# Refs for TQC and SI

- TQC: B. Bradlyn, L. Elcoro, J. Cano, M. G. Vergniory, Z. Wang, C. Felser, M. I. Aroyo, and B. A. Bernevig, *Topological Quantum Chemistry*, Nature 547, 298 (2017).
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- From SI to invariants: **Z.-D. Song**, T. Zhang, Z. Fang, and C. Fang, *Quantitative Mappings between Symmetry and Topology in Solids*, Nature Communications 9, 3530 (2018).
- From SI to invariants: **Z.-D. Song**, T. Zhang, and C. Fang, *Diagnosis for Nonmagnetic Topological Semimetals in the Absence of Spin-Orbital Coupling*, Phys. Rev. X 8, 031069 (2018).
- From SI to invariants: **Z.-D. Song**, S.-J. Huang, Y. Qi, C. Fang, and M. Hermele, *Topological States from Topological Crystals*, Science Advances 5, eaax2007 (2019).
- Materials: M. G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B. A. Bernevig, and Z. Wang, *A Complete Catalogue of High-Quality Topological Materials*, Nature 566, 480 (2019).
- Materials: T. Zhang, Y. Jiang, **Z.-D. Song**, H. Huang, Y. He, Z. Fang, H. Weng, and C. Fang, *Catalogue of Topological Electronic Materials*, Nature 566, 475 (2019).
- Materials: Tang, F., Po, H. C., Vishwanath, A., & Wan, X. (2019). Comprehensive search for topological materials using symmetry indicators. *Nature*, *566*(7745), 486-489.
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arXiv.2307.10364, accepted in PRX

# Spin-Space Groups: Full Classification and Applications

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[1] Z. Xiao, J. Zhao, Y. Li, R. Shindou, and Z.-D. Song, Spin Space Groups: Full Classification and Applications, arXiv:2307.10364 (2023), accepted in PRX

***Related works:***

[2] Y. Jiang, Z. Song, T. Zhu, Z. Fang, H. Weng, Z.-X. Liu, J. Yang, and C. Fang, Enumeration of Spin-Space Groups: Towards a Complete Description of Symmetries of Magnetic Orders, arXiv:2307.10371 (2023).

[3] J. Ren, X. Chen, Y. Zhu, Y. Yu, A. Zhang, J. Li, C. Li, and Q. Liu, Enumeration and Representation of Spin Space Groups, arXiv:2307.10369 (2023).

[4] H. Watanabe, K. Shinohara, T. Nomoto, A. Togo, and R. Arita, Symmetry Analysis with Spin Crystallographic Groups: Disentangling Spin-Orbit-Free Effects in Emergent Electromagnetism, arXiv:2307.11560 (2023).

[5] H. Schiff, A. Corticelli, A. Guerreiro, J. Romhányi, and P. McClarty, The Spin Point Groups and Their Representations, arXiv:2307.12784 (2023).

[6] K. Shinohara, A. Togo, H. Watanabe, T. Nomoto, I. Tanaka, and R. Arita, Algorithm for Spin Symmetry Operation Search, arXiv:2307.12228 (2023).

[7] X. Chen, J. Ren, J. Li, Y. Liu, and Q. Liu, Spin Space Group Theory and Unconventional Magnons in Collinear Magnets, arXiv:2307.12366 (2023).

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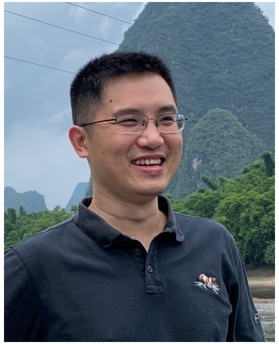

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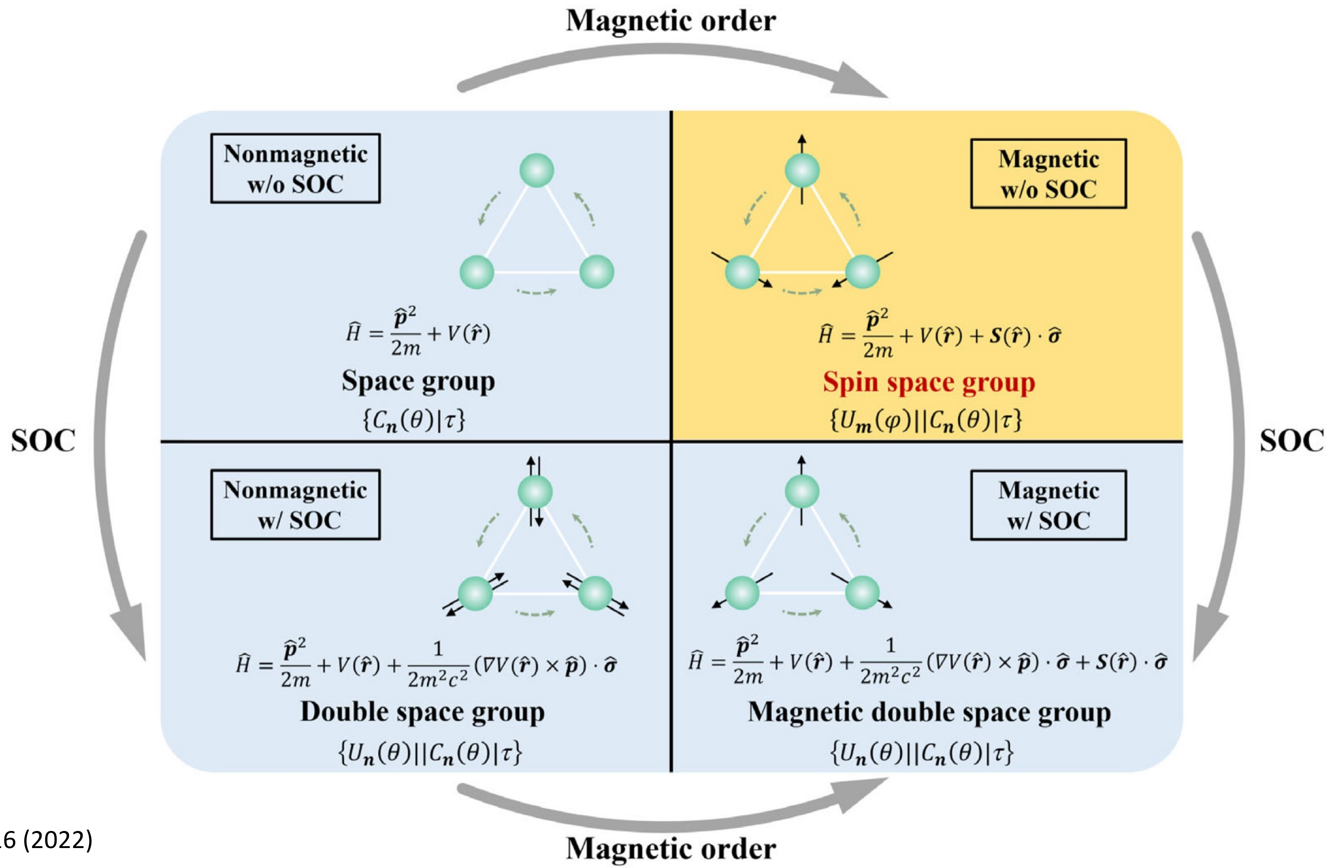
# Spin-space groups




Liu et al, PRX 12, 021016 (2022)

# Spin-space groups

Theory of spin-space groups

By W. F. Brinkman† and R. J. Elliott

*Department of Theoretical Physics, University of Oxford, England*

*(Communicated by R. E. Peierls, F.R.S.—Received 14 February* 1966)

SPIN GROUPS

D. B. LITVIN and W. OPECHOWSKI

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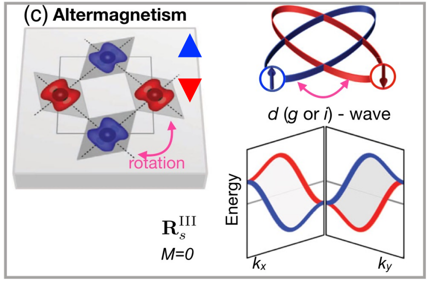
Received 4 June 1974




**Alter-magnetism**

*Šmejkal et al., PRX 12, 040501 (2022)*

*Liu, Multi-functional AFM (2021)*

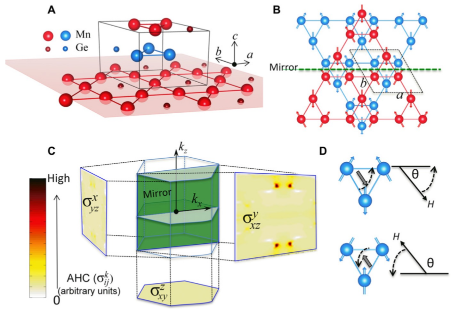
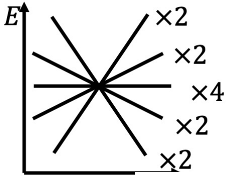



Fig. 1 Crystal structure, magnetic structure, and Berry curvature of $Mn_3Ge$. (A) Crystal structure showing the two layers of Mn-Ge atoms stacked along the c(z) axis. Red and blue spheres represent atoms lying in the z = 0 and z = c/2 planes, respectively. Large and small spheres represent Mn and Ge atoms, respectively. In each layer, the Mn atoms form a Kagome-type lattice. (B) Calculated 120° antiferromagnetic configuration in the z = 0 and z = c/2 planes, respectively. Only the Mn atoms are shown, with their moments represented by arrows. The green dashed line indicates the mirror plane (that is, the xz plane). Corresponding mirror reflection plus a translation by c/2 along the z axis transforms the system back into itself, by exchanging two magnetic planes. (C) First Brillouin zone and momentum-dependent

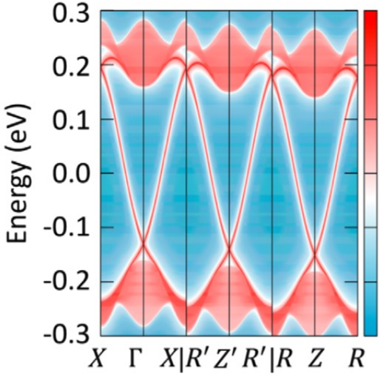
**Large AHE in weak SOC system: Mn3Ge**

*sciadv.1501870 (2016)*



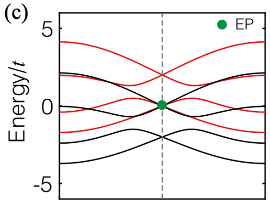

**12fold Dirac fermion in 3D**

*Yang & Fang et al., arXiv:2105.12738 (2021).*



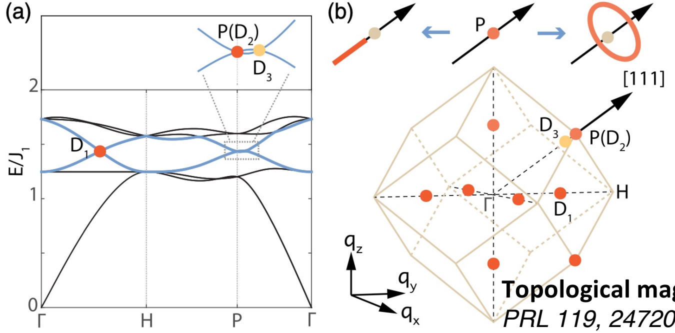

**New TI states**

Liu et al, PRX 12, 021016 (2022)




**8fold Dirac fermion in 2D**

*Guo & Lu et al., PRL 127, 176401 (2021)*




**Topological magnon**

*PRL 119, 247202 (2017)*

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# Group Structure

**Spin Space Group:** $\mathcal{G} = \{\{X \cdot U|R|\boldsymbol{v}\} \mid \{X \cdot U|R|\boldsymbol{v}\} \cdot \boldsymbol{S} = \boldsymbol{S}\}$

$$\boldsymbol{S}'(\boldsymbol{r}_i) = s(X) \cdot U \cdot \boldsymbol{S}(\{R|\boldsymbol{v}\}^{-1}\boldsymbol{r}_i)$$

U: SO(3) spin-rotation
X: I or T (time-reversal)
s(I)=1, s(T)= -1

**Parent Space Group:** $P = \{\{R|\boldsymbol{v}\} \mid \{X \cdot U|R|\boldsymbol{v}\} \in \mathcal{G}\}$

***All subgroups of $P \times O(3)$***

- Non-coplanar

  Local symmetry: None

  For every $g \in P$, assign a spin operation $X_g U_g \in O(3)$

  **$\mathcal{G}$: a 3D real representation of $P$**

- Coplanar, $\mathcal{G} = \mathcal{S} \times G$

  Local symmetry: $\mathcal{S} = \{\{\{I|1|\mathbf{0}\}, \{T \cdot U_z(\pi)|1|\mathbf{0}\}\} = \mathcal{S}_{Z_2^T}$

  For every $g \in P$, assign a spin operation $X_g U_g \in O(2)$

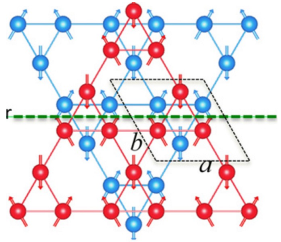
  **$G$: a 2D real representation of $P$**

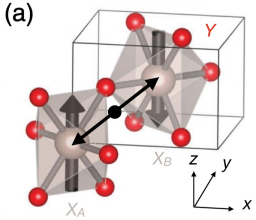
- Collinear, $\mathcal{G} = \mathcal{S} \times G$

  Local symmetry: $\mathcal{S} = \mathcal{S}_{Z_2^T} \ltimes \mathcal{S}_{U(1)}$

  For every $g \in P$, assign a spin operation $X_g U_g = \pm 1 \in O(1)$

  **$G$: a 1D real representation of $P$**



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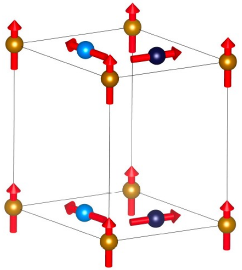
# O(3): Examples (P=P3,non-coplanar)

**GM1**
**(identity)**

Pure spatial symmetry



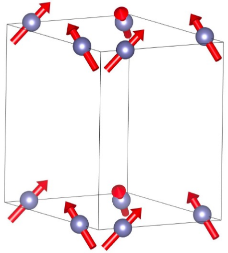
**GM2GM3, L=+-1 rep**

$D(t) = 1 \oplus 1, \quad D(C_{3z}) = e^{i\omega} \oplus e^{-i\omega} \quad \left(\omega = \frac{2\pi}{3}\right)$

➔ *3D real rep*

$X_t U_t = \mathbb{I}_{3\times3}$

$$X_{C_3} U_{C_3} = \begin{pmatrix} \cos\omega & -\zeta\cdot\sin\omega & 0 \\ \zeta\cdot\sin\omega & \cos\omega & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \left(\omega = \frac{2\pi}{3}\right)$$



*A global spin rotation may change* $\zeta$ ➔ $\zeta = \pm 1$ *correspond to the same SSG*
$\zeta = 1$ *corresponds to MSG P3'*
$\zeta = -1$ *corresponds to SSG symmetry (SOC=0)*

**A1 (k=00pi)**

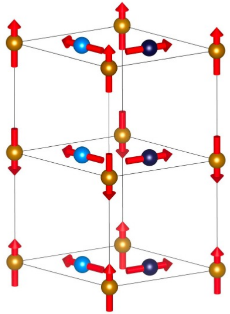
$D(C_{3z})$ =1

$D(t) = e^{i\pi t_3}$

➔ *3D real rep*

$X_{C_3} U_{C_3} = \mathbb{I}_{3\times3}$

$$X_t U_t = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\pi t_3} \end{pmatrix}$$



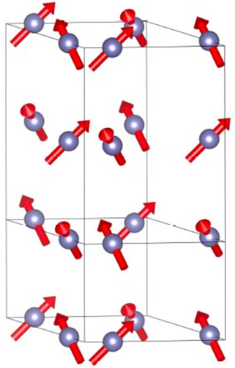
**DT2 $\oplus$ DU2,** k=$(00u\pi), (00, -u\pi)$

$D(t) = e^{iu\pi t_3} \oplus e^{-iu\pi t_3}, \quad D(C_{3z}) = e^{i\omega} \oplus e^{-i\omega} \quad \left(\omega = \frac{2\pi}{3}\right)$

➔ *3D real rep*

$$X_t U_t = \begin{pmatrix} \cos u\pi t_3 & -\zeta\cdot\sin u\pi t_3 & 0 \\ \zeta\cdot\sin u\pi t_3 & \cos u\pi t_3 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$X_{C_3} U_{C_3} = \begin{pmatrix} \cos\omega & -\zeta\cdot\sin\omega & 0 \\ \zeta\cdot\sin\omega & \cos\omega & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \left(\omega = \frac{2\pi}{3}\right)$$



***$u\pi$ is spiral angle!***

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# All O(*N*) representations

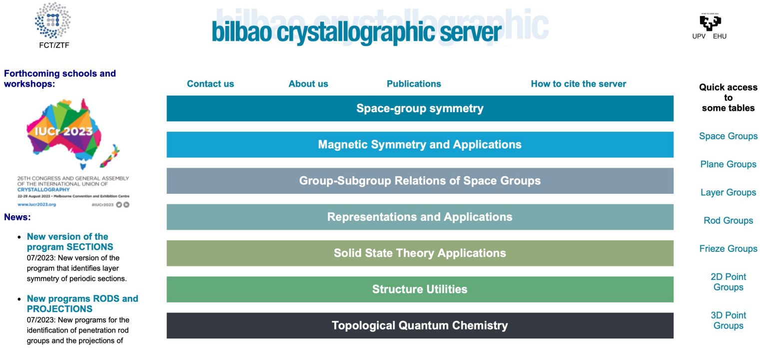
- O(N) (N=1,2,3) rep decomposes into
  - (N-m) trivial (identity) representations
  - A nontrivial O(m) rep consisting of
    - Real irrep of *P*
    - Complex irrep and its conjugation
    - (No pseudo-real irrep, because they at least induce 4D real rep)
- Real irrep $\rho_k$, $[\rho_k \uparrow P]^r_{d=1,2,3}$ *(d: dimension)*
  - k must be TRS-invariant
  - $|P|/|P_{\boldsymbol{k}}|$=1, 2, 3 (k-star)
- Complex irrep $\rho_k$, $[\rho_k \uparrow P]^c_1 \oplus [\rho^*_k \uparrow P]^c_1$
  - k can be TRS-invariant **or *not***
  - $|P|/|P_{\boldsymbol{k}}|$=1
  - Spiral magnetism if fixed points of Pk form line/plane/bulk

O(1): Types I – II
O(2): Types I – VIII
O(3): Types I – XVI

**All types of nontrivial O(m) reps**

| $n$ | Type | Irreps | $\lvert P\rvert/\lvert P^{\boldsymbol{k}}\rvert$ | TRS | HSP |
|---|---|---|---|---|---|
| 0 | I | 1 | 1 | ✓ | ✓ |
| 1 | II | $[\rho_{\boldsymbol{k}} \uparrow P]^r_1$ | 1 | ✓ | ✓ |
| 2 | III | II ⊕ II | - | - | - |
|  | IV | $[\rho_{\boldsymbol{k}} \uparrow P]^c_1 \oplus [\rho^*_{\boldsymbol{k}} \uparrow P]^c_1$ | 1 | ✓or ✗ | ✓ |
|  | V | $[\rho_{\boldsymbol{k}} \uparrow P]^c_1 \oplus [\rho^*_{\boldsymbol{k}} \uparrow P]^c_1$ | 1 | ✗ | ✗ |
|  | VI | $[\rho_{\boldsymbol{k}} \uparrow P]^r_2$ | 1 | ✓ | ✓ |
|  | VII | $[\rho_{\boldsymbol{k}} \uparrow P]^r_2$ | 2 | ✓or ✗ | ✓ |
|  | VIII | $[\rho_{\boldsymbol{k}} \uparrow P]^r_2$ | 2 | ✗ | ✗ |
| 3 | IX-XIV | II ⊕ (III-VIII) | - | - | - |
|  | XV | $[\rho_{\boldsymbol{k}} \uparrow P]^r_3$ | 1 | ✓ | ✓ |
|  | XVI | $[\rho_{\boldsymbol{k}} \uparrow P]^r_3$ | 3 | ✓ | ✓ |

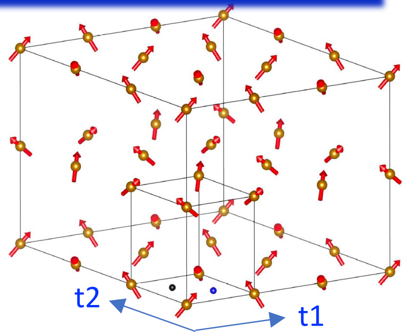
$\rho_k$'s are available on the ***Bilbao Crystallographic Server***



# Equivalence & O(3) rep classes

- A. Coordinate transformation in spin space
  - ➔ Equivalent O(3) reps define the same SSG
- B. Coordinate transformation in real space
  - ➔Example, P*i* ⨁ PC*i* (*i*=1,2,3), $P = (\frac{\pi}{3}, \frac{2\pi}{3}, \nu\pi)$

P1 ⨁ PC1




P*i* ⨁ PC*i* have the same rep of translations

$$U_{t_1} = \begin{pmatrix} \cos\pi/3 & -\sin\pi/3 & 0 \\ \sin\pi/3 & \cos\pi/3 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad U_{t_2} = \begin{pmatrix} \cos 2\pi/3 & -\sin 2\pi/3 & 0 \\ \sin 2\pi/3 & \cos 2\pi/3 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad U_{t_3} = \begin{pmatrix} \cos\nu\pi & -\sin\nu\pi & 0 \\ \sin\nu\pi & \cos\nu\pi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

P*i* ⨁ PC*i* have different reps of C3

$$U_{c_3} = \begin{pmatrix} \cos\omega & -\sin\omega & 0 \\ \sin\omega & \cos\omega & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \omega = \frac{(i-1)2\pi}{3}$$

Re-choice of origin: C3 → t2*C3, D(C3) changes accordingly ➔ PC1 ~= PC2 ~= PC3

- C. Continuous change of spiral angle
  - ➔Example, v in the P1PC1 rep.

***O(3) reps related by the equivalences are in the same class.***

***Distinct O(3) classes define disticnt SSGs***

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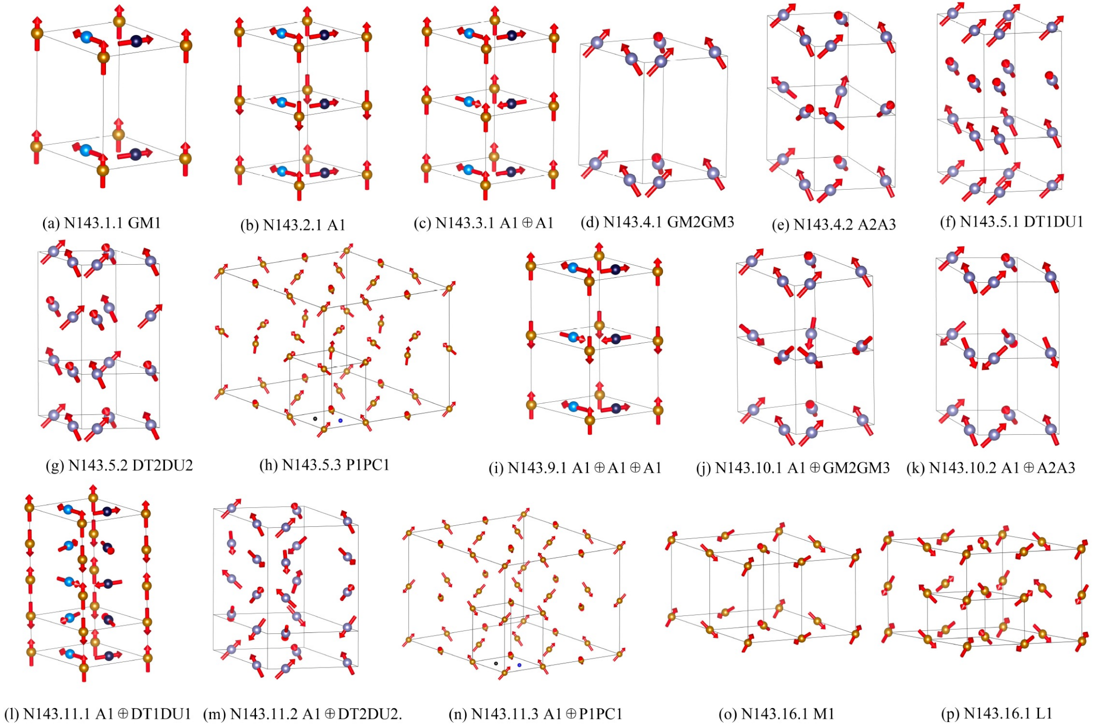
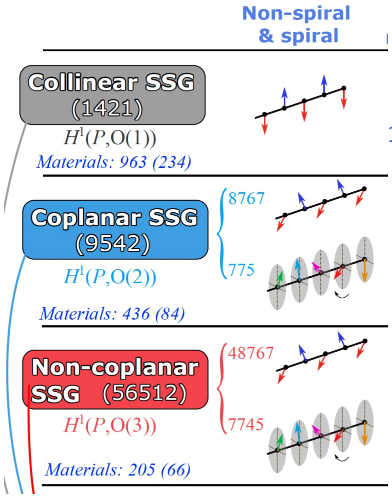
# Complete classification

## All (16) non-coplanar SSGs with the parent SG P3



(a) N143.1.1 GM1 (b) N143.2.1 A1 (c) N143.3.1 A1⊕A1 (d) N143.4.1 GM2GM3 (e) N143.4.2 A2A3 (f) N143.5.1 DT1DU1
(g) N143.5.2 DT2DU2 (h) N143.5.3 P1PC1 (i) N143.9.1 A1⊕A1⊕A1 (j) N143.10.1 A1⊕GM2GM3 (k) N143.10.2 A1⊕A2A3
(l) N143.11.1 A1⊕DT1DU1 (m) N143.11.2 A1⊕DT2DU2. (n) N143.11.3 A1⊕P1PC1 (o) N143.16.1 M1 (p) N143.16.1 L1




1421= #MSGs of types I, III, IV

**Naming convention:** $\alpha I.J.K\ \rho$

$\alpha$ =**L, P, N** (for collinear, coplanar, non-coplanar)

$I$ =**1…230** (parent SG)

$J$ =**1…16** (type of the SSG)

$K$ =**1…** (SSG index for given $\alpha I.J$)

$\rho$ = GM1, A1 ⋯ (name of the irreps)

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# Electronic band theory in SSG

- Electrons are spin-1/2 particles ➔ They form projective rep of SSG

$$\mathcal{H} = \frac{\hat{\boldsymbol{p}}^2}{2m}\sigma_0 + V(\boldsymbol{r})\sigma_0 + J\boldsymbol{S}(\boldsymbol{r})\cdot\boldsymbol{\sigma}$$

- It has SSG symmetry $\{XU|R|\boldsymbol{v}\}$, $XU \in O(3)$ if $V(\boldsymbol{r}) = V(\{R|\boldsymbol{v}\}^{-1}\boldsymbol{r}), \quad \boldsymbol{S}(\boldsymbol{r}) = s(X)U\boldsymbol{S}(\{R|\boldsymbol{v}\}^{-1}\boldsymbol{r})$
- When acting on electron states, $g = \{XU|R|\boldsymbol{v}\}$ ➔ $\hat{g} = \{\hat{X}\hat{U}|R|\boldsymbol{v}\}$
  - $\hat{X} = 1, i\sigma_y K$ for $X = I, T$
  - For $U = U_{\boldsymbol{n}}(\theta)$, $\hat{U} = \exp\left(-i\frac{\theta}{2}\boldsymbol{n}\cdot\boldsymbol{\sigma}\right)$ (axis: $\boldsymbol{n}$; angle: $\theta$)

$$(\hat{g}\cdot\psi)(\boldsymbol{r}) \equiv \hat{X}_g\hat{U}_g\psi(\boldsymbol{r}')$$
$$\hat{g}\cdot\mathcal{H}\cdot\hat{g}^{-1} = \mathcal{H}$$

$\psi(\boldsymbol{r})$ at each **r** is a two-by-one vector

- ***$\hat{g}$'s form projective rep of the SSG***
  - If $g_1 g_2 = g_3$, then

$$\hat{g}_1\cdot\hat{g}_2 = \omega_2(g_1, g_2)\hat{g}_3 \qquad \omega_2(g_1,g_2) = e^{-i\frac{\theta_3}{2}\boldsymbol{n}_3\cdot\boldsymbol{\sigma}}\cdot e^{i\frac{\theta_2}{2}\boldsymbol{n}_2\cdot\boldsymbol{\sigma}}\cdot e^{i\frac{\theta_1}{2}\boldsymbol{n}_1\cdot\boldsymbol{\sigma}}\cdot\hat{X}_{g_3}\cdot\hat{X}_{g_2}^{-1}\cdot\hat{X}_{g_1}^{-1}$$

# Electronic band theory in SSG

- **Collinear SSG**: electrons form ***linear rep of grey groups***

  If SSG is given by the trivial 1D irrep $\mathcal{G} = G_0 \times [\mathcal{S}_{Z_2^T} \ltimes \mathcal{S}_{U(1)}]$

  If SSG is given by nontrivial 1D irrep $\mathcal{G} = (G_0 + h \cdot G_0) \times [\mathcal{S}_{Z_2^T} \ltimes \mathcal{S}_{U(1)}]$

  *$h \cdot G_0$ are those represented by D(g)=-1, spin flipping operations.*

  In each spin sector, symmetry group is the grey group $G_0 \times \mathcal{S}_{Z_2^T}$

- **Coplanar SSG**:

  $\mathcal{S} = \{\{\{I|1|\mathbf{0}\}, \{T \cdot U_{\boldsymbol{z}}(\pi)|1|\mathbf{0}\}\} = \mathcal{S}_{Z_2^T}$

  - Isomorphic to grey MSG, $X_g U_g$ chosen to be unitary, $T_{eff}^2 = 1$
  - Projective rep is given by **$H^2(M, U(1))$, M: type-II MSG (grey group)**

- **Non-coplanar SSG**:
  - Isomorphic to type-I, III, IV MSG
    - g with $X_g = T$ correspond to anti-unitary operations in MSGs
    - g with $X_g = I$ correspond to unitary operations in MSGs
  - Projective rep is given by **$H^2(M, U(1))$, M: type-I, III, IV MSG**

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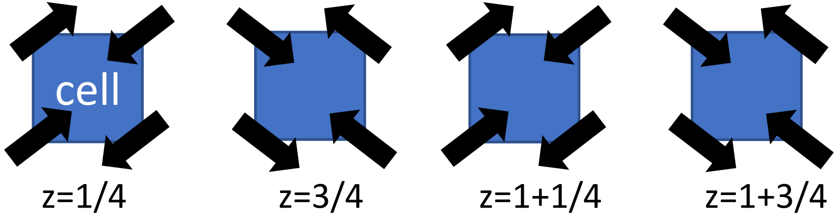
# SSG Brillouin zone

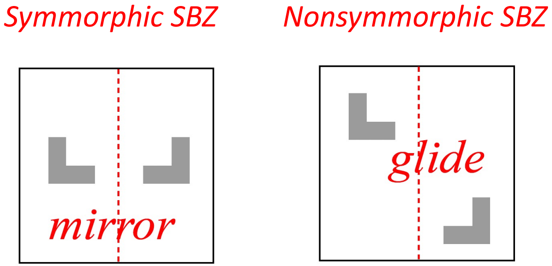
- (Unitary) spin-space translations $\hat{t}_i$ (*i=1,2,3*), may involve nontrivial spin rotations
- Commuting $\{\hat{t}_i\}$: *8635 of 9542 coplanar SSGs, 53107 of 56512 non-coplanar SSGs*
  - ➔ SSG Brillouin zone (SBZ) , $\hat{t}_i \cdot |\psi_k\rangle = e^{ik_i}|\psi_k\rangle$
  - **Nonsymmorphic SBZ**:

$$g^{-1}t_i g = \tau \qquad \hat{g}^{-1}\hat{t}_i\hat{g} = e^{i2\pi q_i(g)}\hat{\tau} \qquad \hat{g}\cdot|\psi_k\rangle \propto |\psi_{k'}\rangle, \qquad \boldsymbol{k}' = s_g(R_g\boldsymbol{k} + \boldsymbol{q}_g)$$

**fractional translation in SBZ**

  - Example: **glide in SBZ**
    - $\hat{t}_1 = \{\sigma_z|1|100\},\ \hat{t}_2 = \{\sigma_0|1|010\},\ \hat{t}_3 = \{\sigma_0|1|001\},\ \widehat{M}_z = \{\sigma_x|m_z|000\}$
    - $\widehat{M}_z\hat{t}_1\widehat{M}_z^{-1} = -\hat{t}_1,$ Mz: $(k_1, k_2, k_3) \rightarrow (k_1 + \pi, k_2, -k_z)$



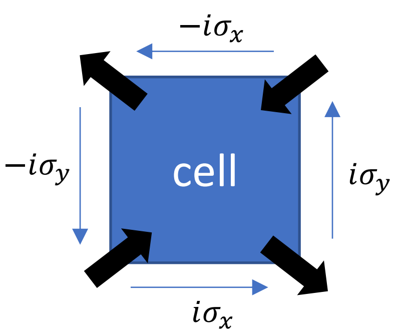

*3501 of 8635 coplanar SBZs are nonsymmorphic*
*15300 of 53107 non-coplanar SBZs are nonsymmorphic*

# SSG Brillouin zone

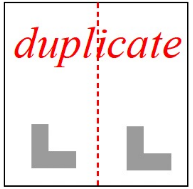
- Non-commuting $\{\hat{t}_i\}$: *907 of 9542 coplanar SSGs, 3405 of 56512 non-coplanar SSGs*
  - $\{t_1, t_2\} = 0, \quad [t_{1,2}, t_3] = 0,$ **effective pi flux** along t3
  - $\{t_1, t_{2,3}\} = 0, \quad [t_2, t_3] = 0,$ **effective pi flux** along t2 and t3
  - $\{t_i, t_j\} = 0\ (i \neq j),$ **effective pi flux along** t1, t2, and t3
  - **Example:**

$$\hat{t}_1 = \{i\sigma_x|1|100\},\ \hat{t}_2 = \{i\sigma_y|1|010\},\ \hat{t}_3 = \{\sigma_0|1|001\}$$

$$\hat{t}_1 \cdot \hat{t}_2 \cdot \hat{t}_1^{-1} \cdot \hat{t}_2^{-1} = \sigma_x\sigma_y\sigma_x\sigma_y = -1$$




*Non-commuting SBZ*




Bands should be labeld by eigenvalues of $\{\hat{t}_1, \hat{t}_2^2, \hat{t}_3\}$

$$\hat{t}_{1,3}\left|\psi(\tilde{\boldsymbol{k}})\right\rangle = e^{i\tilde{k}_{1,3}}\left|\psi(\tilde{\boldsymbol{k}})\right\rangle,\ \hat{t}_2^2\left|\psi(\tilde{\boldsymbol{k}})\right\rangle = e^{i\tilde{k}_2}\left|\psi(\tilde{\boldsymbol{k}})\right\rangle$$

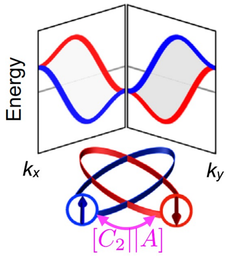
Suppose $|\psi(\boldsymbol{k})\rangle$ has energy $E(\boldsymbol{k})$, then $\hat{t}_2|\psi(\boldsymbol{k})\rangle$ is another state at $\boldsymbol{k} + \frac{1}{2}\boldsymbol{b}_2$ with the same energy

$$\hat{t}_1\hat{t}_2\left|\psi(\tilde{\boldsymbol{k}})\right\rangle = -\hat{t}_2\hat{t}_1\left|\psi(\tilde{\boldsymbol{k}})\right\rangle = e^{i(\tilde{\boldsymbol{k}}+\frac{1}{2}\boldsymbol{b}_1)\cdot\boldsymbol{a}_1}\hat{t}_2\left|\psi(\tilde{\boldsymbol{k}})\right\rangle$$

Thus ***the SBZ is duplicated*** as in pi-flux models

# Spin texture

- **Collinear SSG**, *442 of 1421 have nontrivial spin texture*
  - There must be $E_s(\boldsymbol{k}) = E_s(-\boldsymbol{k})$ $(s = \uparrow, \downarrow)$ as each spin sector respects grey group $G_0 \times \mathcal{S}_{Z_2^T}$
  - If SSG is given by trivial rep, then it's ferromagnetic, no spin texture
  - If SSG is given by nontrivial rep $\mathcal{G} = (G_0 + h \cdot G_0) \times [\mathcal{S}_{Z_2^T} \ltimes \mathcal{S}_{U(1)}]$
    - h is translation ➔ $E_\uparrow(\boldsymbol{k}) = E_\downarrow(\boldsymbol{k})$, no spin texture
    - h is inversion ➔ $E_\uparrow(\boldsymbol{k}) = E_\downarrow(-\boldsymbol{k}) = E_\downarrow(\boldsymbol{k})$, no spin texture
    - Otherwise ➔ ***Nontrivial spin texture***, d-,g-,i-wave-like




*Šmejkal et al., PRX 12, 040501 (2022)*

- **Non-collinear SSG**, *3920 (37807) coplanar (non-coplanar) symmorphic SBZ has nontrivial spin texture*
  - Span of $S(\boldsymbol{k})$ in SBZ $d_{\mathrm{SBZ}}$
  - Span of $S(\boldsymbol{k})$ in BZ (crystal momenta) $d_{\mathrm{BZ}}$
  - $d_{\mathrm{SBZ/BZ}}$ could be 0,1,2,3 for coplanar or non-coplanr SSGs
  - SSG has a ***nontrivial spin texture if $d > 0$ and $S_{tot} = 0$***
  - In symmorphic BZ/SBZ, S(k) is characterized by a rep

TABLE III. The dimensions $d_{\mathrm{SBZ}}/d_{\mathrm{BZ}}$ of the span of spin texture $\tilde{\boldsymbol{S}}(\tilde{\boldsymbol{k}})/\vec{S}(\boldsymbol{k})$ in the SBZ/BZ of non-collinear SSGs. Columns and rows specify spin-rotations that accompany translations ($t_i$) and space-time reversion $\mathcal{PT}$, respectively. $\{U_{t_i}\} = \{U_{\boldsymbol{n}}(\theta_i)\}$ means that all the translations are accompanied by spin rotations along the same axis $\boldsymbol{n}$ by $\theta_i$ $(i = 1, 2, 3)$, and at least one $\theta_i$ is nonzero.

| $U_{\mathcal{PT}}$ \ $\{U_{t_i}\}$ | Identity | $\{U_{\boldsymbol{n}}(\theta_i)\}$ | Non-commuting |
|---|---|---|---|
| Absent | 3/3 | 1/1 | 1/0 |
| Identity | 0/0 | 1/0 | 1/0 |
| $U_{\boldsymbol{m}}(\pi)$ | 2/2 | 1/1 $(\boldsymbol{m} \perp \boldsymbol{n})$<br>1/0 $(\boldsymbol{m} \parallel \boldsymbol{n})$ | 1/0 |

arXiv.2307.10364, accepted in PRX

# SSG Tables

TABLE 437: Non-coplanar SSGs with parent space group $P3$ (No. 143).

| SSG | Commute | $d_{\mathrm{SBZ}}$ | $d_{\mathrm{BZ}}$ | Symmorphic SBZ | Sym of $\tilde{\boldsymbol{S}}(\tilde{\boldsymbol{k}})$ | Representation |
|---|---|---|---|---|---|---|
| N143.1.1 GM1 | √ | 3 | 3 | √ | 3 | A1 ⊕ A1 ⊕ A1 |
| N143.2.1 A1 | √ | 3 | 3 | √ | $\bar{3}$ | $\mathrm{A_g} \oplus \mathrm{A_g} \oplus \mathrm{A_u}$ |
| N143.3.1 A1 ⊕ A1 | √ | 1 | 1 | √ | 3 | A1 |
| N143.4.1 GM2GM3 | √ | 3 | 3 | √ | 3 | $\mathrm{A1} \oplus {}^2\mathrm{E} \oplus {}^1\mathrm{E}$ |
| N143.4.2 A2A3 | √ | 1 | 1 | √ | 3 | A1 |
| N143.5.1 DT1DU1 | √ | 1 | 1 | √ | 3 | A1 |
| N143.5.2 DT2DU2 | √ | 1 | 1 | √ | 3 | A1 |
| N143.5.3 P1PC1 | √ | 1 | 1 | √ | 3 | A1 |
| N143.9.1 A1 ⊕ A1 ⊕ A1 | √ | 3 | 3 | √ | $\bar{3}$ | $\mathrm{A_u} \oplus \mathrm{A_u} \oplus \mathrm{A_u}$ |
| N143.10.1 A1 ⊕ GM2GM3 | √ | 3 | 3 | √ | $\bar{3}$ | $\mathrm{A_u} \oplus {}^2\mathrm{E_g} \oplus {}^1\mathrm{E_g}$ |
| N143.10.2 A1 ⊕ A2A3 | √ | 3 | 3 | √ | $\bar{3}$ | $\mathrm{A_u} \oplus {}^2\mathrm{E_u} \oplus {}^1\mathrm{E_u}$ |
| N143.11.1 A1 ⊕ DT1DU1 | √ | 1 | 1 | √ | $\bar{3}$ | $\mathrm{A_u}$ |
| N143.11.2 A1 ⊕ DT2DU2 | √ | 1 | 1 | √ | $\bar{3}$ | $\mathrm{A_u}$ |
| N143.11.3 A1 ⊕ P1PC1 | √ | 1 | 1 | √ | $\bar{3}$ | $\mathrm{A_u}$ |
| N143.16.1 M1 | × | - | - | - | - | - |
| N143.16.2 L1 | × | - | - | - | - | - |

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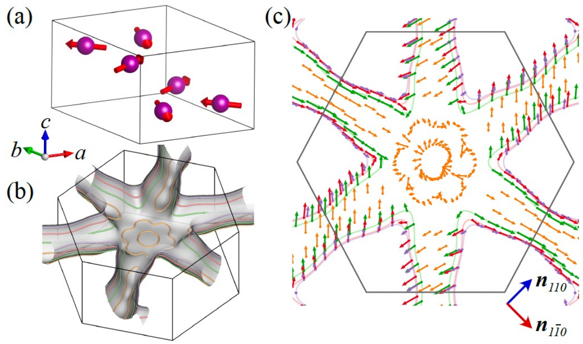
# Magnetic materials

- **MAGNDATA** on the ***Bilbao Crystallographic Server***
  - Excluding entries with non-integer occupations, there are ***1604*** experimental magnetics structures
  - We identify SSG for each of them
  - Properties such as SBZ, $d_{\mathrm{SBZ}}$, $d_{\mathrm{BZ}}$, spin-textures are immediately identified (*without referring to microscopic detail*)

| BCSID | Chemical formula | MSG | Trans from parent structure | PSG | Rep | SSG |
|---|---|---|---|---|---|---|
| 0.328 | $KMnF_4$ | No. 14.5.90 $P2_1'/c'$ | $-c, b, a; 0, 0, 0$ | No. 14 $P2_1/c$ | $GM2^+$ | P14.2.2 $GM2^+$ |
| 0.377 | $Mn_3Ge$ | No. 63.8.518 $Cm'cm'$ | $a, b, c; 0, 0, 0$ | No. 194 $P6_3/mmc$ | $GM5^+$ | P194.6.1 $GM5^+$ |
| 0.385 | $LiCoPO_4$ | No. 14.4.89 $P2_1/c'$ | $a, b, c; 0, 0, 0$ | No. 62 $Pnma$ | $GM2^- \oplus GM3^-$ | P62.3.16 $GM2^- \oplus GM3^-$ |
| 0.387 | $Fe_3BO_5$ | No. 26.3.170 $Pm'c2_1'$ | $b, c, a; 0, 0, 0$ | No. 62 $Pnma$ | $GM2^-$ | P62.2.3 $GM2^-$ |
| 0.425 | $Na_2CoP_2O_7$ | No. 33.3.228 $Pn'a2_1'$ | $a, b, c; 0, 0, 0$ | No. 33 $Pna2_1$ | $GM2 \oplus GM3$ | P33.3.2 $GM2 \oplus GM3$ |
| 0.579 | $Na_2NiFeF_7$ | No. 74.6.655 $Imm'a'$ | $a, b, c; 0, 0, 0$ | No. 74 $Imma$ | $GM4^+$ | P74.2.4 $GM3^+$ |
| 0.580 | $Na_2NiFeF_7$ | No. 74.6.655 $Imm'a'$ | $a, b, c; 0, 0, 0$ | No. 74 $Imma$ | $GM4^+$ | P74.2.4 $GM3^+$ |
| 0.583 | $Fe_2F_5(H_2O)_2$ | No. 74.6.655 $Imm'a'$ | $a, b, c; 0, 0, 0$ | No. 74 $Imma$ | $GM3^+$ | P74.2.4 $GM3^+$ |

1. Commuting Symmorphic SBZ
2. $d_{\mathrm{SBZ}} = d_{\mathrm{BZ}} = 2$
3. Spin texture: E2g of 6/mmm



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# Material examples

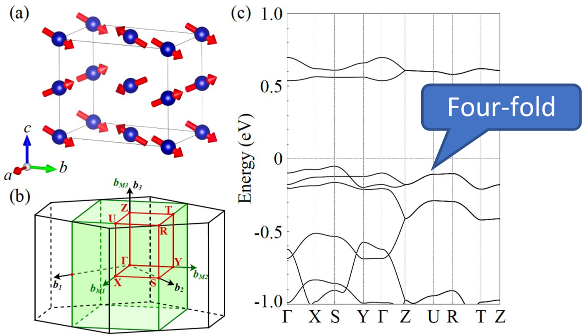


FIG. 5. (a) The magnetic structure of $CoSO_4$ showing only the magnetic atoms (Co). (b) The first BZs in the SSG reciprocal lattice $\boldsymbol{b}_i$'s (black lines) and MSG reciprocal lattice $\boldsymbol{b}_{Mi}$'s (green region). (c) The energy bands obtained from the first-principle calculation. At every $\boldsymbol{k}$, $E(\boldsymbol{k})$ is at-least two-fold degenerate.

Non-symmorphic SBZ ➔ extra degeneracy

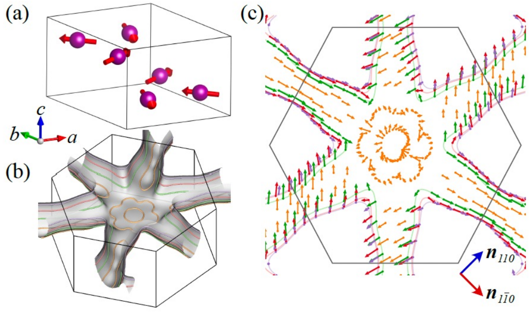


FIG. 7. (a) The magnetic structure of $Mn_3Ge$ showing only the magnetic atoms (Mn). (b) The Fermi surface of $Mn_3Ge$, which is centered at A ($\boldsymbol{k} = (0, 0, \pi)$) point. Only the lower half is shown, and the full Fermi surface is symmetric with respect to $k_z = \pi$. Different colors represent equal-$k_z$ lines. (c) The spin texture $\vec{S}(\boldsymbol{k})$ on equal-$k_z$ lines labeled in (b). Arrows represent the directions of $\vec{S}(\boldsymbol{k})$.

Nontrivial spin texture (E2g of 6/mmm)

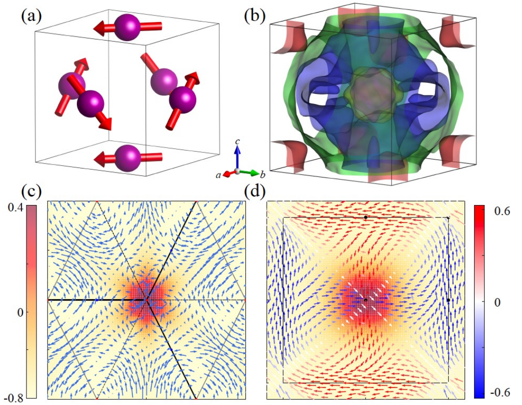


FIG. 8. (a) Magnetic structure of $Mn_3GaN$ showing only the magnetic atoms (Mn). (b) The Fermi surface of $Mn_3GaN$. (c), (d) The spin texture $\vec{S}(\boldsymbol{k})$ on the 111 plane ($k_x + k_y + k_z = 0$) and 001 plane ($k_z = 0$) in the momentum space. The background colors denote the values of $E(\boldsymbol{k})$ (see the left color bar). The outer hexagon in (c) and the square in (d) denoted the boundary of the first BZ projected to these planes. In (c), $\vec{S}(\boldsymbol{k})$'s are coplanar on the 111 plane. In (d), $\vec{S}(\boldsymbol{k})$'s are not confined to the 001 plane, and the red or blue color (the right color bar) represents the value of $S_z(\boldsymbol{k})$.

Nontrivial spin texture (Eg of Oh)

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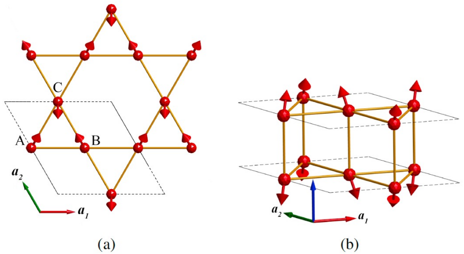
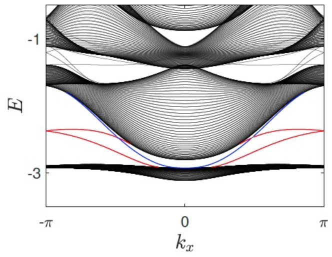
# Topological states

### SOC-free and TRS-free 2D Z2 TI

$\widehat{M}_z\widehat{T}$ squares to -1
Hoppings are real
SOC=0
Topology comes from non-collinear magnetism

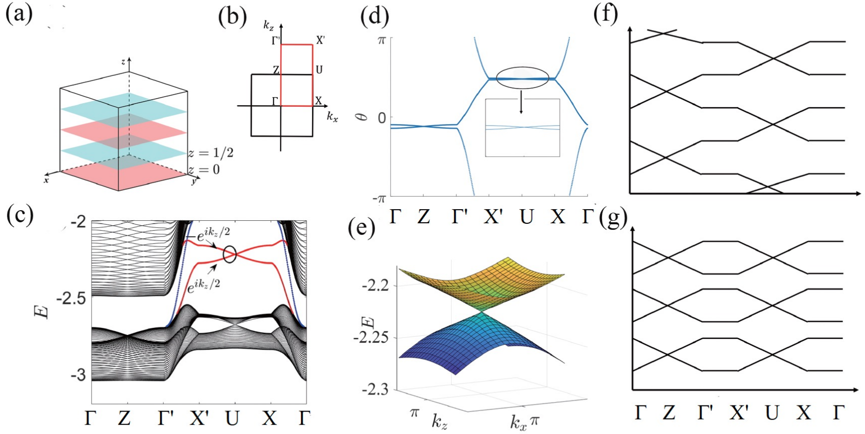
*See also [Liu et al, PRX 12, 021016 (2022)]*



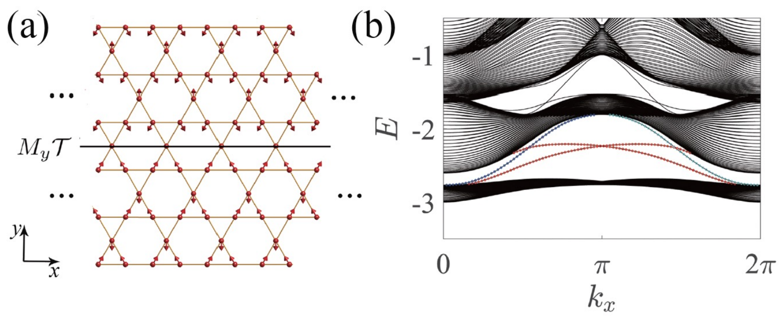

### SOC-free and TRS-free 3D Z2 TI (with double Dirac cone on surface)

Protected by $\widehat{M}_z\widehat{T}$ (squares to −1) and glide $\{M_{100}|0,0,1/2\}$




### Topological domain wall

$\widehat{M}_y\widehat{T}$ related magnetic domains



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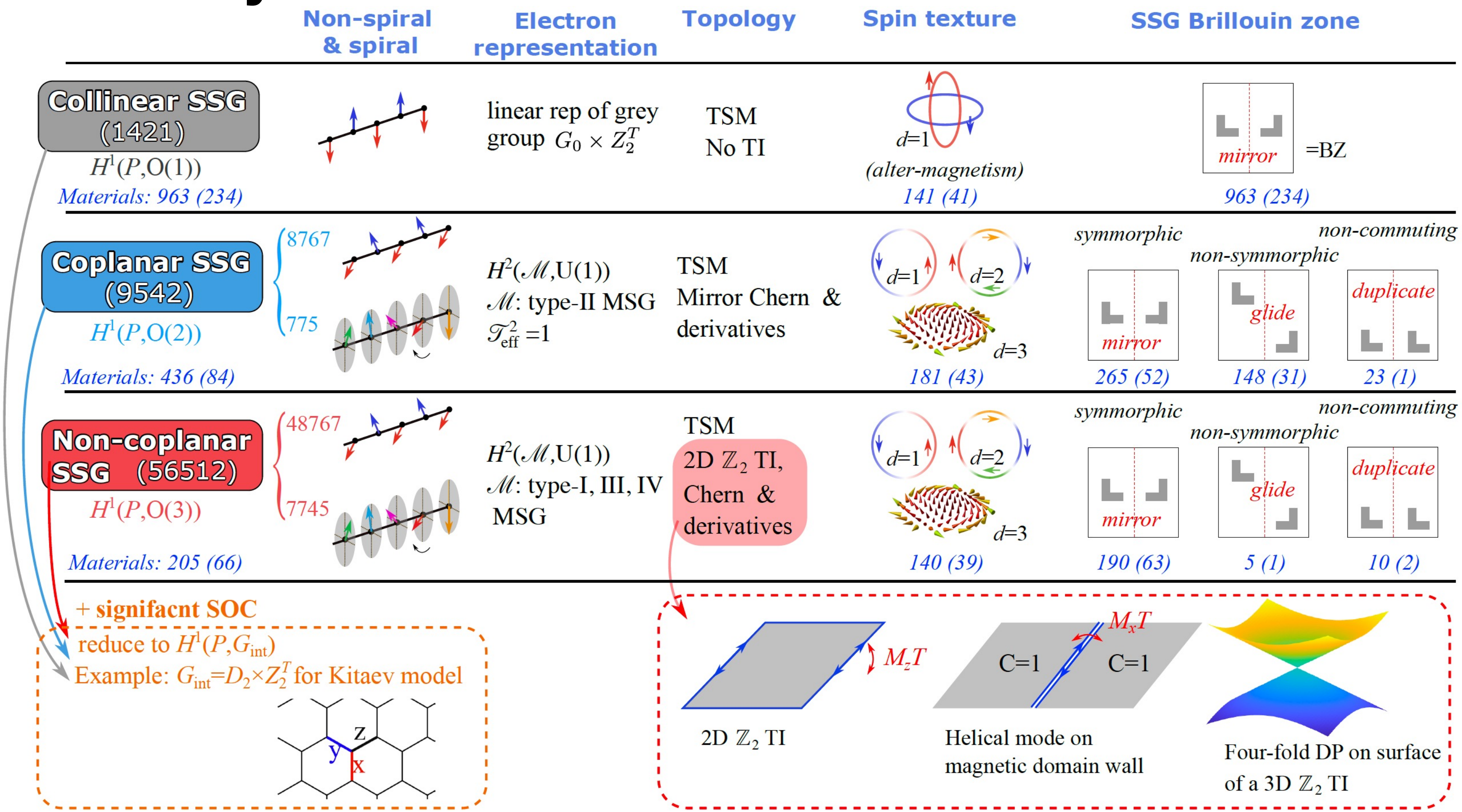
# Summary



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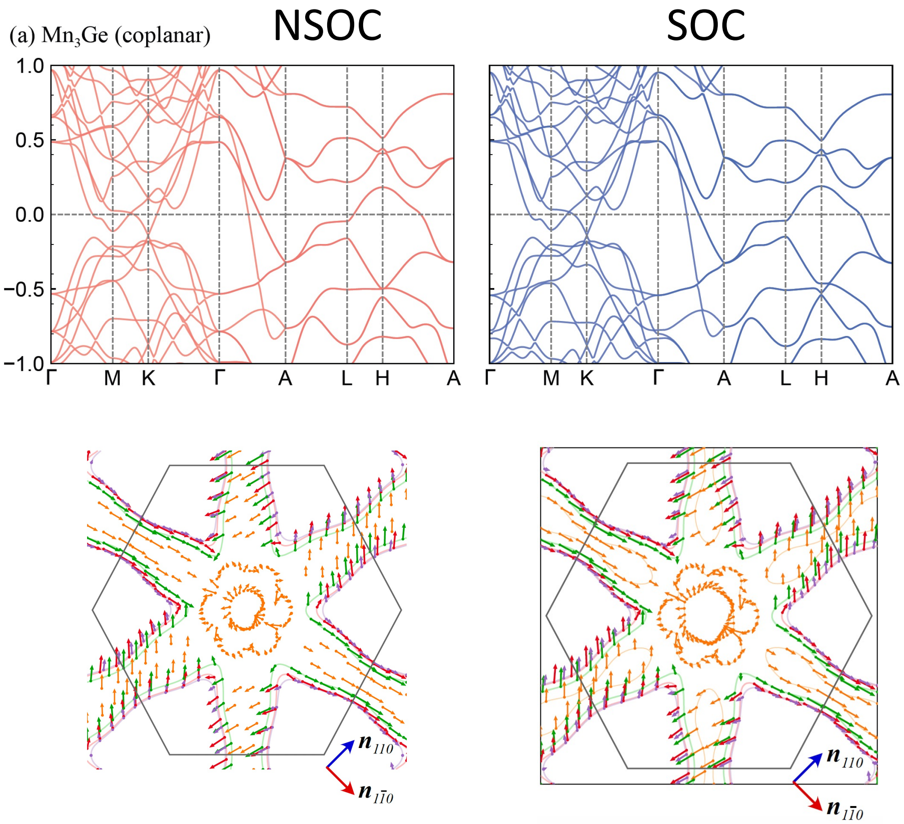
# Effects of SOC




## Kitaev spin model

- Symmetry $G_{latt} \times G_{int}$, $G_{int} = D_2 \times Z_2^T \cong Z_2^3$
- Little groups of SSB state: $H^1(G_{latt}, Z_2^3)$
- $H^1(G_{latt}, Z_2^3)$ are given by three 1D real irreps
  = types I, II, III, IX SSGs

***Some SSGs are still valid***