{L} \parallel [100]$. As a matter of fact, for magnetic point group $2/m$ with $\hat{L} \parallel [100]$, σ_{xz} and σ_{zx} are two independent tensors. Nevertheless, their magnitudes are almost identical as shown in Fig. 11, which leads to a negligible antisymmetric contribution that can give observable XMCD responses.

APPENDIX D: ADDITIONAL SYMMETRY RELATIONS

The demonstration of the site-resolved antisymmetric part A_{xz}^i ($i = 1, 2$ for atomic sites Fe1 and Fe2) in Fig. 12 supports

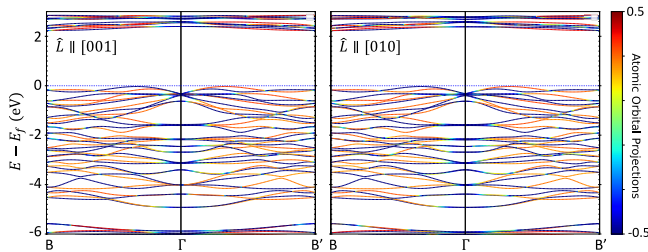


FIG. 7. Band structures of α -Fe₂O₃ calculated using DFT + U + SOC for Néel vectors along the [001] (left panel) and [010] (right panel) directions. The color code indicates the projected spin momentum along the directions of the Néel vectors.

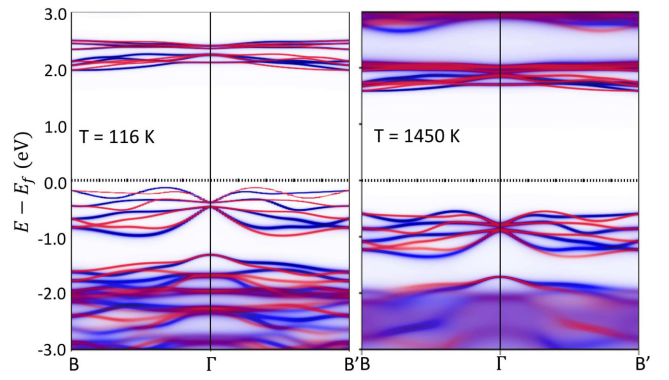


FIG. 8. Band structures of α -Fe₂O₃ calculated using DFT + DMFT at $T = 116$ K (left panel) and $T = 1450$ K (right panel).

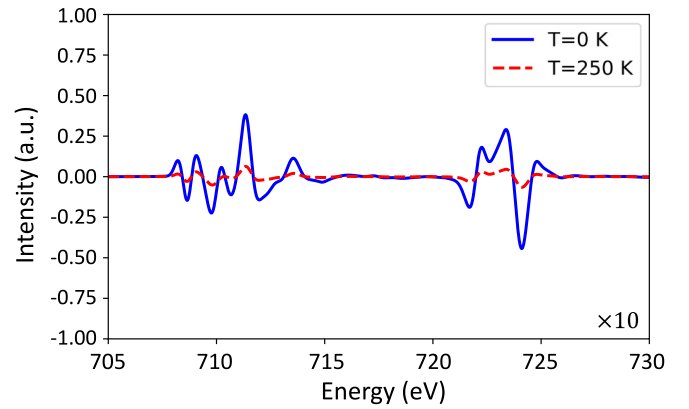


FIG. 9. The XMCD spectra with $\hat{L} \parallel [010]$ and $\hat{k} \parallel [001]$ at $T = 0$ K and $T = 250$ K.

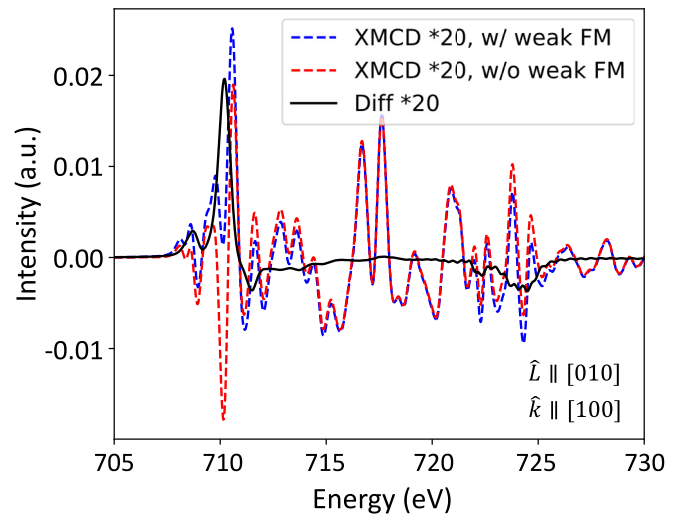


FIG. 10. The total XMCD responses for $\hat{L} \parallel [010]$ and $\hat{k} \parallel [100]$ in two different configurations with (blue dashed line) and without (red dashed line) the weak ferromagnetic component. The difference between the two calculated XMCD spectra is shown by the black solid line.

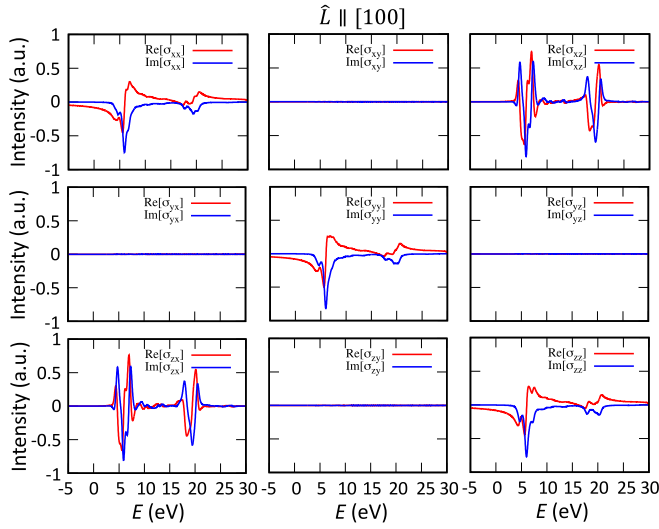


FIG. 11. X-ray absorption spectroscopy of the Fe $L_{2,3}$ edge in the form of the conductivity tensor for Néel vector $\hat{L} \parallel [100]$.

the argument in Sec. III B 2 that although the bulk symmetry forbids the manifestation of the antisymmetric contribution ($\sigma_{xz} = \sigma_{zx}$), intrinsically, the site-resolved contribution is not

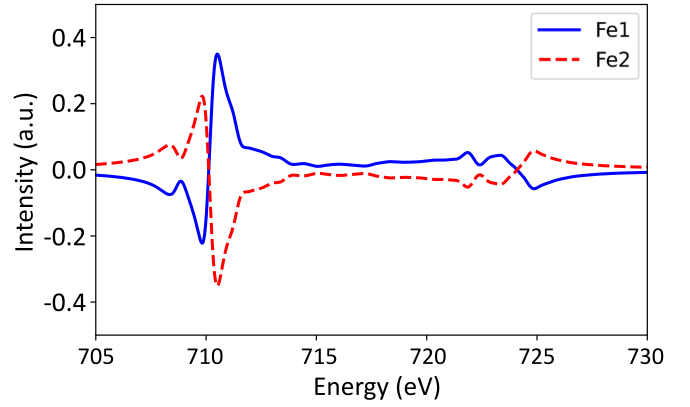


FIG. 12. The site-resolved antisymmetric part A^i_{xz} ($i = 1, 2$) for atomic sites Fe1 and Fe2 for $\hat{k} \parallel [001]$ with $\hat{L} \parallel [010]$.

zero and can manifest if a symmetry-breaking perturbation is introduced.

The specific form of $h_{mm'}^{CF}$ can be extracted from the Wannier functions constructed in FPLO. However, it is originally expressed in the real basis [Eq. (D1)], and one needs to apply a basis transformation from real to the angular momentum basis:

$$h_{mm'}^{CF} = \begin{pmatrix} -0.65 & 0 & 0 & 0.01 + 0.11i & 0 \\ 0 & -0.62 & 0 & 0 & -0.01 - 0.11i \\ 0 & 0 & 0 & -0.78 & 0 \\ 0.01 - 0.11i & 0 & 0 & 0 & -0.62 \\ 0 & -0.01 + 0.11i & 0 & 0 & -0.65 \end{pmatrix}. \quad (D1)$$

- [1] L. Šmejkal, R. González-Hernández, T. Jungwirth, and J. Sinova, Crystal time-reversal symmetry breaking and spontaneous Hall effect in collinear antiferromagnets, *Sci. Adv.* **6**, eaaz8809 (2020).
- [2] L. Šmejkal, A. H. MacDonald, J. Sinova, S. Nakatsuji, and T. Jungwirth, Anomalous Hall antiferromagnets, *Nat. Rev. Mater.* **7**, 482 (2022).
- [3] R. D. Gonzalez Betancourt, J. Zubáč, R. Gonzalez-Hernandez, K. Geishendorf, Z. Šobáň, G. Springholz, K. Olejník, L. Šmejkal, J. Sinova, T. Jungwirth, *et al.*, Spontaneous anomalous Hall effect arising from an unconventional compensated magnetic phase in a semiconductor, *Phys. Rev. Lett.* **130**, 036702 (2023).
- [4] M. Naka, Y. Motome, and H. Seo, Anomalous Hall effect in antiferromagnetic perovskites, *Phys. Rev. B* **106**, 195149 (2022).
- [5] K. Samanta, M. Ležaić, M. Merte, F. Freimuth, S. Blügel, and Y. Mokrousov, Crystal Hall and crystal magneto-optical effect in thin films of SrRuO₃, *J. Appl. Phys.* **127**, 213904 (2020).
- [6] A. Hariki, A. Dal Din, O. Amin, T. Yamaguchi, A. Badura, D. Kriegner, K. W. Edmonds, R. P. Campion, P. Wadley, D. Backes, *et al.*, X-ray magnetic circular dichroism in altermagnetic α -MnTe, *Phys. Rev. Lett.* **132**, 176701 (2024).
- [7] A. Hariki, Y. Takahashi, and J. Kuneš, X-ray magnetic circular dichroism in RuO₂, *Phys. Rev. B* **109**, 094413 (2024).
- [8] N. Sasabe, M. Mizumaki, T. Uozumi, and Y. Yamasaki, Ferroc order for anisotropic magnetic dipole term in collinear antiferromagnets of $(t_2g)^4$ system, *Phys. Rev. Lett.* **131**, 216501 (2023).
- [9] M. Hu, O. Janson, C. Felser, P. McClarty, J. van den Brink, and M. G. Vergniory, Spin Hall and Edelstein effects in chiral non-collinear altermagnets, *Nat. Commun.* **16**, 8529 (2025).
- [10] H. Watanabe, K. Shinohara, T. Nomoto, A. Togo, and R. Arita, Symmetry analysis with spin crystallographic groups: Disentangling effects free of spin-orbit coupling in emergent electromagnetism, *Phys. Rev. B* **109**, 094438 (2024).
- [11] I. Dzyaloshinsky, A thermodynamic theory of “weak” ferromagnetism of antiferromagnetics, *J. Phys. Chem. Solids* **4**, 241 (1958).
- [12] I. E. Dzialoshinskii, The problem of piezomagnetism, *J. Exptl. Theoret. Phys.* **33**, 807 (1958) [*Sov. Phys. JETP* **6**, 621 (1958)].
- [13] I. Dzyaloshinskii, On the magneto-electrical effect in antiferromagnets, *J. Exptl. Theoret. Phys.* **37**, 881 (1959) [*Sov. Phys. JETP* **37**, 628 (1959)].
- [14] E. Turov, *Kinetic, Optical, and Acoustic Properties of Antiferromagnets* (Izd. Ural. Otd. Akad. Nauk, Sverdlovsk, USSR, 1990).
- [15] I. Solovyev, Hidden ferromagnetism of centrosymmetric antiferromagnets, *arXiv:2509.00369*.

- [16] J. Kuneš, Néel vector dependence of x-ray magnetic circular dichroism in altermagnets, *Phys. Rev. B* **112**, 184415 (2025).
- [17] A. Hariki, T. Okauchi, Y. Takahashi, and J. Kuneš, Determination of the Néel vector in rutile altermagnets through x-ray magnetic circular dichroism: The case of MnF_2 , *Phys. Rev. B* **110**, L100402 (2024).
- [18] A. Hariki, K. Sakurai, T. Okauchi, and J. Kuneš, Separating altermagnetic and ferromagnetic effects in x-ray magnetic dichroism of rutile NiF_2 , *npj Quantum Mater.* **10**, 49 (2025).
- [19] X. Wan, S. Mandal, Y. Guo, and K. Haule, High-throughput search for metallic altermagnets by embedded dynamical mean field theory, *Phys. Rev. Lett.* **135**, 106501 (2025).
- [20] F. Morin, Magnetic susceptibility of $\alpha\text{-Fe}_2\text{O}_3$ and $\alpha\text{-Fe}_2\text{O}_3$ with added titanium, *Phys. Rev.* **78**, 819 (1950).
- [21] T. Moriya, Anisotropic superexchange interaction and weak ferromagnetism, *Phys. Rev.* **120**, 91 (1960).
- [22] L. Šmejkal, J. Sinova, and T. Jungwirth, Beyond conventional ferromagnetism and antiferromagnetism: A phase with nonrelativistic spin and crystal rotation symmetry, *Phys. Rev. X* **12**, 031042 (2022).
- [23] X. Chen, Y. Liu, P. Liu, Y. Yu, J. Ren, J. Li, A. Zhang, and Q. Liu, Unconventional magnons in collinear magnets dictated by spin space groups, *Nature (London)* **641**, E1 (2025).
- [24] R. Hoyer, P. P. Stavropoulos, A. Razpopov, R. Valentí, L. Šmejkal, and A. Mook, Altermagnetic splitting of magnons in hematite $\alpha\text{-Fe}_2\text{O}_3$, *Phys. Rev. B* **112**, 064425 (2025).
- [25] V. Baltz, A. Manchon, M. Tsoi, T. Moriyama, T. Ono, and Y. Tserkovnyak, Antiferromagnetic spintronics, *Rev. Mod. Phys.* **90**, 015005 (2018).
- [26] R. Lebrun, A. Ross, S. Bender, A. Qaiumzadeh, L. Baldrati, J. Cramer, A. Brataas, R. Duine, and M. Kläui, Tunable long-distance spin transport in a crystalline antiferromagnetic iron oxide, *Nature (London)* **561**, 222 (2018).
- [27] A. Ross, R. Lebrun, O. Gomonay, D. A. Grave, A. Kay, L. Baldrati, S. Becker, A. Qaiumzadeh, C. Ulloa, G. Jakob, *et al.*, Propagation length of antiferromagnetic magnons governed by domain configurations, *Nano Lett.* **20**, 306 (2020).
- [28] M. W. Haverkort, M. Zwierzycki, and O. O. Andersen, Multiplet ligand-field theory using Wannier orbitals, *Phys. Rev. B* **85**, 165113 (2012).
- [29] P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G. K. Madsen, and L. D. Marks, WIEN2k: An APW+lo program for calculating the properties of solids, *J. Chem. Phys.* **152**, 074101 (2020).
- [30] K. Haule, C.-H. Yee, and K. Kim, Dynamical mean-field theory within the full-potential methods: Electronic structure of CeIrIn_5 , CeCoIn_5 , and CeRhIn_5 , *Phys. Rev. B* **81**, 195107 (2010).
- [31] K. Haule, Quantum Monte Carlo impurity solver for cluster dynamical mean-field theory and electronic structure calculations with adjustable cluster base, *Phys. Rev. B* **75**, 155113 (2007).
- [32] G. Kresse and J. Furthmüller, Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set, *Phys. Rev. B* **54**, 11169 (1996).
- [33] S. L. Dudarev, G. A. Botton, S. Y. Savrasov, C. J. Humphreys, and A. P. Sutton, Electron-energy-loss spectra and the structural stability of nickel oxide: An LSDA+U study, *Phys. Rev. B* **57**, 1505 (1998).
- [34] K. Koepernik and H. Eschrig, Full-potential nonorthogonal local-orbital minimum-basis band-structure scheme, *Phys. Rev. B* **59**, 1743 (1999).
- [35] I. Opahle, K. Koepernik, and H. Eschrig, Full-potential band-structure calculation of iron pyrite, *Phys. Rev. B* **60**, 14035 (1999).
- [36] K. Koepernik, O. Janson, Y. Sun, and J. van den Brink, Symmetry-conserving maximally projected Wannier functions, *Phys. Rev. B* **107**, 235135 (2023).
- [37] L. Šmejkal, A. Marmodoro, K.-H. Ahn, R. González-Hernández, I. Turek, S. Mankovsky, H. Ebert, S. W. D'Souza, O. Šipr, J. Sinova, *et al.*, Chiral magnons in altermagnetic RuO_2 , *Phys. Rev. Lett.* **131**, 256703 (2023).
- [38] M. Tahir, M. Fakhar-e Alam, M. Atif, G. Mustafa, and Z. Ali, Investigation of optical, electrical and magnetic properties of hematite $\alpha\text{-Fe}_2\text{O}_3$ nanoparticles via sol-gel and co-precipitation method, *J. King Saud Univ. Sci.* **35**, 102695 (2023).
- [39] A. Hill, F. Jiao, P. Bruce, A. Harrison, W. Kockelmann, and C. Ritter, Neutron diffraction study of mesoporous and bulk hematite, $\alpha\text{-Fe}_2\text{O}_3$, *Chem. Mater.* **20**, 4891 (2008).
- [40] A. S. Belozеров, I. Leonov, and V. I. Anisimov, Magnetism of iron and nickel from rotationally invariant Hirsch-Fye quantum Monte Carlo calculations, *Phys. Rev. B* **87**, 125138 (2013).
- [41] A. Borovik-Romanov and H. Grimmer, Magnetic properties, in *International Tables for Crystallography, Vol. D: Physical Properties of Crystals*, edited by A. Authier (Springer, Dordrecht, 2006), pp. 105–149.
- [42] M. Winder, A. Hariki, and J. Kuneš, X-ray spectroscopy of the rare-earth nickelate LuNiO_3 : LDA+DMFT study, *Phys. Rev. B* **102**, 085155 (2020).
- [43] P. Kuiper, B. G. Searle, P. Rudolf, L. H. Tjeng, and C. T. Chen, X-ray magnetic dichroism of antiferromagnet Fe_2O_3 : The orientation of magnetic moments observed by Fe 2p x-ray absorption spectroscopy, *Phys. Rev. Lett.* **70**, 1549 (1993).
- [44] H. Jani, J. Linghu, S. Hooda, R. V. Chopdekar, C. Li, G. J. Omar, S. Prakash, Y. Du, P. Yang, A. Banas, *et al.*, Reversible hydrogen control of antiferromagnetic anisotropy in $\alpha\text{-Fe}_2\text{O}_3$, *Nat. Commun.* **12**, 1668 (2021).
- [45] Y. Lu, M. Höppner, O. Gunnarsson, and M. W. Haverkort, Efficient real-frequency solver for dynamical mean-field theory, *Phys. Rev. B* **90**, 085102 (2014).
- [46] A. E. Bocquet, T. Mizokawa, T. Saitoh, H. Namatame, and A. Fujimori, Electronic structure of 3d-transition-metal compounds by analysis of the 2p core-level photoemission spectra, *Phys. Rev. B* **46**, 3771 (1992).
- [47] Y. Ishii, N. Sasabe, and Y. Yamasaki, Altermagnetic XMCD in hematite distinct from weak ferromagnetic contributions, [arXiv:2603.00442](https://arxiv.org/abs/2603.00442).
- [48] www.nhr-verein.de/unserepartner.