

Identifying oriented spin space groups and related physical properties using an online platform FINDSPINGROUP

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ABSTRACT

Unconventional magnets combining antiferromagnetic structures with ferromagnetic-like responses are essential for the development of next-generation spintronics. Their emergent properties are fundamentally dictated by the interplay between exchange-driven magnetic geometry and spin-orbit coupling, described by spin space groups and magnetic space groups, respectively. However, the lack of direct correspondence between these frameworks hinders the systematic tracking of symmetry evolution of these intertwined physical contributions. Here we introduce FINDSPINGROUP, an online platform based on the oriented spin space group framework to unify spin space group and magnetic space group descriptions. By automating the tracking of symmetry-breaking pathways from the absence to the presence of spin-orbit coupling effects, FINDSPINGROUP enables the classification of magnetic phases and the derivation of symmetry-constrained tensors for phenomena such as momentum-dependent spin splitting and the anomalous Hall effect. By standardizing data exchange through the spin crystallographic information file, FINDSPINGROUP establishes a computational infrastructure for the high-throughput discovery and design of unconventional magnets.

Keywords: unconventional magnets, oriented spin space group, online platform, spin-orbit coupling, spin polarization, anomalous Hall effect

INTRODUCTION

The exploration of magnetic materials with high storage density, ultrafast dynamics, and electric controllability is central to next-generation spintronic devices [1,2]. In recent years, unconventional magnets that combine ferromagnetic-like responses with antiferromagnetic structures have emerged as promising candidates [3]. These systems host diverse emergent phenomena arising from two distinct physical sources: the magnetic geometry governed by exchange interactions and the spin-orbit coupling (SOC) effect. Here, the magnetic geometry refers to the spatial distribution of magnetic moments. However, the textbook magnetic space group (MSG) framework assumes complete locking between lattice and spin spaces [4], which naturally conflates effects driven by magnetic geometry with those solely induced by SOC. Recently, the spin space group (SSG) theory has emerged as an extended framework to provide a comprehensive description of magnetic geometry by decoupling symmetry operations in lattice and spin spaces [5-16]. This has led to a new symmetry paradigm for understanding the physical effects of unconventional magnets, such as spin splitting, anomalous Hall effect (AHE), and magnetoelectric coupling [12,17-28], i.e., employing SSG to describe the effects induced by magnetic order and MSG to characterize the SOC effects.

Despite this conceptual framework, its practical implementation for real materials remains hindered by the lack of a unified platform. In practice, different conventions between SSG and MSG frameworks, such as cell choices and coordinate systems, often hinder direct comparisons of physical responses across regimes with and without SOC. Without a unified convention, reconciling these two symmetry descriptions requires manual realignment, which is inefficient and error-prone. While existing tools can identify SSG operations [29-31], they lack an automated workflow to bridge the SSG and MSG descriptions and analyze physical properties. Consequently, tracing the symmetry-breaking pathways of physical properties under SOC has remained largely manual, limiting systematic and high-throughput discovery of unconventional magnetism.

In this work, we address these challenges by introducing FINDSPINGROUP, an open-source platform for the automated identification of magnetic symmetry, magnetic phases, and various symmetry-constrained physical properties. Specifically, the platform is built on the recently developed oriented spin space group (OSSG) framework [32], which unifies the SSG and MSG frameworks and explicitly elucidates the symmetry-breaking pathways from SSG to MSG. FINDSPINGROUP generates standardized outputs, including magnetic cells, spin Wyckoff positions, spin site-symmetry groups, the spin Brillouin zone, and spin little co-groups. This automated workflow enables a systematic investigation of how various physical properties evolve as magnetic order and SOC are sequentially introduced, covering fundamental properties such as magnetizations, electric polarization, and spin polarization, as well as transport tensors. Beyond these capabilities, the practical utility of this workflow is demonstrated by its integration with other tools such as STensor [33] and TensorSymmetry [34]. This interoperability, along with its widespread adoption [20,21,23,32-37], establishes FINDSPINGROUP as a computational infrastructure for investigating unconventional magnets.

SYMMETRY FRAMEWORK AND IMPLEMENTATION

Spin space group and oriented spin space group

The symmetry operations of the SSG can be expressed as $\{g_s || g_l | \tau\}$, where $g_s \in \{U_m(\varphi), TU_m(\varphi)\}$ consists of spin rotations $U_m(\varphi)$ and the time reversal T that simultaneously reverses spin and momentum, while $g_l \in \{C_n(\theta), PC_n(\theta)\}$ comprises lattice rotations $C_n(\theta)$ and the spatial inversion P . A magnetic structure is characterized by specifying the atomic positions (r) and magnetic moments (m). The action of an SSG operation on the tuple (r, m) is defined as:

$$\{g_s || g_l | \tau\}(r, m) = (D(g_l)r + \tau, D(g_s)m). \quad (1)$$

Here, $D(g_l)$ denotes the matrix representation of the lattice operation g_l in the lattice coordinate basis of r , while $D(g_s)$ denotes the orthogonal matrix representing the spin operation g_s in the Cartesian spin basis of m . And the product of two SSG operations

is defined as:

$$\{g_{s_1}||g_{l_1}|\tau_1\}\{g_{s_2}||g_{l_2}|\tau_2\} = \{g_{s_1}g_{s_2}||g_{l_1}g_{l_2}|g_{l_1}\tau_2 + \tau_1\}. \quad (2)$$

The general form of an SSG, denoted by G_{SS} , can be expressed as the direct product of a nontrivial SSG G_{NS} and the spin-only group G_{SO} [8]:

$$G_{SS} = G_{NS} \times G_{SO}. \quad (3)$$

where G_{NS} denotes the nontrivial SSG that every spin operation is combined with a spatial operation, except for the identity element. The spin-only group G_{SO} consists of pure spin operations $\{g_s||E|0\}$ and reflects whether the magnetic configuration is collinear, coplanar, or noncoplanar. Based on the nomenclature of SSGs developed in Ref. [14], we extend the four-index nomenclature ($L_0, G_0, i_k, index$) of the nontrivial SSG G_{NS} to Chen-Liu nomenclature ($G_0, L_0, i_k, index, L/P$) of the full SSG G_{SS} , where G_0 , L_0 , i_k , and $index$ represent the parent space group, sublattice space group, cell-expansion factor, and mapping sequence in the database, respectively. The additional fifth index L or P represents a collinear or coplanar spin-only group, respectively, and is omitted for noncoplanar configurations. The complete database of all SSGs, with their standard nomenclatures, is available on the FINDSPINGROUP website.

When considering SOC effects, operations in lattice and spin spaces become completely locked. Only the SSG operations that satisfy $U_m(\varphi) = C_n(\theta)$ are retained in the corresponding MSG, where the spin-space operations are encoded within the lattice operations and are thus not separately expressed. Although the SSG and MSG provide comprehensive descriptions of magnetic geometry and SOC effects, respectively, an SSG alone does not specify the physical orientations of its spin-space operations relative to the crystallographic frame (Fig. 1a). This ambiguity prevents a direct mapping from the SSG to the MSG, and hence a systematic comparison of physical properties with and without SOC remains elusive.

Historically, the characterization of phase transitions has relied on group-subgroup relationships, in which the symmetry-breaking path from a parent to a daughter phase is typically labeled by the irreducible representations of the parent group. For example,

magnetic representations are adopted to characterize the symmetry descent from a paramagnetic space group to an MSG [38,39]. Intriguingly, the symmetry descent from an SSG to its MSG subgroup can be established without introducing additional representations by selecting an oriented representative from the equivalent SSGs related by global spin rotations.

Physically, while the SSG describes an exchange-driven regime where spin space is isotropic and decoupled from the lattice space, it fundamentally represents an equivalence class under global spin rotations. To simultaneously describe the magnetic order and SOC effects, the OSSG framework establishes a physical orientation of the spin-space operations relative to the crystallographic frame by selecting a specific oriented representative from the equivalence class (Fig. 1b). This alignment explicitly introduces magnetic anisotropy into the symmetry description, thereby delineating the symmetry-breaking pathway from SSG to MSG [32]. Finally, in the full SOC limit where operations in lattice and spin spaces are completely locked, the corresponding MSG is naturally obtained by retaining only those OSSG operations compatible with the constraint $U_m(\varphi) = C_n(\theta)$.

In collinear and coplanar systems, the oriented representative further specifies the physical orientation of the spin-only group relative to the crystallographic frame. The crystallographic direction $[\alpha\beta\gamma]$ is used to label the principal axis of the magnetic moment in collinear systems, ${}^{\infty}\alpha\beta\gamma m1$, and the normal direction of the spin plane in coplanar systems ${}^m\alpha\beta\gamma 1$, respectively. Based on these, the connection between OSSG and the corresponding MSG can be established (Fig. 1c).

Take two altermagnets, CrSb and MnTe, as examples. They share the same underlying SSG $P^{-1}6_3/-^1m^1m^{-1}c^{\infty m}1$ (194.164.1.1.L), but can be distinguished by distinct OSSGs depending on their Néel order relative to the lattice. Specifically, both systems can be expressed by the general OSSG form $P^{-1}6_3/-^1m^1m^{-1}c^{\infty\alpha\beta\gamma m}1$, where the easy axis $[\alpha\beta\gamma]$ corresponds to $[001]$ and $[210]$, respectively. These fixed orientations dictate the completely locked operations from which the corresponding

MSGs are identified. For CrSb, the six-fold screw symmetry is preserved via the completely locked operation $\{-1 \cdot 6_{001}^1 \| 6_{001}^1 | \tau\}$. Combined with two operations $\{-1 \cdot 2_{001} \| m_{001} | \tau\}$ and $\{-1 \cdot 2_{210} \| m_{210} | \tau\}$ (where $\tau = (0,0,1/2)$), the system yields the hexagonal MSG $P6_3'/m'm'c$. In contrast, the in-plane Néel order of MnTe along $[210]$ axis is non-coaxial with the six-fold screw rotation along $[001]$ axis in lattice space. This misalignment breaks the six-fold rotation symmetry in the full SOC limit, as shown in Fig. 1c, thereby reducing the symmetry to the orthorhombic MSG $Cm'c'm$, which can be obtained from $\{-1 \cdot m_{001} \| m_{001} | \tau\}$, $\{-1 \cdot 2_{210} \| m_{210} | \tau\}$.

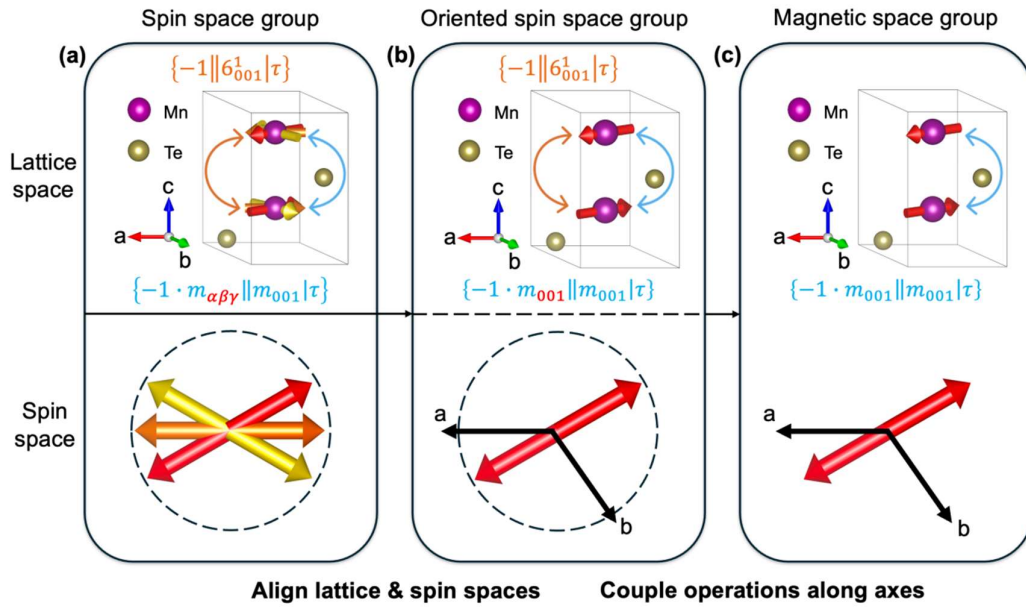


Figure 1. Evolution from SSG to MSG via the oriented framework. (a) In the SSG, the solid line in the middle separates two spaces, indicating that lattice and spin spaces are independent and have an arbitrary relative orientation. The multicolored spin arrows and dashed circle represent equivalent realizations related by global spin rotations, reflecting the absence of a uniquely selected physical orientation relative to the crystallographic frame. (b) In the OSSG, the dashed line indicates that the two spaces are aligned to define a material-specific orientation of magnetic orders, but the operations remain decoupled. (c) Upon introducing full SOC effects, the disappearance of the central line indicates complete coupling between spin and lattice spaces, and the magnetic moments are constrained along specific crystallographic axes. Only the subset of OSSG operations compatible with spin-lattice locking is preserved, yielding the

corresponding MSG. The orientational degeneracy is removed, and the dashed circle therefore disappears. This construction integrates descriptions regarding magnetic geometry and SOC effects, along with their symmetry evolution pathways, into a unified framework. For visual clarity, the atomic motif is shown with the origin shifted by $(0,0,1/4)$ relative to the standard setting. Note that all symmetry operations are defined with respect to the standard setting. For example, the glide mirror $\{-1 \cdot m_{001} || m_{001} | \tau\}$ is located at $z = 1/4$ in the standard setting, which corresponds to the $z = 1/2$ plane here.

Identification and standardization

Systematic identification of the OSSG requires a standard numerical framework to ensure consistency across regimes with and without SOC. In FINDSPINGROUP, the OSSG of a magnetic structure is determined by evaluating the symmetry operations within the direct product of the parent space group and the point group in spin space [14]. Throughout this work, the crystallographic part of the spin-group setting, including the basis vectors, cell setting, and origin choice, is expressed in the standard space-group convention of the Bilbao Crystallographic Server [40]. Besides, we introduce the .scif format, termed SpinCIF (spin crystallographic information file). Analogous to the .mcif format for MSGs, the .scif format records magnetic structures together with their OSSG descriptions. The coordinate conventions associated with the symmetry data are retained, supporting data exchange across different settings and reuse by compatible tools, including tensor-symmetry analysis with STensor [33] and visualization with tools such as Jmol and VESTA [41,42]. Detailed information on identification and the SpinCIF representation is provided in the Methods section.

Following the space groups and MSGs, the spin Wyckoff positions and spin site-symmetry groups are introduced to evaluate the Wyckoff-position splitting induced by magnetic order. Notably, the spin site-symmetry groups of an OSSG are always isomorphic to a subset of the 941 spin point groups. This isomorphism ensures that site-dependent effects can be exhaustively classified; for instance, only 375 spin point

groups allow local magnetic moments. In reciprocal space, the OSSG dictates the symmetry of the spin Brillouin zone. While collinear and coplanar systems are characterized by the 24 centrosymmetric arithmetic crystal classes, noncoplanar SSGs correspond to all 73 arithmetic classes [43]. The construction of spin Wyckoff positions, the associated spin site-symmetry groups, and the little co-groups of wave vectors within the OSSG convention are discussed in the Methods section. This ensures the precise identification of high-symmetry wavevectors, providing a comprehensive description of momentum-dependent spin physics.

SYMMETRY-DICTATED PHYSICAL PROPERTIES

According to Neumann's principle, the symmetry of any physical property of a crystal must include the symmetry operations of its point group [44]. Consequently, crystallographic and magnetic point groups are often employed to impose symmetry constraints on physical properties such as ferroelectricity, magnetic moments, and various transport effects [45,46]. However, unlike space groups and MSGs, which strictly reduce to finite 32 point groups and 122 magnetic point groups upon removing translations, SSGs can reduce to a much wider class of spin point groups than those derived from crystallographic constraints. Since spin and lattice spaces are decoupled, an SSG naturally permits spin propagation of the form $\{g_s || E | \tau\}$, where g_s can be a non-crystallographic spin rotation. Consequently, the 598 nontrivial spin point groups [9] and 941 spin point groups [10], which constitute finite catalogs defined under crystallographic constraints, are insufficient to provide an exhaustive description of SSGs. To bridge this gap, we directly employ the OSSG to impose symmetry constraints and trace the symmetry-breaking pathways as the system transitions into the regime with SOC, where the locking of spin and lattice spaces can permit previously forbidden physical responses.

For a tensor O , the transformation under a symmetry operation of OSSG can be expressed as:

$$O'_{ijk...} = \omega d_{il} d_{jm} d_{kn} \dots O_{lmn...} \quad (4)$$

where the indices $i, j, k, l, m, n, \dots$ refer to Cartesian components x, y , and z . Following standard conventions [14], the Cartesian x -axis is parallel to a , the y -axis lies in the ab plane in the direction orthogonal to a with a positive projection onto b , and the z -axis completes a right-handed orthonormal frame. The coefficients $d_{il}, d_{jm}, d_{kn} \dots$ correspond to elements of the representation matrix $D(g_s)$ or $D(g_l)$ derived from the symmetry operation $\{g_s || g_l | \tau\}$, depending on whether the index belongs to spin or lattice space. The factor ω accounts for the parity under spatial inversion and time reversal.

Based on whether they change sign under spatial inversion and time reversal, tensors are classified as either polar or axial, and as time-reversal-odd (T -odd) and time-reversal-even (T -even), respectively. Therefore, ω is determined by the determinants of the symmetry operations in lattice and spin spaces:

$$\omega = \begin{cases} 1 & T\text{-odd polar vector} \\ \det(D(g_l)) & T\text{-odd axial vector} \\ \det(D(g_s)) & T\text{-even polar vector} \\ \det(D(g_l))\det(D(g_s)) & T\text{-even axial vector} \end{cases} \quad (5)$$

where $\det(D(g_l))$ and $\det(D(g_s))$ denote the determinant of the operations in lattice and spin spaces, respectively. Improper rotations yield a determinant of -1 and correspond to rotations combined with spatial inversion in lattice space or time reversal in spin space.

The overall workflow of FINDSPINGROUP is illustrated in Fig. 2. Starting from structure files (.cif, .mcif, .scif), the program identifies the OSSG, assigns the corresponding standardized database index, and derives outputs such as conventional and primitive magnetic cells, spin Wyckoff positions, and the spin Brillouin zone. By applying the tensor constraints defined in Eq. (4), FINDSPINGROUP evaluates a range of physical properties, including magnetization, electric polarization, spin splitting, and various transport effects such as AHE and nonlinear Hall effect. The relationships between these transport tensors and the underlying Berryology-related physical quantities are also provided on the online platform. Representative applications to these classes of physical properties are discussed below.

ORIGINAL UNEDITED MANUSCRIPT

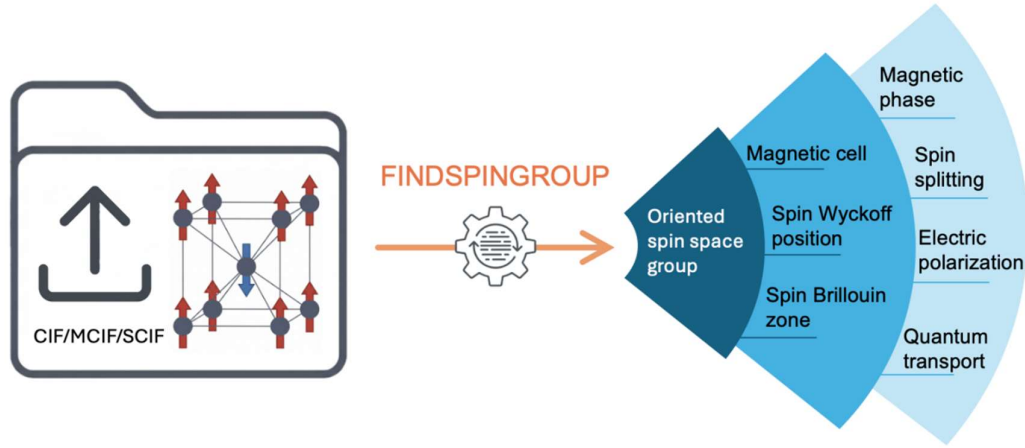


Figure 2. Overview of the workflow of FINDSPINGROUP. Starting from magnetic-structure input in CIF, MCIF, or SCIF format, FINDSPINGROUP identifies the OSSG and uses it as the working convention for downstream analysis. Within this unified framework, the platform determines the magnetic cell, spin Wyckoff positions, and spin Brillouin zone, and further evaluates symmetry constraints on magnetic phase, spin splitting, electric polarization, and quantum transport in the presence or absence of spin-orbit coupling.

Magnetization and electric polarization

As discussed before, the OSSG framework, which reconciles the SSG description of the phenomenological dichotomy between ferromagnetism and antiferromagnetism [32] with the MSG description of SOC effects, is employed to design time-reversal-odd physical responses in unconventional magnets. Below, we begin with the net magnetization M , a T -odd axial vector, to show how the OSSG establishes a symmetry classification of magnetism.

Symmetry analysis can be applied separately to the spin magnetization M^S and the orbital magnetization M^O in the absence of SOC effect. Although both are T -odd axial vectors, M^S is governed by the spin-space operation g_s while M^O is constrained by the lattice-space operation g_l and the time reversal component in g_s . Specifically, the spin-space point group, formed by all spin-space operations in OSSG, constrains M^S . In contrast, M^O is constrained by the effective magnetic point group,

which is obtained by mapping the operation $\{g_s||g_l|\tau\}$ to g_l and Tg_l for proper and improper spin-space operation g_s , respectively. The respective transformation relations are expressed as:

$$M_i^S = \sum_j D(g_s)_{ij} M_j^S, \quad (6)$$

$$M_i^O = \det(D(g_s)) \det(D(g_l)) \sum_j D(g_l)_{ij} M_j^O. \quad (7)$$

This distinction leads to different physical consequences. The symmetry-protected zero M^S defines the boundary between ferromagnets/ferrimagnets (FMs/FiMs) and antiferromagnets (AFMs) [32], serving as a prerequisite for exploring unconventional magnets with time-reversal-odd physical responses. On the other side, the spin-mirror operation in collinear and coplanar magnets enforces a zero M^O in the absence of SOC, while noncoplanar magnets can support a nonzero M^O originating from the magnetic geometry without SOC. Furthermore, the symmetry requirements for M^O are identical to those of the anomalous Hall conductivity, which corresponds to the antisymmetric part of the conductivity tensor and thus an axial pseudovector [47]. This implies that a magnetic-geometry-induced AHE can only emerge in noncoplanar magnets [48,49]. In contrast, for collinear and coplanar systems, the AHE originates solely from SOC effects.

The classification procedure of magnetic phases under OSSGs is summarized in Fig. 3. A polar spin-space point group, defined as a subgroup of ∞m , supports a nonzero M^S . Systems with a nonzero M^S are further distinguished by their spin Wyckoff positions (SWPs), of which a single type identifies an FM and multiple inequivalent types indicate a FiM. In the case of FiM, when the magnetization vanishes, the system is further classified as a compensated ferrimagnet (cFiM). Conversely, nonpolar spin-space point groups correspond to AFMs. Unlike FMs, which maintain a net magnetization regardless of whether SOC is considered, AFMs are further distinguished by their response to SOC. If there exists a net magnetization induced by SOC effects in an AFM, i.e., allowed by the fully coupled operations in its OSSG, it is further classified as spin-orbit magnetism (SOM) [32]. Such a unique class of AFM

manifests FM-like properties related to finite magnetization, such as the AHE, anomalous Nernst effect, and magneto-optical Kerr effect. In contrast, the recently emergent 'new magnetism', such as altermagnets and odd-parity magnets, categorizes magnets based on the momentum-space spin polarization. These distinct classes of magnetism do not necessarily encompass one another, though they can overlap under specific symmetry conditions (see Extended Data Fig. 3 of Ref. [32]).

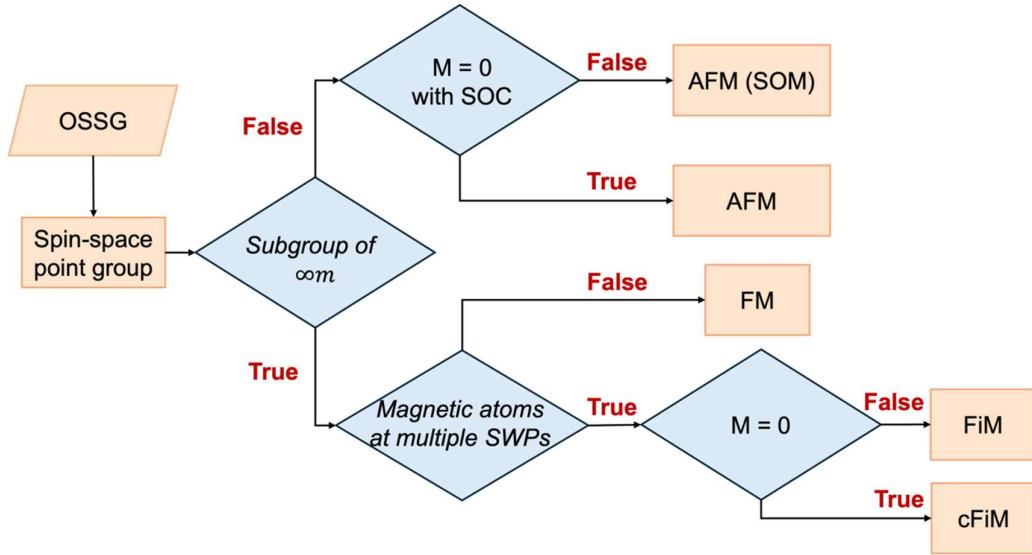


Figure 3. Symmetry classification of magnetic phases based on the spin magnetization. In the absence of spin-orbit coupling (SOC), the spin-space point group governs whether a macroscopic spin magnetization is symmetry-allowed. If allowed, the system is classified as ferromagnetic (FM), ferrimagnetic (FiM), or compensated ferrimagnetic (cFiM) based on its spin Wyckoff positions (SWPs) and net magnetization. If forbidden, the system is classified as antiferromagnetic (AFM). Within the AFM class, spin-orbit magnetism (SOM) specifies systems whose MSG allows a net magnetization under SOC.

Beyond magnetic classification, the OSSG framework also provides a fundamental basis for studying coexisting ferroic orders and their correlations, which are essential for understanding multiferroic couplings in unconventional magnets. For example, this analysis extends naturally to the macroscopic electric polarization [23-25], which is a T -even polar vector. In addition to conventional lattice-driven

ferroelectricity, the OSSG distinguishes two distinct physical origins of ferroelectricity related to magnetic order. In a non-polar lattice, spin-induced ferroelectricity occurs when magnetic ordering breaks spatial symmetry into a polar group. In comparison, SOC-induced ferroelectricity is identified when a polar group forms upon the inclusion of SOC. By evaluating these symmetry constraints, FINDSPINGROUP determines whether the ferroelectric state is driven by lattice order, magnetic order, or SOC effects.

Spin splitting and spin polarization

Besides macroscopic properties, the OSSG evaluates how magnetic geometry governs the spin-polarized band structure in reciprocal space, where the wave vector k is treated as a T -odd polar vector and remains invariant under proper spin rotations. In FMs, FiMs, and cFiMs, the spin-space point group is polar, leading to Zeeman-type splitting in such systems. In AFMs, the SSG protects a vanishing net magnetization, corresponding to the absence of spin polarization at the Γ point in momentum space. Away from Γ , when the spin space part of the k -little co-group is polar, the momentum-dependent spin splitting is allowed. This condition requires breaking the combination of spatial inversion and time reversal (PT), which is also an MSG operation. In addition, such spin splitting requires the absence of the D_∞ or D_2 group in spin space, which could occur in collinear and noncollinear magnetic configurations, respectively [14]. This analysis also distinguishes between spin-polarization components at any k -point induced by magnetic geometry and the additional contributions that emerge only upon the introduction of SOC. For collinear AFMs that support momentum-dependent spin splitting without SOC, FINDSPINGROUP explicitly assigns the label "altermagnet" [12].

This method can also be applied to two-dimensional spin-split AFMs. Compared with three-dimensional cases, a prerequisite step is to identify the orientation of the non-periodic direction of the structural input and then to apply constraints on the spin polarization. In practice, the three-dimensional OSSG is first determined. By removing the k -point components along the non-periodic direction, the two-dimensional spin

Brillouin zone, high-symmetry k -points, and spin little co-groups for any k -points are identified. The reduction in dimensionality can induce additional symmetry-protected degeneracies, i.e., the spin polarization at general k -points can be further constrained by improper spin rotation coupled with lattice rotation C_{2z} , or proper spin rotations associated with the mirror operation M_z [50,51].

EXAMPLES

To illustrate the functionality of our algorithm and program, we present several examples in which FINDSPINGROUP is used to identify OSSGs and analyze their associated physical properties.

Altermagnet V_2Se_2O

The full symmetry of two-dimensional (2D) altermagnet V_2Se_2O (Fig. 4(a)) [19,52,53] is described by the OSSG $P^{-1}4/1m^1m^{-1}m^{\infty_{a\beta\gamma}}1$ (123.47.1.1.L), where $[a\beta\gamma]$ denotes the easy axis under SOC. This system is classified as an AFM due to its spin-space point group $\infty/m\bar{m}$ (Fig. 4(c)). In the absence of SOC, this SSG belongs to the arithmetic crystal class $4/m\bar{m}mP$, the corresponding irreducible spin Brillouin zone is constructed with all high-symmetry k -points identified by the red triangle in Fig. 4b. Symmetry analysis reveals that this collinear AFM is an altermagnet in the absence of SOC, characterized by momentum-dependent spin splitting. The spin polarization consists of only the S_x component, while the electronic bands along the Γ -M direction remain spin degenerate due to the $\{2_{010}||m_{1-10}\}$ symmetry operation. Furthermore, the $\{2_{010}||4_{001}\}$ operation enforces a sign reversal of the spin texture under a four-fold lattice rotation in momentum space, thereby dictating the d -wave spin texture and the spin-polarized Fermi surfaces as shown in Fig. 4d.

Upon the introduction of SOC, the $[100]$ easy axis breaks the four-fold lattice rotation symmetry, yielding an OSSG subgroup that corresponds to the MSG $Pmm'm'$. As a result, the system is further classified as an SOM. Notably, a nonzero net magnetization emerges parallel to the Néel vector, which is distinct from the conventional ferromagnetic canting induced by Dzyaloshinskii-Moriya interactions,

where the net magnetization is perpendicular to the Néel vector. This effect arises from SOC-induced Wyckoff splitting, in which the symmetry equivalence between two opposite-spin sublattices is lifted. The two V atoms at spin Wyckoff position $2f$ are split into two different magnetic Wyckoff positions, $1c$ and $1e$.

The symmetry breaking also leads to an expansion of the irreducible Brillouin zone where the high-symmetry Γ -M path reduces to a set of general k -points (Fig. 4b). This reduction lifts spin degeneracy throughout the whole Brillouin zone, allowing the emergence of spin polarization S_x . Although the $\{2_{100}||m_{100}\}$ symmetry ensures that the spin polarization at all high-symmetry points remains restricted to the S_x component, the further reduction of symmetry enables the emergence of an additional S_y component at general k -points, while S_z remains strictly forbidden by the $\{m_{001}||2_{001}\}$ symmetry. While MSG permits a uniform S_x distribution across the Brillouin zone, the d -wave character remains dominant because of the negligible SOC (Fig. 4d). The small S_y projection observed in the DFT calculations with SOC is also consistent with the symmetry analysis. This evolution explains how the OSSG captures the symmetry-breaking pathway and the resulting modulation of momentum-dependent spin textures, providing a microscopic foundation for the design of tunneling magnetoresistance, piezomagnetism, and spin-splitting torque.

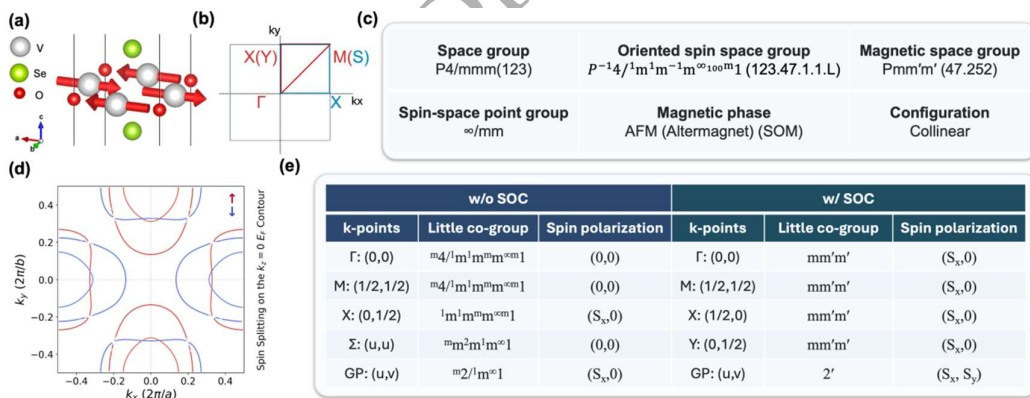


Figure 4. Symmetry analysis of 2D altermagnet V_2Se_2O . (a) Magnetic structures, (b) spin Brillouin zone, and (c) group information of 2D altermagnet V_2Se_2O . The region enclosed by the red lines is the irreducible spin Brillouin zone of SSG, and the blue one

is the irreducible magnetic Brillouin zone of MSG. (d) DFT-calculated spin splitting on the $k_z = 0$ plane at the Fermi level in the absence of SOC. (e) Momentum-dependent spin splitting in V_2Se_2O without and with SOC. All the information except panel (d) can be output by FINDSPINGROUP.

Spin-induced ferroelectricity in altermagnet $MnSe_2$

The OSSG framework, implemented in FINDSPINGROUP, also facilitates the identification of coexisting ferroic orders and the exploration of magnetic switching mechanisms. As stated before, this approach effectively distinguishes between spin-induced and SOC-induced ferroelectricity, enabling the electric control of unconventional magnets [23-26]. For example, the non-magnetic state of $MnSe_2$ [54] crystallizes in the centrosymmetric space group $Pa\bar{3}$, which forbids spontaneous electric polarization. However, the emergence of a supercell antiferromagnetic order leads to a symmetry reduction as illustrated in Figs. 5(a) and 5(b). Symmetry analysis indicates that the spatial part of the SSG is $Pca2_1$, a polar group that permits a spontaneous electric polarization along z direction. This mechanism differs from traditional multiferroics governed by exchange striction models, such as MnS_2 and Cu_2MnSnS_4 , where spatial inversion is broken while the $T\tau$ symmetry is preserved, resulting in hidden altermagnets [55,56]. In contrast, the magnetic ordering in $MnSe_2$ simultaneously breaks both, allowing a macroscopic ferroelectric state and enabling momentum-dependent spin splitting.

Beyond the coexistence of ferroic orders, FINDSPINGROUP enables the systematic identification of switching trajectories between symmetry-related domain states. By excluding the continuous global spin rotations within $O(3)$ in spin space that leave both the electric polarization and collinear spin polarization invariant in the absence of SOC, the switching pathways are determined by combining the 18 lattice domains with the binary factor from time reversal, and 36 potential switching paths are identified. Here, 18 lattice domains arise from a factor of 6 determined by the ratio of the orders of the point group part, combined with a factor of 3 from the supercell expansion. Subsequent calculations can be employed to identify the trajectories with the lowest energy barriers. For instance, considering the operations $\{-1||-1|0,0.5,0\}$

and $\{1||-1|0,0.5,0\}$ (Figs. 5d and 5e), the former represents a path where the spin polarization remains invariant during ferroelectric switching, whereas the latter corresponds to the simultaneous switch of electric polarization and spin splitting. Such symmetry analysis facilitates the design of spin-induced ferroelectricity and the prediction of whether the ferroelectric state can control coexisting FM-like responses. By distinguishing between this exchange-driven mechanism and the more common SOC-induced ferroelectricity, the OSSG framework provides a microscopic roadmap for designing multiferroic materials where electric and magnetic degrees of freedom are coupled.

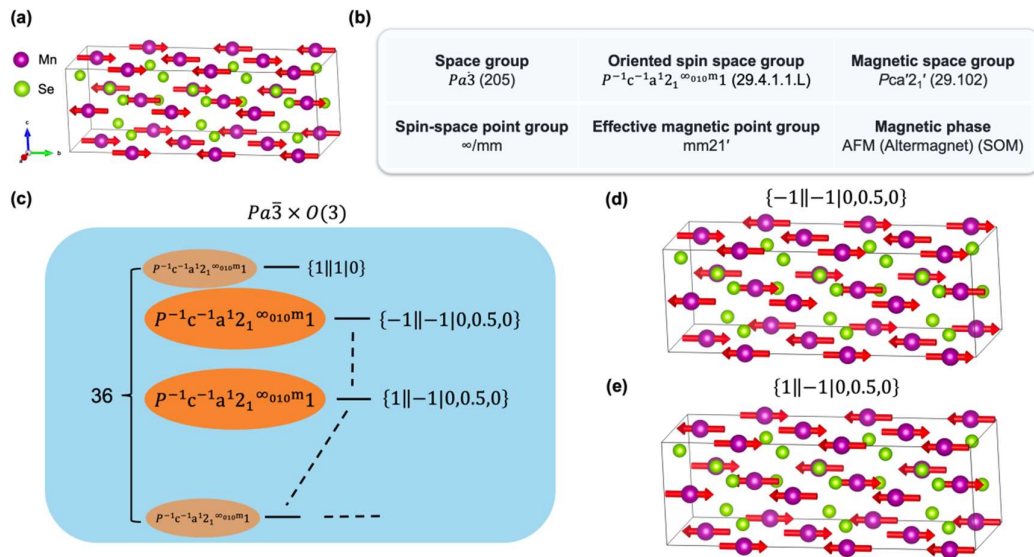


Figure 5. Symmetry analysis of ferroelectric altermagnet MnSe₂. (a) Magnetic structures and (b) group information of altermagnet MnSe₂. (c) Schematic illustration of 36 possible pathways obtained by considering only the binary time-reversal operation within $O(3)$ in spin space that switches the collinear spin polarization in momentum space. Panels (d) and (e) represent the magnetic phases obtained via operations $\{-1||-1|0,0.5,0\}$ and $\{1||-1|0,0.5,0\}$ from (a), respectively.

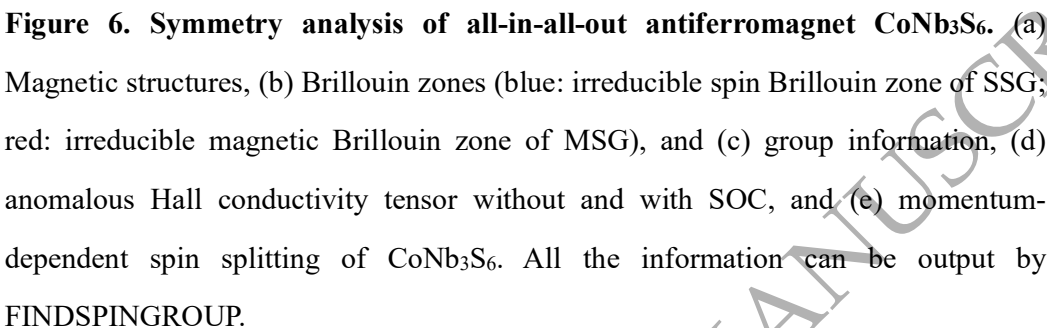
All-in-all-out antiferromagnet CoNb₃S₆

The all-in-all-out AFM CoNb₃S₆ (Fig. 6a) represents a typical case where OSSG captures the coexistence of spin degenerate bands and the magnetic geometry induced AHE. It is described by the OSSG $P^{32}_{001}6_3m_{100}2m_{010}2|(2_{12-\gamma}, 2_{21\gamma}, 1)$ (182.4.4.2). A

distinct feature of this OSSG is the coexistence of a hexagonal space group $P6_322$ with a tetrahedral spin-space point group $\bar{4}3m$, whose point-group components are incompatible (Fig. 6c). Such a configuration goes beyond the description of 941 spin point groups and can only be characterized by the SSG or OSSG. This example demonstrates that spin point groups alone cannot exhaustively characterize the physical properties of magnetic geometry, unlike classification using conventional point groups and magnetic point groups.

Despite the absence of PT symmetry, the spin little co-group at the general k -point is $^{222}1$, which strictly forbids the spin polarization throughout the whole Brillouin zone [14,16,57,58]. However, while the electronic band structure of CoNb_3S_6 remains spin degenerate in the absence of SOC, it supports a nonzero AHE without SOC since its OSSG corresponds to the ferromagnetic effective magnetic point group $62'2'$ (Fig. 6c and 6d). This AHE originates from the noncoplanar magnetic geometry, while such a response is forbidden in collinear and coplanar AFMs due to the presence of effective time reversal symmetry from the spin-only group. The coexistence of spin degeneracy and the AHE indicates that the physical origins and symmetry requirements of these two effects are distinct [3].

When SOC is included, the OSSG corresponds to the chiral MSG $P32'$, which allows the emergence of a net magnetization along the $[001]$ direction and reclassifies the magnetic phase as SOM. Furthermore, SOC breaks the spin-translation group $^{222}1$, leading to the emergence of SOC-induced spin polarization as shown in Fig. 6e. Specifically, the presence of the 3^1_{001} operation dictates that, for the Γ -A and H-K paths, only the S_z component is permitted. In contrast, on the $k_x = 0$ plane, the presence of the $T2_{100}$ symmetry allows for the S_y and S_z components, while at general k -points, spin polarization in arbitrary directions is permitted.



The FINDSPINGROUP platform provides a systematic computational framework for symmetry analysis and the exploration of physical properties in unconventional magnets. By implementing the OSSG framework, it treats magnetic geometry and SOC effects within a single workflow and combines standardized structural conventions, spin site-symmetry groups, spin Brillouin zones, and spin little co-groups. Based on the OSSG framework, the platform enables automated tracking of symmetry-breaking pathways across regimes with and without SOC, facilitating the symmetry classification of magnetic phases and the disentanglement of physical origins for emergent phenomena such as spin splitting and the AHE. This scheme provides a clear physical picture for understanding the interplay between magnetic geometry and SOC effects. Furthermore, the introduction of the SCIF format standardizes spin-group symmetry analysis in a manner analogous to conventional crystal structure analysis,

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enhancing the efficiency of high-throughput screening and design of unconventional magnets. Overall, the FINDSPINGROUP platform offers physical navigation for the high-throughput discovery of unconventional magnets, facilitating the future development of spintronic devices.

METHODS

Identification, equivalence, and index

From the input magnetic structure, we determine a magnetic primitive cell and the crystallographic operations preserving it using spglib [59]. The site moments are then used to classify the magnetic configuration as collinear, coplanar, or noncoplanar and to determine the admissible spin-space operations. The identified symmetry is the set of all operations $\{g_s \parallel g_l \mid \tau\}$ that leave the magnetic structure invariant, with action (1).

Classification is performed on the equivalence class of this operation set under orientation-preserving affine changes of lattice-space coordinates, together with proper rotations of spin space. Writing an affine transformation as $(A, a) \in \text{Aff}^+(3)$ and a spin-space rotation as $Q \in \text{SO}(3)$, two SSG descriptions are equivalent if their operations are related by conjugation,

$$\{g_s \parallel g_l \mid \tau\} \rightarrow \{Qg_sQ^{-1} \parallel Ag_lA^{-1} \mid A\tau + a - Ag_lA^{-1}a\}. \quad (8)$$

This removes basis, origin, and spin-frame choices while preserving the magnetic symmetry.

The nomenclature is assigned only after reduction to the canonical database representative of this equivalence class at database.findspingroup.com. Thus, the reported label identifies an equivalence class rather than a raw input-dependent realization. For certain coplanar families, especially those associated with a nontrivial spin-space point group 2 or 222, the coarse suffix P does not uniquely specify the full group $G_{\text{SS}} = G_{\text{NS}} \times G_{\text{SO}}$. Although the nontrivial part G_{NS} is fixed, extending it by the coplanar spin-only part G_{SO} can yield, under the equivalence defined above, up to

three inequivalent full-group representatives. These refined coplanar representatives are distinguished in the database by the suffixes P1, P2, and P3. For example, the SSGs 2.1.1.2.P1 and 2.1.1.2.P2 share the same nontrivial part $P^{2_{001}\bar{1}}$, yet incorporate distinct spin-only groups $m_{001}1$ and $m_{100}1$, respectively. In 2.1.1.2.P1, the spin mirror is perpendicular to the twofold rotation axis in spin space, yielding the spin-space point group $2/m$, which forbids a nonzero magnetization. Conversely, in 2.1.1.2.P2, the mirror plane is parallel to the twofold rotation axis in spin space, yielding $mm2$, which permits a net magnetization along $[001]$. These two full SSGs thus belong to the AFM and FM classes, respectively, illustrating why the coarse coplanar suffix P must be refined.

Spin Wyckoff positions and spin Brillouin zones

Spin Wyckoff positions are obtained as site orbits under the OSSG. For a representative site, the associated spin site-symmetry group is the subgroup of OSSG operations that leaves the site invariant, and it determines the symmetry-allowed moment components at that site. This fixes the splitting chain from the parent space group to the OSSG and then to the corresponding MSG in one convention.

The spin Brillouin zone is constructed from the effective reciprocal-space action of the OSSG. For an OSSG operation $\{g_s||g_l|\tau\}$, its action on a wave vector is

$$\{g_s||g_l|\tau\} : k \rightarrow \det(D(g_s)) ((D(g_l))^{-1})^T k. \quad (9)$$

The resulting effective k -space operations are reduced to an arithmetic crystal class, which fixes the spin Brillouin-zone type, the standardized primitive transformation and the tabulated high-symmetry k -points. For a given wave vector k , the spin little group is obtained from the subset of OSSG operations that preserves k under the same action, modulo reciprocal lattice translations. The corresponding spin little co-group is defined by removing the translational part of this little group. The same procedure is applied separately to the OSSG and its corresponding MSG, providing results for the cases without and with SOC, respectively. FINDSPINGROUP determines the symmetry-allowed spin-polarization components at each k -point, where (0,0,0) indicates that spin

polarization is symmetry-forbidden. In this way, the spin Brillouin zone, its labeled high-symmetry points, and the associated spin little co-groups and magnetic little co-groups are determined in the same oriented convention as the lattice space symmetry.

SpinCIF representation

FINDSPINGROUP exports magnetic structures and their identified OSSGs in .scif format. The files record symmetry-independent atomic sites and spin moments, together with the lattice setting and the spin frame relative to the crystallographic frame. Each listed symmetry operation specifies the spatial and spin transformations separately, unlike .mcif, where the moment transformation is determined by the spatial operation and its time-reversal sign. The complete magnetic structure can be reconstructed by applying the reported operations to the representative sites and moments; additional OSSG symmetries can reduce the number of independent sites required. A preliminary specification and example files are available in the Committee for the Maintenance of the CIF Standard (COMCIFS) spinCIF repository [60].

Tolerance parameters

The default tolerance parameters of the current implementation are used throughout: $\text{space_tol} = 0.02 \text{ \AA}$, $\text{mtol} = 0.02 \mu_B$, $\text{meigtol} = 2 \times 10^{-5}$, $\text{matrix_tol} = 0.01$, and $\text{parser_atol} = 0.02$. Here, space_tol is the lattice space distance tolerance used for crystallographic symmetry matching, space-group determination, and standard-setting construction; mtol is the magnetic-moment tolerance used for moment matching and for classifying the magnetic configuration as collinear, coplanar, or noncoplanar; meigtol is the eigenvalue tolerance used in point-group candidate construction; matrix_tol is the tolerance used to compare operation matrices during standardization and equivalence reduction; and parser_atol is the absolute tolerance used in SCIF expansion to check whether symmetry-generated moments assigned to the same crystallographic site remain numerically consistent. Symmetry matching uses separate tolerances in lattice and spin spaces. Positional deviations are controlled by space_tol , whereas mtol measures the vector difference between symmetry-mapped magnetic moments and the input moments, thus accounting for both their directions and

magnitudes. A candidate operation is retained only when both criteria are satisfied. Excessively large tolerances risk overestimating the symmetry, while excessively small values may interpret numerical noise as symmetry breaking. Users are therefore advised to test a range of reasonable tolerance values and verify that the resulting OSSG label and identification index remain unchanged.

Comparison with related tools

Spinspg searches for the spin-symmetry operations, MOM2SSG and SSGReps focus on identifying SSGs and calculating band representations, and amcheck determines whether a collinear compensated magnet belongs to the altermagnet. In contrast, FINDSPINGROUP offers a comprehensive OSSG-based workflow. Beyond operation searching, it standardizes material-specific OSSGs, generates corresponding OSSG symmetry-guided crystallographic information files, provides an OSSG-based classification of magnetism and enables physical property analysis both without and with SOC.

DFT calculations

All DFT calculations were performed using the projector augmented-wave method as implemented in the Vienna *ab initio* simulation package [61,62]. The generalized gradient approximation of Perdew-Burke-Ernzerhof-type exchange-correlation potential [63] was adopted. A plane-wave cutoff energy of 520 eV and an electronic convergence criterion of 10^{-7} eV were used. The self-consistent calculations were performed with a Γ -centered $15 \times 15 \times 1$ k -mesh, and the spin texture was calculated with a Γ -centered $101 \times 101 \times 1$ mesh.

CODE AVAILABILITY

FINDSPINGROUP is an open-source platform, with the source code available at <https://github.com/LiuQH-lab/FindSpinGroup>. The online platform is available at <https://findspingroup.com>.

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AUTHOR CONTRIBUTIONS

Q.L. conceived the project. Y.Y. and X.C. developed the theoretical framework and core codebase and built the database. Y.Z. developed the code labelling spin space group. Y.H.L. calculated and curated the spin-Wyckoff-position data. R.X. calculated and curated the spin-space-group operations data. J.L. provided theoretical guidance on higher-order nonlinear tensors. Y.T.L. provided guidance on magnetic classification. Y.Y., X.C., and Q.L. wrote the manuscript. All authors discussed the results and approved the manuscript.

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