The Chirality of Phonons: from symmetry constraints to experimental validation

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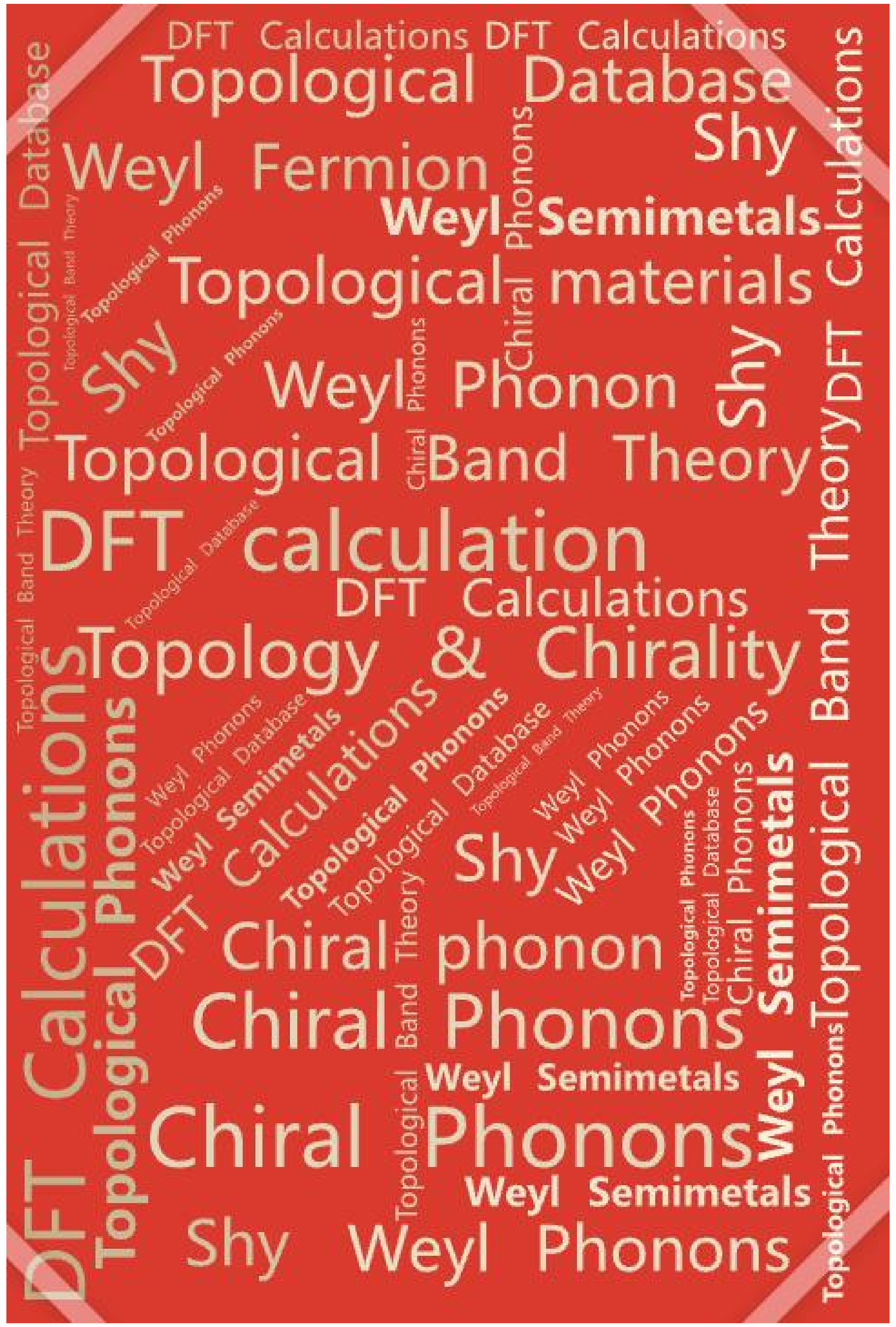
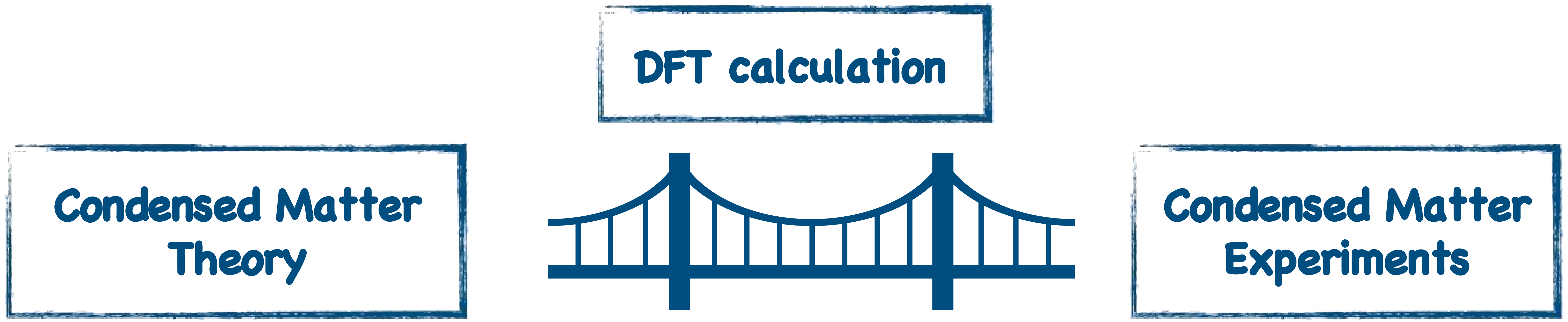
Zhang et al., PRL 120, 016401(2018)
Zhang et al., PRL 123, 245302 (2019)
Zhang et al., PRB 102, 125148 (2020)
Zhang et al., PRR 4, L012024 (2022)
Komiyama, et al. PRB 106, 184104 (2022)
Ishito, et al. Nat. Phys. 19, 142-142 (2023)
Zhang et al., Nano Lett., 23, 7561–7567 (2023)
npj Comput Mater 10, 264 (2024)
NatCommun 16, 3560 (2025)
PRL 134, 196905 (2025)
PRL 134, 196906 (2025)
arXiv:2503.22794 (2025)
arXiv:2505.06179 (under review in RMP)

Research Background





Research interests

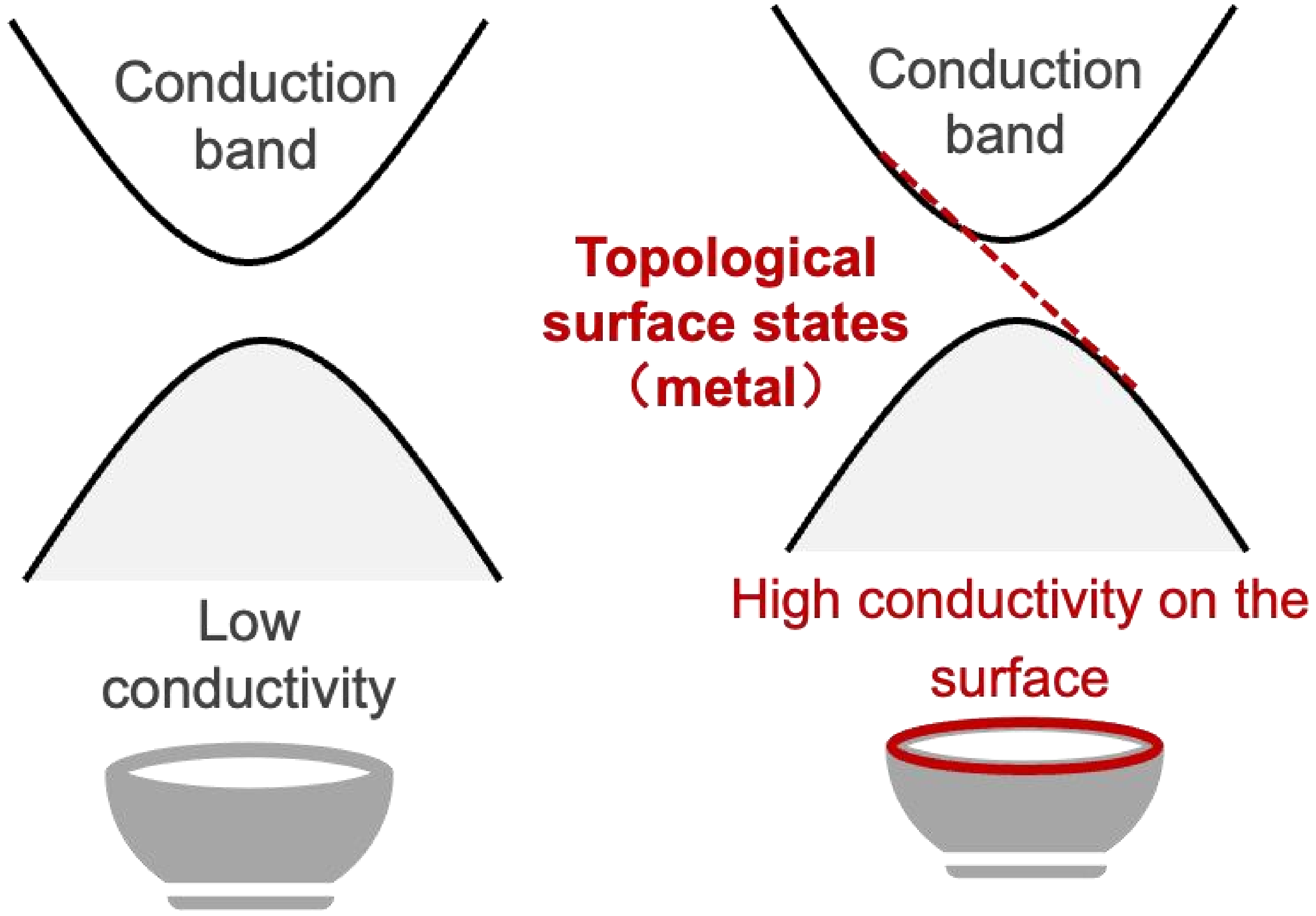
- Topological band theory
- DFT calculations (electrons & phonons)

Background I: Topological electronic materials

Topological invariant Is the key

Bulk-surface correspondence

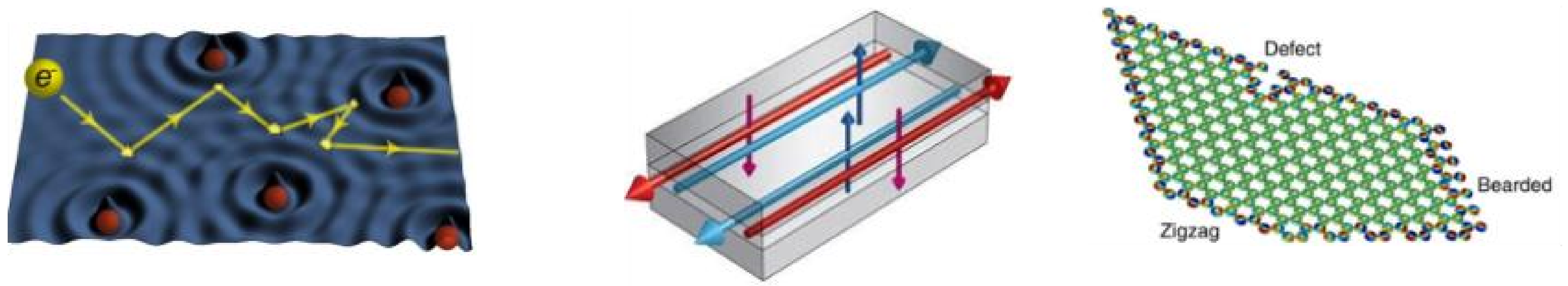
Trivial insulator | **Topological insulator**



Topological classifications

- **Topological insulators, topological crystalline insulators …**
- **Topological semimetals:** Weyl semimetal, Dirac semimetal, node-line semimetal…

application

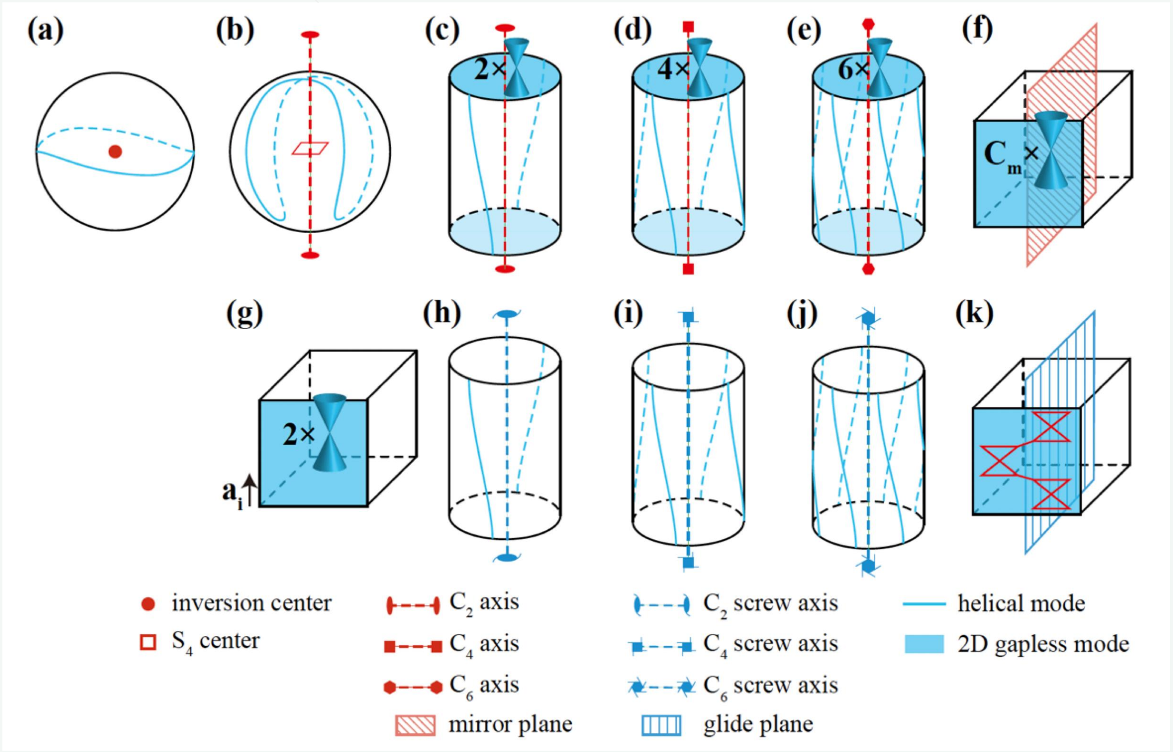


- **Spintronic devices, low-loss devices, topological quantum computation**

Background I: Topological electronic materials

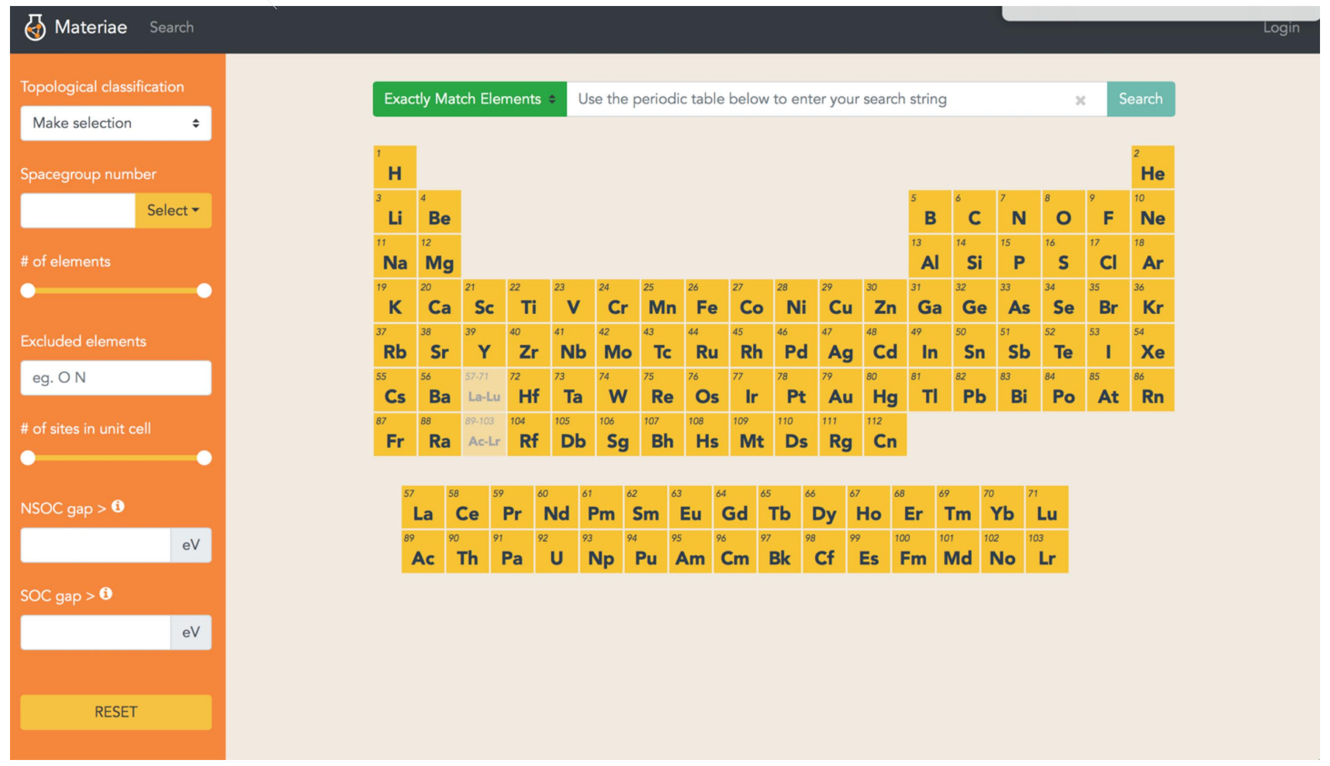
- **Complete** the classification of topological states, **reduce** the computation volume ($10^1 \sim 10^4$) of topological invariants for 230 space groups
- Design an algorithm, high-throughput calculation on non-magnetic materials, discovered 8000+ topological materials, build the **first topological database.** (http://cmpdc.materiae.iphy.ac.cn/)
- Prediction on topological electronic materials, **all of them have been experimentally verified**

Topological band theories



Song, Zhang, et al. ***NatCommu*** (2018)
Song, Zhang, et al. ***PRX*** (2018)
Zhang*, et al. ***PRR*** (2020)

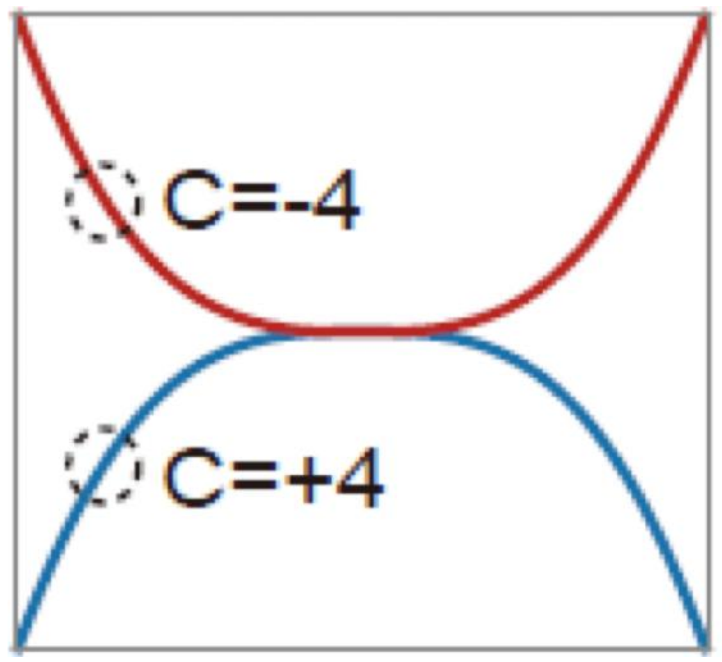
Topological material database



Tiantian Zhang, et al., Nature, 566, 475–479 (2019)

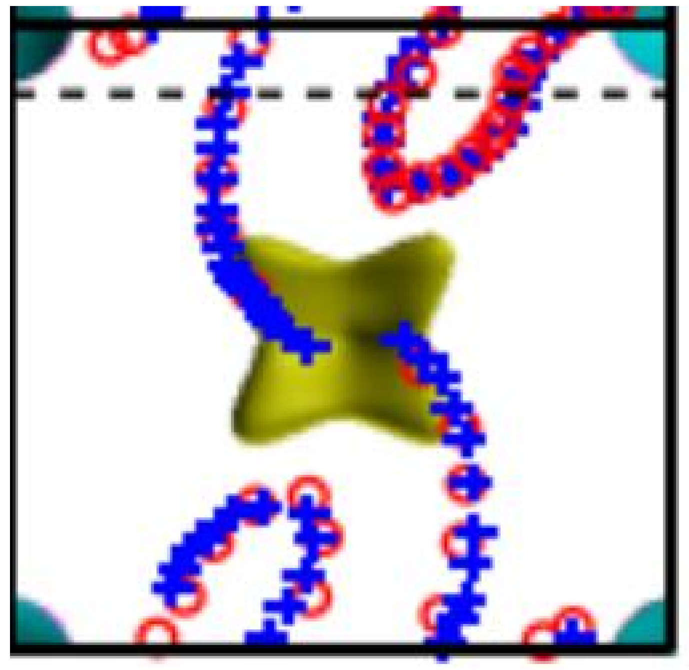
Zhang, et al. ***Nature*** 566, 475-479 (2019)

Topological materials (Prediction)



PRB 102, 125148 (2020)
npjComputMater 8, 155 (2022)
Adv.Mater. 2309803 (2024)

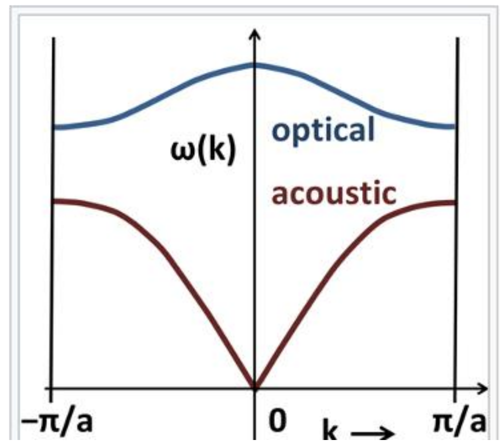
Topological materials (Observation)



Nature 567, 496–499 (2019)
Sci.Adv. eaau6459 (2019)

Background II: topological and chiral phonons

Harmonic approximation

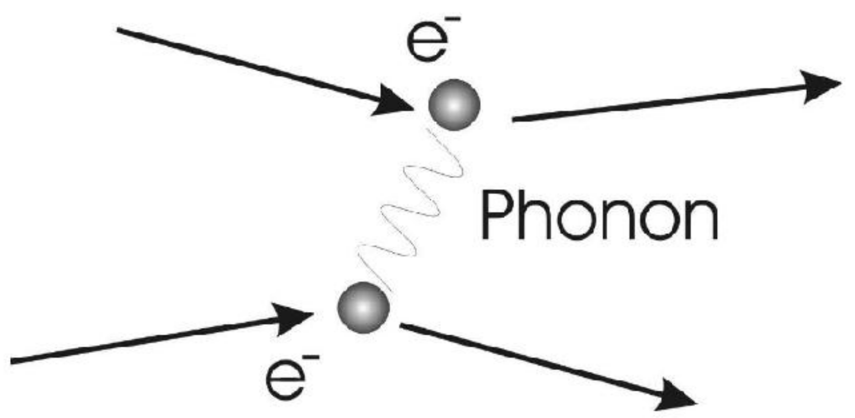


phonon: quantum description of lattice vibrations

photon-phonon coupling

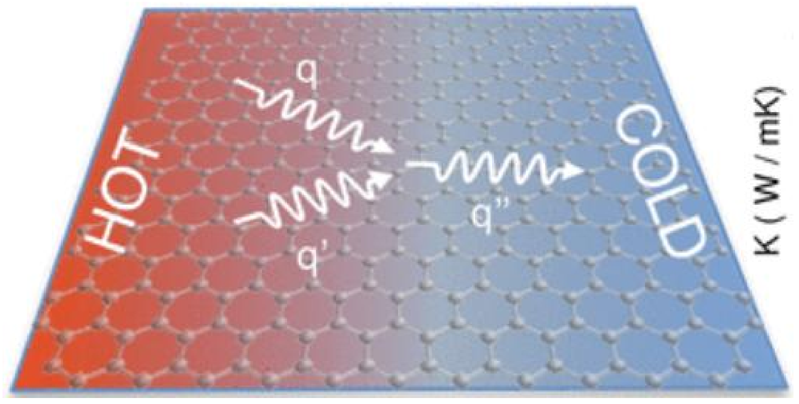
Electron-phonon coupling

- Resistivity in (semi-)metals
- Charge-density waves
- Superconductivity

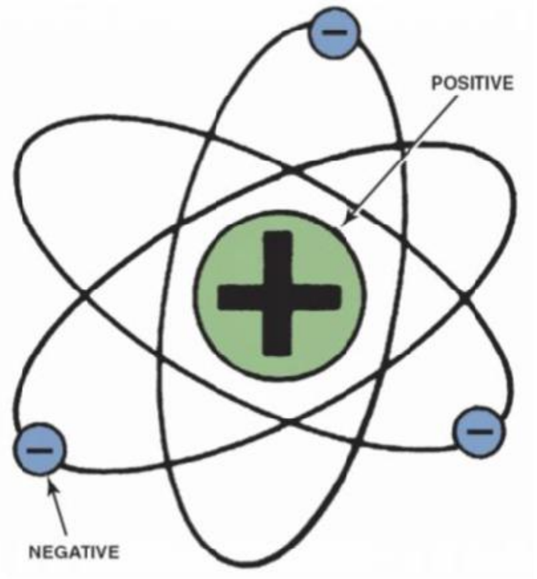


Anharmonic effects

- Phonon lifetime
- Phonon thermal conductivity
- Anomalous thermal expansion
- Mechanical Properties



Electrons v.s. Phonons: ways to control

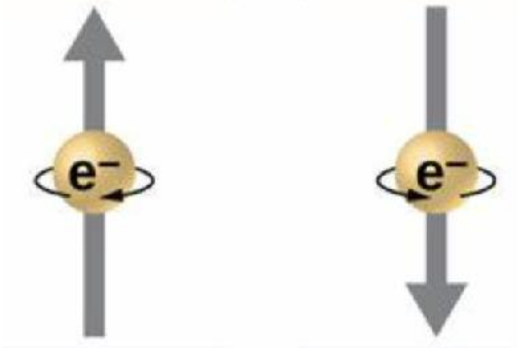


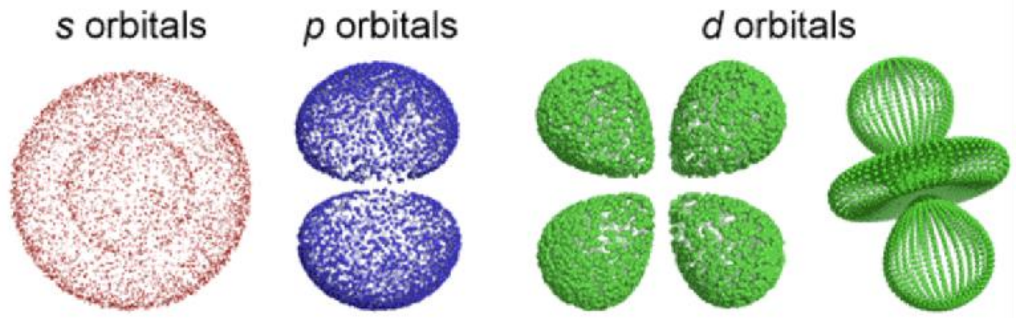
Charge

Electrons

Spin

Orbital





Other DOF?

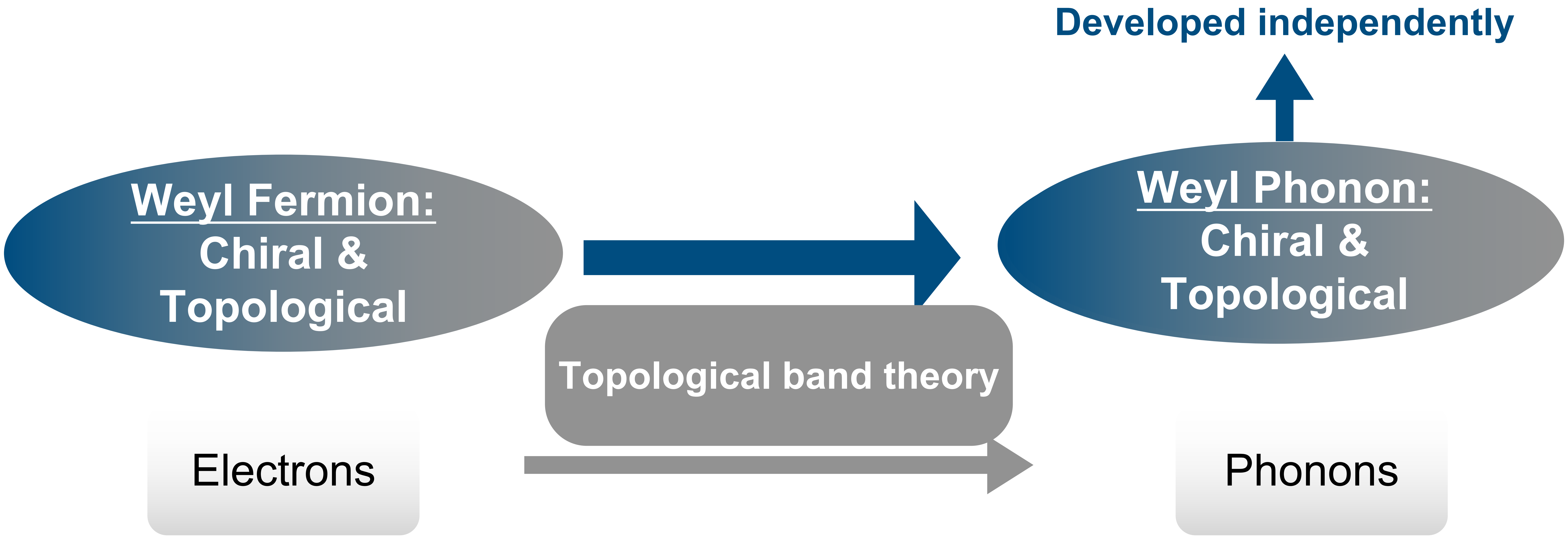
Charge neutral

Phonons

Spin zero

Orbital free

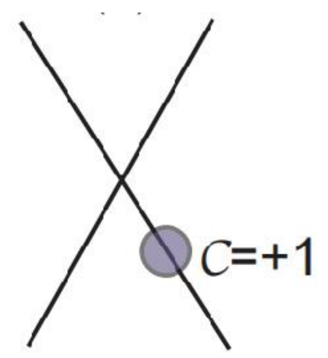
Electrons v.s. Phonons: ways to control



Zhang et al. NatCommun 16, 3560 (2025)

Weyl phonons: Topology&Chiral

Topological invariant: Chern number



Weyl point

$$C_n = \frac{1}{2\pi}\int_S \Omega_n(\mathbf{k})\cdot dS$$

$$\Omega_n(\mathbf{k}) = i\langle \nabla_{\mathbf{k}} u_{n\mathbf{k}}| \times |\nabla_{\mathbf{k}} u_{n\mathbf{k}}\rangle$$

C≠0

Topology: Nonzero Chern number

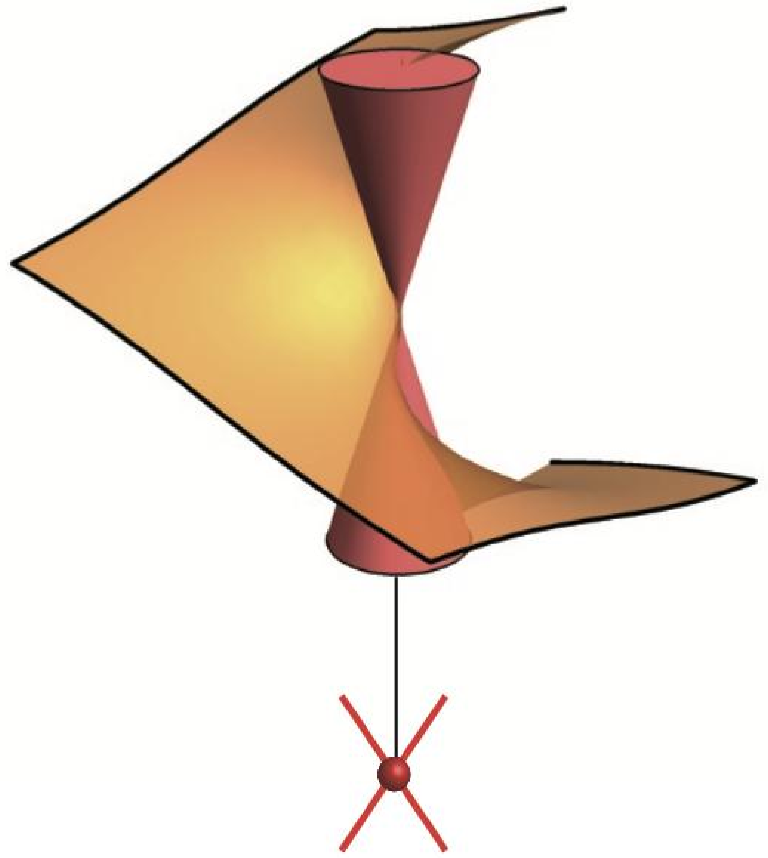
***k*-space Chirality:**

The sign of Chern number

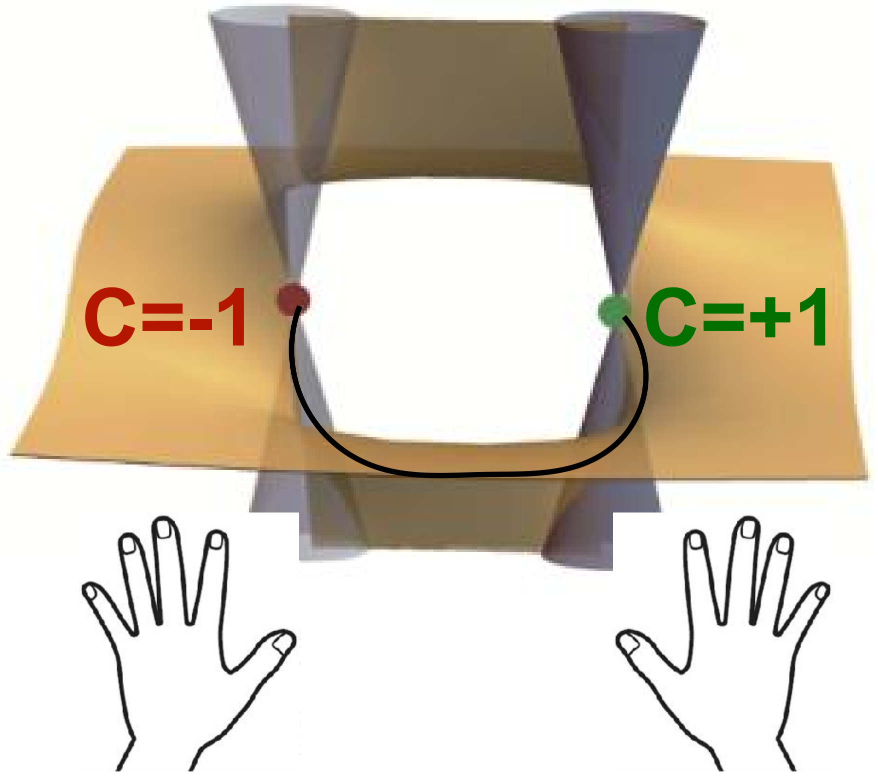
Pseudospin texture (wrapping number)

Helicoid surface states

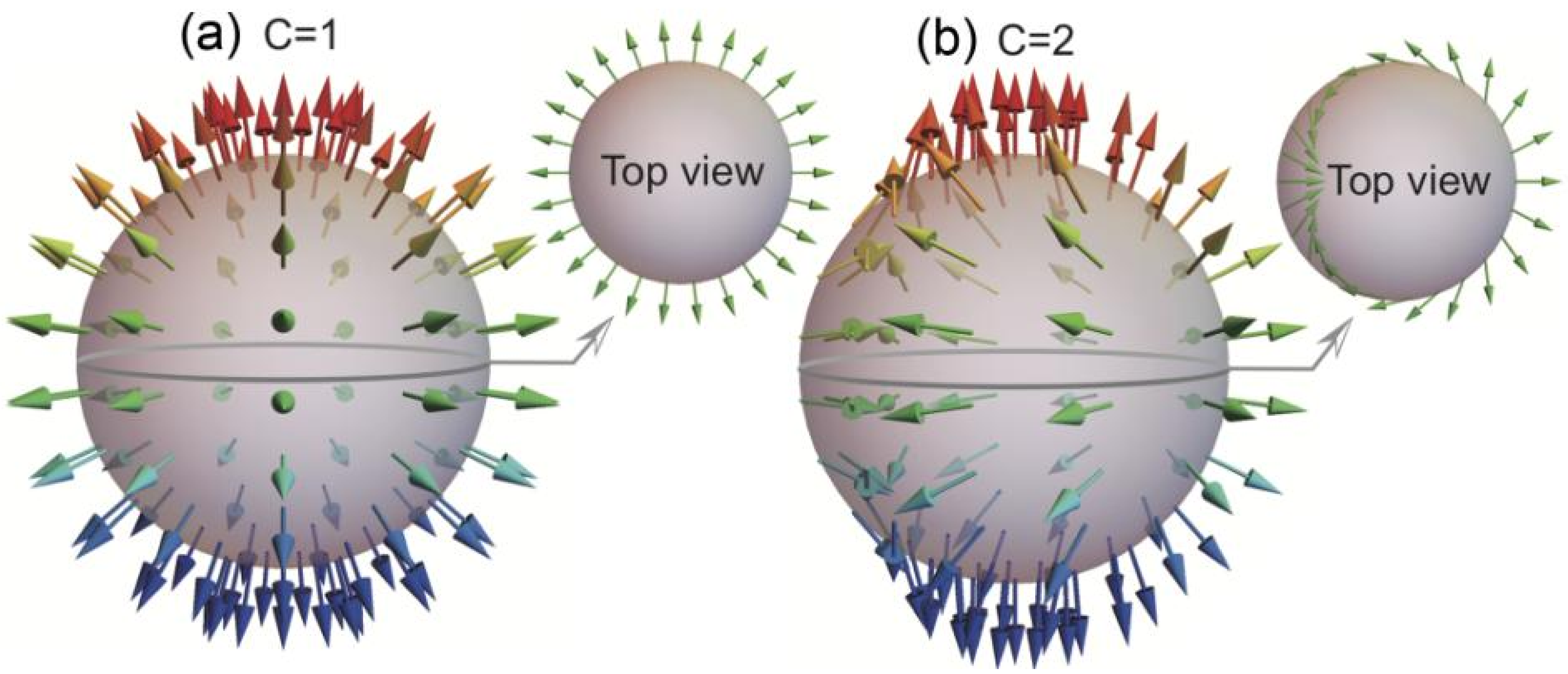
Chiral surface state



Surface arc



Pseudospin texture



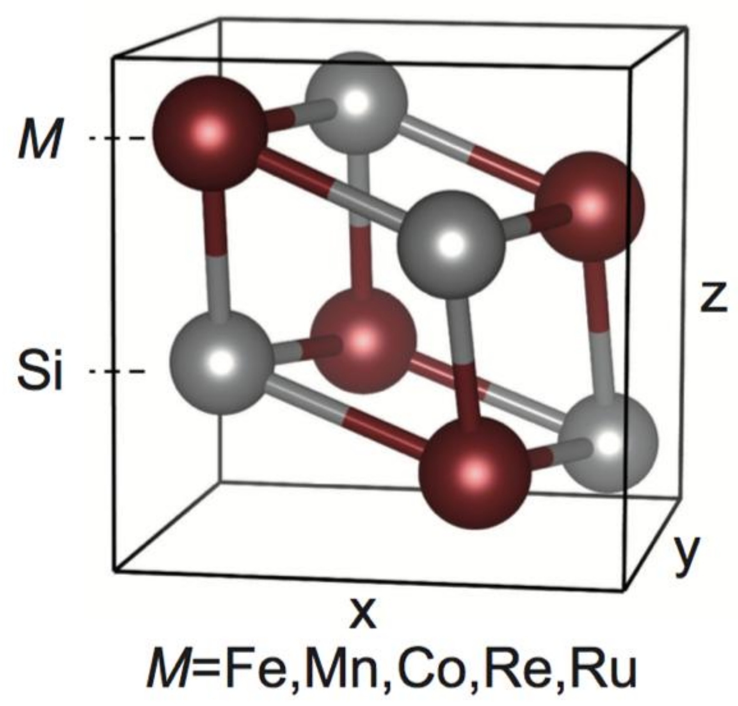
C. Fang, et al, Nat. Phys. 12, 936 (2016)

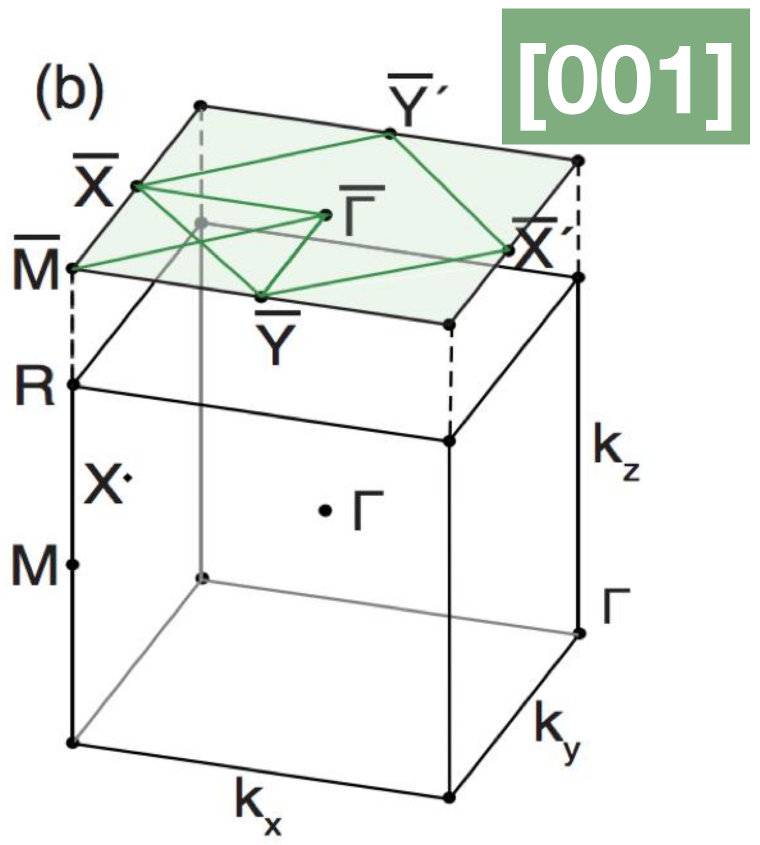
Zhang et al., PRB 102, 125148 (2020)

First Weyl phonon in FeSi family: prediction

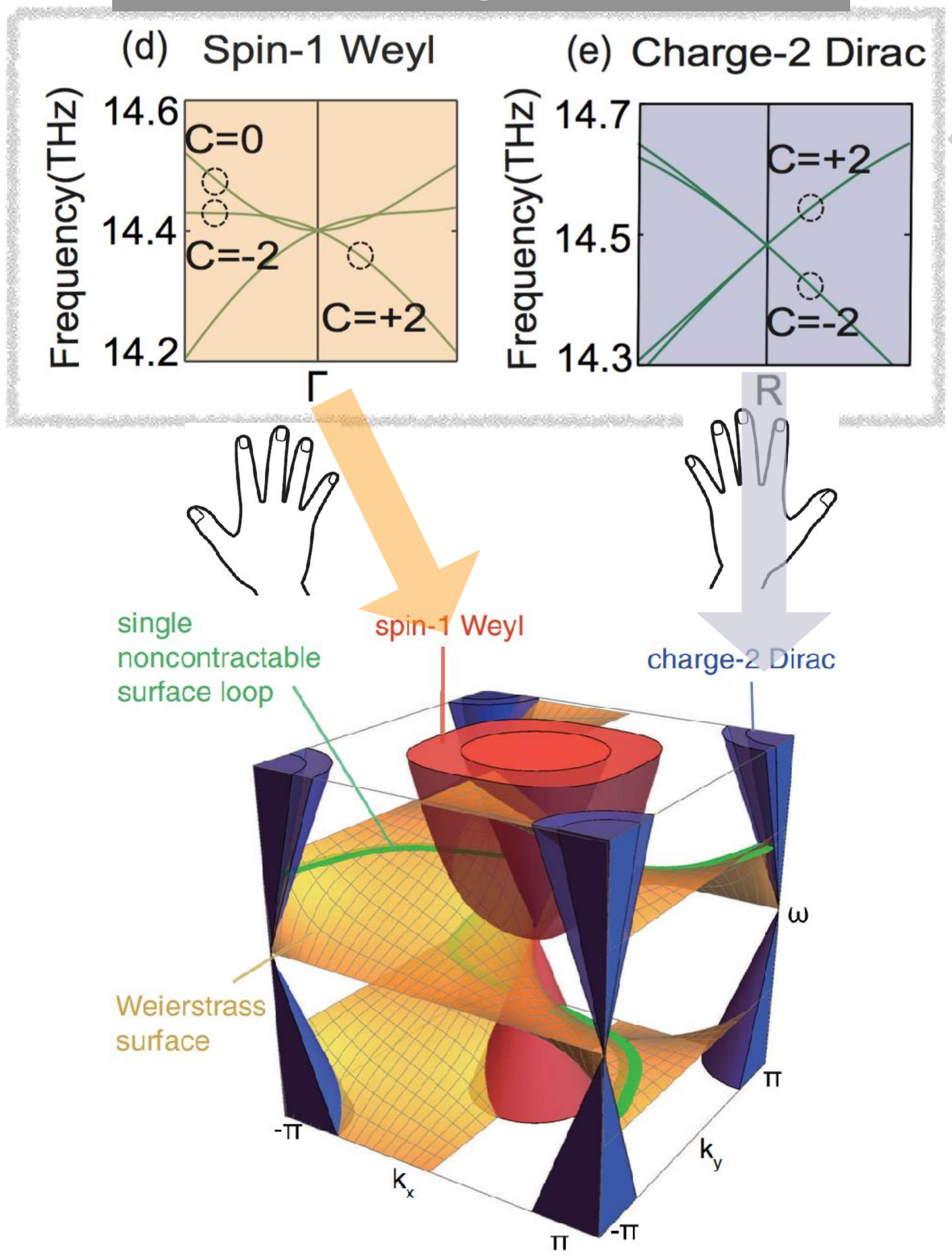
Zhang et al. PRL **120**, 016401(2018)
Miao, Zhang, et al. PRL **121**, 035302(2018)

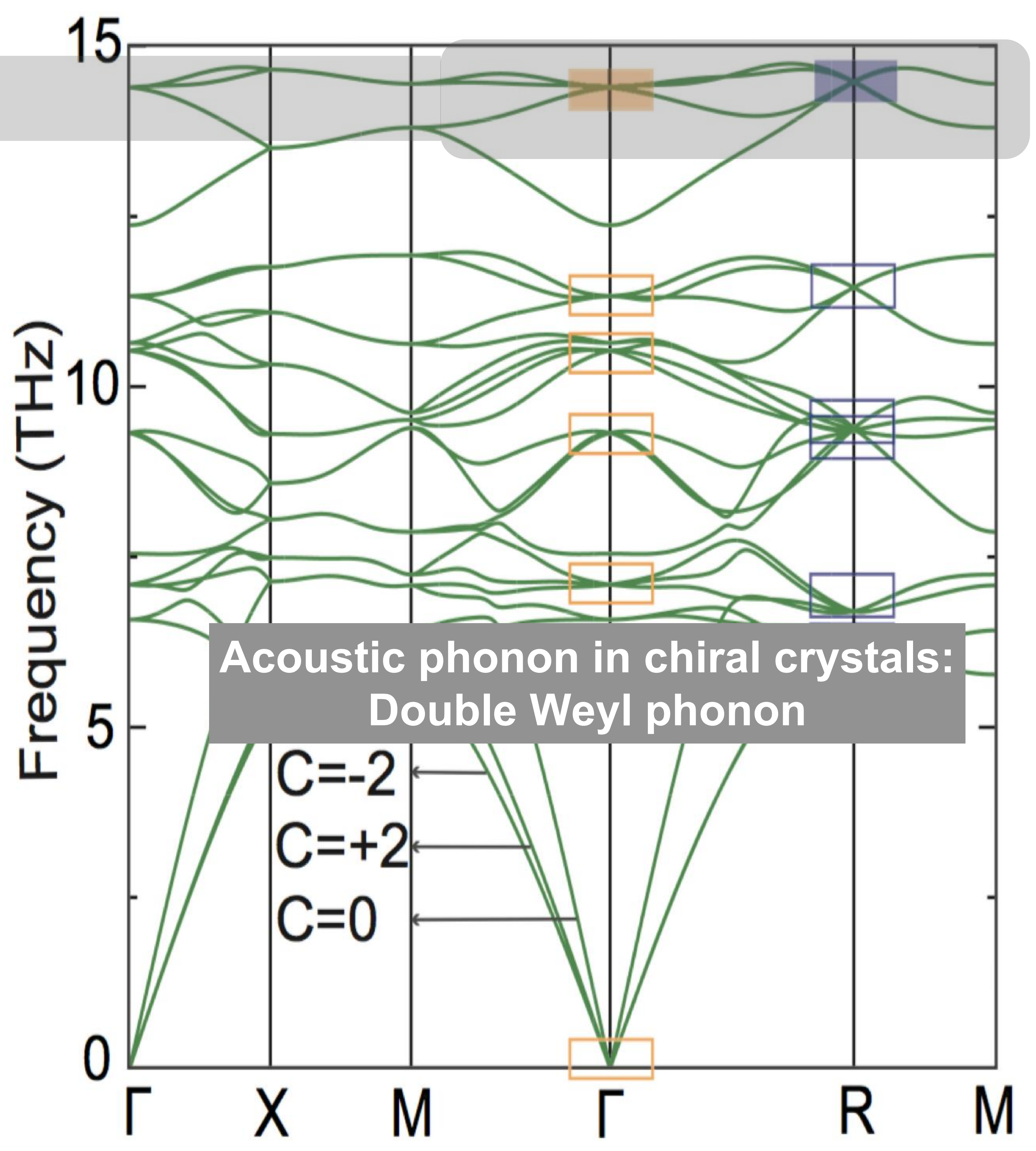
Space group No. 198





Double Weyl phonons

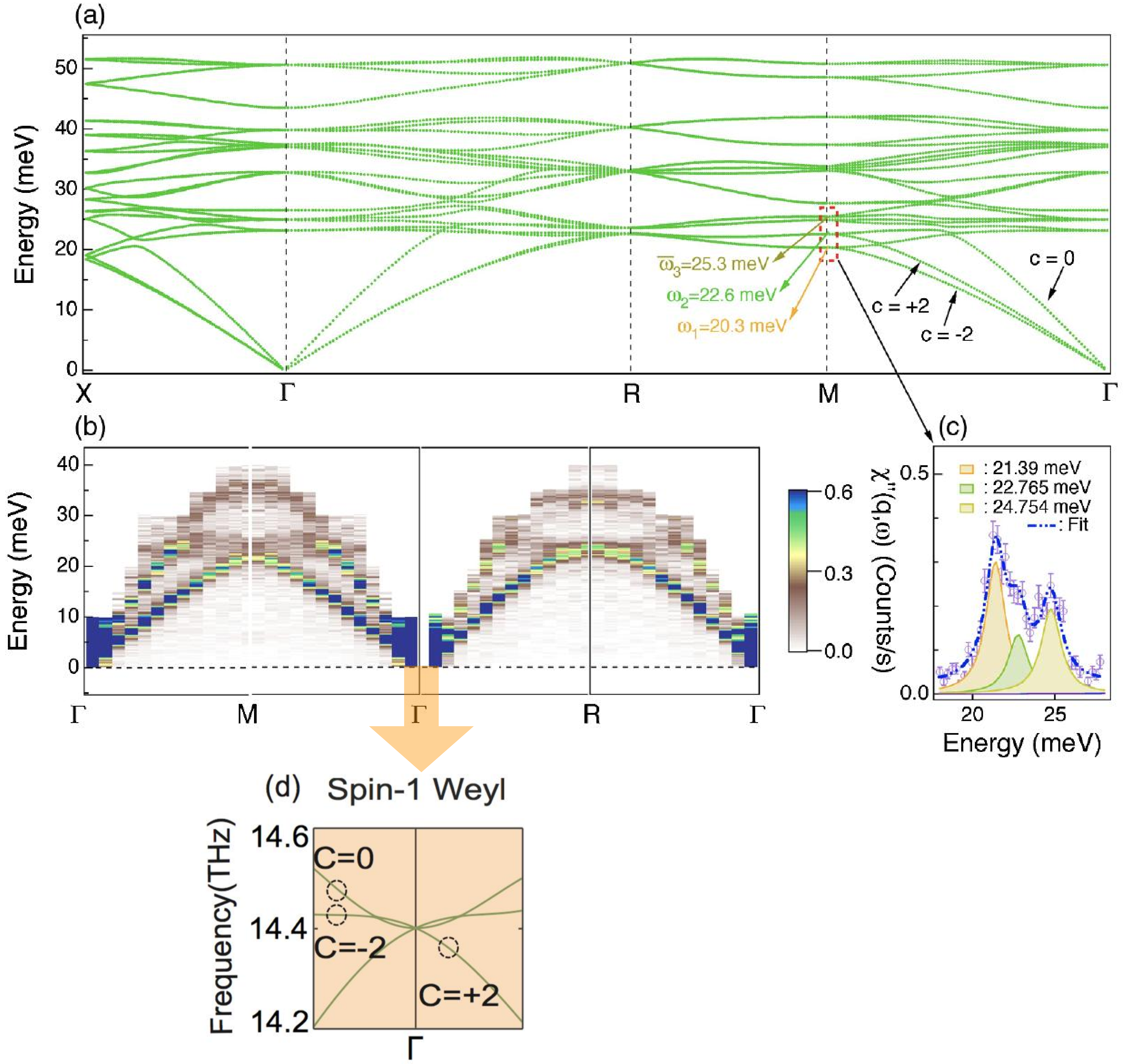


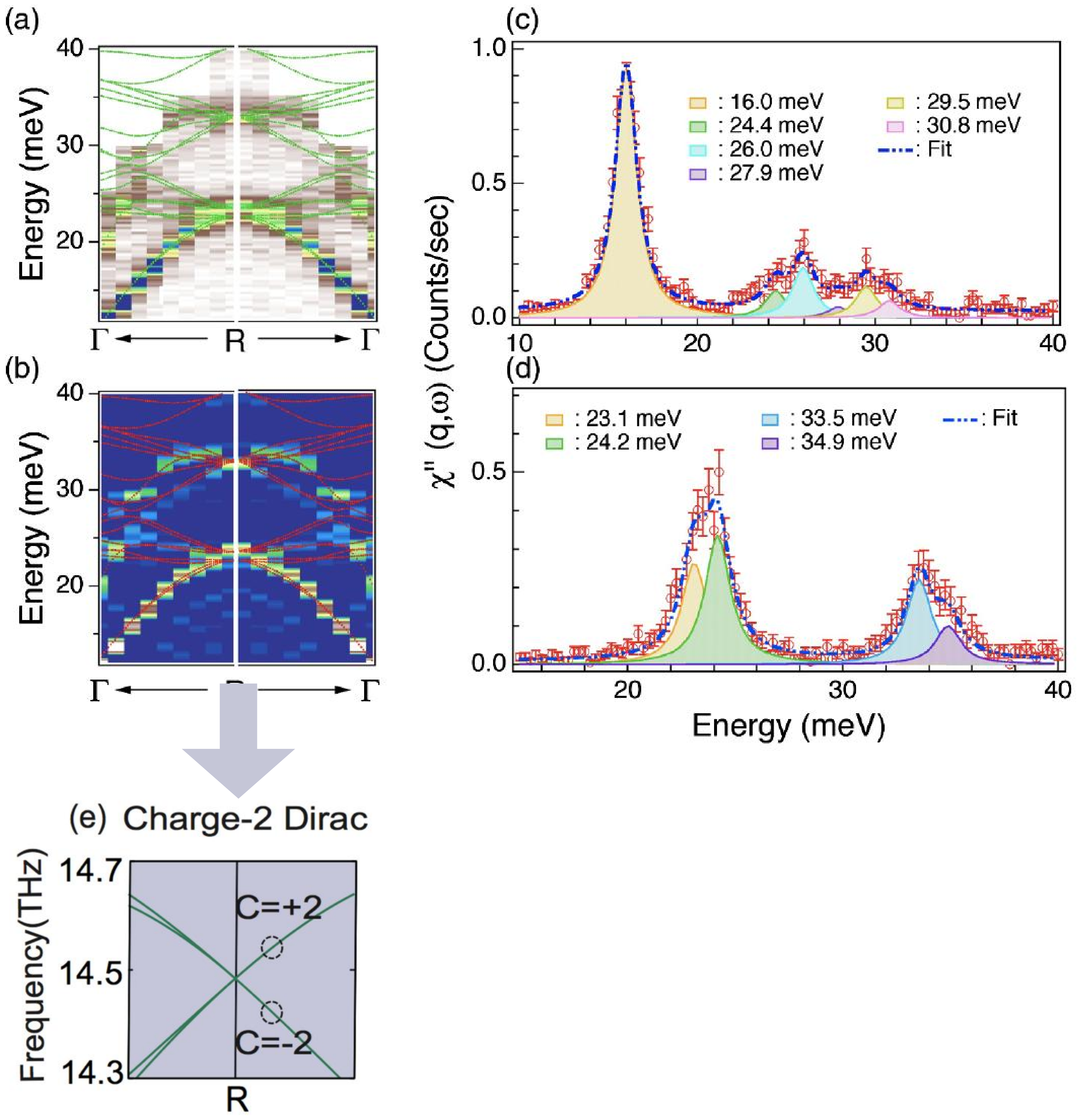


First Weyl phonon in FeSi family: observation

Zhang et al. PRL **120**, 016401(2018)
Miao, Zhang, et al. PRL **121**, 035302(2018)

Weyl phonons observed in FeSi by inelastic X-ray





r-space chirality in phonon spectra

Atomic motion

Depends on symmetry

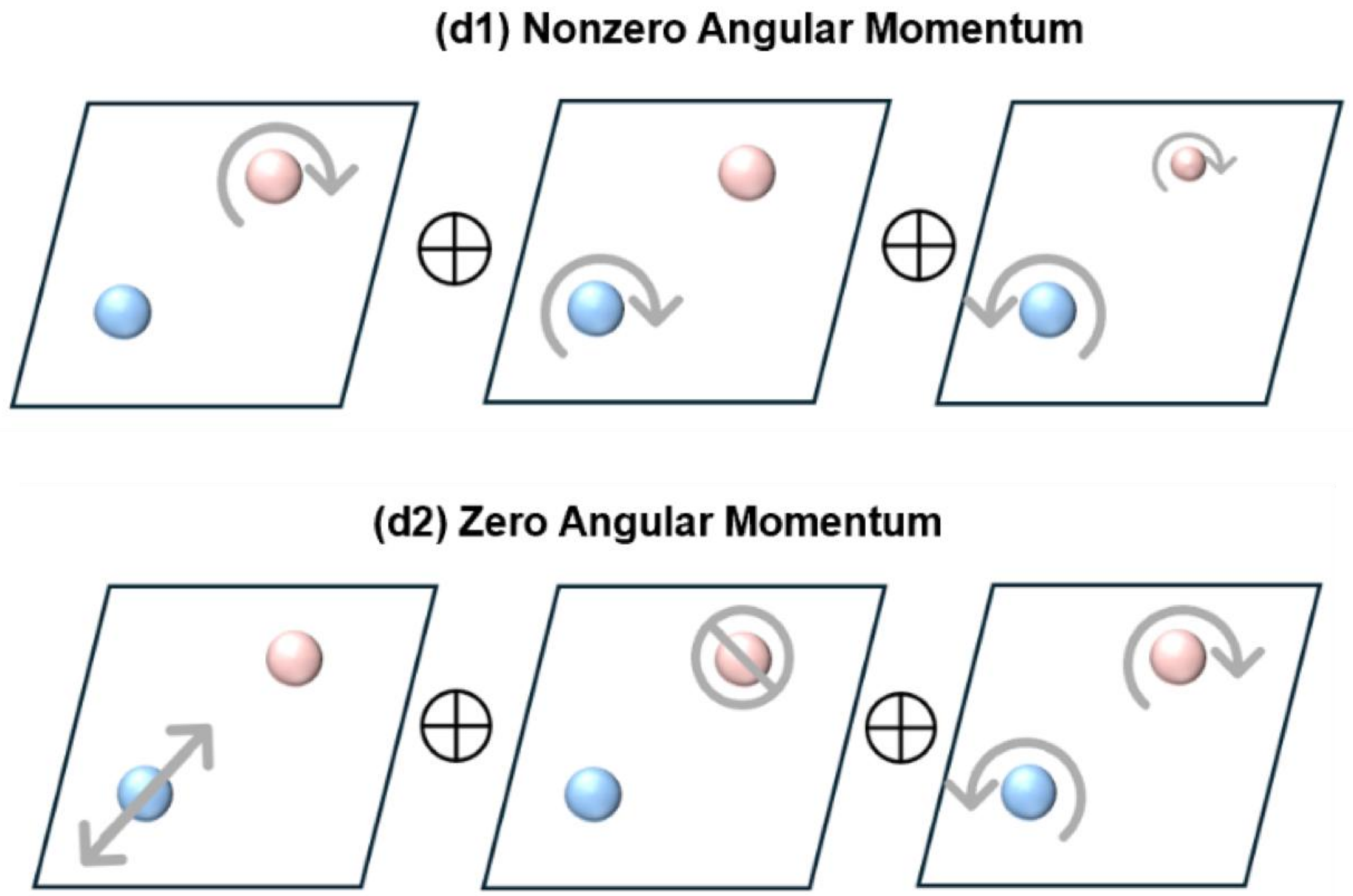
- Linearly polarized motion
- Circularly polarized motion
- Certain atoms keep stationary

→ ***r*-space chirality** ←

Angular momentum

$$l_{\nu,z}(q) = \sum_{\kappa}^{Na} u_{\nu q}^{\kappa} \times \dot{u}_{\nu q}^{\kappa} = e_{\nu q}{}^{\dagger} M_z e_{nq}$$

Assume z+ as the propagating direction, since chirality need 3 degrees of freedom



—> most widely exist in solids

—> symmetry restrict AM=0

Last century:

"Circularly polarized phonon"

"Rotational vibration"

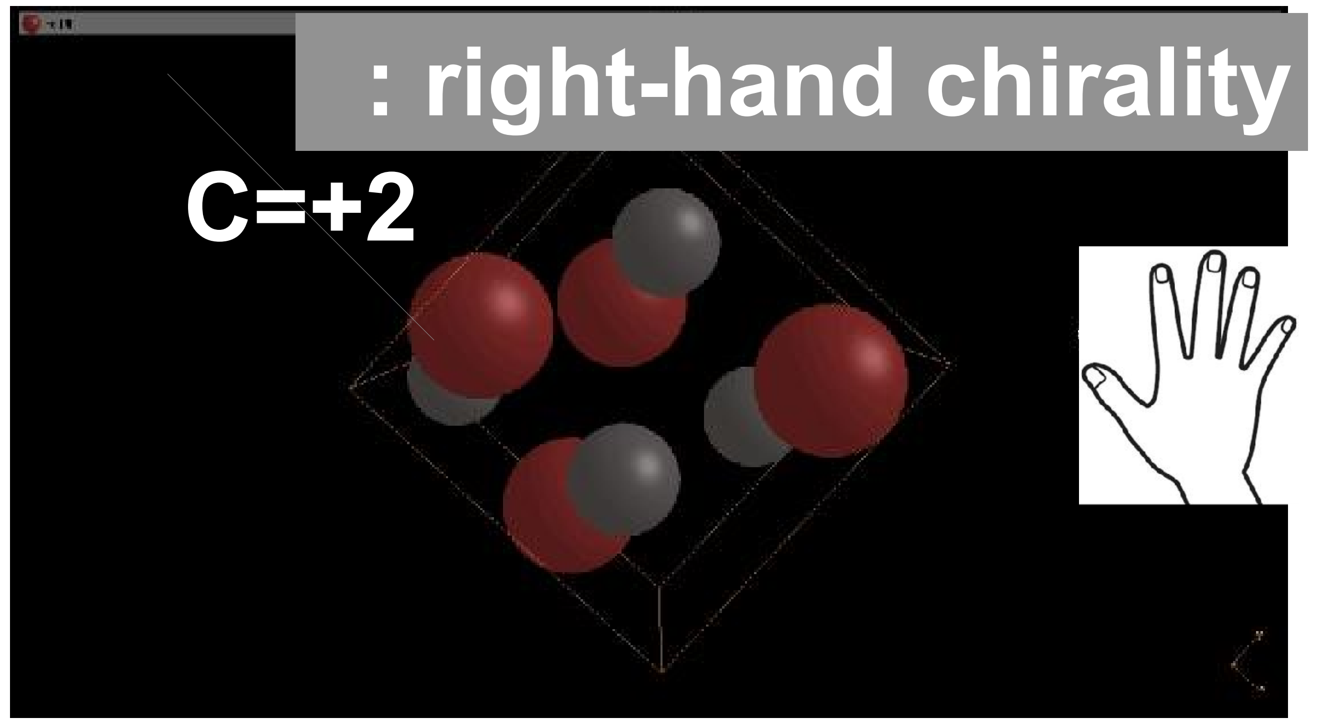
After 2008:

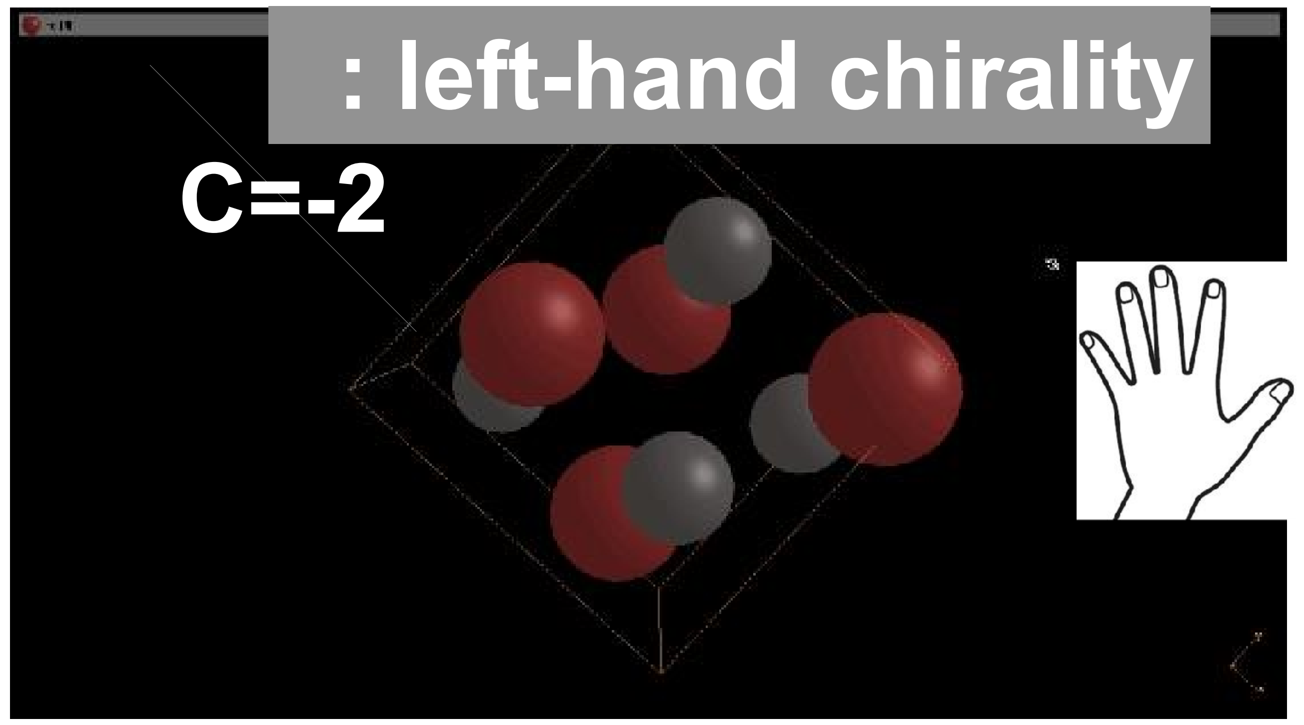
"Chiral phonon"

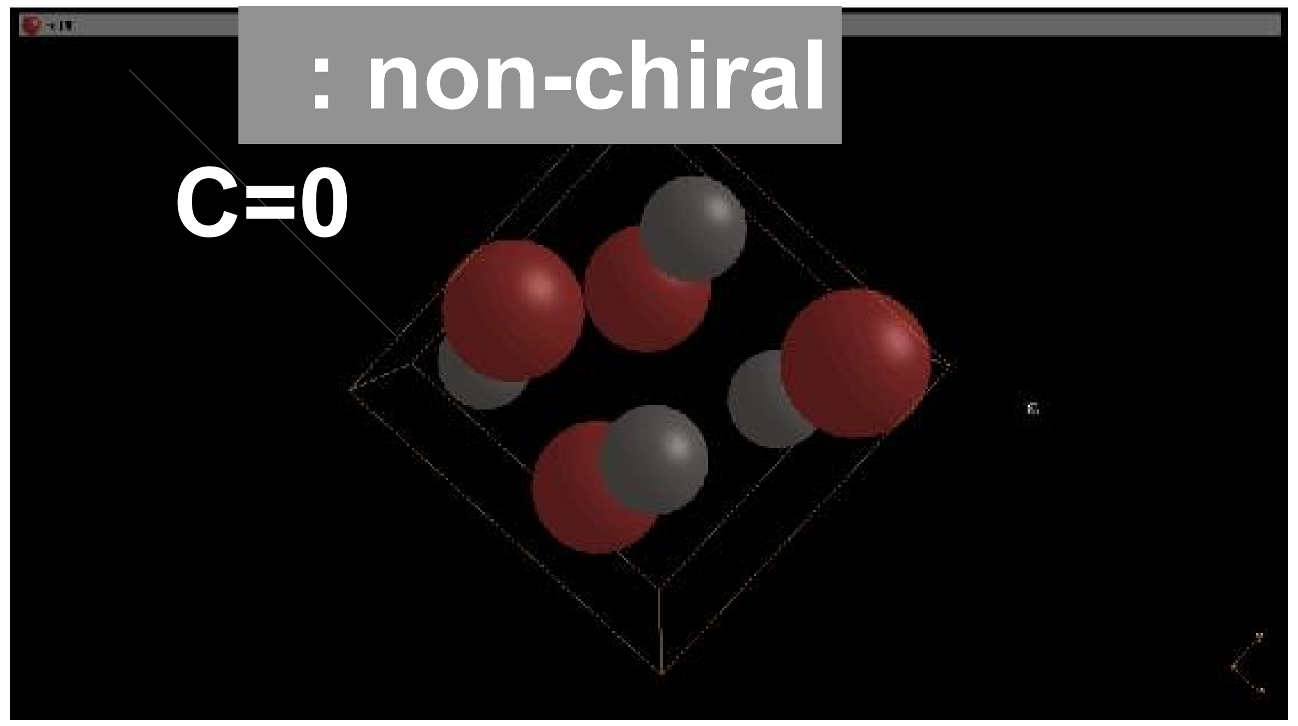
Zhang et al., arXiv:2503.22794

R. C. Johnson, Angular momentum on a lattice. Phys. Lett. B 114, 147–151 (1982)
Yu. T. Rebane. Zh. Eksp. Teor. Fiz. 84,2323-2328 (1983)
A Bermudez and M A Martin-Delgado, J. Phys. A: Math. Theor. 41 485302 (2008)
A Bermudez, et al., Phys. Rev. A 77, 063815 (2008)
Zhang and Niu, Phys. Rev. Lett. 112, 085503 (2014)

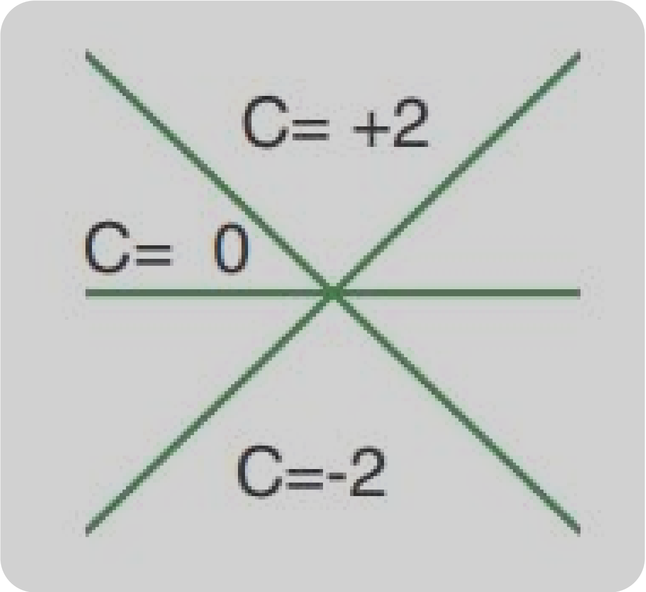
Weyl phonons are both topological and chiral





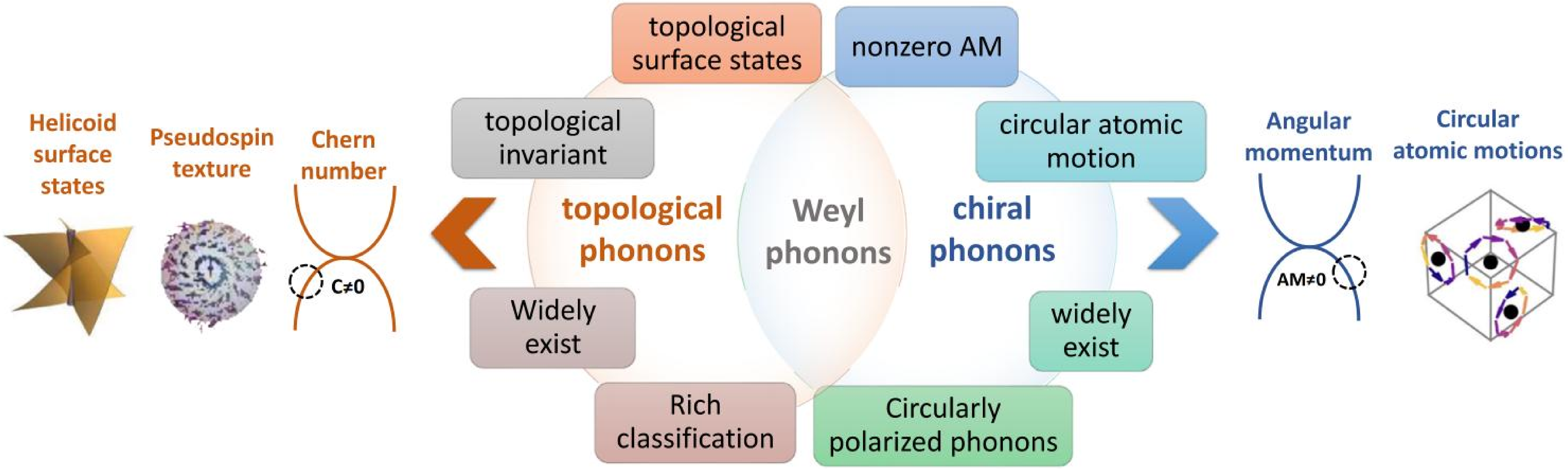


Spin-1 Weyl phonons in FeSi



Zhang et al. PRL 120, 016401(2018)
Zhang et al. PRB 102, 125148 (2020)
Zhang et al. NatCommun 16, 3560 (2025)

Weyl phonons are topological and chiral (*k*&*r*-space)



Topological band theory for Weyl phonons: symmetry vs. diagnosis

C_n rotation symmetry

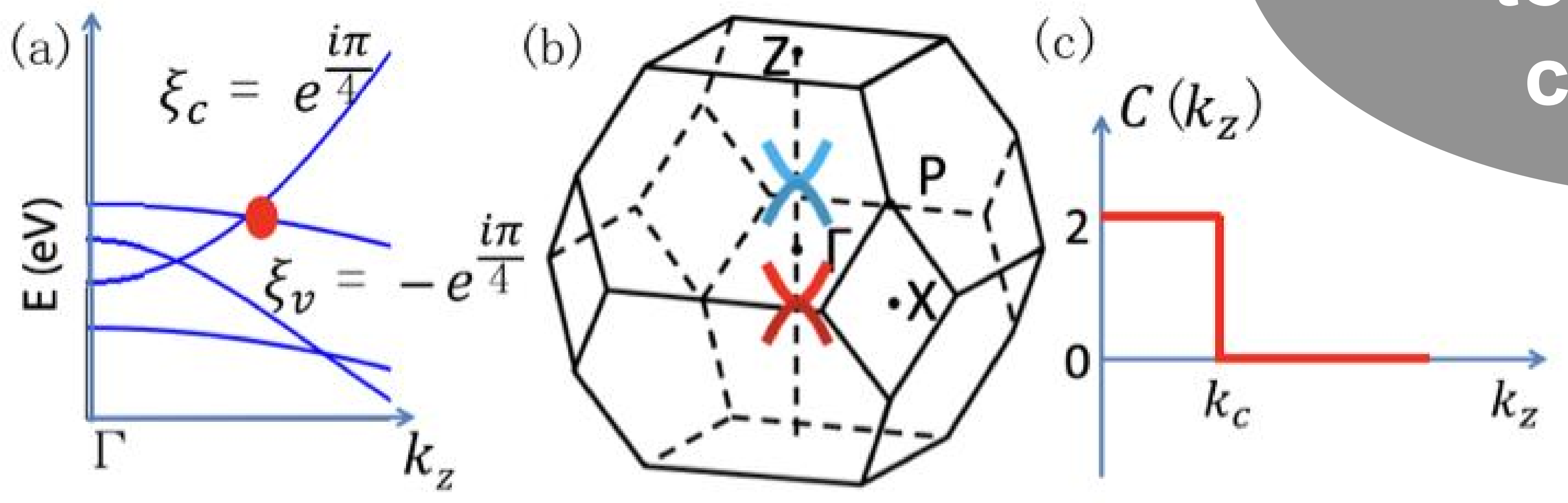
$$C_n u_q = C_n \sum_{l,\kappa,\alpha} e_q^{\kappa\alpha} u_\alpha(R_l, \tau_\kappa) e^{ik(R_l+\tau_\kappa)} = e^{2\pi i \frac{l_{rot}}{n}} u_q$$

$$l_{ph} = l_{rot}$$

pseudo-angular momentum: l_{ph} is an integer, modulus n

Tarantul, A., & Tsukerblat, B. *Inorganica Chimica Acta*, *363*, 4361-4367 (2010)
Zhang, L., & Niu, Q. PRL, *115*, 115502 (2015)

$$C: \ (l_{ph}^{up}, l_{ph}^{dn})$$



C Fang, et al. PRL 108, 266802 (2012)
C Fang, et al. PRB 86, 115112 (2012)

How to observe phonon topology & chirality?

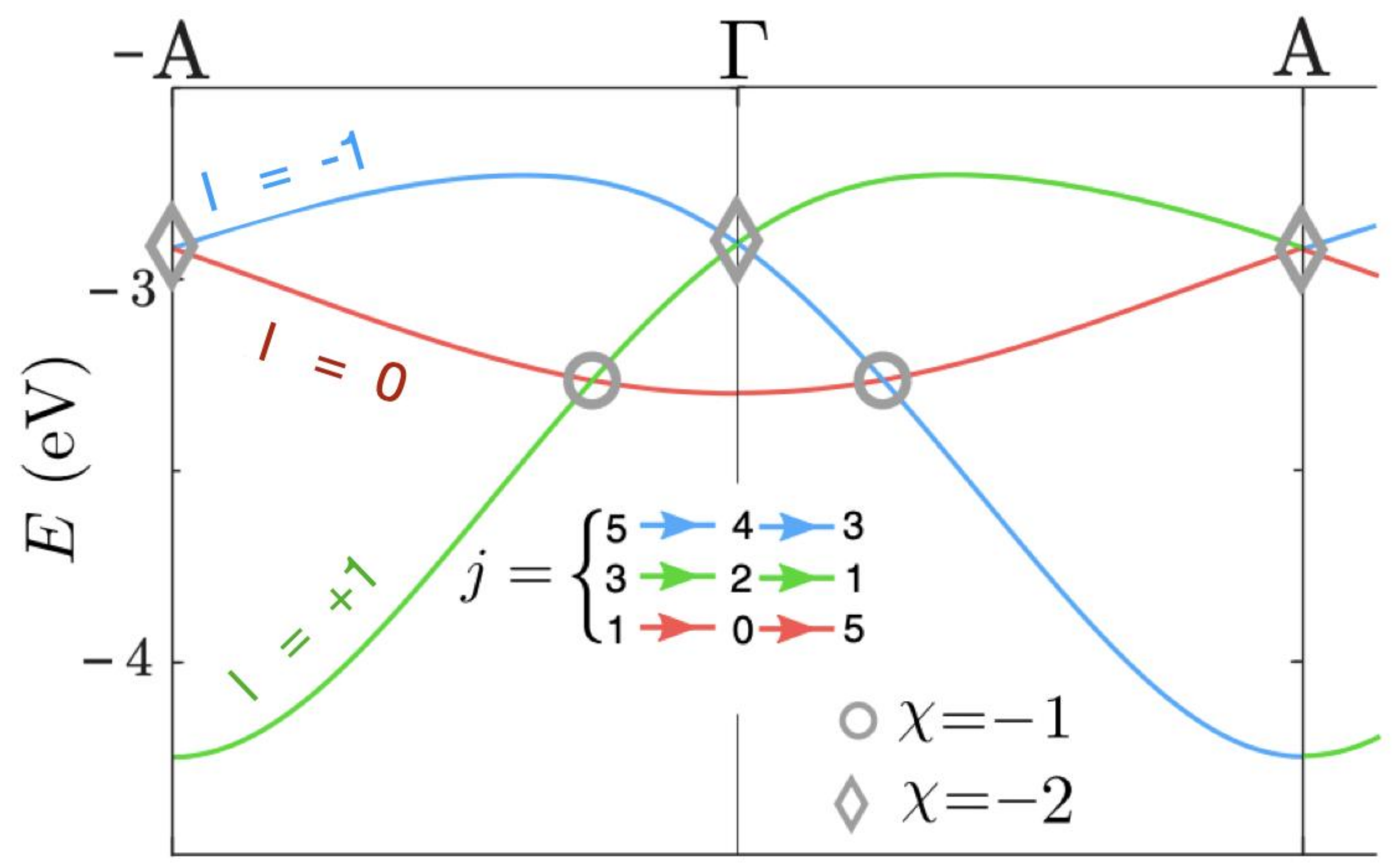
C_3^1 screw rotation symmetry

$$C_n' u_{nq} = C_n P_\tau u_{nq} u_{nq} = e^{2\pi i \frac{l_{rot}}{n}} \cdot e^{iq\cdot\tau} u_{nq}$$

$$l_{ph} = l_{rot} + \frac{q\cdot\tau}{2 * \pi/n}$$

l_{ph} is q-dependent, modulus n

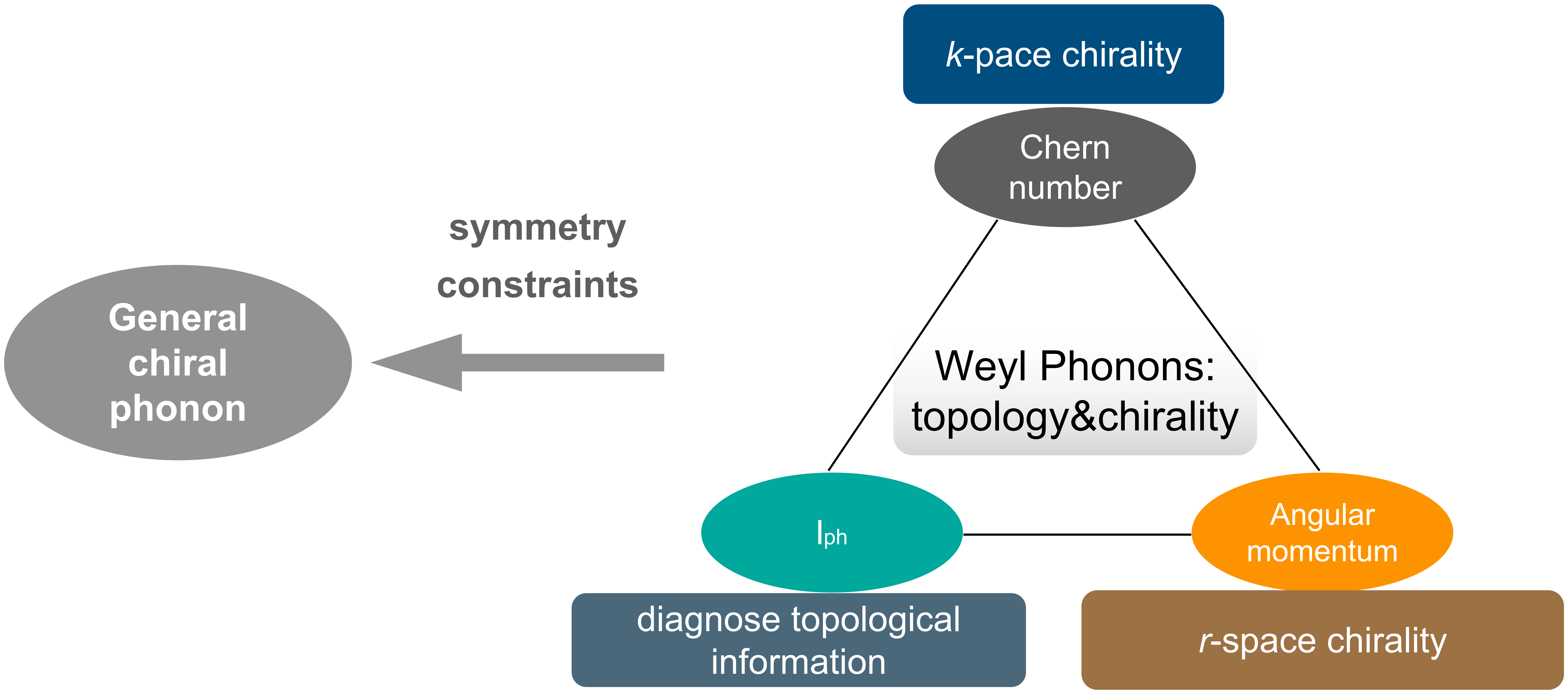
Zhang and Murakami, PRR. 4, L012024 (2022)



Stepan et al., PRB 96, 045102 (2017)

Rotational Symmetries (PAM) can diagnosis Weyl phonons

Weyl phonon: topological & chiral



AM and PAM (l_{ph}) are not inherently related, DFT calculations/symmetry analysis are needed

Symmetry constrains on the chirality of phonons @ q

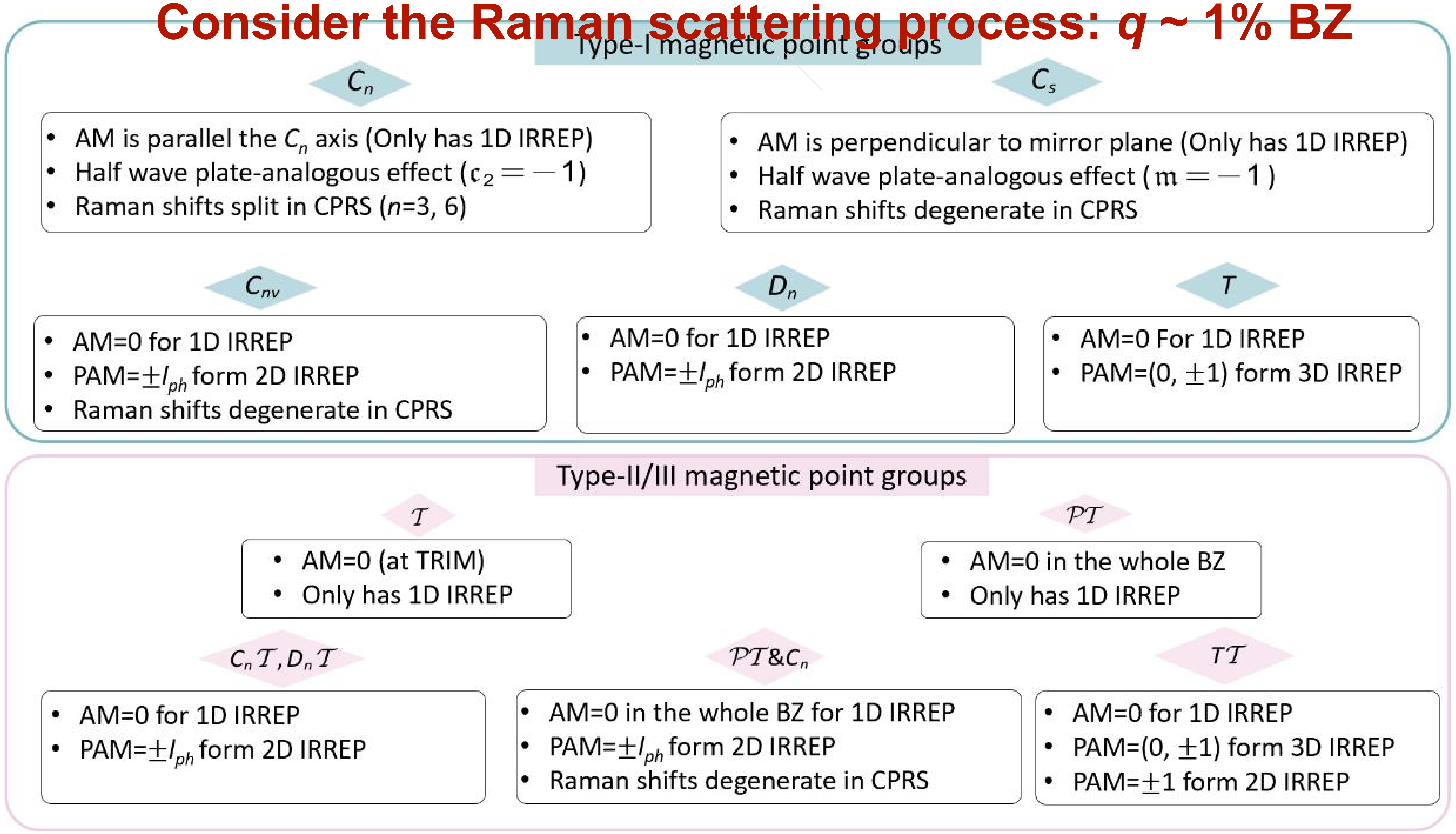
phonon degeneracy, AM, PAM, experimental benchmark…

General chiral phonons

symmetries

+

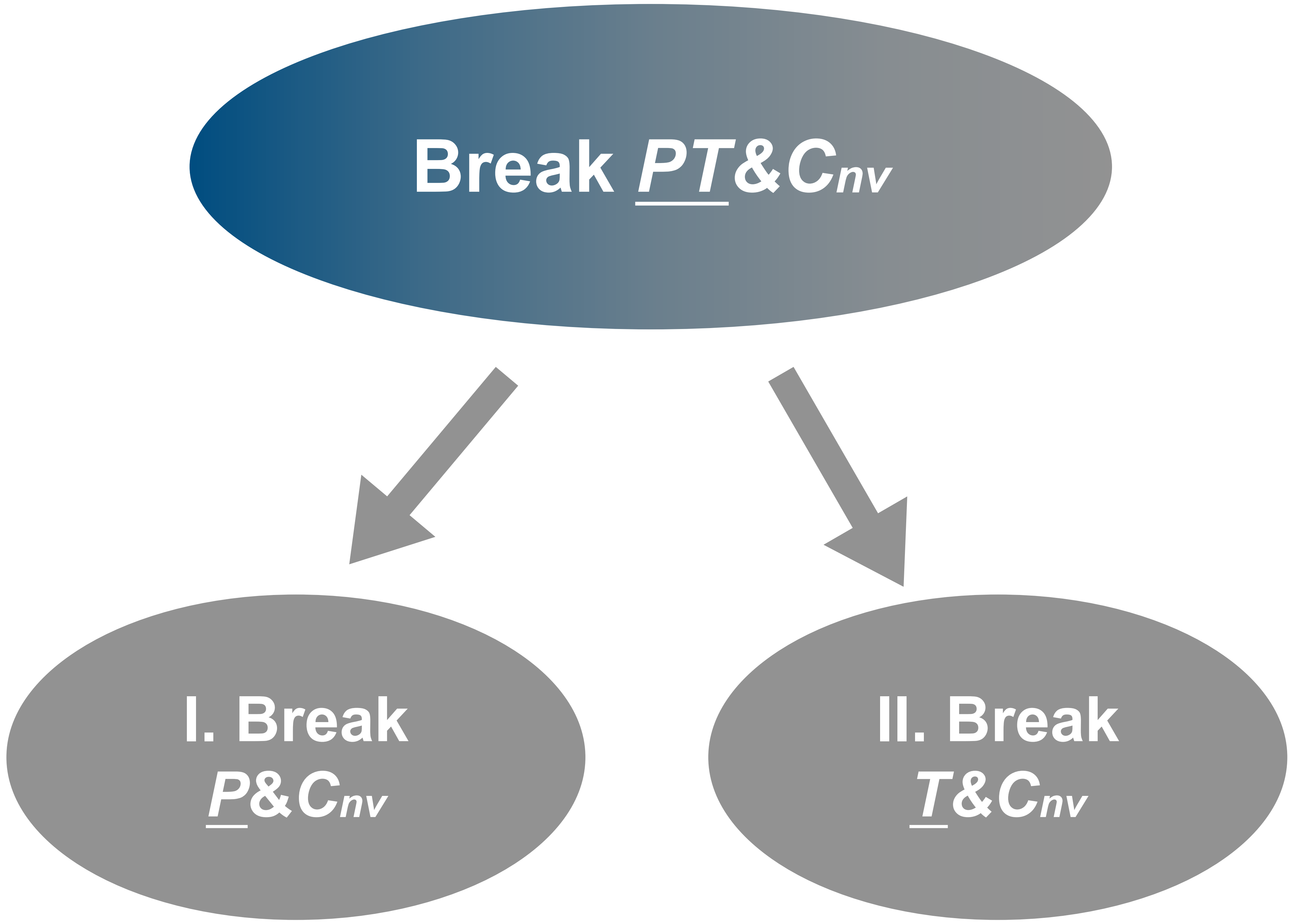
Consider the Raman scattering process: q ~ 1% BZ



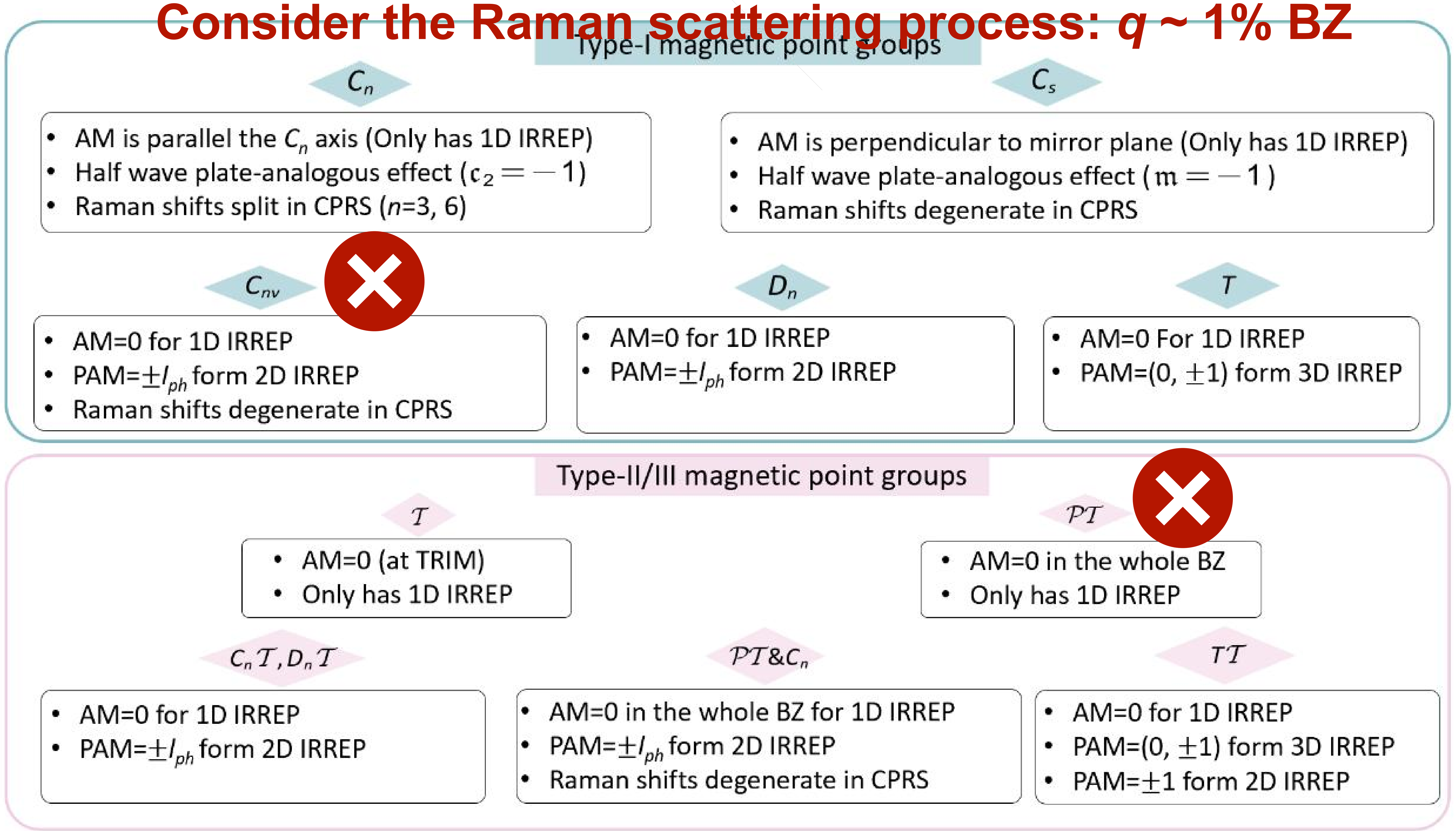
Zhang et al., arXiv:2503.22794

Symmetry constrains on the chirality of phonons @ q

AM and PAM (l_{ph}) are not inherently related, DFT calculations/symmetry analysis (below) are needed



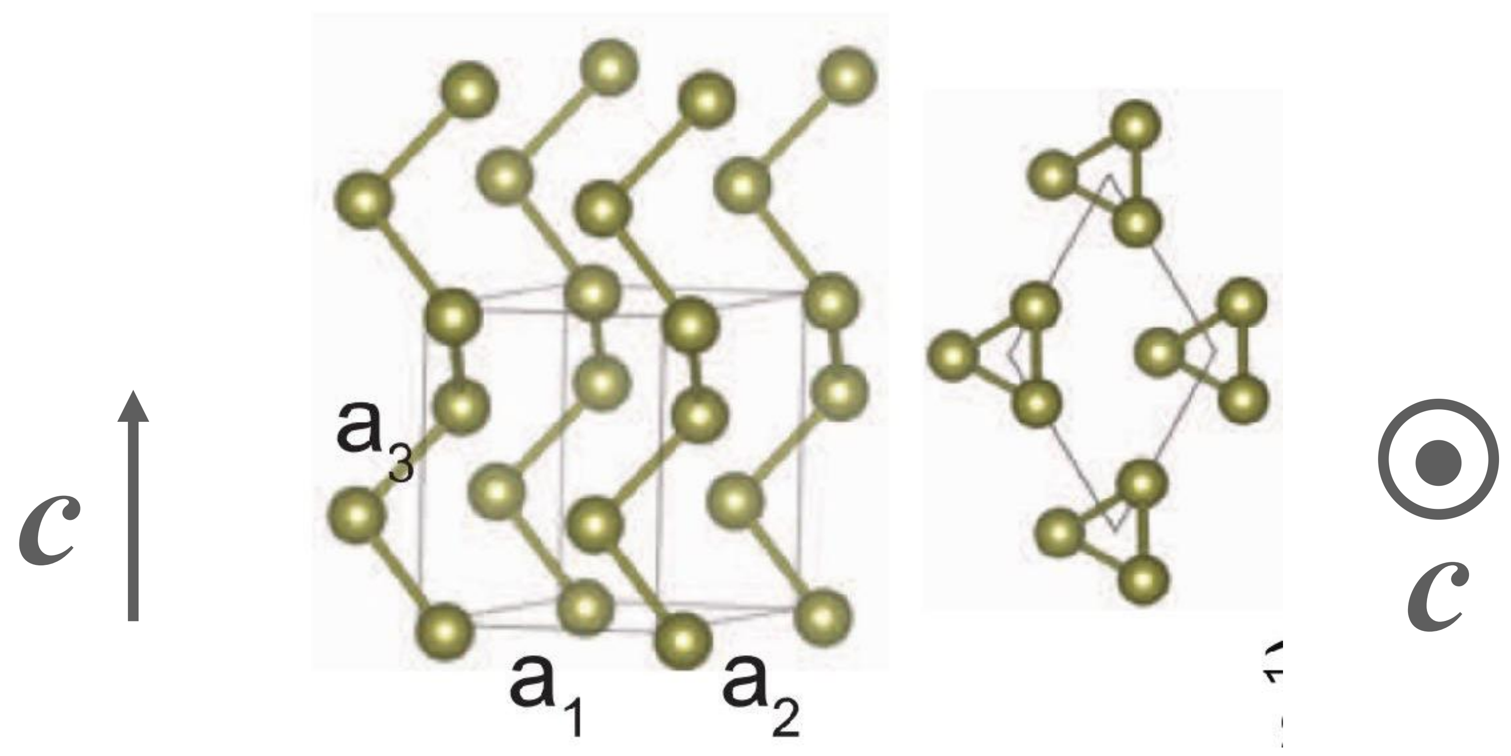
Consider the Raman scattering process: q ~ 1% BZ



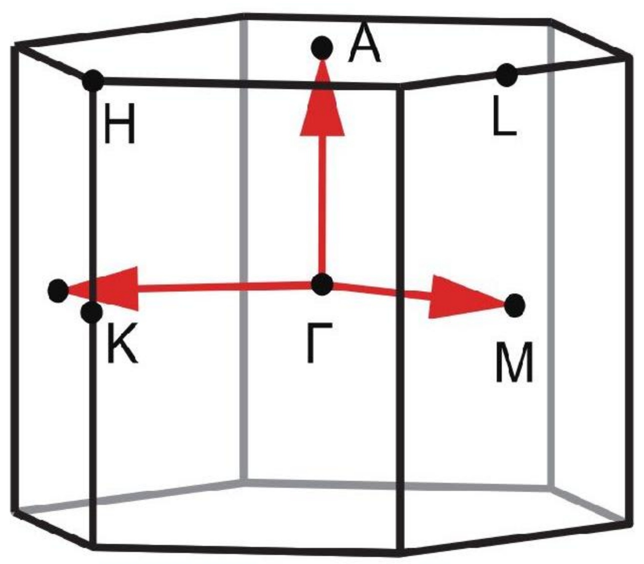
Zhang et al., arXiv:2503.22794

I. Break P&C_{nv} : Weyl phonon in chiral crystal (Te)

Chiral crystal Te:
C_3^1 screw rotation symmetry

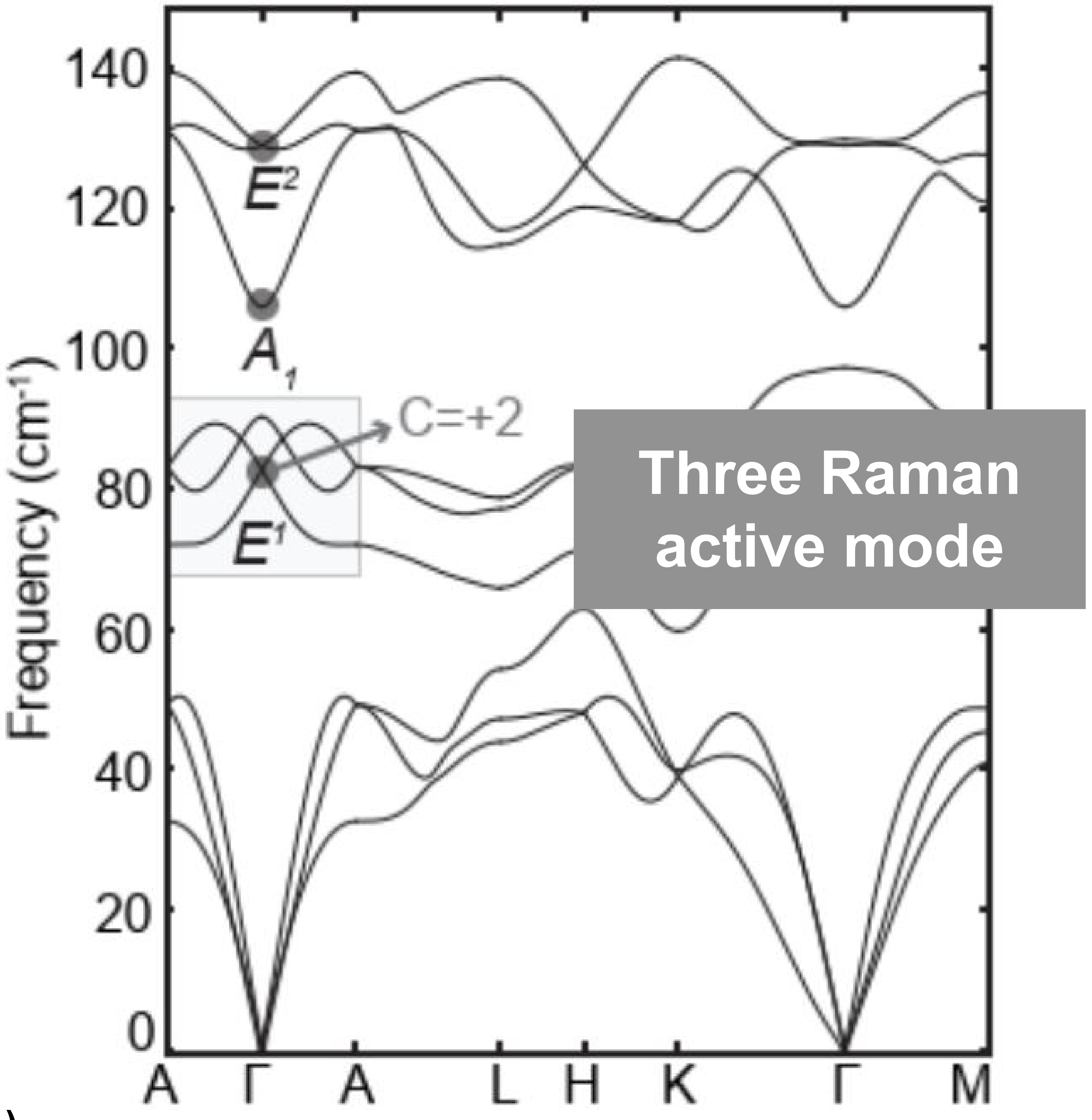


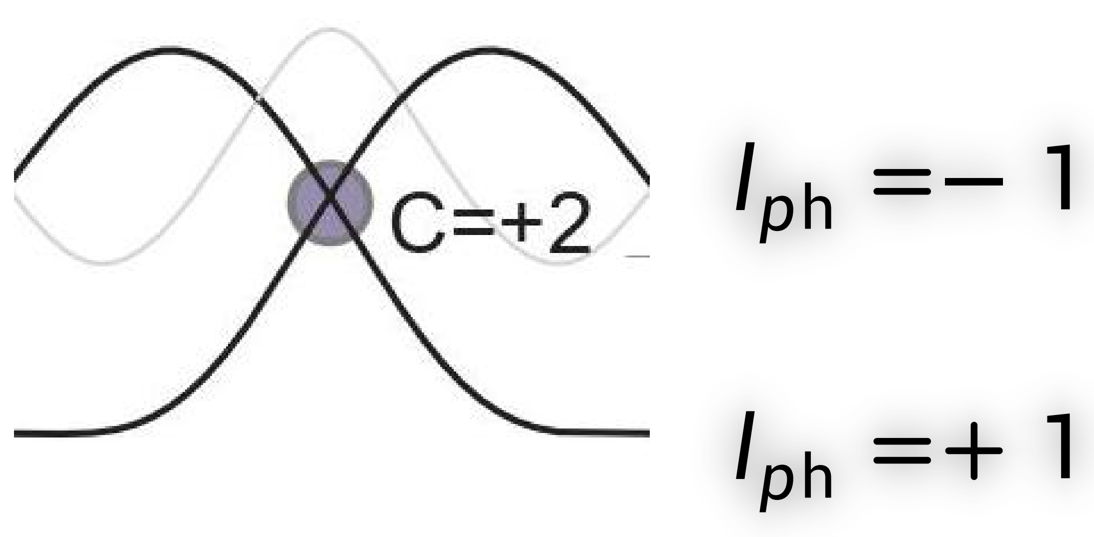
BZ of Te



Zhang and Murakami, PRR. 4, L012024 (2022)
Zhang et al., Nano Lett., 23, 7561–7567 (2023)

Phonon spectra of Te





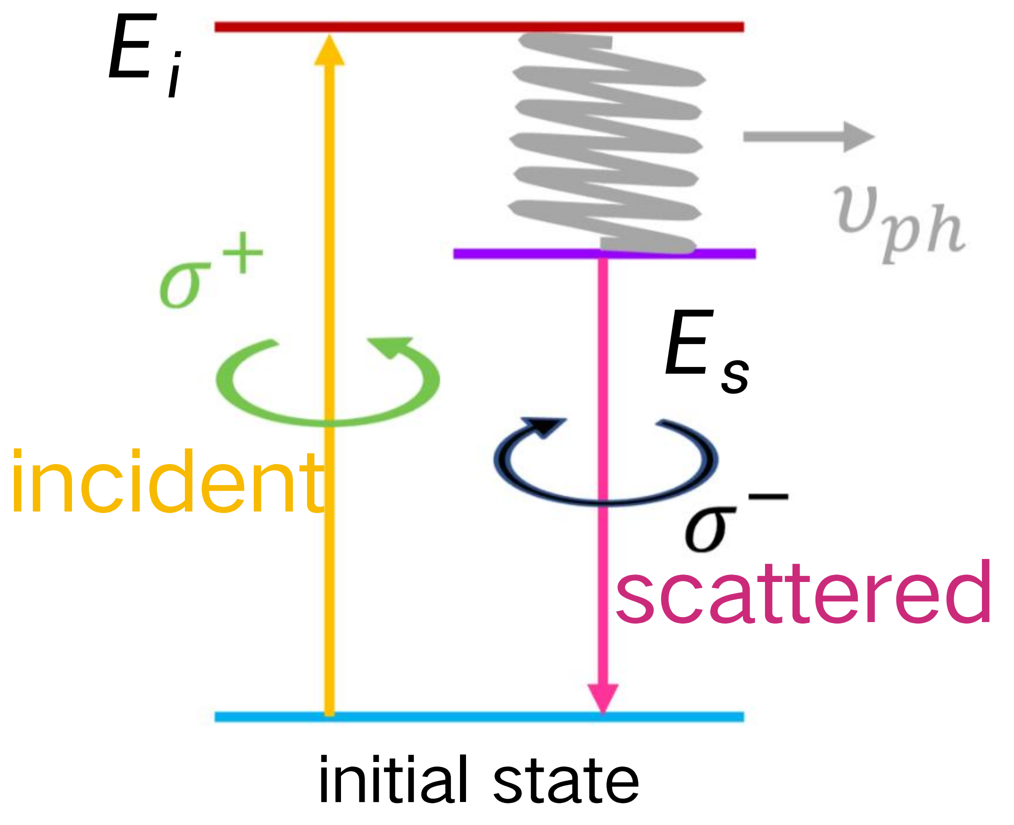
$C_\Gamma = 2$

How to observe/selectively excite phonons by I_{ph}?

C Fang, et al. PRL 108, 266802 (2012)
C Fang, et al. PRB 86, 115112 (2012)
Stepan et al., PRB 96, 045102 (2017)

I. Break P&Cnv : Weyl phonon in chiral crystal (Te)

Cross circular polarized Raman spectroscopy (c−CPRS)



conservation rules:

(1) momentum

(2) energy

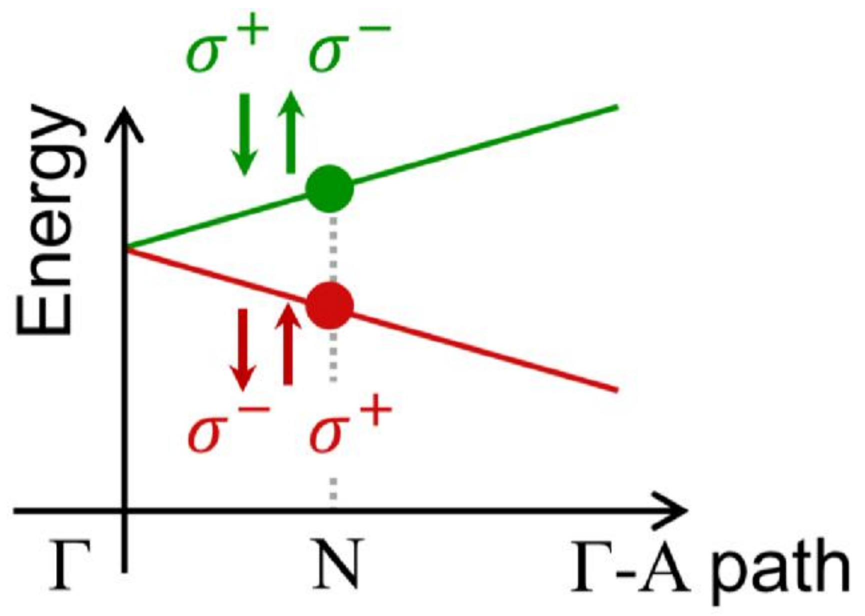
(3) pseudoangular momentum l_{ph}

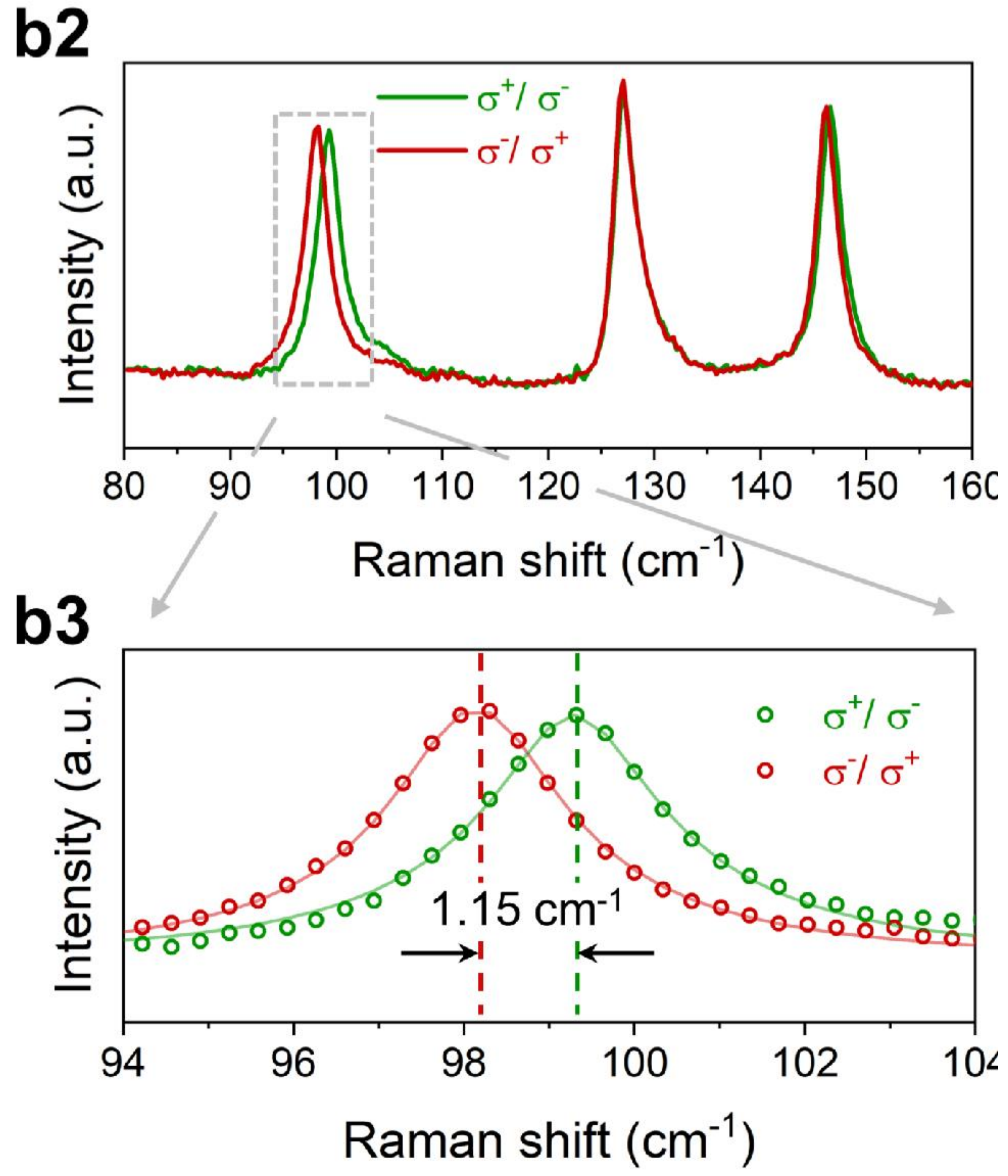
$k_{photon} = k_{ph}$

Raman shift = Weyl phonon frequency

$\triangle l_{photon} = l_{ph}$ (modulus n)

c-CPRS on Te: E¹ mode





Zhang, and Murakami. PRR 4, L012024 (2022)

Zhang et al., Nano Lett., 23,

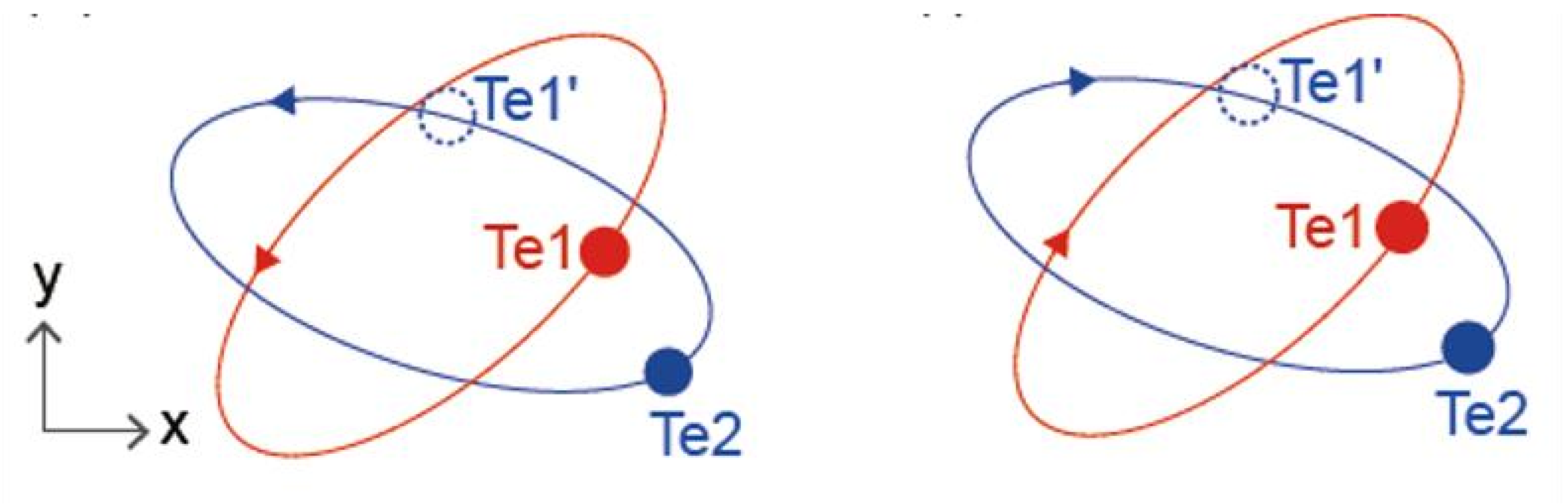
I. Break P&Cnv : Weyl phonon in chiral crystal (Te)

PAM: the relative phase between neighboring atoms.

The phase of Te1' is advanced/delayed comparing to Te2, so l_{ph} =+1/-1.

l_{ph} =+1 @momentum N

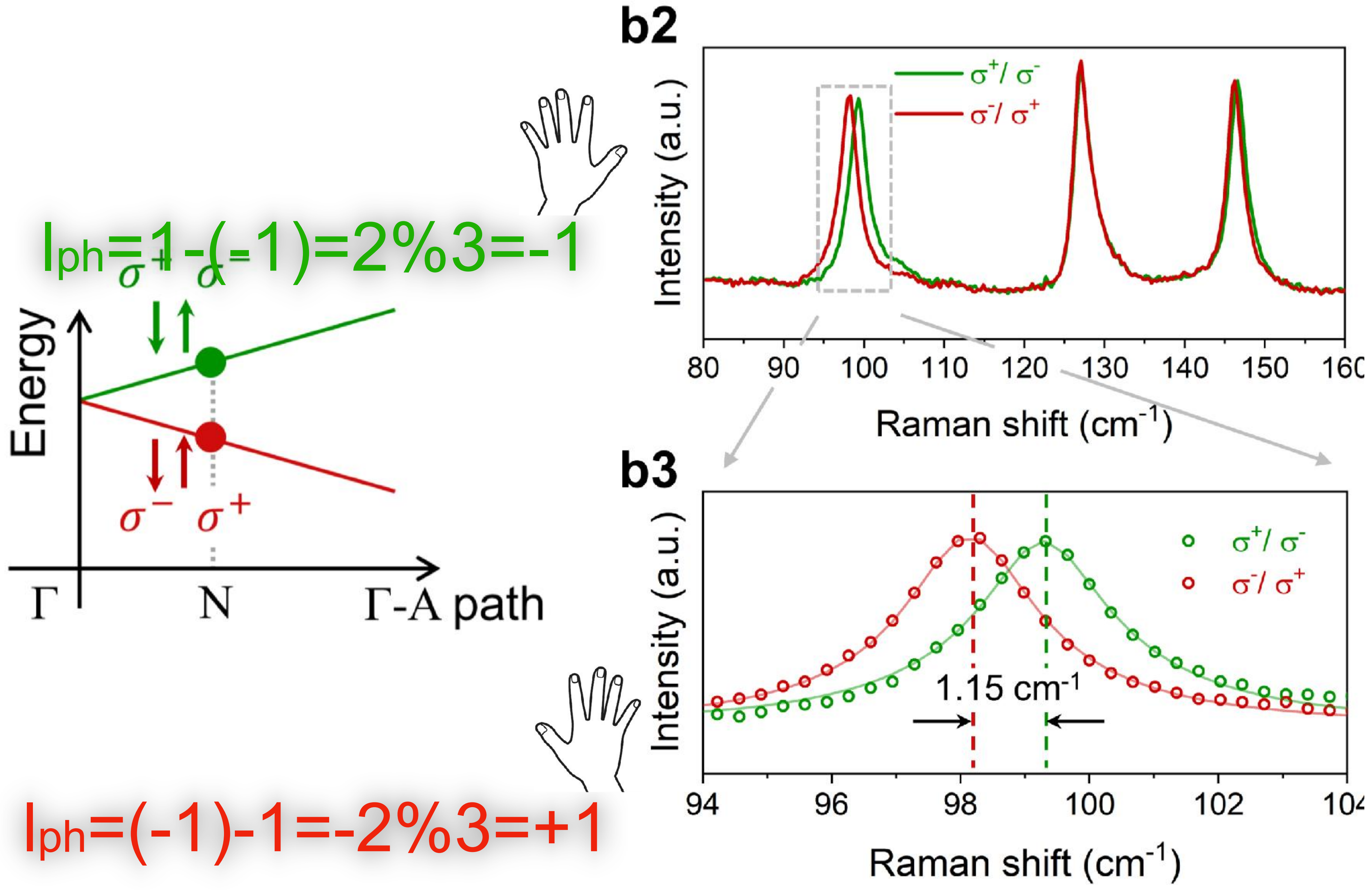
l_{ph} =-1 @ momentum N



$k_{photon} = k_{ph}$
Raman shift = Weyl phonon frequency
$\triangle l_{photon} = l_{ph}$ (modulus n)

c-CPRS on Te: E¹ mode

l_{ph}=1-(-1)=2%3=-1



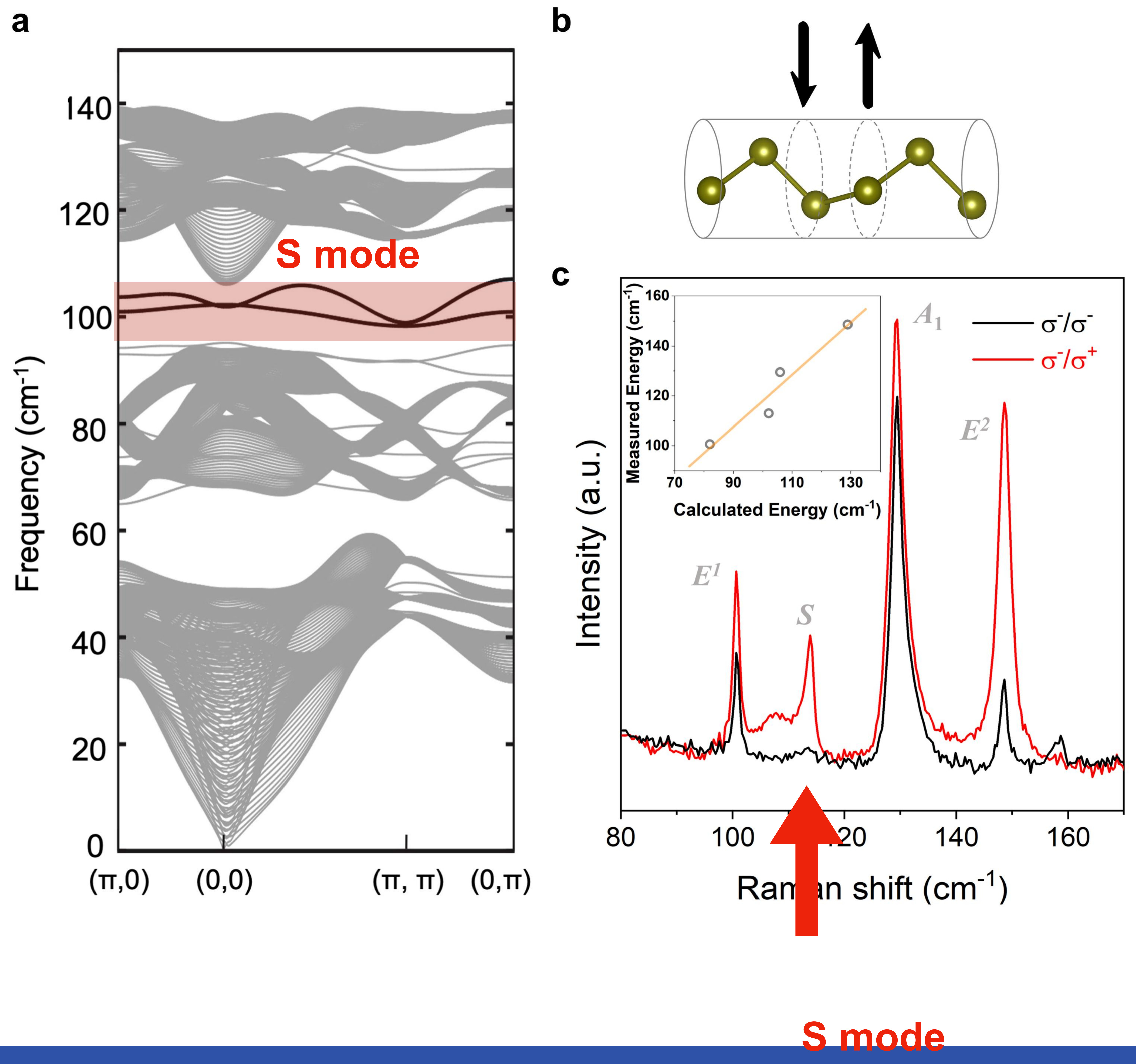
l_{ph}=(-1)-1=-2%3=+1

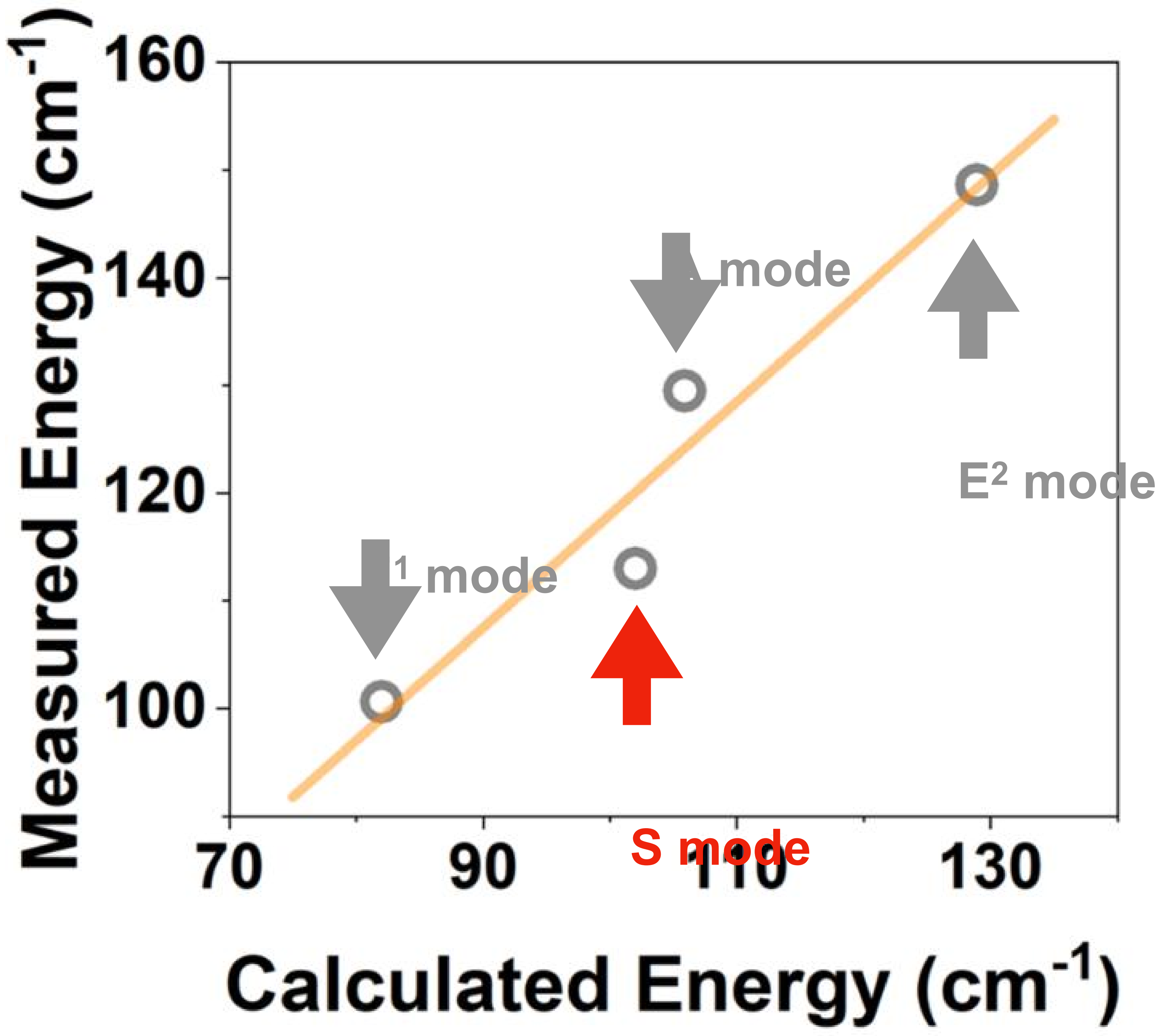
selectively screening phonons

Zhang, and Murakami. PRR 4, L012024 (2022)
Zhang et al., Nano Lett., 23, 7561–7567 (2023)

Observation for obstructed surface phonons in Te

“Obstructed atomic insulator”-like surface phonon

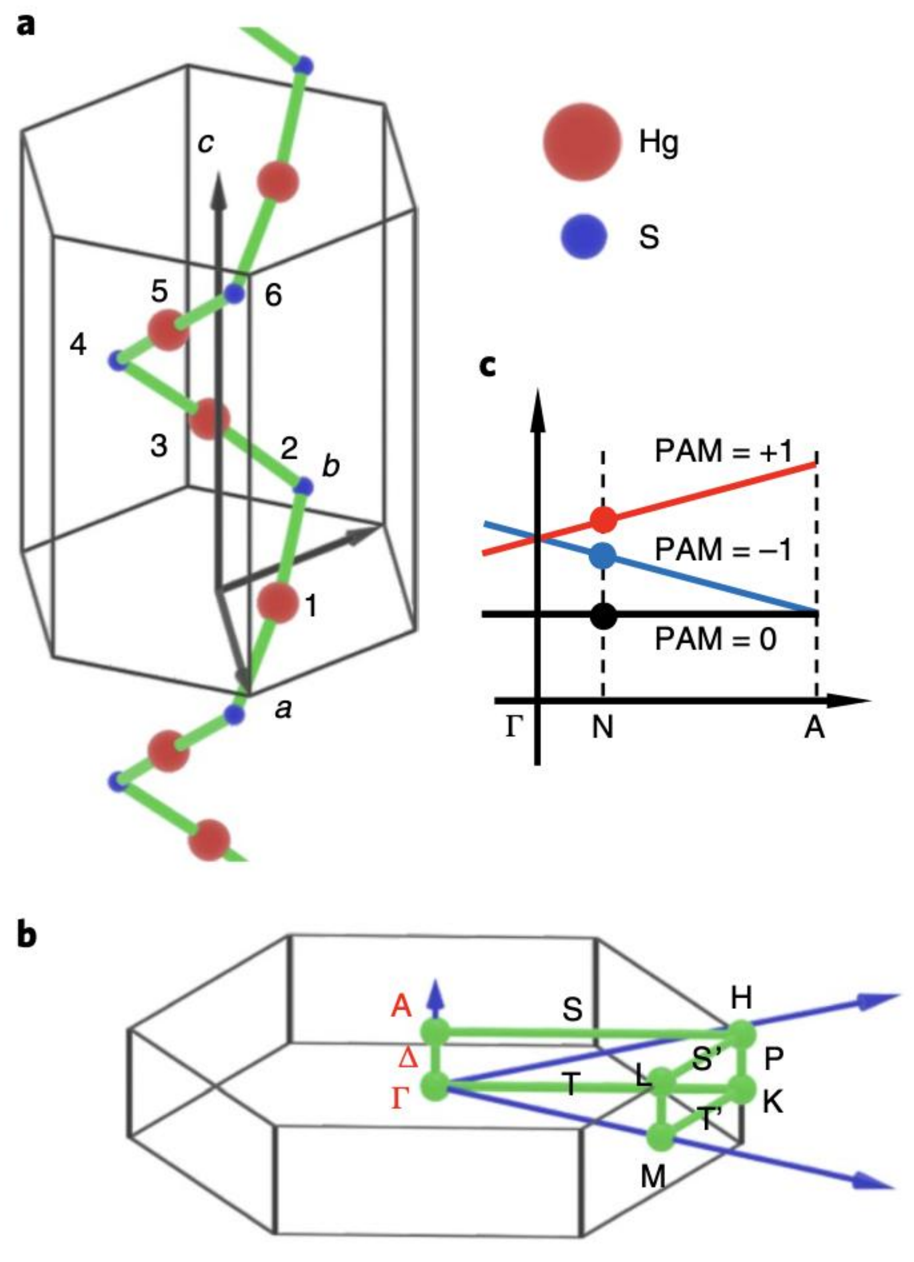


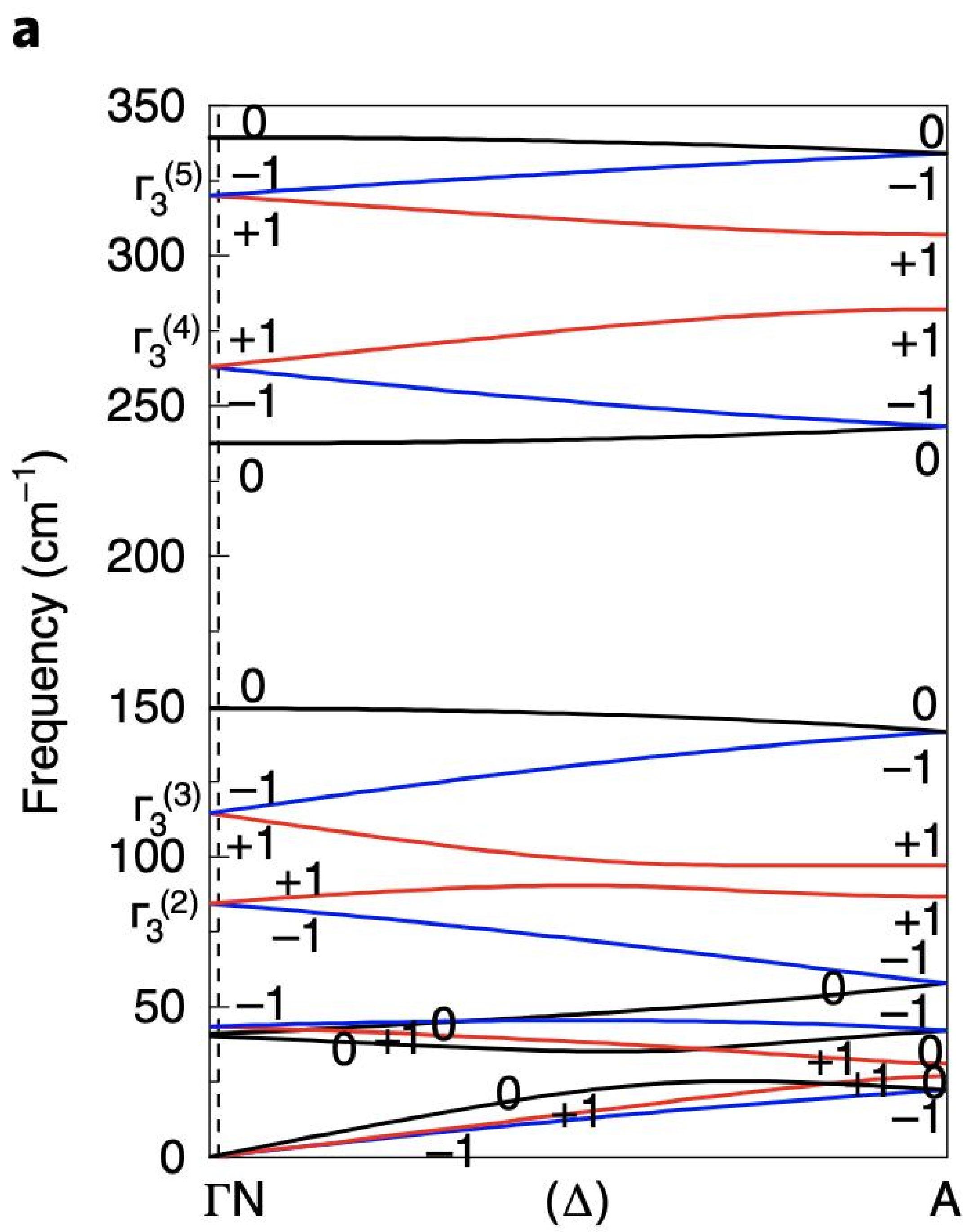


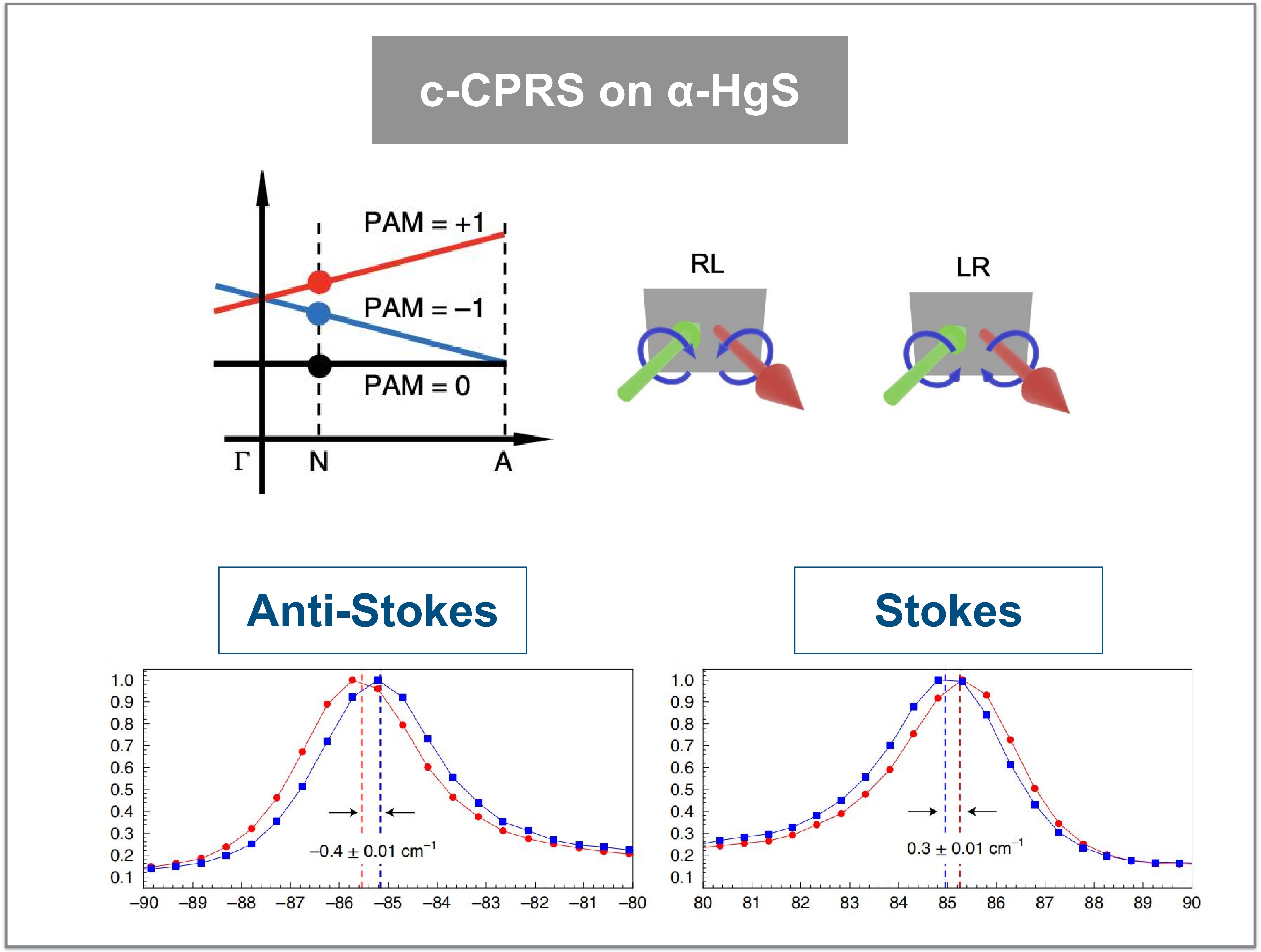
Zhang and Murakami, PRR. 4, L012024 (2022)
Zhang et al., Nano Lett., 23, 7561–7567 (2023)

I. Break P&Cnv : Weyl phonon in chiral crystal (α-HgS)

- Same space group with Te, chiral crystal
- C_3^1 screw rotation symmetry



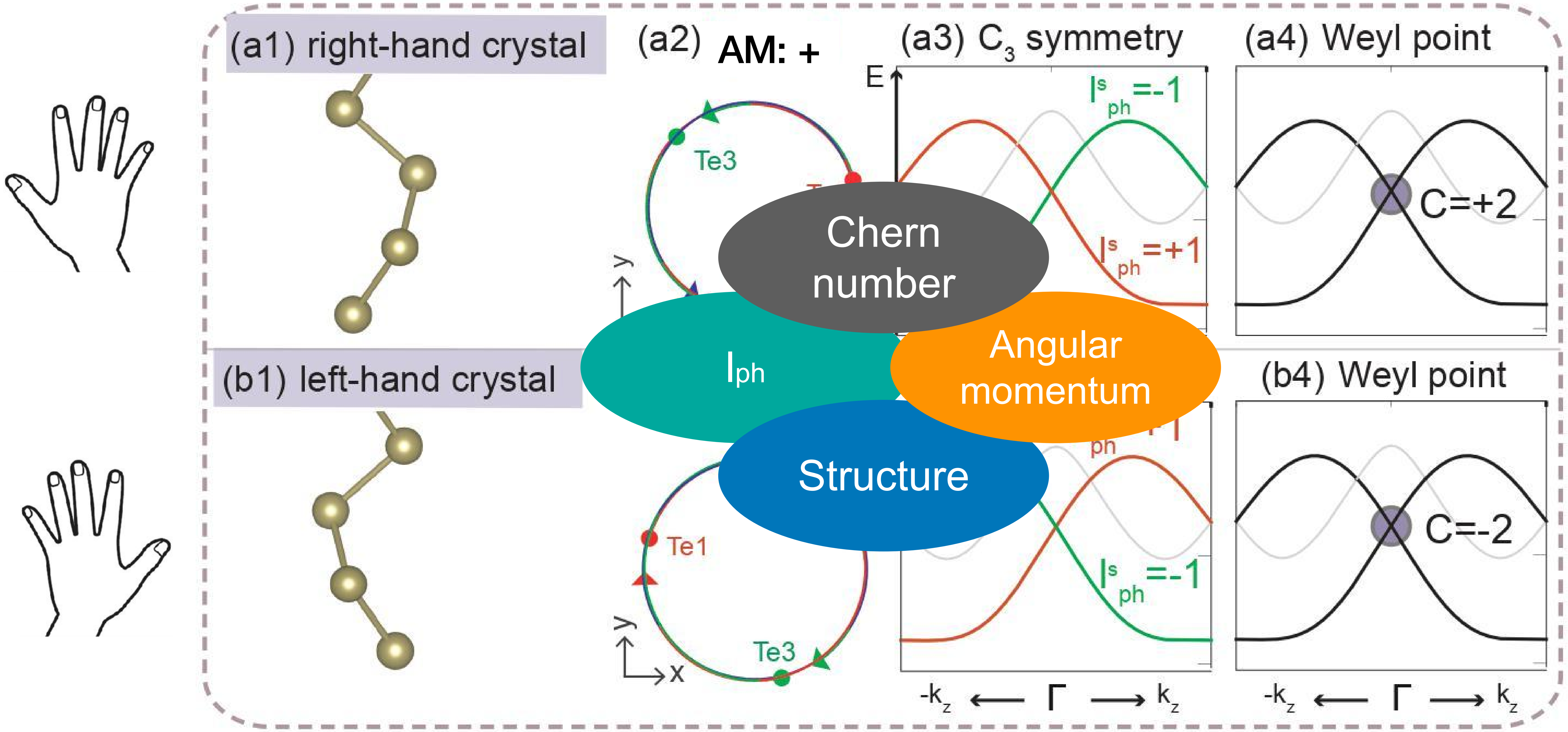




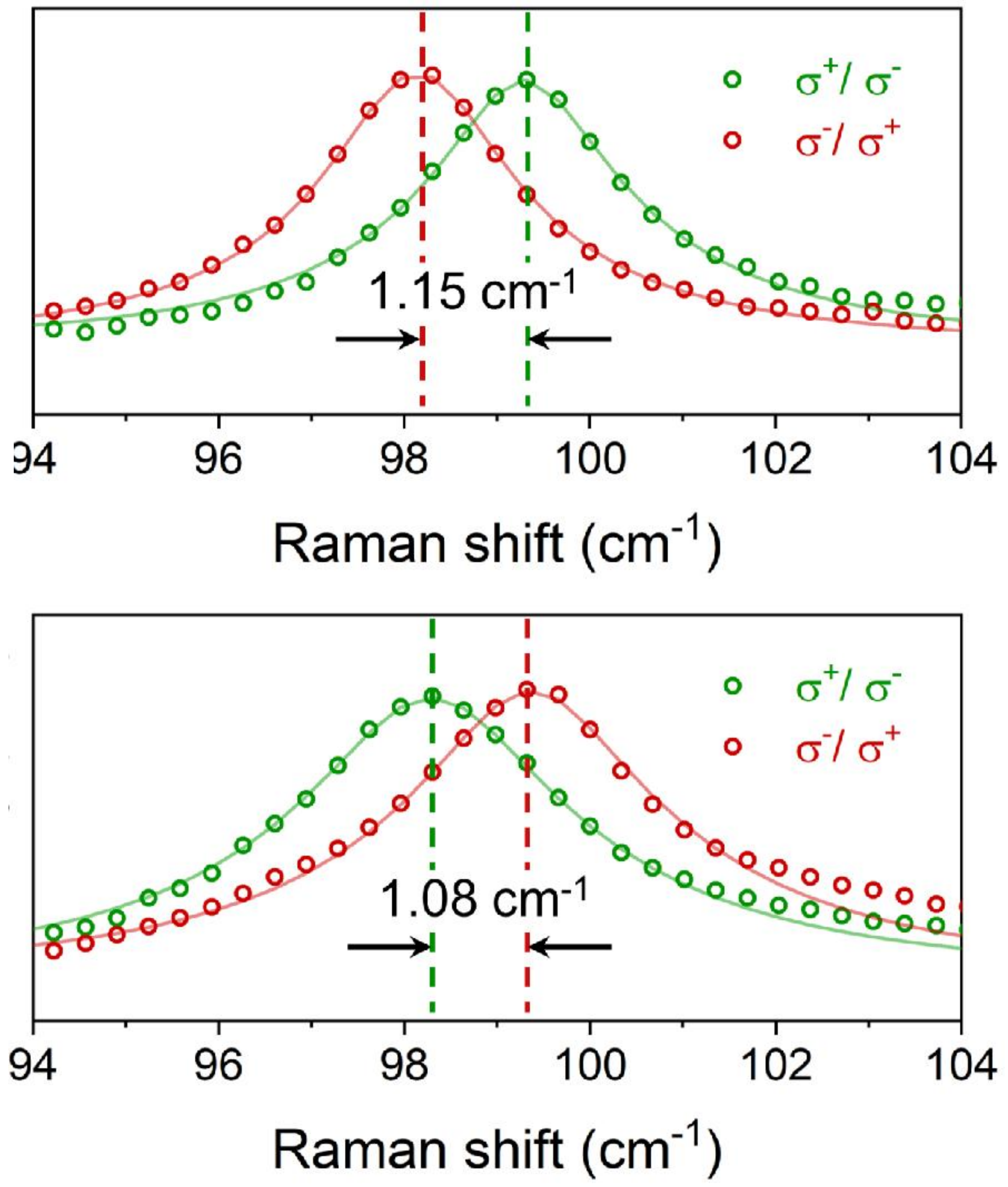
Ishito, … Zhang … et al. Nat. Phys. 19, 35–39 (2023)
Ishito K, Mao H, Kobayashi K, et al. Chirality, 35: 338-345 (2023)

Two enantiomers for Te

Zhang and Murakami. PRR 4, L012024 (2022)
Zhang et al., Nano Lett., 23, 7561–7567 (2023)

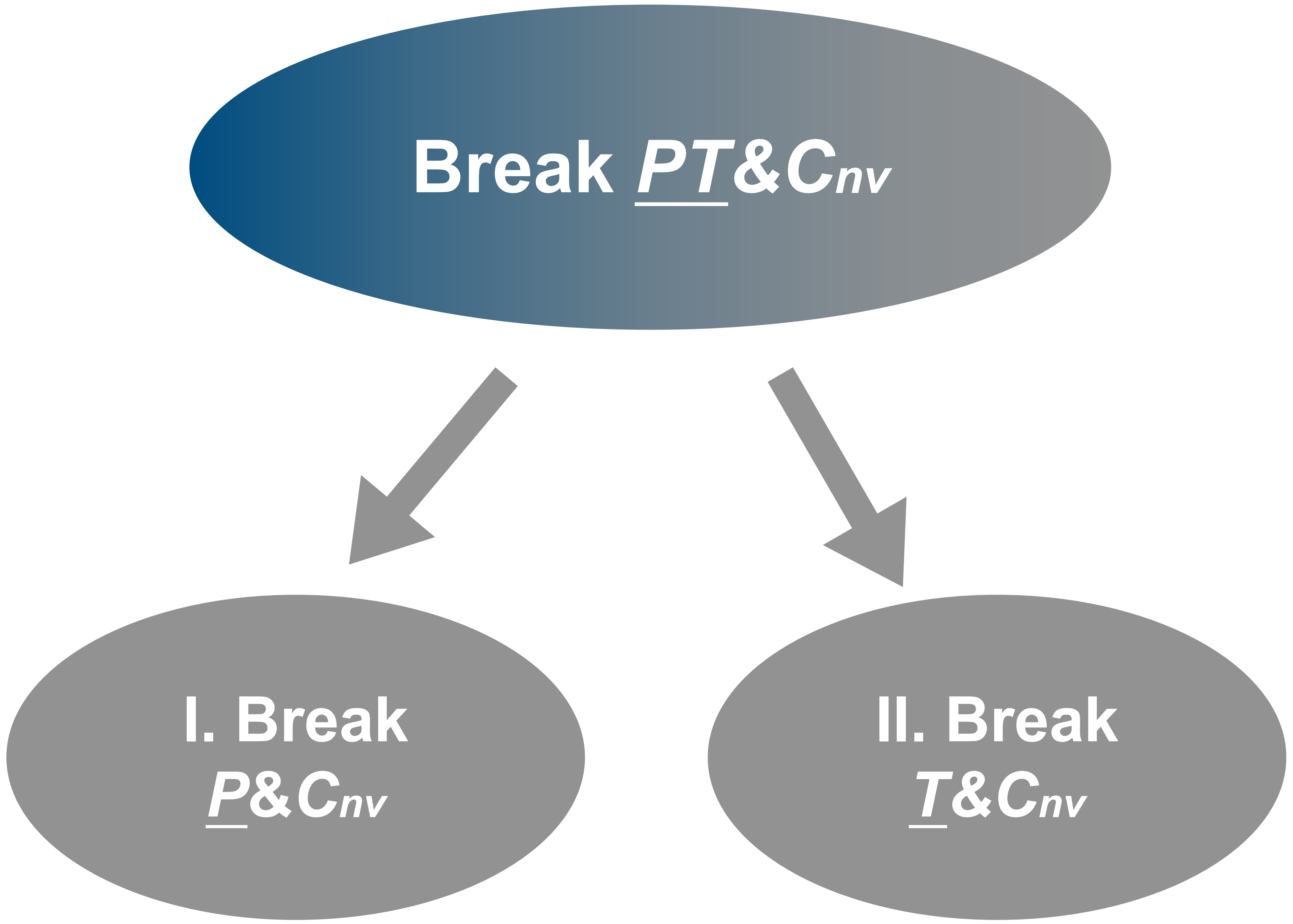


c-CPRS on Te

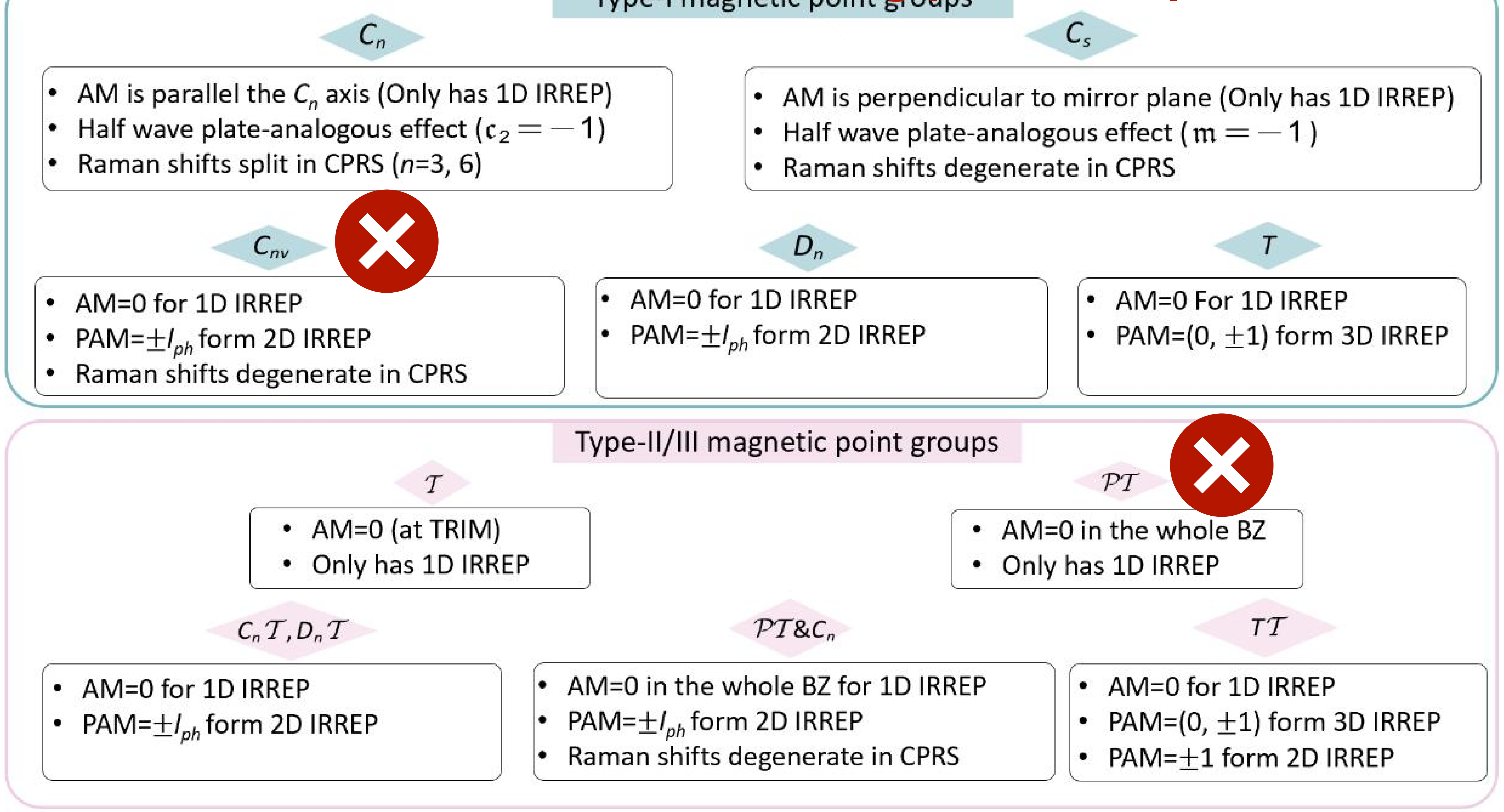


One can use any of the quantities above to identify the chirality of crystals

Way to obtain circularly polarized phonons



Consider the Raman scattering process: *q* ~ 1% BZ

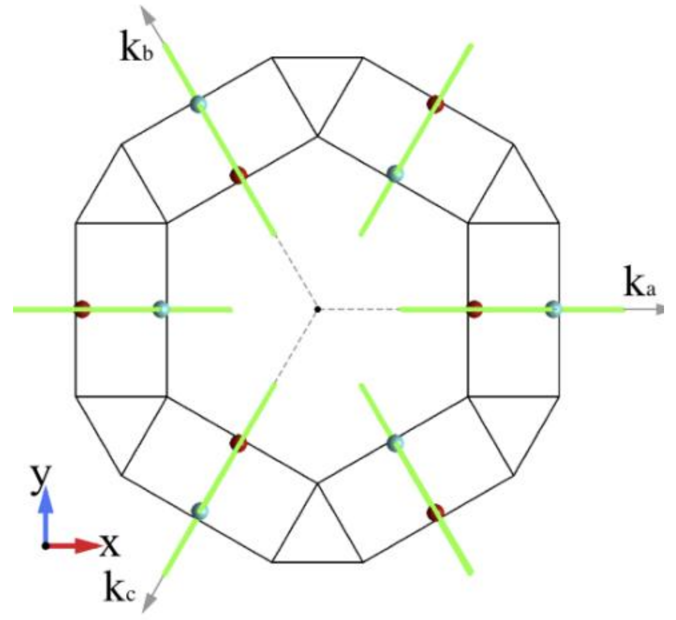


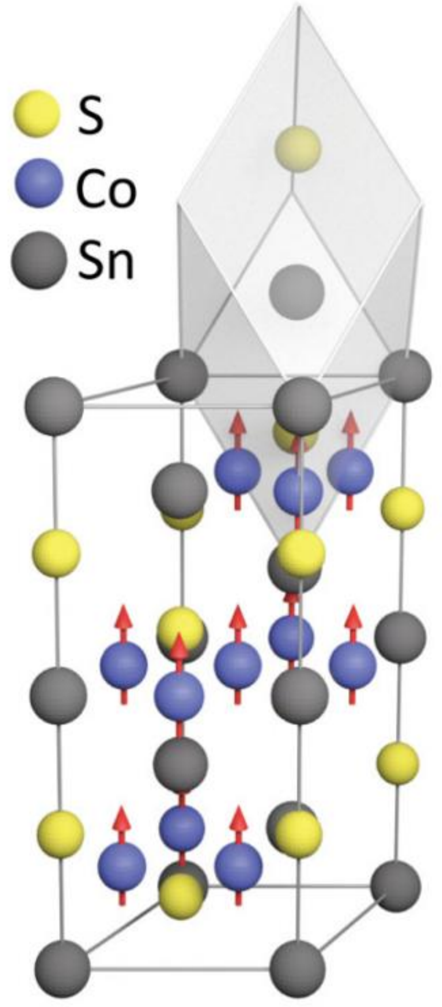
Zhang et al., arXiv:2503.22794

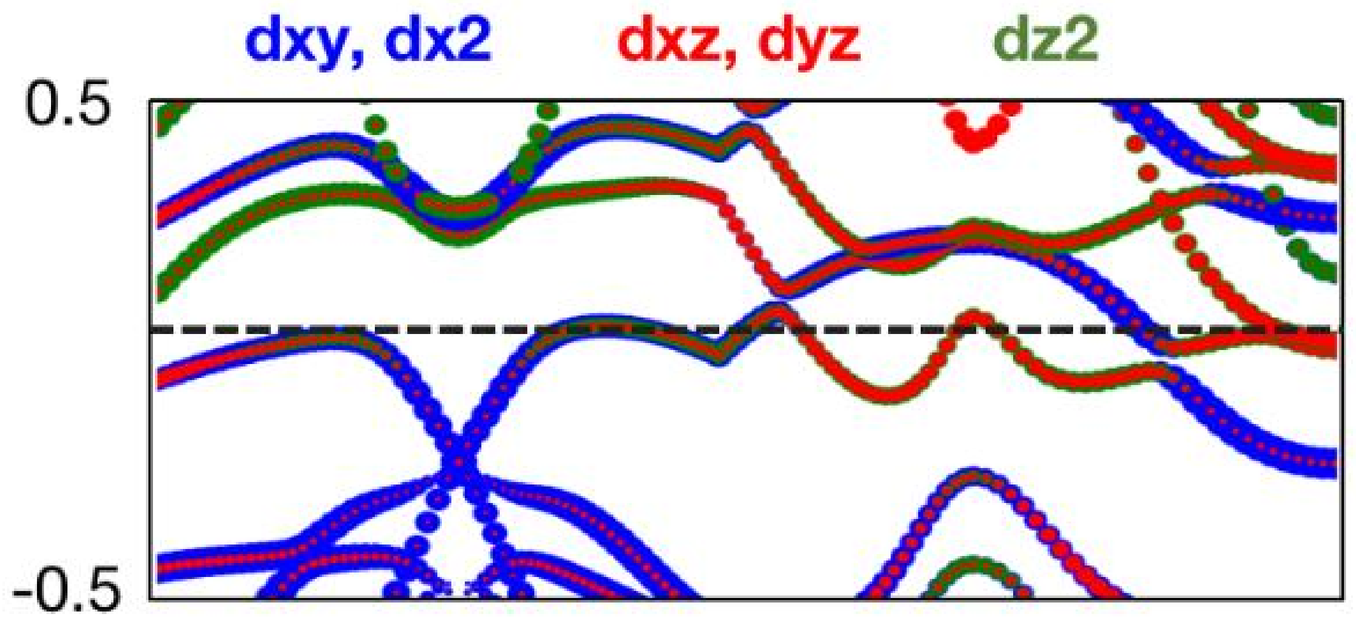
II. Break T&Cnv : Magnetic order-induced phonon splitting in Weyl semimetal

Co3Sn2S2 #166, R-3m

FM Weyl semimetal
Tc~177K

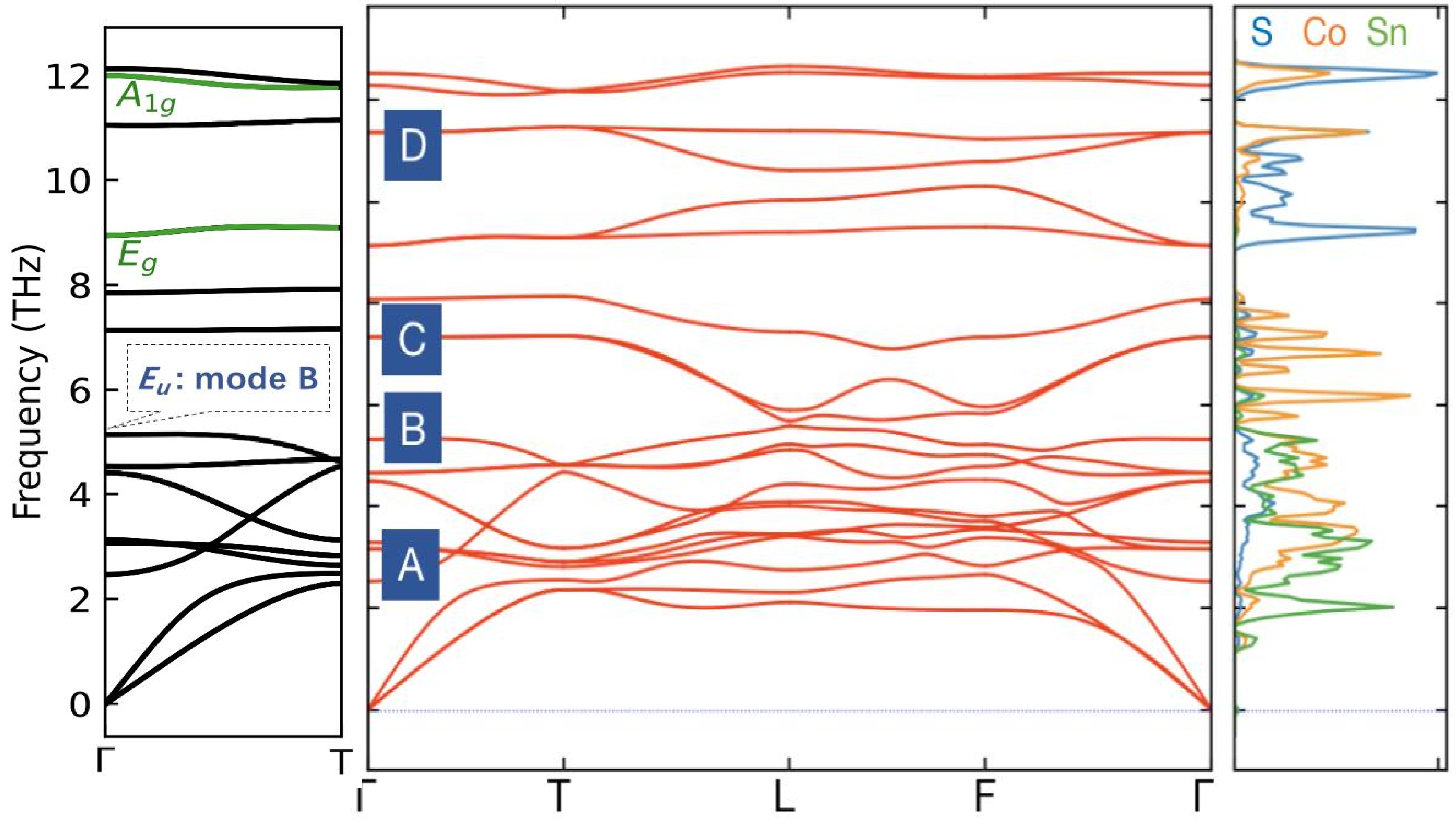






Inversion-symmetric

2 Raman active + 9 infrared active

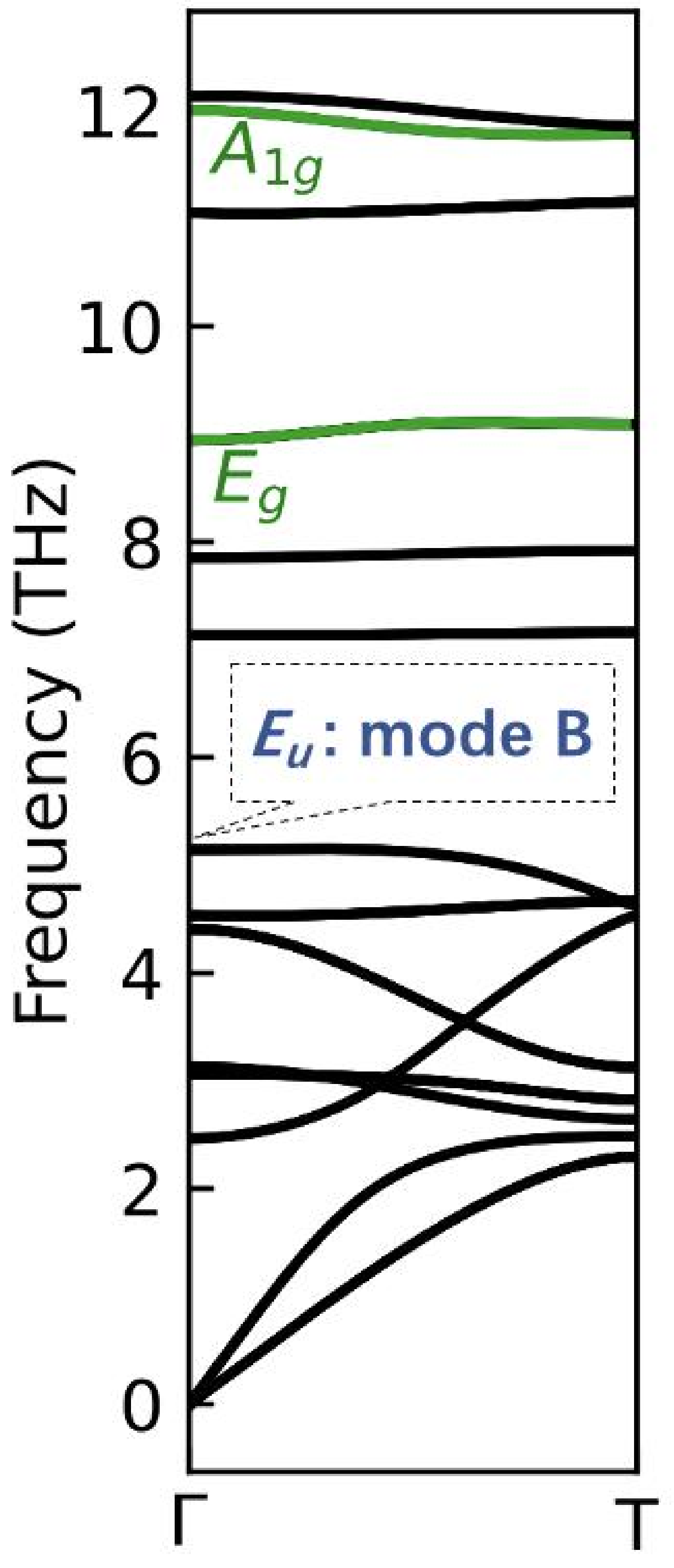


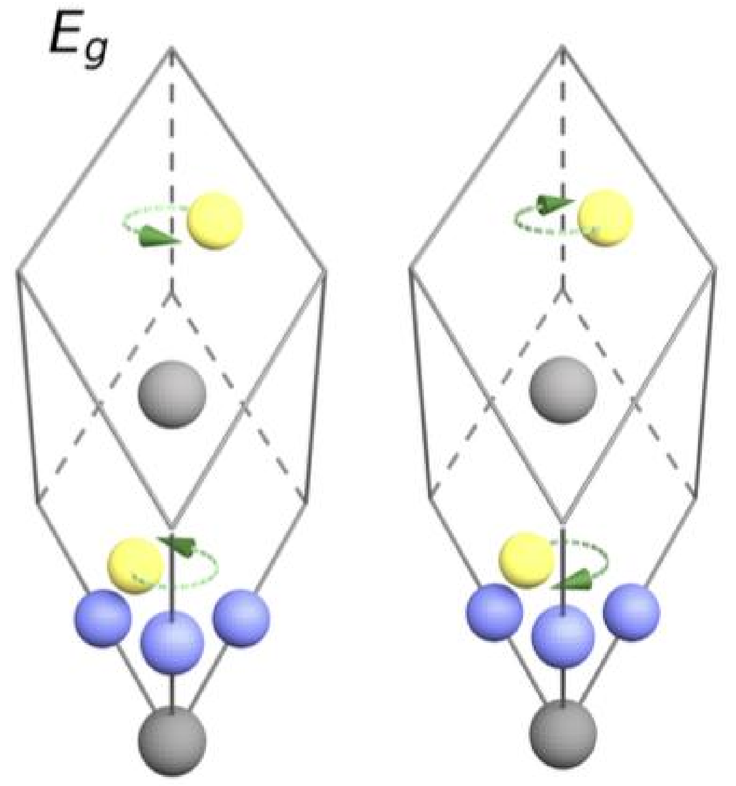
Xu et al., PRB 97, 235416 (2018)
Wang, et al., NatCommun, 9, 1-8 (2018)
Liu, et al., Science, 365, 1282-1285 (2019)

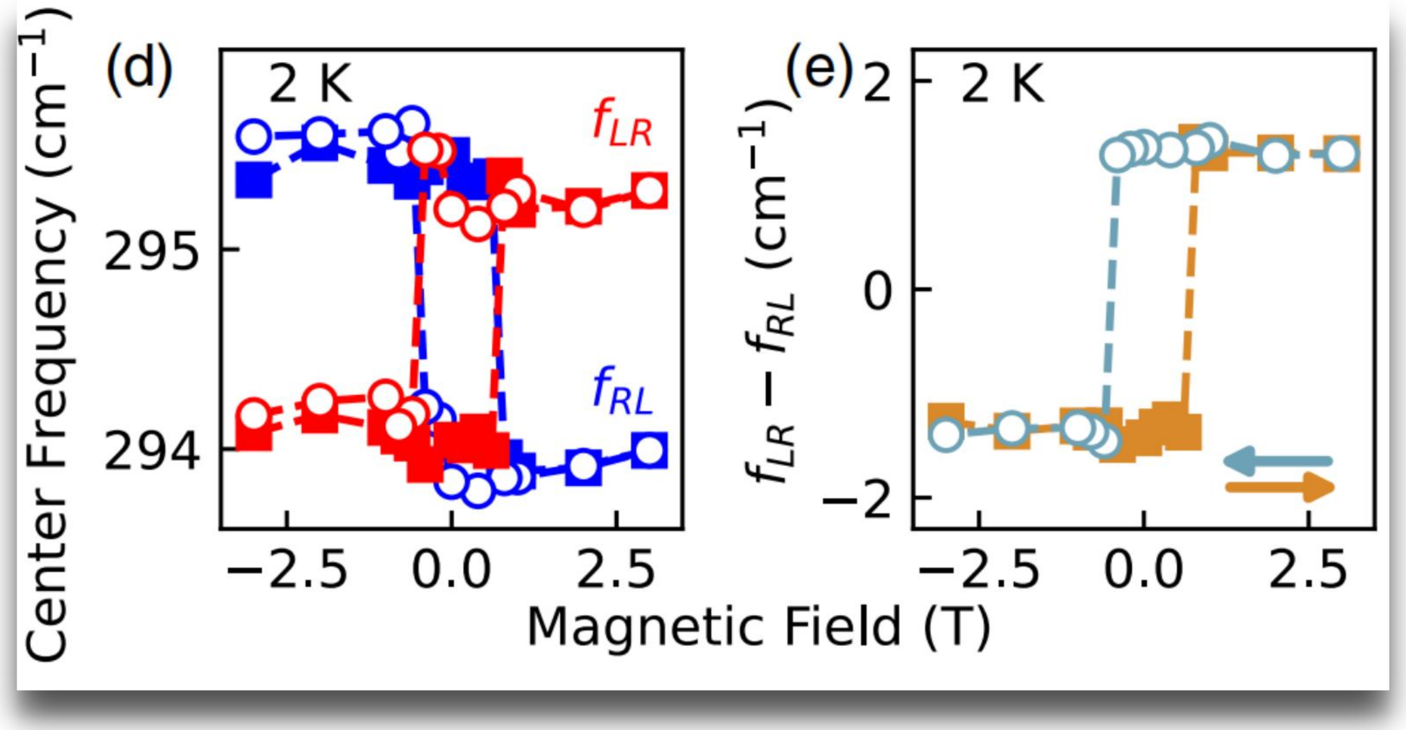
Yang, … Zhang*, Dressel*, PRL 134, 196905 (2025)
Che, … Zhang*, Yang*, PRL 134, 196906 (2025)

Phonon splitting on Raman active modes: Eg

Raman active modes: E_g+A_{1g}

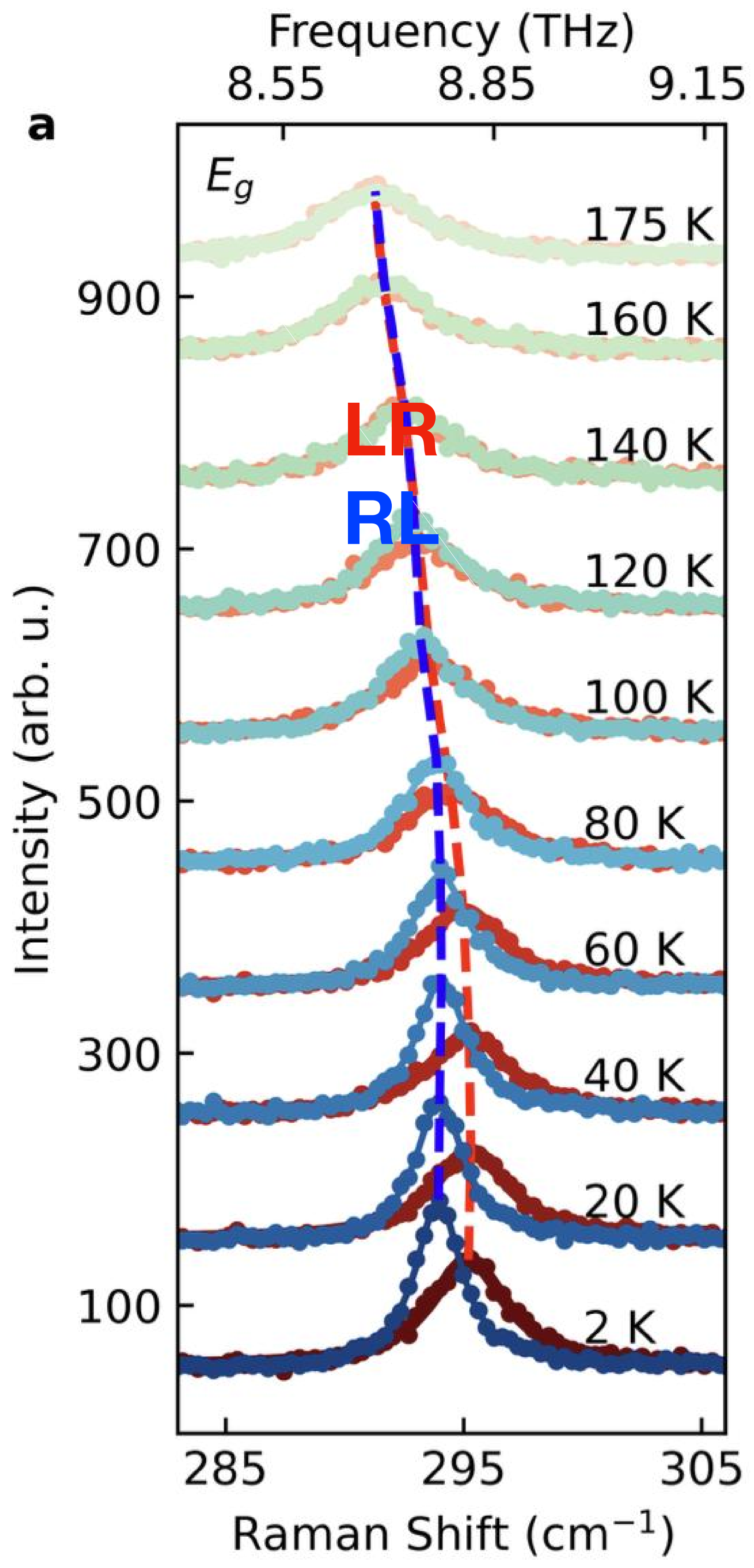


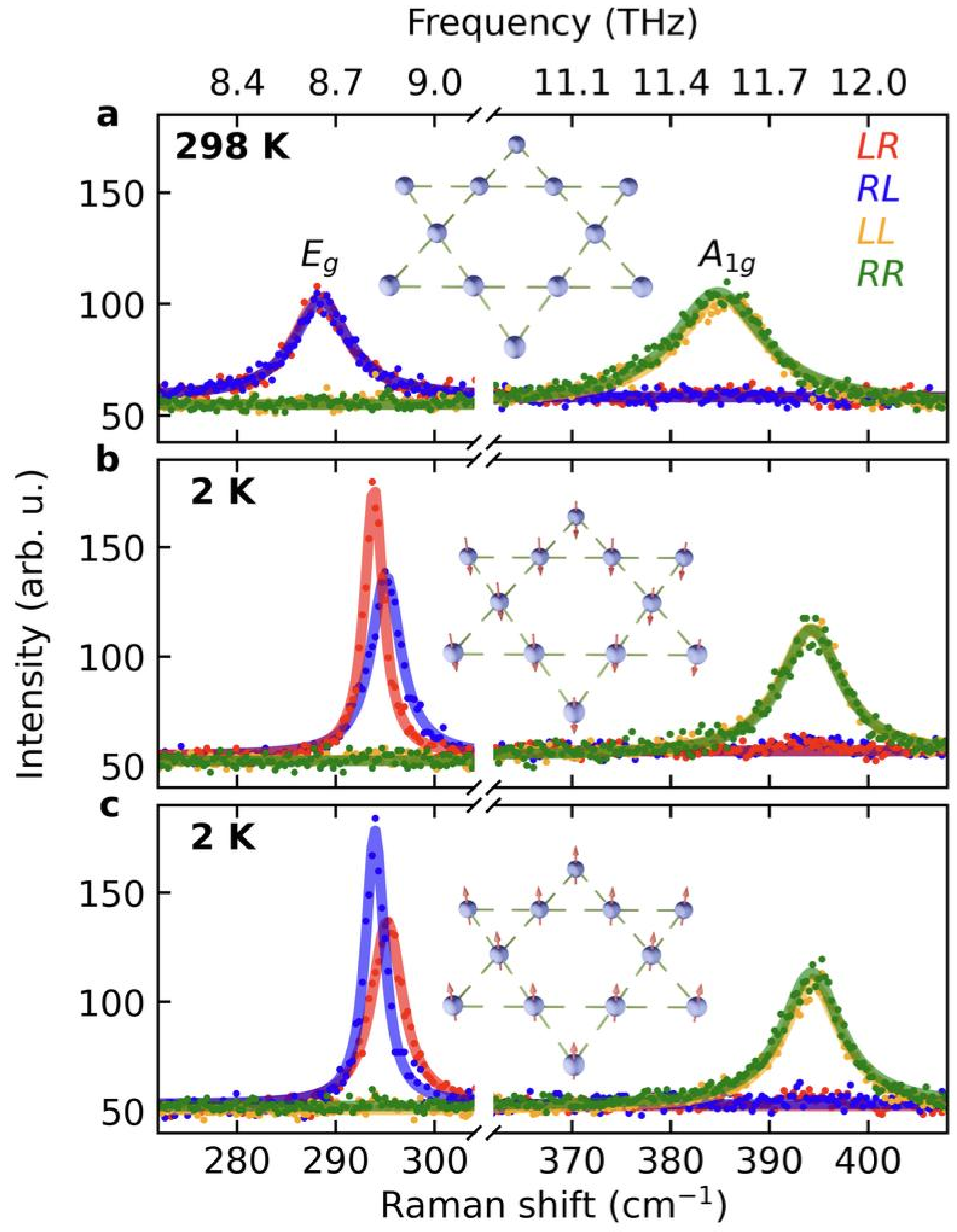




Break T&C3v

Magnetic ordered induced phonon splitting
Different from CeCl3、Fe2Mo3O8、CoTiO3, et al.

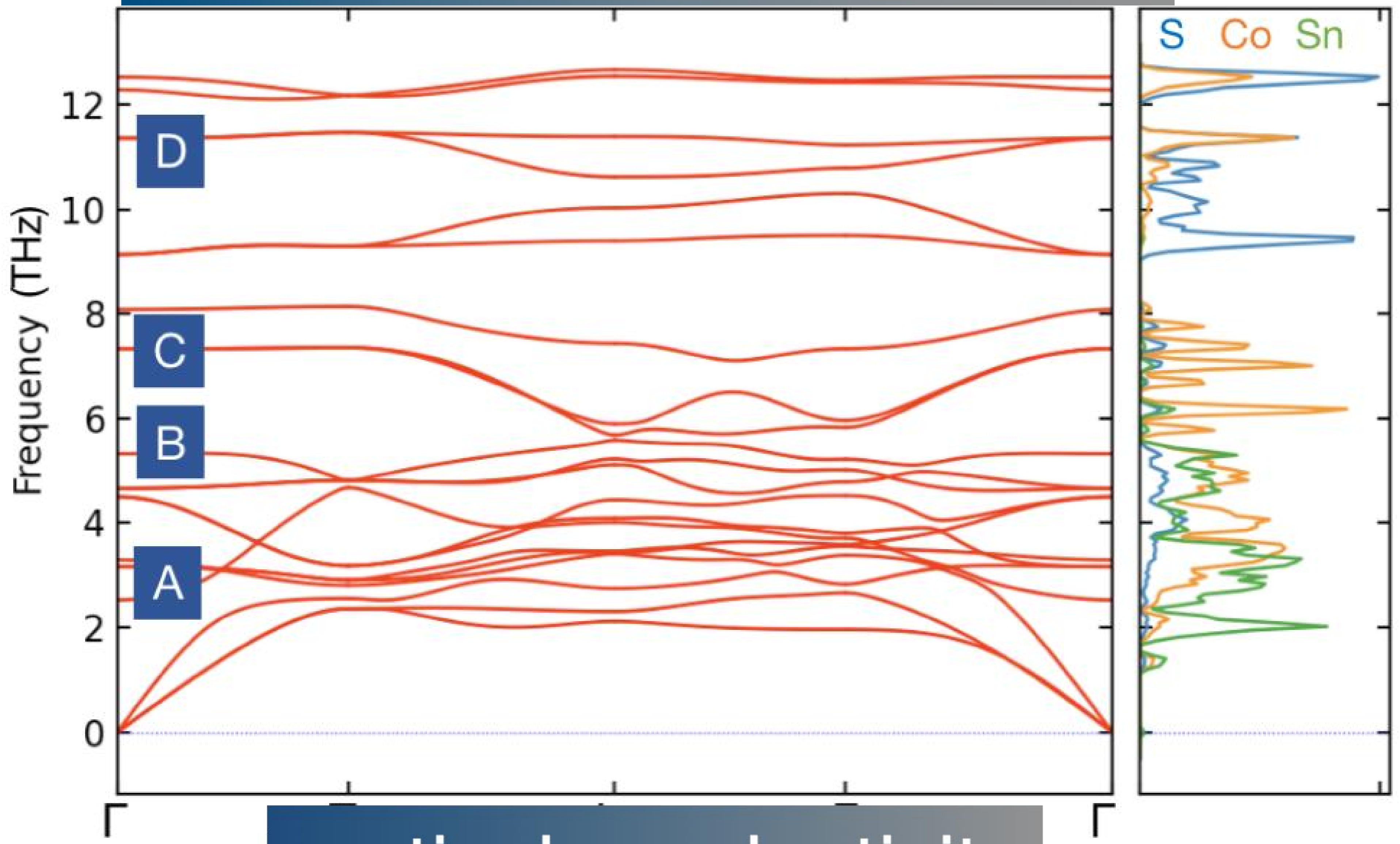




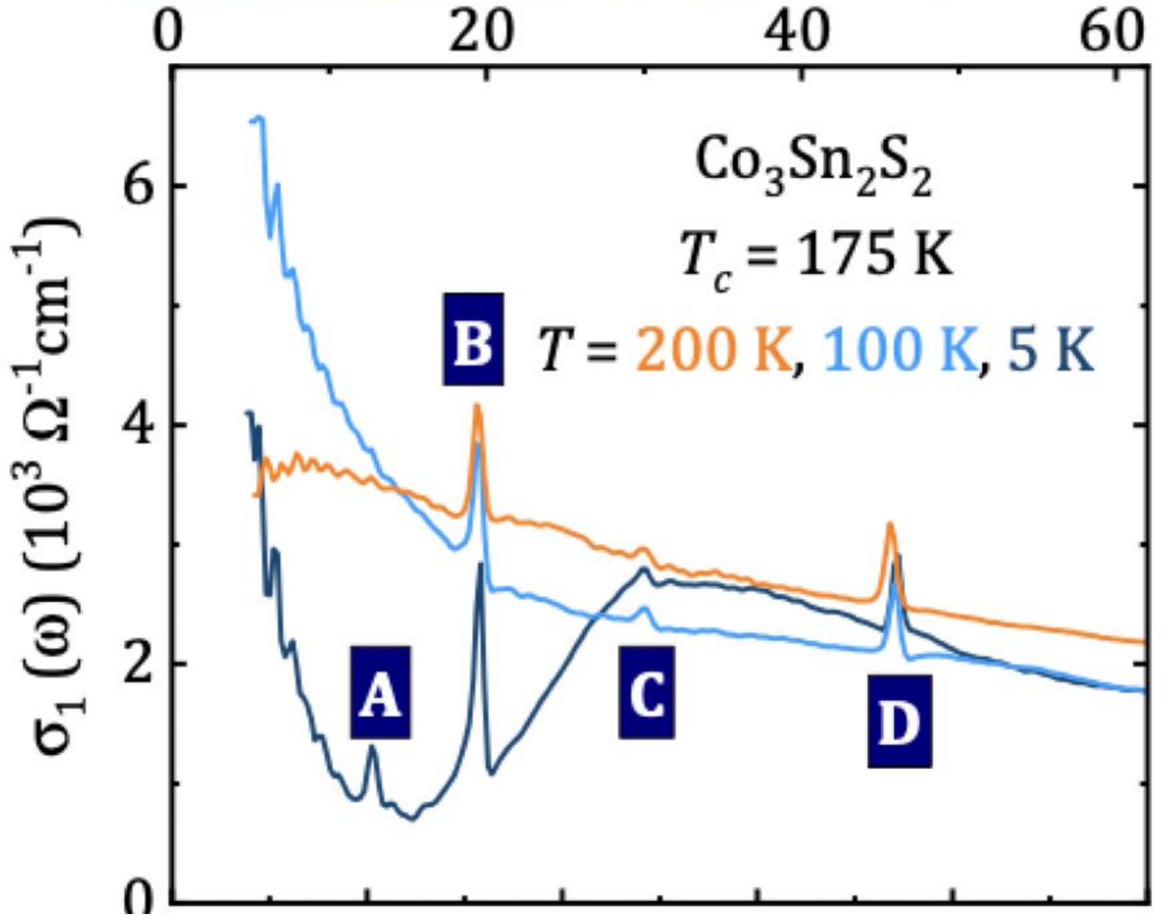
Che, … Zhang*, Yang*, PRL 134, 196906 (2025)
Zhang et al., arXiv:2503.22794 (2025)

Phonon splitting on infrared active modes: Eu

Infrared active modes: E_u



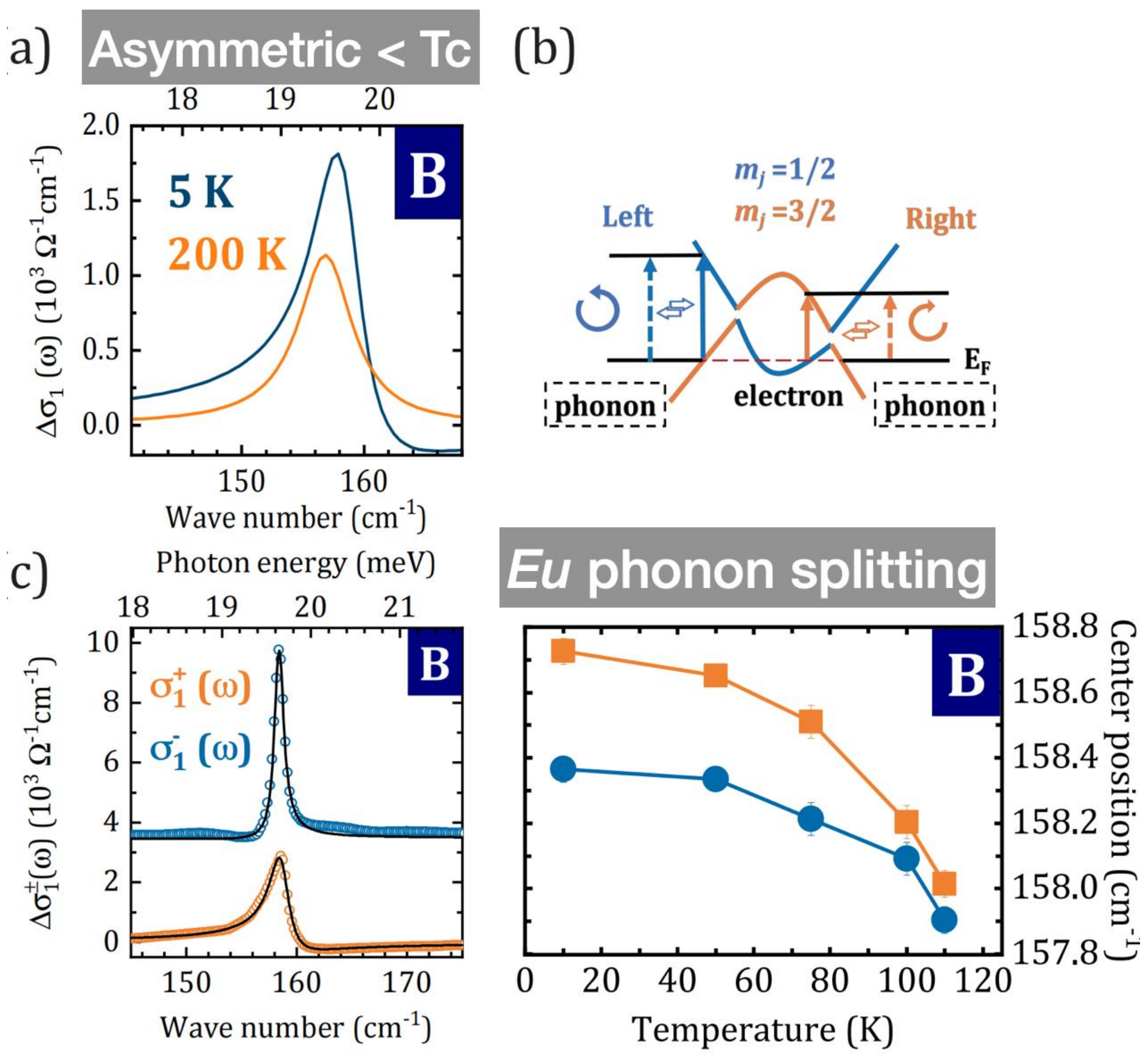
optical conductivity



circular dichroism (<Tc)

Strong
ele-ph coupling

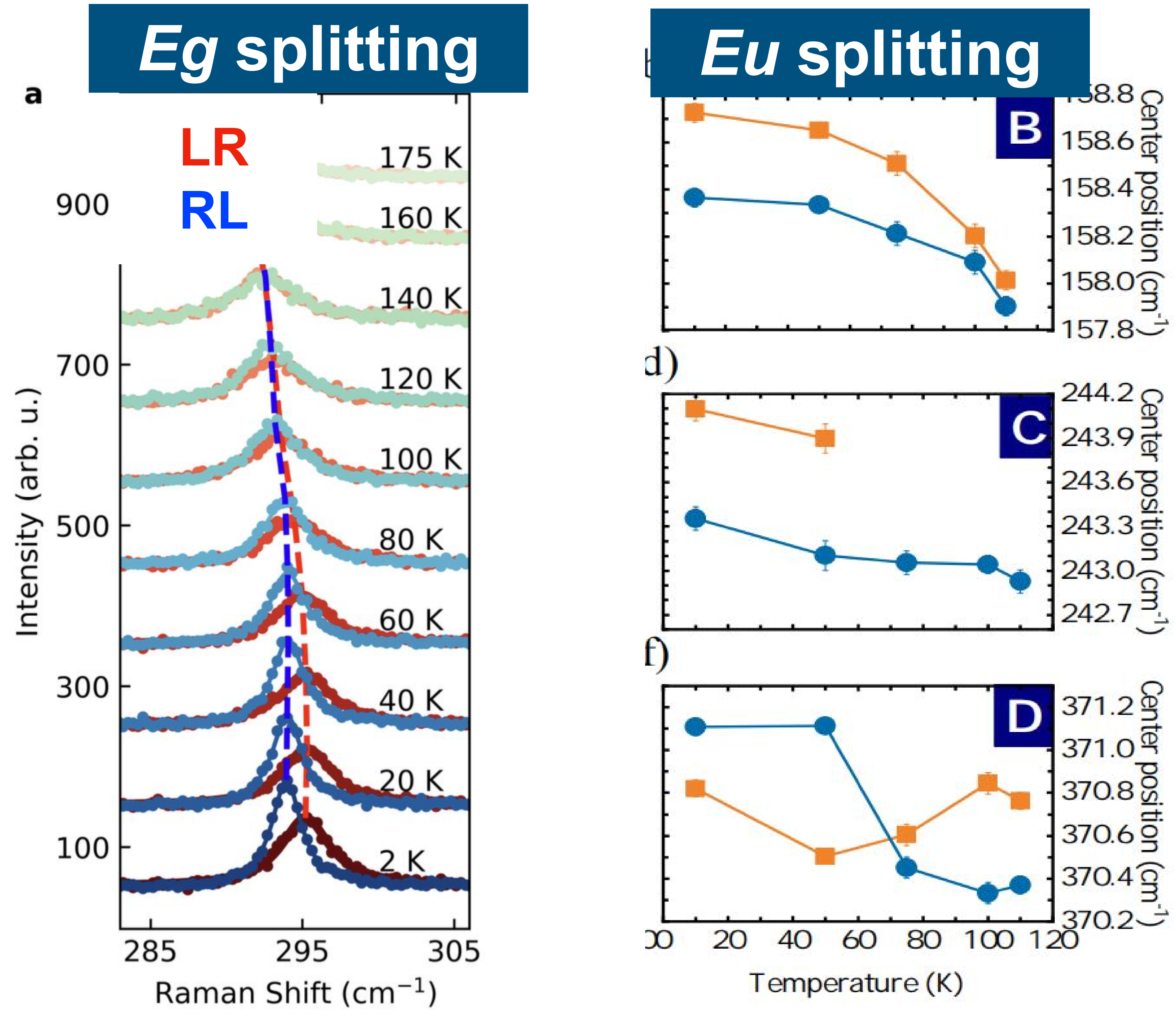
Eu splits,
two chiral phonons have
Diferent frequency,
ele-ph coupling



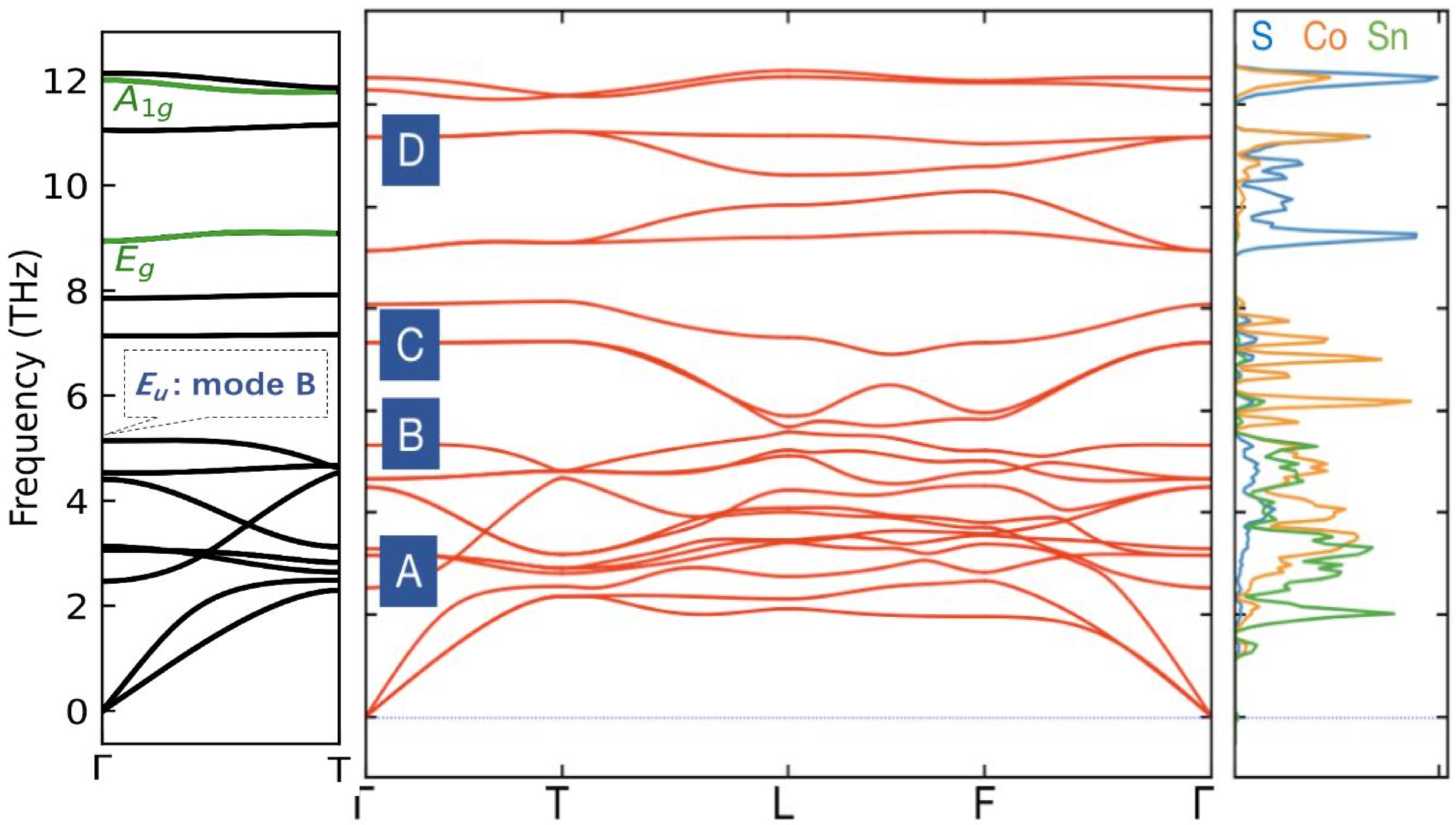
Yang, … Zhang*, Dressel*, PRL 134, 196905 (2025)
Zhang et al., arXiv:2503.22794 (2025)

Phonon splitting in Co3Sn2S2

FM order → Strong EPC —> chiral phonon splitting



2 Raman active + 9 infrared active



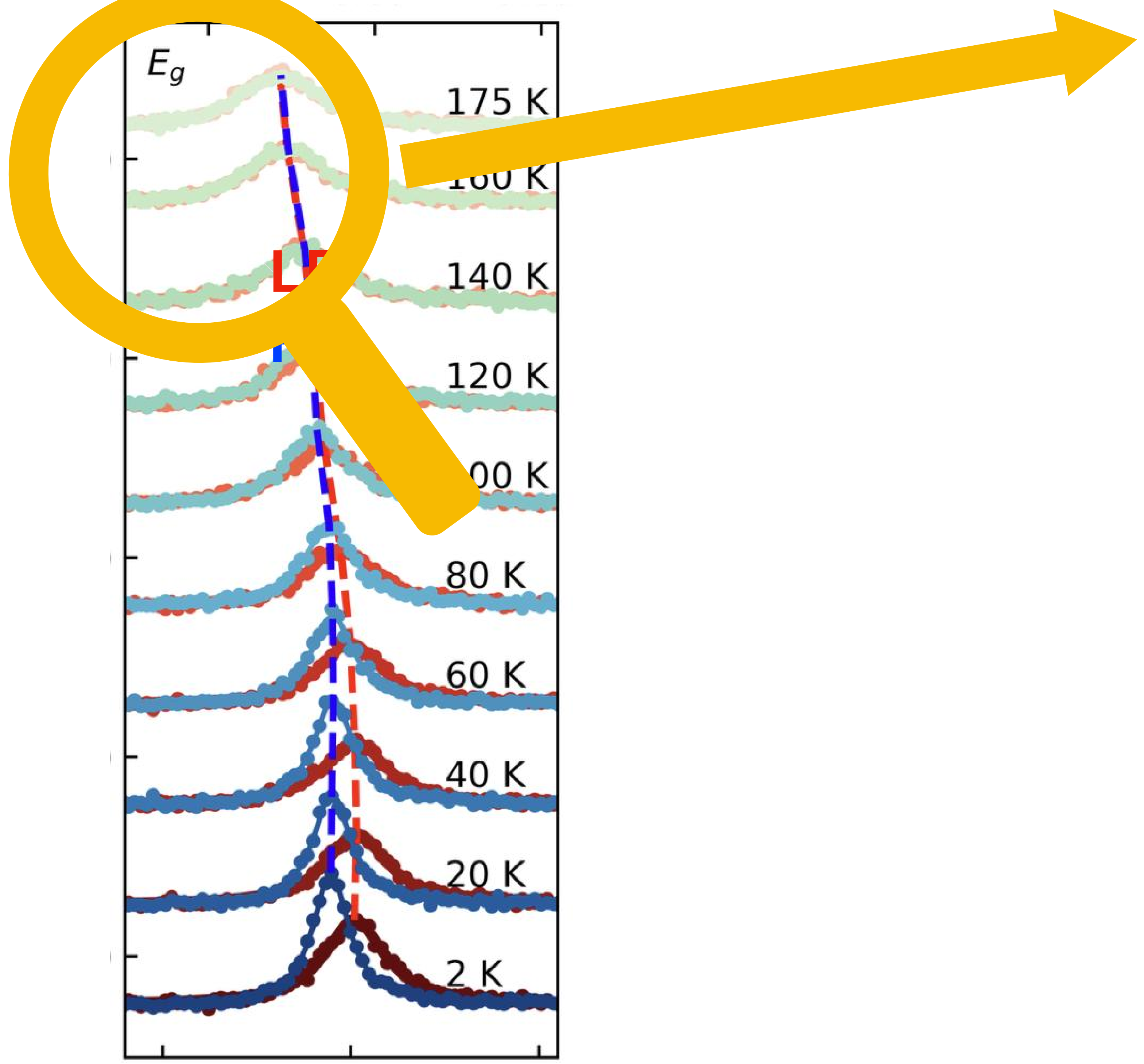
DFT algorithm on the phonon splitting is in preparation, based on the molecular Berry curvature theory.

Yang, … Zhang*, Dressel*,PRL 134, 196905 (2025)
Che, … Zhang*, Yang*, PRL 134, 196906 (2025)
Zhang, … Zhang*, arXiv:2503.22794 (2025)

Symmetry constrains on Eg mode under Cn

AM and PAM (l_{ph}) are not inherently related, DFT calculations/symmetry analysis (below) is needed

Co3Sn2S2，C3 @ q



Zhang et al., arXiv:2503.22794 (2025)

Type-I magnetic point groups

C_n

- AM is parallel the C_n axis (Only has 1D IRREP)
- Half wave plate-analogous effect ($c_2 = -1$)
- Raman shifts split in CPRS (n=3, 6)

C_s

- AM is perpendicular to mirror plane (Only has 1D IRREP)
- Half wave plate-analogous effect ($m = -1$)
- Raman shifts degenerate in CPRS

C_{nv}

- AM=0 for 1D IRREP
- PAM=$\pm l_{ph}$ form 2D IRREP
- Raman shifts degenerate in CPRS

D_n

- AM=0 for 1D IRREP
- PAM=$\pm l_{ph}$ form 2D IRREP

T

- AM=0 For 1D IRREP
- PAM=(0, $\pm$1) form 3D IRREP

Type-II/III magnetic point groups

$\mathcal{T}$

- AM=0 (at TRIM)
- Only has 1D IRREP

$\mathcal{PT}$

- AM=0 in the whole BZ
- Only has 1D IRREP

$C_n\mathcal{T}, D_n\mathcal{T}$

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- PAM=$\pm l_{ph}$ form 2D IRREP

$\mathcal{PT}$&C_n

- AM=0 in the whole BZ for 1D IRREP
- PAM=$\pm l_{ph}$ form 2D IRREP
- Raman shifts degenerate in CPRS

$T\mathcal{T}$

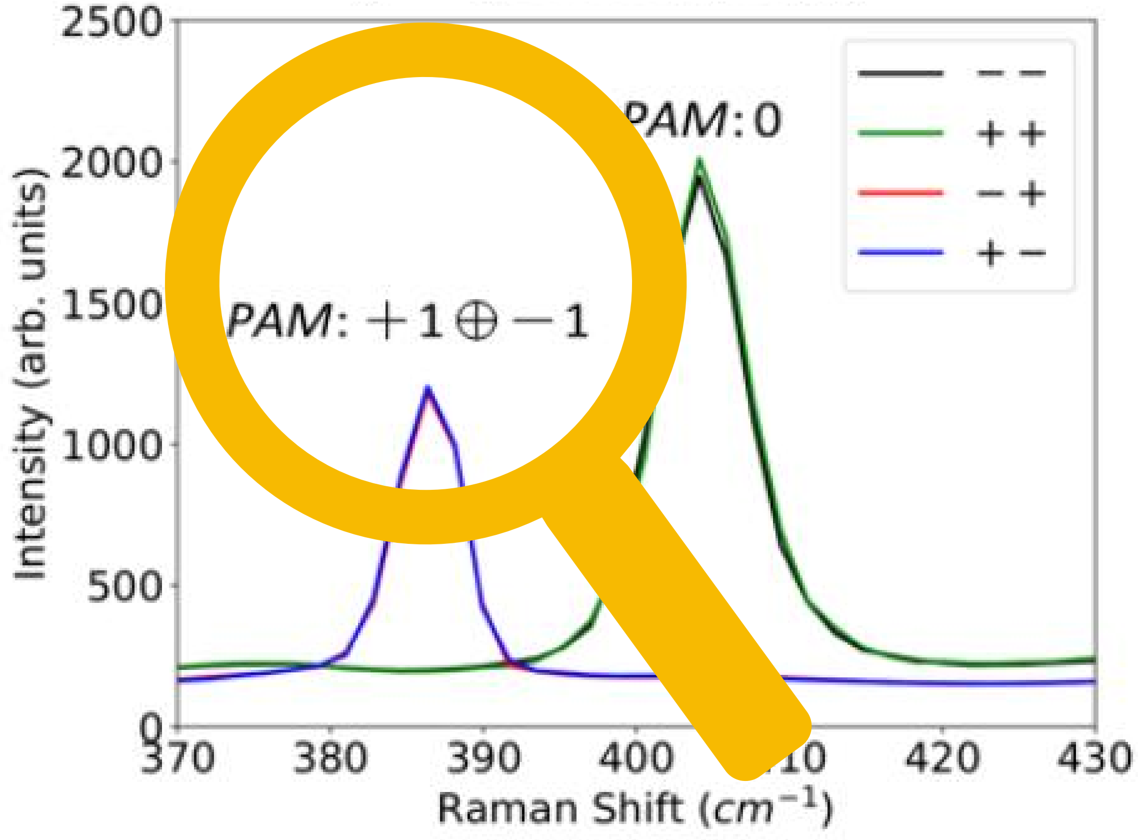
- AM=0 for 1D IRREP
- PAM=(0, $\pm$1) form 3D IRREP
- PAM=$\pm$1 form 2D IRREP

Experiments on PAM with Cnv

Preserve
PT or C_{nv} ?

AM and PAM (l_{ph}) are not inherently related, DFT calculations/symmetry analysis (below) is needed

MoS_2, C3v @ q



$\triangle l_{photon} = l_{ph}$ (modulus n)

Zhang et al., arXiv:2503.22794

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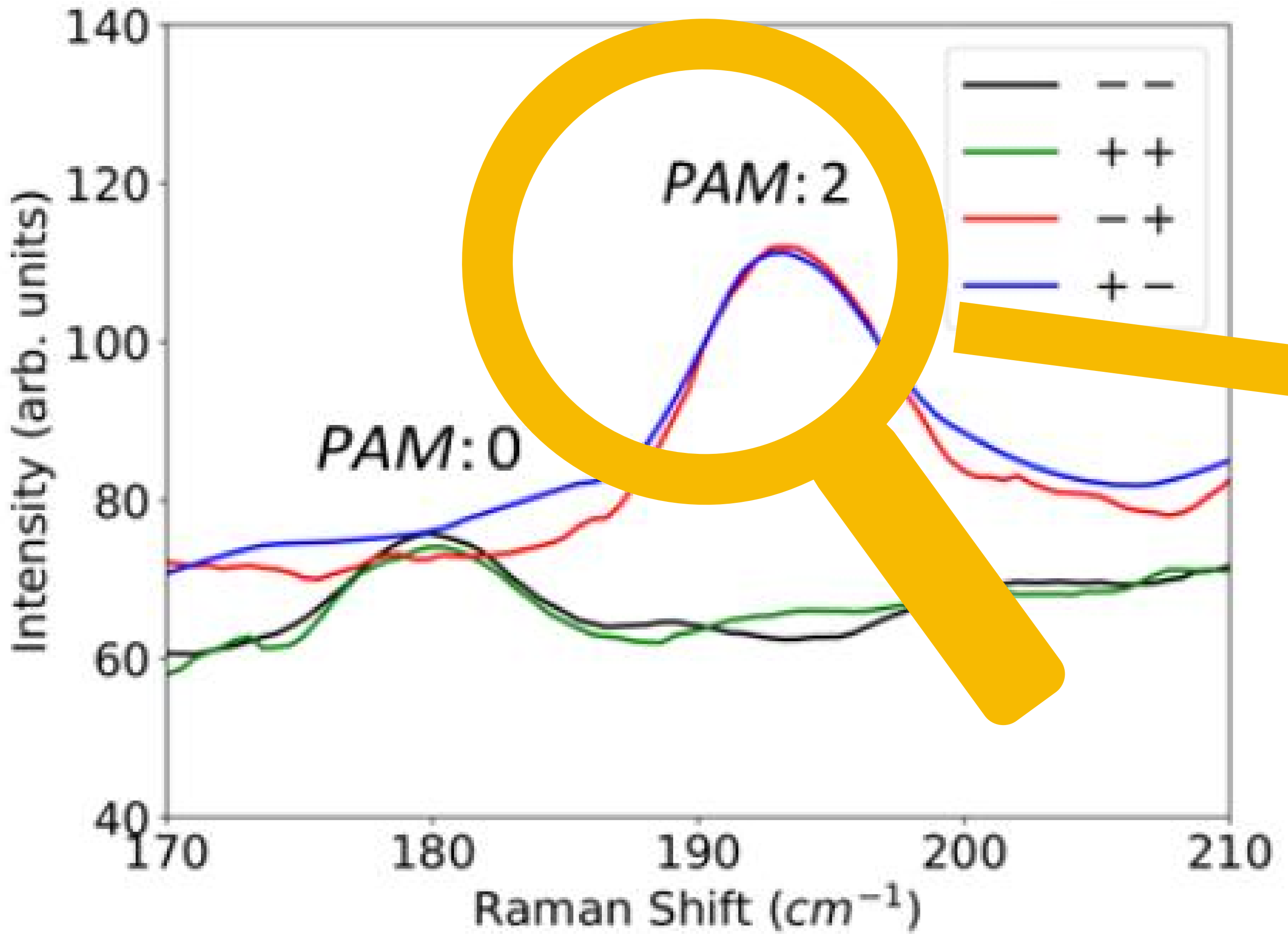
Preserve
PT or C_{nv} ?

AM and PAM (l_{ph}) are not inherently related, DFT calculations/symmetry analysis (below) is needed

FeSe, C4v @ q



$\triangle l_{photon} = l_{ph}$ (modulus n)

Zhang et al., arXiv:2503.22794

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- Raman shifts degenerate in CPRS

$T\mathcal{T}$
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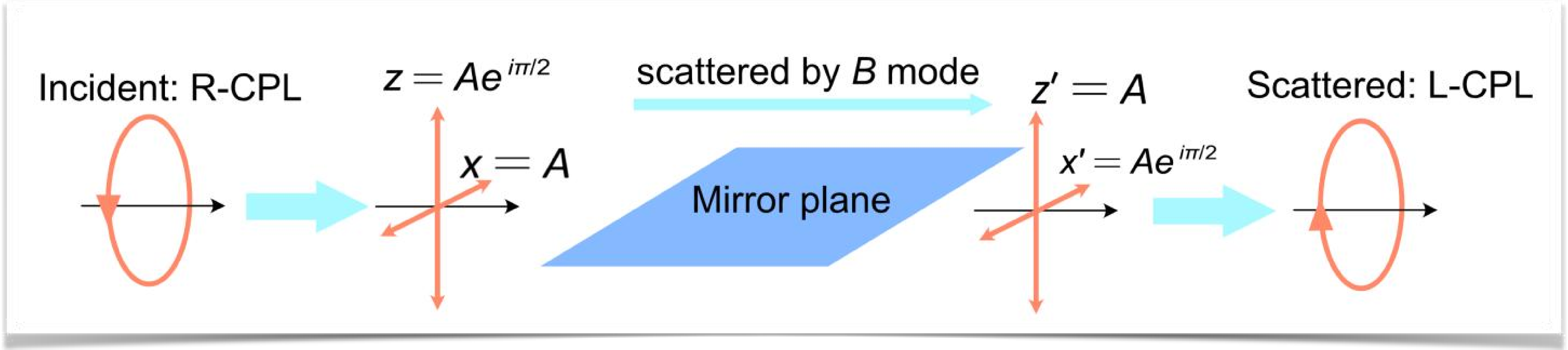
- PAM=(0, $\pm$1) form 3D IRREP
- PAM=$\pm$1 form 2D IRREP

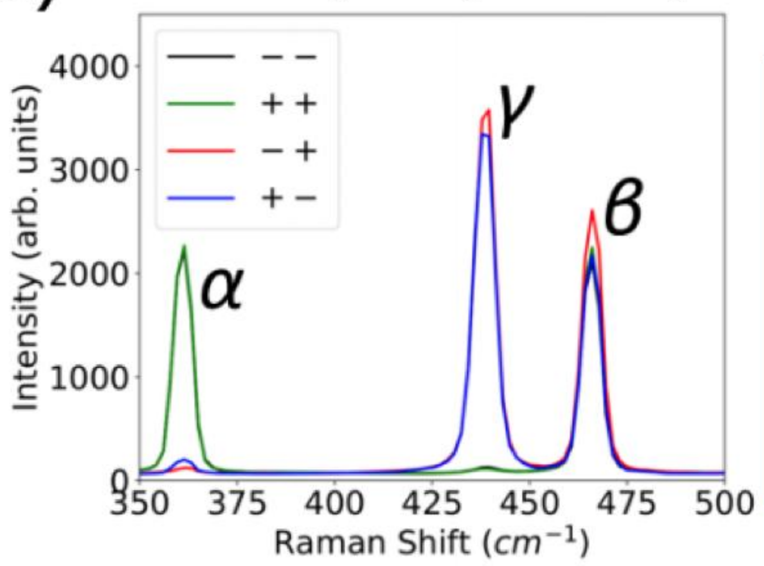
Mirror/C_2 odd phonon: half-wave plate



New discovery

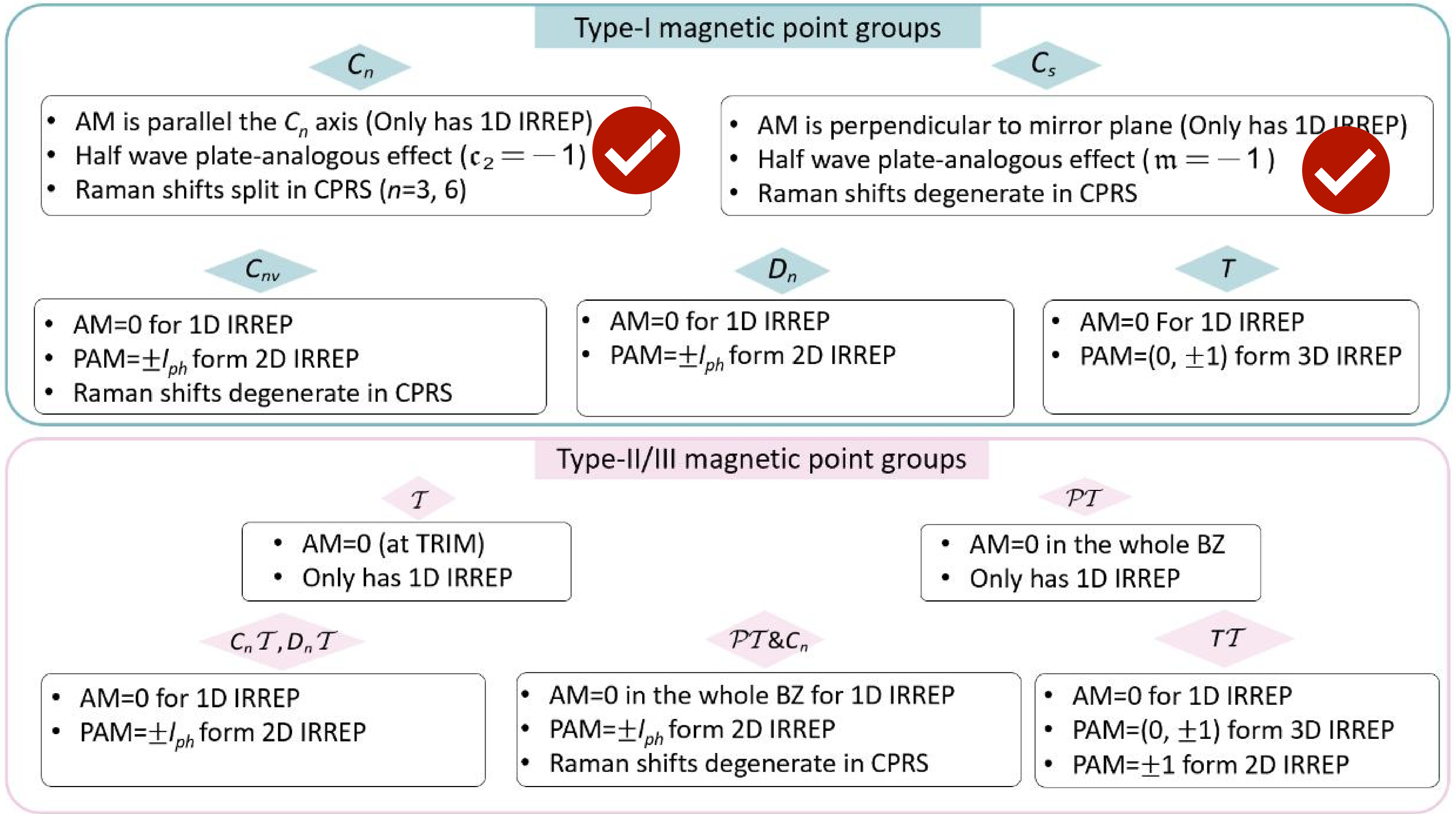
Half-wave plate effect

(a) **Black phosphorus (D2h/C2v)**



- Propagate ∥ mirror plane, or ⊥C2 axis
- B_{2g} (m = –1, C_2 =-1)： half-wave plate
- Can not explained by PAM

Label	Irrep.	Mirror eigenvalues			selection rules in CPRS	
		m_z	m_x	m_y	$\sigma^+/\sigma^-, \sigma^-/\sigma^+$	$\sigma^+/\sigma^+, \sigma^-/\sigma^-$
α	A_g	+1	+1	+1	Yes	No
γ	B_{2g}	-1	-1	+1	Yes	No
β	A_g	+1	+1	+1	Yes	No

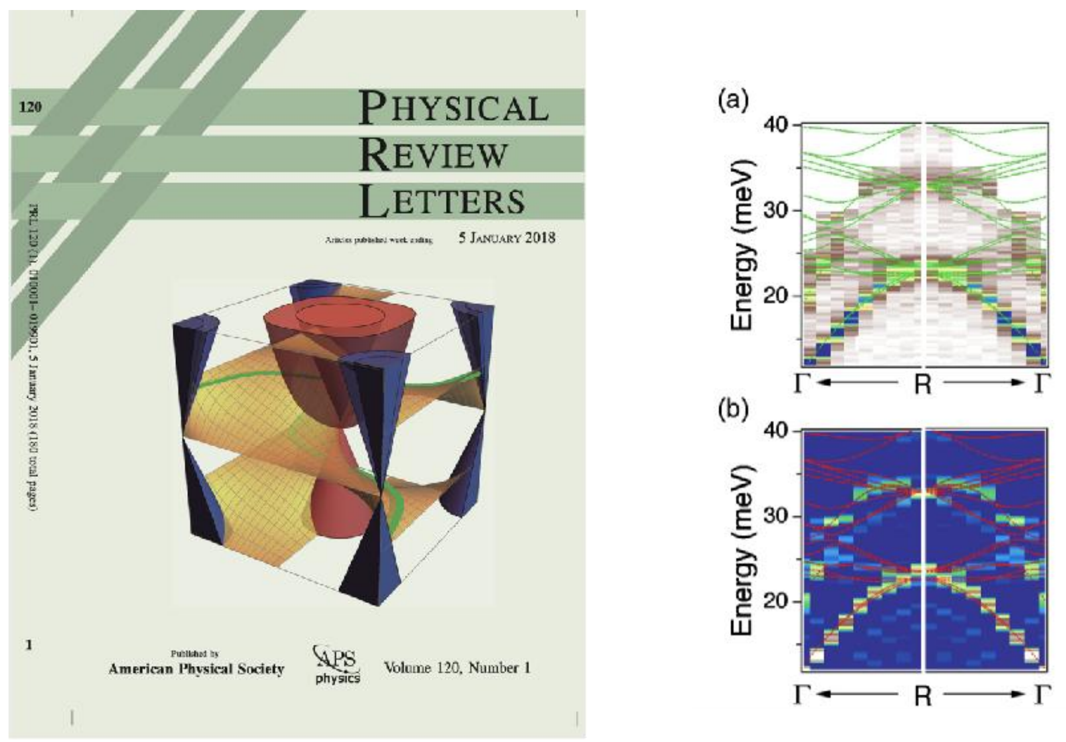


Zhang et al., arXiv:2503.22794

Conclusion: the "topology" and "chirality" of phonons

- We study and built the connection of topology and chirality in Weyl phonons.
- We predicted several topological phonon materials, all verified experimentally, including the first topological phonon material FeSi
- We proposed either break P (Te, α-HgS) or T ($Co_3Sn_2S_2$) can obtain chiral phonons.

Topological phonon materials

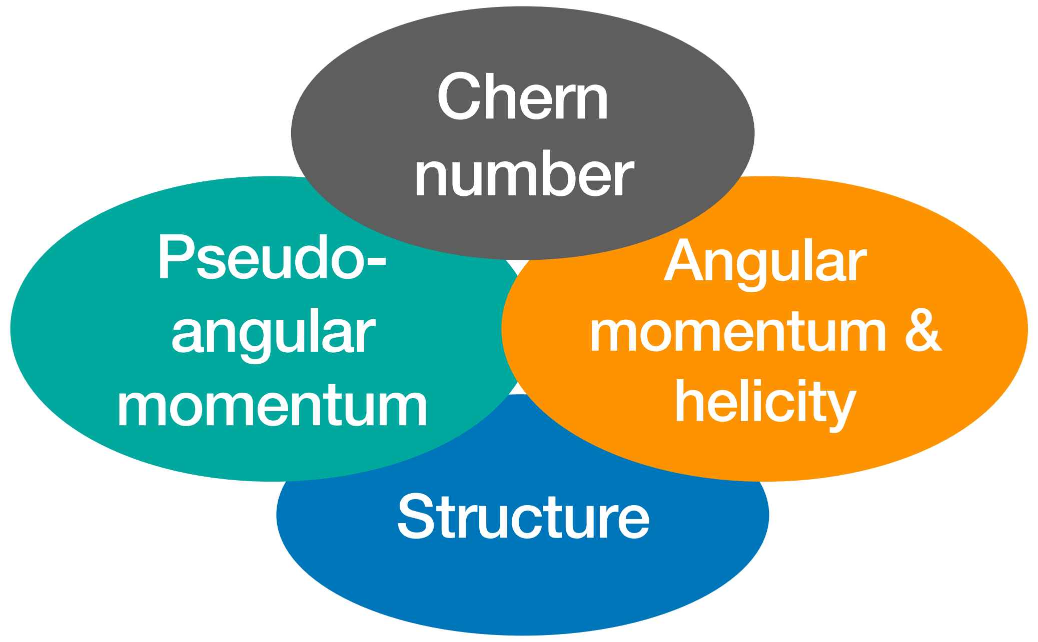


PRL 120, 016401 (2018)
PRL 121, 035302 (2018)
PRL 123, 245302 (2019)

Comments are welcomed !

arXiv:2505.06179 (under review in RMP)

Weyl/Chiral phonons in 3D



Sci. Adv. 6, eabd1618 (2020)
PRR. 4, L012024 (2022)
PRB 106, 184104 (2022)
Nat. Phys. , 19, 142-142 (2023)
Nano Lett., 23, 7561–7567 (2023)
npj Comput Mater 10, 264 (2024)
NatCommun 16, 3560 (2025)
PRL 134, 196905 (2025)
PRL 134, 196906 (2025)

Thank you!

- **Theoretical/Numerical collaborators:**

Shuichi Murakami (Tokyo U), Shuai Zhang (ITP)、Chen Fang(IOP)、Hongming Weng(IOP)、Zhong Fang(IOP)

- **Experimental collaborators：**

Hu Miao(ORNL)、Mark Dean(BNL)、Luojun Du(IOP)、Takuya Satoh (TokyoTech)、Luyi Yang (Tsinghua U)、Run Yang (Eastsouth U)、Martin Dressel (Stuttgart U)

Students & Postdocs are welcomed !

NSFC

中国科学院

JAPAN SOCIETY FOR THE PROMOTION OF SCIENCE
日本学術振興会

中华人民共和国科学技术部
Ministry of Science and Technology of the People's Republic of China