Magnetic-structure generation based on oriented spin space groups

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Ab-initio magnetic-structure search needs good candidates

The self-consistent calculation converges near its initial guess; the candidates decide the outcome.

Context: SDFT now searches magnetic structures

- **AFM spintronics** established: no stray field, ultrafast dynamics
- New classes: **noncollinear AFMs (Mn_3Sn, Mn_3Ge)**, **altermagnets** ▶ ferromagnet-like responses (e.g. anomalous Hall effect)
- Large-scale ground-state searches: **SDFT** (spin density functional theory); configuration space is large

▶ **The missing step: systematic candidate generation** [1-3]

this talk: candidates from symmetry

recent works in the same direction: [1] Y. Jiang *et al.*, PRX **14**, 031039 (2024); [2] H. Zhou *et al.*, arXiv:2601.01617; [3] Y. Li *et al.*, arXiv:2512.21672

The standard framework and a remaining difficulty

Representation analysis with isotropy subgroups does not guarantee equal moments; spin space groups do.

The standard: representation analysis (RA) with isotropy subgroups [1-4]

nonmagnetic structure + propagation vector q ▶ irreducible representations (IRs) + isotropy subgroups ▶ maximal **magnetic space groups (MSGs)** (ISODISTORT / MAXMAGN)

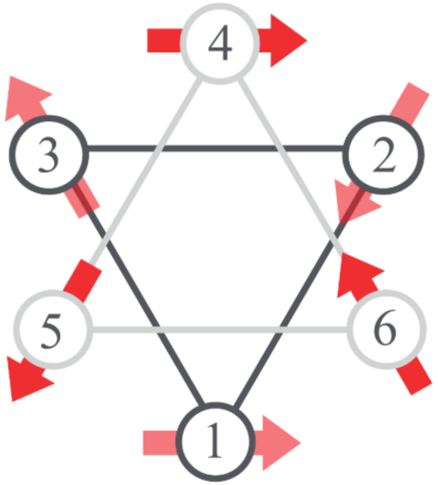
The difficulty: equal moments not guaranteed

MSG: $\{1,4\} \nsim \{2,3,5,6\}$, magnitudes unrelated

experiment: all six equal

SSG: $\{1,2,\ldots,6\}$, one orbit ▶ equal $|\mathbf{m}|$

Mn_3Sn, a triangular kagome structure (right)



MSG / REPRESENTATION ANALYSIS

equal moments not guaranteed

SSG

equal moments by construction

[1] Bertaut, Acta Cryst. A **24**, 217 (1968); [2] Ascher, J. Phys. C **10**, 1365 (1977); [3] Stokes and Hatch (1989); [4] Rodriguez-Carvajal and Perez-Mato, Acta Cryst. B **80**, 370 (2024)

Spin space groups in brief

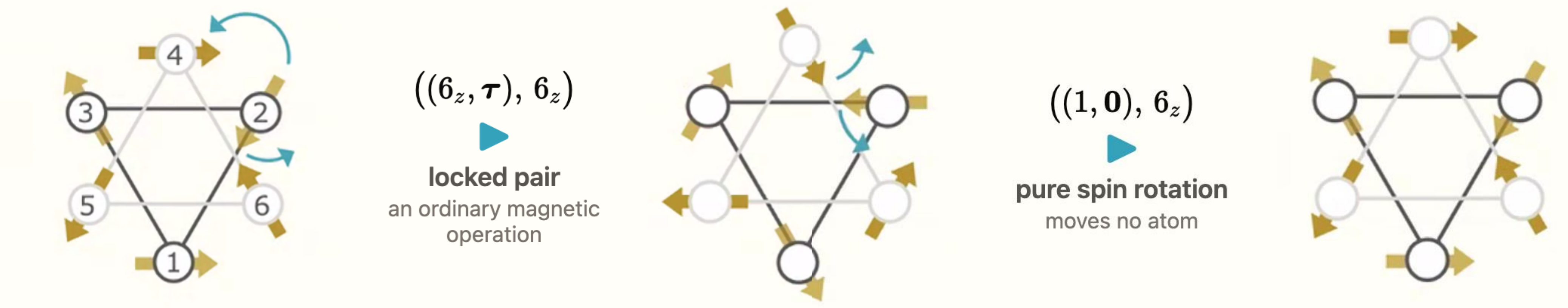
A spin space group decouples spatial operations from spin rotations.

Definition: space and spin decoupled

- SSG operation (g, U): spatial g, spin $U \in O(3)$, **independent** (an MSG locks them)
- **Approximate symmetry** for weak spin-orbit coupling (SOC)
- Subgroups $\mathcal{X} \leq G \times O(3)$, spatial parts covering all of G

Example: one operation, in two steps

$((6_z, \boldsymbol{\tau}),\ 3_z) \in \mathcal{X}$ spatial 6_z · spin 3_z



spatial 6_z vs spin 3_z ▶ **not a magnetic operation** (an MSG locks the two); only an SSG contains it

Enumerating spin space groups

One coset decomposition organizes an SSG; three inputs give the finite list.

Anatomy: one coset decomposition

$$\mathcal{X} = \bigcup_{I=1}^{N_t} \bigcup_{m=1}^{N_k} \left(g_{i_I}(\mathbf{I}, \mathbf{t}_m),\ \mathbf{U}_{Im}\right) (\mathcal{H} \times \mathcal{B}_{\mathrm{so}})$$

N_k ▶ **k-index**: magnetic-cell enlargement

$\mathcal{B}_{\mathrm{so}}$ ▶ **spin-only group**: **collinear** $(C_{\infty v})$ / **coplanar** (C_s) / **noncoplanar** (C_1); $d = 1, 2, 3$

$\mathcal{X}$ **is an extension of** G: the spatial parts cover all of G, each operation decorated with a spin rotation

ESTABLISHED [1-3]

inputs (G, spin-only type, N_k) ▶ a **finite list of SSGs**

SSG framework and full classification: [1] Z. Xiao *et al.*, PRX **14**, 031037 (2024); [2] X. Chen *et al.*, PRX **14**, 031038 (2024); [3] Y. Jiang *et al.*, PRX **14**, 031039 (2024)

Spin-symmetry-adapted (SSA) structures

Crystallographic orbits stay intact under the enumerated SSGs: equal moment magnitudes, naturally.

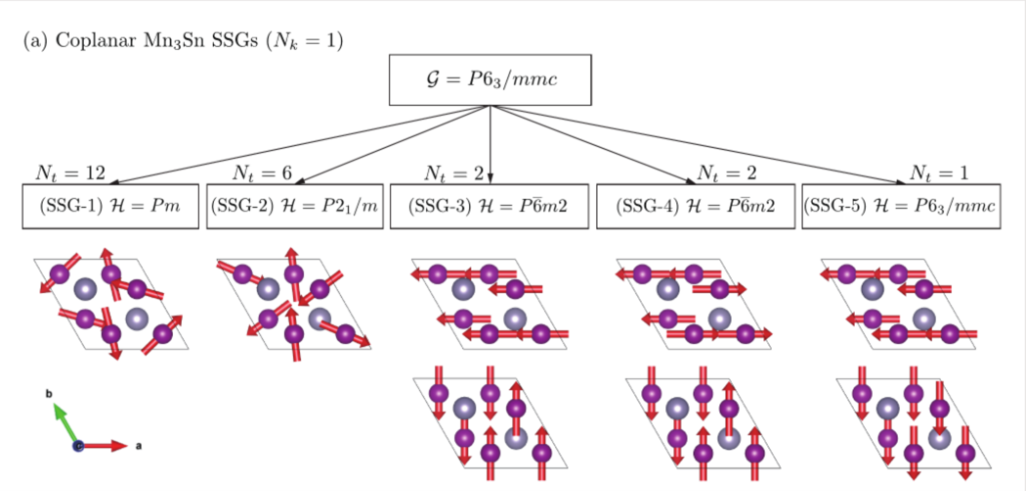
Action g moves sites, U rotates moments

SSA structures: equal moments, naturally

SSA structure = invariant moments, $(g, U)\,\mathbf{m} = \mathbf{m}$: totally symmetric rep, by projection

$$\textbf{one orbit and } |U\mathbf{m}| = |\mathbf{m}| \;\; \blacktriangleright \;\; \textbf{equal } |\mathbf{m}|$$

every operation of G persists in the SSG, so each parent orbit stays one orbit; a consequence, not an ansatz



Mn_3Sn Mn sites = one orbit (Wyckoff $6h$ of $P6_3/mmc$) ▶ equal $|\mathbf{m}|$ on all six sites; structures per box = basis vectors (one: SSG-1, 2; two: SSG-3-5)

RA / isotropy subgroups: subgroups of $G \times \mathbb{Z}_2$ ($\mathbb{Z}_2 = \{1, \theta\}$, time reversal); SSA: subgroups of $G \times O(3)$, a straightforward generalization

Oriented spin space groups: pinning the spin axis

SOC often pins spin axes; oriented SSGs give each pinned case its magnetic space group.

Motivation: SOC often selects the spin axis

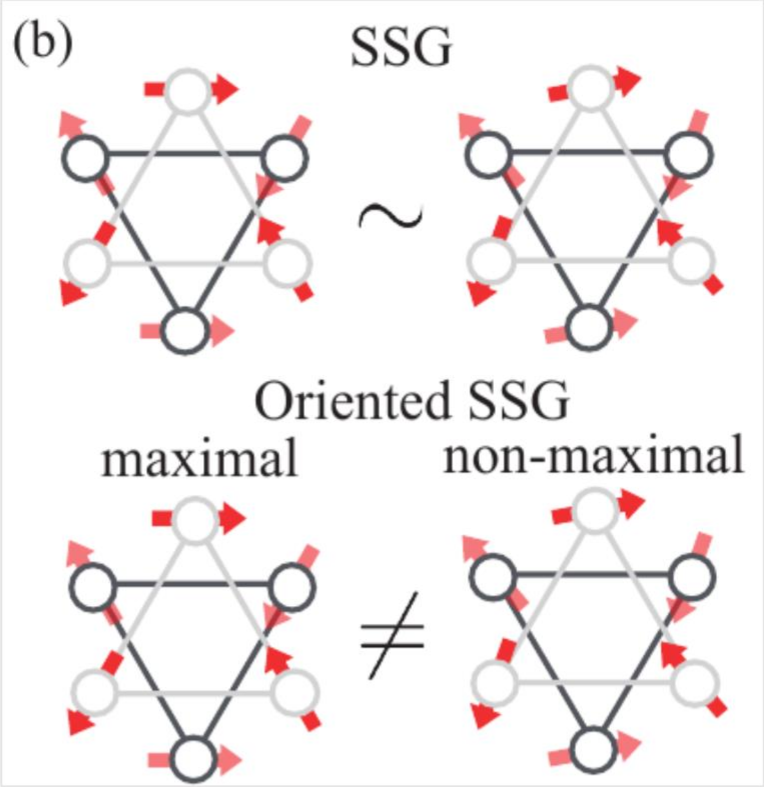
- SSA fixed only up to a global spin rotation $Q \in O(3)$ (figure, top row)
- Fix Q, keep the **maximal** induced MSGs ▶ **oriented SSGs** (concept and name by Liu *et al.* [1]): SSG + BNS symbol, one object

Condition: spin operation survives as magnetic

$$(\det R)\, R \;=\; (\det U)\, U$$

from the **SOC Hamiltonian**: spin locked to the lattice

same SSG: equivalent up to a global spin rotation ($\sim$); orientation fixed: maximal vs non-maximal MSG ($\neq$)

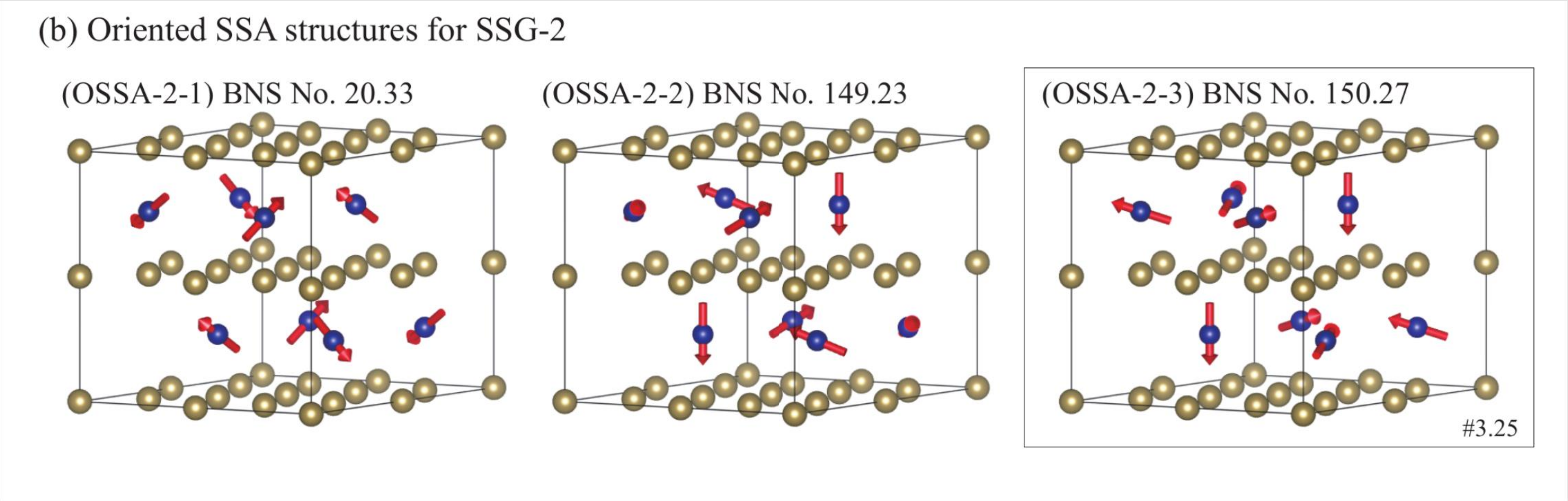


[1] the oriented-SSG concept and name are due to Y. Liu, X. Chen, Y. Yu, J. Etxebarria, J. M. Perez-Mato, and Q. Liu, Nature **652**, 869 (2026)

Example: $CoTa_3S_6$, one SSG, three oriented SSGs

One SSG, three pinned orientations: three maximal magnetic space groups.

$CoTa_3S_6$ (noncoplanar, all-in-all-out): BNS labels in the panels; boxed = reported (MAGNDATA #3.25)



Oriented SSGs from a manifold of rotations

The induced MSG lives on a manifold of rotations Q; special points give maximal symmetry.

The idea: generic Q ▶ low symmetry; **special points** ▶ **maximal MSGs** $=$ the oriented SSGs, like special Wyckoff positions

1 **enumerate subgroups** $\mathcal{Y}$ of the SSG — candidates for the surviving magnetic symmetry

2 **solve for the orientation**: one Q, **all elements simultaneously** ▶ $Q =$ a **real intertwiner**

$$D_{\text{space}}(g, U) = (\det R)\, R, \qquad D_{\text{spin}}(g, U) = (\det U)\, U$$

$$D_{\text{space}}(g_i, U_i) \;=\; Q^{-1}\, D_{\text{spin}}(g_i, U_i)\, Q \qquad \text{for all } i$$

3 **fix** Q ▶ the operations satisfying the condition survive as magnetic ▶ the **induced MSG**

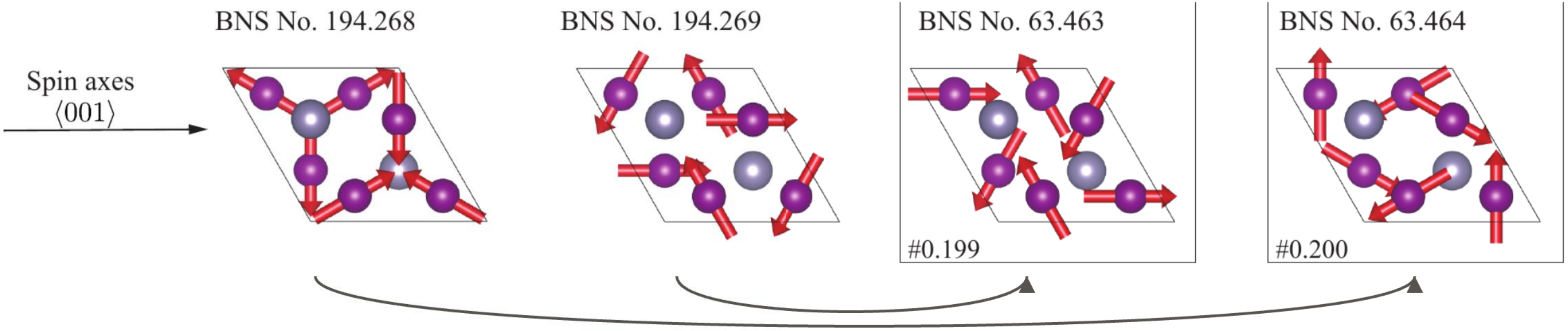
4 **keep the maximal** ▶ the **finite list of oriented SSGs**

$CoTa_3S_6$ SSG-2: its three oriented SSGs

Spin chirality, motivated by Mn_3Sn: the reported structures escape the plain enumeration

Mn_3Sn's reported structures never appear as maximal in the plain enumeration.

kept as maximal | **reported, missed**



a global spin rotation superposes each inverse structure onto its normal partner

No chirality condition imposed ▶ only the **normal** pair kept as maximal

THE DISCREPANCY
reported = the **inverse** pair, missed as non-maximal

▶ **distinguish normal from inverse by symmetry**

Existing chirality notions do not carry over

Neither existing notion names the normal-inverse difference.

Vector spin chirality $\mathbf{S}_i \times \mathbf{S}_j$: defined case by case, not general

The time-reversal analog of spatial chirality: compare the SSG with its time-reversed counterpart ▶

$$\bar{\mathbf{1}}^{-1}\, U\, \bar{\mathbf{1}} \;=\; U$$

for every spin rotation U

▶ the comparison names nothing

We need a refinement that names the mirror difference

Spin-planochirality: comparing an SSG with its enantiomorph

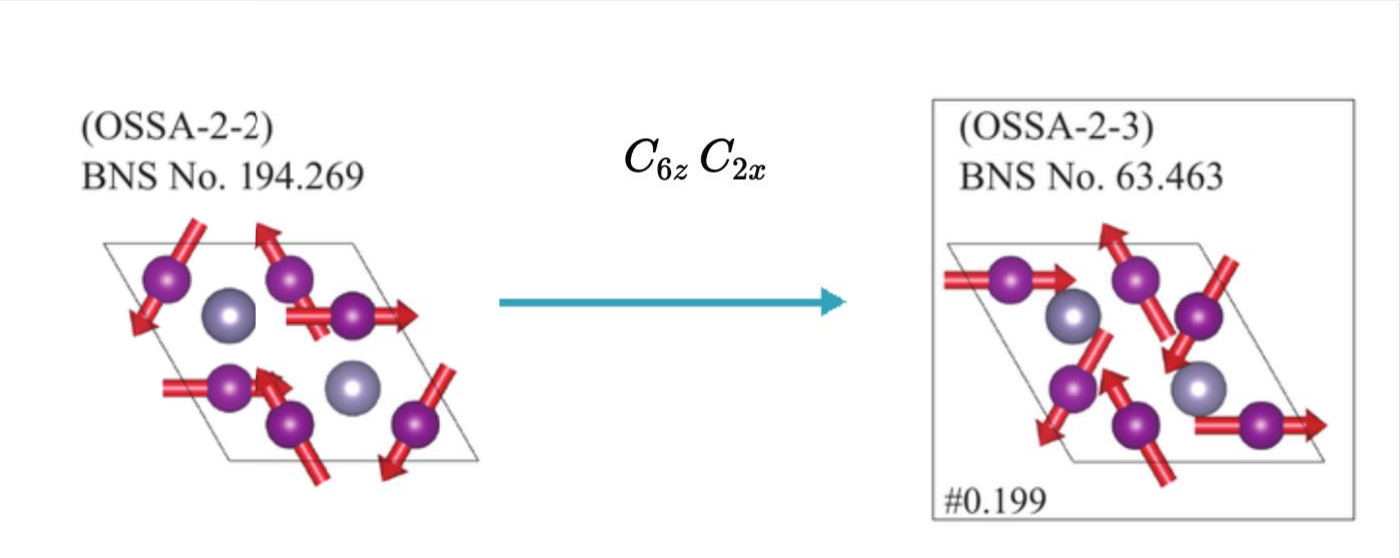
Compare the SSG with its enantiomorph, only through in-plane rotations.

$$\mathcal{X}_{\mathrm{e}} \;=\; (1,\sigma)^{-1}\,\mathcal{X}\,(1,\sigma), \qquad \sigma:\ \text{a mirror flipping the spin plane}$$

$$\textbf{spin-planochiral} \iff \textbf{no in-plane proper rotation} \text{ maps } \mathcal{X} \text{ onto } \mathcal{X}_{\mathrm{e}}$$

comparison domain $Q \in SO(d) \oplus \mathbf{I}_{3-d}$, rotations fixing the spin plane/axis; plane ▶ axis for the collinear case

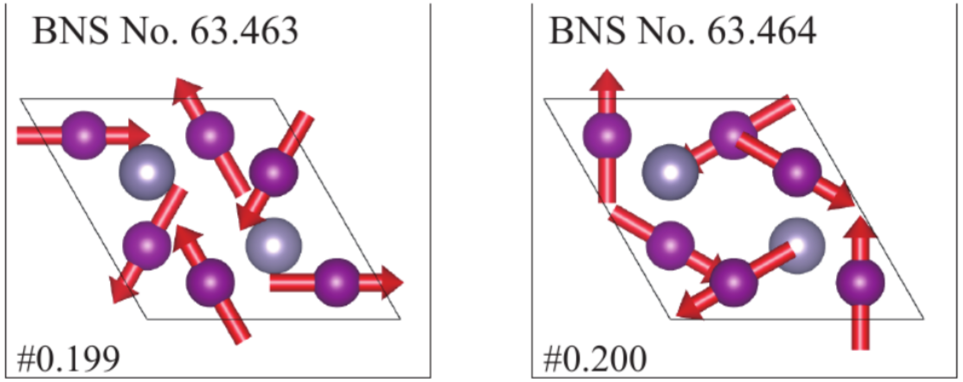
Example: the normal ▶ inverse map needs $C_{6z}C_{2x}$; the in-plane C_{6z} is allowed, the plane-flip C_{2x} is excluded ▶ the pair stays distinct



Classification results: only spin-planochirality survives

Refined per spin dimension, **only the coplanar case survives:**
spin-planochirality

recovered



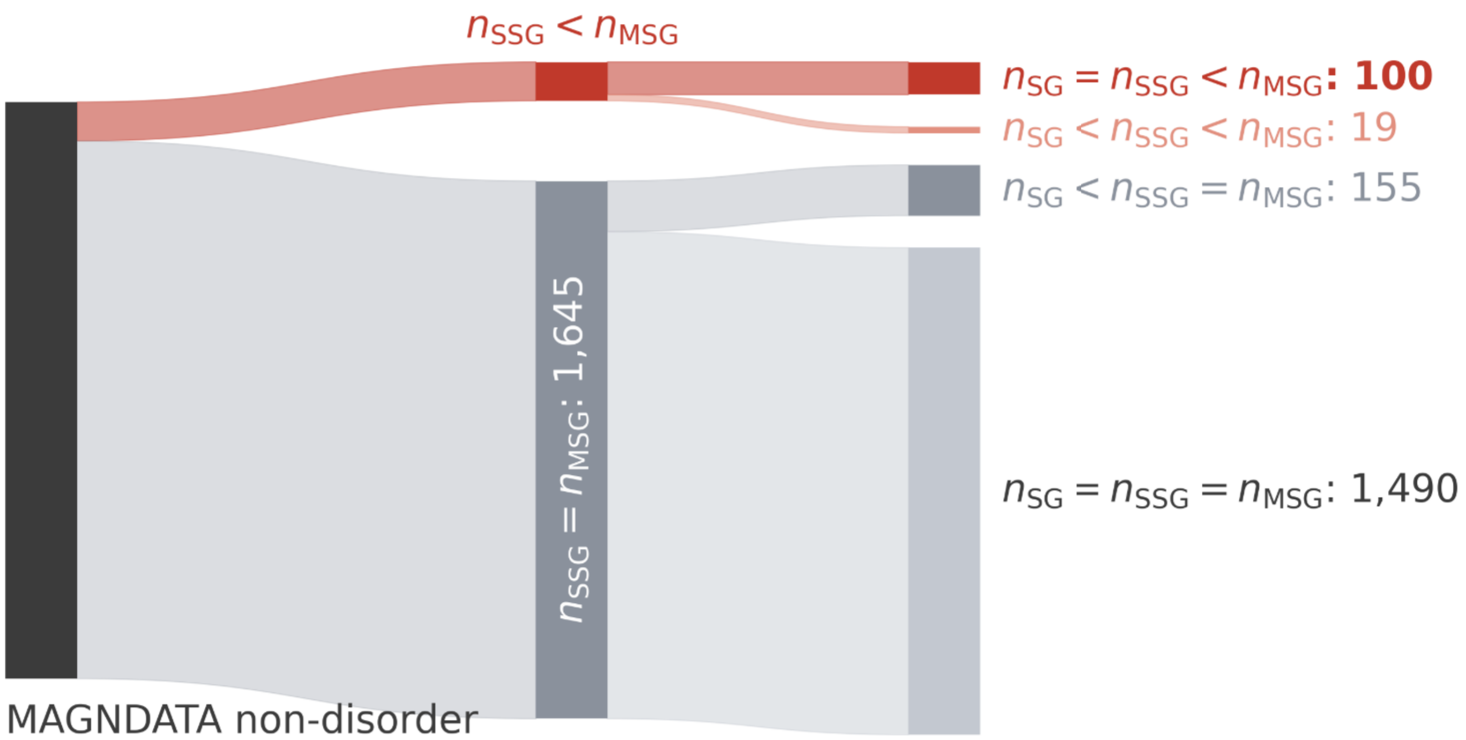
Mn_3Sn's reported inverse-triangular pair (MAGNDATA #0.199 / #0.200)

CONSEQUENCE

chiral SSG ▶ enumerated **with its enantiomorph** ▶ Mn_3Sn's reported inverse pair recovered

MAGNDATA statistics show the equal-moment constraint at work

in **119** / 1,764 reported structures, the MSG **splits equal-moment sites**; the SSG keeps them equivalent



magnetic-site orbits under the nonmagnetic SG / the SSG / the MSG;
finer only splits:
$n_{SG} \leq n_{SSG} \leq n_{MSG}$

Mn_3Sn #0.199:
$n_{SG} = n_{SSG} = 1 < n_{MSG} = 2$
({1,4} / {2,3,5,6})

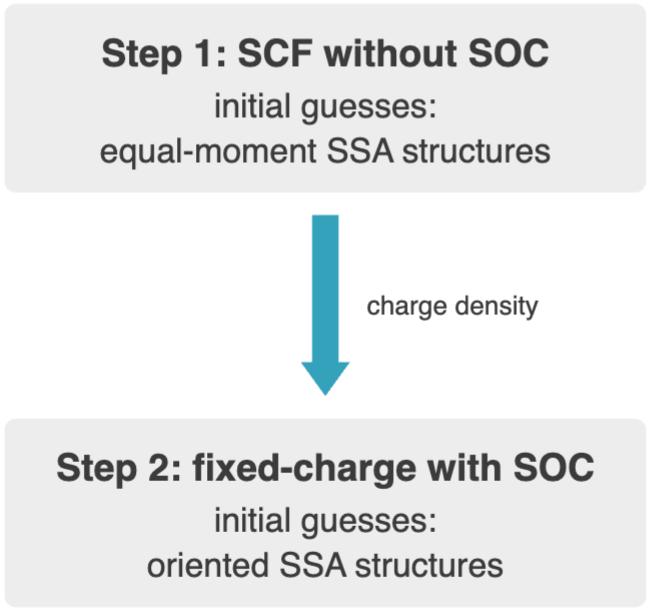
the survey covers MAGNDATA as collected at the research time (2,186 entries), keeping all 1,764 non-disorder structures (no partially occupied sites)

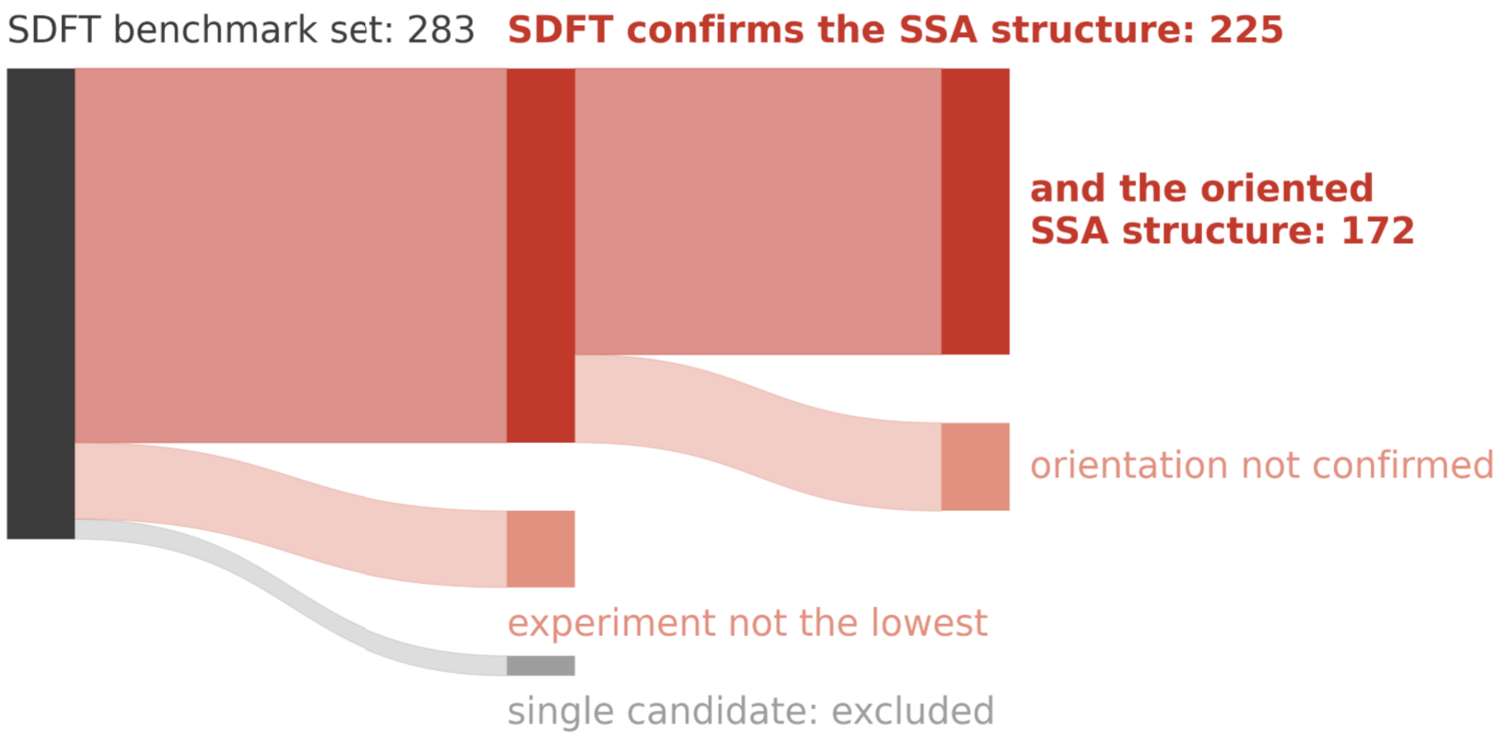
SDFT recovers the reported structures

Used as SDFT initial guesses, the candidates recover the reported structures across a 283-material benchmark.

Dataset curation: MAGNDATA, symmetry-related magnetic atoms (1,023) ▶ SSA-reproducible, SDFT-tractable:
283 materials

Two-step SDFT



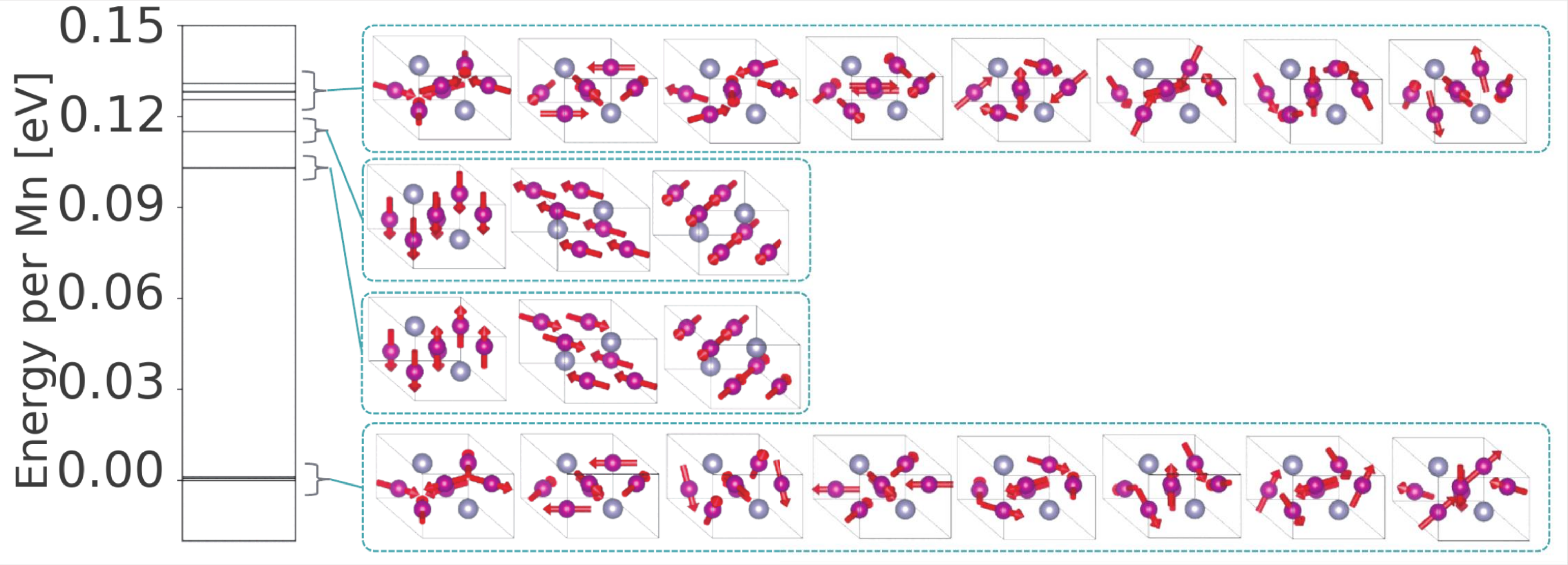


multiple inequivalent Wyckoff positions: not symmetry-related; still an initial guess, but symmetry alone cannot determine the structure

The energy hierarchy behind the two-step scheme

Spin-orbit splitting within one SSG is ~300x smaller than the spacing between symmetry-adapted structures.

0.3 meV (SOC, within an SSG) vs **100 meV** (between SSAs), per magnetic atom ▶ **~300x**



Mn_3Sn check: lowest dashed box = the SSG-2 structures from the enumeration example

CLOSING

Takeaway and next work

Oriented SSGs give each candidate its magnetic space group; determination against diffraction data is next.

Generation	SSA structures; **equal moments, naturally**
Oriented SSGs	the **magnetic space group** determined (BNS symbol), ready for refinement
Spin-planochirality	recovers Mn_3Sn's reported pair
Validation	MAGNDATA statistics; 283-material SDFT benchmark

OUTLOOK **Next work: magnetic structure determination**

Few-parameter fits against $F(Q)$ ▶ Rietveld integration: an **additional generation option alongside ISODISTORT**

arXiv:2601.15735

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Software ecosystem

Everything runs on the spglib ecosystem; spinforge will be released on publication.

SpinForge — magnetic-structure generation, built on moyopy — release on publication

Generation [6]

[6] spinforge: arXiv:2601.15735 (this work)

`spinspg` — identification; produced the MAGNDATA statistics

`spgrep` — irreps and physically irreducible representations of finite groups and space groups

Domain tools [4,5]

[4] spinspg: Shinohara, Togo, Watanabe, Nomoto, Tanaka, and Arita, Acta Cryst. A **80**, 94 (2024); github.com/spglib/spinspg · [5] spgrep: Shinohara, Togo, and Tanaka, J. Open Source Softw. **8**, 5269 (2023); github.com/spglib/spgrep

`spglib` → moyo — moyo / moyopy, next-generation Rust successor

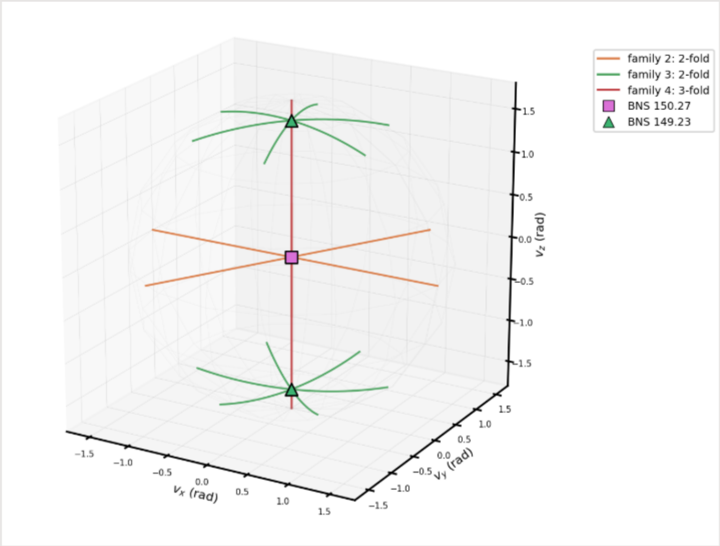
Foundation [1-3]

spglib (C; originally developed and maintained by A. Togo, NIMS): [1] Togo, Shinohara, and Tanaka, Sci. Technol. Adv. Mater., Meth. **4**, 2384822 (2024); [2] Shinohara, Togo, and Tanaka, Acta Cryst. A **79**, 390 (2023) · [3] spglib.github.io/moyo

read bottom up: foundation ▶ domain tools ▶ generation

The $SO(3)$ chart of $CoTa_3S_6$

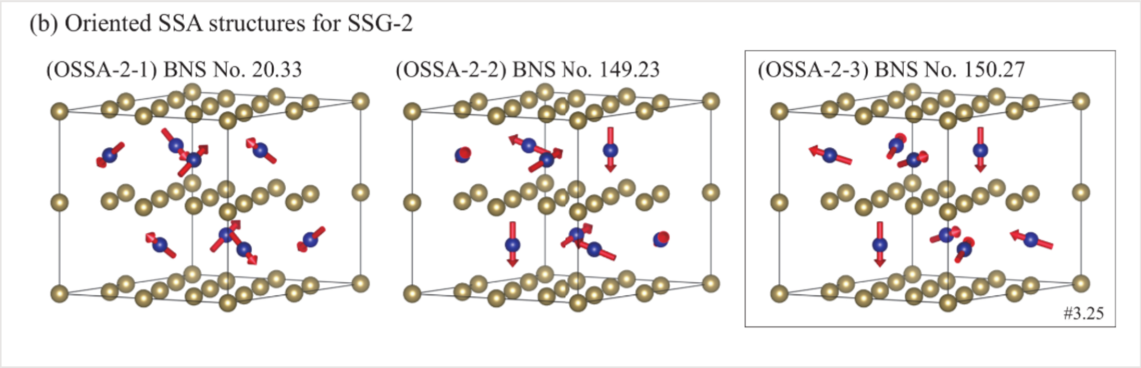
A local chart of the rotation manifold: constraint curves cross at the oriented SSGs.



A local chart of the rotation manifold around the BNS 150.27 solution of $CoTa_3S_6$ SSG-2; each compatible operation constrains Q to a curve, and the high-symmetry (maximal) MSGs, the oriented SSGs, sit where the curves cross.

On the chart: the center crossing = BNS 150.27 (reported); the crossings at $|v| = \pi/2$ = BNS 149.23; the third oriented SSG, BNS 20.33, lies outside this patch.

the chart draws only the solutions at the center's spin direction and the curves through them; improper Q folded onto proper ones by sign; half the operations admit no compatible Q (never magnetic operations, e.g. pure spin rotations)



the structures the crossings stand for: boxed OSSA-2-3 (BNS 150.27, #3.25) = the center crossing; OSSA-2-2 (BNS 149.23) = the $|v| = \pi/2$ crossings

Spin chirality, formal

Conjugating by an improper spin rotation, and comparing by proper rotations of the d spin dimensions, makes $d = 2$ the single nontrivial case, provided the spin representation is physically irreducible.

Refinement: enantiomorph by a mirror, comparison by a proper rotation

- The enantiomorphic SSG: $\mathcal{X}_\mathrm{e} = (1, \sigma)^{-1}\, \mathcal{X}\, (1, \sigma)$, with σ an improper spin rotation
- $\mathcal{X}$ is chiral iff **no proper** $Q \in SO(d) \oplus \mathbf{I}_{3-d}$ intertwines $\mathcal{X}$ and $\mathcal{X}_\mathrm{e}$

The parity argument: why only $d = 2$ survives

- An intertwiner always exists: σ itself intertwines $\mathcal{X}$ and $\mathcal{X}_\mathrm{e}$ **by construction** (it is improper)
- $-\mathbf{1}_d$ commutes with every spin part, so it is a **self-intertwiner**, with $\det(-\mathbf{1}_d) = (-1)^d$
- Odd d (1, 3): composing an intertwiner with $-\mathbf{1}_d$ flips its parity ▶ a proper intertwiner can always be chosen ▶ achiral
- $d = 2$: $\det(-\mathbf{1}_2) = +1$, so $-\mathbf{1}_2$ no longer flips the parity ▶ **spin-planochirality** is decided by whether the spin representations of $\mathcal{X}$ and $\mathcal{X}_\mathrm{e}$ admit **only** $\det = -1$ intertwiners

The $d = 2$ parity is fixed iff the spin representation is physically irreducible

- The parity is fixed iff every **self-intertwiner** is proper: composing an intertwiner with an improper self-intertwiner would flip its parity
- Reducible case: the 2D spin representation splits into two 1D ones, so $\mathbf{1} \oplus (-\mathbf{1})$ is an **improper self-intertwiner** ▶ achiral
- **Physically irreducible** (irreducible over $\mathbb{R}$): by the real Schur lemma the self-intertwiners form $\mathbb{R}$ (real type) or $\mathbb{C}$ (complex type), and every nonzero element has $\det > 0$ ▶ the parity is fixed
- Hence a spin-planochiral SSG carries a **physically irreducible** 2D spin representation (SSG-2 of Mn_3Sn: the E irrep of C_{3v})

preprint Appendices C and D

Spin-planochirality in action: the full Mn_3Sn payoff

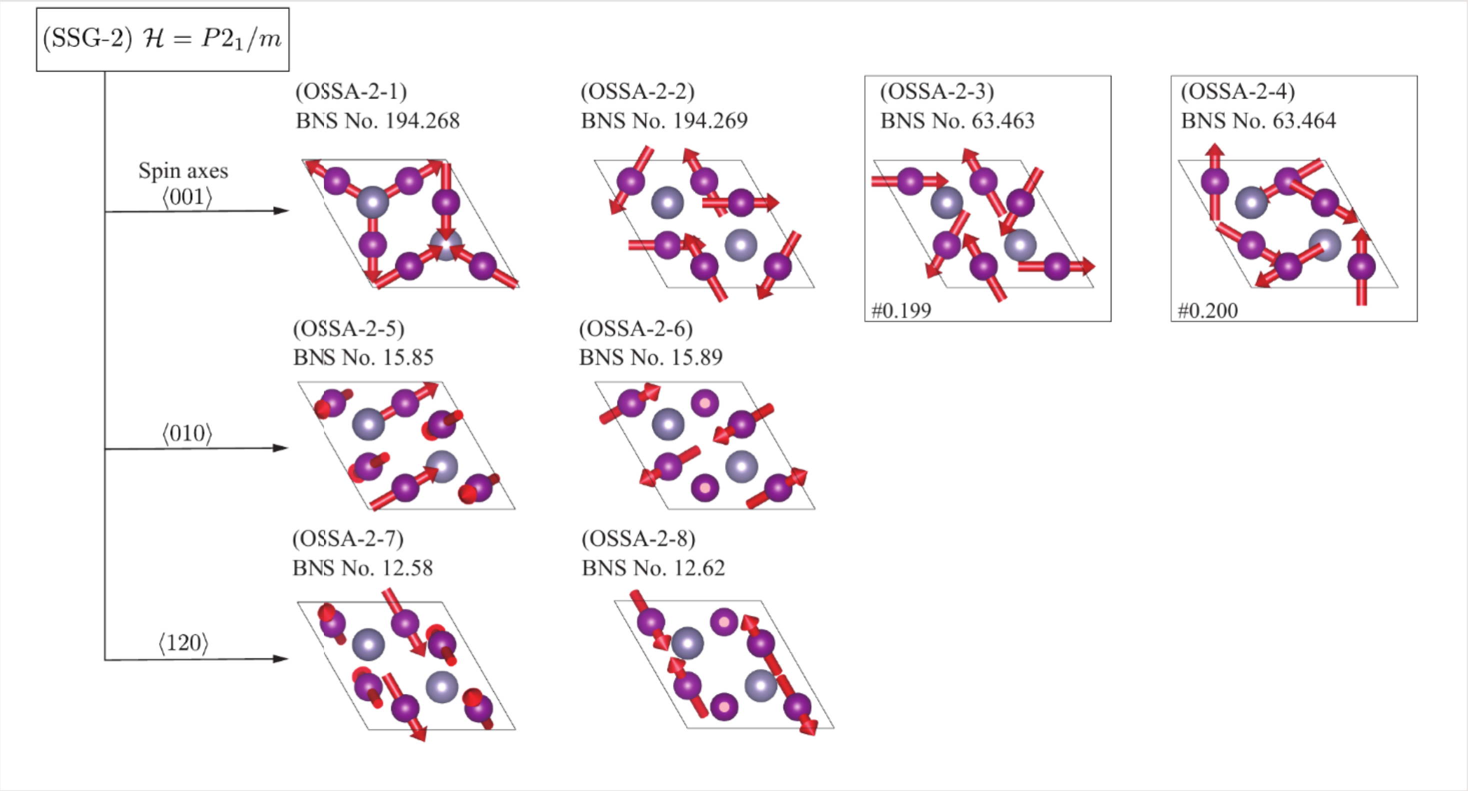
SSG-2 is spin-planochiral; enumerating its enantiomorph adds Mn_3Sn's reported inverse-triangular pair.

Setup

- **SSG-2 is spin-planochiral**: spin rotations realize the 2D E irrep of $G/\mathcal{H} \cong C_{3v}$
- Enumerate from **both** SSG-2 and its enantiomorph, group up to conjugacy

Result: new structures only along $\langle 001 \rangle$

- $\langle 010 \rangle$ / $\langle 120 \rangle$: unchanged; $\langle 001 \rangle$: **doubles** ▶ the reported pair #0.199 / #0.200 (BNS 63.463 / 63.464)
- $C_{6z}C_{2x}$ (a spin-plane mirror) pairs each inverse with its normal partner



the oriented-SSA tree of SSG-2 and its enantiomorph; the $\langle 001 \rangle$ row carries the $C_{6z}C_{2x}$ pairing

Conclusion: MSGs treat inverse = normal; **spin-planochirality distinguishes them and recovers the reported pair**

their MSGs are orthorhombic (BNS 63.x); the SSG keeps the hexagonal spin operations, holding all six $6h$ sites in one orbit

BACKUP · Q&A ONLY

Generation-method comparison

Given the same input, a family space group and a propagation-vector star, established symmetry-based generation cannot guarantee equal moments or leaves the global spin axis unresolved; SSA structures with oriented SSGs provide both, and the closest concurrent workflow (Li *et al.*) awaits a detailed comparison.

METHOD	CONSTRUCTION	LIMITATION
RA	the $3N$ magnetic degrees of freedom decomposed into IRs; basis vectors as candidates	multi-dimensional IRs: the combination underdetermined; equal moments not guaranteed
RA + isotropy subgroups (ISODISTORT / MAXMAGN)	epikernel principle: the combinations yielding maximal MSGs	highest symmetry within each IR, still no equal-moment guarantee by construction
Cluster multipole (CMP)	multipole-based symmetry-adapted basis, mapped from a virtual cluster	same MSG framework as RA ▶ same limitation; a basis construction, not a distinct symmetry framework
Jiang *et al.*	SSG enumeration; per-Wyckoff refinement constraints	refinement-oriented, not yet a generation scheme; the global spin axis stays unresolved, fixed externally
Li *et al.*	hierarchical SSG-to-MSG workflow, ranked by two-step DFT	conceptually closest to ours; the SSG-to-MSG step is public only at a high level, detailed comparison ongoing
Ours	**SSA structures (totally symmetric rep of the SSG) ▶ oriented SSGs fix the global orientation**	**equal moments by construction; the magnetic space group determined**

RA: Bertaut, Acta Cryst. A **24**, 217 (1968); Izyumov and Naish, J. Magn. Magn. Mater. **12**, 239 (1979). Isotropy subgroups: Ascher, J. Phys. C **10**, 1365 (1977); Stokes and Hatch, *Isotropy Subgroups of the 230 Crystallographic Space Groups* (1989); ISODISTORT: Campbell, Stokes, Tanner, and Hatch, J. Appl. Crystallogr. **39**, 607 (2006); MAXMAGN (Bilbao magnetic tools): Perez-Mato *et al.*, Annu. Rev. Mater. Res. **45**, 217 (2015); Zhou *et al.*, arXiv:2601.01617 (same framework, with a practical high-symmetry-direction rule). CMP: Suzuki *et al.*, Phys. Rev. B **95**, 094406 (2017); Suzuki *et al.*, Phys. Rev. B **99**, 174407 (2019); Yanagi *et al.*, Phys. Rev. B **107**, 014407 (2023). SSG: Jiang *et al.*, PRX **14**, 031039 (2024); Li *et al.*, arXiv:2512.21672. Ours: arXiv:2601.15735; the oriented-SSG concept: Liu *et al.*, Nature **652**, 869 (2026)