

Structural and magnetic phases of topological kagome metal Fe_3Sn_2 under pressure

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We investigate the pressure-induced evolution of crystal structure and magnetism in the kagome ferromagnet Fe_3Sn_2 by combining x-ray diffraction, x-ray emission spectroscopy, x-ray magnetic circular dichroism, and spin-polarized density functional theory calculations. X-ray diffraction reveals a structural phase transition above ~ 20 GPa, which coincides with a pronounced reduction of the local Fe magnetic moment evidenced by x-ray emission spectroscopy, indicating a high-spin to low-spin transition. While x-ray emission spectroscopy probes the amplitude of the local moment, XMCD provides direct information on the orientation of the ordered magnetic moments and uncovers a rich pressure-temperature magnetic phase diagram. At room temperature, a collinear ferromagnetic phase with moments aligned along the c axis persists up to the structural transition. At low temperature, a tilted magnetic configuration remains stable to significantly higher pressures, while at intermediate temperatures pressure stabilizes the low-temperature magnetic phase at the expense of the high-temperature one. Spin-polarized first-principles calculations show that, although isotropic ferromagnetic exchange interactions remain robust under compression, pressure enhances spin-orbit-driven magnetic anisotropy and Dzyaloshinskii-Moriya interactions, favoring noncollinear magnetic configurations. Furthermore, hydrostatic pressure reconstructs the kagome-derived low-energy electronic structure, redistributes the Berry curvature in momentum space, and suppresses the intrinsic anomalous Hall conductivity despite the preservation of the metallic state. Our results demonstrate that pressure simultaneously reshapes the magnetic energy landscape of Fe_3Sn_2 and Berry-phase electronic transport by coupling lattice, spin state, and relativistic magnetic interactions, establishing hydrostatic pressure as an effective control parameter to engineer magnetic anisotropy and electronic topological phases in kagome materials.

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I. INTRODUCTION

Magnetic structure and its evolution under external perturbations are central topics in the study of quantum materials. In particular, kagome lattices, with their geometry of corner-sharing triangles, provide a unique platform in which magnetic interactions and electronic topology are intertwined. While magnetic frustration was initially the main focus in kagome systems, leading to proposals of exotic ground states such as quantum spin liquids [1,2], it has become clear that kagome materials also host topologically nontrivial band structures with flat bands and Dirac cones [3,4]. The orientation of the magnetic moments, and more generally the magnetic structure, plays a crucial role in determining the electronic topology, including the appearance

of Weyl nodes, Chern gaps, and anomalous Hall effects [5,6]. Therefore, controlling and understanding changes in magnetic orientation provide a powerful route to engineer emergent topological and correlated phases.

Among kagome compounds, Fe-Sn based materials stand out as key systems hosting this interplay of magnetism and topology. FeSn , with its simple crystal structure, has been widely investigated as a model kagome magnet [7–10]. In contrast, Fe_3Sn_2 exhibits a more complex bilayer kagome structure and richer physics. It is a soft ferromagnet with a high Curie temperature ($T_C = 657$ K) [11] and exhibits a giant anomalous Hall effect arising from Berry curvature associated with Dirac-like bands [5]. At ambient pressure, Fe_3Sn_2 displays a rich magnetic phase diagram as a function of temperature. Below T_C , the magnetic moments are predominantly aligned along the c axis (out of plane). Upon cooling, the system undergoes a spin-reorientation transition around 80 K [12], where the moments progressively tilt away from the c axis toward the kagome ab plane. This temperature-driven

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spin reorientation reflects the competition between exchange interactions and magnetocrystalline anisotropy (MAE), and is intimately connected to the electronic topology of the material. Recent studies have shown that the spin orientation in Fe_3Sn_2 strongly affects its electronic structure [13], even tuning the system into Weyl semimetallic phases [14]. This connection has been directly evidenced by optical spectroscopy, where the low-temperature spin reorientation was shown to open a gap in the Dirac-like bands, consistent with the emergence of additional Weyl nodes [15]. Complementary magneto-optical measurements of the Hall conductivity spectra have further traced the momentum-space helical volumes associated with these band features, directly linking the anomalous Hall response to the underlying Berry curvature generated by spin-orbit-coupled kagome bands [16]. Furthermore, real-space topological textures such as skyrmions have been observed [17], highlighting the coexistence of reciprocal and real-space topology. Beyond the magnitude of the magnetic moment, spin-orbit coupling (SOC) and magnetocrystalline anisotropy play a central role in kagome ferromagnets, as they control the orientation of the magnetic moments and enable nontrivial electronic topology. In Fe_3Sn_2 , subtle changes in crystal symmetry or lattice parameters can therefore strongly modify the balance between collinear and noncollinear magnetic configurations.

A key challenge is to explore how the magnetic orientation and amplitude respond to external parameters. Magnetic field has already been shown to induce spin reorientations in Fe_3Sn_2 thin films [14]. Strain has been theoretically proposed as an alternative tuning parameter in kagome systems, capable of acting as an effective magnetic field and modifying exchange interactions and lattice symmetry [18]. Among the different external stimuli, hydrostatic pressure is particularly powerful because it directly modifies interatomic distances, bandwidths, and exchange pathways, potentially coupling structural and magnetic degrees of freedom [19]. Pressure can induce structural phase transitions that dramatically reshape the magnetic structure or even quench the magnetic moment [20]. Despite its importance, the pressure dependence of magnetism in kagome magnets remains largely unexplored.

In this context, Fe_3Sn_2 constitutes an ideal platform to investigate how magnetic structure, in particular, spin orientation and magnetic moment amplitude, evolve under pressure. Its layered kagome-based structure, intrinsic ferromagnetism, and strong spin-orbit coupling make it highly sensitive to lattice distortions. Moreover, the close interplay between crystal symmetry and electronic topology suggests that pressure could unlock alternative magnetic or topological phases. Previous works have hinted at a possible structural transition at high pressure [21], but the magnetic consequences of such a transition have not been addressed experimentally.

In this paper, we combine x-ray diffraction (XRD), x-ray Magnetic Circular Dichroism (XMCD), X-ray emission spectroscopy (XES), and density functional theory (DFT) calculations to systematically investigate the pressure evolution of structure and magnetism in Fe_3Sn_2 . We focus on the modification of magnetic orientation and the collapse of ferromagnetism across the pressure-induced structural transition. We demonstrate that pressure stabilizes distinct magnetic regimes and induces a transformation of the magnetic state

intimately linked to structural changes. By disentangling the evolution of the local magnetic moment amplitude from that of magnetic anisotropy and spin orientation, we provide a comprehensive picture of how pressure reshapes the magnetic energy landscape of this kagome compound. Combining spectroscopy, diffraction, and spin-polarized first-principles calculations, we show that pressure not only drives a spin-state transition but also enhances spin-orbit-driven anisotropic interactions, stabilizing distinct magnetic configurations over extended pressure–temperature ranges.

II. X-RAY DIFFRACTION

The high-resolution XRD was carried out at the PSICHE beamline of the SOLEIL synchrotron with a photon energy of 23 keV ($\lambda = 0.3738$ Å). Fe_3Sn_2 powder sample was mounted in a Diamond Anvil Cell with 300- μm culet diamonds, equipped with Rhenium gasket and ethanol:methanol mixture in 1:4 volumic proportion as pressure transmitting medium [22]. Gold powder was also put in the chamber to monitor the pressure, using the measured lattice parameter and the Au equation of state [23]. Measurements were performed at room temperature (300 K) between 0 and 35 GPa. The results are presented in the color map of Fig. 1(a). Beyond the expected contraction of the lattice visible by the continuous shift of the peaks to high angles, we observe a structural transition around 22 GPa confirming what was observed in a previous publication [21]. This transition corresponds to a symmetry lowering toward a lower-symmetry ($Pnma$) high-pressure phase, whose average crystallographic symmetry will be discussed in connection with DFT calculations.

The structural transition from the rhombohedral $R\bar{3}m$ phase to the orthorhombic $Pnma$ phase is first order in nature. This conclusion is supported by two key observations. First, there is no group–subgroup relationship between $R\bar{3}m$ and $Pnma$; such a reconstructive transition inherently involves a discontinuous change in lattice symmetry, which is a hallmark of a first-order process. Second, our XRD data clearly show a coexistence of the two phases over a pressure range of approximately 20 to 25 GPa, evidenced by the simultaneous presence of diffraction peaks from both structures. This phase coexistence is a classic experimental signature of a first-order transition involving nucleation and growth. The high-pressure $Pnma$ phase differs significantly from the ambient $R\bar{3}m$ phase: whereas the rhombohedral structure features perfectly hexagonal and highly symmetric kagome layers, the orthorhombic phase involves a substantial distortion of the kagome network. The Fe–Fe bond lengths are no longer equivalent, leading to stretched or compressed triangles within the kagome planes. The transition also implies a change in the stacking sequence and the relative alignment of the bilayers along the compression axis, driven by the need to optimize packing under high pressure. The diffraction peak widths at low pressure are found to be instrument limited, consistent with the resolution determined by CeO_2 calibration. Near the structural transition, an excess physical broadening of the peaks is observed, attributable to the onset of phase coexistence and microstrain accumulation.

We represent in Figs. 1(b) and 1(c) the extracted lattice parameters using the Le Bail method and the evolution of the

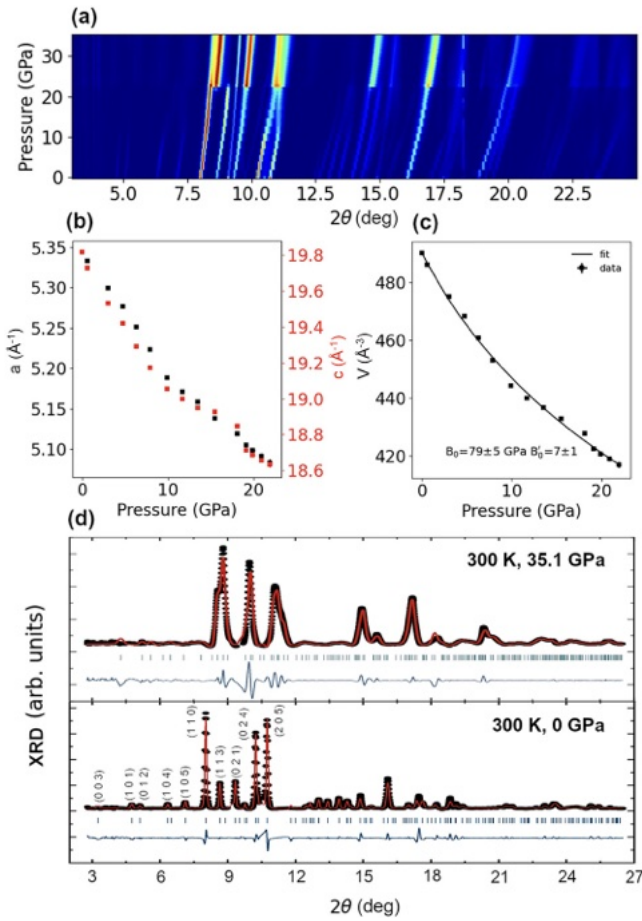


FIG. 1. High-pressure x-ray diffraction analysis. (a) Color map showing the pressure evolution of x-ray diffraction patterns, revealing the emergence of additional peaks above 22 GPa, indicative of a structural phase transition. (b) Pressure dependence of the refined lattice parameters a (black symbols) and c (red symbols) obtained from Le Bail refinement using the $R\bar{3}m$ space group up to the transition pressure. (c) Unit cell volume as a function of pressure (black squares) fitted with a third-order Birch–Murnaghan equation of state (solid black line). (d) Experimental ambient and high pressure (35.1 GPa) diffractogram (black points) together with Le Bail fit (red line) using $R\bar{3}m$ and $Pnma$ space group, respectively. The blue line is the difference between experimental data and fitted curve.

unit cell volume fitted by a Birch–Murnaghan equation [24]. The results are similar to the one obtained previously, with $B_0 = 79 \pm 5$ GPa and $B'_0 = 7 \pm 1$ for the bulk modulus and its derivative, respectively. A very slight deviation in the c parameter is visible near 20 GPa; we attribute this to the early-stage interference of the emerging $Pnma$ phase, which slightly perturbs the $R\bar{3}m$ Le Bail fit just before the transition becomes unmistakable. This improved interpretation does not significantly alter the extracted physical constants.

III. DENSITY FUNCTIONAL THEORY CALCULATIONS

To further characterize the high pressure structure, we carried out a structural search using the evolutionary algorithm implemented in the USPEX package [25–27] in variable-

composition mode. The population size was set to 60, with an initial pool of 100 randomly generated structures and evolution continued for up to ten generations. Structural candidates were ranked based on their enthalpy, and the selection and variation of structures were governed by heredity (50%), random symmetric structures (20%), soft mutation (20%), lattice mutation (10%), and permutation (10%). Structures containing between 15 and 30 atoms were allowed, and the search was unconstrained with respect to the crystallographic space groups. The USPEX code interfaced with QUANTUM ESPRESSO, using scalar relativistic pseudopotentials from PSLibrary. The local density approximation was used for the electron exchange and correlation energy, following the projector augmented wave formalism of Kresse and Joubert [28]. The plane-wave cutoff for the DFT calculation was set to 50 Ry for the plane-wave expansion of the wave functions.

For each generation of structures, DFT calculations were conducted over four sequential calculations, each employing increasingly stringent convergence criteria and relaxation settings. The convergence thresholds and electronic smearing widths were progressively tightened across these stages to ensure numerical stability and reliable identification of the lowest-enthalpy candidates. In the last calculation, the Brillouin zone was sampled using Monkhorst-Pack grids generated to a reciprocal-space resolution of $0.5 \text{ \AA}^{-1}$. The self-consistent DFT calculation was considered converged when the total energy difference between successive iterations dropped below 10^{-6} Ry. Ionic relaxations were performed using the Broyden–Fletcher–Goldfarb–Shanno quasi-Newton algorithm, until the forces on all atoms were smaller than 10^{-3} Ry/Bohr and the residual pressure deviated by less than 0.5 kbar from the target external pressure of 45 GPa. This pressure, which exceeds the 35 GPa used in the diffractogram, was chosen to ensure that the system had fully undergone the intended phase transition.

In our structural search using USPEX, we identified a low-enthalpy structure with orthorhombic symmetry, belonging to the $Pnma$ space group. To assess its relevance to experiment, we used it as the basis for XRD analysis. A Le Bail fit of the experimental XRD data was performed using only the space group symmetry ($Pnma$) and the optimized lattice parameters ($a = 6.6283 \text{ \AA}$, $b = 4.8723 \text{ \AA}$, $c = 7.6609 \text{ \AA}$), yielding excellent agreement with the measured XRD spectrum [Fig. 1(d)]. The high-pressure $Pnma$ phase represents a clear departure from the ambient-pressure $R\bar{3}m$ phase, which fails to reproduce key features of the observed diffraction pattern. This $Pnma$ assignment is consistent with the earlier high-pressure study by Gieffers and Nicol [21], which identified a structural transition at similar pressures but did not definitively assign a specific space group to the high-pressure phase. Our results agree with their reported lattice evolution and equation-of-state parameters (B_0 and B'_0) within experimental uncertainties. The present work goes further by proposing the $Pnma$ symmetry as a robust structural model, supported both by our high-resolution synchrotron XRD refinements and by the DFT evolutionary structural search. This supports a pressure-induced structural transition, which we will further correlate with other spectroscopic signatures in XMCD and x-ray absorption spectroscopy (XAS) measurements. The fact that the atomic positions of the predicted structure do not fully

reproduce the experimental diffraction pattern suggests that the real high-pressure phase may involve additional degrees of freedom, such as superstructural modulations, disorder, or fractional occupancies [29], which are not captured in the present model.

IV. X-RAY EMISSION SPECTROSCOPY

To probe the evolution of the local magnetic moment under pressure, we performed x-ray emission spectroscopy at the RIXS endstation of the GALAXIES beamline at synchrotron SOLEIL [30,31]. Pressure was applied using a membrane-driven diamond anvil cell equipped with 1.2-mm-thick diamonds featuring 300- μm culets. Multiple Fe_3Sn_2 single crystals were placed in a 150- μm hole within a stainless steel gasket, along with ruby chips for in situ pressure measurement [32], and Daphne oil as the pressure-transmitting medium [22]. XES were performed at room temperature (300 K) in transmission geometry, employing a 1-meter-radius spherically bent Ge(620) crystal analyzer and an avalanche photodiode detector arranged in the Rowland circle geometry. The total energy resolution at the $\text{Fe K}\beta$ line (7057 eV, $\theta_B = 79^\circ$) was 1.1 eV as determined by the full width at half maximum of the elastic line. The XES spectra were collected using incident x-rays at 10 keV. The XES spectra are presented in Fig. 2(a). As now well established [33–36], the XES $\text{K}\beta$ line is a sensitive probe of the local spin state along with metal valence and chemical environment. More precisely, the $\text{K}\beta'$ satellite intensity reflects the $3p$ – $3d$ exchange interaction and is related to the amplitude of the local spin magnetic moment. When the local Fe magnetic moment decreases, spectral weight is transferred from the $\text{K}\beta'$ satellite to the main peak, which narrows slightly as the total spectral weight is conserved. In Fig. 2(a), the spectra are normalized to the maximum of the main $\text{K}\beta_{1,3}$ peak so the pressure-induced changes in the $\text{K}\beta'$ satellite are more easily observed. We observe two pressure ranges for which all the spectra overlap: below (blue curves) and above (red curves) ~ 20 GPa. The reduction in spectral weight at the low-energy shoulder indicates a decrease in the amplitude of the local magnetic moment of iron. This amplitude can be plotted as a function of pressure using the integrated absolute difference (IAD) method [36,37] where $\text{IAD}(P) = \int |\text{XES}(P, E) - \text{XES}(P_0, E)| dE$ with $\text{XES}(P, E)$ the $\text{K}\beta$ spectrum at a pressure P and P_0 a reference pressure, as shown in Fig. 2(b) (black circles). A clear high-spin to low-spin transition is observed around 20 GPa. While XES provides a robust signature of this spin-state crossover—the abrupt jump in IAD and the collapse of the $\text{K}\beta'$ satellite intensity are characteristic hallmarks—a precise quantitative determination of the final spin state or absolute moment value is not straightforward in this intermetallic system, owing to the lack of a reference compound with identical crystallographic environment. Our results therefore emphasize the significant reduction of the local Fe $3d$ moment rather than an absolute transition to a specific spin- S value. This transition coincides with the pressure-induced structural transition identified by x-ray diffraction and supported by DFT calculations, demonstrating a strong coupling between lattice degrees of freedom and the local spin state. The slight shift in the transition pressure between the

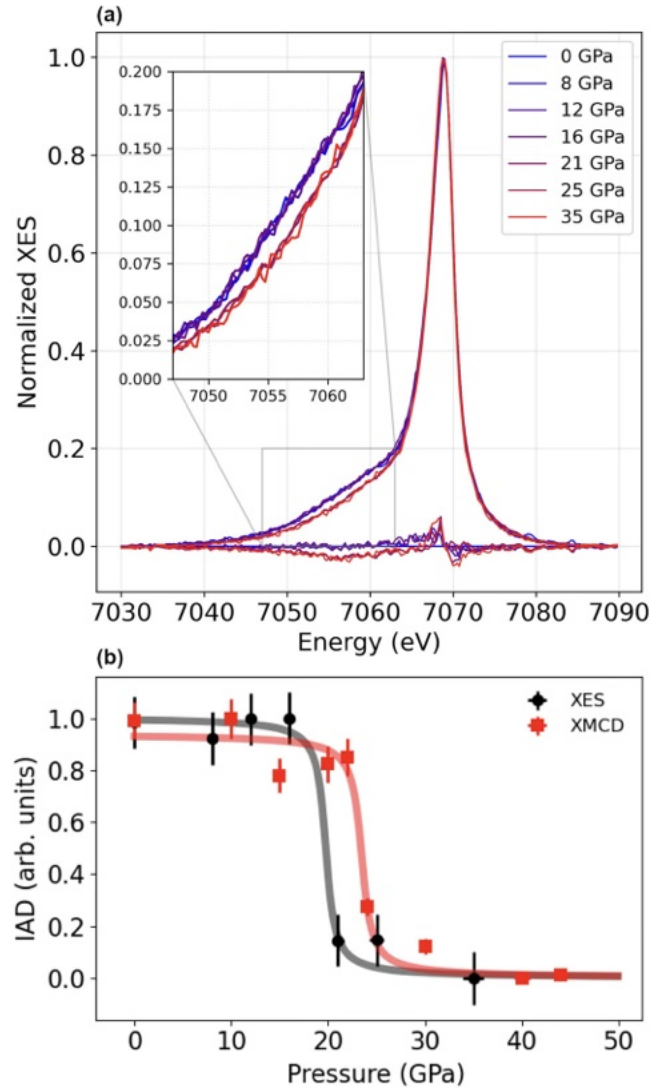


FIG. 2. (a) $\text{Fe K}\beta$ x-ray emission in Fe_3Sn_2 as a function of pressure measured at 300 K. Spectra are normalized to the maximum of the main $\text{K}\beta_{1,3}$ peak. The curves near the baseline correspond to the difference spectra relative to the 0 GPa reference. Inset: zoom on the $\text{K}\beta'$ line showing two distinct clusters of curves for the low- and high-pressure regimes. (b) Evolution of the Integrated Absolute Difference (IAD) of the XES spectra as a function of pressure (black circles) compared to the evolution of the XMCD signal (red squares). Thick lines are guides to the eyes.

XES and XMCD measurements, of approximately 2 GPa, can be attributed to the different pressure-transmitting media used (Daphne oil for XES and an ethanol:methanol mixture for XMCD, respectively). Such a coupling is expected in kagome systems where changes in Fe–Fe and Fe–Sn bonding strongly affect bandwidths and exchange interactions. Nonetheless, as a local probe, XES only provides access to the amplitude of the local moment and not to its orientation. To address this point, we turn to X-ray Magnetic Circular Dichroism.

V. X-RAY MAGNETIC CIRCULAR DICHROISM

XMCD is sensitive to the projection of the magnetic moment along the x-ray propagation direction and therefore

provides direct information on the magnetic orientation. In this sense, XMCD is complementary to XES and DFT: while the latter establish the existence and amplitude of the local magnetic moment, XMCD resolves how this moment is oriented with respect to the crystal axes and how magnetic anisotropy evolves under pressure. XMCD measurements on Fe_3Sn_2 single crystals were performed at the ODE beamline of the SOLEIL synchrotron, focusing on the Fe K-edge [38,39]. Pressure was applied using a diamond anvil cell equipped with diamonds with 300- μm -culet size. The Fe_3Sn_2 crystals were loaded into a rhenium gasket with a 150- μm diameter and 40- μm -thick hole, along with a ruby chip for pressure monitoring via standard ruby fluorescence calibration [32]. Fe_3Sn_2 crystals naturally grow with a highly two-dimensional, platelike habit, with the large faces corresponding to the (*ab*) kagome planes. When loading the sample, these plates naturally lie flat against the culet of the diamond anvil, so the *c* axis of every crystal piece is inherently oriented parallel to the compression axis and collinear with the incident x-ray beam. While the in-plane *a* and *b* axes of the various crystal pieces may be randomly rotated around the *c* axis, this does not affect the XMCD signal, since XMCD at normal incidence probes only the projection of the magnetic moment along the photon propagation direction (the *c* axis in our geometry). The statistical coalignment of the *c* axes is therefore the only requirement for a reliable measurement, and this geometric alignment is highly reproducible. An ethanol:methanol mixture in a 1:4 volumetric ratio was employed as the pressure-transmitting medium [22]. Data were collected in three separate experiments at constant temperatures of 30 K, 100 K, and room temperature (300 K), with pressure progressively increased. The XMCD signal was measured by reversing a 1.3 T magnetic field, with approximately a dozen cycles performed for each pressure point. The absorption spectra were normalized to unity at high energy, and the dichroic signal was similarly normalized. XAS spectra, alongside the XMCD signal (magnified by a factor of 500 for clarity), are shown in Figs. 3(a)–3(c).

A. 300 K: High-temperature magnetic phase

At ambient temperature, Fe_3Sn_2 is known to have a ferromagnetic (FM) structure with moments aligned nearly parallel to the *c* axis. Our XMCD data confirm that the dichroic signal remains strong and positive up to ~ 20 GPa, indicating that the magnetic moments retain their orientation along the *c* axis in this pressure range. At around 20 GPa, the XMCD intensity collapses sharply. This collapse coincides with both the spin-state transition observed by XES and the structural transition revealed by XRD, indicating that at 300 K a single magnetic phase with $M \parallel c$ is stable up to the pressure-induced structural instability.

B. 30 K: Low-temperature tilted phase

At 30 K and ambient pressure, Fe_3Sn_2 adopts a magnetic configuration in which the spins are tilted away from the *c* axis. In our XMCD geometry, this results in a reduced dichroic signal. Remarkably, this signal persists up to at least 33 GPa, with no clear transition detected up to the

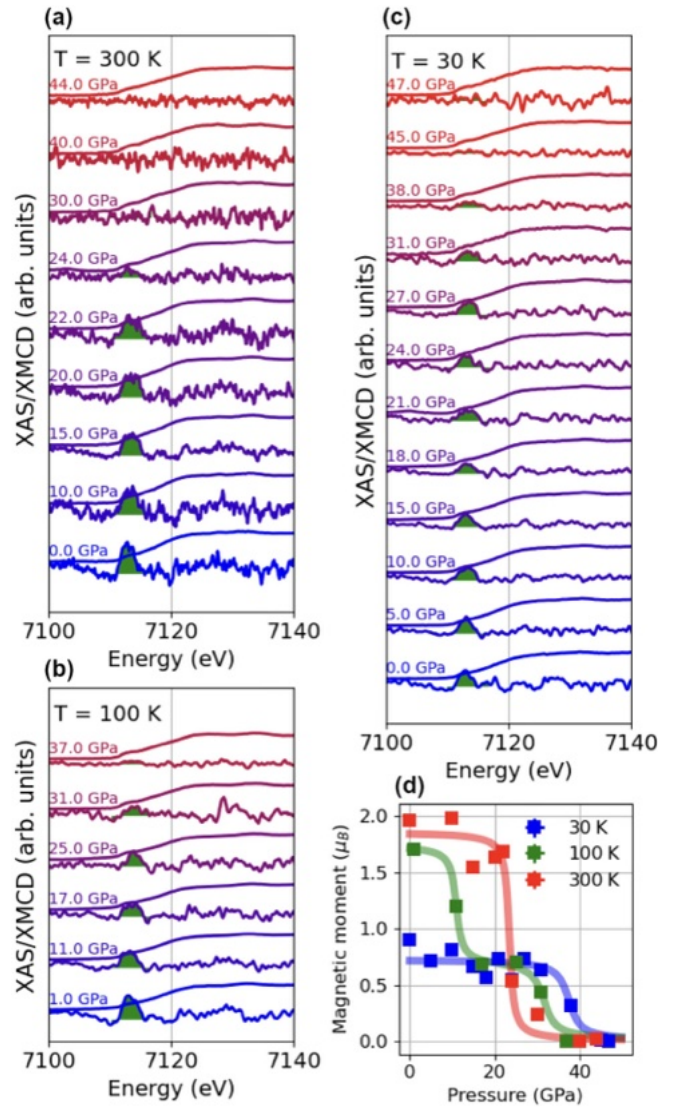


FIG. 3. (a)–(c) X-ray absorption spectra and associated dichroic signal at Fe K-edge, performed at 1.3 T and 300, 30, and 100 K, respectively. Dichroic signals are multiplied by a factor of 500 for a sake of visibility. The green area corresponds to the intensity reported in panel (d). (d) Evolution of the ferromagnetic component along the *c* axis deduced from the dichroic area [in green in (a)–(c)] and normalized to $2 \mu_B$ at ambient condition (300 K and 0 GPa), for 30 K (blue), 100 K (green), and 300 K (red). Thick lines are guides to the eyes.

highest pressure point measured (39 GPa). The significantly higher transition pressure at low temperature suggests that the low-temperature magnetic phase is more robust against compression, consistent with the general increase of structural transition pressures at low temperature. This robustness may also be related to a pressure-induced modification of magnetic anisotropy, expected when the crystal symmetry is reduced, as suggested by the DFT results.

C. 100 K: Intermediate regime

At 100 K, an intermediate behavior is observed. At low pressure, the XMCD signal resembles that at 300 K, indicating

moments aligned close to the c axis. However, around 10 GPa, the XMCD amplitude decreases and stabilizes at a value comparable to that of the low-temperature tilted phase. This demonstrates that under pressure the low-temperature magnetic configuration becomes stabilized at significantly higher temperatures than at ambient pressure. This phase remains stable up to ~ 30 GPa.

D. Pressure–temperature magnetic phase diagram

Altogether, XMCD reveals that pressure destabilizes the high-temperature collinear magnetic phase in favor of the low-temperature tilted configuration. Under compression, the phase boundary between these two magnetic states shifts to higher temperatures, indicating that pressure reshapes the magnetic anisotropy landscape. This behavior highlights a strong spin–lattice coupling in Fe_3Sn_2 , reminiscent of other iron-based kagome compounds such as Fe_3Ge [40].

VI. SPIN-POLARIZED DFT

To gain microscopic understanding of the observed pressure-induced evolution of the magnetic behaviors in Fe_3Sn_2 , we performed spin-polarized DFT calculations within the plane-wave pseudopotential formalism, as implemented in the VASP package [41,42]. The exchange–correlation effects were treated using the generalized gradient approximation (GGA), and the on-site Coulomb interaction on Fe-3d orbitals was incorporated through the GGA+ U approach to account for electronic correlation effects beyond conventional DFT. Two representative values of the Hubbard parameter, $U = 2$ eV and $U = 4$ eV, were considered to assess the influence of electronic correlations on structural and magnetic properties. The experimentally determined rhombohedral crystal structure (space group $R\bar{3}m$) was used as the starting geometry, with lattice parameters $a = b = 5.34$ Å and $c = 19.80$ Å at ambient pressure [21]. To simulate the effect of hydrostatic pressure, we uniformly scaled the lattice parameters while maintaining a constant c/a ratio to preserve the symmetry. The unit cell volume (V) was systematically varied from -5% ($\frac{V-V_0}{V_0}$) to 0% relative to the ambient experimental value (V_0). For each volume, all internal atomic coordinates were fully relaxed until the residual Hellmann–Feynman forces on every atom were smaller than 10^{-3} eV/Å. This computational strategy enabled us to track the evolution of electronic structure and magnetic order as a function of pressure, thereby providing theoretical insight complementary to the experimental observations.

To understand the microscopic magnetic interactions in Fe_3Sn_2 and their evolution under pressure, we computed all relevant terms of the effective spin Hamiltonian—namely, the isotropic Heisenberg exchange, the antisymmetric Dzyaloshinskii–Moriya (DM) interaction, and the symmetric anisotropic exchange. These quantities were evaluated at both the ambient equilibrium volume and under 5% hydrostatic compression to assess the pressure dependence of magnetic couplings. To capture spin-orbit-driven anisotropic interactions, the Lichtenstein–Katsnelson–Antropov–Gubanov methodology was extended to its relativistic form using the Korringa–Kohn–Rostoker Green’s-function framework im-

TABLE I. Equilibrium lattice parameters obtained from GGA and GGA+ U calculations compared with experimental results. The experimental bulk modulus (B) is not available (NA).

Method	a (Å)	c (Å)	V (Å ³)	B (GPa)
GGA	5.33	19.78	488.26	102.8
GGA+ U ($U = 2$ eV)	5.38	19.97	502.09	81.6
GGA+ U ($U = 4$ eV)	5.45	20.21	520.42	80.1
Experiment	5.34	19.80	488.89	NA

plemented in RSPt code. This method has been discussed in details in Refs. [43,44] and shown to provide a reliable description of magnetic interactions in transition metal compounds. This yields the full exchange tensor $J_{ij}^{\alpha\beta}$, from which the isotropic exchange, DM interaction vectors, and symmetric anisotropic exchange components are extracted. The single-ion anisotropy was computed independently from fully relativistic total-energy calculations with the magnetic quantization axis constrained along different crystallographic directions.

A. Optimized lattice parameters

We first examined the magnetic stability by computing the total energies of two representative spin configurations, namely, FM and antiferromagnetic states. The results obtained from both GGA and GGA+ U ($U = 2$ and 4 eV) formalisms show FM configuration remained energetically favored. This theoretical result is consistent with experimental XMCD measurements, which indicate a predominantly ferromagnetic character in ambient condition. Further, we computed total energies as a function of volume for both GGA and GGA+ U ($U = 2$ eV and 4 eV) approaches in the ferromagnetic state. The resulting energy–volume data were fitted using the third-order Birch–Murnaghan equation of state [24,45], from which equilibrium lattice parameters and bulk moduli were obtained as shown in Table I. The equilibrium lattice parameters derived from GGA calculations show excellent agreement with experimental values, while the use of Hubbard U leads to a moderate lattice expansion. Consequently, the GGA approximation was chosen for subsequent pressure-dependent analyses.

In addition to the energy–volume analysis, the pressure corresponding to each compressed volume was obtained directly from the derivative of the third-order Birch–Murnaghan equation of state. This allowed us to construct the theoretical pressure–volume (p – V) curve and compare it quantitatively with the available experimental data. As shown in Fig. 4(a), the p – V relation calculated within the GGA framework reproduces the experimental trend remarkably well over the entire pressure range studied, indicating that the chosen exchange–correlation treatment captures the underlying compressibility and elastic response of Fe_3Sn_2 with high fidelity. Furthermore, the individual lattice parameters $a(p)$ and $c(p)$, extracted at each volume, exhibit pressure dependence consistent with experimental observations [see Fig. 4(b)]. The close agreement between theory and experiment reinforces the reliability of the structural description obtained within GGA. The combination of GGA-based total-energy calculations and equation-of-state

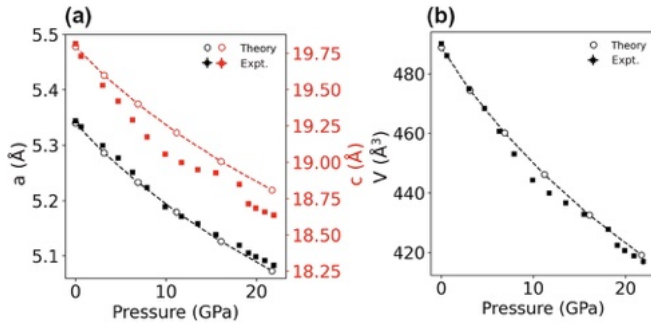


FIG. 4. Comparison between experimental and theoretical structural parameters of Fe_3Sn_2 under pressure. (a) Pressure dependence of the lattice parameters. (b) Pressure dependence of the unit-cell volume. Experimental data are compared with results obtained from density functional theory calculations, highlighting the agreement across the pressure-induced structural transition.

analysis thus provides a solid microscopic foundation for exploring the pressure-induced evolution of structural, electronic, and magnetic degrees of freedom in Fe_3Sn_2 .

B. Magnetism under application of pressure

To observe the evolution of magnetic behavior, we first examined the pressure dependence of the magnetic couplings (shown in Fig. 5) and the local Fe magnetic moment (shown in Fig. 6). A gradual decrease in the moment, in line with the XES outcome, is observed with increasing pressure, indicating a weakening of the exchange splitting as Fe-Fe distances shrink and orbital hybridization strengthens. This trend reflects the suppression of the ferromagnetic component within the rhombohedral phase and provides the microscopic basis for understanding the subsequent SOC-driven anisotropic effects that emerge at higher pressures.

Next, the inter-atomic exchange interactions were evaluated for two representative structures: ambient condition and 21.7 GPa pressure (-5% volume change). The results are summarized in Table II. All three leading couplings J_1 , J_2 , and

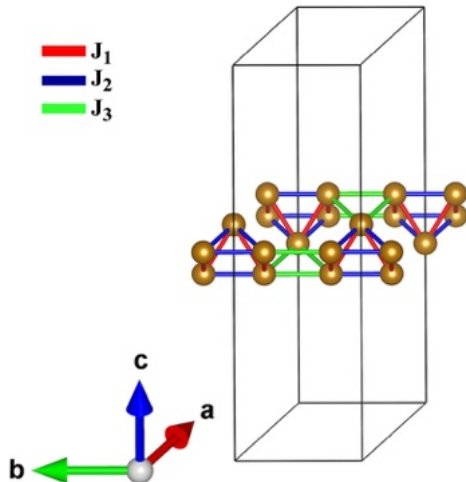


FIG. 5. Color representation of dominant exchange interactions in the unit cell of Fe_3Sn_2 .

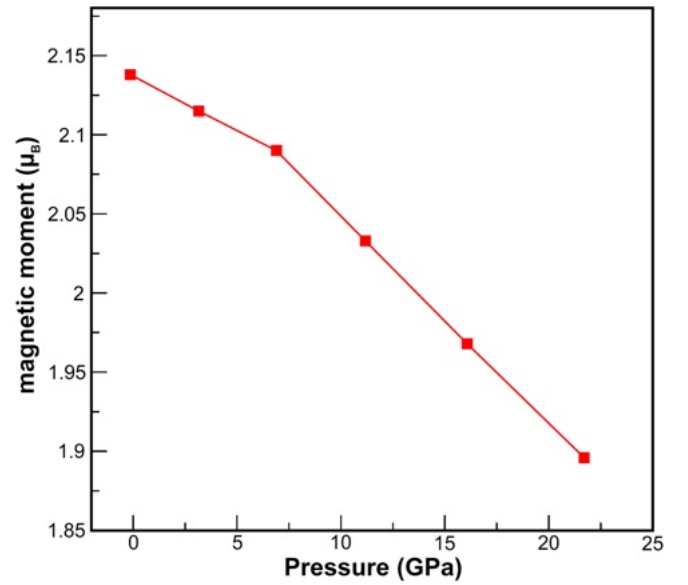


FIG. 6. Pressure dependence of the calculated local Fe magnetic moment in Fe_3Sn_2 , showing a gradual reduction of the moment amplitude under compression.

J_3 (as indicated in Fig. 5) are ferromagnetic and remain positive under compression. Upon applying hydrostatic pressure, the Fe-Fe distances decrease and the exchange interactions, particularly J_2 , become stronger. This enhancement reflects the increased orbital overlap between neighboring Fe atoms.

Following the strengthening of the isotropic exchange interactions, we next examined the evolution of the MAE under pressure to assess the role of SOC. As summarized in Table III, Fe_3Sn_2 exhibits an in-plane easy axis at ambient conditions, with the a - and b -axis spin orientations lying lower in energy than the c axis by 0.86 meV. Upon applying hydrostatic pressure (corresponding to 21.7 GPa), this energy difference increases to 1.32 meV, while the a - and b -axis energies remain degenerate. The larger magnitude of the MAE clearly indicates a strengthening of SOC-driven anisotropy under pressure, reinforcing the stabilization of an in-plane magnetic alignment relative to the out-of-plane (c -axis) direction. Such an enhancement of SOC with compression is further manifested in the behavior of the anisotropic exchange interactions. Our calculations suggest that the symmetric anisotropic exchange components C_{ij} s are very weak and we can ignore them in setting up spin Hamiltonian of this

TABLE II. Exchange interactions (J_i) between Fe-Fe ions in Fe_3Sn_2 at different hydrostatic strain values. Distances are in Å and exchange strengths in meV.

p (GPa)	Interaction	Distance (Å)	J_i (meV)
0 (ambient)	J_1	2.48	16.18
	J_2	2.54	22.37
	J_3	2.80	23.61
21.7 (-5%)	J_1	2.39	16.83
	J_2	2.52	25.88
	J_3	2.55	17.36

TABLE III. Comparison of magnetocrystalline anisotropy energy (MAE) values at ambient conditions and under applied pressure. The c axis is taken as the reference axis.

Pressure (GPa)	Spin-axis energy (meV)		
	c axis	b axis	a axis
Ambient (0)	0.00	−0.86	−0.86
21.7 (−5%)	0.00	−1.32	−1.32

system. However, as listed in Table IV, the antisymmetric DM vectors D_{ij} increase in magnitude for several Fe-Fe pairs, most notably for the second-nearest neighbors, where $|D_y|$ grows substantially from 0.42 to 0.83 meV, accompanied by an increase in $|D_z|$. The magnitude of D_{ij} for the second neighbor almost gets doubled due to the application of pressure of 21.7 GPa. Since DM interaction originates exclusively from SOC, their growth under compression provides a microscopic description of the pressure-enhanced SOC strength inferred from MAE trends. The amplification of DM interactions, in particular, favors a canting of the Fe spins promoting noncollinear or weakly canted configurations within the kagome bilayers. This theoretical trend is consistent with our XMCD measurements, which reveal a progressive tilting of the ferromagnetic component away from the c axis under pressure. Thus, the combined evolution of MAE and anisotropic exchange couplings under pressure establishes SOC-enhanced spin canting as a key precursor to the experimentally observed suppression of long-range ferromagnetic order. Taken together, these results indicate that pressure does not immediately suppress ferromagnetism through a collapse of isotropic exchange, but instead progressively reshapes the magnetic anisotropy landscape through enhanced spin-orbit coupling. This mechanism naturally explains why a tilted ferromagnetic configuration remains stable over a broad pressure range before the eventual disappearance of long-range magnetic order observed experimentally.

C. Pressure-induced evolution of the electronic structure and Berry-phase transport

To elucidate the microscopic origin of the pressure-induced evolution of the electronic and topological properties of Fe_3Sn_2 , we examine the spin-polarized electronic structure within the rhombohedral phase. The orbital-resolved partial density of states (PDOS) for the Fe-3d states at ambient pressure and under 5% lattice volume compression (corresponding to ~ 21.7 GPa) is shown in Fig. 7. In both cases, finite Fe-3d spectral weight persists at the Fermi level, confirming that

TABLE IV. Antisymmetric anisotropic Dzyaloshinskii–Moriya (DM) interaction strengths (D) at ambient conditions and under applied pressure. Values are in meV.

Neighbor	0 GPa	$ D_{ij} $	21.7 GPa (−5%)	$ D_{ij} $
First	(0.14, 0.08, 0.14)	0.21	(0.16, 0.09, 0.02)	0.18
Second	(0.00, −0.42, −0.25)	0.48	(0.00, −0.83, −0.40)	0.92
Third	(0.00, 0.39, −0.09)	0.40	(0.00, 0.11, −0.52)	0.53

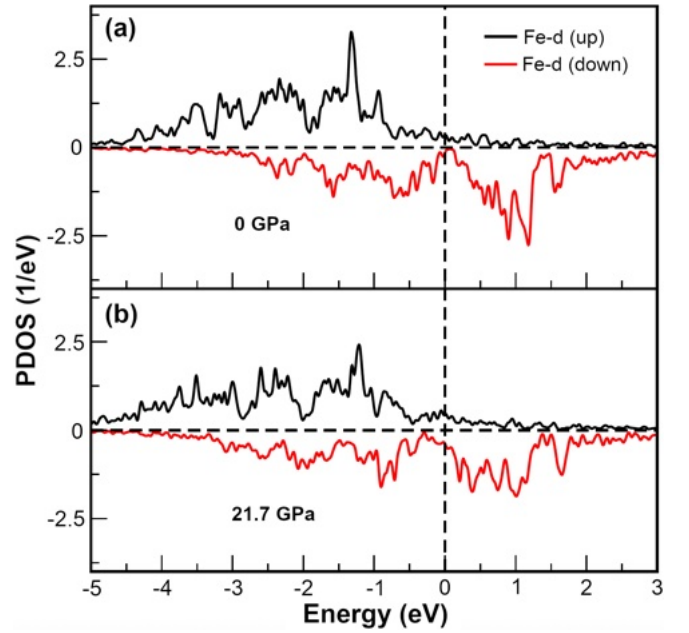


FIG. 7. Partial density of states (PDOS) obtained from GGA calculations for Fe-3d orbital at (a) ambient (0 GPa) conditions and (b) at 21.7 GPa (−5%).

Fe_3Sn_2 remains metallic throughout the investigated pressure range. The low-energy electronic states continue to be dominated by Fe-3d orbitals, while pressure induces a moderate broadening of the 3d bandwidth, reflecting enhanced Fe-Fe orbital overlap and stronger hybridization. Such an increase in electronic bandwidth is consistent with the gradual reduction of the local magnetic moment discussed in the previous section and provides the microscopic basis for the subsequent reconstruction of the low-energy kagome-derived electronic structure.

Fe_3Sn_2 is one of the prototypical magnetic kagome metals, where the interplay between the kagome lattice geometry, ferromagnetism, and SOC gives rise to massive Dirac fermions and a large intrinsic anomalous Hall effect originating from Berry curvature concentrated near SOC-gapped band crossings [3,5]. Since pressure modifies both the electronic bandwidth and the spin-orbit-driven magnetic interactions, it is expected to influence the momentum-space distribution of Berry curvature and the associated topological transport response. To quantify these effects, the topological electronic structure was investigated using a Wannier-function-based tight-binding Hamiltonian constructed from spin-polarized GGA+SOC calculations. Maximally localized Wannier functions were generated using the WANNIER90 package [46], with projections chosen to accurately reproduce the Fe-3d dominated bands around the Fermi level. The intrinsic Berry curvature and anomalous Hall conductivity (AHC) were subsequently evaluated within the Kubo formalism [47–49]. The relevant Berry curvature component $\Omega_z(\mathbf{k})$, which contributes directly to σ_{xy} , is evaluated using the following formula:

$$\Omega_z(\mathbf{k}) = -2 \text{Im} \sum_{m \neq n} \frac{\langle u_{n\mathbf{k}} | v_x | u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | v_y | u_{n\mathbf{k}} \rangle}{(E_{m\mathbf{k}} - E_{n\mathbf{k}})^2}, \quad (1)$$

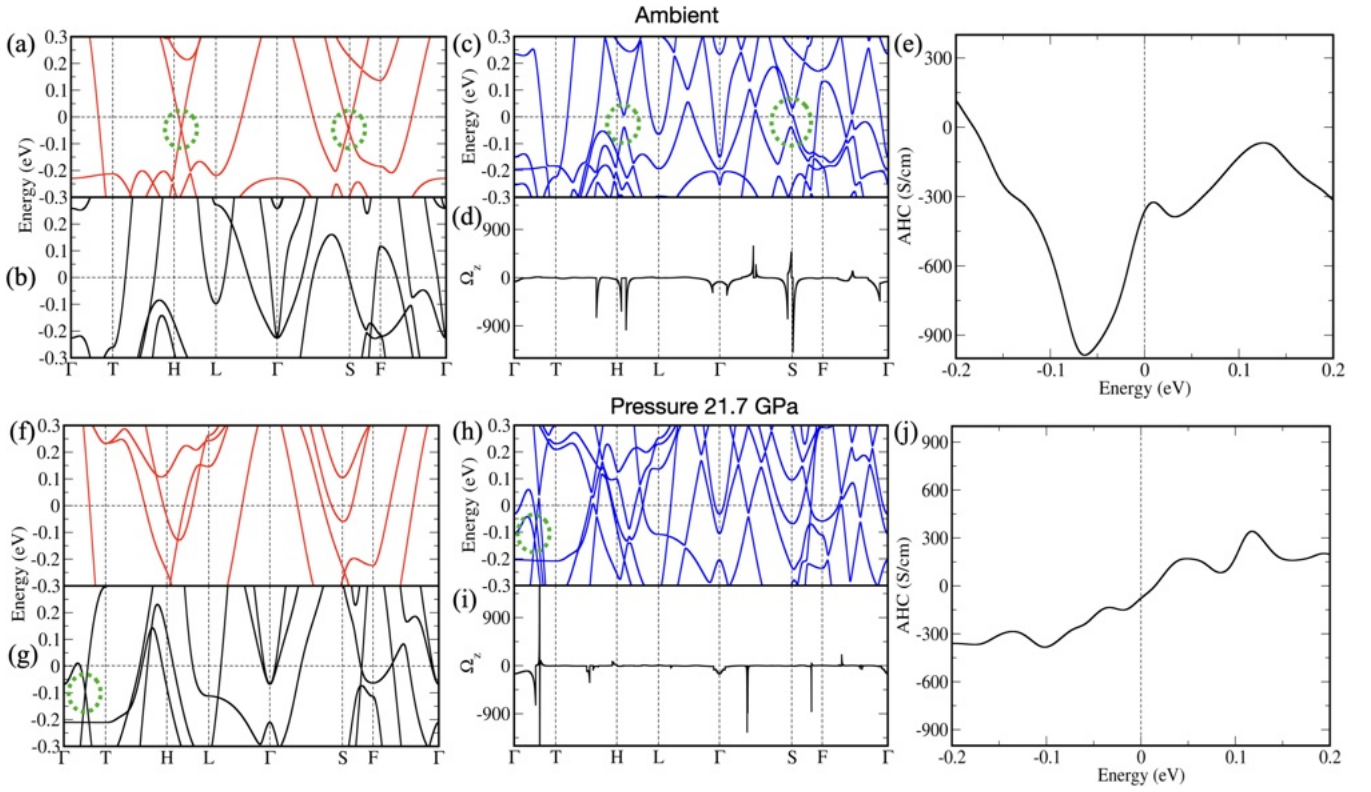


FIG. 8. Band dispersion at ambient pressure within GGA approach for (a) minority-spin (red), (b) majority-spin (black), (c) total (blue) after incorporating SOC (GGA+SOC approach), corresponding (d) Berry curvature, $\Omega_z(\mathbf{k})$, along the high-symmetry path, and (e) energy-dependent intrinsic anomalous Hall conductivity (AHC). Band dispersion at 21.7 GPa pressure (5% lattice volume compression) within GGA approach for (f) minority-spin (red), (g) majority-spin (black), (h) total (blue) after incorporating SOC (GGA+SOC approach), corresponding (i) Berry curvature, $\Omega_z(\mathbf{k})$, along the high-symmetry path, and (j) energy-dependent intrinsic AHC.

where $E_{n\mathbf{k}}$ and $|u_{n\mathbf{k}}\rangle$ are the eigenvalues and periodic parts of the Bloch eigenstates, respectively, and $v_\alpha = \frac{1}{\hbar} \frac{\partial \mathcal{H}(\mathbf{k})}{\partial k_\alpha}$ is the velocity operator. The total $\mathbf{k}$ -resolved Berry curvature was obtained by summing over all occupied bands. The intrinsic anomalous Hall conductivity was calculated by integrating the Berry curvature over the full Brillouin zone using the following equation:

$$\sigma_{xy} = -\frac{e^2}{\hbar} \sum_n \int_{\text{BZ}} \frac{d^3k}{(2\pi)^3} f_{n\mathbf{k}} \Omega_z(\mathbf{k}), \quad (2)$$

where $f_{n\mathbf{k}}$ is the Fermi-Dirac occupation factor. A dense $200 \times 200 \times 200$ uniform $\mathbf{k}$ -mesh was used for the Brillouin zone integration. The energy-dependent AHC was obtained by shifting the chemical potential from -0.2 to $+0.2$ eV relative to the Fermi level, allowing us to examine how pressure modifies the Berry-phase transport associated with the low-energy electronic structure.

The calculated electronic band structure at ambient pressure is presented in Figs. 8(a)–8(c). In the absence of SOC, several kagome-derived band crossings appear close to the Fermi level, particularly around the H and S high-symmetry points in the minority spin channel [see dotted circle in Fig. 8(b)]. These crossings originate from the characteristic Dirac-like bands of the kagome lattice. Upon inclusion of SOC, small gaps open at these crossing points [Fig. 8(c)]. These characteristic features of the bands act as

intense sources of Berry curvature, giving rise to pronounced momentum-space hotspots, as illustrated in Fig. 8(d). Consequently, Fe_3Sn_2 exhibits a large intrinsic anomalous Hall conductivity of $\sigma_{xy} = -364.72$ S/cm at the Fermi level, while the magnitude reaches a maximum value of -986.05 S/cm around $E - E_F = -0.06$ eV. The strong energy dependence of the Hall conductivity demonstrates that the Berry-phase response is extremely sensitive to the precise location of the chemical potential, in agreement with previous theoretical and experimental studies attributing the giant anomalous Hall effect of Fe_3Sn_2 to Berry curvature generated by SOC-gapped kagome-derived massive Dirac bands [3,5].

Application of hydrostatic pressure substantially reconstructs the low-energy electronic structure while preserving the overall metallic character of the system. As shown in Figs. 8(f)–8(h), compression shifts several Fe-3d bands relative to the Fermi level and redistributes the SOC-induced avoided crossings throughout the Brillouin zone. In particular, new avoided-crossing features emerge near the T point in the majority spin channel [Fig. 8(g)], while the prominent crossings around the H and S points are significantly modified [Fig. 8(f)]. These changes originate from enhanced Fe-Fe hybridization under compression, which alters the dispersion of the kagome-derived bands and consequently changes the location and strength of the SOC-induced band anti-crossings responsible for generating Berry curvature. The evolution of the Berry curvature clearly reflects this electronic

reconstruction. At ambient pressure, the Berry curvature is dominated by a few intense hotspots associated with the SOC-gapped Dirac crossings. Under compression, however, these hotspots are redistributed over different regions of momentum space [Fig. 8(i)]. Consequently, the intrinsic anomalous Hall conductivity is dramatically reduced, yielding $\sigma_{xy} = -77.95$ S/cm at 21.7 GPa, corresponding to an approximately 79% suppression relative to the ambient-pressure value.

We note here that pressure reduces the anomalous Hall conductivity not by destroying the kagome-derived electronic states or the metallic character of Fe_3Sn_2 but by reconstructing the low-energy band structure and consequently redistributing the Berry curvature throughout the Brillouin zone. The present Berry-curvature calculations are restricted to the compressed rhombohedral phase and therefore describe the evolution of the electronic topology as the system approaches the structural transition. Overall, our results demonstrate that hydrostatic pressure provides an effective means of tuning the Berry-phase transport in Fe_3Sn_2 by reconstructing the SOC-gapped kagome bands and their associated Berry-curvature distribution, thereby strongly suppressing the intrinsic anomalous Hall response.

VII. DISCUSSION AND CONCLUSION

In this work, we have experimentally investigated the interplay between crystal structure and magnetism in the kagome compound Fe_3Sn_2 under high pressure. Using a combination of x-ray diffraction, x-ray Magnetic Circular Dichroism, X-ray emission spectroscopy, and density functional theory calculations, we have shown that Fe_3Sn_2 undergoes a pressure-induced structural transition toward a lower-symmetry phase, which coincides with a drastic modification of its magnetic properties.

By combining X-ray Emission Spectroscopy and XMCD, we were able to disentangle the evolution of the amplitude of the local Fe magnetic moment from that of its orientation. XES reveals a clear high-spin to low-spin transition occurring around 20 GPa, concomitant with the structural transition identified by XRD and supported by evolutionary structural searches. This result demonstrates a strong coupling between lattice degrees of freedom and the local spin state, highlighting the sensitivity of the Fe 3d electrons to pressure-induced changes in bonding and bandwidth.

XMCD measurements further show that, while XES captures the collapse of the local moment amplitude, the magnetic orientation follows a distinct pressure–temperature evolution. At 300 K, the magnetic structure with moments aligned predominantly along the c axis remains stable up to the structural transition around 20 GPa. At low temperature (30 K), a tilted magnetic configuration persists up to much higher pressures, reaching at least 33 GPa, indicating an enhanced robustness of the low-temperature magnetic phase against compression. At intermediate temperature (100 K), pressure stabilizes the low-temperature tilted phase already around 10 GPa, and this phase remains stable up to approximately 30 GPa. These results demonstrate that pressure destabilizes the high-temperature magnetic phase in favor of the low-

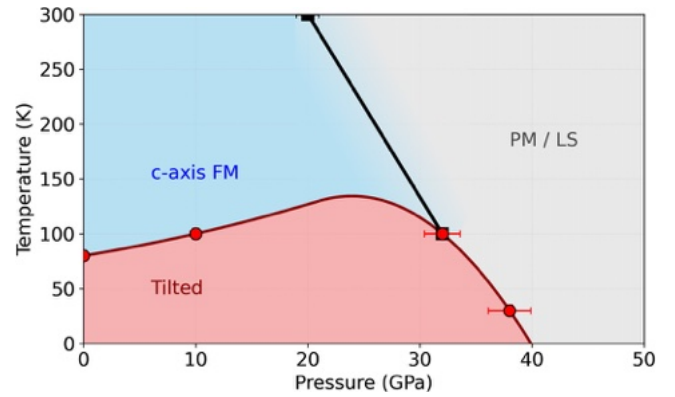


FIG. 9. Pressure–temperature phase diagram of Fe_3Sn_2 determined from XMCD, XES, and XRD measurements and DFT calculations. The diagram delimits the high-spin rhombohedral ($R\bar{3}m$) phase with a collinear ferromagnetic state (moments aligned along the c axis, in blue) and a low-temperature tilted magnetic configuration phase (in red). Under pressure, both phases transition to a low-spin state concomitant with a lower-symmetry $Pnma$ orthorhombic structure (in grey).

temperature one, shifting the magnetic phase boundary to higher temperatures.

Spin-polarized DFT calculations provide a microscopic framework for understanding these experimental observations. While the isotropic ferromagnetic exchange interactions remain robust and even slightly enhanced under compression, the local Fe magnetic moment gradually decreases with pressure, in agreement with the XES results. More importantly, our calculations reveal a pronounced enhancement of spin-orbit-coupling-driven anisotropic interactions under pressure, manifested by an increase of the magnetocrystalline anisotropy energy and a substantial amplification of the Dzyaloshinskii-Moriya interaction. These effects favor a canting of the magnetic moments away from the c axis and provide a natural explanation for the pressure-induced stabilization of the tilted magnetic phase observed by XMCD. To summarize our findings, we present in Fig. 9 the full pressure–temperature schematic phase diagram of Fe_3Sn_2 as determined from the combined XMCD, XES, and XRD measurements and DFT calculations.

The identified structural transition from the rhombohedral $R\bar{3}m$ phase to the orthorhombic $Pnma$ phase at ~ 22 GPa also carries profound implications for the topological electronic structure of Fe_3Sn_2 . This ambient-pressure picture has been independently confirmed by magneto-optical spectroscopy, which traced the anomalous Hall response directly to helical volumes of low-energy band crossings in momentum space, providing a momentum-resolved signature of the same SOC-gapped kagome-derived bands identified in our Berry curvature calculations [16]. Our results show that pressure redistributes precisely these features: the Berry curvature hotspots near the H and S points at ambient conditions are relocated toward the Γ -T region under compression, with the emergence of compensating positive and negative contributions that explain the observed 79% suppression of the AHC. This redistribution is consistent with a momentum-space reconfiguration of the same helical band structure rather

than its outright destruction at 21.7 GPa, suggesting that the full collapse of the anomalous Hall response—and the associated loss of Weyl node protection—is more directly tied to the subsequent $Pnma$ transition than to the rhombohedral compression alone. Our results show that the $Pnma$ transition involves a significant symmetry reduction and a distortion of the kagome layers. This structural degradation is expected to lift the protection of the Dirac nodes, potentially opening gaps or annihilating the Weyl points that characterize the topological phase at low pressure. Furthermore, our XMCD data and DFT calculations reveal that pressure strengthens the DM interaction and the magnetocrystalline anisotropy, favoring a tilted or in-plane magnetic configuration over the c -axis alignment. Because the position and stability of Weyl nodes in magnetic topological insulators are highly sensitive to the magnetization direction, this pressure-induced spin reorientation serves as a tuning knob to relocate these nodes in reciprocal space or to drive a topological phase transition toward a trivial metallic state. Finally, the high-spin to low-spin transition observed via XES at the structural boundary suggests a radical modification of the Fe $3d$ orbital hybridization. In fact, our first-principles calculations reveal that hydrostatic pressure reconstructs the kagome-derived low-energy electronic structure, redistributes the Berry curvature in momentum space, and suppresses the intrinsic anomalous Hall conductivity.

Taken together, our results establish pressure as a powerful tuning parameter that reshapes the magnetic as well as electronic energy landscapes of Fe_3Sn_2 by simultaneously acting on structural symmetry, spin state, and magnetic anisotropy. The pressure-induced reduction of crystal symmetry and the concomitant enhancement of spin-orbit coupling destabilize the high-temperature collinear magnetic phase in favor of a canted configuration that becomes stable over an extended pressure–temperature region.

The fact that the high-pressure structure is only partially captured by DFT suggests that additional structural complexity, such as disorder, superstructural modulations, or subtle atomic rearrangements, may play a role in stabilizing the observed magnetic phases. More broadly, our findings highlight the central role of spin-lattice coupling in kagome magnets and demonstrate how external pressure can be used to selectively tune magnetic orientation independently from the local moment amplitude. Given the strong impact of spin orientation on the topological electronic structure of kagome systems, these results open perspectives for pressure-driven control of topological and magnetic phases in Fe_3Sn_2 and related materials.

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DATA AVAILABILITY

The data that support the findings of this article are available from the corresponding author upon reasonable request.

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