ORAL TALK
Thu Aug 13, 11:30 AM
MS-023 Spin groups & magnetic symmetry

Magnetic-Structure Generation Based on Oriented Spin Space Groups

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01 Introduction

- Spin density functional theory (SDFT): convergence near the initial guess; candidate structures decide the search outcome.
- Standard route [1,2], database-scale searches on it [3]: representation analysis with isotropy subgroups, yielding maximal magnetic space groups (MSGs); equal moments on equivalent sites not guaranteed by construction.

CONTRIBUTION **Candidate magnetic structures from spin space groups: equal moments by construction; each candidate with its magnetic space group.**

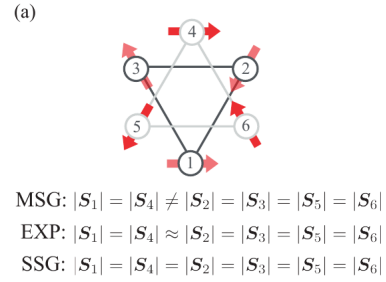


Figure 1. Mn_3Sn, a triangular kagome structure; $|m|$ on the six Mn sites. MSG: sites {1,4} and {2,3,5,6} constrained separately; experiment; SSG.

02 SSA structures from spin space groups

- Spin-space-group (SSG) operation (g, U): spatial operation g and **independent** spin rotation $U \in O(3)$, locked in an MSG; approximate symmetry for weak spin–orbit coupling (SOC) [4–6].
- **Spin-symmetry-adapted (SSA) structure**: the arrangement invariant under every SSG operation; totally symmetric representation, by projection.
- **Equal magnitudes, naturally**: orbits intact, spin rotations length-preserving; a consequence, not an ansatz.

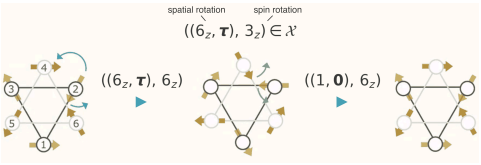


Figure 2. One SSG operation, $((6_z, \tau), 3_z)$, in two steps: the locked pair, then a pure spin rotation.

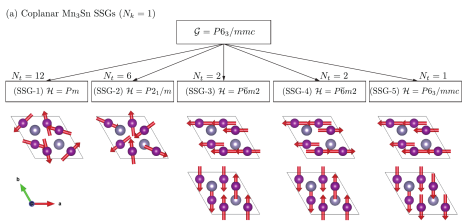


Figure 3. Coplanar SSGs of Mn_3Sn ($G = P6_3/mmc$) with their SSA structures. One Mn orbit (Wyckoff 6h); per box = basis vectors.

03 Oriented SSGs: fixing the spin axis

- SSA structure fixed only up to a global spin rotation Q; the spin axis pinned by SOC.
- **Oriented SSGs**, concept and name due to Liu *et al.* [7]: Q fixed, maximal induced MSGs kept; one object with both the SSG and its BNS symbol.

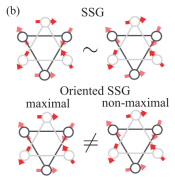


Figure 4. Same SSG, equivalent up to a global spin rotation (~); orientation fixed, maximal vs non-maximal induced MSG (≠).

Survival condition, from the SOC Hamiltonian [8]:

$$(\det R)\, R = (\det U)\, Q^{-1} U\, Q$$

Q constructed as a real intertwiner.

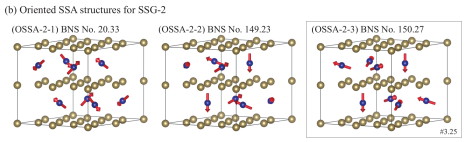
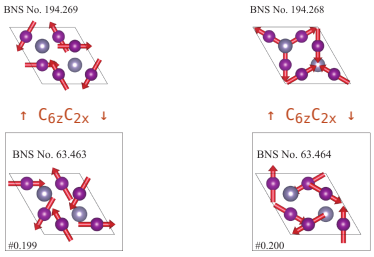


Figure 5. $CoTa_3S_6$ (all-in-all-out), one SSG: three orientations, three maximal MSGs (BNS 20.33 / 149.23 / 150.27); boxed = reported (MAGNDATA #3.25).

04 Spin-planochirality: the reported Mn_3Sn pair

NORMAL TRIANGULAR · KEPT AS MAXIMAL spin axis (001)



INVERSE TRIANGULAR · REPORTED, RECOVERED

Figure 6. The four (001)-pinned structures of Mn_3Sn SSG-2, normal pair and inverse pair.

- Mn_3Sn, spin axis (001): reported inverse-triangular pair (#0.199 / #0.200) mapped onto the more symmetric normal pair by a global spin rotation; absent from the plain maximal enumeration.
- Enantiomorph $X_e = (1, \sigma)^{-1} X (1, \sigma)$; comparison by proper rotations $Q \in SO(d) \oplus I_{3-d}$ only.

Both enantiomorphs enumerated: the reported pair recovered; inverse and normal identical as MSGs.

SPIN DIMENSION	CHIRALITY	EXISTS?
collinear (d = 1)	spin-axichirality	none
coplanar (d = 2)	spin-planochirality	yes
noncoplanar (d = 3)	(unrestricted, SO(3))	none

05 Results: database-scale validation

- **MAGNDATA orbit statistics** (spinspg [8]): **119 / 1,764** structures with $n_{SSG} < n_{MSG}$; equal-moment sites split by the MSG.

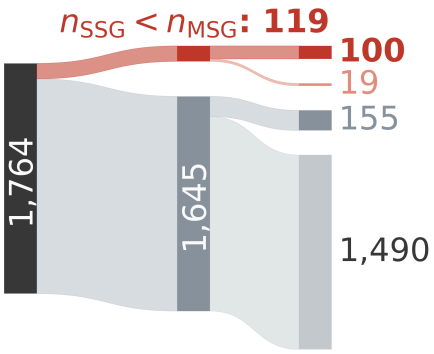
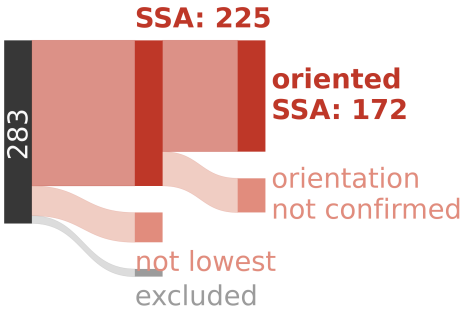


Figure 7. Accent branch = the decisive case (100 of the 119, every nonmagnetic orbit intact).

- **SDFT benchmark**: 283 materials; reported structure recovered for 225 of the 271 assessed at the SSA level, 172 also at the oriented level.



SSA: 225 = reported structure lowest in energy at the SSA level; oriented SSA: 172 = lowest at the oriented level too; pale = not the lowest; gray excluded = the 12 materials with only one SSA candidate.

Figure 8. Two-step SDFT: self-consistent without SOC (SSA), then fixed-charge with SOC (oriented SSA). Per magnetic atom: ~100 meV between SSA structures, ~0.3 meV within a manifold.

06 Outlook: magnetic structure determination

- Oriented SSA structures as **few-parameter initial models**: a nonmagnetic structure and a propagation vector as input; sign, magnitude, and spin angle fitted against $F(Q)$, ranked by R-factor.
- Collaboration with experimentalists underway; Rietveld integration (FullProf, JANA2020, GSAS-II) as an additional option alongside ISODISTORT.

07 Conclusions

- SSA structures: equal moment magnitudes, naturally.
- Oriented SSGs determine each candidate's magnetic space group, ready for refinement.
- Spin-planochirality recovers Mn_3Sn's reported pair.
- Validated across MAGNDATA and a 283-material SDFT benchmark.

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