

Effect of applied pressure on the nonrelativistic spin splitting of the altermagnet FeSb₂: A first-principles study

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We have investigated the pressure-dependent electronic structure, phonon stability, and anomalous Hall response of the recently discovered altermagnet FeSb₂ from density functional theory (DFT) and Wannier function analysis. From density functional perturbation theory (DFPT) calculations, we have found that FeSb₂ remains dynamically stable up to 10 GPa, evidenced by positive phonon frequencies. Our spin-polarized band structure reveals that the crossing nodes between the spin-up and spin-down bands near the Fermi energy occur precisely at the Γ and Z high-symmetry points. The Fermi crossing is mostly exhibited by band-24, band-25, and band-26. The nonrelativistic spin-splitting (NRSS) along $M'-\Gamma-M$ and $A-Z-A'$ high symmetry paths is attributed to the symmetry operation $[C_2||C_{2v}t]$ and broken time-reversal symmetry ($\mathcal{T}$). Significant changes in the band structure are observed under applied pressure, as evidenced by the shift of the crossing node between bands 24 and 26 toward higher energies. The NRSS exhibited by band-24 along $M'-\Gamma-M$ symmetry is notably small. Although the strength of NRSS associated with band-26 along the $A-Z-A'$ path is substantial, it decreases under applied pressure. We have calculated and presented the anomalous Hall conductivity (AHC) over the energy range from -1.5 to 1.5 eV. The pronounced positive AHC peak at ambient pressure becomes spectrally broadened, and changes sign at 10 GPa as a result of pressure-induced modifications to the band structure and the associated redistribution of Berry curvature near the Fermi level. Furthermore, we quantify the orbital magnetization within the modern theory framework, which reaches a magnitude of $0.29 \mu_B$ at zero pressure. Our results identify FeSb₂ as a tunable altermagnetic candidate, where applied pressure can modulate both topological transport and dynamical stability, opening new avenues for strain-engineered Hall responses in compensated magnetic systems.

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I. INTRODUCTION

Altermagnetism garners significant interest in condensed matter physics due to its potential applications in spintronics, particularly magnetic sensing and scalable data storage [1–3]. Altermagnets (AMs) are a new class of collinear magnetic materials that exhibit time reversal $\mathcal{T}$ symmetry breaking spin-split electronic bands despite having zero net

magnetization. This symmetry-protected spin splitting arises from the combined rotational and spatial symmetries [1–5]. Uniquely, this spin splitting does not rely on spin-orbit coupling (SOC), but instead stems from motif-pair anisotropy, enabling unconventional spin polarization [1,6–17]. Altermagnets thus bridge the gap between ferromagnets (FMs) and antiferromagnets (AFMs), offering the spin functionality of the former and the stability of the latter. Recently identified AMs with collinear AFM order and nonrelativistic spin splittings (NRSS) from the experiments include MnTe [18–20], CrSb [21–24], KV₂Se₂O [25], CoNb₄Se₈ [26,27], and others. While RuO₂ has been proposed as a potential altermagnet, its magnetic nature remains under debate [28–32]. Some of us recently managed to give a new perspective on the emergence of altermagnetism in RuO₂ by exploring the case of ultrathin films made on this material [33].

Recently, we conducted first-principles electronic structure studies of FeSb₂ [34], revealing distinct asymmetry between spin-up and spin-down states in the spin-polarized electronic

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bands. Notably, the presence of NRSS in this collinear AFM provides a clear signature of altermagnetism in FeSb₂. Three bands cross the Fermi level (E_F), forming the Fermi surface of FeSb₂, and the band-resolved Fermi pockets exhibit d -wave symmetry with evident spin asymmetry. Furthermore, the quantum oscillation frequencies derived from the extremal cross-sectional areas of the Fermi surface are in good agreement with experimental de Haas–van Alphen (dHvA) frequencies.

While the intrinsic magnetic and topological properties of AMs have recently attracted significant attention, their response to external stimuli such as pressure or strain remains relatively underexplored. Pressure engineering, a well-established technique in condensed matter physics, offers a clean and effective way to tune interatomic distances, lattice symmetry, and crystal-field environments without introducing chemical disorder [35–37]. This method has proven to be a powerful tool for modulating electronic, magnetic, and topological properties across a wide range of quantum materials. For instance, Devaraj *et al.* employed first-principles calculations and spin-group analysis to demonstrate tunable altermagnetism in α -MnTe and γ -MnTe under pressure, revealing enhanced spin-splitting and anomalous Hall conductivity (AHC) in various antiferromagnetic configurations with values exceeding 370 S/cm and 400 S/cm, respectively [37]. Similarly, Fan *et al.* reported stable altermagnetic ordering in MnF₂ across a pressure range of 0–20 GPa, with spin-splitting tunable up to 307.5 meV [36]. In FeSe, applied pressure enhances superconductivity from 8 K to over 35 K by modifying the nematic order and reconstructing the Fermi surface [38]. In Mn₃Sn, uniaxial strain has been shown to control both the magnitude and sign of the AHC by reshaping the Berry curvature distribution [39]. Likewise, the Dirac semimetal Cd₃As₂ undergoes a topological phase transition under pressure, driven by Dirac node annihilation [40]. More recently, electrical switching and the Coulomb drag effect have also been reported on the altermagnetic materials [41,42].

This study investigates the impact of external pressure on the electronic and phononic properties of FeSb₂ using first-principles calculations. Our phonon dispersion analysis reveals that FeSb₂ maintains positive phonon modes up to 10 GPa, confirming the system’s dynamical stability within this pressure range. Additionally, electronic band structure calculations show a gradual suppression of spin splitting near E_F as pressure increases up to 10 GPa. We also examine how pressure influences the evolution of the Fermi surface, AHC, and spin Hall conductivity (SHC). Finally, we quantify the orbital magnetization on the basis of the modern theory based on the Berry phase.

II. COMPUTATIONAL DETAILS

For the spin-polarized electronic structure calculation, we have used density functional theory as implemented in quantum espresso [43–45]. A scalar nonrelativistic pseudopotential within the projector augmented wave with Perdew-Burke-Ernzerhof formalism of the generalized gradient approximation (GGA) is employed for the exchange and correlation potential [46,47]. A kinetic energy cutoff of 70 Ry and an electron density cutoff of 750 Ry is used. The threshold

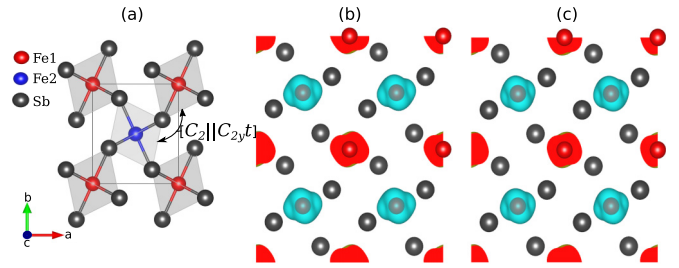


FIG. 1. (a) Unit cell structure of FeSb₂ with an anisotropic local environment. Spin density at (b) 0.25 GPa and (c) 10 GPa with an isosurface value of 0.004 a.u. red clouds represent spin-down ($\downarrow$) and cyan clouds represent spin-up ($\uparrow$), associated with the Fe1 and Fe2 atoms, respectively.

(for the self-consistent simulations) is set to 10^{-6} Ry. For the integration of the first Brillouin zone, we have used the k mesh of $12 \times 12 \times 12$ within a Monkhorst-Pack scheme [48]. Structural optimization was performed with the option ‘vc-relax’ within the Broyden-Fletcher-Goldfarb-Shanno algorithm [49–52]. The optimized lattice parameters were adopted for the calculations of the various properties explored in the current study. The unit cell and the associated magnetic configurations are illustrated in Fig. 1. The dependence of the lattice parameter and unit cell volume as a function of the applied pressure is shown in Fig. S1 of the Supplemental Material [53]. The computed value of equilibrium lattice parameter ($a = 5.8193$ Å, $b = 6.5323$ Å, $c = 3.2008$ Å) is in fairly good agreement with the experimental reports [54,55].

To account for the electronic correlation effects of the Fe $3d$ electrons, the Hubbard U parameters were calculated within density-functional perturbation theory across the investigated pressure range, following Ref. [56]. These parameters were subsequently employed within the GGA + U approach. Although previous studies report increasing [57] and decreasing [58] trends of U under pressure, we find an increase in U (see Fig. S2 of the Supplemental Material [53]), indicating an intricate behavior. Consistent with constrained random phase approximation results, this trend arises despite enhanced bandwidth and orbital overlap under compression. The dominant effect is the increase in transition energies between occupied and unoccupied states, which suppresses the electronic polarization and weakens screening [57].

To verify the structural and thermodynamic stability, we have calculated the phonon dispersion [59]. FeSb₂ is found to be stable with the lowest energy in the antiferromagnetic state at ambient conditions, consistent with the experimental report [34,60]. This behavior is maintained as a function of pressure, as shown in Fig. S3(a) of the Supplemental Material [53], after proceeding to a fit based on the Murnaghan equation [35,61–63] [see Fig. S3(b) of the Supplemental Material [53]]. Including spin-orbit coupling, we also performed ground-state energy calculations for various magnetic orientations at high pressure (10 GPa) and found that the most preferable state corresponds to the spin magnetization aligned along the c axis (see Table S1 of the Supplemental Material [53]).

Furthermore, along with the electronic structure calculation, we have extended our calculations to explore the magnetotransport properties of this Material, such as the

anomalous and spin Hall conductivities, using Wannier functions as implemented in Wannier90 [64]. From the interpolated Wannier bands, a geometrical phase of the wave functions can be extracted, which gives the Berry curvature [given by Eq. (1)] [65,66]. The AHC σ_{xy}^{AHC} and SHC σ^{SHC} for all occupied bands were evaluated by integrating the Berry curvature in the Brillouin zone over a dense $\mathbf{k}$ -point mesh using Kubo's formula within linear response theory given by Eqs. (2) and (3), respectively [65,67,68].

$$\Omega_n^z(\mathbf{k}) = -2, \text{Im} \sum_{m \neq n} \frac{\langle u_{n\mathbf{k}} | \hat{v}_x | u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | \hat{v}_y | u_{n\mathbf{k}} \rangle}{(E_{m\mathbf{k}} - E_{n\mathbf{k}})^2}, \quad (1)$$

where $\Omega_n^z(\mathbf{k})$ is the Berry curvature for band (n), $u_{n\mathbf{k}}$ are the cell-periodic parts of Bloch functions, $\hat{v}_x$ and $\hat{v}_y$ are velocity operators, $E_{n\mathbf{k}}$ are the band energies:

$$\sigma_{xy}^{\text{AHC}} = -\frac{e^2}{\hbar} \int_{\text{BZ}} \frac{d\mathbf{k}}{(2\pi)^3} \sum_n^{\text{occ}} \Omega_n^z(\mathbf{k}), \quad (2)$$

where e is the electron charge, $\hbar$ the reduced Planck constant, and the sum runs over the occupied bands:

$$\sigma^{\text{SHC}} = \frac{\hbar}{2e} \times \int_{\text{BZ}} \frac{d\mathbf{k}}{(2\pi)^3} \sum_n^{\text{occ}} \Omega_n^{s,z}(\mathbf{k}), \quad (3)$$

where $\Omega_n^{s,z}(\mathbf{k})$ is the spin Berry curvature, computed similarly to the Berry curvature but incorporating spin operators.

In practice, we assume a dense $\mathbf{k}$ grid of $150 \times 150 \times 150$, and the magnetization is considered along the [001] direction to compute the AHC and SHC. To address the orbital moments using the modern theory of orbital magnetization, we follow Refs. [69–75], and assumed a $\mathbf{k}$ grid of $100 \times 100 \times 100$ points for the calculations.

III. RESULTS AND DISCUSSION

A. Crystal structure and phonon analysis

The crystal structure of FeSb₂, having space group $Pnmm(58)$ with two antiferromagnetically coupled Fe1 and Fe2 atoms, each carrying a magnetic moment along the c axis, is shown in Fig. 1(a). The constant spin density around the two magnetic atoms is represented by a transparent cloud showing anisotropy between spin-up and spin-down atoms (denoted by cyan and red colors) [see Figs. 1(b) and 1(c)]. Due to the reduction of the magnetic moment per atom as a function of pressure (see Table S2 of the Supplemental Material [53]) induced by strong hybridization of the Fe-3d/Sb-5p orbitals, the plotted spin density experiences a reduced volume.

For further analysis of the dynamical stability, we have performed phonon calculations. The dispersion of phonons and the associated projected density of states (DOS) of FeSb₂ under external pressures ranging from 0 to 10 GPa reveal a pressure-dependent evolution of vibrational stability in this altermagnetic system. At ambient pressure (0 GPa), the phonon spectrum does not show imaginary frequencies in the Brillouin zone, confirming dynamical stability. The acoustic modes below 100 cm^{-1} and the distinct optical branches up to 270 cm^{-1} are well separated, with DOS projections indicating dominant Sb contributions in the lower frequency region, consistent with the mass and bonding asymmetries as

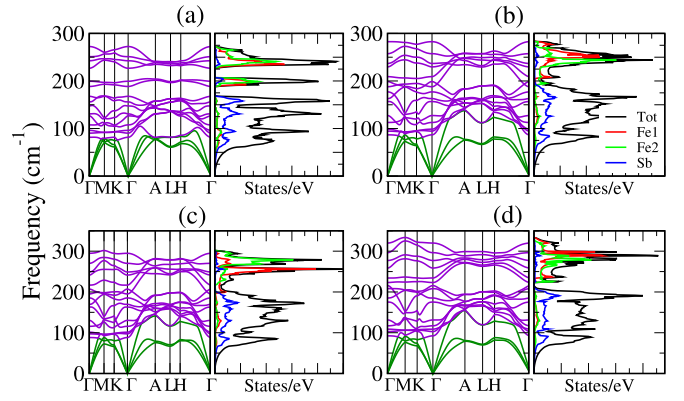


FIG. 2. Phonon dispersion relations and phonon density of states (DOS) for FeSb₂ under hydrostatic pressures of (a) 0 GPa, (b) 1 GPa, (c) 4 GPa, and (d) 10 GPa. The absence of imaginary frequencies in all panels confirms the dynamical stability of FeSb₂ across this pressure range.

in Fig. 2(a). As pressure increases to 1 GPa, the entire phonon spectrum exhibits a moderate blue shift, reflecting a stiffening of the lattice and a compression-induced enhancement of interatomic force constants. The structure of the phonon band remains real-valued with no soft modes, indicating that FeSb₂ retains its dynamical stability in this low-pressure regime. At 4 GPa, the phonon branches shift further upward in frequency, and the optical modes become slightly more dispersive, especially along the Γ -A and L-H directions, which can be seen in Fig. 2(c). Despite the increasing pressure, the absence of imaginary phonon modes confirms that the Material remains dynamically stable up to this pressure threshold. When pressure is further increased to 10 GPa, no imaginary phonon modes were still observed, a point indicating stiffening of the interatomic force constant and dynamical stability. The highest optical mode at Γ point is around 320 cm^{-1} [see Fig. 2(d)]. The total and projected DOS of the phonon continue to show significant Sb character in low-frequency modes, with notable Fe1 and Fe2 contributions at intermediate frequencies, suggesting enhanced lattice participation of iron atoms under compression. Our predictions indicate the mechanical robustness of FeSb₂ and highlights the potential resilience of its crystalline phase against the external perturbations.

B. Electronic properties

The antiferromagnetic ground state of FeSb₂ at ambient pressure has already been confirmed by experimental observations [34], and the comparison in terms of energy between different magnetic (AFM and FM) configurations from our density functional theory calculations is shown in Fig. S3(a) of the Supplemental Material [53].

To investigate the influence of external pressure on the electronic structure and the emergence of altermagnetism in FeSb₂, we computed its spin-resolved band structures under various pressures (0.25–10 GPa), as shown in Fig. 3 and examined the resulting pressure dependence of the NRSS, as shown in Fig. 4. Under ambient conditions, FeSb₂ exhibits motif pair anisotropy accompanied by collinear antiferromagnetic coupling between the two Fe atoms. The local

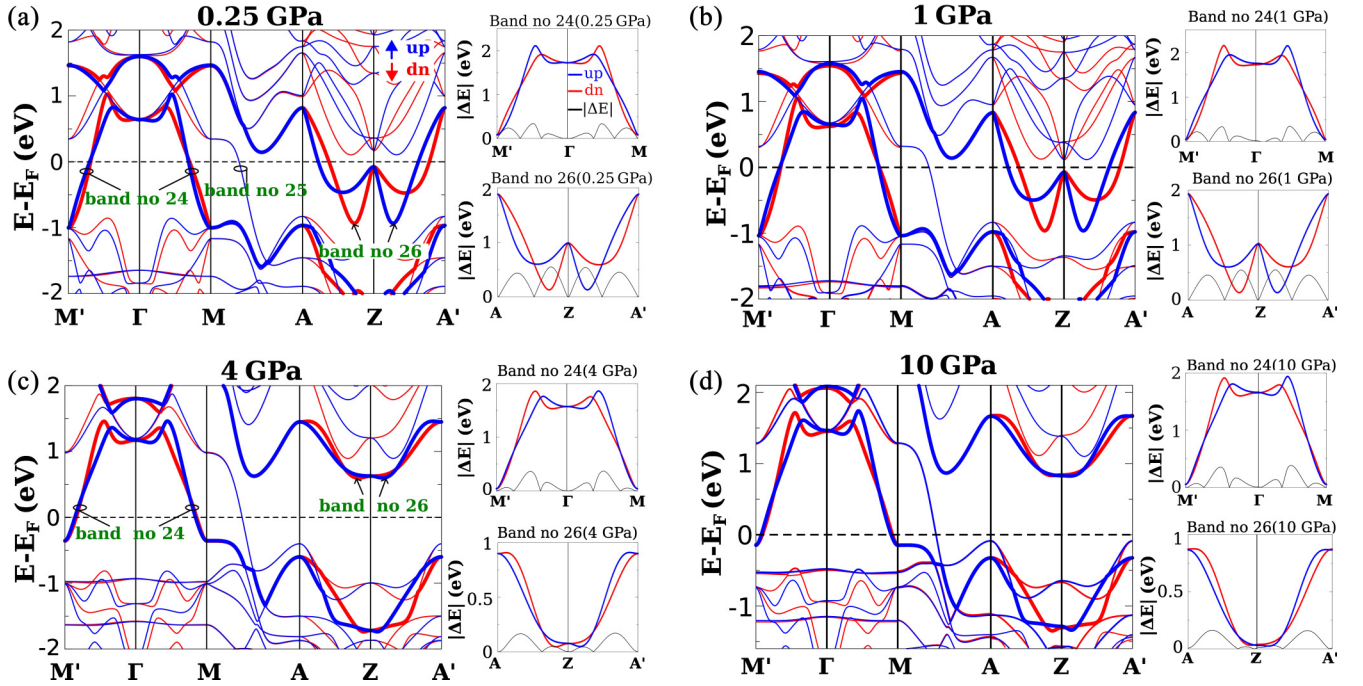


FIG. 3. Spin-resolved electronic band structures of FeSb₂ under varying hydrostatic pressure: (a) 0.25 GPa, (b) 1 GPa, (c) 4 GPa, and (d) 10 GPa. Blue and red lines represent spin-up and spin-down states, respectively. Spin splitting in the absence of net magnetization indicates the presence of altermagnetic order. The evolution of band dispersion and spin splitting with increasing pressure highlights the pressure dependence of altermagnetism in FeSb₂. E_F is set to zero.

environments surrounding the Fe1 and Fe2 atoms are related by a twofold rotational symmetry around the [010] direction, followed by half a unit cell translation [$C_2||C_{2y}t$], while the $\mathcal{T}$ symmetry flips the spin quantization axis in the nonrelativistic limit [60]. This combined action of spatial and $\mathcal{T}$ symmetries underpins the altermagnetic order observed in the system. The complete analysis of the electronic structure of FeSb₂ at ambient conditions has already been performed using spin-polarized and SOC approaches and reported as a potential altermagnet candidate [34]. The dispersion of the band was evaluated along the optimal path connecting high symmetry points within the first Brillouin zone, specifically

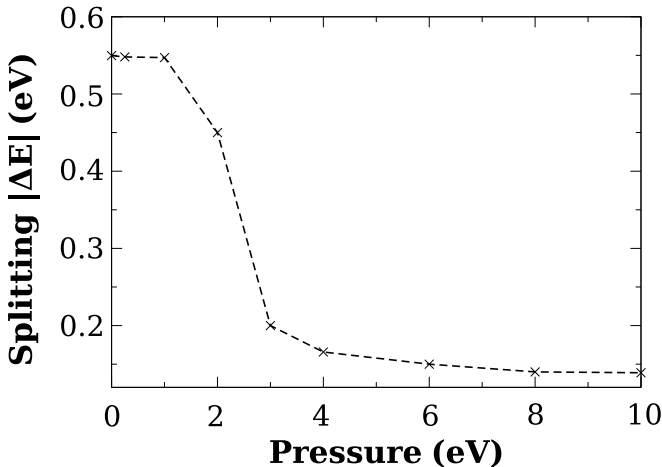


FIG. 4. Variation of splitting energy under applied pressure in the range of 0 to 10 GPa for band-26.

$M'-\Gamma-M-A-Z-A'$, as illustrated in Fig. 5(a). This path was selected to capture the key features of the electronic profile illustrating the altermagnetic behavior. Indeed, the presence of NRSS near the high-symmetry points in the fully compensated magnetic system in the absence of SOC constitutes a hallmark of AM ordering. The strength of the NRSS ($|\Delta E|$) near-Fermi energy is determined from the energy difference between the spin-up and spin-down states, i.e., $|\Delta E| = E(\uparrow) - E(\downarrow)$ [1,2,6–8].

At 0.25 GPa, bands 24, 25, and 26 contribute to the Fermi surface topology since they cross the E_F , see Fig. 3(a). These bands exhibit prominent spin splitting around the E_F with a clear separation between spin-up and spin-down states, supporting altermagnetic behavior. Band 26 exhibits the largest splitting along the A-Z symmetry, followed by band 24 along

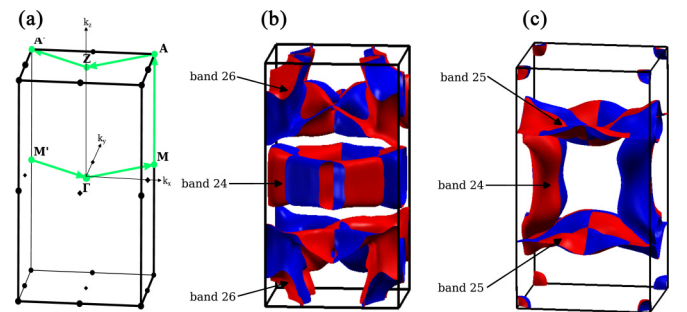


FIG. 5. (a) First Brillouin-zone with high symmetry points $M'-\Gamma-M-A-Z-A'$ and Fermi surface of FeSb₂ calculated at (b) 0.25 GPa and (c) 10 GPa [displaying two distinctive colors in each band representing spin-up (blue) and spin-down (red) bands].

Γ -M, while band 25 shows moderate splitting above the Fermi energy. The maximum value of NRSS along Γ -M (band-24) and A-Z (band 26) symmetries are $|\Delta E| = 0.3397$ eV and $|\Delta E| = 0.5497$ eV, respectively. From the analysis of the orbital-projected PDOS we have noticed that these bands are predominantly derived from Fe-3*d* orbitals, particularly d_{yz} orbital (see Fig. S4 of the Supplemental Material [53]).

On increasing the pressure up to 1 and 4 GPa, the NRSS of bands 24 and 26 preserves its spin splitting. However, the strength of NRSS decreases, while the crossing between opposite-spin bands, defining a node, shifts to higher energies [see Fig. 3(b)]. This trend becomes more prominent above 4 GPa, where the NRSS separation further decreases, and the bands begin to overlap more, indicating a suppression of altermagnetic effects under pressure [see Figs. 3(a)–3(c)]. On further increasing the pressure up to 10 GPa, the $|\Delta E|$ value drops from ~ 0.55 to ~ 0.14 eV (see Fig. 4). Notably, the reduction is more pronounced for band 26 than for band 24, where $|\Delta E|$ remains nearly constant over the same pressure range (0.25–10 GPa). This behavior indicates a stronger sensitivity of band 26 to external pressure compared to band 24.

The diminishing *d*-orbital character near the E_F with the applied pressure can be attributed to the suppression of the spin splitting, consistent with the previous reports [36,37,76]. At ambient pressure, the electronic states near E_F are predominantly derived from Fe-3*d* orbitals. As pressure increases, the Fe-3*d* contribution gradually decreases, while the contribution from Sb-5*p* orbitals increases near E_F (see Fig. S4 of the Supplemental Material [53]), indicating enhanced Fe-3*d*/Sb-5*p* hybridization. Furthermore, the magnitude of NRSS can be expressed qualitatively in terms of exchange interaction energy as $|\Delta E| \propto \frac{J_{\text{ex}}}{J_{\text{ex}}}$ [36,77]. In this framework, t_1 and t_2 correspond to the *d*-orbital hopping integrals, representing intraorbital (intrasublattice) and interorbital (intersublattice) hopping between two nearest neighboring atoms. Our results show that J_{ex} increases with pressure (see Fig. S5 of the Supplemental Material [53]), which in turn suppresses NRSS. The node of band-26 at Zpoint shifts above the Fermi energy, showing no E_F crossing at 10 GPa, whereas the bands 24 and 25 still cross the Fermi energy [see Fig. 3(d)]. On the other hand, the $|\Delta E|$ value has been significantly suppressed and nearly degenerate, especially along the A-Z directions. Within the investigated pressure range, we find no evidence of a structural phase transition, consistent with previous reports [54]. This result shows the role of applied pressure in reducing the exchange splitting in FeSb₂ and diluting the essence of altermagnetism. The variations in band structures across the entire investigated pressure range are shown in Fig. S6 of the Supplemental Material [53].

Figure 5, illustrates the Fermi surface of FeSb₂ at 0.25 GPa and 10 GPa, highlighting bands 24, 25, and 26 with spin-resolved pockets. At 0.25 GPa, band-24 forms a distinct red- and blue-colored pocket near the zone center, primarily derived from Fe-3*d* orbitals. However, band 26 disappears entirely at 10 GPa, indicating a pressure-induced band shift above E_F and leading to anisotropic hole pockets. Band-25, with contributions from both Fe-3*d* and Sb-5*p* orbitals, shows red (spin-down) and blue (spin-up) colored lobes that evolve into more coherent structures under pressure, suggesting en-

hanced hybridization. The observed Fermi surface evolution underlines the sensitivity of orbital contributions to external pressure and the potential tunability of altermagnetic features in FeSb₂.

C. Anomalous and spin Hall effect

The AHE serves as a macroscopic probe of $\mathcal{PT}$ (where $\mathcal{P}$ inversion or parity)-symmetry breaking in magnetic systems. Traditionally associated with ferromagnets and noncollinear antiferromagnets, AHE has recently been observed in AMs in the presence of SOC. The intrinsic AHE arises from a finite Berry curvature generated by SOC in magnetic systems whose symmetries permit a nonvanishing Brillouin-zone-integrated Berry curvature. In altermagnets, crystallographic rotational symmetry gives rise to characteristic spin-split band structures, while SOC acts on these bands to produce a finite Berry curvature and consequently a nonzero AHC. Unlike ferromagnets, where AHE is allowed in symmetry in all orientations, altermagnets display AHE only for specific Néel vector directions relative to the crystal axes. In α -MnTe, for instance, AHE emerges when the Néel vector aligns with $\langle 1\bar{1}00 \rangle$ axes, showing hysteresis and remanent signal [16]. In tetragonal RuO₂, the AHE has been observed in (110)-oriented thin films when the Néel vector is aligned along the [001] axis [78].

The incorporation of relativistic SOC gives rise to a finite orbital magnetic moment calculated with the modern theory of orbital magnetization. The moment has a dominant component $|M_z^{\text{orb}}|$ of approximately 0.29 (μ_B/cell) in FeSb₂, as shown in Fig. S7 (at 0 GPa) of the Supplemental Material [53]. This orbital contribution mediates a weak ferromagnetic component, thereby establishing SOC-induced ferromagnetism as the microscopic origin of the AHE [69].

Likewise, spin Hall effect plays a key role in spin-to-charge conversion that converts a charge current into spin current [68]. In FeSb₂, SHC is driven by spin-orbit entanglement of the Fe-3*d* and Sb-5*p* states, especially where spin-up and spin-down components are spatially separated due to SOC.

In the following, we address and present the AHC and SHC spectra of FeSb₂, considering the ground state orientation of the magnetization ([001] direction) under applied pressures of 0–10 GPa (see Fig. 6).

Figure 6(a) shows the AHC and SHC at ambient pressure (0 GPa). We observe the highest AHC peak of approximately 129.0 S/cm at -0.07 eV, while the AHC at the Fermi energy (E_F) is approximately 100 S/cm, which is in fairly good agreement with the previously reported value [60]. The maximum value of SHC is about 36.0 ($\hbar/e \times \text{S/cm}$) at 0.055 eV, indicating strong Berry curvature contributions from altermagnetic band crossings, and the SHC at E_F is ~ 32.5 ($\hbar/e \times \text{S/cm}$).

These features correspond to sharp Berry curvature contributions from nodal structures near E_F , consistent with our prior analysis of altermagnetic band crossings, as shown in Fig. 3. Figure 6(b) depicts AHC and SHC at 1 GPa, showing broader and more asymmetric features. The AHC peak near -1.19 eV, which is around 131.0 (S/cm), and the value at E_F is 50.9 (S/cm). Such large values of AHC are often desired in spintronics functionalities [60]. The maximum value of SHC is around 26.0 ($\hbar/e \times \text{S/cm}$) at -1.33 eV, and its

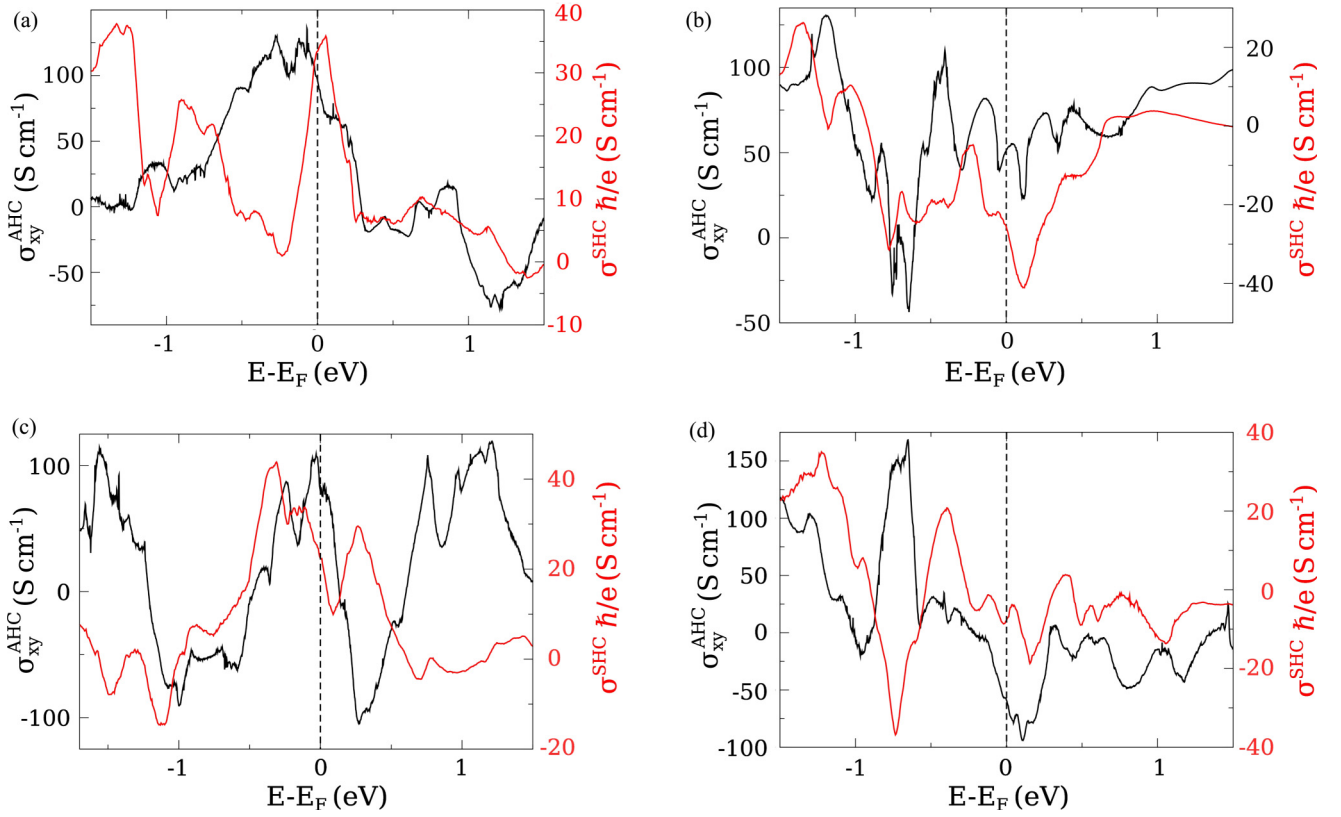


FIG. 6. Anomalous Hall conductivity (Scaling on the left side) and Spin Hall conductivity (Scaling on the right side) of FeSb₂ calculated at different pressures: (a) 0 GPa, (b) 1 GPa, (c) 4 GPa, and (d) 10 GPa. The AHC, σ_{xy}^{AHC} , is plotted as a function of energy relative to the E_F . At ambient pressure, sharp peaks reflect strong Berry curvature near the E_F , consistent with altermagnetic band topology. With increasing pressure, the spectral features evolve significantly, showing redistribution, suppression, and broadening of AHC signatures, indicative of pressure-tuned topological transitions in the electronic structure.

value is approximately $6.5 (\hbar/e \times \text{S/cm})$ at E_F . On further increasing the pressure to 4 GPa, the peak value of AHC is reduced to 119.0 (S/cm) at 1.21 eV and 110.7 (S/cm) at E_F [see Fig. 6(c)]. The SHC is found to be $43.5 (\hbar/e \times \text{S/cm})$ at around 0.3 eV and $26.0 (\hbar/e \times \text{S/cm})$ at E_F . The reduction in AHC suggests a pressure-induced suppression of spin-orbit-driven transport where the dominant topological features are modified. At 10 GPa, spectral weight shifts into the negative-energy region. The maximum value of AHC is 168.0 (S/cm) at -0.7 eV, however, the AHC at E_F has been decreased to -79.2 (S/cm) as compared to the one at 4 GPa. Meanwhile, the maximum value of SHC is around $35.0 (\hbar/e \times \text{S/cm})$ and lies at -1.21 eV while it goes down to $-8.6 (\hbar/e \times \text{S/cm})$ at E_F [see Fig. 6(d)]. Interestingly, the sign of the conductivities at E_F changes under pressure. This suggests enhanced Berry curvature contributions from deeper-lying bands, owing to pressure-induced band inversions [39,79,80]. Here, we observe an overall increase in $|\sigma_{xy}^{\text{AHC}}|_{\text{max}}$, while $|\sigma_{xy}^{\text{AHC}}|_{E_F}$ and $|\sigma^{\text{SHC}}|$ exhibit complex variation under compressive pressure. Despite the spectral complexity, a significant AHC persists, implying robust topological character even under high compression. The coexistence and tunability of both AHC and SHC highlight the dual spin-charge transport nature of this material and its potential for pressure-controlled spintronic functionalities.

IV. SUMMARY

In this study, we have systematically explored the effect of pressure on the electronic, magnetic, and transport properties of FeSb₂, a recently proposed altermagnetic material [34,60]. Our first-principles calculations predict that the system remains dynamically stable up to 10 GPa, as confirmed by phonon dispersion analysis. With increasing pressure, FeSb₂ undergoes a significant reconstruction of its electronic structure near the E_F , accompanied by pronounced changes in the Fermi surface topology and anomalous transport response.

Our calculations further reveal the microscopic origin of these pressure-induced phenomena. The reduction of lattice parameters and unit-cell volume under pressure decreases interatomic distances, leading to stronger Fe-3d/Sb-5p hybridization and an increase in the exchange interaction energy. The resulting modification of the spin-split electronic structure associated with the altermagnetic order drives a redistribution of Berry curvature throughout the Brillouin zone (see Fig. S8 of the Supplemental material [53]). Consequently, the anomalous Hall conductivity evolves from a sharply peaked positive response at ambient pressure to a spectrally broadened and predominantly negative response at higher pressures. The inclusion of spin-orbit coupling further gives rise to weak ferromagnetism through slight spin canting and produces finite orbital magnetization, providing a micro-

scopic explanation for the emergence of the anomalous Hall effect in FeSb₂.

These findings establish a direct connection between lattice compression, orbital hybridization, exchange interactions, Berry curvature, and anomalous transport in FeSb₂. More broadly, our results demonstrate that pressure provides an effective route for tuning altermagnetic electronic properties and Berry-phase-driven transport phenomena, highlighting FeSb₂ as a promising platform for the exploration and engineering of pressure-controlled altermagnetic spintronic functionalities.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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