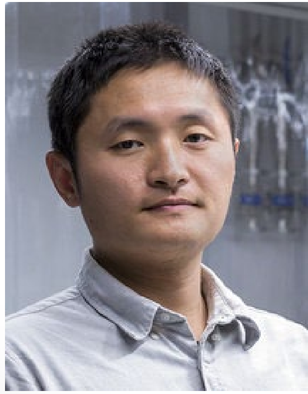
# Quasi-symmetry protected topology in CoSi



Chunyu(Mark) Guo, Jonas Diaz, Carsten Putzke, Philip J. W. Moll

MQM, Max Planck Institute for the Structure and Dynamics of Matter,
Hamburg, Germany

Lunhui Hu, Chaoxing Liu

Department of Physics,
The Pennsylvania State University

B. Andrei Bernevig

Department of Physics,
Princeton University

Kaustuv Manna, Feng-Ren Fan, Yan Sun, Chandra Shekhar, Claudia Felser

Max-Planck-Institute for Chemical Physics of Solids

Nature physics 18, 813–818 (2022)
See also: News & Views,
Nat. Phys. 18, 731-732 (2022)

mqm

MAX-PLANCK-GESELLSCHAFT

FNSNF
FONDS NATIONAL SUISSE
SCHWEIZERISCHER NATIONALFONDS
FONDO NAZIONALE SVIZZERO
SWISS NATIONAL SCIENCE FOUNDATION

EPFL

mqat

Princeton Physics

PennState
Eberly College of Science

# The broken cup

Topology protects characteristics of the band structure against perturbations.

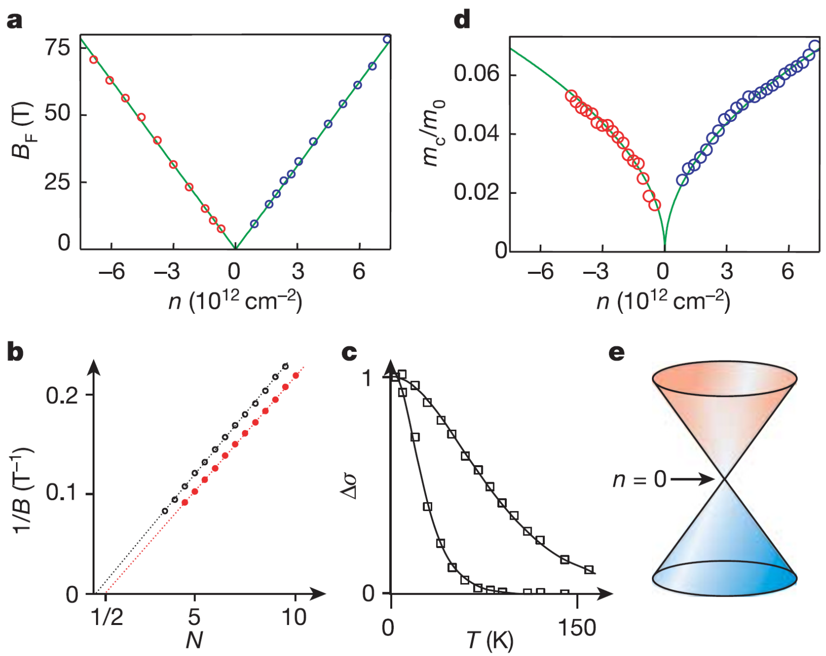
***But what if I need a cup?***

# Outline

- Reminders: Approximate symmetries and hidden symmetries.
- The semi-metal CoSi is too simple
- What is a quasi-symmetry
- Growing classes of quasi-symmetric materials

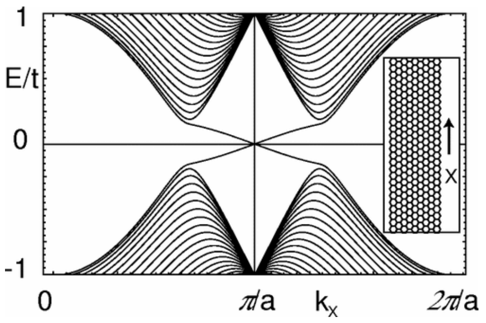
# Massless Dirac Fermions in Graphene

**Carriers in Graphene behave as massless Dirac particles.**

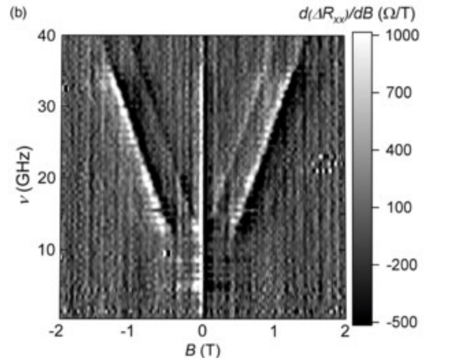



K.S. Novoselov et al., Nature 438, 197 (2005)

**Weak but finite spin-orbit coupling induces a gap of 42 μeV (~0.4K).**




C.L. Kane and E.J. Mele, PRL 95, 226801 (2005)

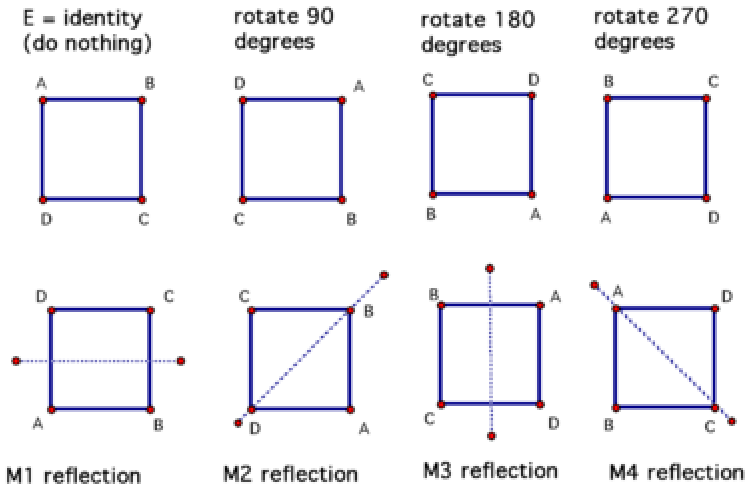



J. Sichau et al., PRL 122, 046403 (2019)

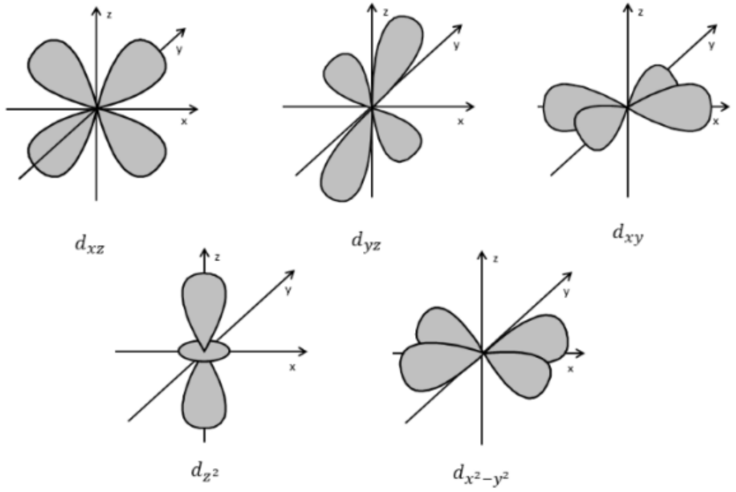
- Topology of electronic spectra is well defined mathematically by the choice of model, which may not resemble nature.
- The model that captures all effects at relevant energy scales will describe reality best.
- Mathematical classification may not be the ultimate judge for novel applications.

# Symmetries simplify physics problems

Symmetry group of the problem $G$




Reduced complexity (*degeneracy*)



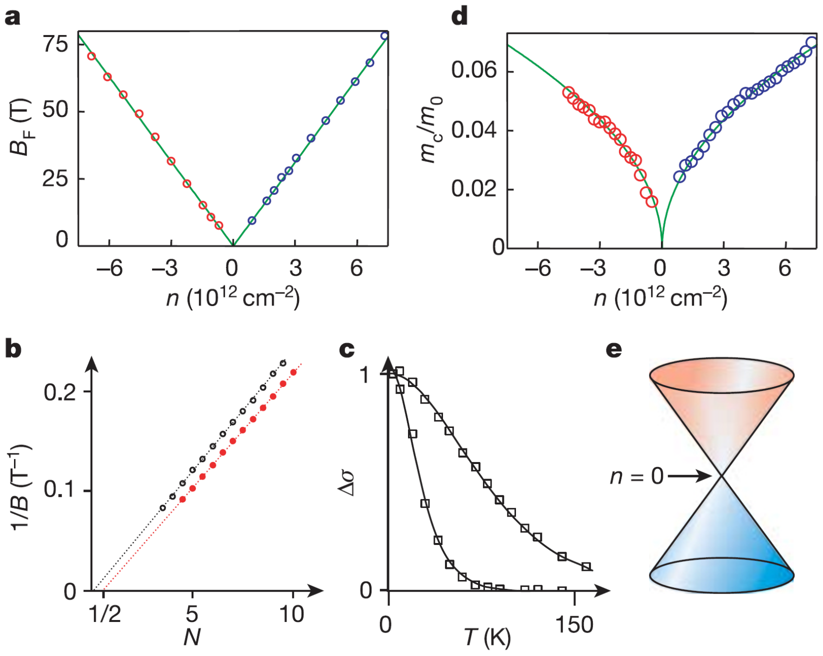
# Approximate symmetry

Too high symmetry of the model: **spin-rotation symmetry**.

But is it relevant? It remains an **approximate symmetry**.

$$H = H_D$$

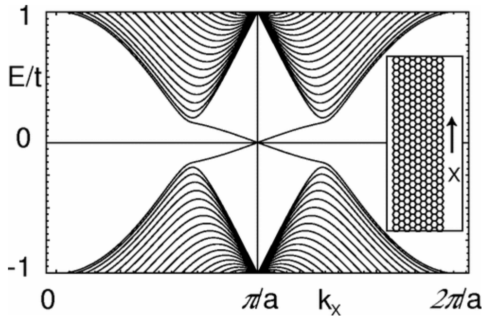
**Carriers in Graphene behave as massless Dirac particles.**



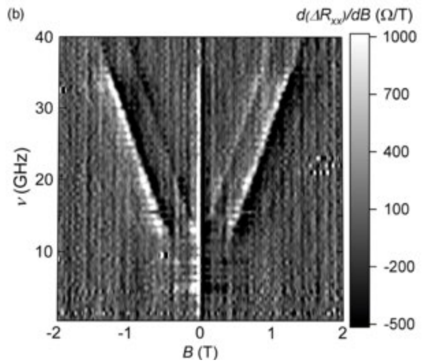

K.S. Novoselov et al., Nature 438, 197 (2005)

$$H = H_D + \mathrm{H_{SOC}}$$

**Weak but finite spin-orbit coupling induces a gap of 42 μeV (~0.4K).**



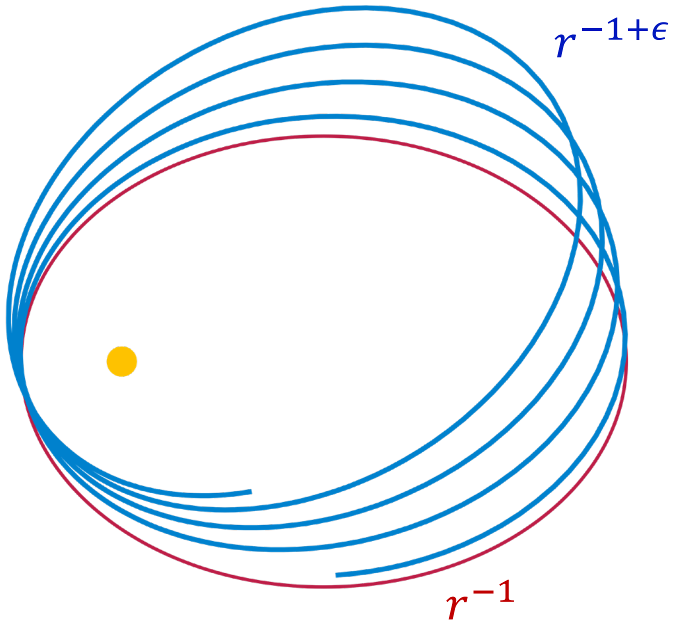

C.L. Kane and E.J. Mele, PRL 95, 226801 (2005)




J. Sichau et al., PRL 122, 046403 (2019)

# Hidden symmetry

Radially symmetric potential V(r) → Symmetry SO(3) → Classical orbits fall in plane perp. to angular momentum.




**Classical gravity**: All solutions of the Kepler problem are ***closed*** ellipses!

Solution: V(r) ~ 1/r has a higher symmetry than SO(3), namely SO(4).

Famous example of a hidden symmetry
and hidden conservation law (Lenz-Runge-Kutta vector)

$$\boldsymbol{A} = \boldsymbol{p} \times \boldsymbol{L} - mk\boldsymbol{e_r}$$

**Not all relevant symmetries are directly apparent. Look out for simpler behavior than symmetry would predict.**

# Hidden, approximate symmetries

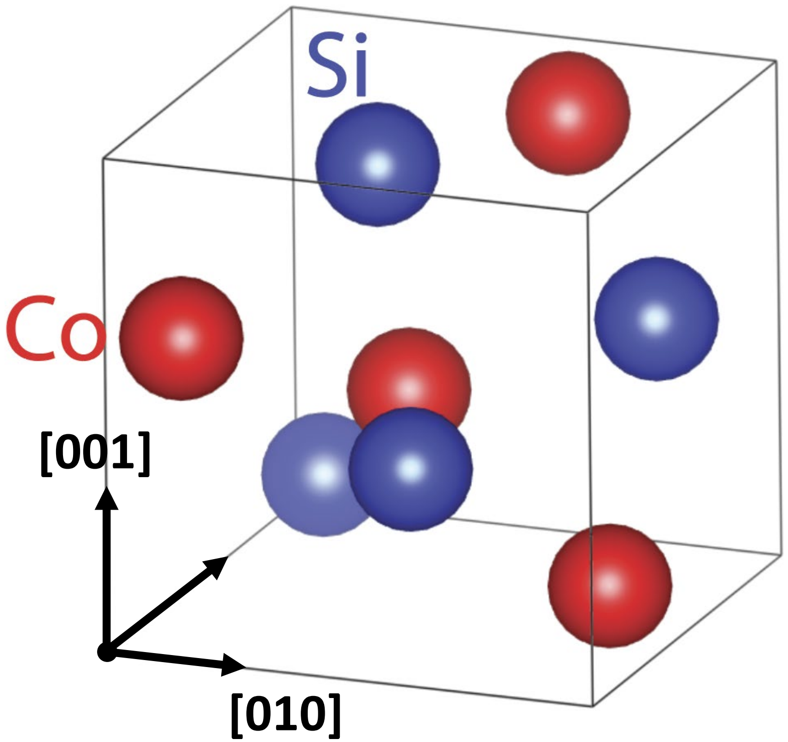
It could be possible that approximate, hidden symmetries stabilize (quasi-)degeneracies that are practically indistinguishable from true symmetries.

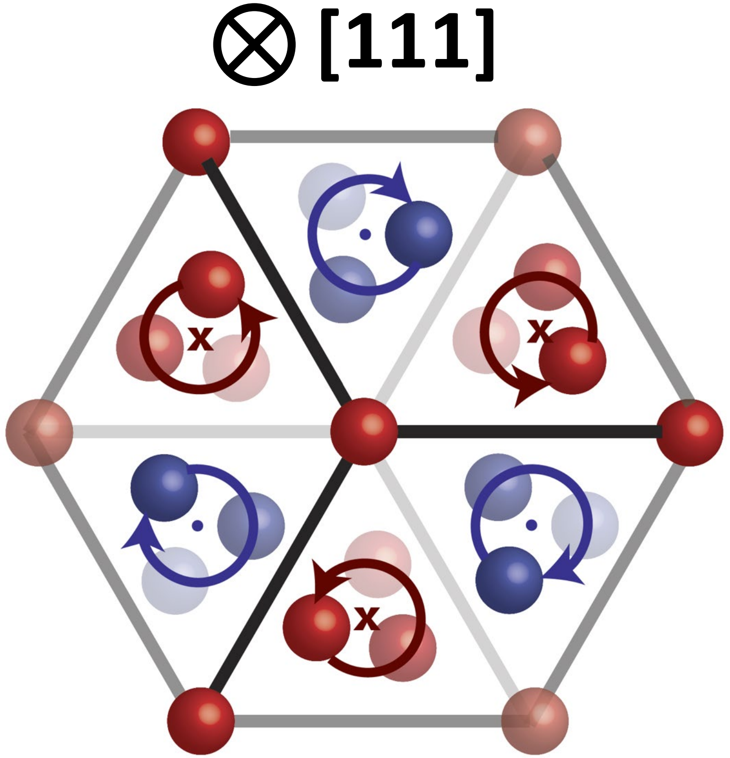
# Outline

- Reminders: Approximate symmetries and hidden symmetries.
- The semi-metal CoSi is too simple
- What is a quasi-symmetry
- Growing classes of quasi-symmetric materials

# Basic properties of CoSi

**Chiral cubic structure**

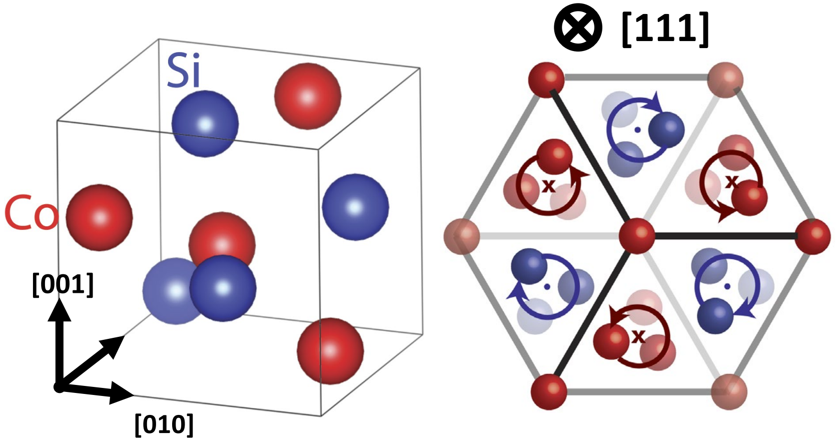


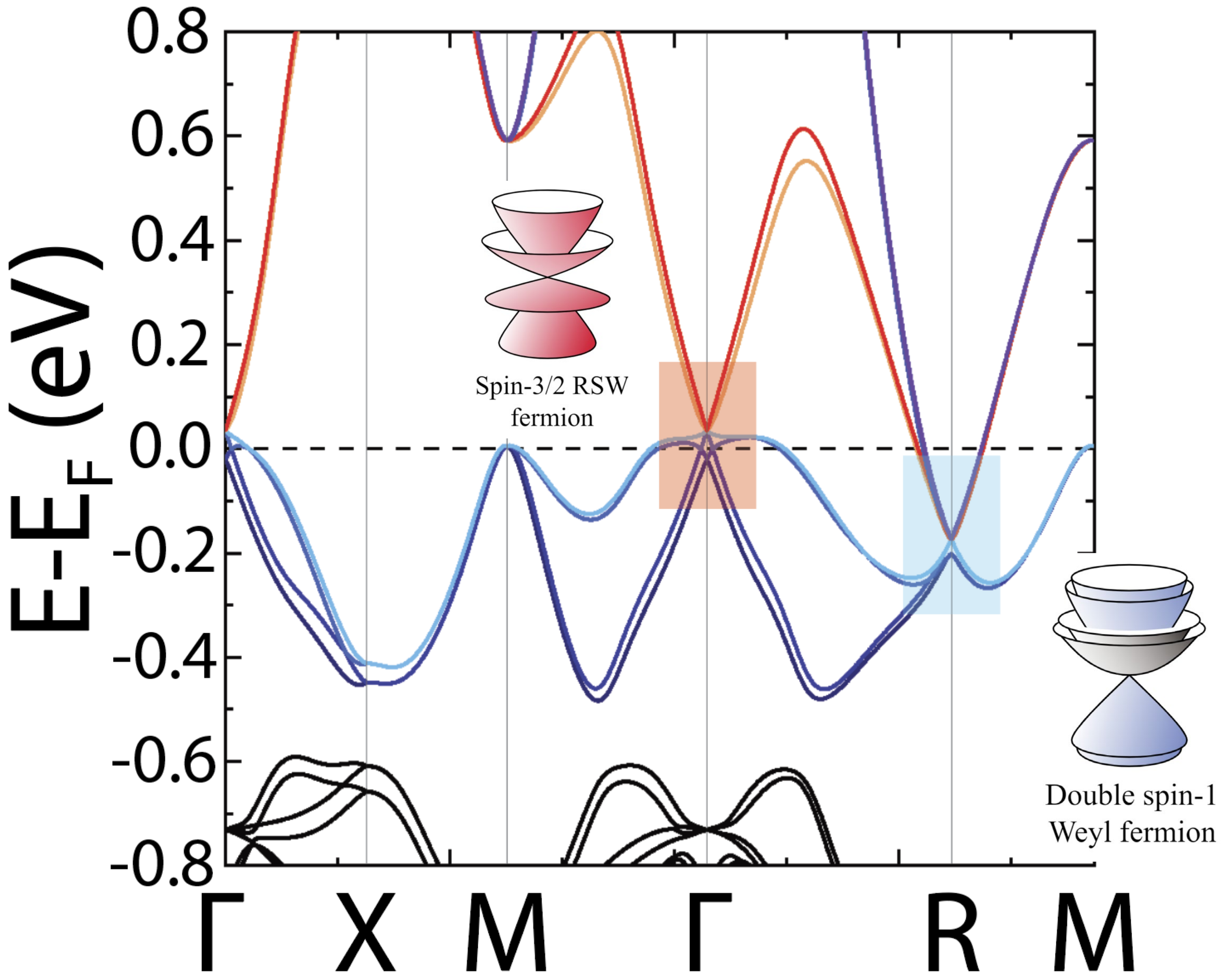

Space group: $P2_13$ (198)
No inversion center
Chiral axis along [111]

# Basic properties of CoSi

**Chiral cubic structure**

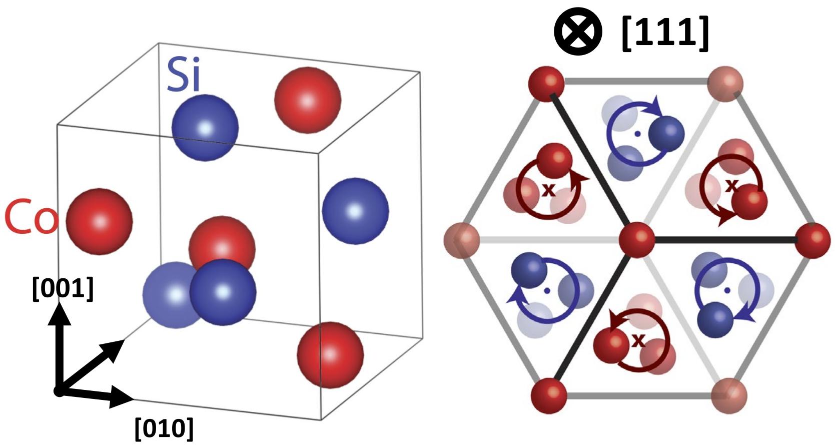



**Band structure from DFT**

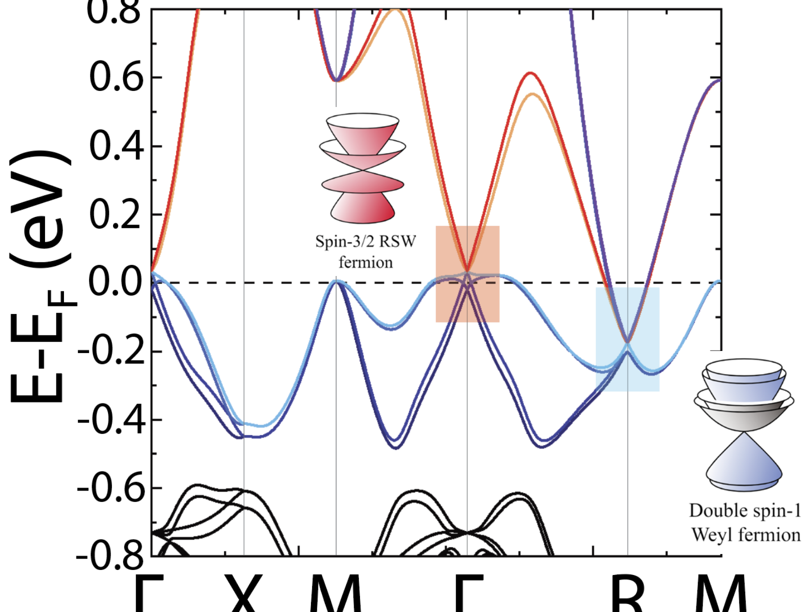


# Basic properties of CoSi

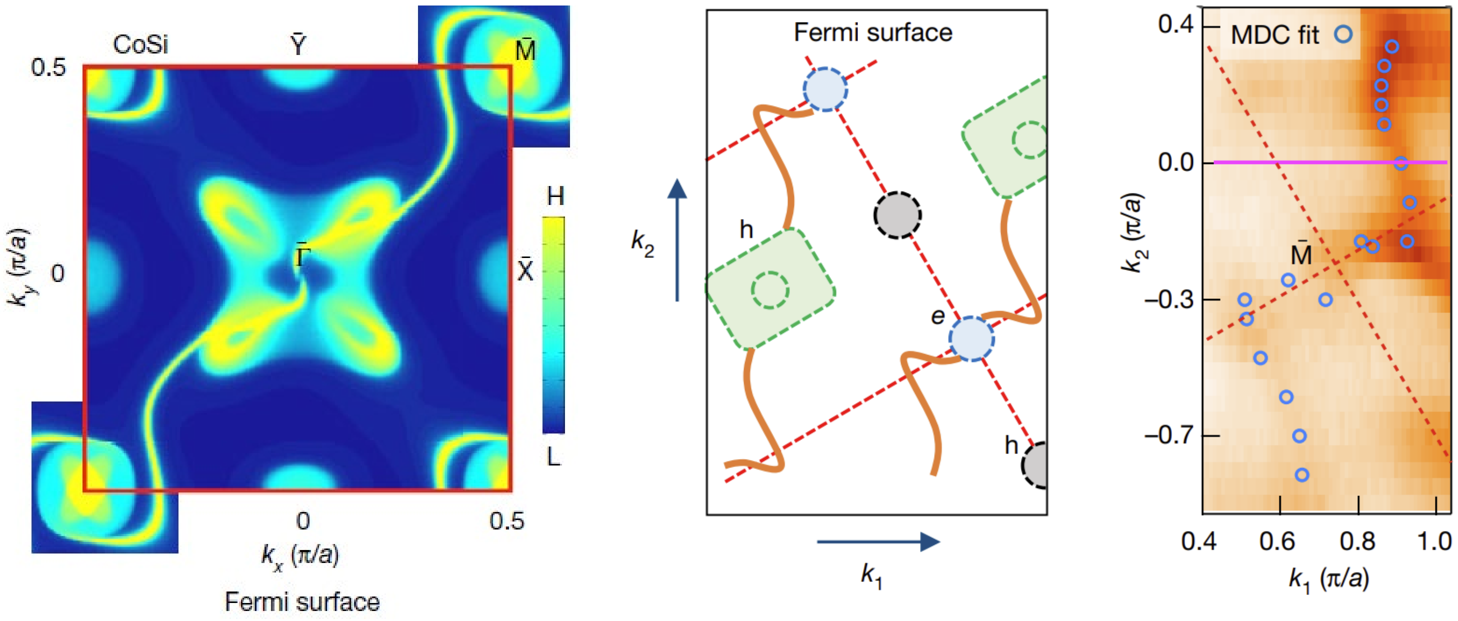
**Chiral cubic structure**




**Band structure from DFT**



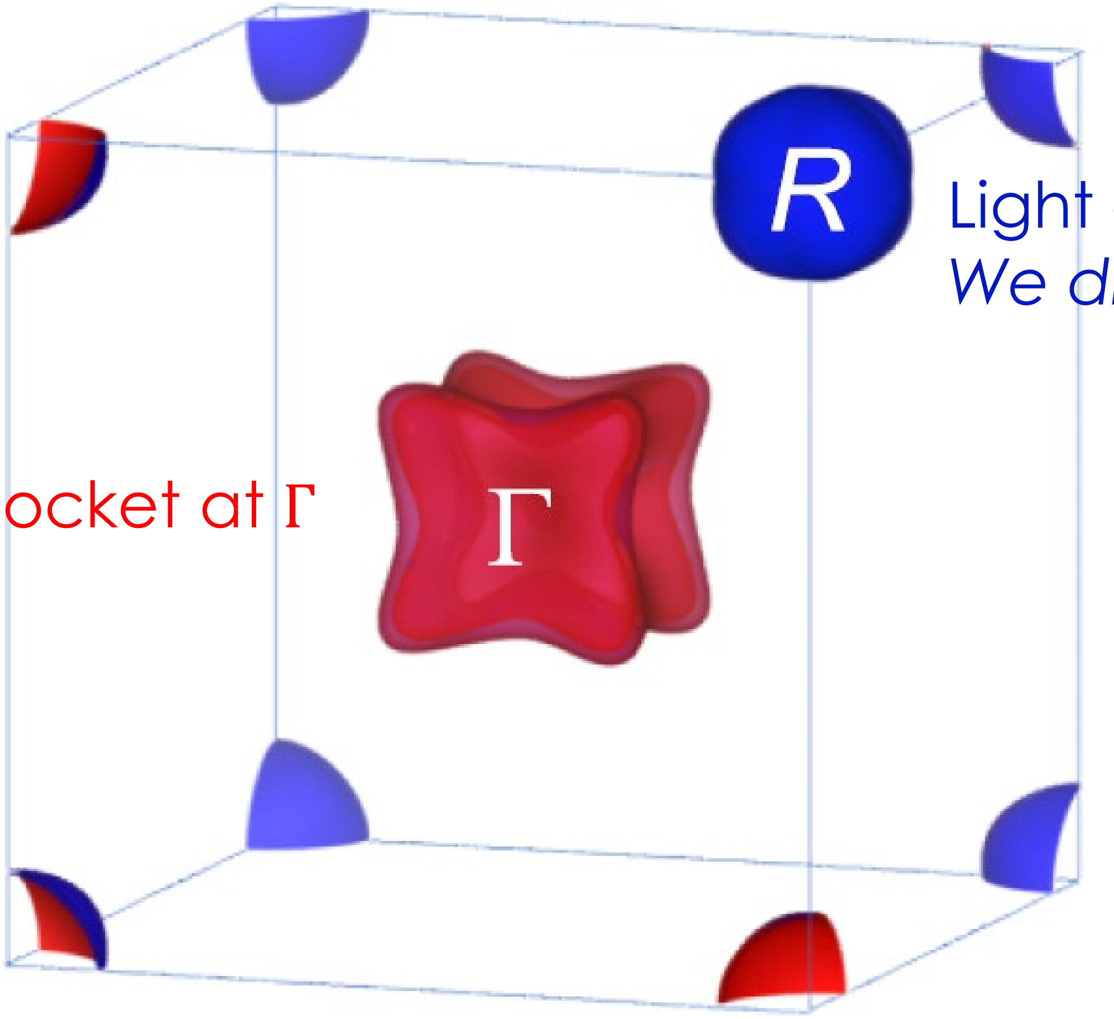

## Long Fermi-arc




Long Fermi-arc observed in ARPES measurements.


[1] Z. Rao et al., Nature 567, 496 (2019).
[2] D. S. Sanchez et al., Nature 567, 500505 (2019).

# Fermi surface overview



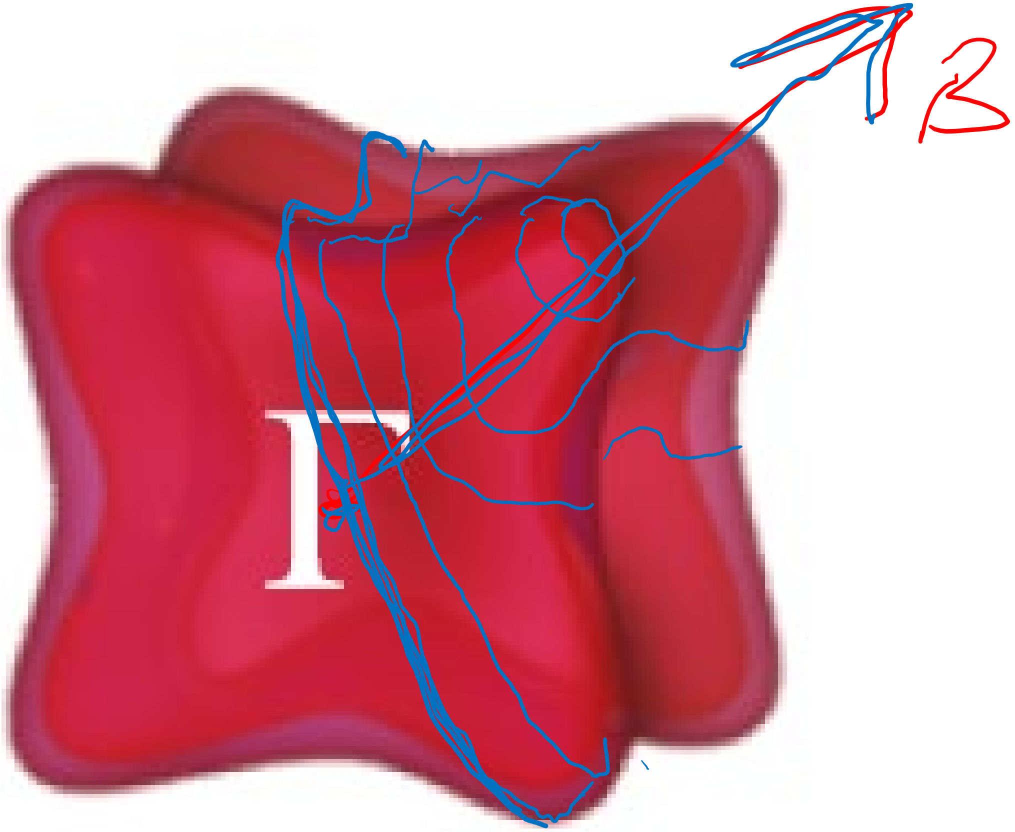

Light electron pocket at R
*We discuss about this one.*

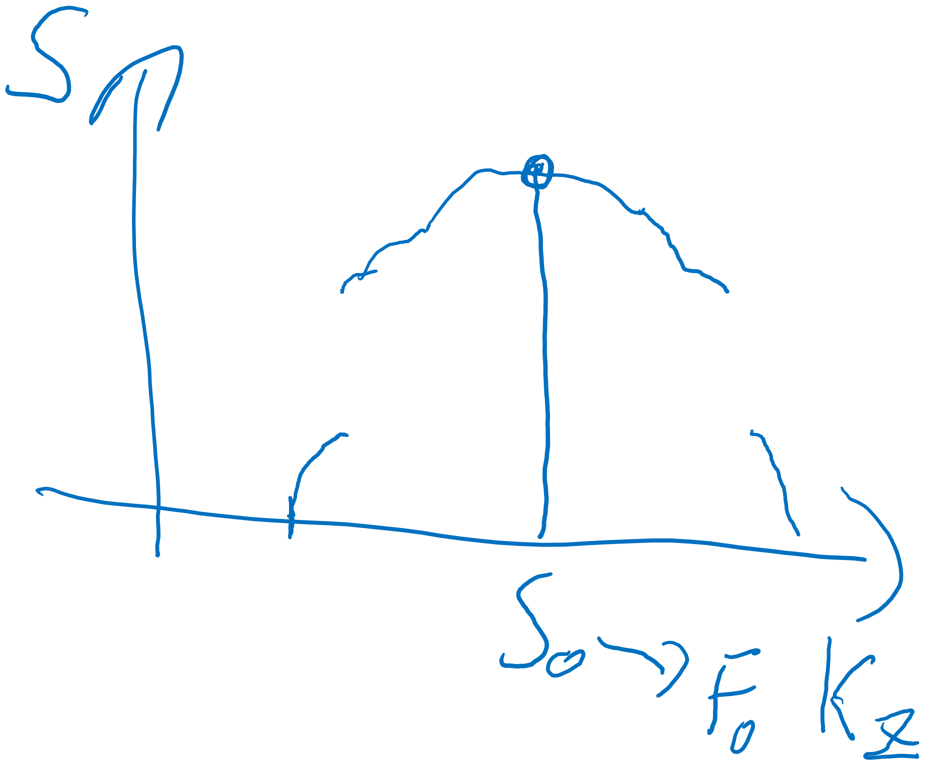
Very heavy hole-pocket at Γ
*Hard to see in QO*

# Fermi surface topology from quantum oscillations

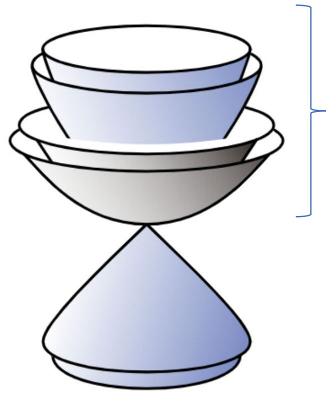
Onsager relation: $F = \dfrac{\hbar}{2\pi e} S$

Frequency of QO (M,R,..) = Extremal cross-section of Fermi surface



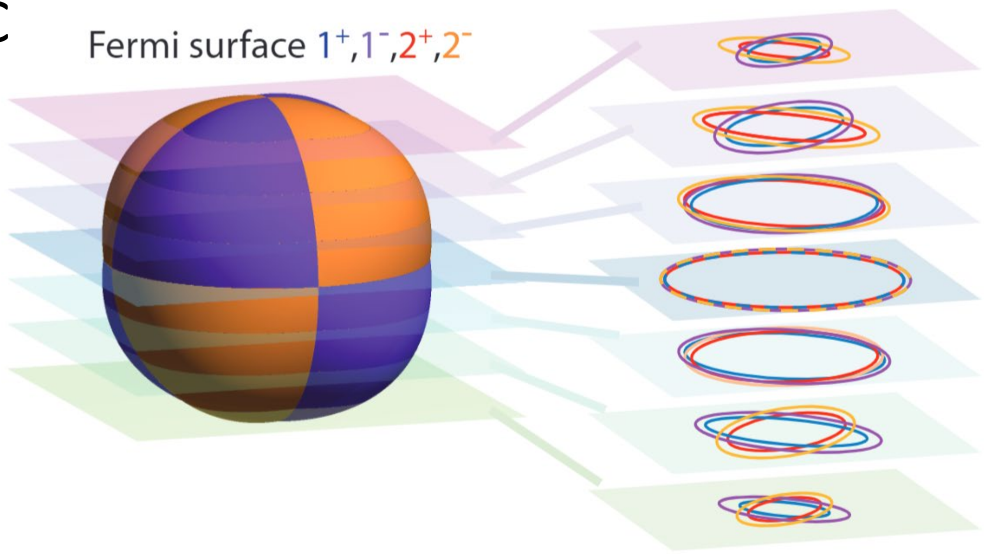



# Fermi surface topology: slice and view

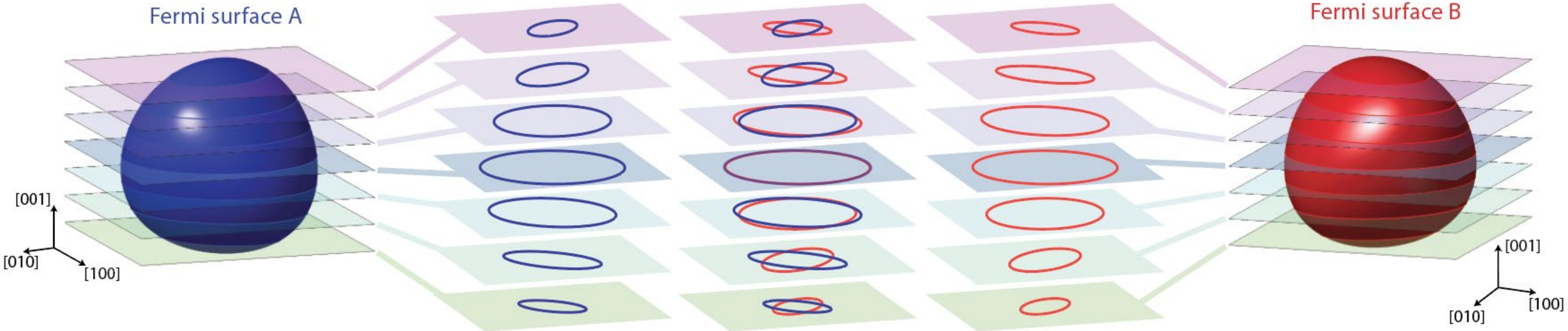



**4 bands**:
2 orbital, 2 spin

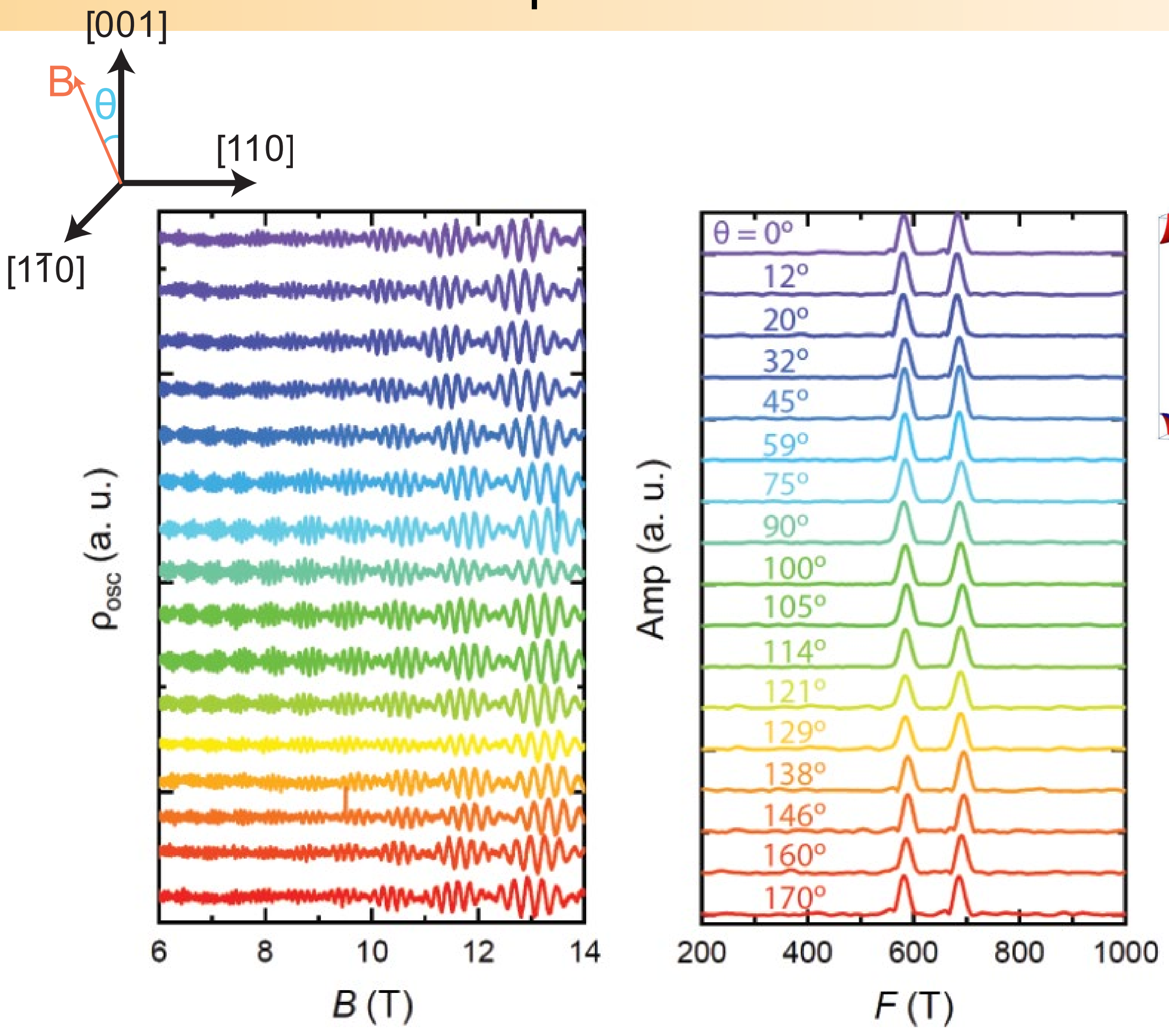
With SOC
Full FS

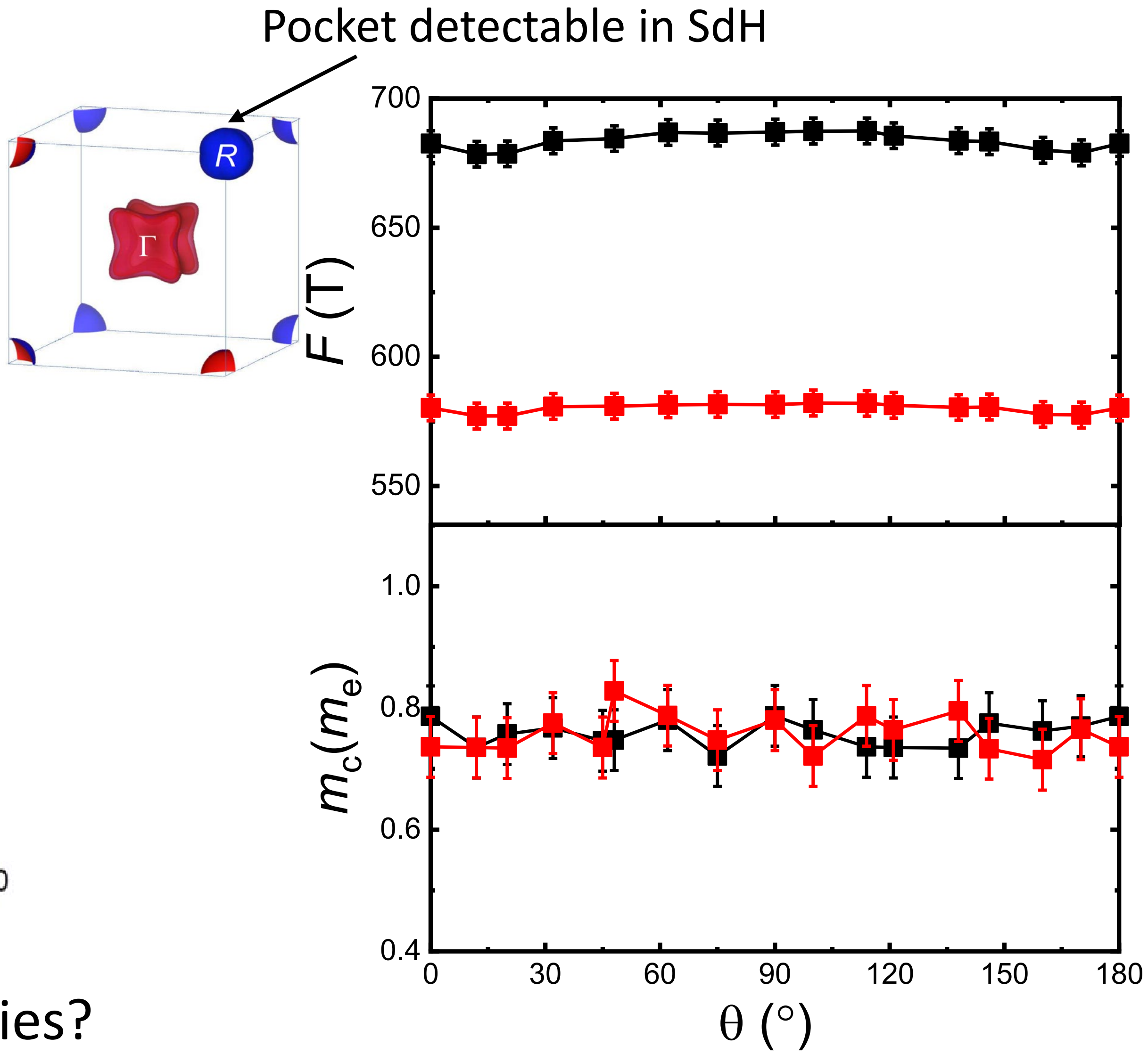



First ignore SOC (only 2 surfaces)



# CoSi is too simple!

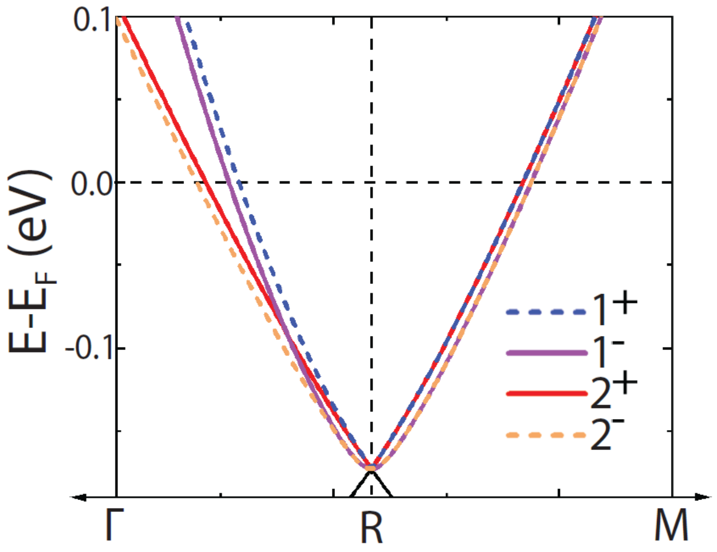


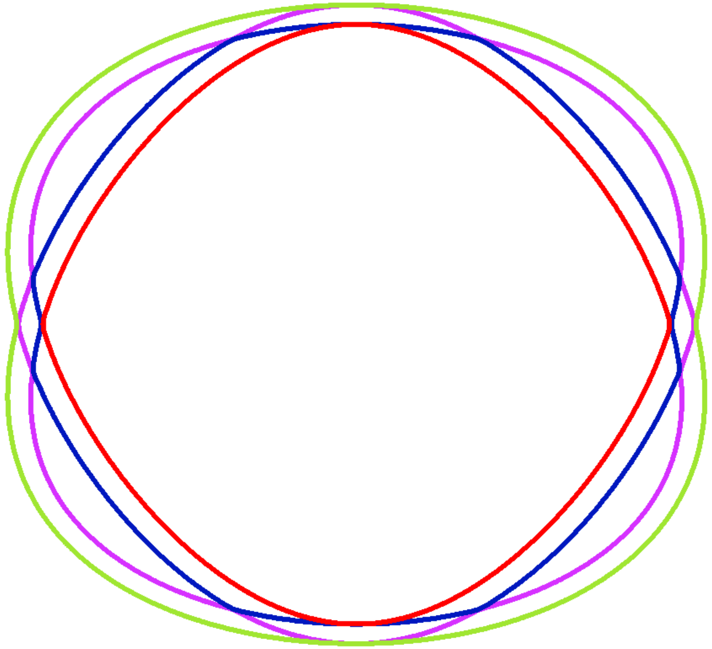

Two angle-independent oscillation frequencies?

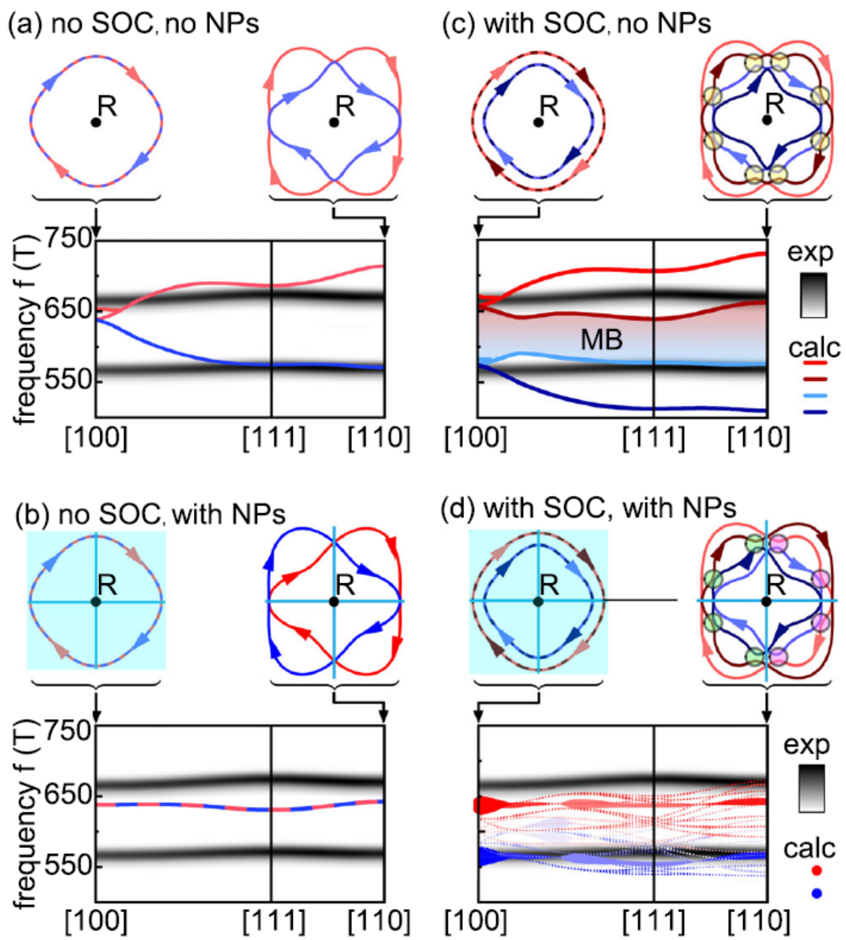
Many before us: D. Wu et al., CPL 36, 077102 (2019); X. Xu et al., PRB 100, 045104 (2019); H. Wang et al., PRB 102, 115129 (2020);…

# Why are the QO so simple?



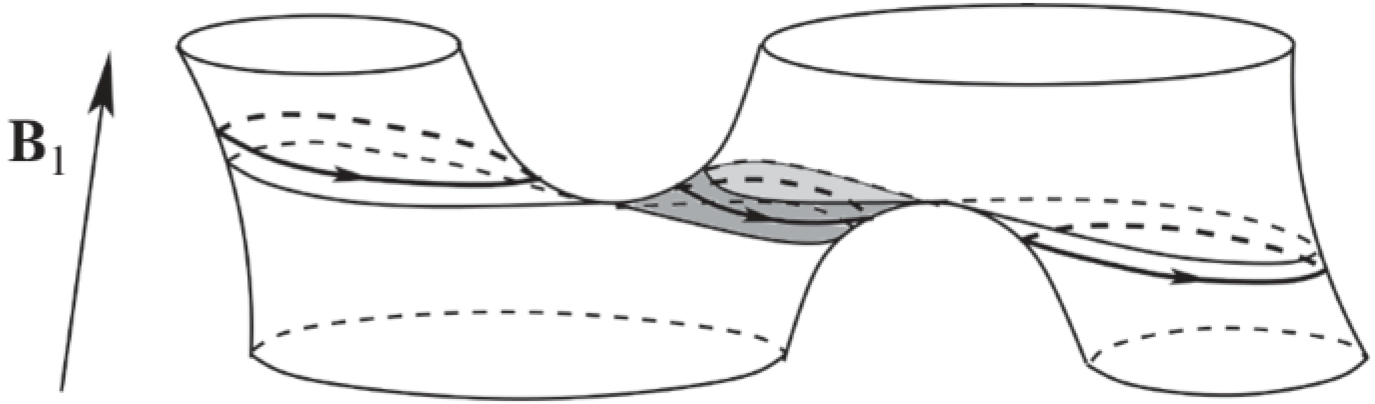

Predicted orbits for B//[110]






N. Huber et al., PRL 129, 026401 (2022)

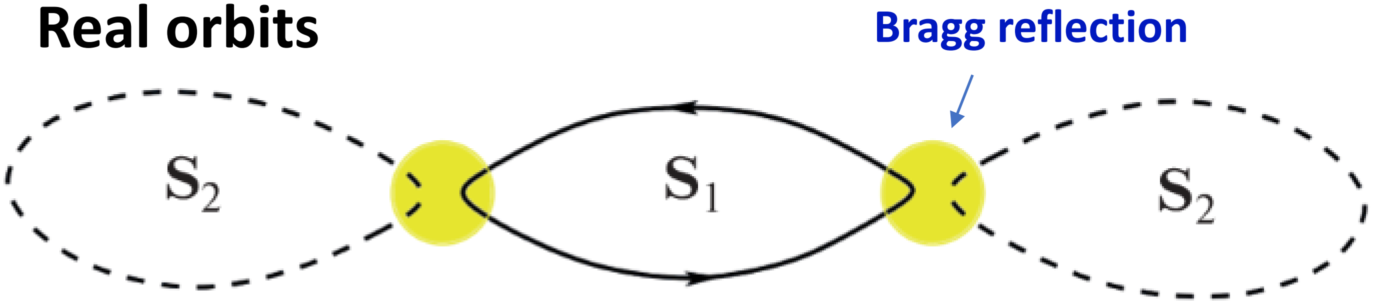
# Magnetic breakdown



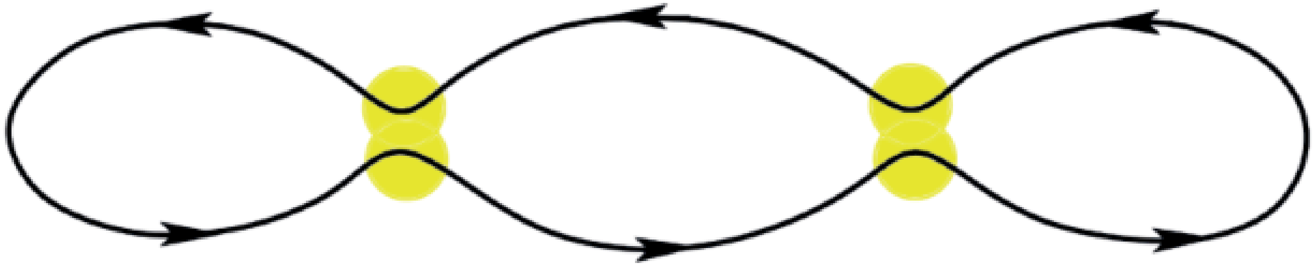

Compare energy with barrier height

$$\hbar\omega_c = \frac{eB}{m_{eff}} \sim \Delta E$$

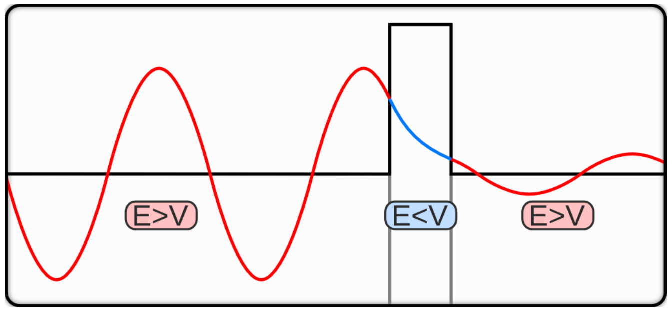
**Real orbits**




**Breakdown orbits**

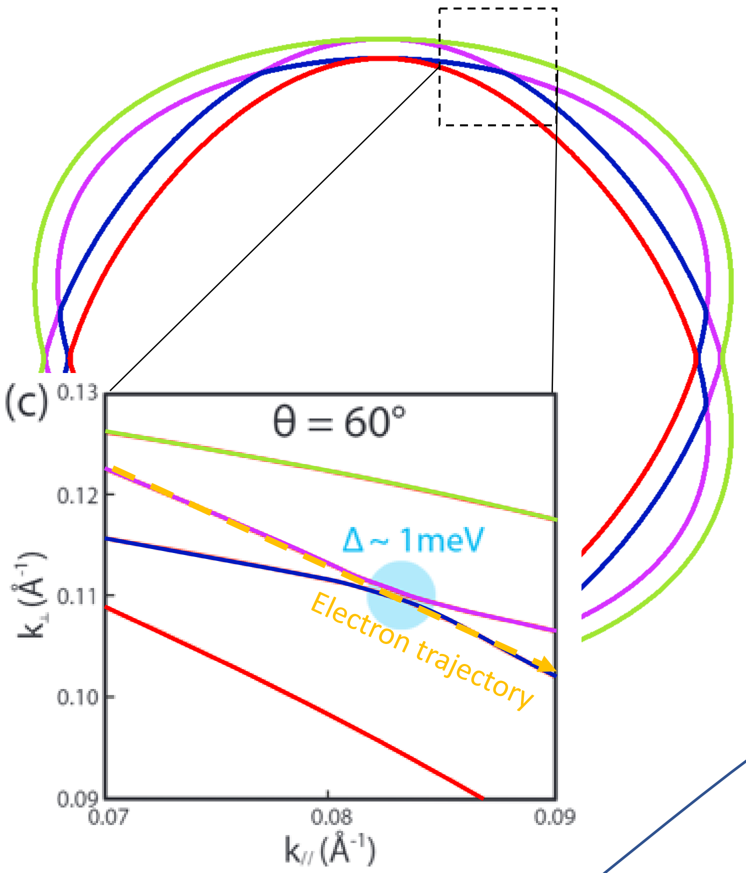


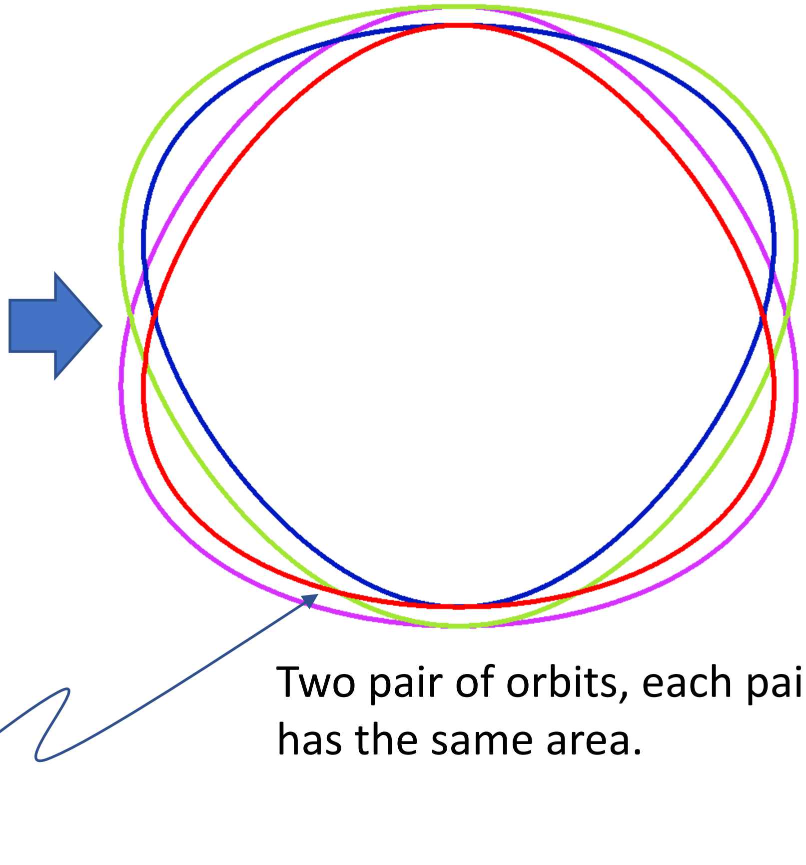
**Tunneling physics**



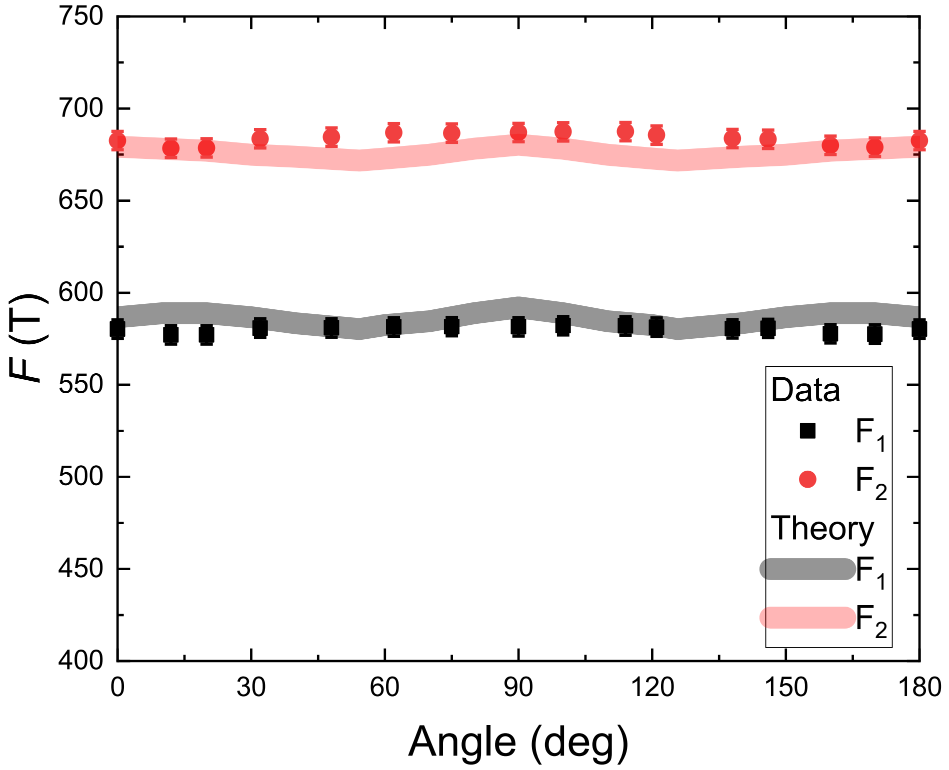
# Hidden in plain sight

Predicted orbits for B//[110]



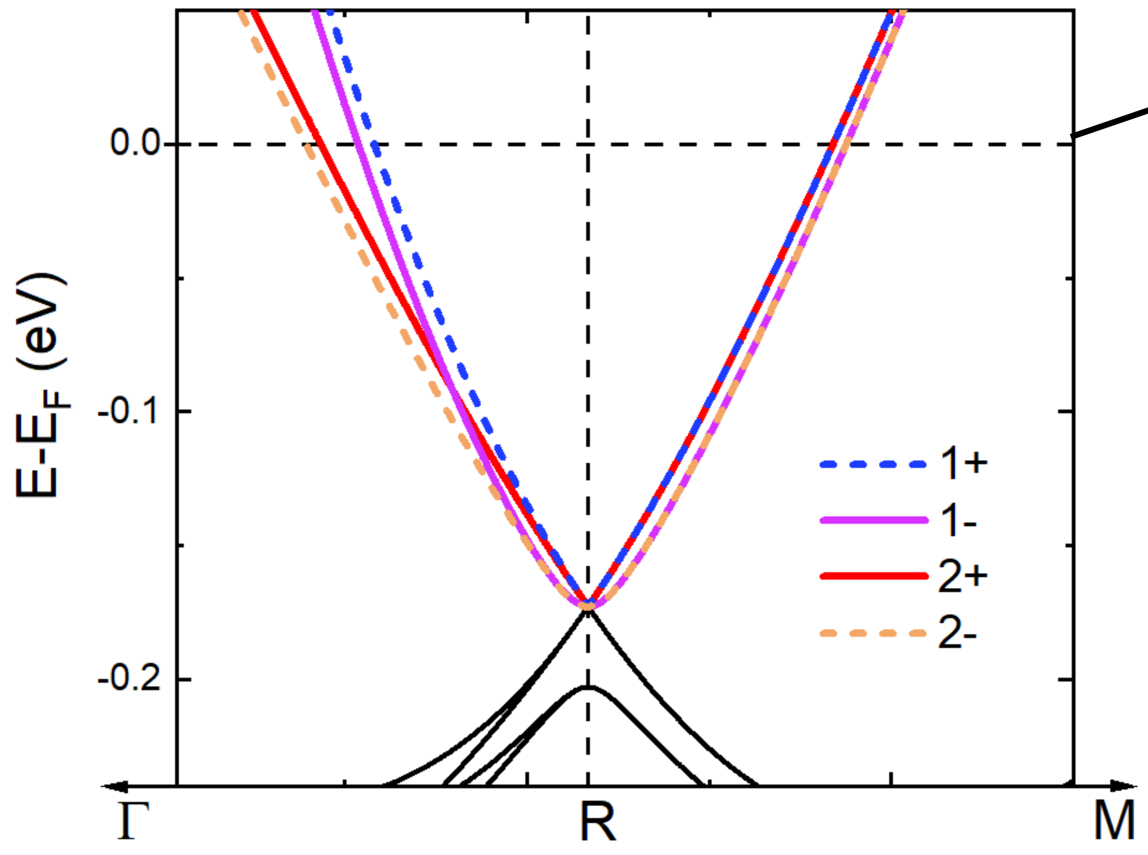



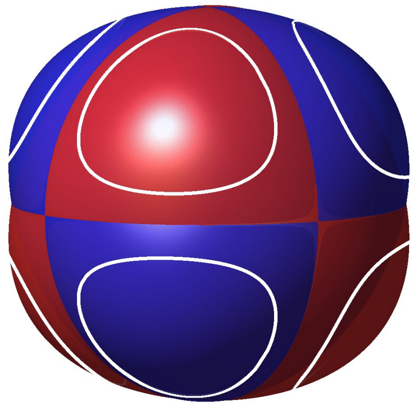
Two pair of orbits, each pair has the same area.




**Why are there tiny gaps all over the place at low-symmetry k-points?**

# Map all crossings at the FS

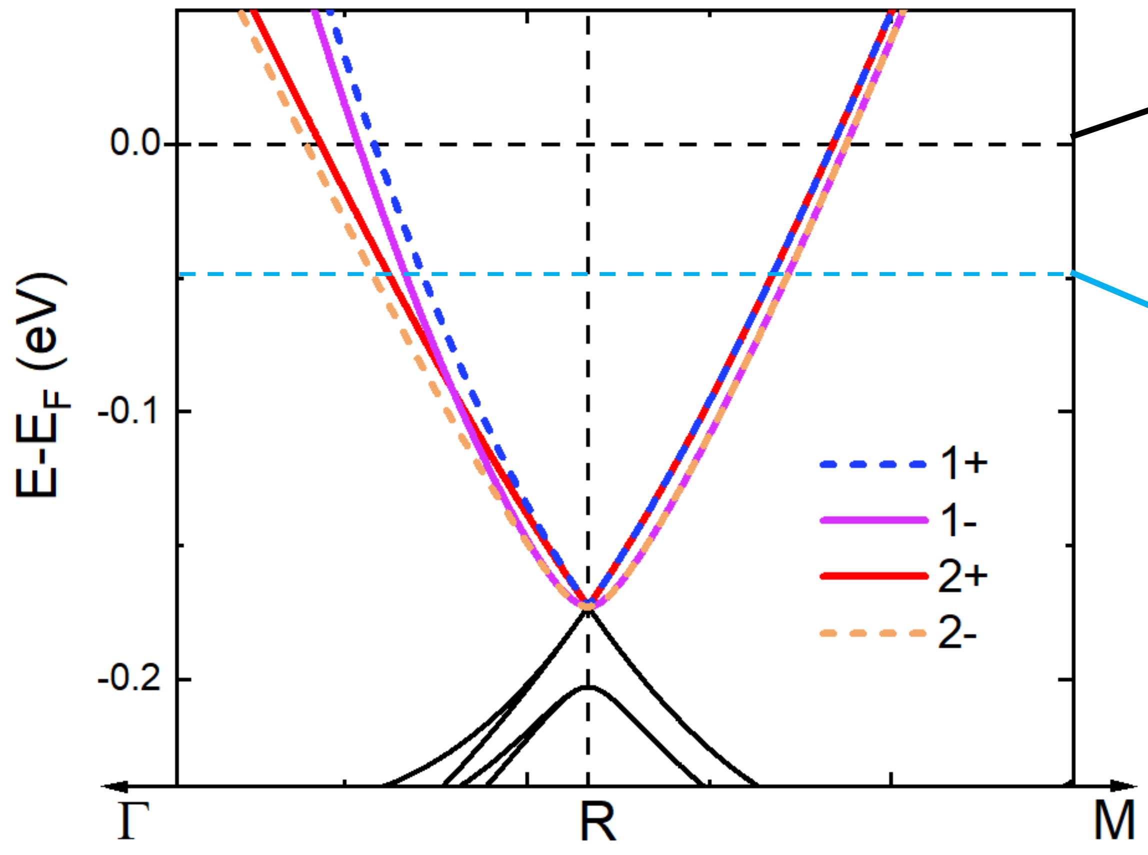


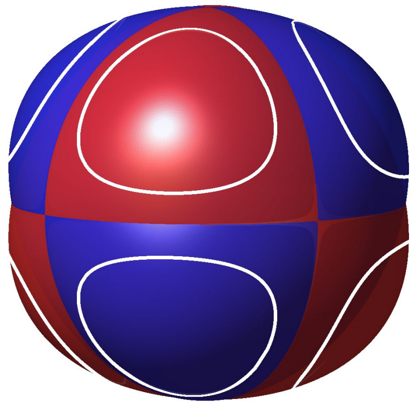



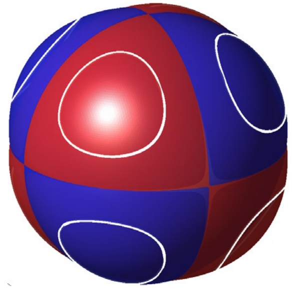
Near-degeneracies fall on
low-symmetry rings on Fermi surface.

# Map all crossings at the FS

Shift chemical potential

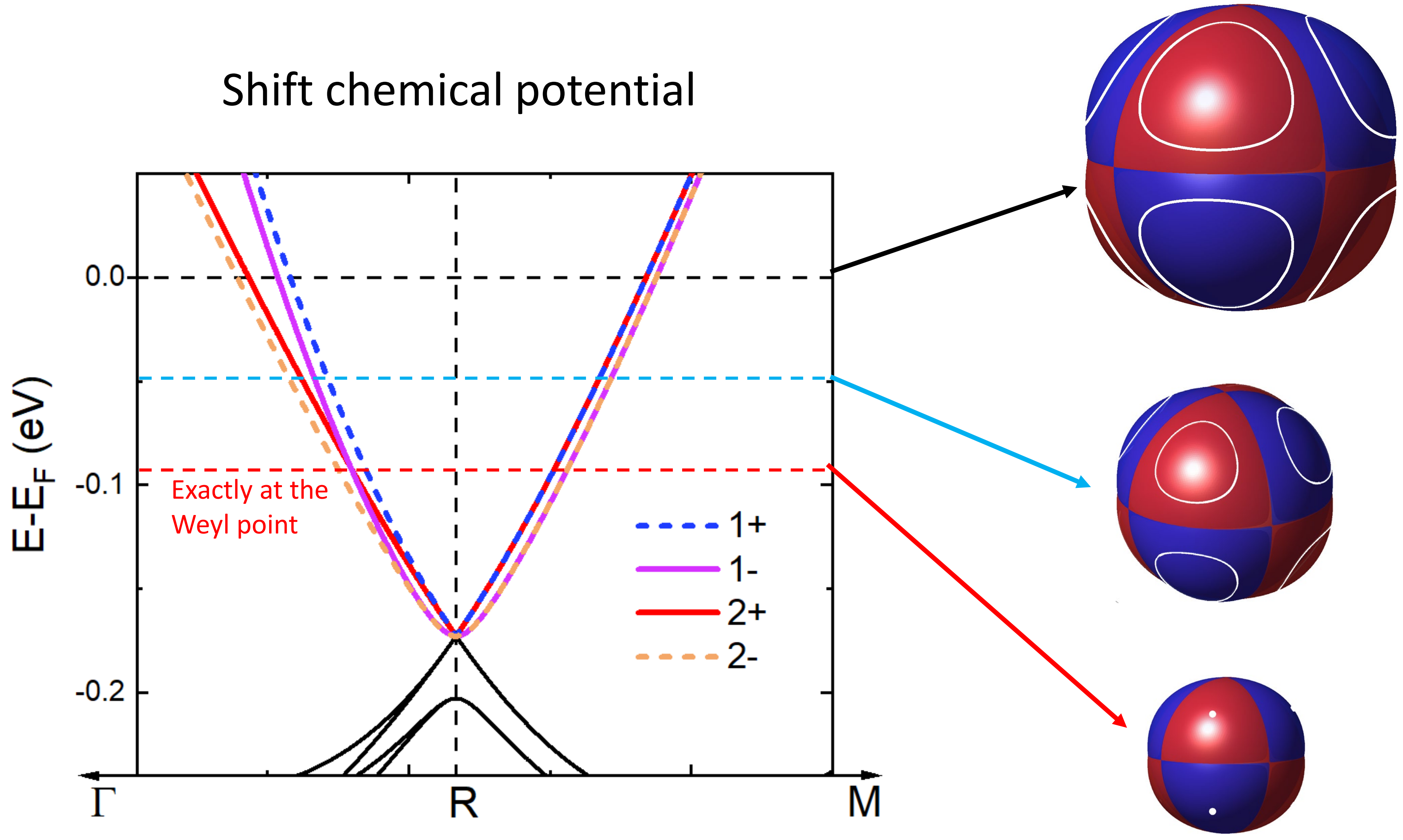




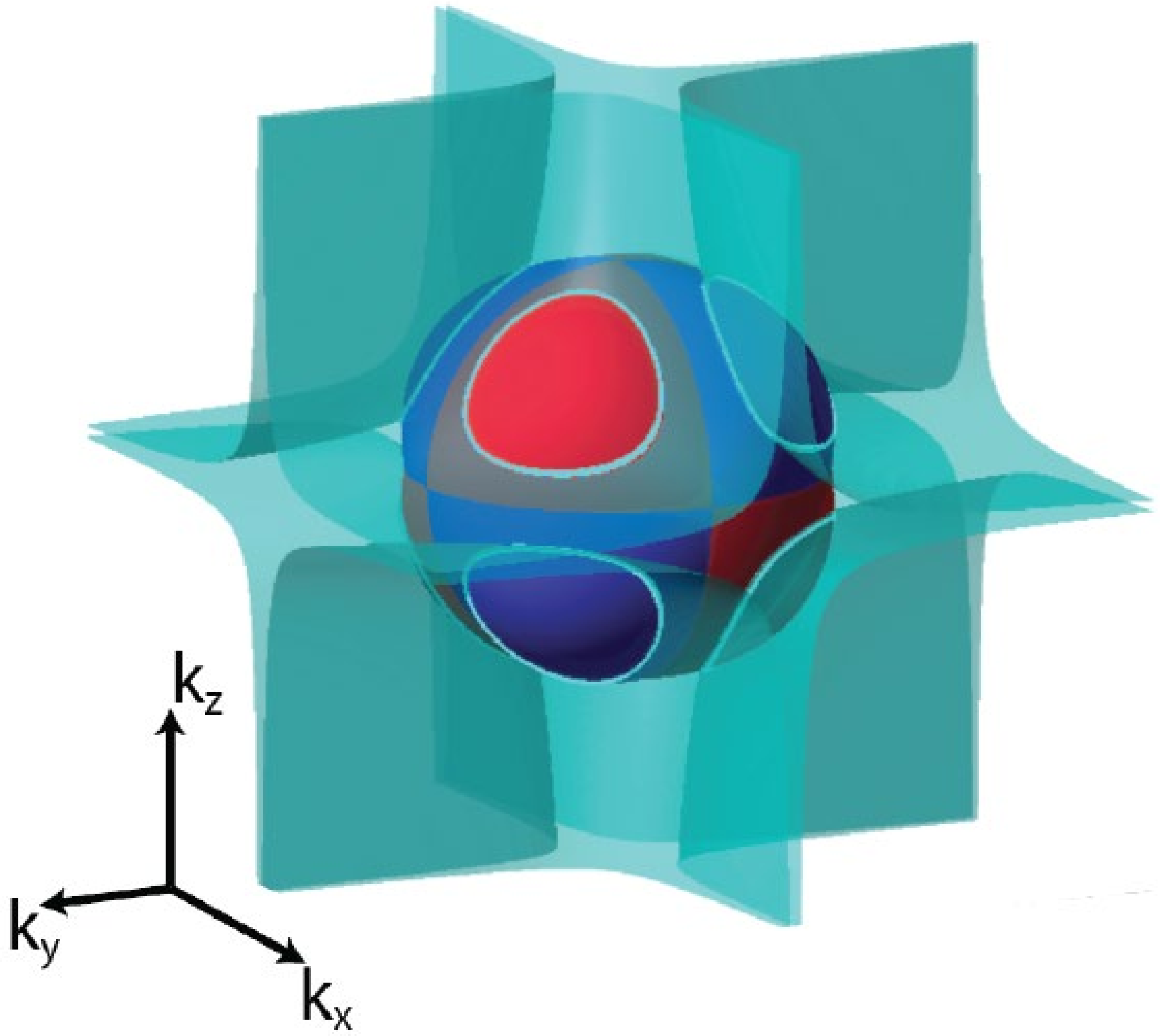
# Map all crossings at the FS

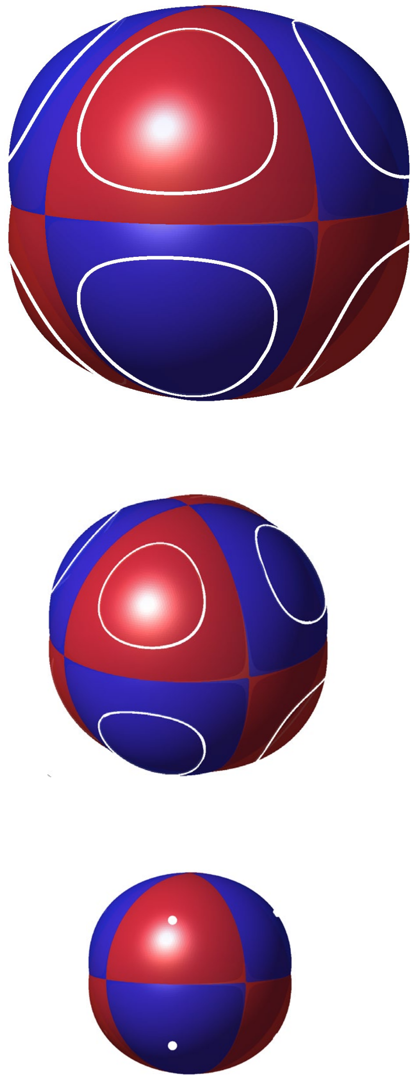
Shift chemical potential




Now we can construct the whole plane in the Brillouin zone!

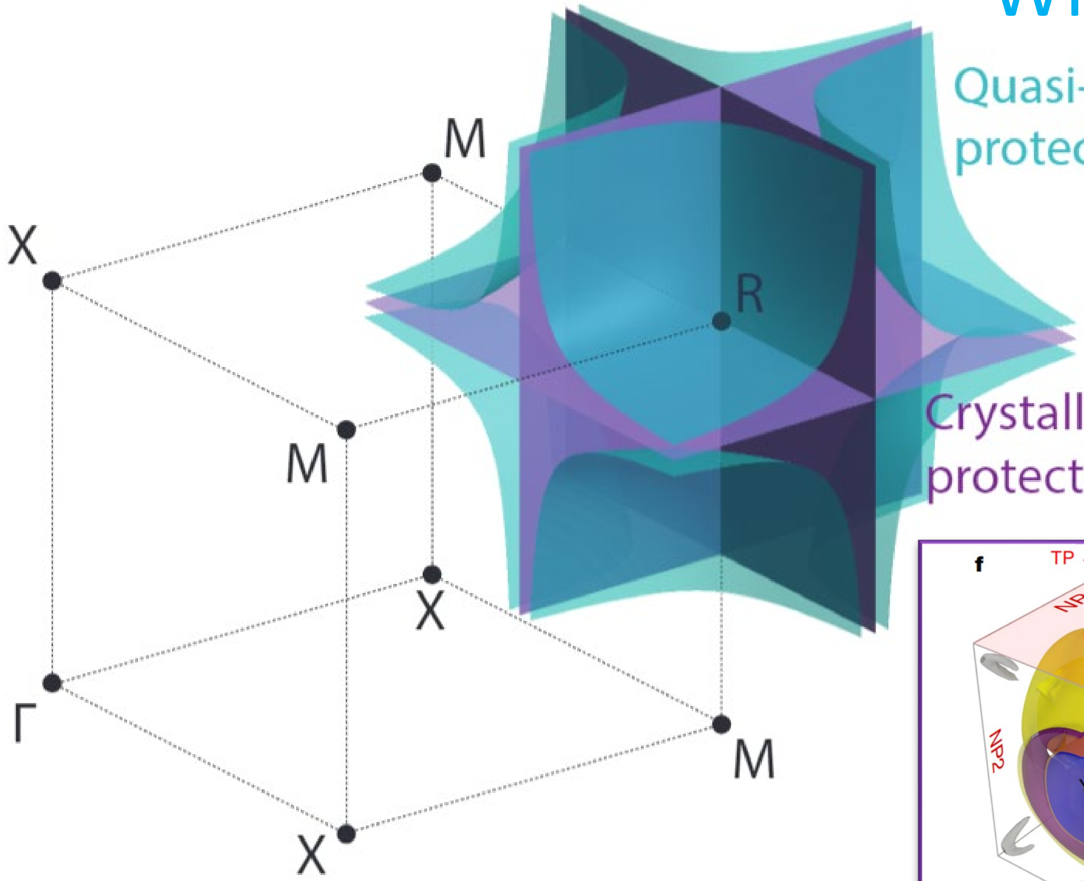
# Map all crossings at the FS



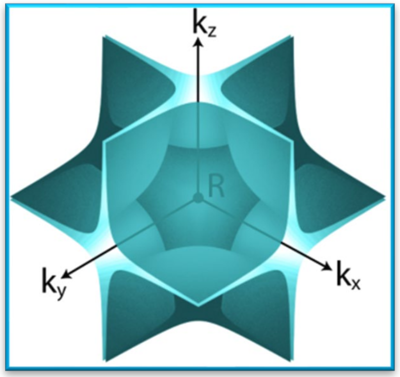



Now we can construct the whole plane in the Brillouin zone!

# Construction of 3D topological planes

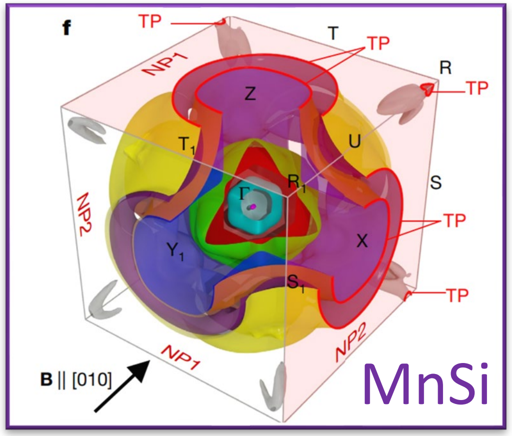



## What is a quasi-symmetry?




Planes of near-degeneracy at low-symmetry k-points that span the entire BZ.

C. Guo et al., Nat. Phys. 18, 813–818 (2022)

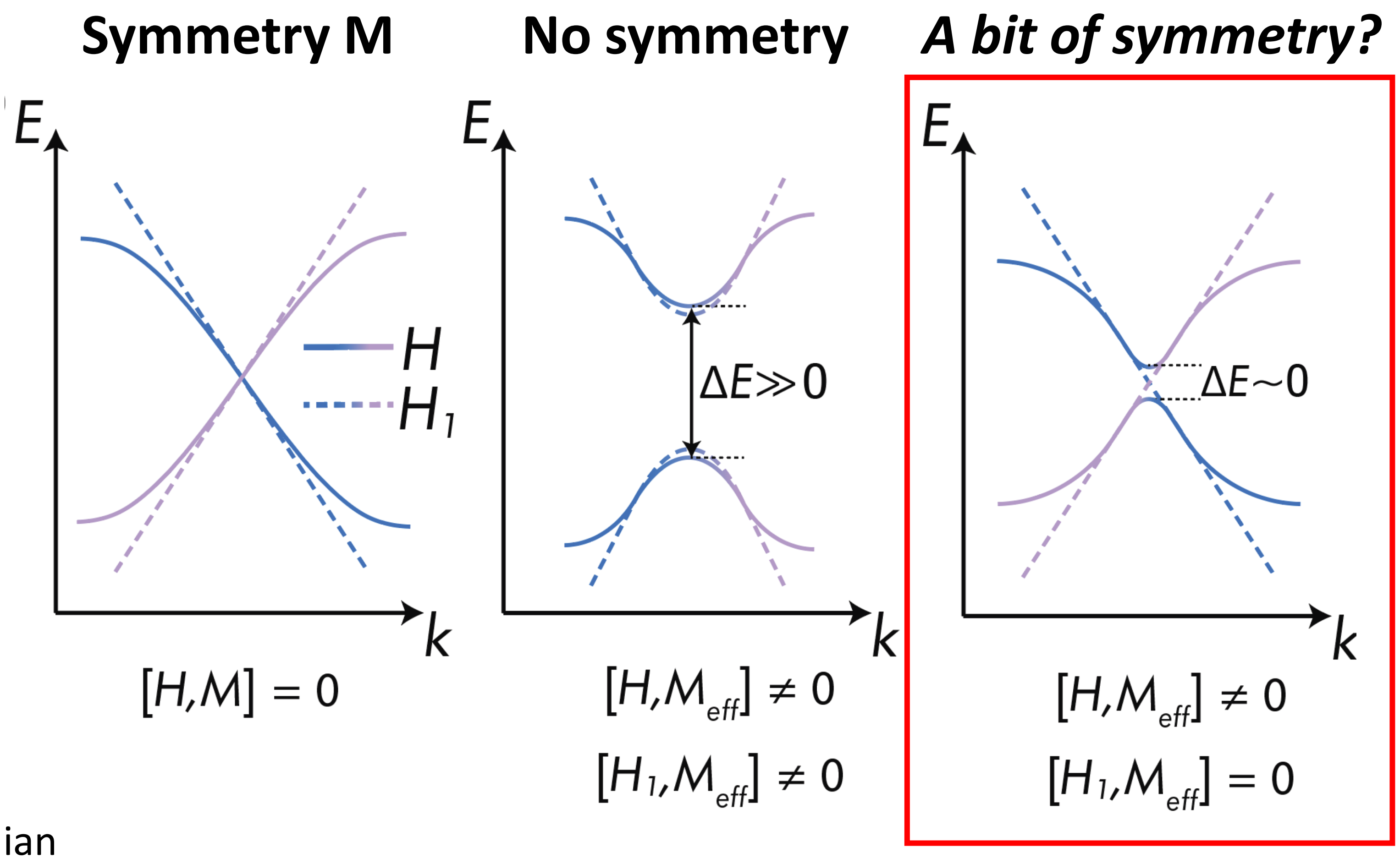



Marc A. Wilde et al., Nature 594,374 (2021)

# Outline

- Reminders: Approximate symmetries and hidden symmetries.
- The semi-metal CoSi is too simple
- What is a quasi-symmetry
- Growing classes of quasi-symmetric materials

# Quasi-symmetry



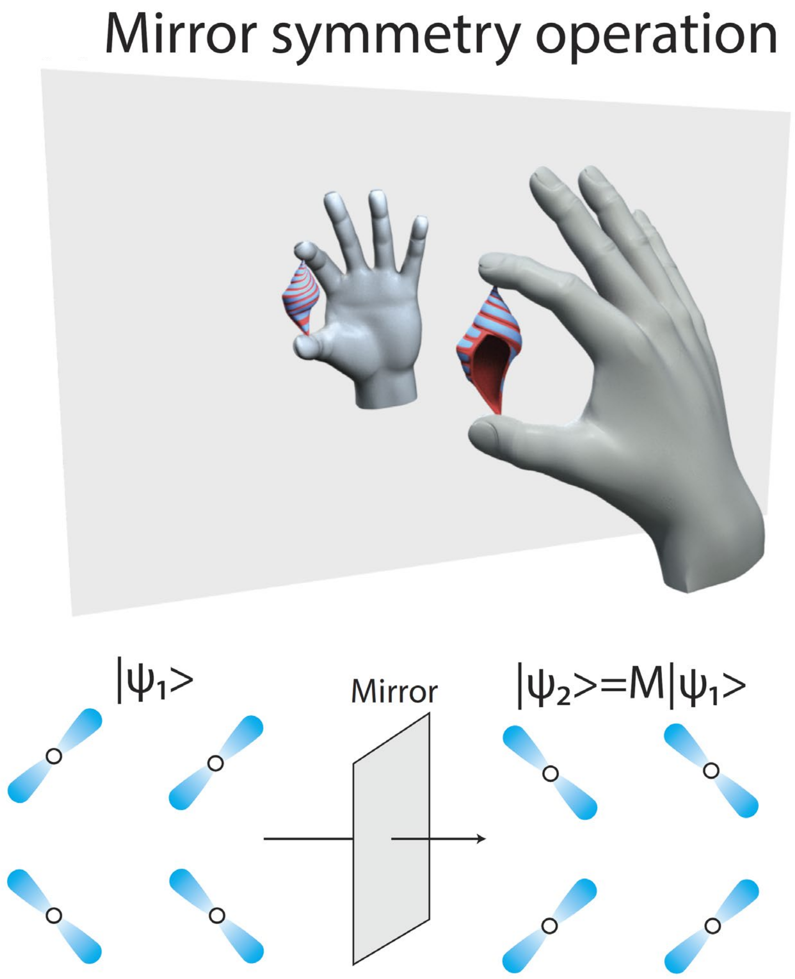

H: full Hamiltonian

$H_1$: dominant part

$H = H_1 + H_2 + \cdots$ (e.g. $k \cdot p$ expansion)

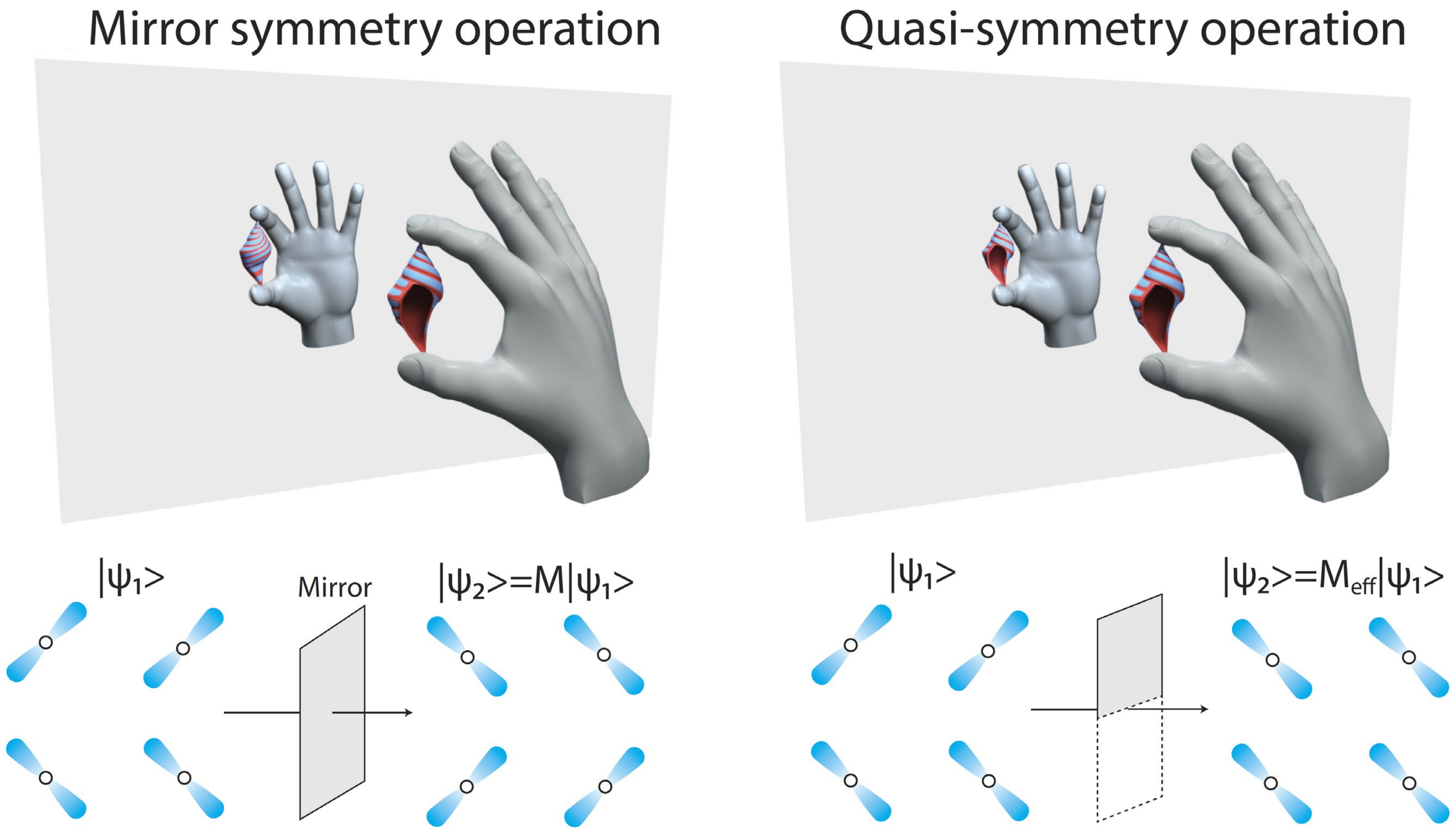
**Quasi-symmetry**: True symmetry of the first order term in a $k \cdot p$ expansion that is not a symmetry of the full Hamiltonian.

# Quasi-symmetry




Mirror symmetry operation: Universal operation on the whole system.

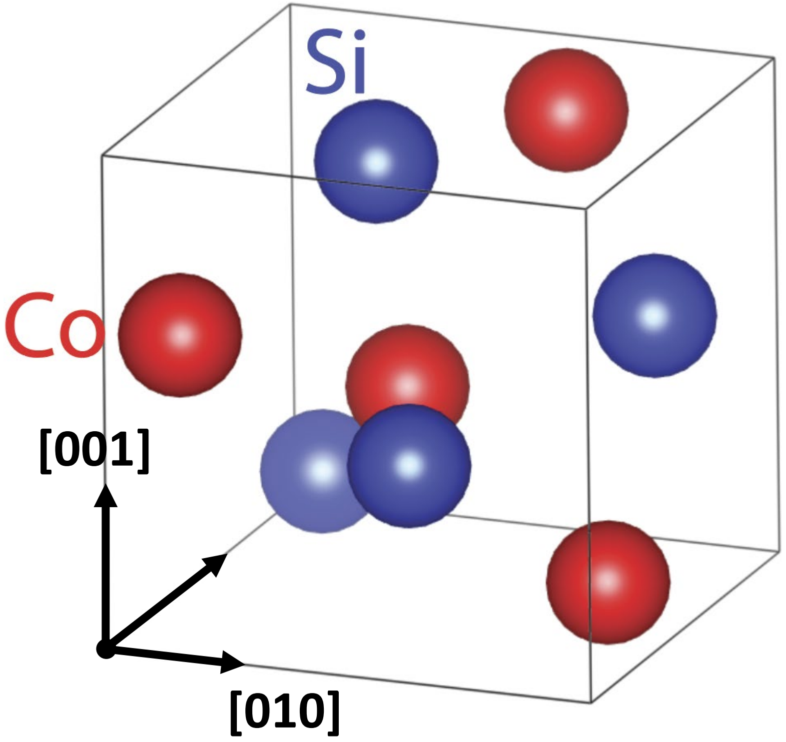
# Quasi-symmetry

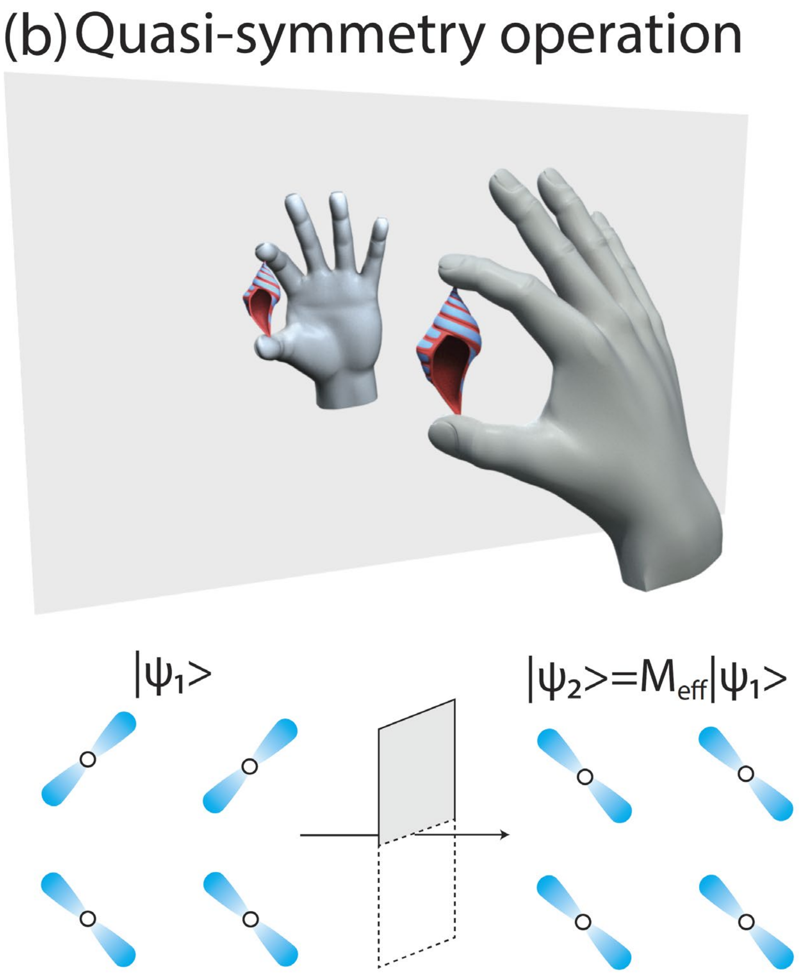



Quasi-symmetry operation: ***Local*** operation on ***part*** of the system.

Lun-Hui Hu, Chunyu Guo et al., PRB 107, 125145 (2023)

# Quasi-symmetry




Quasi-symmetry operation: ***Local*** operation on ***part*** of the system.

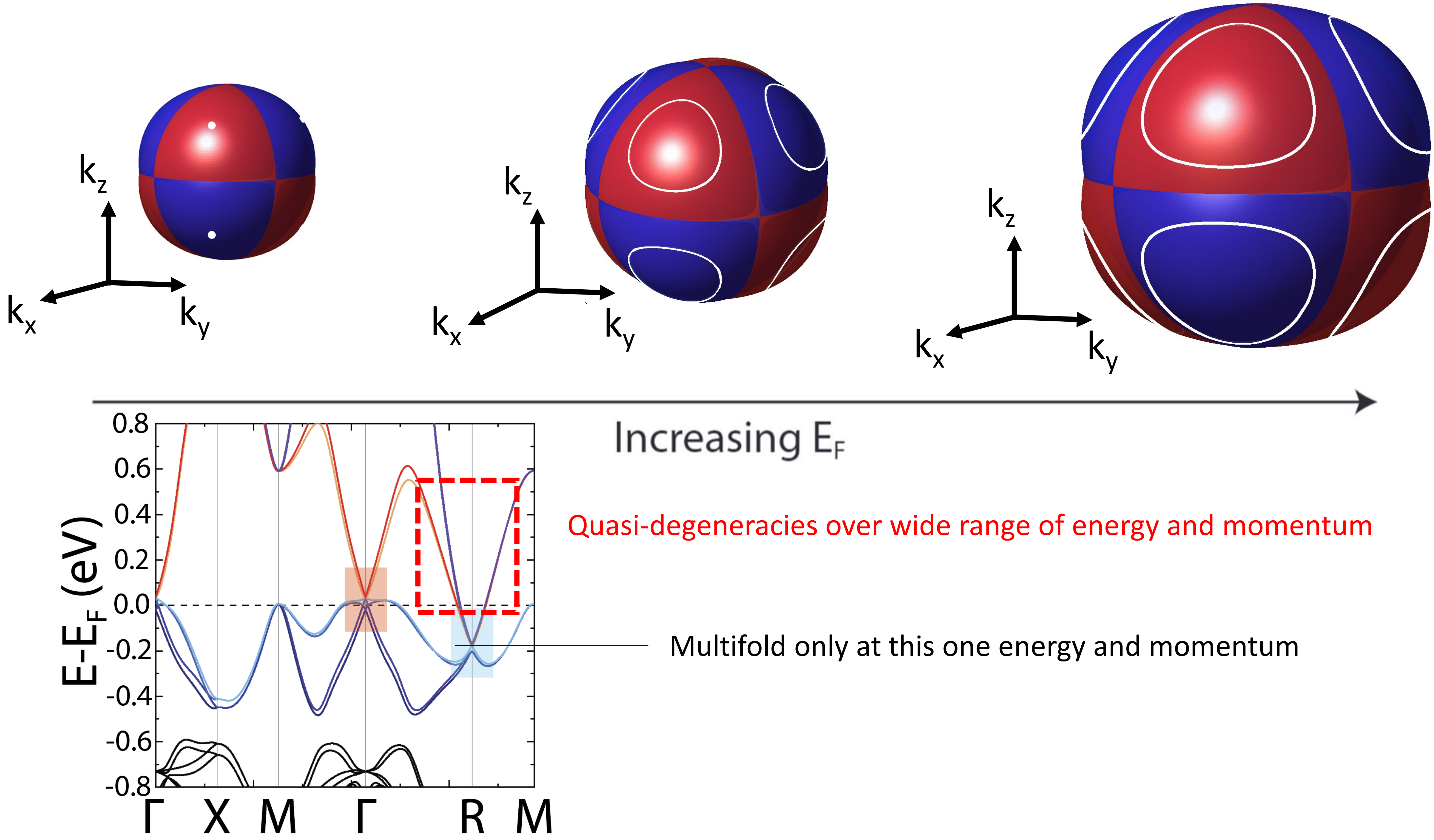
Lun-Hui Hu, Chunyu Guo et al., PRB 107, 125145 (2023)

# Breaking the chains of symmetry

Without the stringent symmetry requirements for real degeneracies, quasi-degeneracies can exist over wide ranges in energy and extended regions of k-space.

*Neumann-Wigner theorem: two level system crossing needs three tuning parameters.*

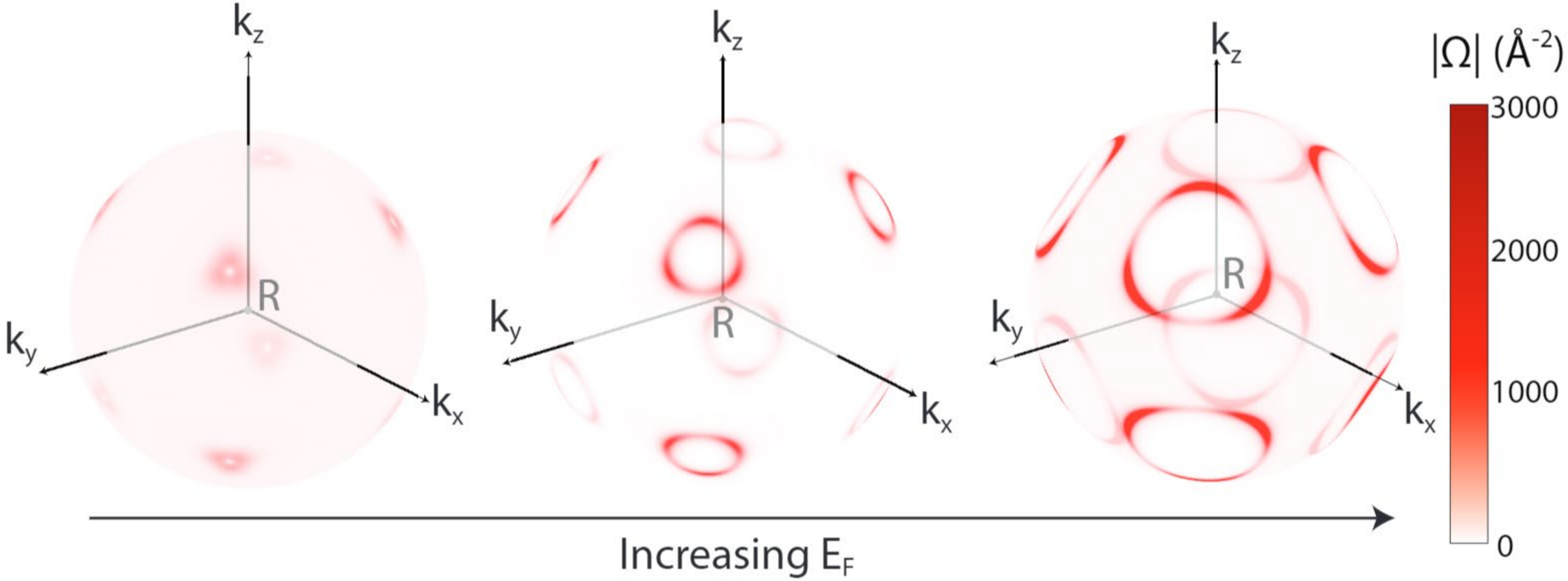
# Importance of quasi-symmetry: giant Berry curvature




Quasi-degeneracies over wide range of energy and momentum

Multifold only at this one energy and momentum

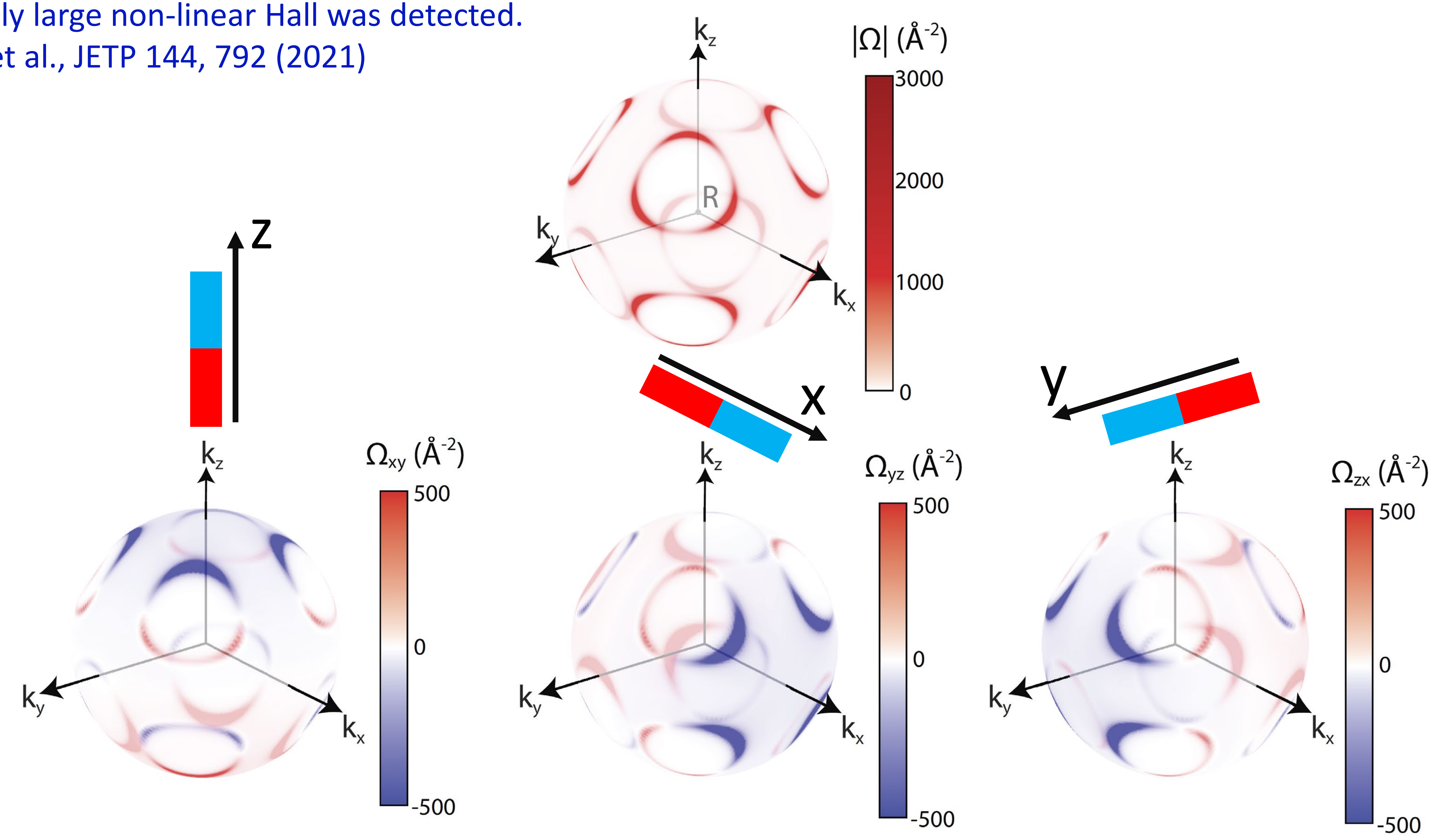
# Importance of quasi-symmetry: giant Berry curvature




***No chemical potential tunning required!***

# Importance of quasi-symmetry: giant Berry curvature *dipole*

Surprisingly large non-linear Hall was detected.
V.D. Esin et al., JETP 144, 792 (2021)



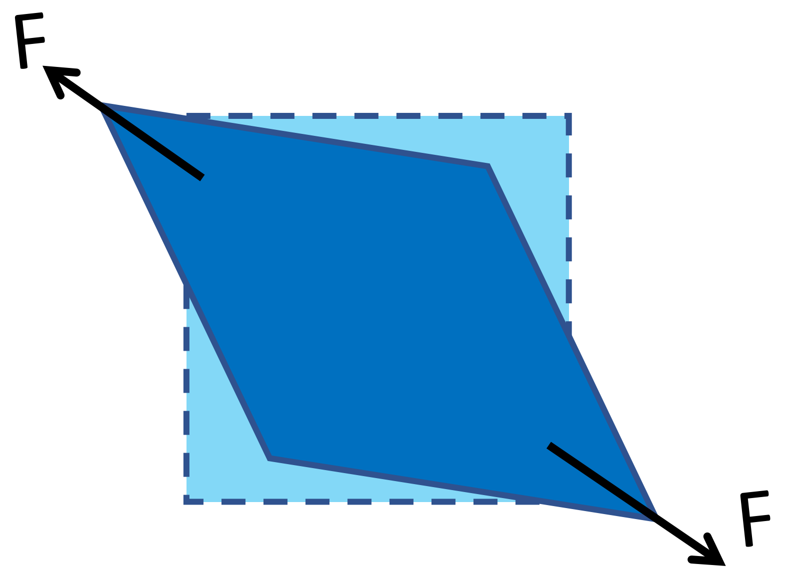

***chiral-distribution of Berry curvature dipole (non-linear Hall effect)***

# Importance of quasi-symmetry: Robust against perturbations

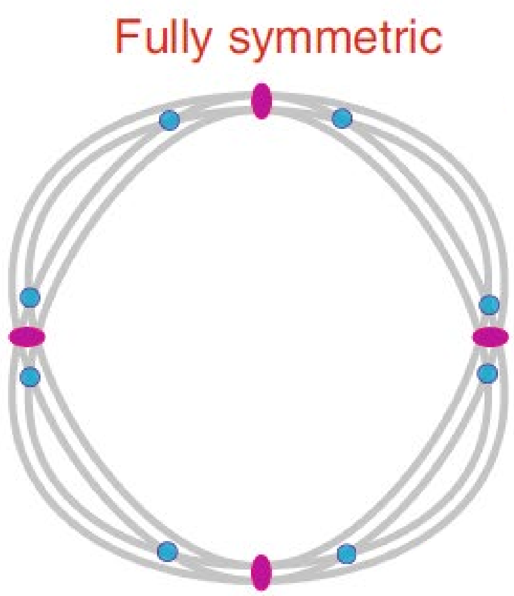
Space group 198

Symmetry operation: $C_{3,111}$ , $C_{2x,2y,2z}$ , $\sigma_d$

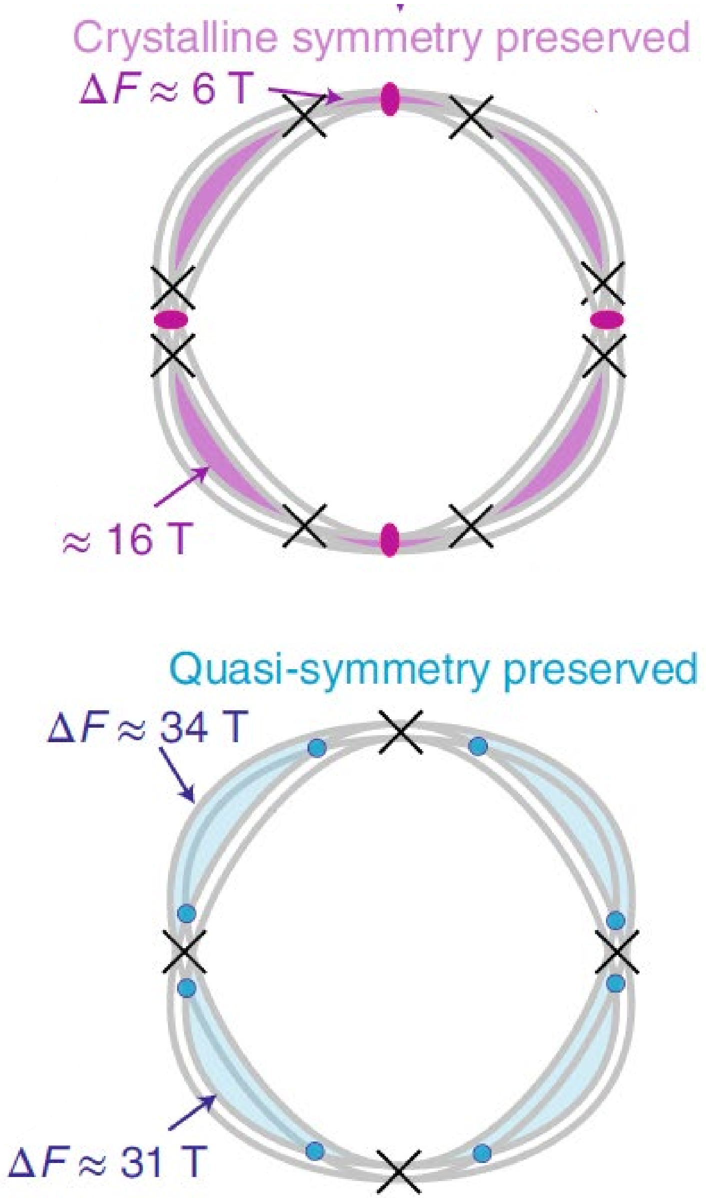
Tensile strain along [11δ]



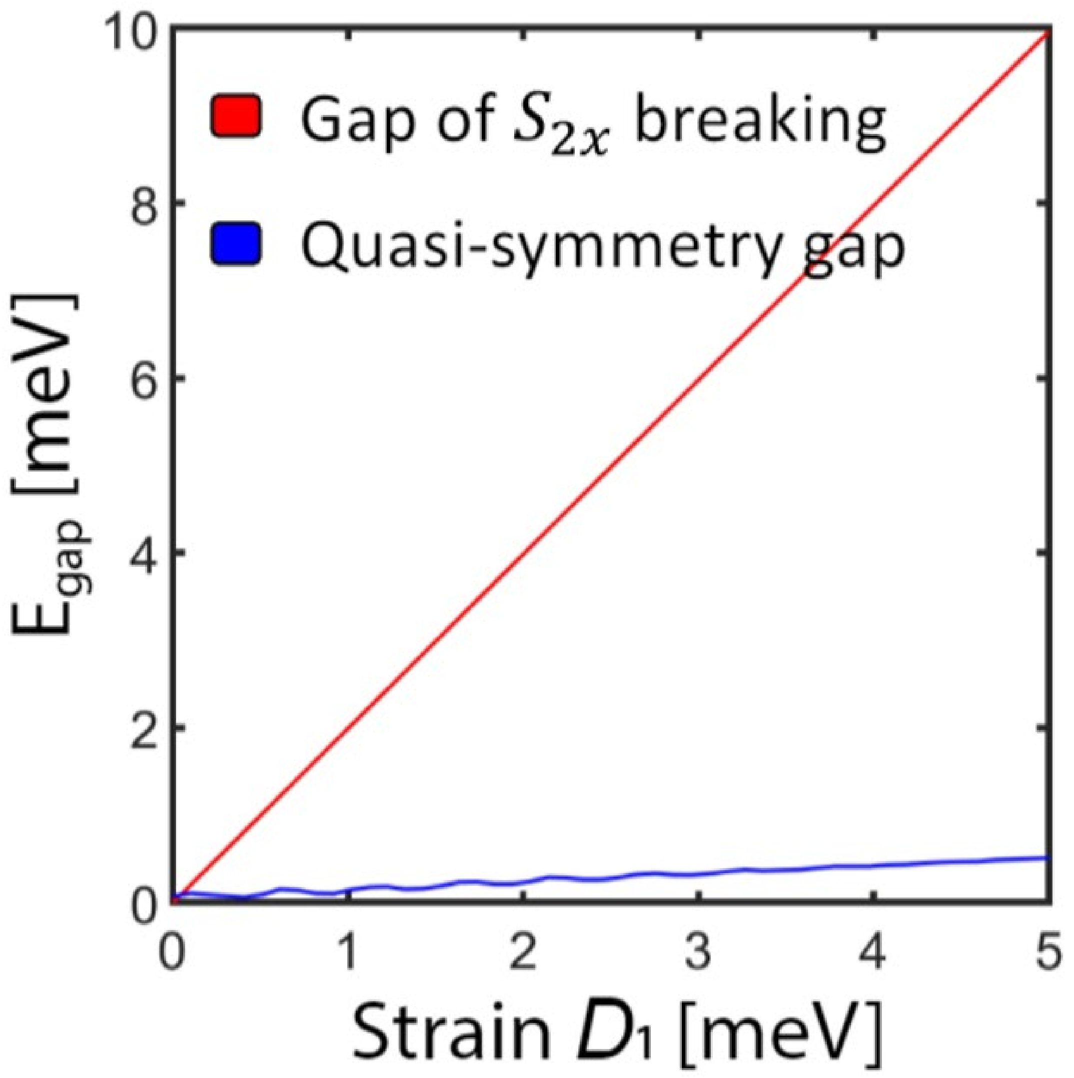

Symmetry-breaking: $C_{3,111}$ $C_{2x,y,z}$

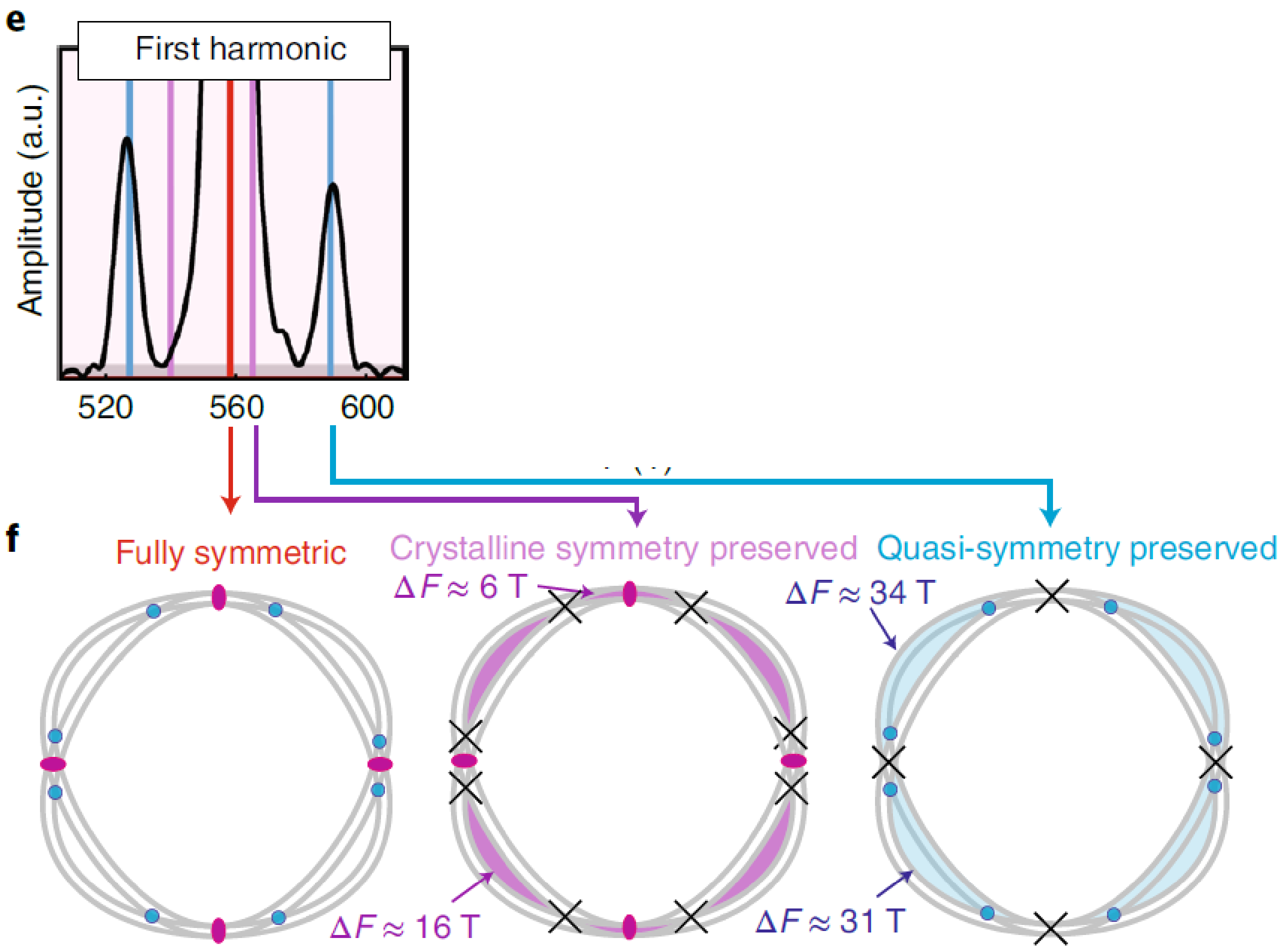



**Expected breakdown orbits**



# Quasi-symmetry robust against perturbations



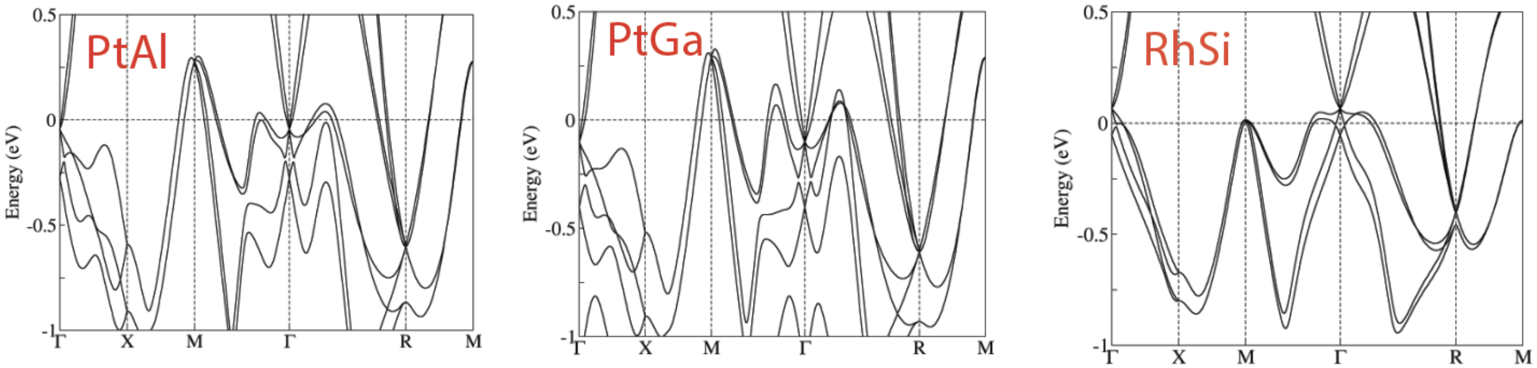



# Outline

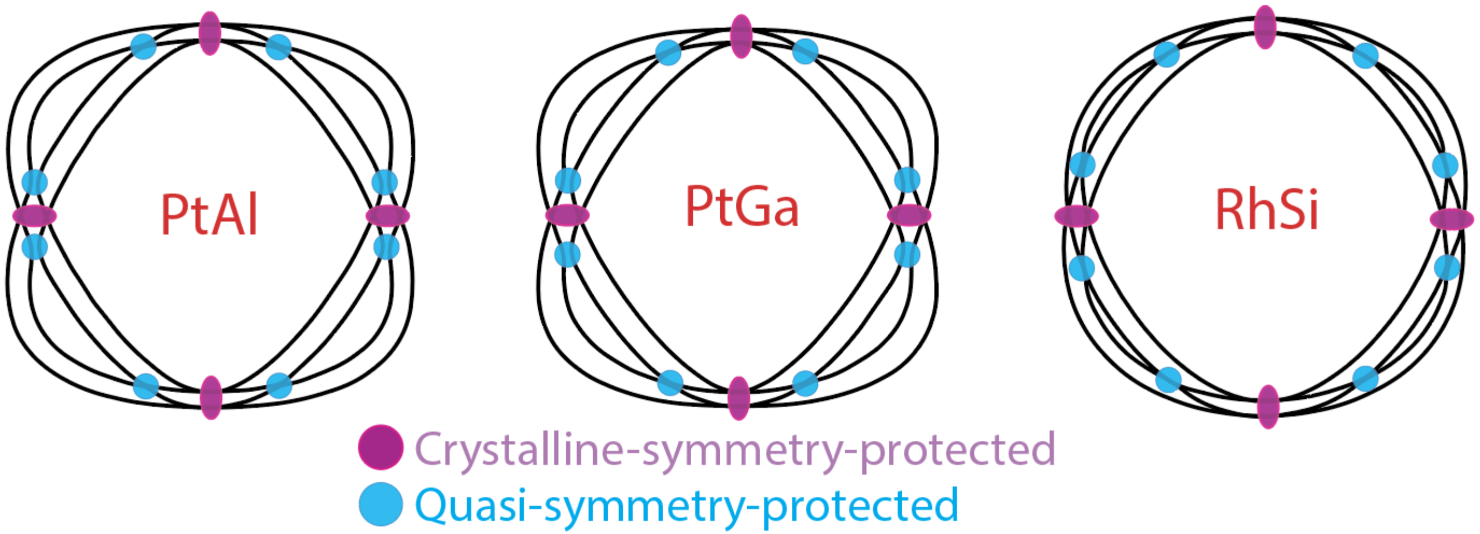
- Reminders: Approximate symmetries and hidden symmetries.
- The semi-metal CoSi is too simple
- What is a quasi-symmetry
- Growing classes of quasi-symmetric materials

# Generality of quasi-symmetry

Band structure




Orbit along [110]




***Natural extension to other 11-compounds with the same crystalline structure.***

| Model/SG | *kp* model | Nodal plane | Material |
| --- | --- | --- | --- |
| I<br>19 R R1#R1 | $\mathcal{H}_1 = A_1 k_x \sigma_3\tau_3 + A_2 k_y \sigma_3\tau_1 + A_3 k_z \sigma_0\tau_2,$<br>$\mathcal{H}_2 = B_1 k_x^2 + B_2 k_y^2 + B_3 k_z^2 + k_x k_y(B_4\sigma_3\tau_2 + B_5\sigma_2\tau_0 + B_6\sigma_1\tau_0)$<br>$+ k_x k_z(B_7\sigma_2\tau_3 + B_8\sigma_0\tau_1 + B_9\sigma_1\tau_3) + k_y k_z(B_{10}\sigma_2\tau_1 + B_{11}\sigma_0\tau_3 + B_{12}\sigma_1\tau_1),$<br>$\mathcal{H}_{\rm soc} = \lambda_1 s_x \sigma_3\tau_3 + \lambda_2 s_y \sigma_3\tau_1 + \lambda_3 s_z \sigma_0\tau_2.$ | $(A_1\lambda_1 k_x)^2 + (A_2\lambda_2 k_y)^2 + (A_3\lambda_3 k_z)^2 = (C_1^2 + C_2^2 + C_3^2)k_x^2 k_y^2 k_z^2.$<br>$C_1 = -A_1B_{12} + A_2B_9 + A_3B_5,\ C_2 = A_1B_{10} - A_2B_7 + A_3B_6$<br>$C_3 = A_1B_{11} + A_2B_8 + A_3B_4.$ | **P7Th**, **GeMn**, **O32P4W8**, **CuErS2**, **CuS2Yb**, **La3MoO7**, **AgErSe2**, **AgSe2Yb**, **Ce2Ga3Ru2**, **C14FeNa**, **H5CuIO7**, **H5CuO5P**, **O8P2Rb2V**, **CuLiO9P3**, **CuNaO4P**, **MoNaO8P2**, **BiFeO9Se3**, **CuO5TiZr**, **BaClCuO4P** |
| II<br>92 A A1#A2<br>96 A A1#A2 | $\mathcal{H}_1 = A_1(k_x\sigma_0\tau_2 - k_y\sigma_3\tau_1) + A_2 k_z \sigma_3\tau_3,$<br>$\mathcal{H}_2 = B_1(k_x^2 + k_y^2) + B_2 k_z^2 + (k_x^2 - k_y^2)(B_3\sigma_2\tau_1 + B_4\sigma_1\tau_1)$<br>$+ k_x k_z(B_5\sigma_0\tau_1 + B_6\sigma_1\tau_0 + B_7\sigma_2\tau_0) + k_y k_z(B_5\sigma_3\tau_2 - B_6\sigma_2\tau_3 + B_7\sigma_1\tau_3).$<br>$\mathcal{H}_{\rm soc} = \lambda_1(s_x\sigma_0\tau_2 - s_y\sigma_3\tau_1) + \lambda_2 s_z\sigma_3\tau_3.$ | $(A_1\lambda_1)^2(k_x^2 + k_y^2) + (A_2\lambda_2)^2 k_z^2 = (C_1^2 + C_2^2)k_x^2 k_y^2 k_z^2$<br>$C_1 = A_1B_6 + A_2B_3$ and $C_2 = -A_1B_7 + A_2B_4$ | **MnO8PbS2**, **Si4V5**, **Ce5Si4**, **La5Si4**, **Mn5Si2**, **Nb5Si4**, **Rh5Si2**, **Si4Ta5**, **Si4Ti5**, **FeK3O2**, **K3NiO2**, **FeNaO2**, **NiO2Rb3**, **Sc2Si4V3**, **Cr3Sc2Si4**, **Re3Sc2Si4**, |
| III<br>198 R R1#R3 | $\mathcal{H}_1 = A_1(k_x\sigma_3\tau_1 - k_y\sigma_0\tau_2 - k_z\sigma_3\tau_3),$<br>$\mathcal{H}_2 = B_1(k_x^2 + k_y^2 + k_z^2) + k_x k_y(-2B_2\sigma_2\tau_1 - B_3\sigma_0\tau_3 + 2B_4\sigma_1\tau_1)$<br>$+ k_x k_z\left[B_2(\sigma_1\tau_0 - \sqrt{3}\sigma_2\tau_0) - B_3\sigma_3\tau_2 + B_4(\sqrt{3}\sigma_1\tau_0 + \sigma_2\tau_0)\right]$<br>$+ k_y k_z\left[B_2(-\sqrt{3}\sigma_1\tau_3 + \sigma_2\tau_3) + B_3\sigma_0\tau_1 + B_4(-\sigma_1\tau_3 - \sqrt{3}\sigma_2\tau_3)\right]$<br>$\mathcal{H}_{\rm soc} = \lambda_1(s_x\sigma_3\tau_1 - s_y\sigma_0\tau_2 - s_z\sigma_3\tau_3).$ | $\lambda_1^2(k_x^2 + k_y^2 + k_z^2) = B_3^2 k_x^2 k_y^2 k_z^2$ | F2Pd, **FeP**, **AlAu4**, AlCu4, AlPd, AlPt, **Al7Sr8**, AuBe, **CoGe**, **CoSi**, GaPd, GaPt, **GeMn**, GeRh, HfSn, **MnSi**, NiSi, ReSi, RhSi, RhSn, SiTc, **NiPS**, **AsNiS**, AsPdS, **BaPPt**, **ClNaO3**, **NiSSb**, **PdSSb**, PtSSb, AlAuBa, **AsNiSe**, AsPdSe, AuBaGa, BaGePt, BaPdSi, BaPtSi, BiNiSe, BiPdSe, BiPdTe, BiPtSe, **BiPtTe**, FePtSb, IrLaSi, IrNdSi, **LaRhSi**, **NiSbSe**, **PdSbSe**, **PdSbTe**, PdSiSr, PtSbSe, **C3H3LiMnO6**, |
| IV<br>198 R R2#R2 | $\mathcal{H}_1 = A_1(k_x\sigma_3\tau_1 - k_y\sigma_0\tau_2 - k_z\sigma_3\tau_3),$<br>$\mathcal{H}_2 = B_1(k_x^2 + k_y^2 + k_z^2) + k_x k_y(B_2\sigma_2\tau_1 + B_3\sigma_0\tau_3 + B_4\sigma_1\tau_1)$<br>$+ k_x k_z(B_2\sigma_1\tau_0 + B_3\sigma_3\tau_2 - B_4\sigma_2\tau_0) + k_y k_z(B_2\sigma_2\tau_3 - B_3\sigma_0\tau_1 + B_4\sigma_1\tau_3).$<br>$\mathcal{H}_{\rm soc} = \lambda_1(s_x\sigma_3\tau_1 - s_y\sigma_0\tau_2 - s_z\sigma_3\tau_3).$ | $\lambda_1^2(k_x^2 + k_y^2 + k_z^2) = 9(B_2^2 + B_3^2 + B_4^2)k_x^2 k_y^2 k_z^2.$ | **SiV**, **Al2Sr3**, **Ba8Ga7**, **CrGe**, **CrSi**, **Ga7Sr8**, HfSb, SbZr, SiTa, **AuGaV3**, BaIrP, **Cu2O4Se**, EuIrP, IrPSr, **AsBaPt**, AuGaNb3, AuGaTa3, CaPtSi, **CeIrSi**, CrPtSb, EuGePt, **EuPdSi**, **EuPtSi**, GePtSr, PtSiSr, |
| V<br>212 R R1#R2<br>213 R R1#R2 | $\mathcal{H}_1 = A_1(k_x\sigma_3\tau_1 - k_y\sigma_0\tau_2 - k_z\sigma_3\tau_3),$<br>$\mathcal{H}_2 = B_1(k_x^2 + k_y^2 + k_z^2) + k_x k_y(B_2\sigma_2\tau_1 + B_3\sigma_1\tau_1)$<br>$+ k_x k_z(B_2\sigma_1\tau_0 - B_3\sigma_2\tau_0) + k_y k_z(B_2\sigma_2\tau_3 + B_3\sigma_1\tau_3),$<br>$\mathcal{H}_{\rm soc} = \lambda_1(s_x\sigma_3\tau_1 - s_y\sigma_0\tau_2 - s_z\sigma_3\tau_3).$ | $\lambda_1^2(k_x^2 + k_y^2 + k_z^2) = 9(B_2^2 + B_3^2)k_x^2 k_y^2 k_z^2$ | **Mo3NPd2**, CAl2Ta3, CAl2Nb3, **Al2NNb3**, Ag3AuS2, **Ga2NV3**, **C7V8**, **C5Zr8**, |
| VI<br>212 R R3<br>213 R R3 | $\mathcal{H}_1 = A_1(k_x\sigma_0\tau_1 - k_y\sigma_3\tau_2 - k_z\sigma_3\tau_3),$<br>$\mathcal{H}_2 = B_1(k_x^2 + k_y^2 + k_z^2) + B_2(k_x k_y\sigma_0\tau_3 + k_x k_z\sigma_0\tau_2 - k_y k_z\sigma_3\tau_1)$<br>$+ B_3\left[2k_x k_y\sigma_1\tau_2 + k_x k_z(\sqrt{3}\sigma_2\tau_3 + \sigma_1\tau_3) + k_y k_z(\sqrt{3}\sigma_1\tau_0 + \sigma_2\tau_0)\right]$<br>$\mathcal{H}_{\rm soc} = \lambda_1(s_x\sigma_0\tau_1 - s_y\sigma_3\tau_2 - s_z\sigma_3\tau_3).$ | $\lambda_1^2(k_x^2 + k_y^2 + k_z^2) = 9B_2^2 k_x^2 k_y^2 k_z^2.$ | Mo3NPt2, **Mo3NNi2**, **Co2Mo3N**, **CMo3Re2**, CRe2W3, **Mn2Zn8**, Mg3Ru2, Fe2Re3, **Au2Nb3**, **Ga2V3**, **Mn**, **C2Na**, **BLi2Pd3**, BLi2Pt3, **Ge3Li2NiO8**, **Li2MgMn3O8**, |

# Generality of quasi-symmetry

Various promising candidates:

Chiral semimetals (SG 198):
**FeP**, AlCu4, AlPd, AlPt, AuBe, **CoGe**, **CoSi**, GaPd, GaPt, **GeMn**, GeRh, HfSn, **MnSi**, NiSi, ReSi, RhSi, RhSn, SiTc…

Kondo semimetals:
$YbCuS_2$, $YbAgSe_2$, $CeRu_2Ga_3$, CeIrSi, EuPtSi…

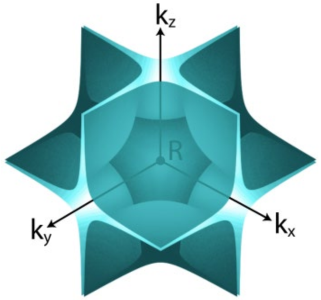
Superconductors:
$Li_2Pd_3B$, $Li_2Pt_3B$, CrAs (@1GPa), LaRhSi, CaPtSi…

# Summary and outlook

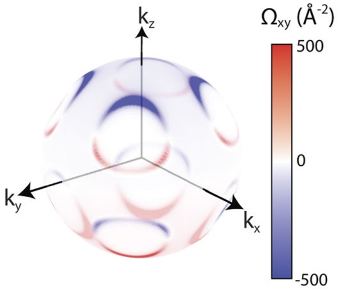
See all our research & find interesting PD and PhD opportunities

## *Quasi-symmetry*

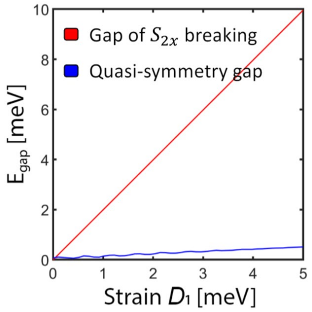
- A new flavor of topological matter.




- A general distribution of Berry curvature dipole.




- A new class of topological materials with remarkable resilience to perturbations (strain etc.).




C. Guo et al., Nature physics 18, 813–818 (2022); See also: News & Views, Nat. Phys. 18, 731-
Lun-Hui Hu, Chunyu Guo et al., PRB 107, 125145 (2023) arXiv:2209.02745; arXiv:2108.02279