SPICE-Workshop on Altermagnetism

Spin crystalline group in magnetic materials

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2023. 5. 9

Phys. Rev. X 12, 021016 (2022)

The Innovation 3, 100343 (2022)

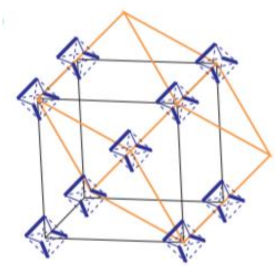
arXiv:2303.04549 (2023)

arXiv:2301.12201 (2023)

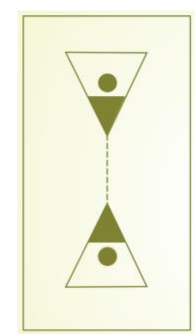
Previous connection to spintronics

- **2012-2013 Northwestern University** (Postdoc with A. Freeman)
- **2013-2018 CU Boulder** (Postdoc with A. Zunger)
- **2018.4 - SUSTech** Associate Professor

High global symmetry + Local symmetry breaking



Hidden Spin Polarization



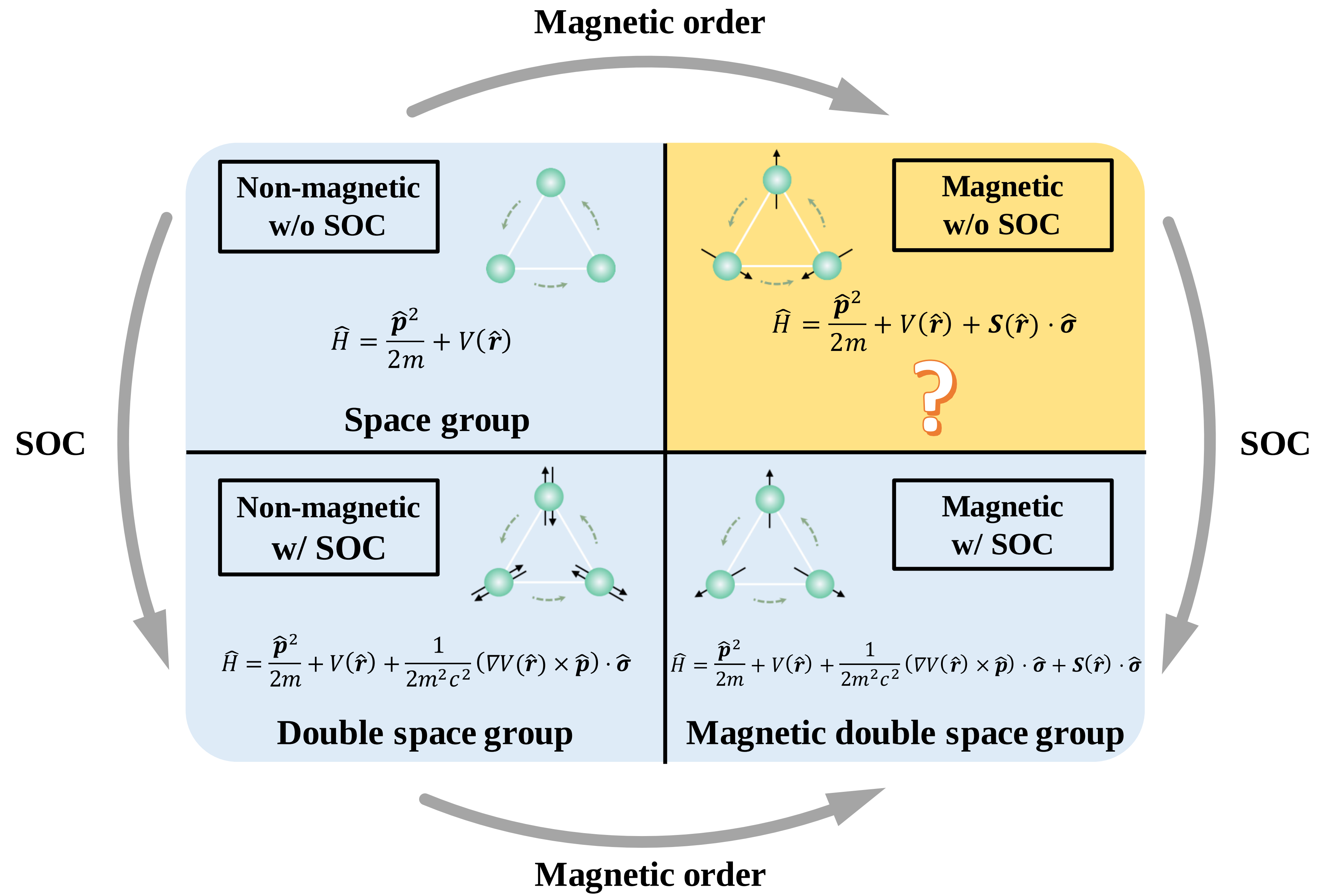
Concept ($LaOBiS_2$):
QL* et al. *Nano Lett.* 13, 5264 (2013)
X. Zhang†, **QL†**, J. Luo*, A. Zunger * et al. *Nat. Phys.* 10, 387 (2014)

New materials:
BiOI: C. Chen*, **QL*** et al. *PRL* 127, 126402 (2021)
CuMnAs: **QL*** et al. *PRL* 129, 276601 (2022)

Outline

- ➢ **Introduction of spin group**
- ➢ **Features of spin point/space group**
- ➢ **Topological phases protected by spin group symmetry**
  - **Kramers degeneracy and Z_2 topological phases**
  - **Chiral Dirac-like semimetal**

Symmetry considerations in crystals – Group Theory



Symmetry considerations in magnetic materials

w/ SOC

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{r}}) + \frac{1}{2m^2c^2}(\nabla V(\hat{\boldsymbol{r}}) \times \hat{\boldsymbol{p}}) \cdot \hat{\boldsymbol{\sigma}} + \boldsymbol{S}(\hat{\boldsymbol{r}}) \cdot \hat{\boldsymbol{\sigma}}$$

$$\widehat{C_{\boldsymbol{n}}(\theta)} \left(\frac{1}{2m^2c^2}(\nabla V(\hat{\mathbf{r}}) \times \hat{\mathbf{p}}) \cdot \hat{\boldsymbol{\sigma}} \right) \widehat{C_{\boldsymbol{n}}(\theta)}^{-1}$$

$$= \frac{1}{2m^2c^2}(R_{\boldsymbol{n}}(\theta)\nabla V(R_{\boldsymbol{n}}(\theta)^{-1}\hat{\mathbf{r}}) \times R_{\boldsymbol{n}}(\theta)\hat{\mathbf{p}}) \cdot \hat{\boldsymbol{\sigma}}$$

$$= \frac{1}{2m^2c^2} R_{\boldsymbol{n}}(\theta)(\nabla V(\hat{\mathbf{r}}) \times \hat{\mathbf{p}}) \cdot \hat{\boldsymbol{\sigma}}$$

$$\widehat{U_{\boldsymbol{n}}(\theta)}\widehat{C_{\boldsymbol{n}}(\theta)} \left(\frac{1}{2m^2c^2}(\nabla V(\hat{\mathbf{r}}) \times \hat{\mathbf{p}}) \cdot \hat{\boldsymbol{\sigma}} \right) \widehat{C_{\boldsymbol{n}}(\theta)}^{-1}\widehat{U_{\boldsymbol{n}}(\theta)}^{-1}$$

$$= \frac{1}{2m^2c^2} R_{\boldsymbol{n}}(\theta)(\nabla V(\hat{\mathbf{r}}) \times \hat{\mathbf{p}}) \cdot R_{\boldsymbol{n}}(\theta)\hat{\boldsymbol{\sigma}}$$

$$= \frac{1}{2m^2c^2}(\nabla V(\hat{\mathbf{r}}) \times \hat{\mathbf{p}}) \cdot \hat{\boldsymbol{\sigma}}$$

Magnetic double group with every spatial rotation operator attached to a spin rotation operator

w/o SOC

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

$$\widehat{C_{\boldsymbol{n}}(\theta)}\boldsymbol{S}(\hat{\boldsymbol{r}}) \cdot \hat{\boldsymbol{\sigma}}\widehat{C_{\boldsymbol{n}}(\theta)}^{-1}$$

$$= \widehat{C_{\boldsymbol{n}}(\theta)}\boldsymbol{S}(\hat{\boldsymbol{r}})\widehat{C_{\boldsymbol{n}}(\theta)}^{-1} \cdot \hat{\boldsymbol{\sigma}}$$

$$= \underline{\boldsymbol{S}(R_{\boldsymbol{n}}(\theta)^{-1}\hat{\boldsymbol{r}})} \cdot \hat{\boldsymbol{\sigma}}$$

$$= \boldsymbol{S}(\hat{\boldsymbol{r}}) \text{ ?}$$

$$\widehat{U_{\boldsymbol{m}}(\varphi)}\widehat{C_{\boldsymbol{n}}(\theta)}\boldsymbol{S}(\hat{\boldsymbol{r}}) \cdot \hat{\boldsymbol{\sigma}}\widehat{C_{\boldsymbol{n}}(\theta)}^{-1}\widehat{U_{\boldsymbol{m}}(\varphi)}^{-1}$$

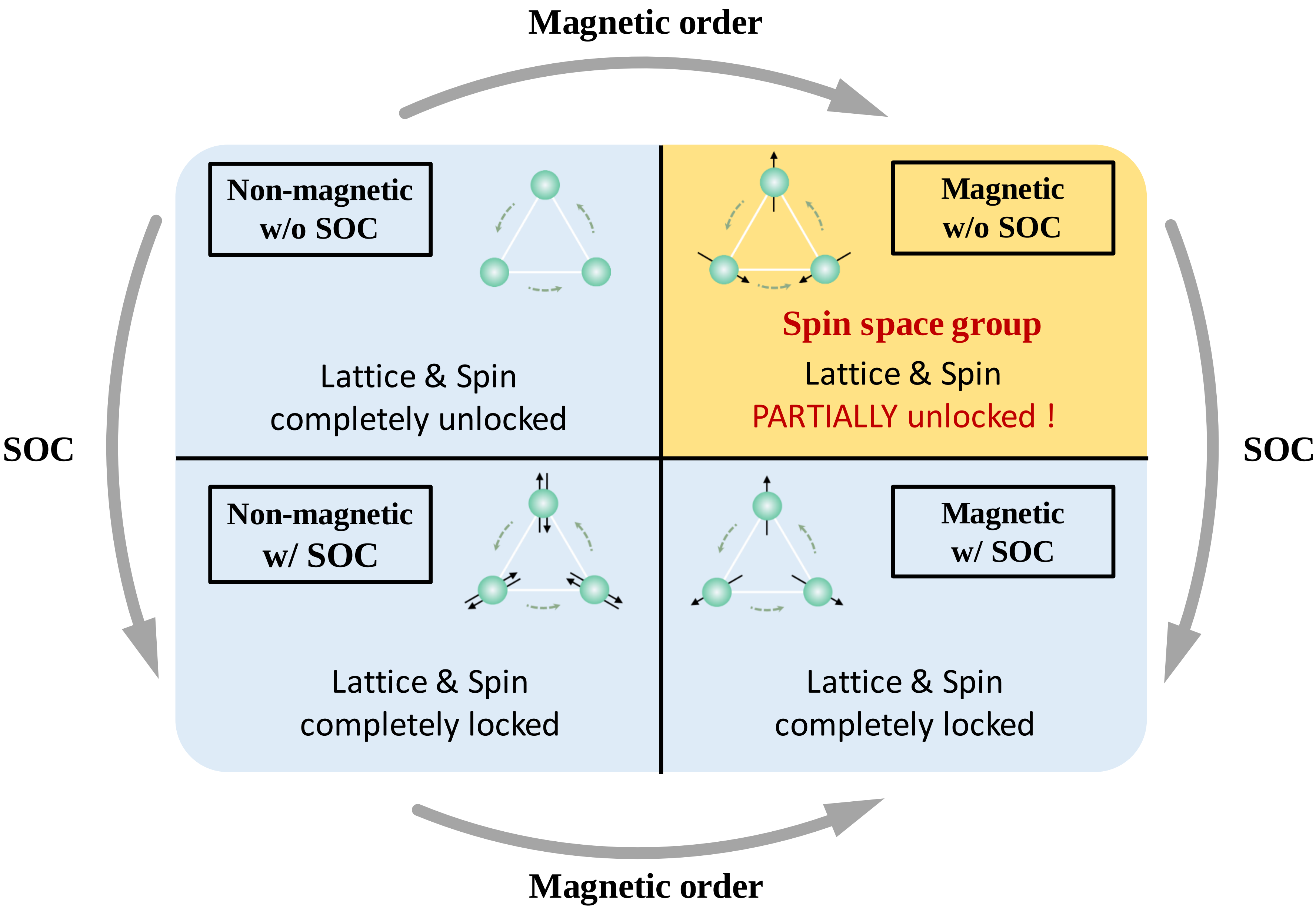
$$= \boldsymbol{S}(R_{\boldsymbol{n}}(\theta)^{-1}\hat{\boldsymbol{r}}) \cdot R_{\boldsymbol{m}}(\varphi)^{-1}\hat{\boldsymbol{\sigma}}$$

$$= \underline{R_{\boldsymbol{m}}(\varphi)\boldsymbol{S}(R_{\boldsymbol{n}}(\theta)^{-1}\hat{\boldsymbol{r}})} \cdot \hat{\boldsymbol{\sigma}}$$

$$= \boldsymbol{S}(\hat{\boldsymbol{r}})$$

Spin group with spin rotation operators detached from spatial rotation operators

Symmetry considerations in crystals – Group Theory



Original works about spin group symmetry

JOURNAL OF APPLIED PHYSICS VOLUME 37, NUMBER 3 1 MARCH 1966

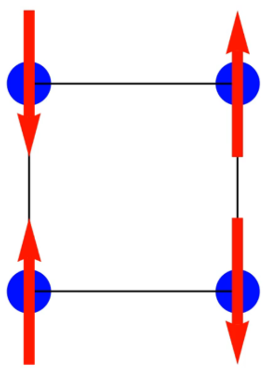
Space Group Theory for Spin Waves

W. Brinkman* and R. J. Elliott†
Department of Theoretical Physics, Oxford University, Oxford, England

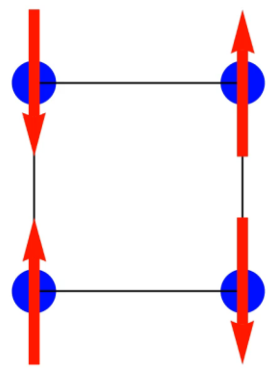
Theory of spin-space groups

By W. F. Brinkman† and R. J. Elliott
Department of Theoretical Physics, University of Oxford, England

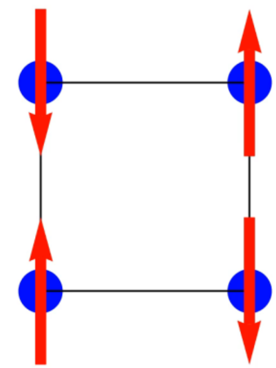
- Multiple-fold degeneracies of spin wave spectrum require an enhanced symmetry group called "spin group", which consider spin rotation and spatial rotation separately.



Consider an AFM
spin arrangement



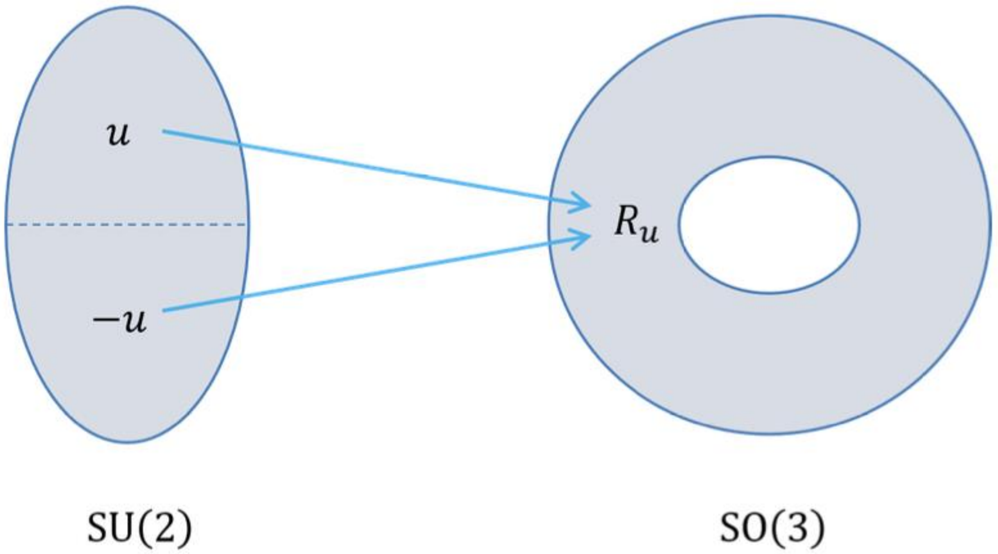
C_2 rotation in
magnetic group



C_2 rotation in
spin group

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

We are talking about spin "crystalline" group



In group theory, spin group is the double cover of SO(N)

Spin(1) = O(1) = {+1, −1}

Spin(2) = U(1) = SO(2)

Spin(3) = SU(2)

Outline

- Introduction of spin group
- **Features of spin point/space group**
- Topological phases protected by spin group symmetry
  - Kramers degeneracy and Z_2 topological phases
  - Chiral Dirac-like semimetal
- Outlook

Separating spin & lattice operation — notations

Spin rotation Lattice rotation

Spin point group: $\{U_{\boldsymbol{m}}(\varphi), TU_{\boldsymbol{m}}(\varphi) || C_{\boldsymbol{n}}(\theta), IC_{\boldsymbol{n}}(\theta)\}$

Spin space group: $\{U_{\boldsymbol{m}}(\varphi), TU_{\boldsymbol{m}}(\varphi) || C_{\boldsymbol{n}}(\theta), IC_{\boldsymbol{n}}(\theta)|\tau\}$

Lattice rotation & translation

There are 598 types of spin point group

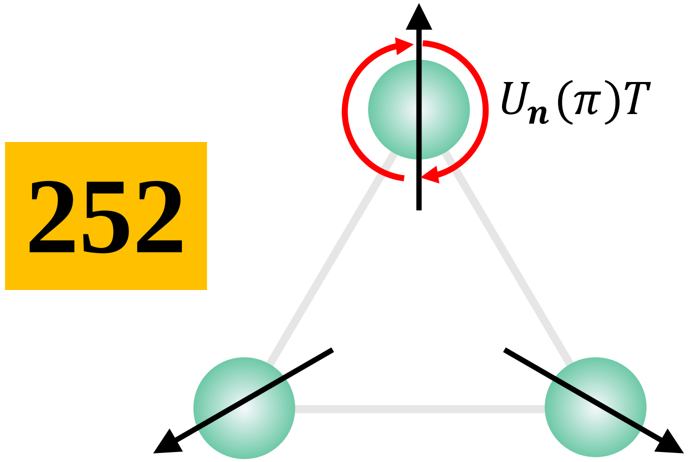
D. B. Litvin and W. Opechowski, Physica **76**, 538 (1974); D. B. Litvin, Acta Crystallogr. A **33**, 279 (1977)

Theory to explore:

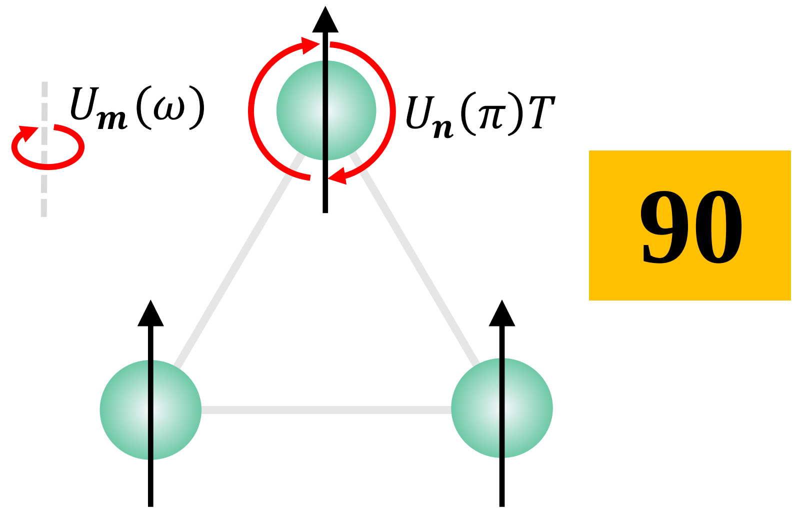
- Spin point groups for specific magnetic configuration?
- Classification of spin space groups?
- Representation theory of spin space groups?
- Application of spin group (Spintronics? Topology?)

Spin groups for collinear and coplanar spin arrangements

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



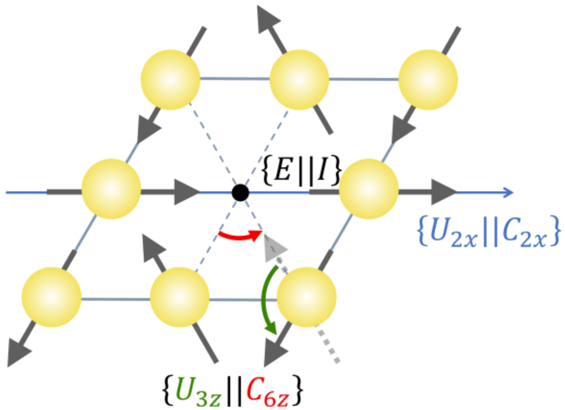
Collinear: $G_{\mathrm{SOP}} = SO(2) \rtimes Z_2^K$

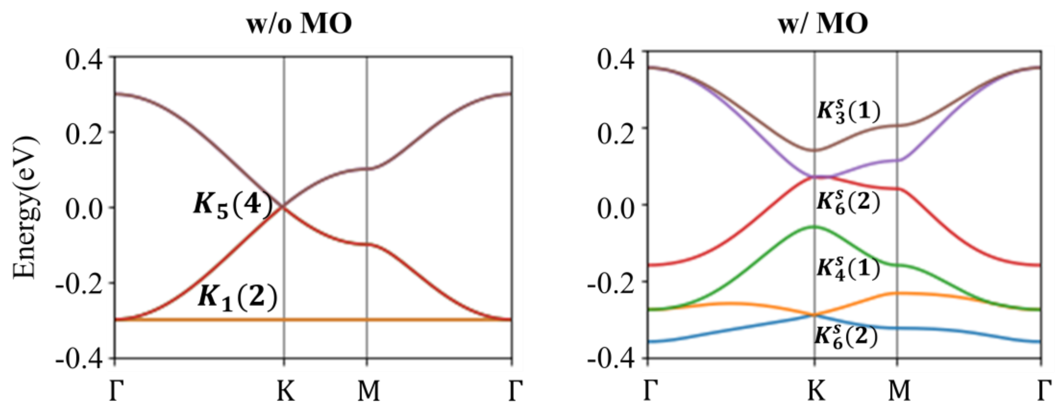


$$Z_2^K = \{\{E||E\},\{TU_{\boldsymbol{n}}(\pi)||E\}\};SO(2) = \{\{U_{\boldsymbol{m}}(\omega)T||E|0\}|\omega \in (0,2\pi]\}$$

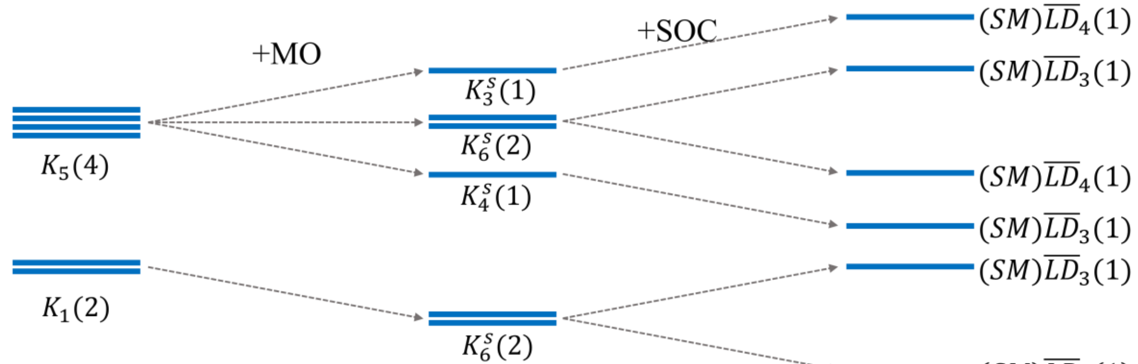
X. Wan*, **<u>QL*</u>** et al. PRX 12, 021016 (2022)

Degeneracies caused by spin space group





Space group	$P6/mmm\otimes SO(3)\otimes Z_2^T$	$P^{3_z}6/^{1}m^{2_x}m^{2_{xy}}m^{m_z}1$	$Cmm'm'$
Little co-group at K	$\bar{6}m2\otimes SO(3)\otimes Z_2^T$	${}^{\bar{6}_z}6/^{1}m^{2_x}m^{m_l}m[\cong 6/mmm(D_{6h})]$	$2'2'2[\cong 222(D_2)]$



- ➢ 2-fold degeneracies occur at K are well explained by spin group symmetry

Applications of spin group symmetry (Before 2022)

Previous discussions

Landau theory of phase transition

Phys. Rev. B **26**, 6947 (1982);
I. A. Izyumov et al., *Phase transitions and crystal symmetry*;…

Neutron scattering

Thorpe, Proc. Phys. Soc. **91**, 903 (1967);
Acta Crystallogr. A **29**, 651 (1973);…

Electronic states of spiral magnet

J. Phys. Condens. Matter **3**, 8565 (1991)

Spin group symmetry

Recent applications

Spin splitting in AFM systems

J. Phys. Soc. Jpn. **88**, 123702 (2019);
Phys. Rev. B **102**, 014422 (2020);
PNAS **118**, e2108924118 (2021)…

Spin Hall effect in AFM systems

Phys. Rev. Lett. **119**, 187204 (2017);
Phys. Rev. Lett. **126**, 127701 (2021);…

Piezomagnetism

Nat. Commun. **12**, 2846 (2021)

Other possible applications ?

Topological phase of matter

- **Introduction of spin group**
- **Features of spin point/space group**
- **Topological phases protected by spin group symmetry**
  - **Kramers degeneracy and Z_2 topological phases**
  - **Chiral Dirac-like semimetal**

Kramers degeneracy and Z_2 topological classification

➢ Kramers degeneracy

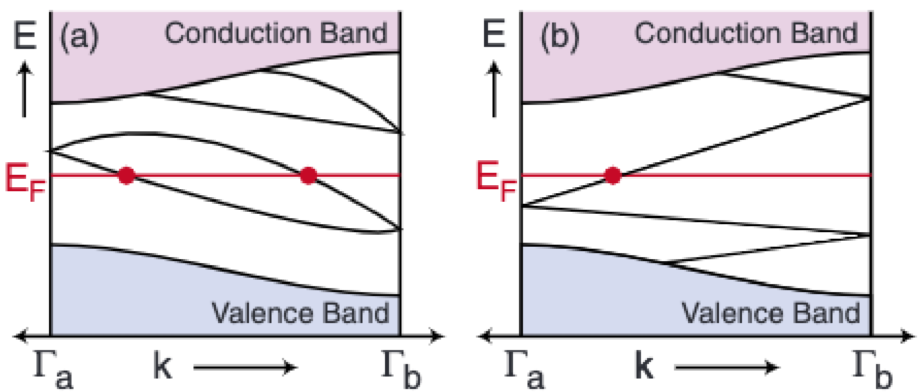
1. An antiunitary symmetry operator Θ (i.e., $\langle \Theta\phi | \Theta\varphi \rangle = \langle \varphi | \phi \rangle$)
2. $\Theta^2 = -1$

➢ Z_2 topological classification in 2D

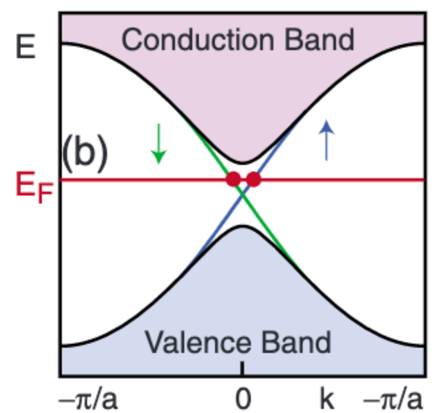
- Time reversal symmetry *T* of electronic system could protect Kramers degeneracy

→ Degeneracy at time reversal invariant momenta (TRIM) for surface states

→ Two types of surface states connection in edges of 2D systems corresponds to Z_2 topological trivial and nontrivial phase (Dirac surface states)



Rev. Mod. Phys. **82**, 3045 (2010)



Kramers degeneracy protected by spin group operations

- Find all symmetries that could protect Kramers degeneracy and are unbroken on certain surfaces

Spin group Symmetry	Momenta with protected 2-fold degeneracy	Surface with the symmetry	Possible surface states
$\{T\|\|E\|\tau_{\boldsymbol{z}/2}\}$	TRIM within $k_z = 0$ plane	(*xy*0)	DP at $(0,0)$ *or* $(\pi,0)$
$\{TU_{\boldsymbol{z}}(\pi)\|\|m_{[001]}\|\tau_{\boldsymbol{x}/2}\}$	$(\pi,0,k_z)$ and (π,π,k_z) lines	(010)	DNL at $k_x = \pi$
$\{T\|\|C_{\boldsymbol{z}}(\pi)\|0\}$	$k_z = 0$ and $k_z = \pi$ planes	(001)	Possible double DP
$\{T\|\|m_{[001]}\|0\}$	$(0,0,k_z), (0,\pi,k_z)$, $(\pi,0,k_z)$ and (π,π,k_z) lines	(*xy*0)	DNL at $k_x = 0$ or $k_x = \pi$
$\{T\|\|m_{[001]}\|\tau_{\boldsymbol{x}/2}\}$	$(0,0,k_z)$ and $(0,\pi,k_z)$ lines	(010)	DNL at $k_x = 0$
$\{TU_{\boldsymbol{n}}(\pi)\|\|m_{[001]}\|\tau_{\boldsymbol{x}/2}\}$	$(\pi,0,k_z)$ and (π,π,k_z) lines	(010)	DNL at $k_x = \pi$
$\{TU_{\boldsymbol{n}}(\pi)\|\|E\|\tau_{\boldsymbol{z}/2}\}$	TRIM within $k_z = \pi$ plane	(*xy*0)	DP at $(0,\pi)$ *or* (π,π)

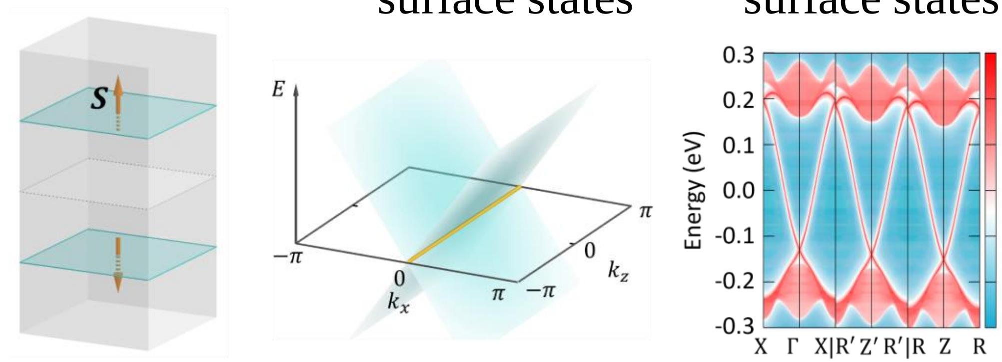
DP—Dirac point; DNL—Dirac nodal line

X. Wan*, **<u>QL*</u>** et al. PRX 12, 021016 (2022)

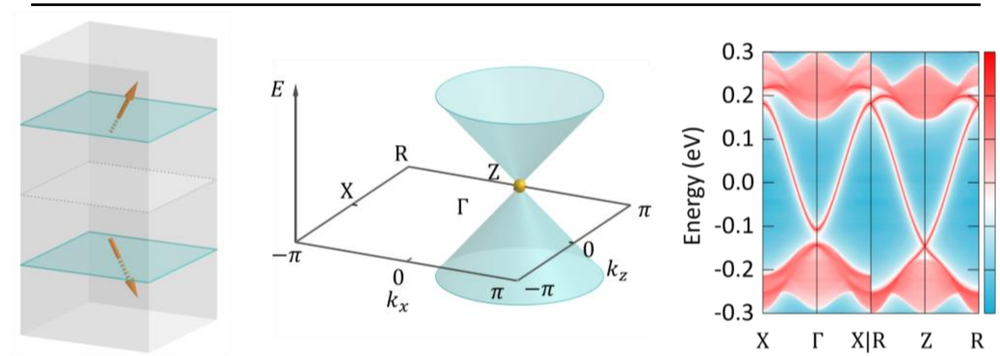
Z_2 topological phases realized by a tight binding model

Structure | Expected surface states | Calculated surface states

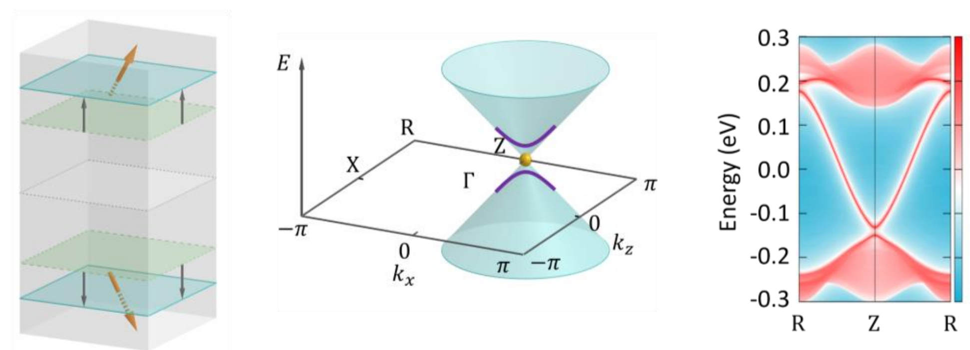
- Z_2Topological insulator protected by $\{T||m_{[001]}|0\}\&\{TU_{\boldsymbol{n}}(\pi)||E|\tau_{\boldsymbol{z}/2}\}$



- Z_2Topological insulator protected by $\{TU_{\boldsymbol{n}}(\pi)||E|\tau_{\boldsymbol{z}/2}\}$



- Trivial insulator



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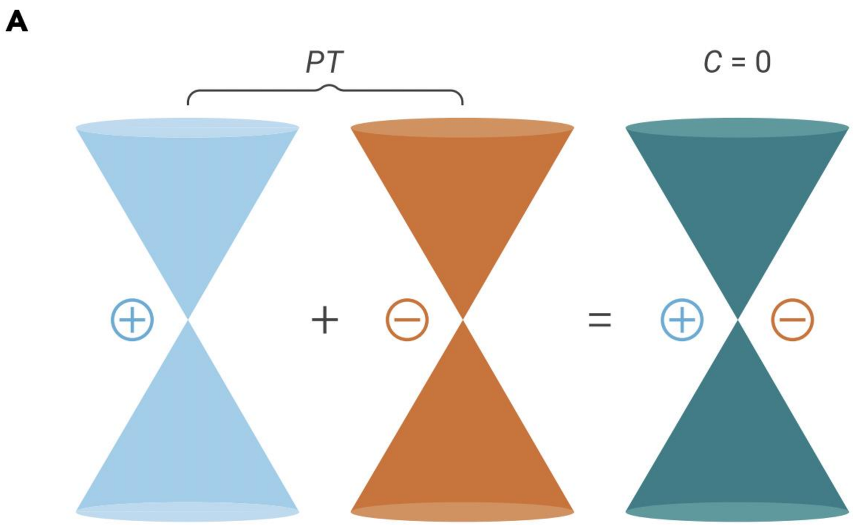
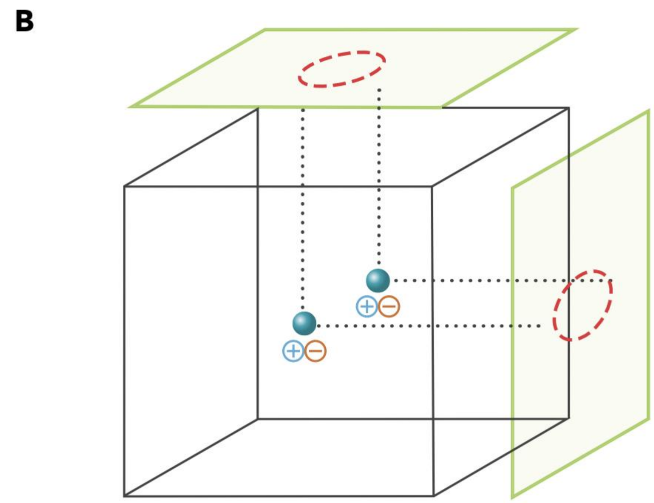
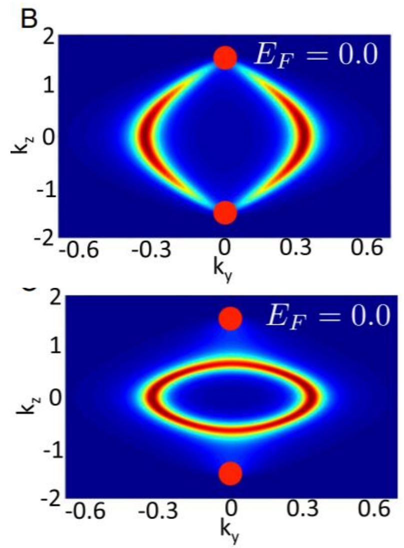
Conventional Dirac semimetal

Surface states



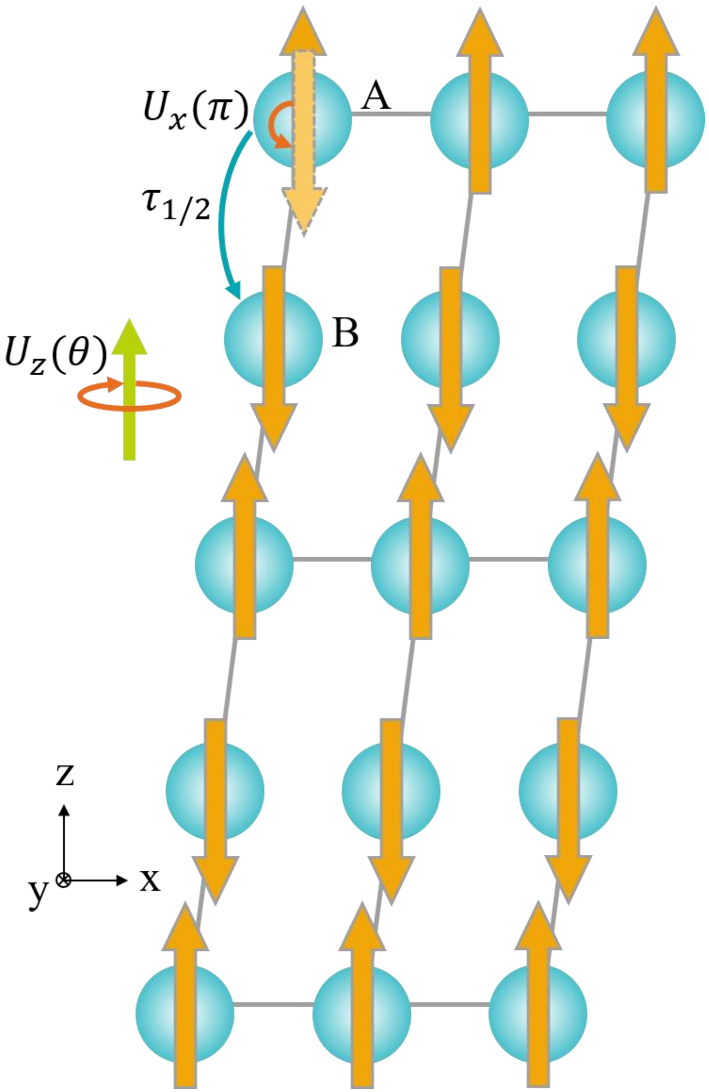




- ➢ A Dirac cone is composed of two Weyl cones with opposite chirality
- ➢ Appear at high-symmetry line/point
- ➢ The surface states are not topologically protected

PNAS **113**, 8648 (2016)

Hidden SU(2) symmetry in certain AFM systems without SOC



- Consider a collinear AFM structure with type-IV magnetic space group.

$$u_{\boldsymbol{x}}^{1/2} \equiv \{U_{\boldsymbol{x}}(\pi)||E|\tau_{1/2}\} = -ie^{-i\boldsymbol{k}\cdot\boldsymbol{\tau}_{1/2}}\tau_x \otimes \sigma_x$$

$$u_{\boldsymbol{y}}^{1/2} \equiv \{U_{\boldsymbol{y}}(\pi)||E|\tau_{1/2}\} = -ie^{-i\boldsymbol{k}\cdot\boldsymbol{\tau}_{1/2}}\tau_x \otimes \sigma_y$$

$$u_{\boldsymbol{z}} \equiv \{U_{\boldsymbol{z}}(\pi)||E|0\} = -i\tau_0 \otimes \sigma_z$$

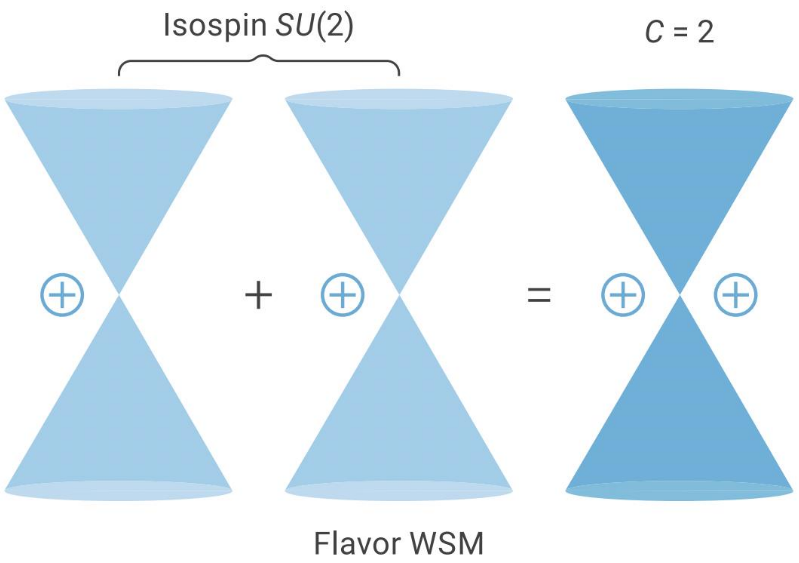
Generators of *su*(2) Lie algebra for an arbitrary ***k***

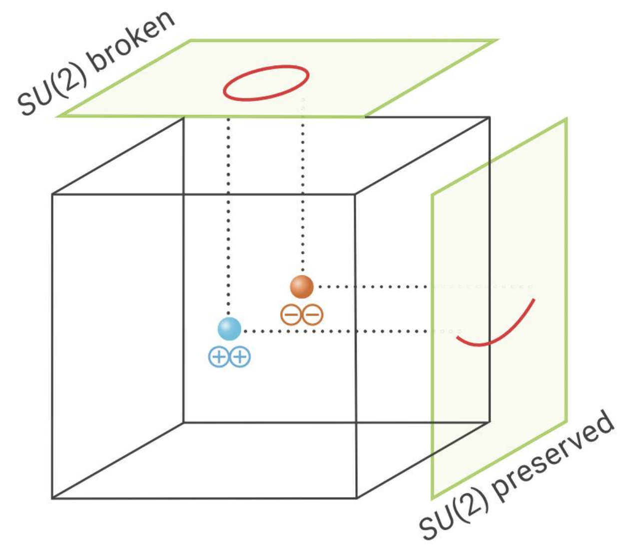
$$SU(2) = \{exp(-i\boldsymbol{\theta}\cdot\boldsymbol{\rho})\},$$

$$\boldsymbol{\rho} = \left(\frac{1}{2}\tau_x\otimes\sigma_x, \frac{1}{2}\tau_x\otimes\sigma_y, \frac{1}{2}\tau_0\otimes\sigma_z\right)$$

QL* et al. The Innovation 3, 100343 (2022)

A Dirac-like fermion but with chirality

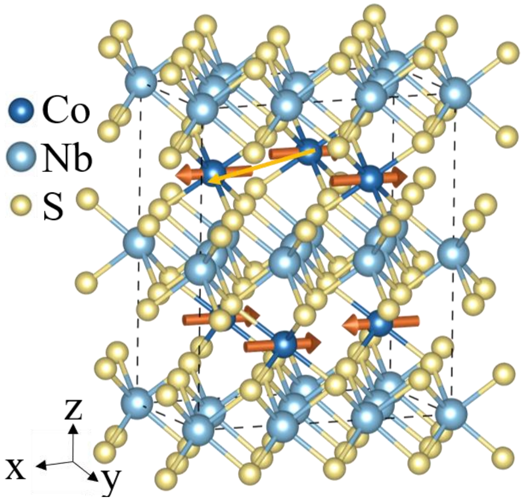


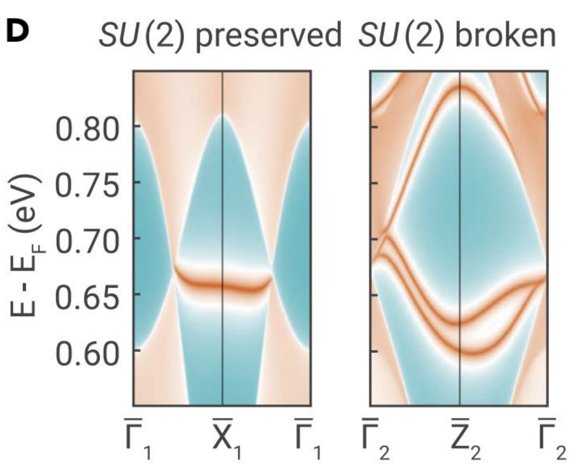


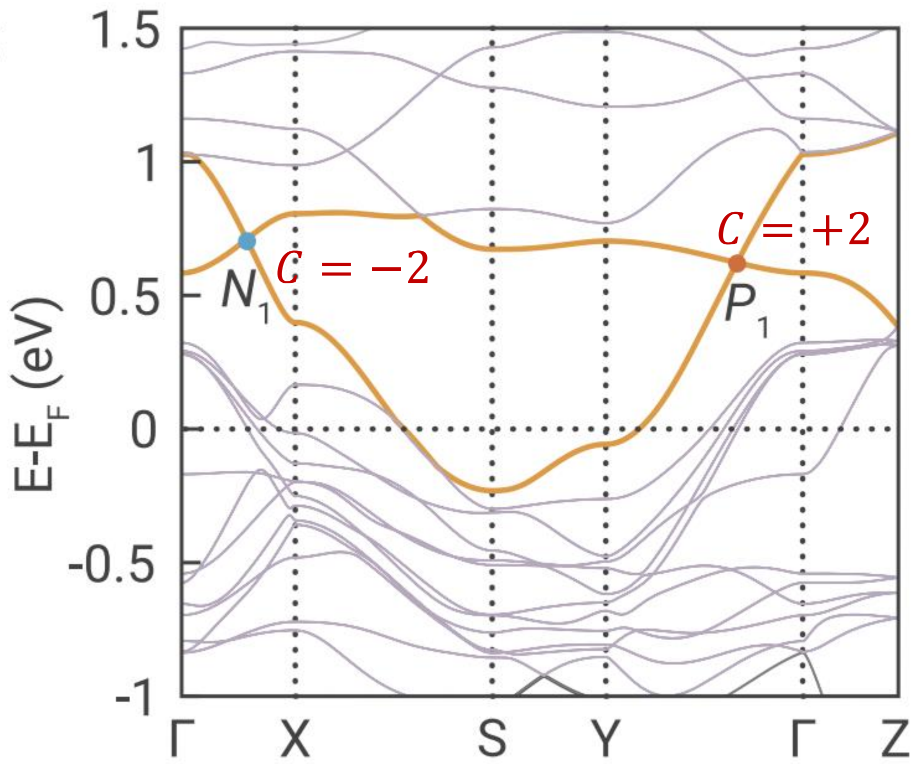
- Two Weyl quasiparticles with same chirality
- Robust Fermi arcs
- Dirac-like on certain surfaces while Weyl-like on other surfaces

Materials realization

- $CoNb_3S_6$ is a representative material of chiral Dirac-like semimetal



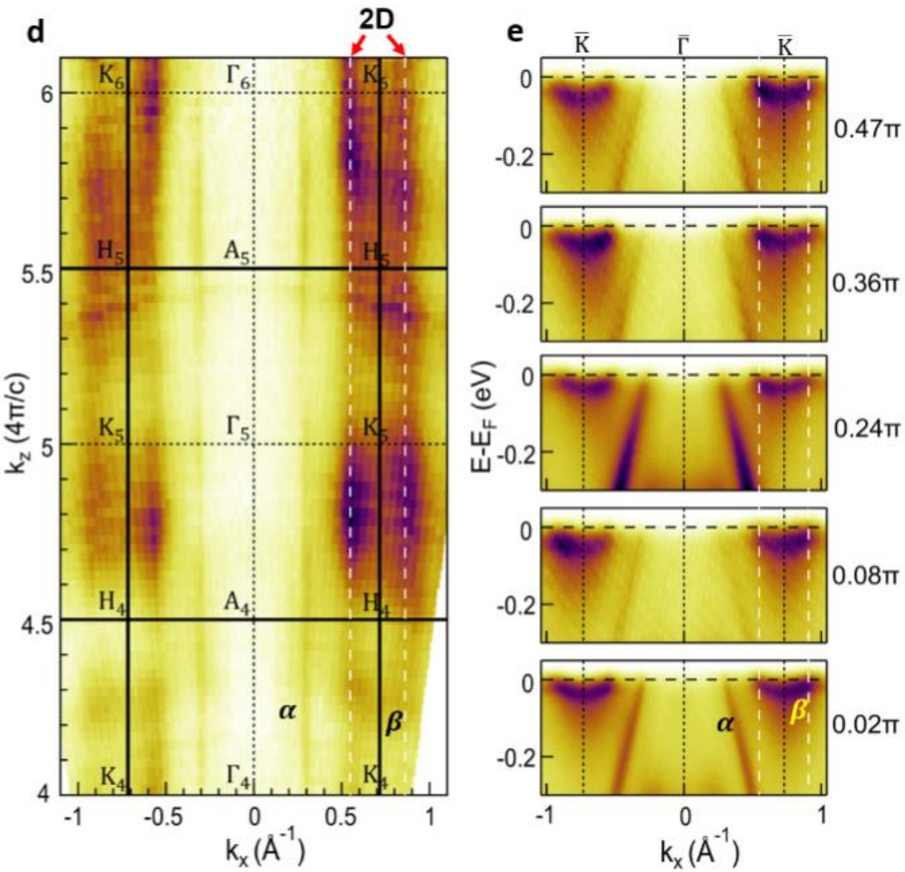


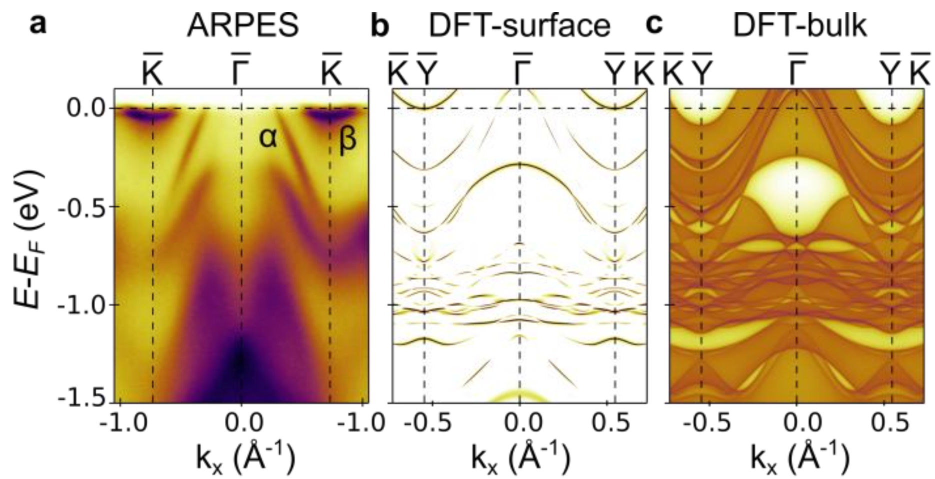


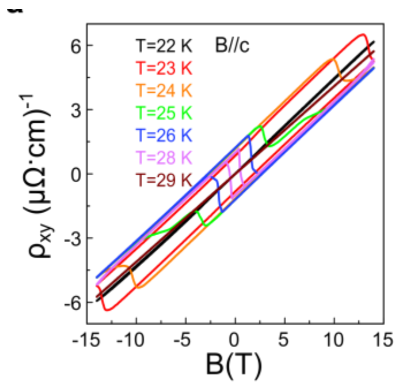
- P_1 and P_2 have chirality $+2$
- N_1 and N_2 have chirality -2.

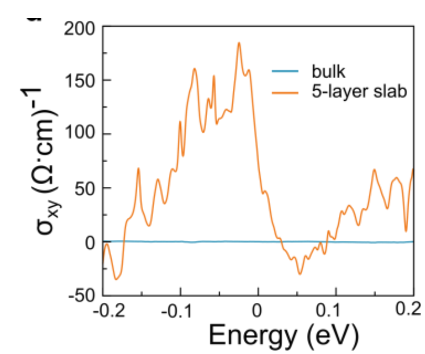
Experimental verification by ARPES and neutron diffraction

- The comparison between ARPES and DFT reveal the Fermi arc surface states of $CoNb_3S_6$









- k_z dispersion shows 2D nature

L. Wu*, C. Chen*, **QL*** et al. arXiv:2303.04549 (2023)

- Mysterious Anomalous Hall effect explained by chiral Dirac fermion

Summary and What's next ?

Spin crystalline group — symmetry description of magnetic materials in SOC-free limit:

1) New symmetry operations, new degeneracies, and new quasiparticles

2) New topological phases and new topological classifications

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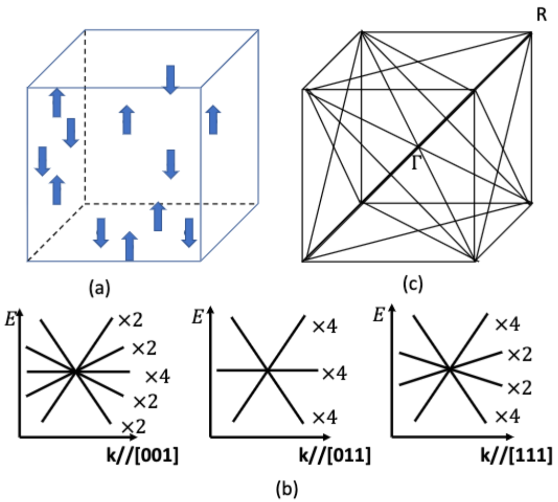
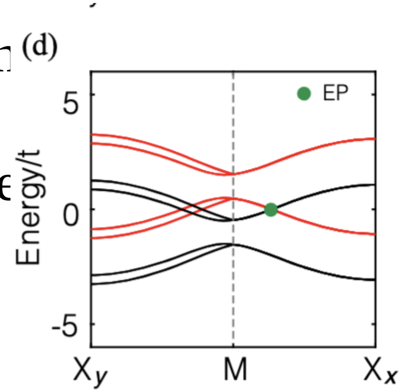
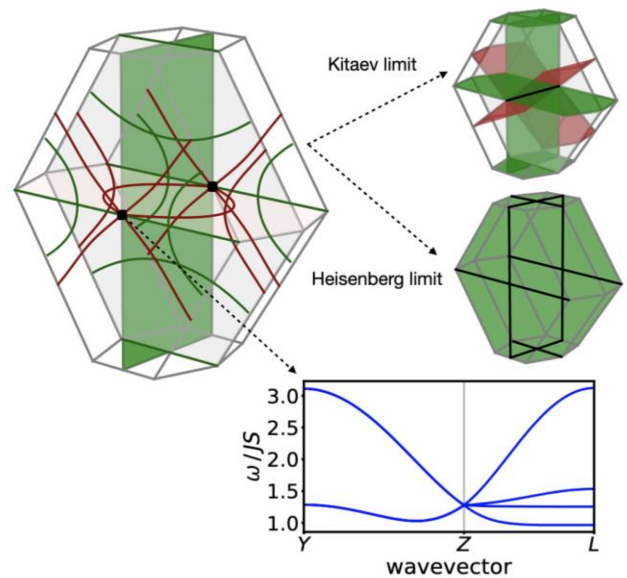


Symmetry invariants
arxiv:2105.12738

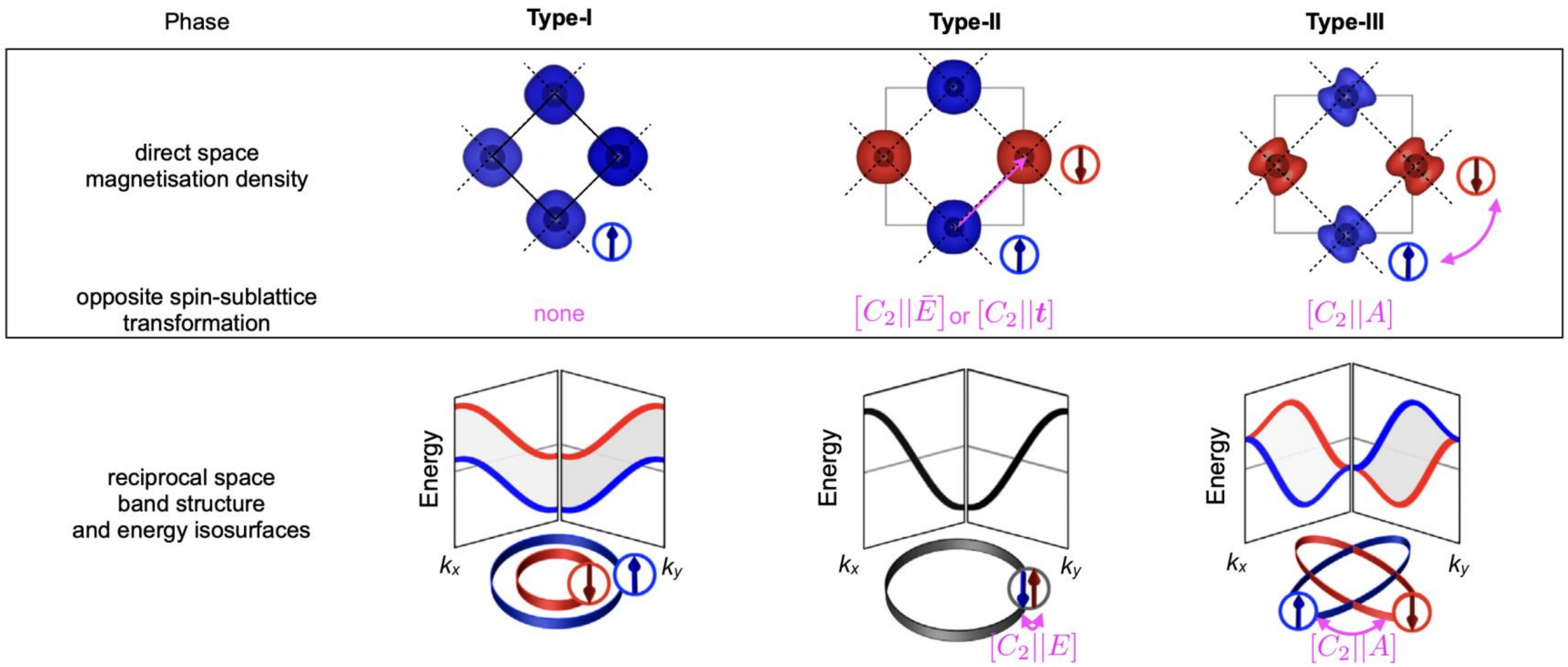


New fermions
PRL 127, 176401 (2021)



Magnon topology
PRB 105, 064430 (2022)

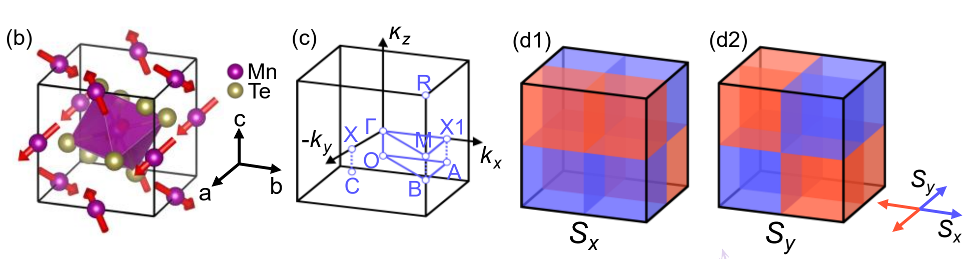
Altermagnetism and spintronics

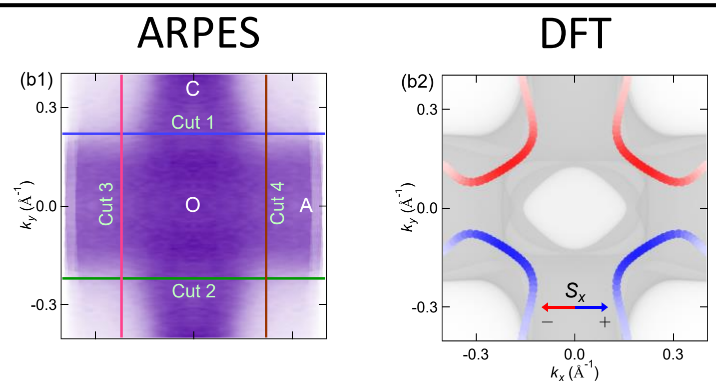


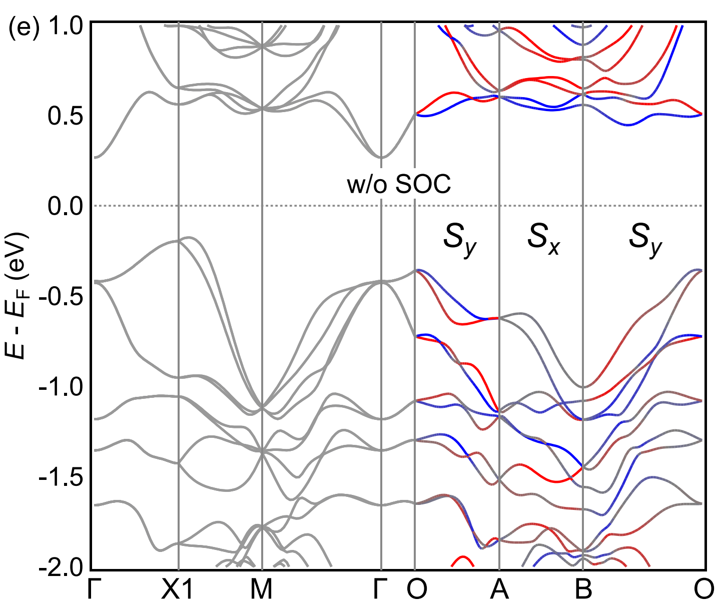
RuO_2, $FeSb_2$, MnF_2, CrSb, MnTe, VNb_3S_6… PRX 12, 031042 (2022); PRX 12, 040501 (2022)

Spin splitting torque	PRL 128, 197202 (2022)
Spin Hall effect	PRL 126, 127701 (2021)
Tunneling Magnetoresistance	PRX 12, 011028 (2022)

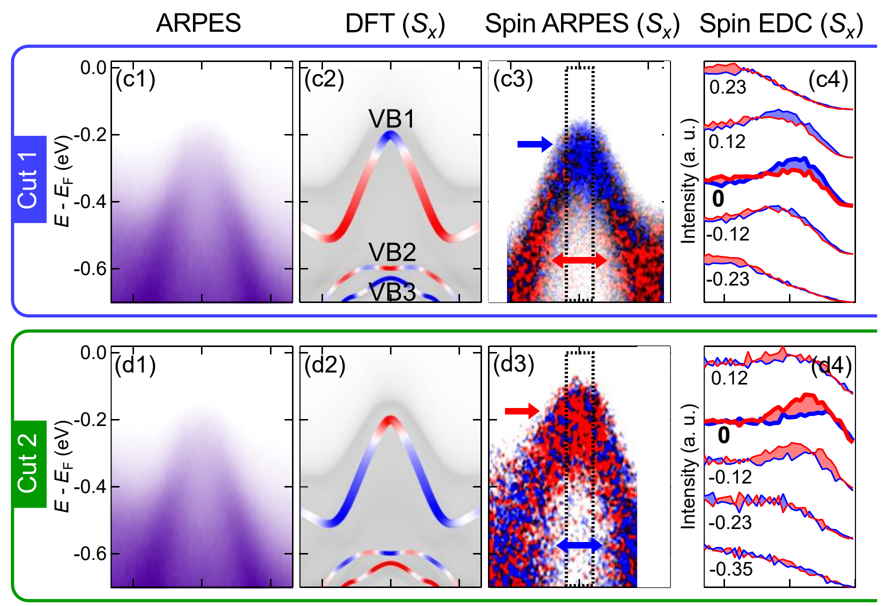
Plaid-like spin splitting in a noncoplanar antiferromagnet $MnTe_2$







Plaid-like spin texture
in the k_z = -0.4 π/c (O-A-B-C) plane



Spin-ARPES shows symmetric/antisymmetric spin polarization along k_x / k_y axes

S. Qiao*, **QL***, C. Liu* et al. arXiv:2303.04549 (2023)

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Thank you for your attention !

Phys. Rev. X 12, 021016 (2022)
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arXiv:2303.04549 (2023)
arXiv:2301.12201 (2023)

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