SPICE-Workshop on Quantum Geometry and Transport of Collective Excitations in (Non-)Magnetic Insulators

Spin Space Group Theory and Unconventional Magnons in Collinear Magnets

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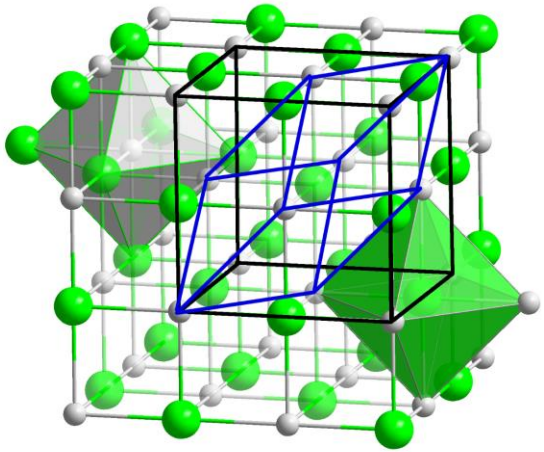
***Phys. Rev. X* 12, 021016 (2022)**
***Phys. Rev. X* 14, 031038 (2024)**
***Nature* 640, 349 (2025)**
Nature 626, 523 (2024)
Nat. Phys. 21, 329 (2025)

Phys. Rev. Lett. 134, 106802 (2025)
Nat. Commun. 13, 919 (2022)
Phys. Rev. Lett. 129, 276601 (2022)
Phys. Rev. Lett. 133, 026402 (2024)
arXiv:2406.03738 (2024)

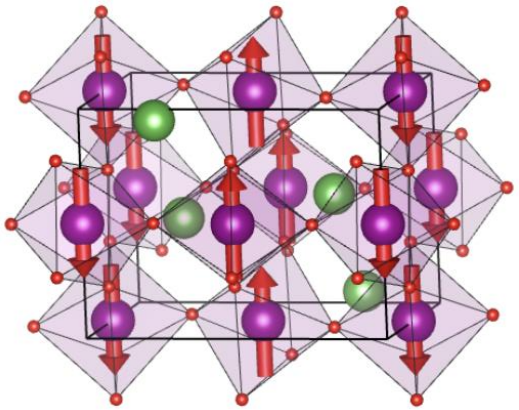
Outline

- **Spin group theory**
- **Unconventional magnons in collinear magnets**
- **Outlook: Unconventional magnetism**

Conventional wisdom of symmetry description for crystals



Nonmagnetic:
Crystallographic point/space groups
Federov, Schoenflies, etc. (1900s)



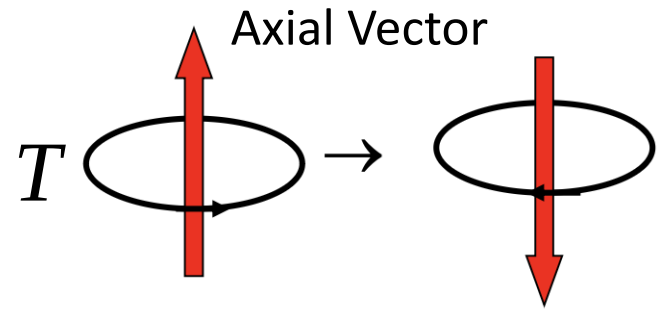
Magnetic ordered:
Magnetic point/space groups
Heesch, Shubnikov, etc. (1950s)

Can magnetic groups completely describe magnetic materials?

Magnetic group: Binary spin operation

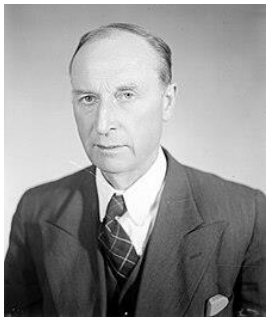
Time reversal = spin reversal

(change the sense of the current)



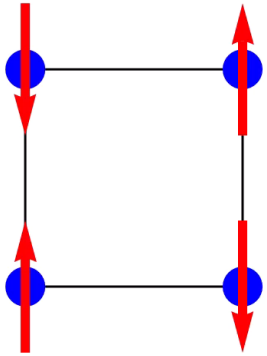
- Crystallographic group operations: C_n, P, M
- Magnetic group operations: C_n, P, M, C_nT, PT, MT

What does C_n mean in a magnetic group?

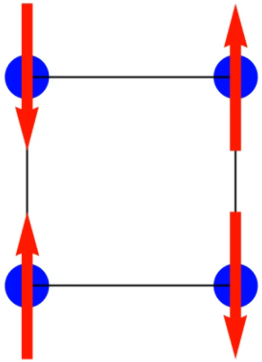


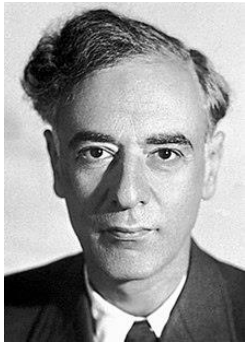
A. V. Shubnikov

C_2 for lattice only



C_2 for lattice & spin





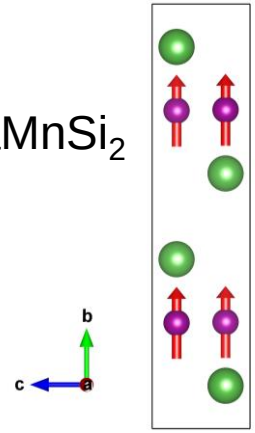
L. Landau

In either way, you can define a “magnetic group” …

Magnetic group is insufficient even in distinguishing FM/AFM

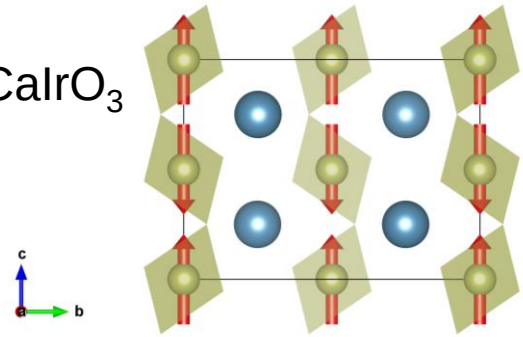
MSG: $Cm'cm'$

$LaMnSi_2$



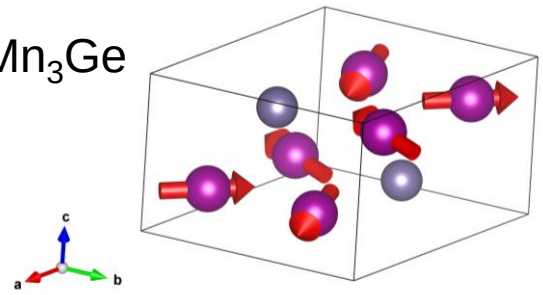
Collinear FM

$CaIrO_3$

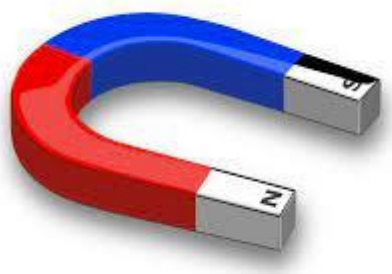


Collinear AFM

Mn_3Ge



Coplanar AFM

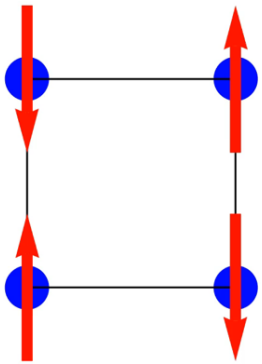


Ferromagnetism
Spin SU(2) symmetry breaking

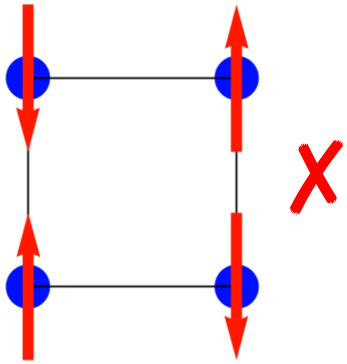
Separate spin and lattice rotations

Spin group

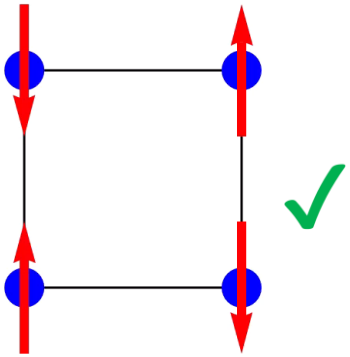
Spin group contains more symmetry operations



Consider an AFM spin arrangement

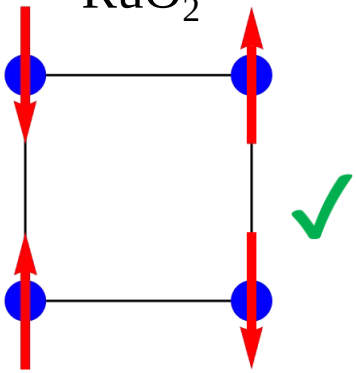


C_2 rotation in magnetic group



Lattice C_2 rotation (spin group)

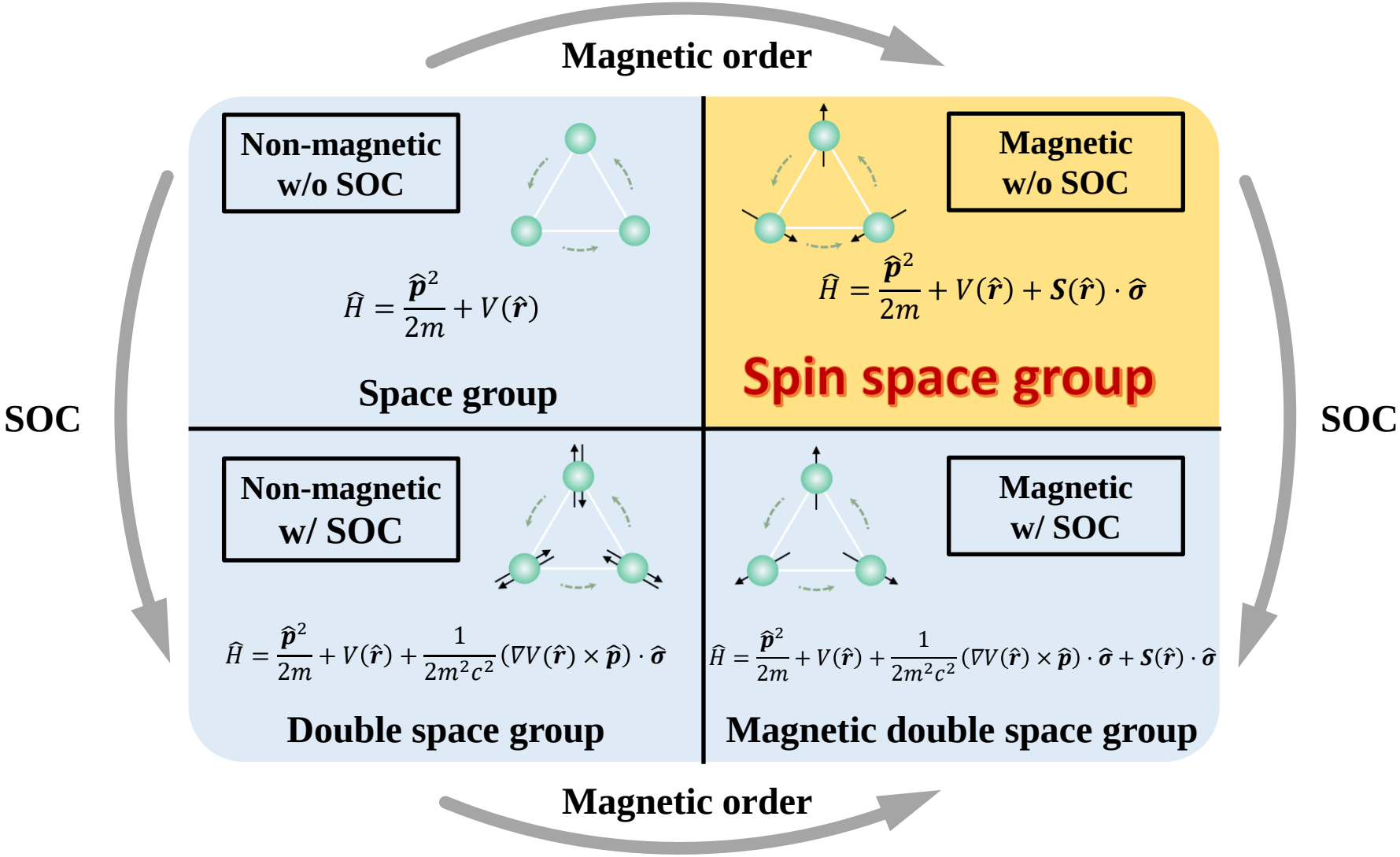
RuO_2



Lattice C_4 + Spin C_2 rotation (spin group)

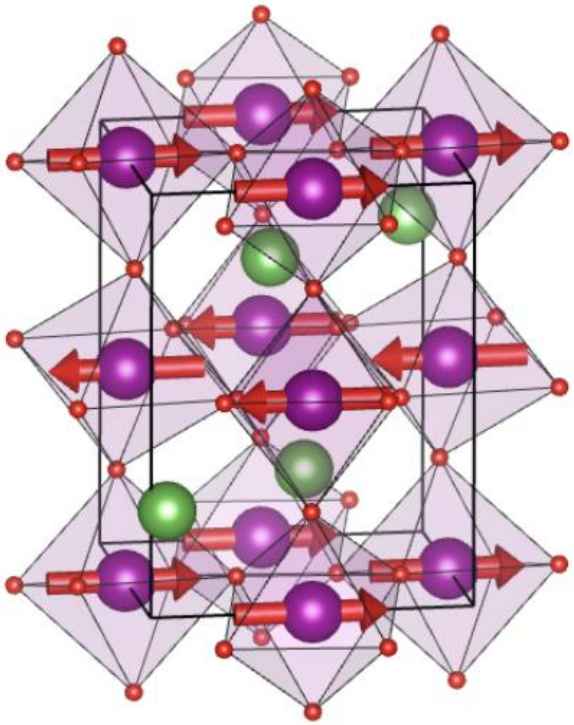
Spin group can completely describe magnetic geometry

Another way to consider: Symmetry of Hamiltonians



X. Wan*, **QL*** et al. PRX 12, 021016 (2022) arXiv:2103.15723

New insight of symmetry description for magnetic crystals



Magnetic order:

SPIN point/space groups

Symmetry breaking

If spin can feel lattice:

Magnetic point/space groups

Original works about spin group symmetry

- Geometry (1963): More "colors" are needed to completely describe the magnetic symmetry.

  V. E. Naish, *Izv. Akad. Nauk SSSR, Ser. Fiz.* **27**, 1496 (1963).

- Hamiltonian (1966): Multiple-fold degeneracies of spin wave spectrum require an enhanced symmetry group called "spin group", which consider spin rotation and spatial rotation separately.

  W. F. Brinkman and R. J. Elliott, *J. Appl. Phys.* **37**, 1457 (1966); *Proc. R. Soc. A* **294**, 343 (1966).

- Group theory (1977): 598 spin point groups are enumerated.

  D. B. Litvin and W. Opechowski, Physica **76**, 538 (1974);
  D. B. Litvin, Acta Crystallogr. A **33**, 279 (1977)

New development of spin group theories

- Spin point groups for specific magnetic configuration?

  PRX 12, 021016 (2022)

- Enumeration of spin space groups?

  PRX 14, 031038 (2024)

- Representation theory of spin space groups?

  Collinear: Nature 640, 349 (2025)
  Noncollinear: PRX 14, 031038 (2024)

- Parallel works on spin group theory:

P. McClarty's group: arXiv:2307.12784 (2023), Phys. Rev. B 105, 064430 (2022)

L. Šmekjal et al.: PRX 12, 031042 (2022)

R. Arita's group: Acta Cryst. A80, 94–103 (2024), Phys. Rev. B 109, 094438 (2024)

Z.-X. Liu and C. Fang's group: PRX 14, 031039 (2024), arXiv:2105.12738 (2021)

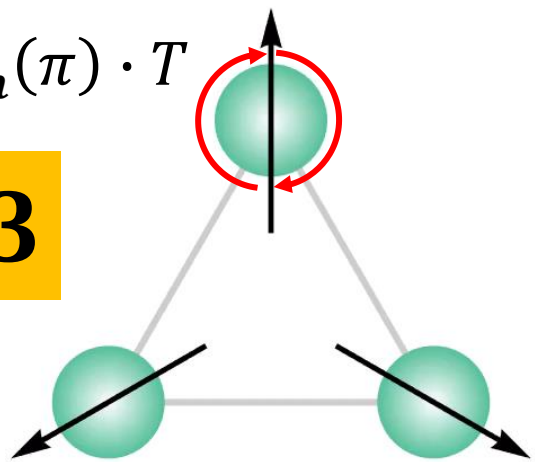
Z. Song's group: PRX 14, 031037 (2024)

Spin point groups for collinear and coplanar configurations

Coplanar: $G_{\mathrm{SO}} = Z_2^K$

$T_{\mathrm{eff}} = U_{\boldsymbol{n}}(\pi) \cdot T$

253

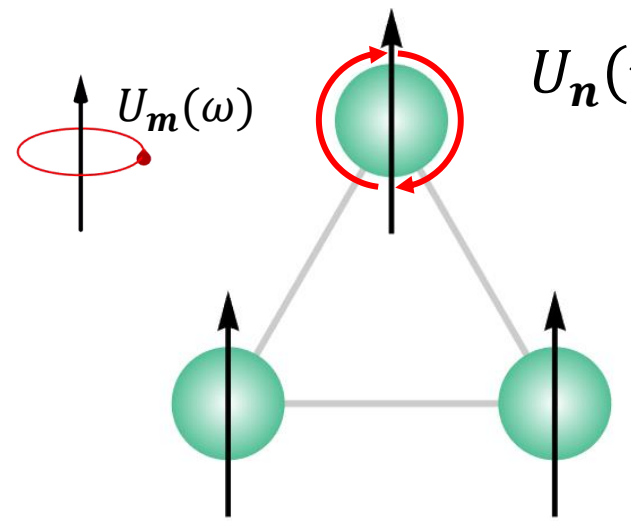


Collinear: $G_{\mathrm{SO}} = SO(2) \rtimes Z_2^K$

$U_{\boldsymbol{m}}(\omega)$

$U_{\boldsymbol{n}}(\pi) \cdot T$

90



Collinear
Coplanar } magnets

✗ Time-reversal T

✓ Effective time-reversal T_{eff}

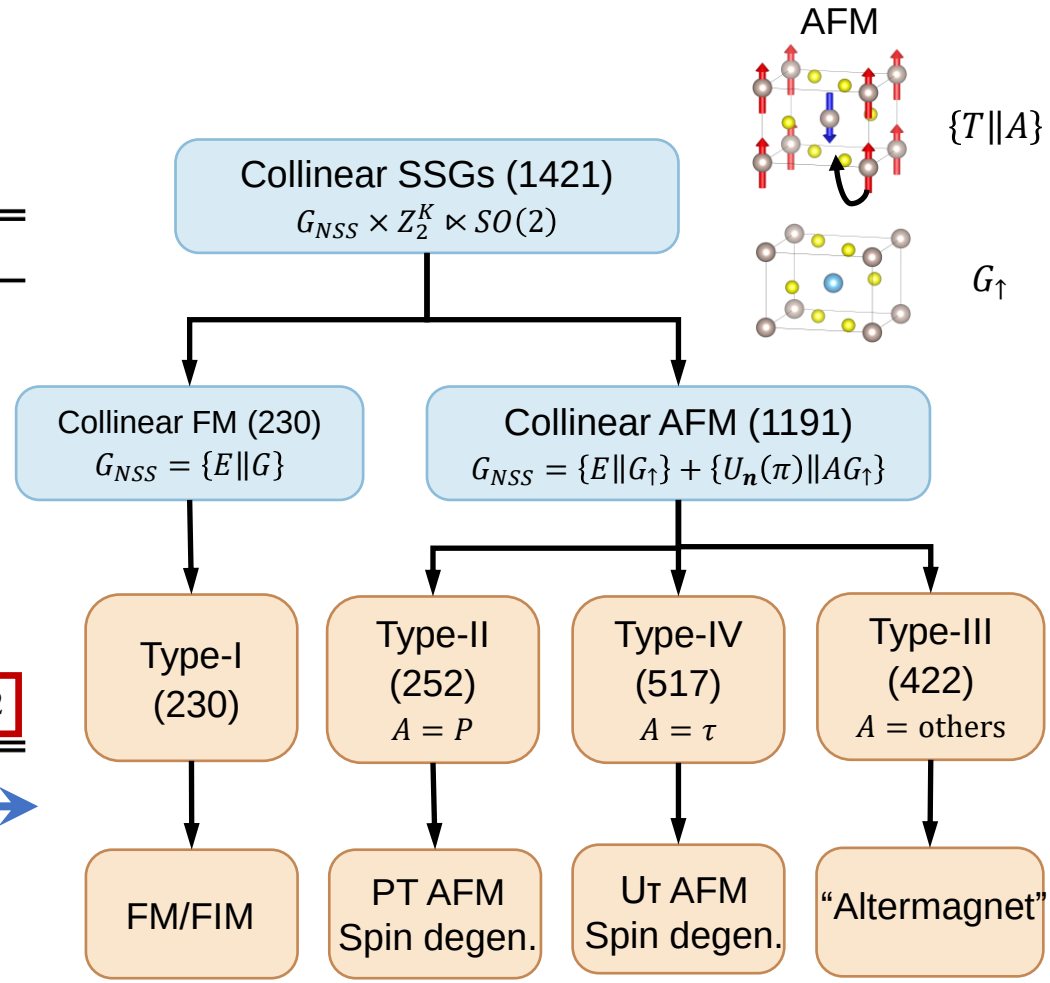
Effective T: NO anomalous Hall effect in col./cop. magnets (w/o SOC)

X. Wan*, **QL*** et al. PRX 12, 021016 (2022) arXiv:2103.15723

Enumeration of spin space group

Cell expansion cutoff: ≤ 8

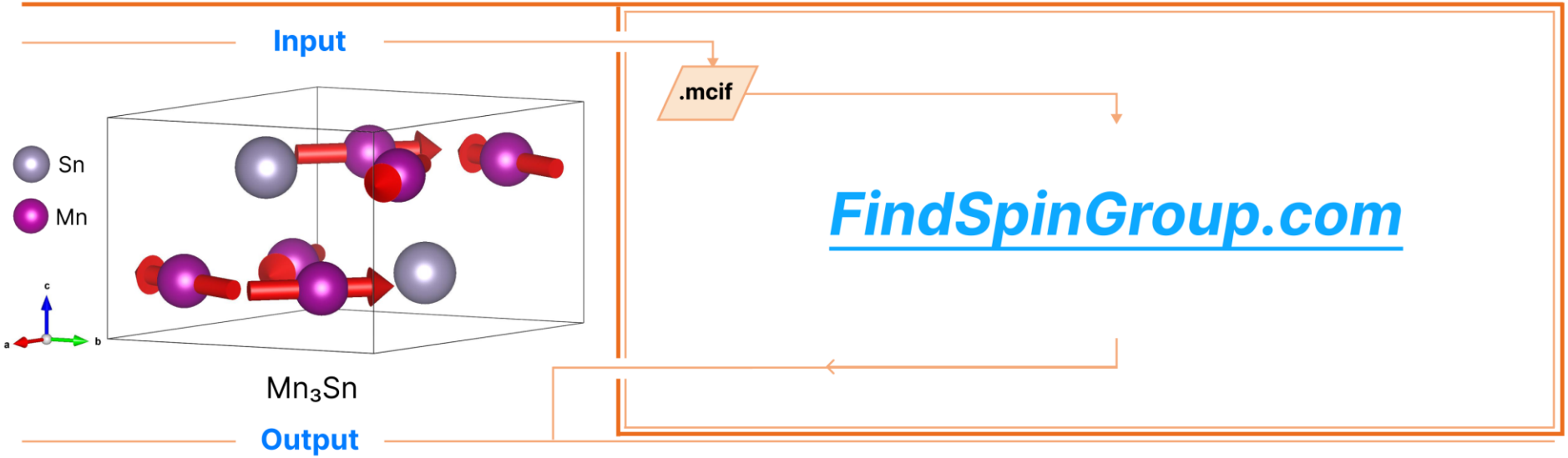
Crystal system	Collinear only	Coplanar	Noncoplanar only	Total
Triclinic (2)	5	55	0	60
Monoclinic (13)	78	3540	0	3618
Orthorhombic (59)	503	53734	0	54237
Tetragonal (68)	502	31185	0	31687
Trigonal (25)	83	2331	62	2476
Hexagonal (27)	137	7149	111	7397
Cubic (36)	113	840	184	1137
Total (230)	1421	98834	357	100612



QL* et al. PRX 14, 031038 (2024)

QL* et al. Nature 640, 349 (2025)

Identification of the spin group symmetries



File Name	Spin Space Group	G0 Symbol	L0 Symbol	it	ik
0.200/Mn₃Sn	$P^{3^1_{001}}6_3/{}^1m^{m\frac{\pi}{3}}m^{m\frac{2\pi}{3}}c^m1$	$P6_3/mmc(194)$	$P2_1/m(11)$	6	1

Space Group	Magnetic Space Group	Spin Part PG	Configuration	Magnetic Phase
$P6_3/mmc(194)$	*Cm'cm'*(63.464) *Type III*	*C3v × Cs = D3h* *3m x 3 = -6m2*	*Coplanar*	*Canting AFM*

Little Cogroup at General Position		Spin Splitting		Effective Magnetic Point Group	Anomalous Hall Effect	
without SOC	with SOC	without SOC	with SOC		without SOC	with SOC
m_{001}-1	1	*k-dependent*	*Yes*	6/mmm1'	*No*	*Yes*

Input:

- .mcif
- Editing data in the program

Output:

- Spin group/magnetic group
- Symmetry operations
- Physical properties

Applications of spin group theory

1) New degeneracies, new quasiparticles, and new topological phases

Chiral Dirac fermion: Theory — The Innovation 3, 100343 (2022)

Experiment — Chin. Phys. Lett. (Express) 40, 126101 (2023)

Z_2 topological phase: PRX 12, 021016 (2022)

Unconventional magnons: Nature 640, 349 (2025)

2) Starting point to investigate SOC effects in magnetic materials

Material search of correlation enhanced SOC: Nat. Commun. 13, 919 (2022)

Multipolar anisotropy: Y. Gao and Q. Niu et al. arXiv:2408.08810 (2024)

3) Emergent effects without the assistance of SOC

AFM induced spin splitting: Nature 626, 523 (2024)

Quantum geometry nonlinear transport: arXiv:2406.03738 to appear in Nat. Commun.

Multiferroicity: PRL 134, 106802 (2025)

4) Classify magnetic phases

Unconventional magnetism [Nat. Phys. 21, 329 (2025)], e.g., altermagnetism

Article

Unconventional magnons in collinear magnets dictated by spin space groups

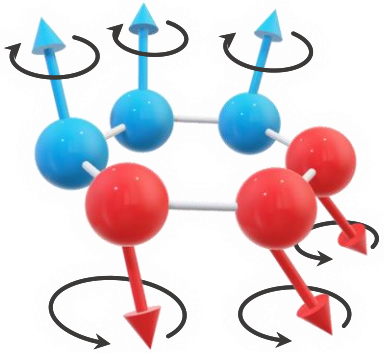
https://doi.org/10.1038/s41586-025-08715-7

Received: 23 July 2023

Accepted: 29 January 2025

Xiaobing Chen[1,2], Yuntian Liu[1], Pengfei Liu[1], Yutong Yu[1], Jun Ren[1], Jiayu Li[1], Ao Zhang[1] & Qihang Liu[1,2,3]

Topological magnons

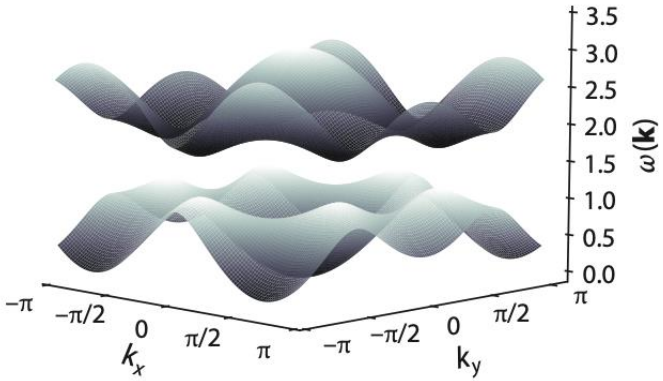


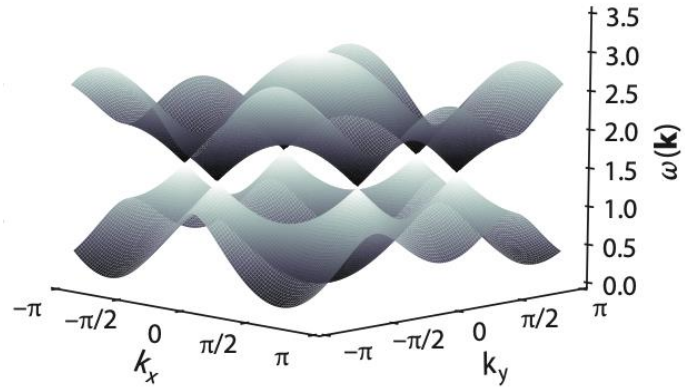
X. Chen, …, **QL*** et al. Nature 640, 349 (2025) arXiv:2307.12366

Topological magnons beyond MSGs

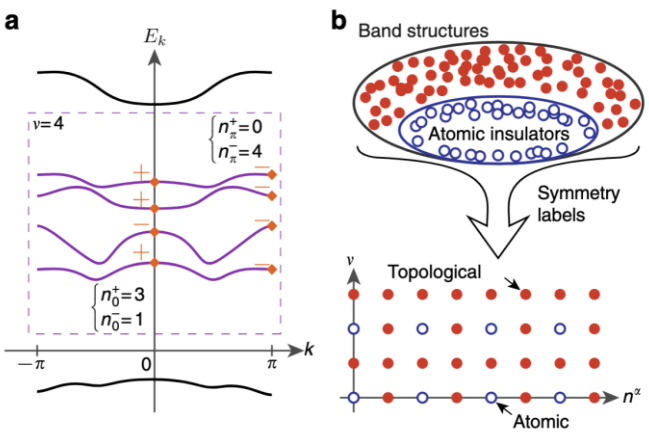
Band topology
(topological insulator)

Node topology
(topological semimetal)





Symmetry indicator (**magnetic group**)



Structure	Materials	Magnon topology
kagome	Cu[1,3-bdc]	Chern insulator
	FeSn, YMn_6Sn_6	Dirac magnon
	Mn_3X (X=Ge, Sn, Pt)	Nodal line
honeycomb	$CrBr_3$, CrI_3, $CrXTe_3$ (X=Si, Ge), α-$RuCl_3$	Chern insulator
	$CrCl_3$, $BaNi_2As_2O_8$	Dirac magnon
	$CoTiO_3$,	Nodal line
	β-Li_2IrO_3,	Nodal plane
	$MnPS_3$	Z_2 topological insulator
pychrocole	$Lu_2V_2O_7$, Cu_2OSeO_3, $Er_2Ir_2O_7$	Weyl magnon
hexagonal	Gd	Nodal plane
tetragonal	$SrCu_2(BO_3)_2$,	Chern insulator
Cubic	Cu_3TeO_6	Dirac and sextuple magnon

A. Mook, et al. PRL (2016); L. Chen, et al. PRX (2018); A. Corticelli et al., PRL (2023); Karaki et al., Sci. Adv. (2023); P. McClarty, Annu. Rev. Condens. Matter Phys. (2022)

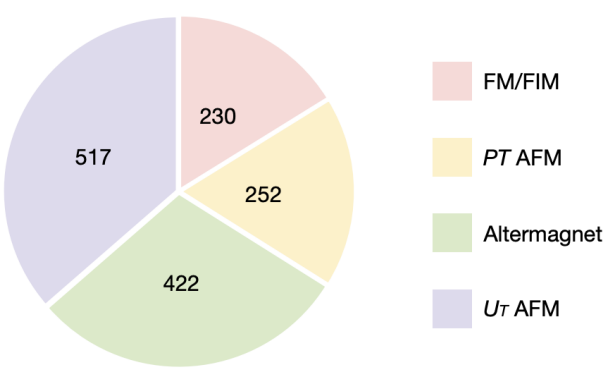
Magnons in collinear magnets largely respect SSG

- Multiple-fold degeneracies of magnon spectrum require "spin group".

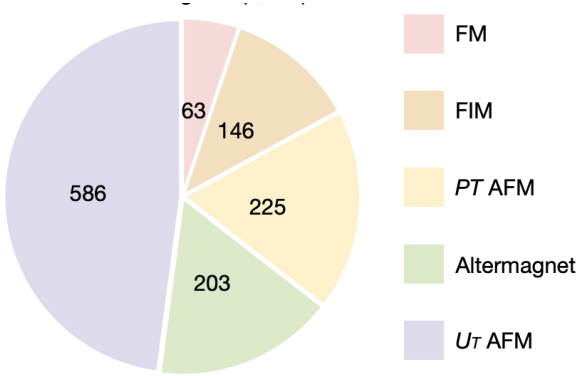
Brinkman et al., JAP 37, 1457 (1966);

$$H = \sum_{\langle ij \rangle} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + A \sum_i (S_i^z)^2 + \sum_{\langle ij \rangle} \boldsymbol{D}_{ij} \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_j) + J^{ani} \sum_{\langle ij \rangle \gamma} S_i^\gamma S_j^\gamma + \sum_{\langle ij \rangle} \Gamma^\gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) + \cdots$$

Heisenberg dominated; Single-ion anisotropy; Dzyaloshinskii Moriya; diagonal anisotropic symmetric; Off-diagonal anisotropic symmetric



Collinear SSGs (**1%**)



Collinear magnets (**62%**)

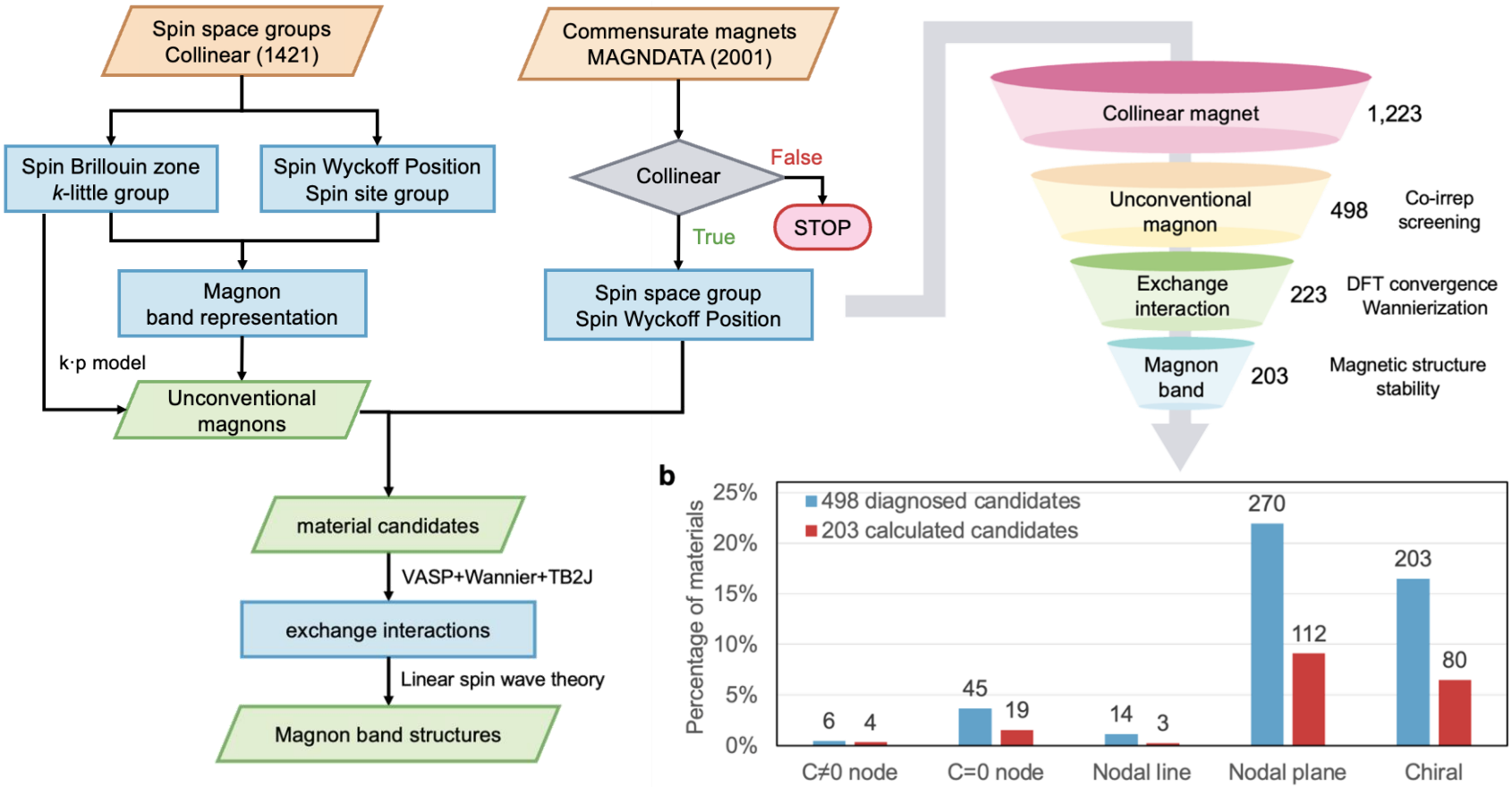
Collinear magnets: $\boldsymbol{J_{ij}} \gg J^{ani}, D, \Gamma$ (generally)

Searching unconventional magnons in collinear magnets

Collinear magnets
(FM / FIM / AFM)

$$H = \sum_{\langle ij \rangle} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

+ Collinear SSGs



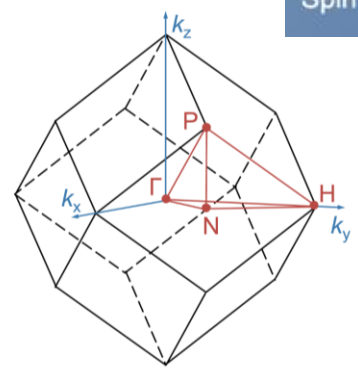
- ~ 500 collinear magnets hosting unconventional magnons
- > 200 magnon band structures w/ and w/o SOC

Band representations in FINDSPINGROUP

- Type I (Collinear Ferromagnet)
- Type II (PT Collinear Antiferromagnet)
- Type III (Altermagnet)
- Type IV (UT Collinear Antiferromagnet)

Wavevector-k	Little co-group
Γ:(0,0,0)	${}^{-1}\mathrm{m}^{-1}\text{-}3^{\infty\mathrm{m}}1$
H:(1,1,1)	${}^{-1}\mathrm{m}^{-1}\text{-}3^{\infty\mathrm{m}}1$
P:(1/2,1/2,1/2)	${}^{-1}\mathrm{m}^{-1}\text{-}3^{\infty}1$
N:(1/2,1/2,0)	${}^{1}2/{}^{2}\mathrm{m}^{\infty\mathrm{m}}1$
Δ:(0,v,0)	${}^{2}\mathrm{m}^{-1}\mathrm{m}^{2}\mathrm{m}^{\infty}1$
Λ:(u,u,u)	${}^{-1}\text{-}3^{\infty}1$
A:(u,v,0)	${}^{m}2/{}^{2}\mathrm{m}^{\infty}1$
D:(1/2,1/2,w)	${}^{1}2/{}^{-1}\mathrm{m}^{\infty}1$
G:(1+u,1-u,1)	${}^{m}2/{}^{2}\mathrm{m}^{\infty}1$
Σ:(u,u,0)	${}^{m}2/{}^{2}\mathrm{m}^{\infty}1$
C:(u,u,w)	${}^{-1}\text{-}1^{\infty}1$
GP:(u,v,w)	${}^{-1}\text{-}1^{\infty}1$

Spin Brillouin Zone



non-magnetic arithmetic crystal class $m\bar{3}I$

Spin Brillouin Zone & k-little co-groups

findspingroup.com

- General Positions
- Wyckoff Positions
- Spin Brillouin Zone & k-little co-groups
- Band Representations (Magnon)

Band Representations

16c

k-vector	k-vector-G↑	A1↑G(8)
Γ:(0,0,0)	Γ:(0,0,0)	$\Gamma_1^S(2)\oplus\Gamma_4^S(6)$
H:(1,1,1)	H:(1,1,1)	$H_1^S(2)\oplus H_4^S(6)$
N:(1/2,1/2,0)	N:(1/2,1/2,0)	$2N_1^S(2)\oplus 2N_2^S(2)$
P:(1/2,1/2,1/2)	P:(1/2,1/2,1/2)	$P_1^S(4)\oplus P_3^S(4)$
D:(1/2,1/2,w)	D:(1/2,1/2,w)	$2D_1^S(2)\oplus 2D_2^S(2)$
Δ:(0,v,0)	Δ:(0,v,0)	$2\Delta_1^S(2)\oplus 2\Delta_2^S(2)$
G:(1+u,1-u,1)	G:(1+u,1-u,1)	$4G_1^S(2)$
Λ:(u,u,u)	Λ:(u,u,u)	$2\Lambda_1^S(2)\oplus\Lambda_2^S(2)\oplus\Lambda_3^S(2)$
Σ:(u,u,0)	Σ:(u,u,0)	$4\Sigma_1^S(2)$
A:(u,v,0)	A:(u,v,0)	$4A_1^S(2)$
C:(u,u,w)	C:(u,u,w)	$4C_1^S(2)$
GP:(u,v,w)	GP:(u,v,w)	$4GP_1^S(2)$

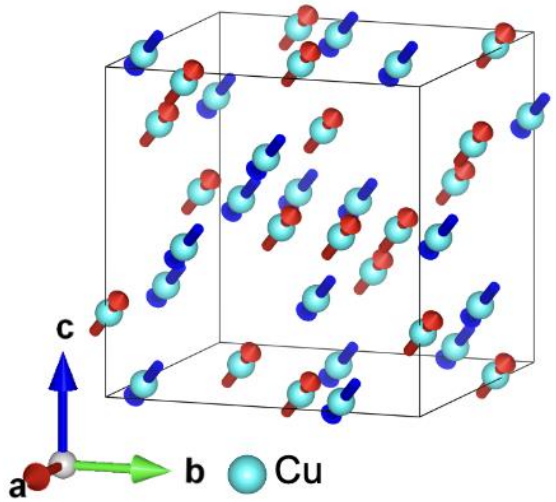
24d

k-vector	k-vector-G↑	A↑G(12)
Γ:(0,0,0)	Γ:(0,0,0)	$\Gamma_1^S(2)\oplus\Gamma_2^S\Gamma_3^S(4)\oplus\Gamma_4^S(6)$
H:(1,1,1)	H:(1,1,1)	$2H_4^S(6)$
N:(1/2,1/2,0)	N:(1/2,1/2,0)	$3N_1^S(2)\oplus 3N_2^S(2)$
P:(1/2,1/2,1/2)	P:(1/2,1/2,1/2)	$P_1^S(4)\oplus P_2^S(4)\oplus P_3^S(4)$
D:(1/2,1/2,w)	D:(1/2,1/2,w)	$3D_1^S(2)\oplus 3D_2^S(2)$
Δ:(0,v,0)	Δ:(0,v,0)	$4\Delta_1^S(2)\oplus 2\Delta_2^S(2)$
G:(1+u,1-u,1)	G:(1+u,1-u,1)	$6G_1^S(2)$
Λ:(u,u,u)	Λ:(u,u,u)	$2\Lambda_1^S(2)\oplus 2\Lambda_2^S(2)\oplus 2\Lambda_3^S(2)$
Σ:(u,u,0)	Σ:(u,u,0)	$6\Sigma_1^S(2)$
A:(u,v,0)	A:(u,v,0)	$6A_1^S(2)$
C:(u,u,w)	C:(u,u,w)	$6C_1^S(2)$
GP:(u,v,w)	GP:(u,v,w)	$6GP_1^S(2)$

48e

k-vector	k-vector-G↑	A↑G(24)
Γ:(0,0,0)	Γ:(0,0,0)	$\Gamma_1^S(2)\oplus\Gamma_2^S\Gamma_3^S(4)\oplus 3\Gamma_4^S(6)$
H:(1,1,1)	H:(1,1,1)	$H_1^S(2)\oplus H_2^S H_3^S(4)\oplus 3H_4^S(6)$
N:(1/2,1/2,0)	N:(1/2,1/2,0)	$6N_1^S(2)\oplus 6N_2^S(2)$
P:(1/2,1/2,1/2)	P:(1/2,1/2,1/2)	$2P_1^S(4)\oplus 2P_2^S(4)\oplus 2P_3^S(4)$
D:(1/2,1/2,w)	D:(1/2,1/2,w)	$6D_1^S(2)\oplus 6D_2^S(2)$
Δ:(0,v,0)	Δ:(0,v,0)	$6\Delta_1^S(2)\oplus 6\Delta_2^S(2)$
G:(1+u,1-u,1)	G:(1+u,1-u,1)	$12G_1^S(2)$
Λ:(u,u,u)	Λ:(u,u,u)	$4\Lambda_1^S(2)\oplus 4\Lambda_2^S(2)\oplus 4\Lambda_3^S(2)$
Σ:(u,u,0)	Σ:(u,u,0)	$12\Sigma_1^S(2)$
A:(u,v,0)	A:(u,v,0)	$12A_1^S(2)$
C:(u,u,w)	C:(u,u,w)	$12C_1^S(2)$
GP:(u,v,w)	GP:(u,v,w)	$12GP_1^S(2)$

Cubic spin space group in collinear AFM: Cu_3TeO_6

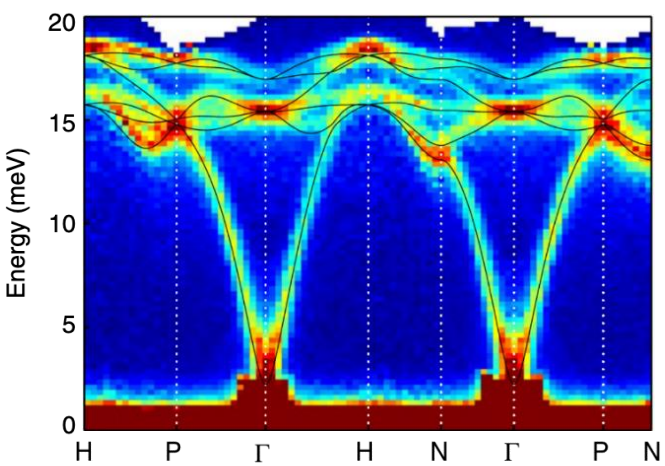


Space group :$Ia\bar{3}$ (Cubic)

Magnetic space group: $R\bar{3}'$ (Rhombohedral)

Spin space group: $I^{\bar{1}}a^{\bar{1}}\bar{3}^{\infty m}1$ (Cubic)

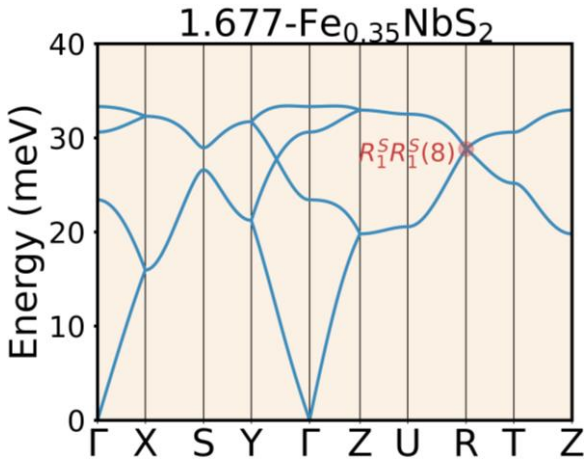
- ✓ Six-fold degenerate points at Γ、H
- ✓ Dirac magnons at Γ、P
- ✓ Doubly-degenerate at arbitrary *k*



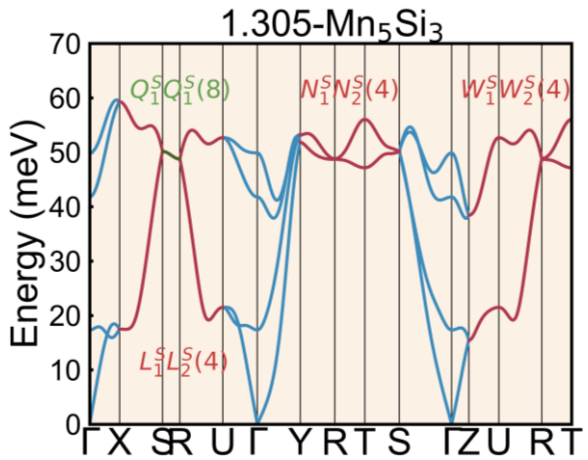
	Magnetic space group $R\bar{3}'$	Spin space group $I^{\bar{1}}a^{\bar{1}}\bar{3}^{\infty m}1$
Band rep	**2A ↑ G (12)**	**A^S ↑ G (12)**
Γ (0, 0, 0)	$4\Gamma_1(1) + 4\Gamma_2\Gamma_3(2)$	$\Gamma_1^S(2) + \Gamma_2^S\Gamma_3^S(4) + \Gamma_4^S(6)$
H (0, 1, 0)	$4H_1(1) + 4H_2H_3(2)$	$2H_4^S(6)$
N (1/2, 1/2, 0)	$12N_1(1)$	$3N_1^S(2) + 3N_2^S(2)$
P (1/2, 1/2, 1/2)	$4P_1(1) + 4P_2P_3(2)$	$P_1^S(4) + P_2^S(4) + P_3^S(4)$
GP (u, v, w)	$12GP_1(1)$	$6GP_1^S(2)$

Yao, et al. Nat. Phys. 14, 1011 (2018)
Bao, et al. Nat. Commun. 9, 2591 (2018)

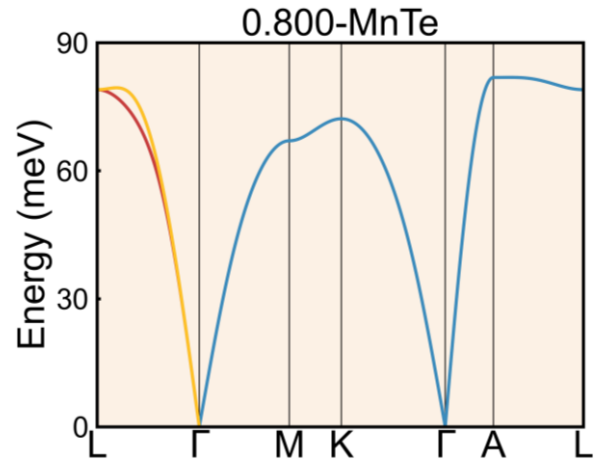
Magnon band database



C-4 Octuple point

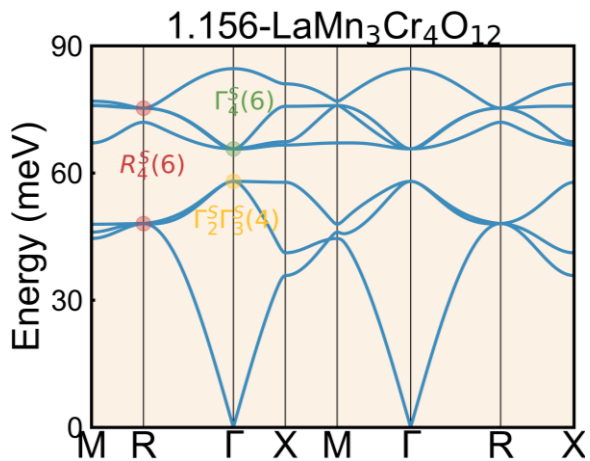


Quadruple nodal plane net
+ Octuple nodal line

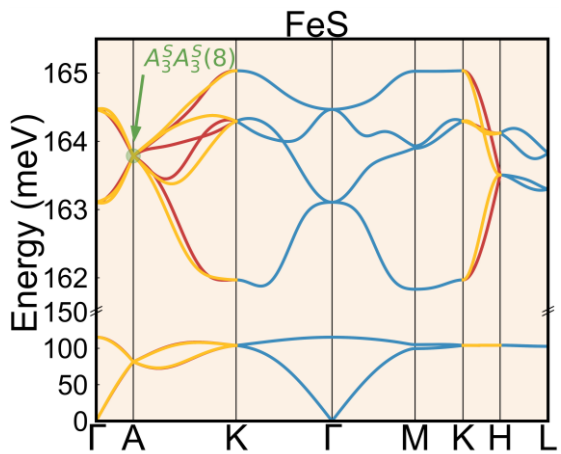


Chiral magnon

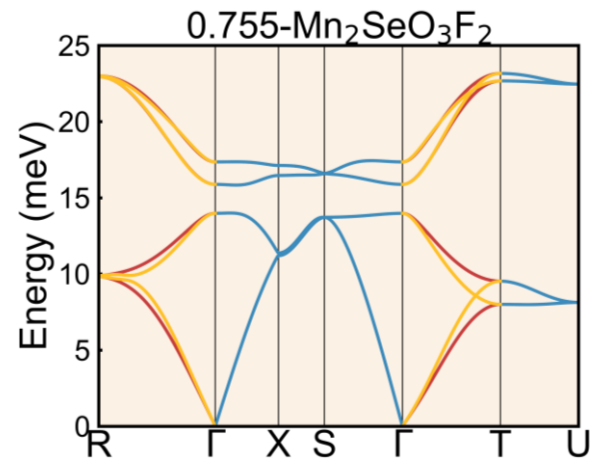
T. Masuda et al., PRL 133, 156702 (2024)



C-4 Sextuple point
C-8 Dirac point



Octuple nodal point
+ Chiral magnon

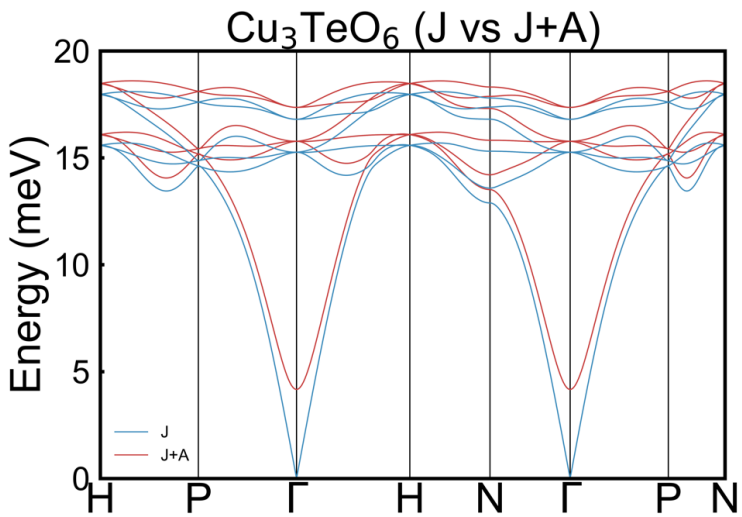


Chiral magnon

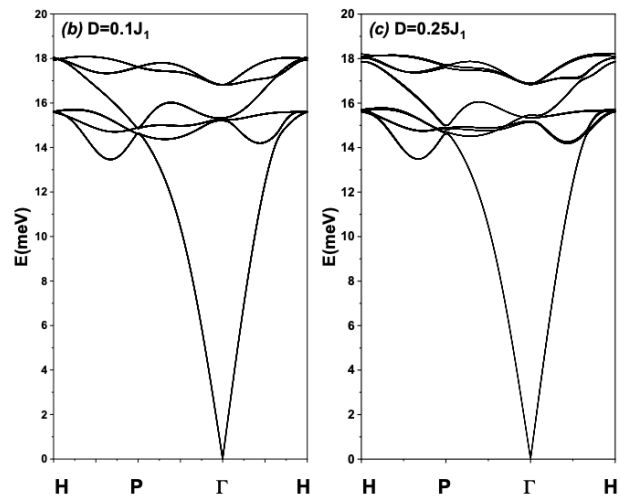
SOC effects

- ~87% 3d, 4d and 4f collinear magnets dominated by SSG

Magnetic ions	Materials	<10% |J|			J dominated
		|D|	|J^{ani}|	|Γ|	
3d	194	175	182	189	169
4d	7	5	5	6	5
4f	12	11	10	11	9
5d	6	1	0	3	0
5f	4	1	0	3	0
Total	223	193	197	212	183



Single-ion anisotropy (A)



Dzyaloshinskii-Moriya interaction (D)

Y. Liu et al., PRB 108, 094427 (2023)

Summary and What's next?

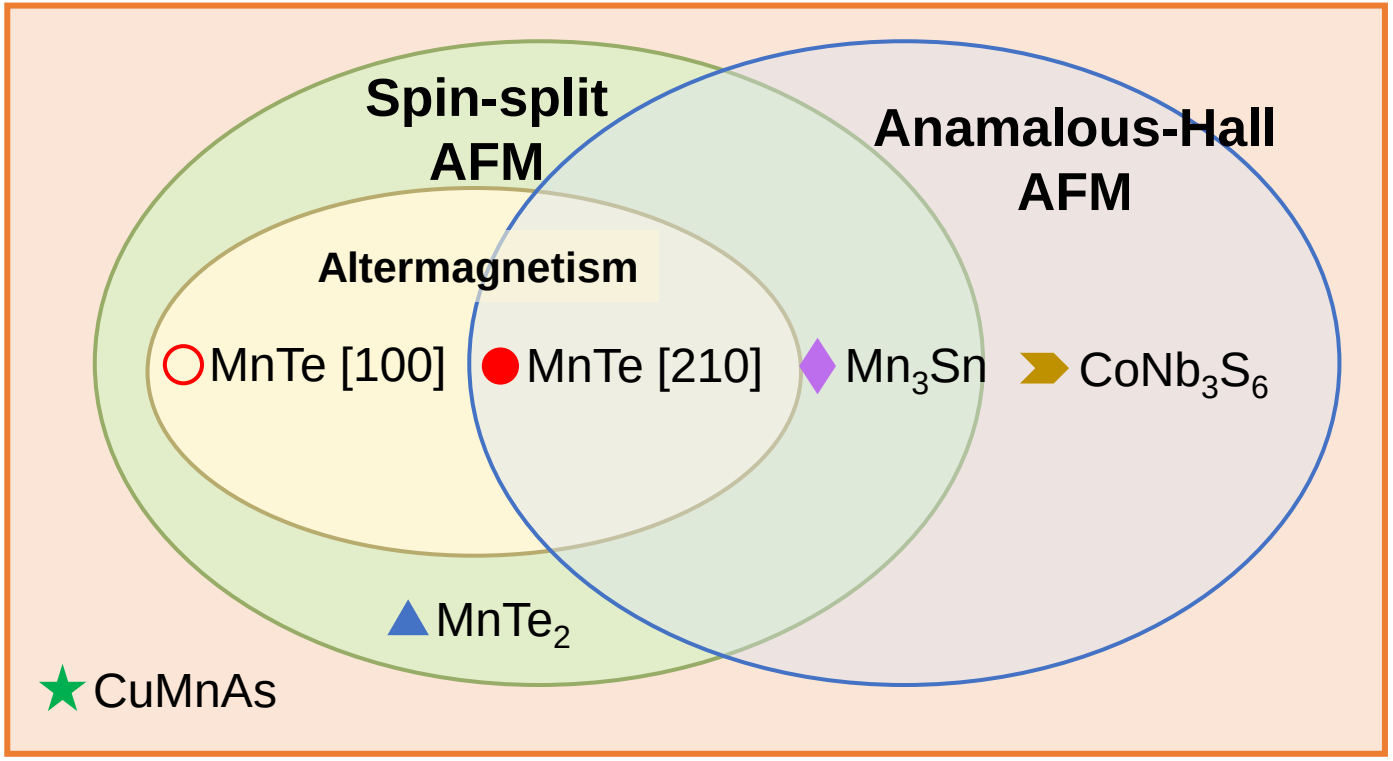
Spin group describes geometry / Magnetic group describes SOC

- Enumeration and representation theory for spin space groups
- Online program FINDSPINGROUP findspingroup.com
- Exploration of general "Unconventional Magnetism"

  Spin splitting, anomalous Hall, multiferroicity, nonlinear transport…

Facets of Unconventional magnetism: dependent on specific properties

Unconventional Magnetism：
AFM configuration with FM properties

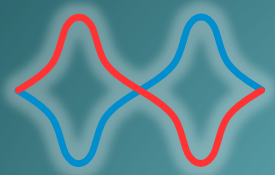


Nakatsuji, S. et al. Nature 527, 212 (2015)
Wadley, P. et al., Science 351, 587 (2016)
G. Betancourt, et al., PRL 130, 036702 (2023)

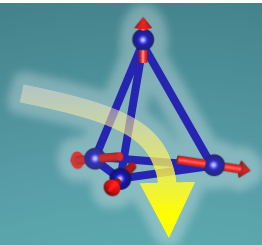
Takagi, H. et al., Nat. Phys. 19, 961 (2023)
Chen, X. et al. PRX 14, 031038 (2024)
Zhu, Y.-P. et al., Nature 626, 523 (2024)

QL* et al. Nat. Phys. 13, 329 (2025)

Landscape of unconventional magnetism

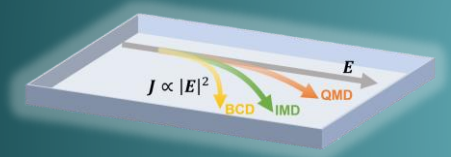


Spin splitting
Nature 626, 523 (2024)

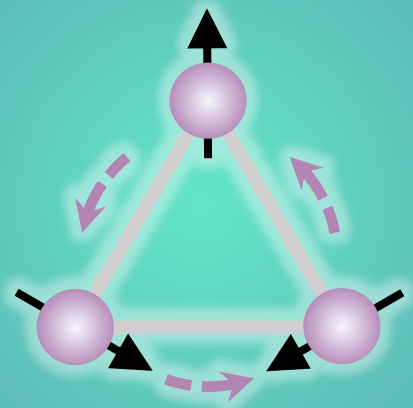


Anomalous Hall
PRX 14, 031038 (2024)
Nano Lett. 23, 8650 (2023)

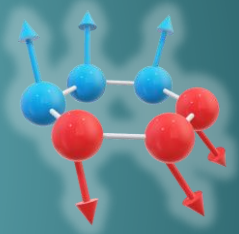
Topological magnets
PRX 12, 021016 (2022)
The Innovation 3, 100343 (2022)



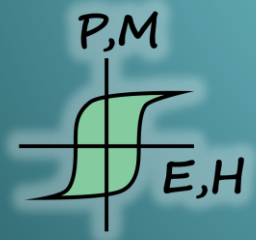
Quantum geometry
PRL 129, 276601 (2022)
Nat. Commun. (2025)



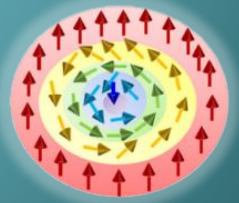
Unconventional Magnets
Nat. Phys. 21, 329 (2025)



Topological magnons
Nature 640, 349 (2025)



Multiferroicity
PRL 134, 106802 (2025)



Skyrmions

Unconventional superconductivity

Acknowledgements

Collaborators

Theory: Xiangang Wan (NJU), Caiheng Li (SUSTech), Xi Dai (HKUST), Stefan Blügel (Jülich, Germany), Alessandro Stroppa (CNR-SPIN, Italy), Kirill Belashchenko (U. Nebraska-Lincoln)

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Thank you for your attention !

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