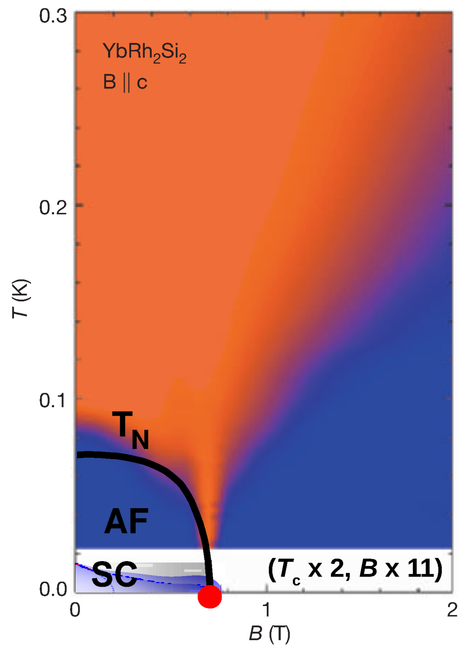
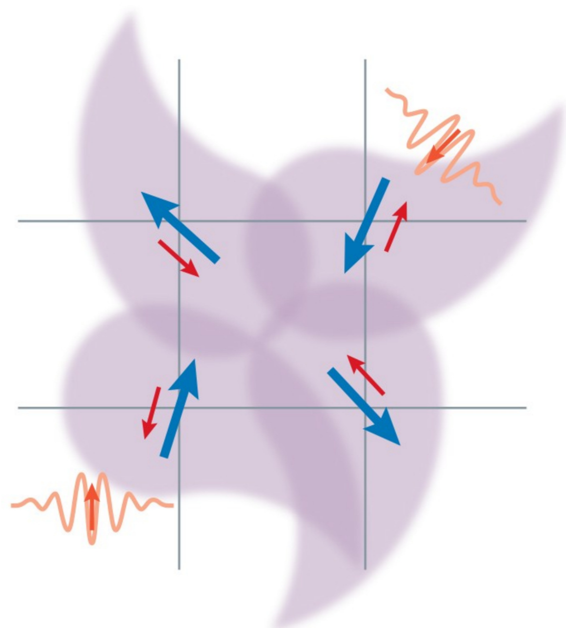
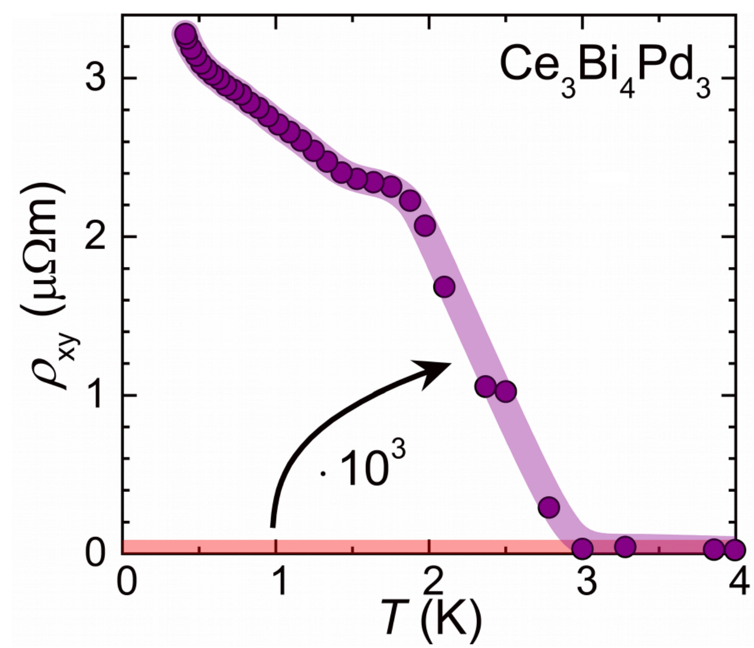
Heavy fermion systems
From quantum criticality to electronic topology

exosup2022 : School on Exotic Superconductivity
13-25 June 2022 Cargèse, Corse (France)

Silke Paschen
Vienna University of Technology







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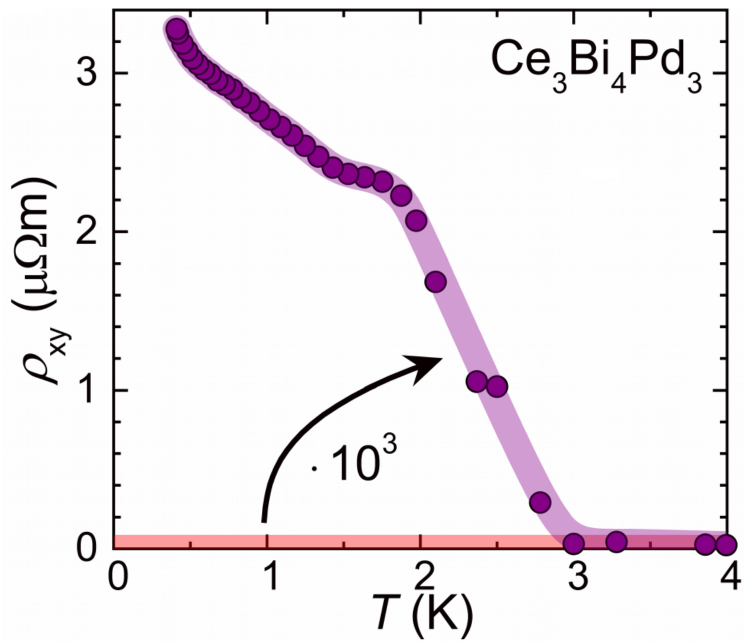

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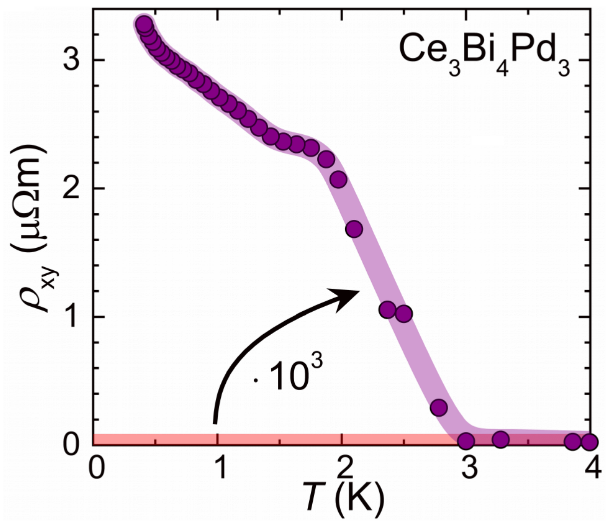

- **Electronic topology: Noninteracting Weyl semimetals**
- **Discovery of the Weyl-Kondo semimetal**
- **Can strongly correlated topology be tuned?**
- **New strongly correlated topological materials**
- **Correlation-driven topology as emergent phase?**

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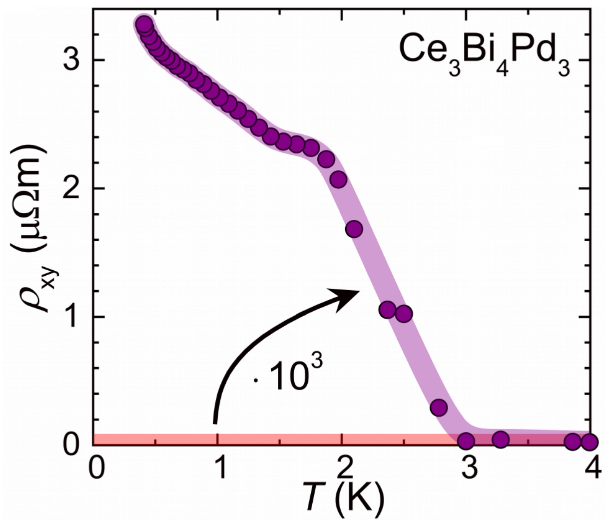

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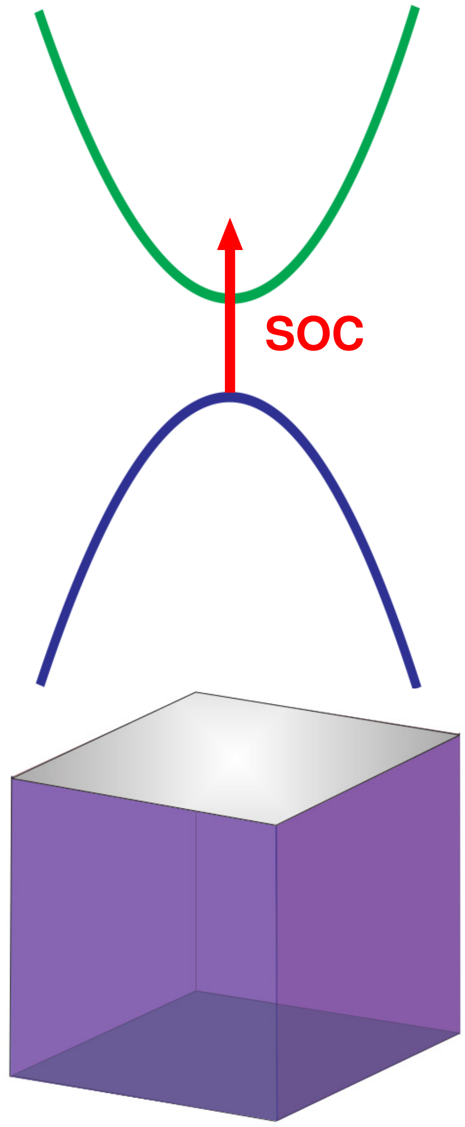
Topological bandstructures via strong spin-orbit coupling

Topological insulators



(Sun et al., PRB 92 (2015) 115428) & SBP

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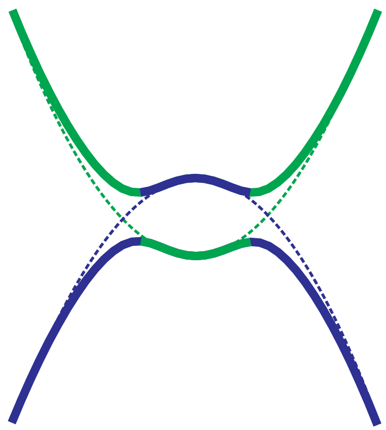

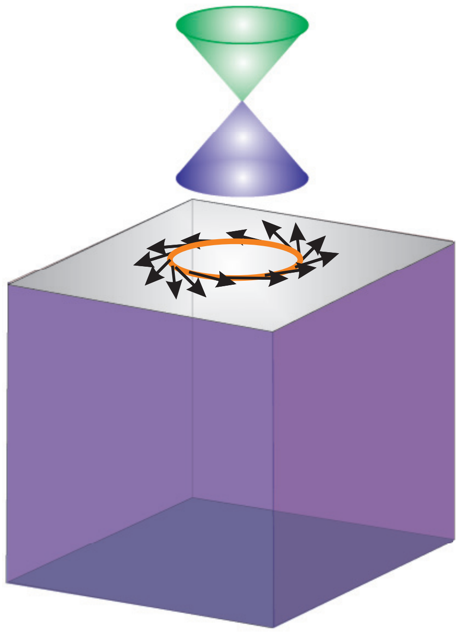

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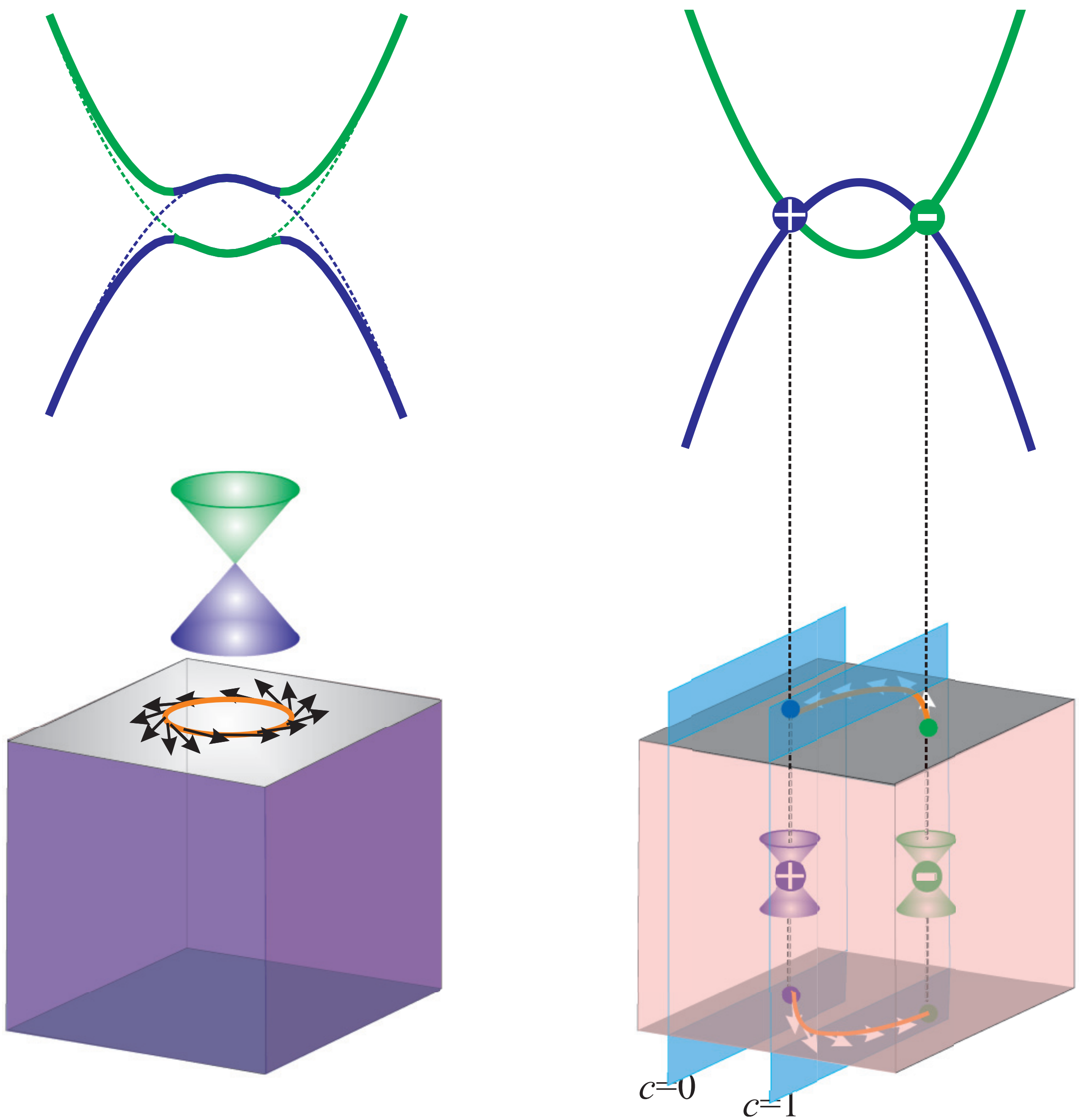


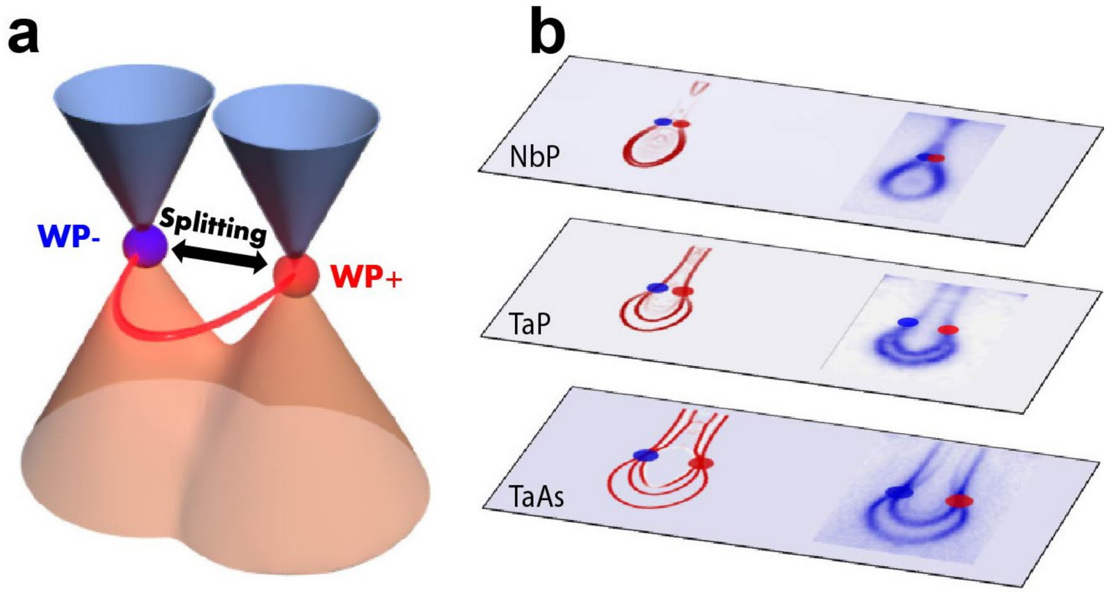
(Sun et al., PRB 92 (2015) 115428)

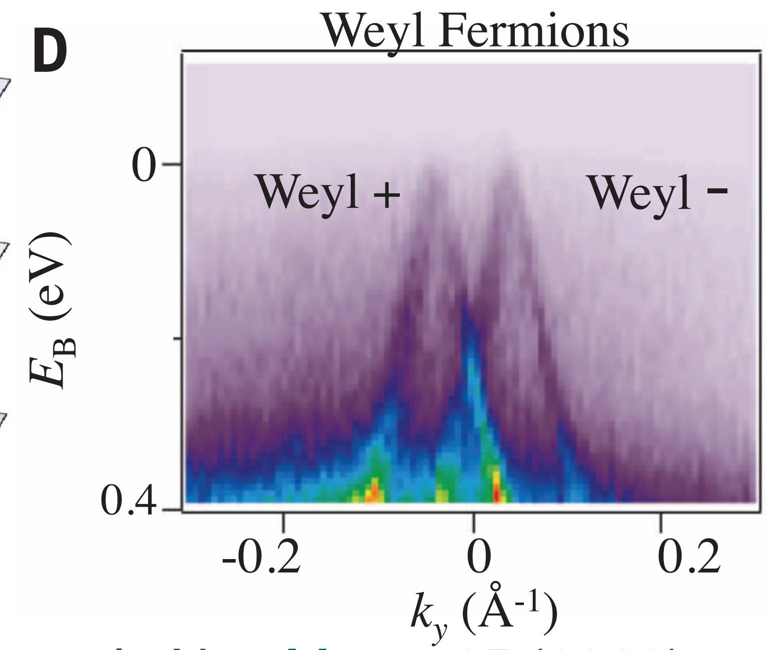
Weyl semimetals:

- **Strong SOC → band inversion**
- **TRS or IS broken → crossing points may remain gapless in the bulk → Weyl nodes**
- **Weyl nodes are sources and sinks of Berry curvature in *k* space ("magnetic monopoles")**

Noninteracting Weyl semimetals

- **Visualization** via ARPES + DFT: Bulk dispersion + surface states





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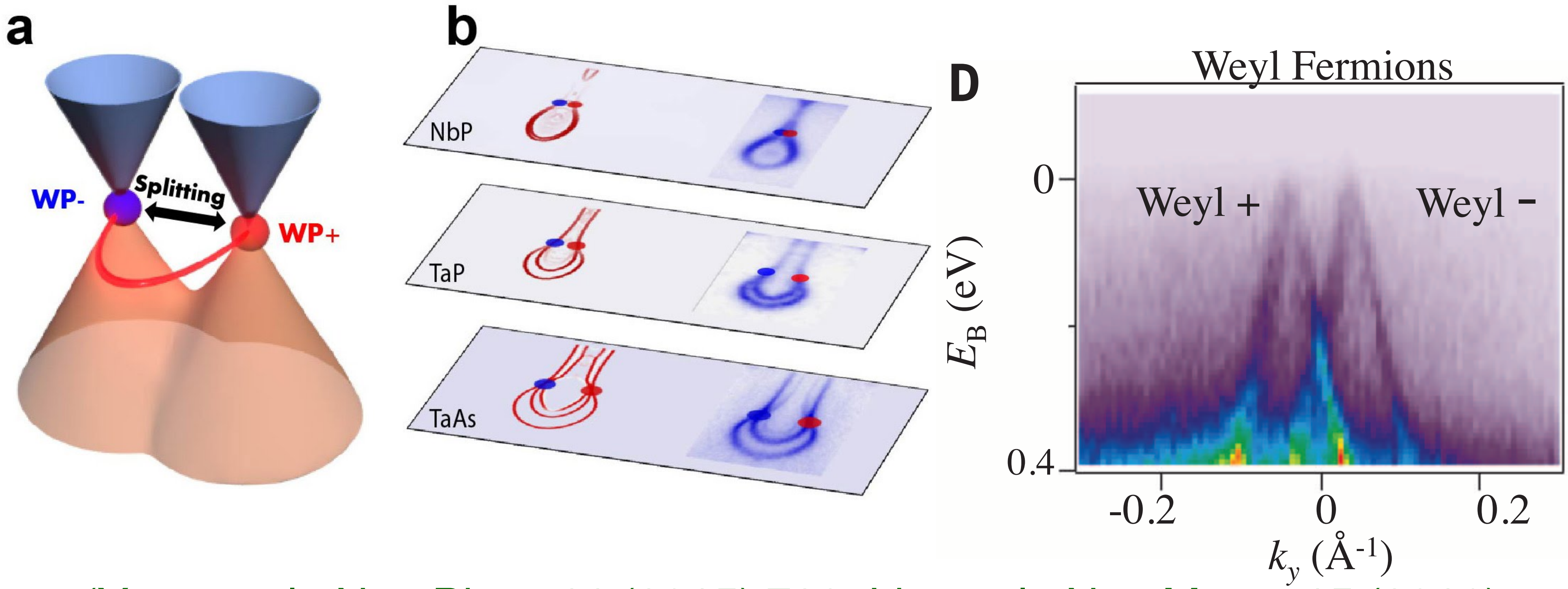
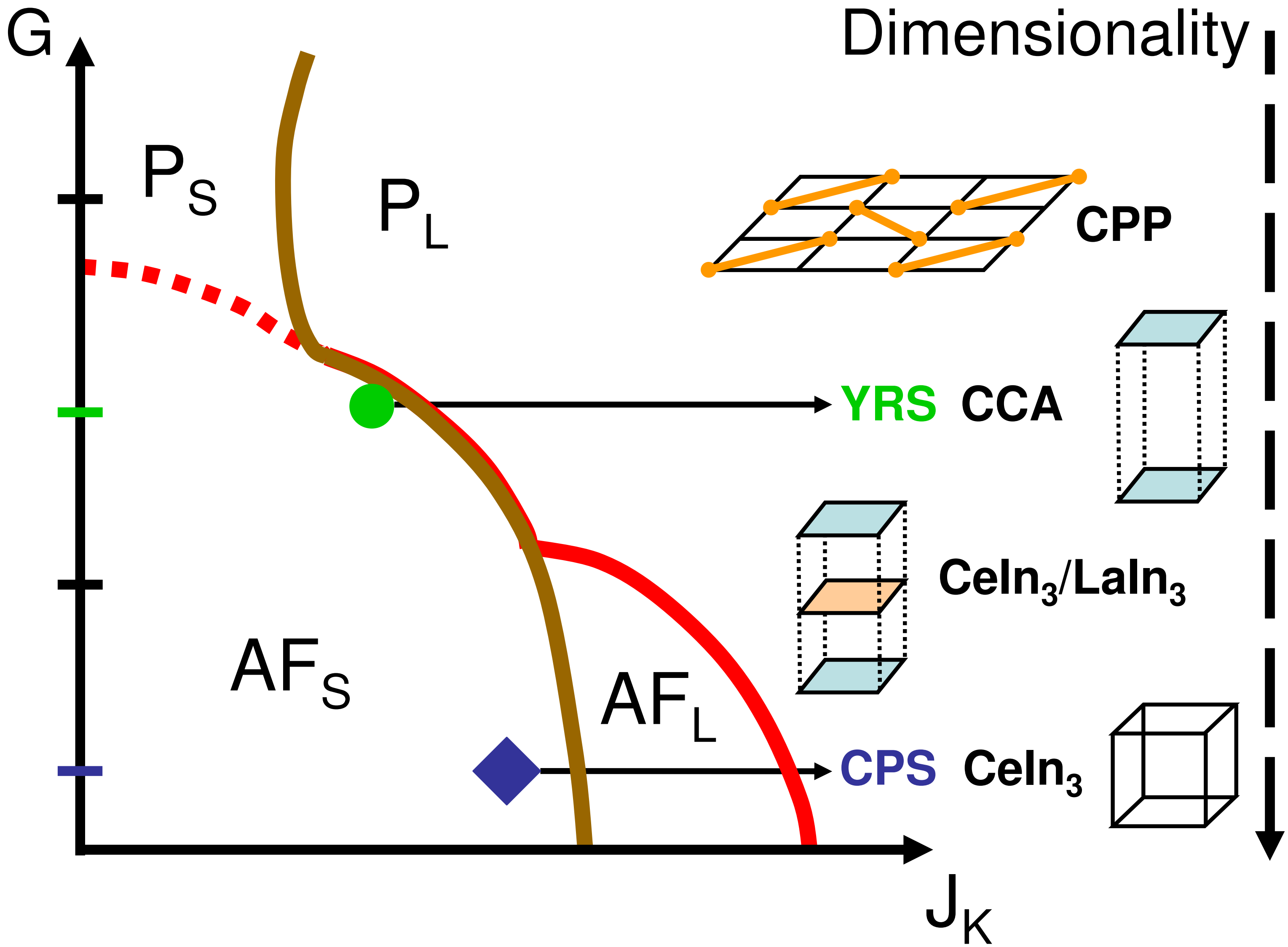


(Yang et al., Nat. Phys. 11 (2015) 728; Liu et al., Nat. Mater. 15 (2016) 27; Xu et al., Science 349 (2015) 613)

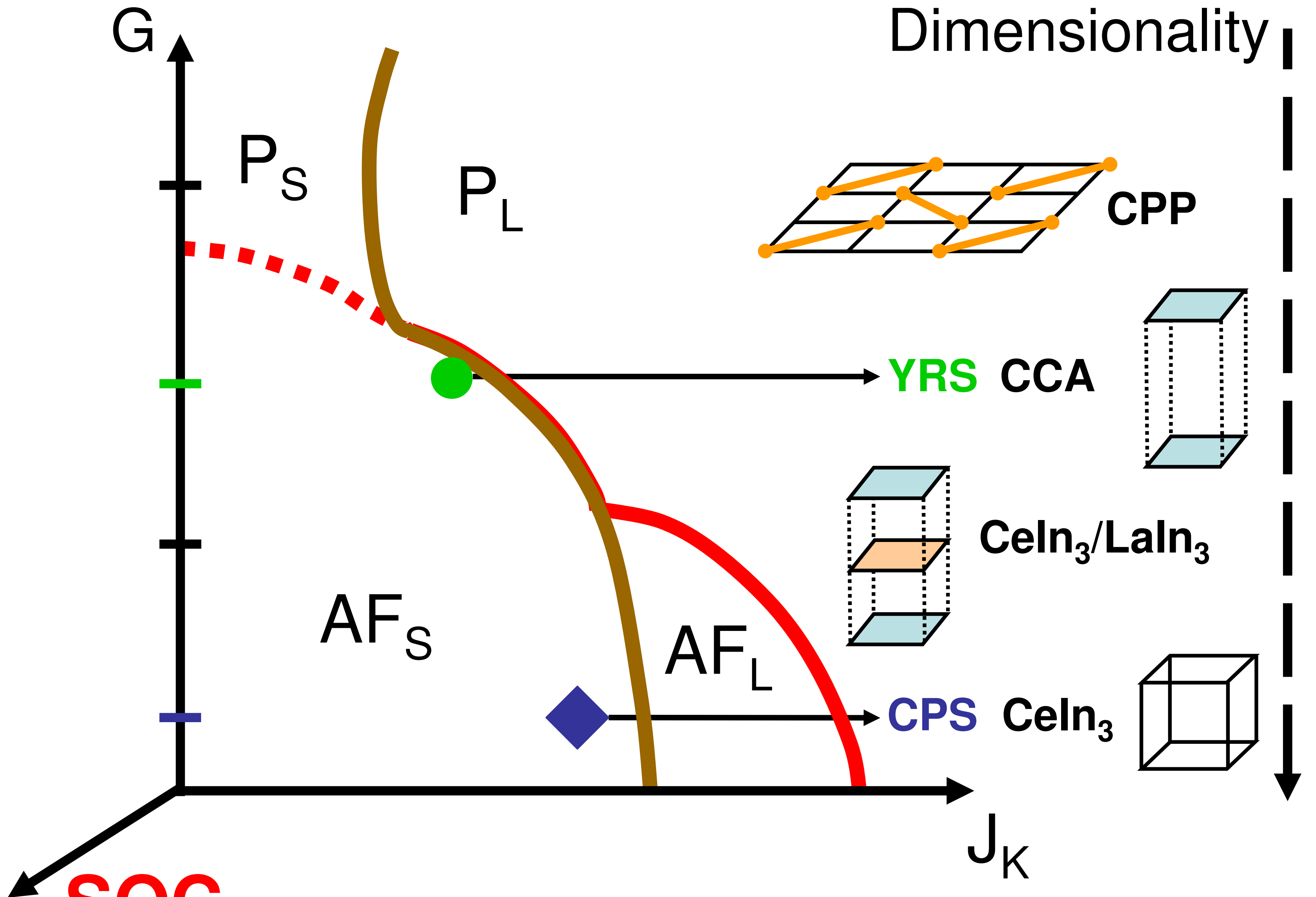
- **Identification** of topological characteristics in transport **challenging**: **Background, current jetting, "normal" semimetal features, "normal" anomalous Hall...**

Heavy fermion phases as starting point?



(Custers et al., Nature Mater. 11 (2012) 189; Si, Physica B 378-380 (2006) 23)

Heavy fermion phases as starting point for robust topology?



(Custers et al., Nature Mater. 11 (2012) 189; Theory: Si et al.)

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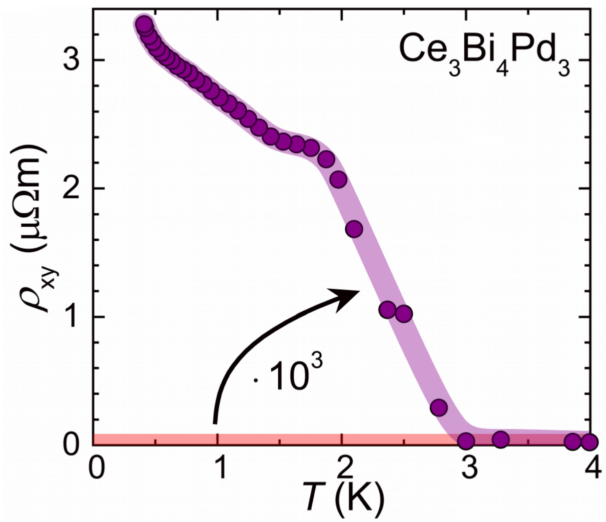

- Electronic topology: Noninteracting Weyl semimetals
- **Discovery of the Weyl-Kondo semimetal**
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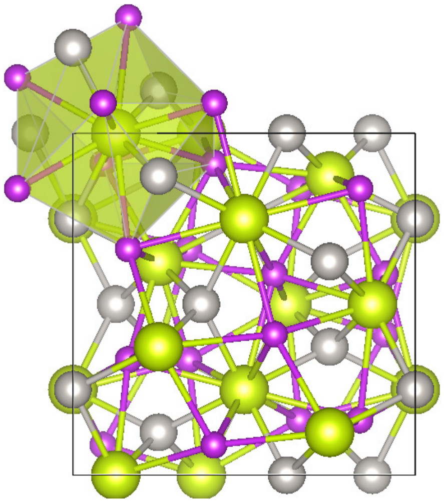
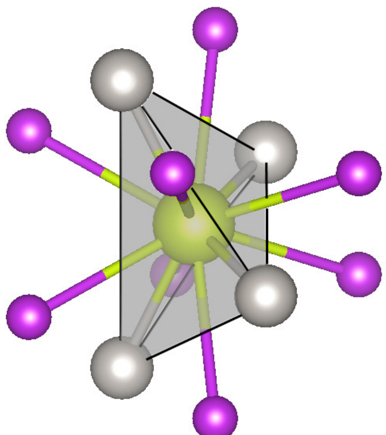
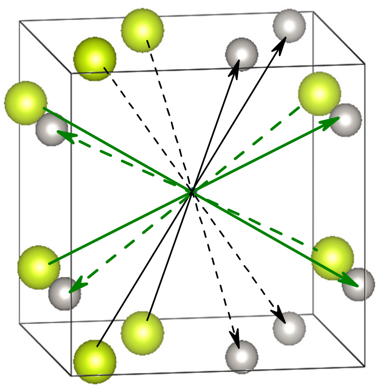
The material: The Kondo semimetal $Ce_3Bi_4Pd_3$

Broken inversion symmetry



$Ce_3Bi_4(Pt,Pd)_3$





Nonsymmorphic

Space group $I\bar{4}3d$

$a \sim 10.055$ Å

4 f.u./u.c.

Z:

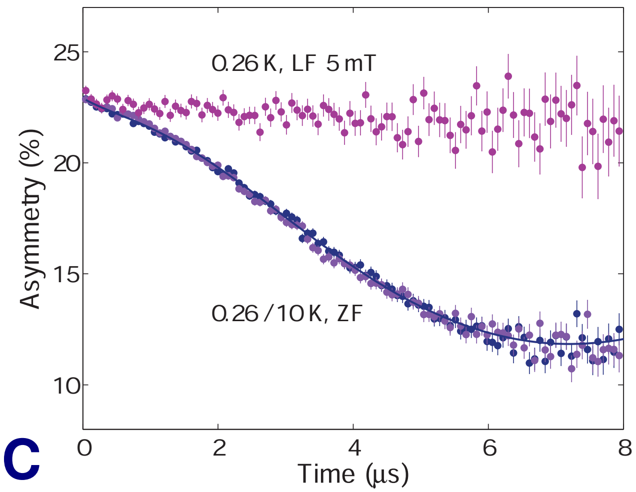
Ce **58**

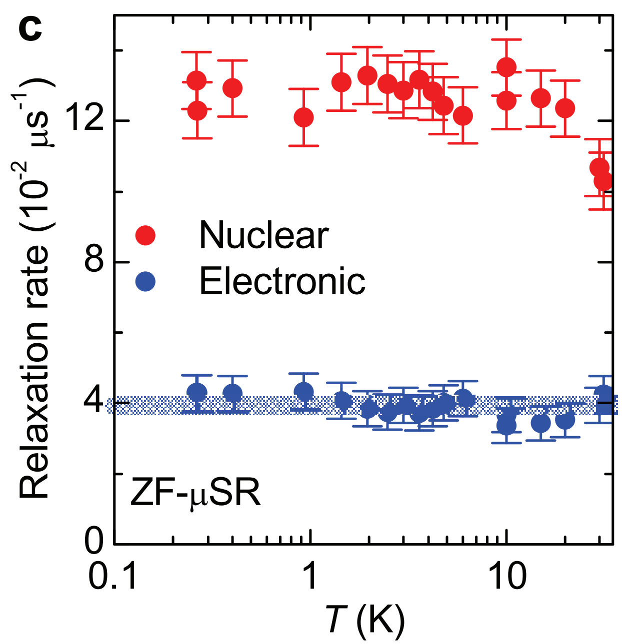
Pt **78**

Bi **83**

Large SOC

Preserved time reversal symmetry

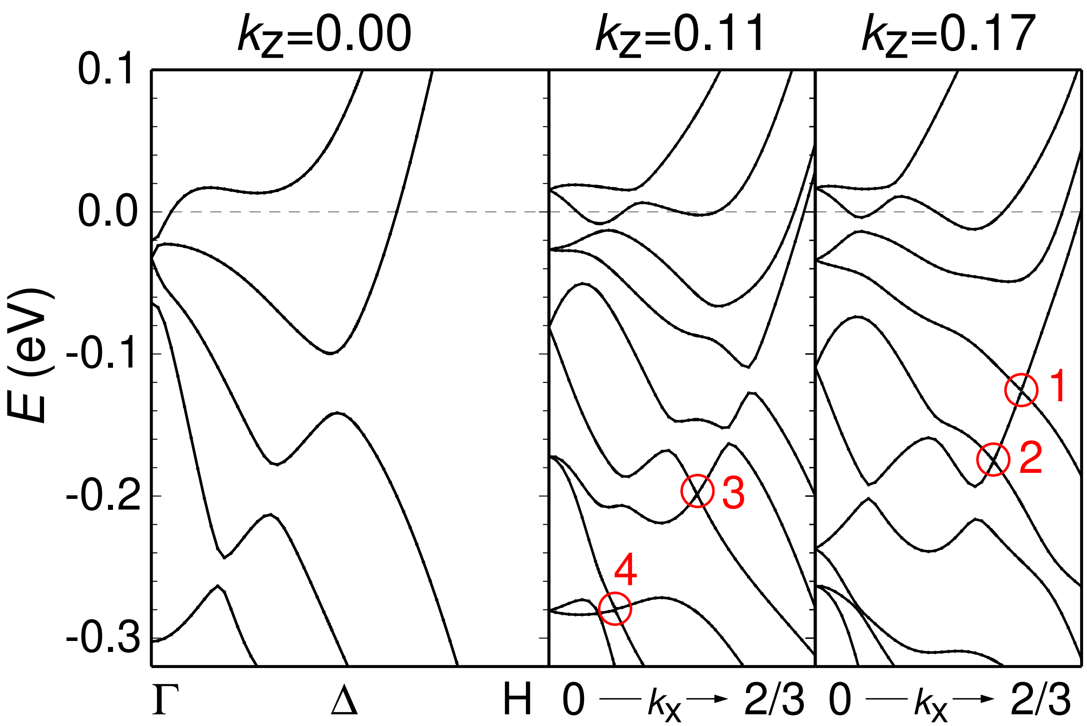




(Dzsaber et al., Phys. Rev. Lett. 118 (2017) 246601 ↑
PNAS 118 (2021) e2013386118 →)

The material: The Kondo semimetal $Ce_3Bi_4Pd_3$

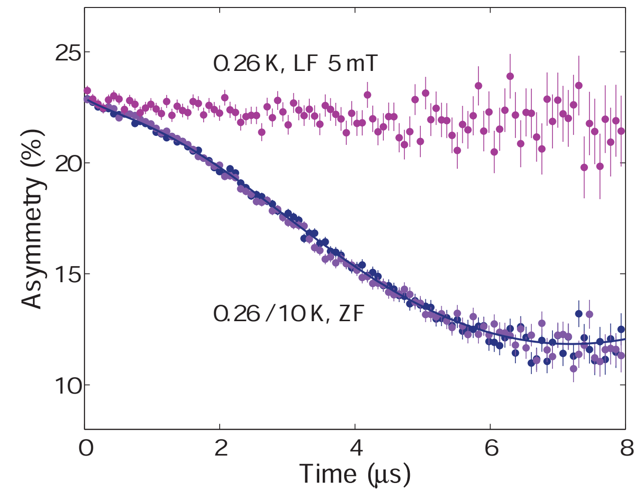
DFT bandstructure

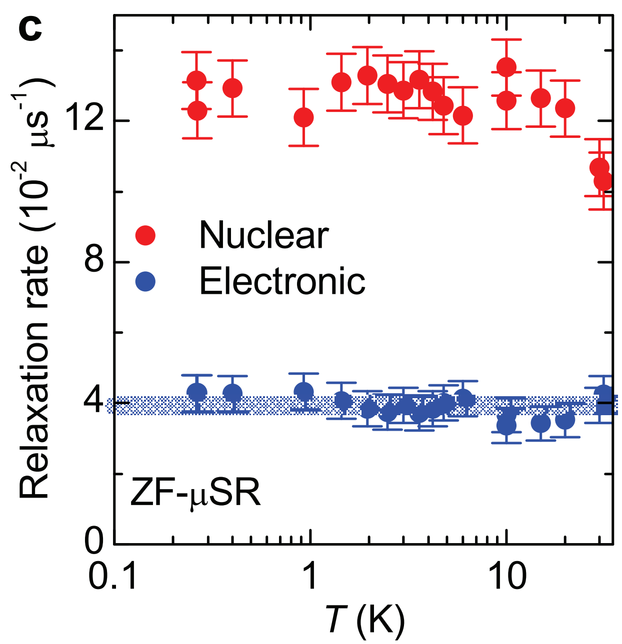


Ce 4f^1 electron in core:
no correlations!

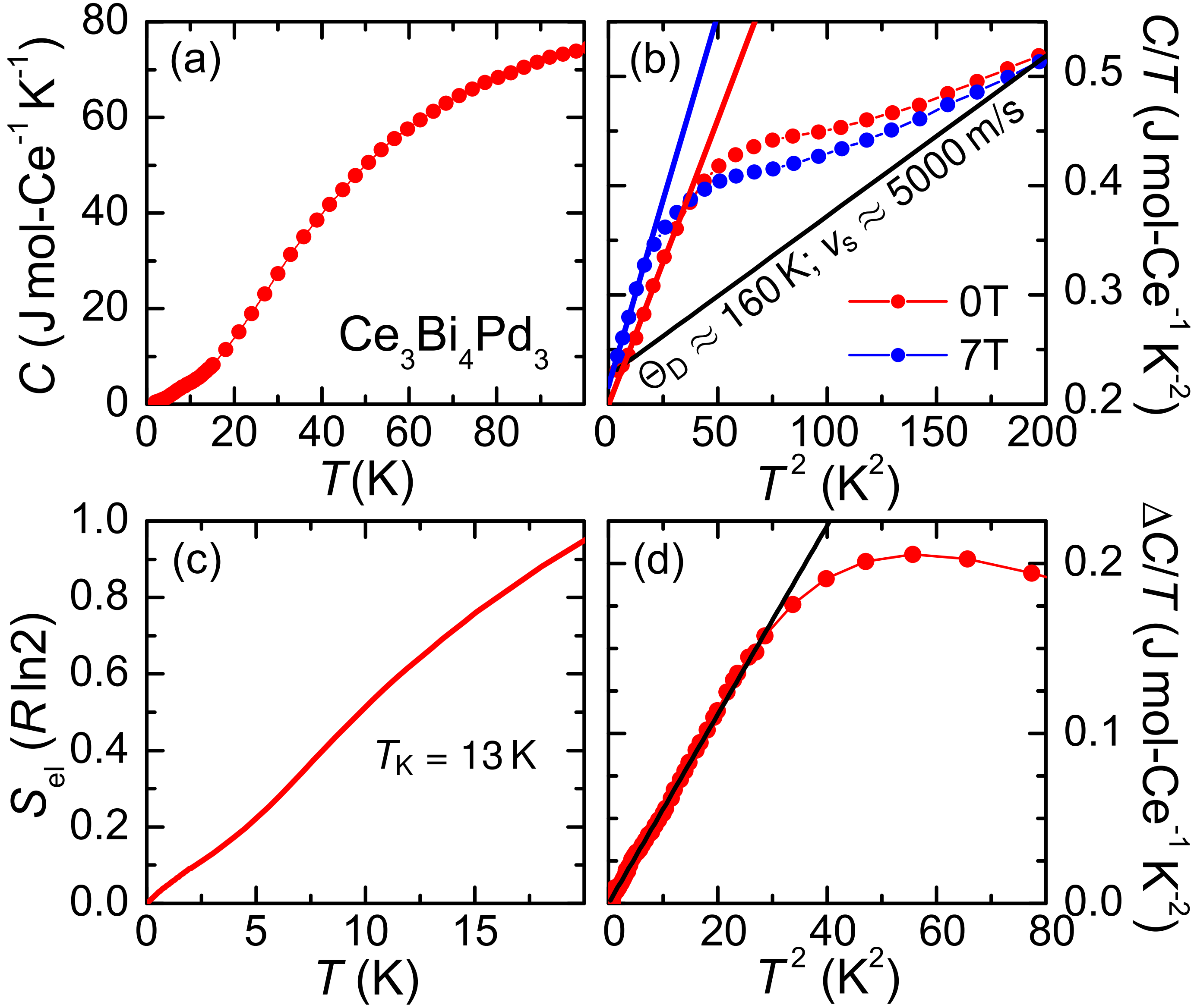
(Dzsaber et al., PNAS 118 (2021) e2013386118)

Preserved time reversal symmetry





Extreme topological response 1: Specific heat



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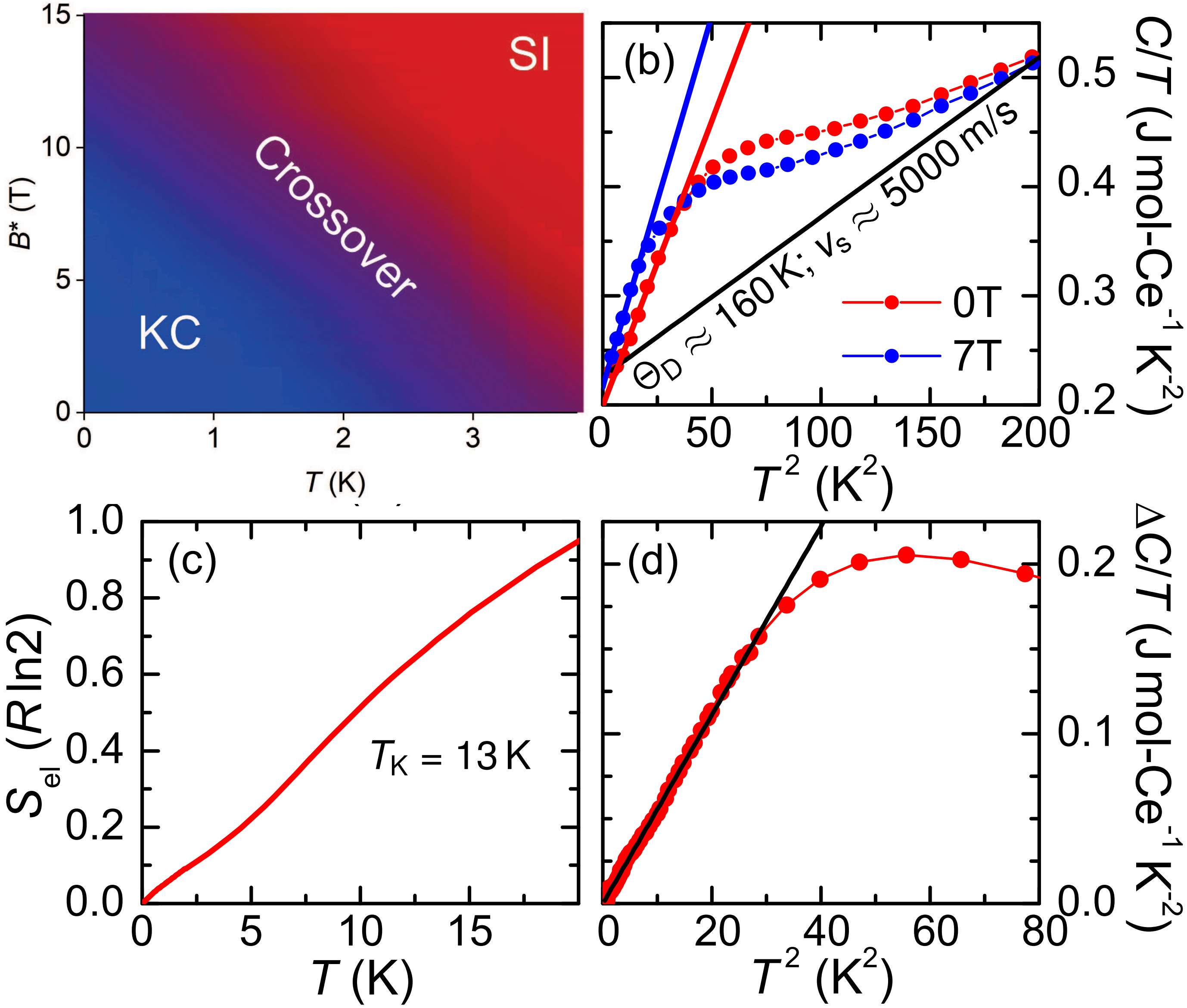

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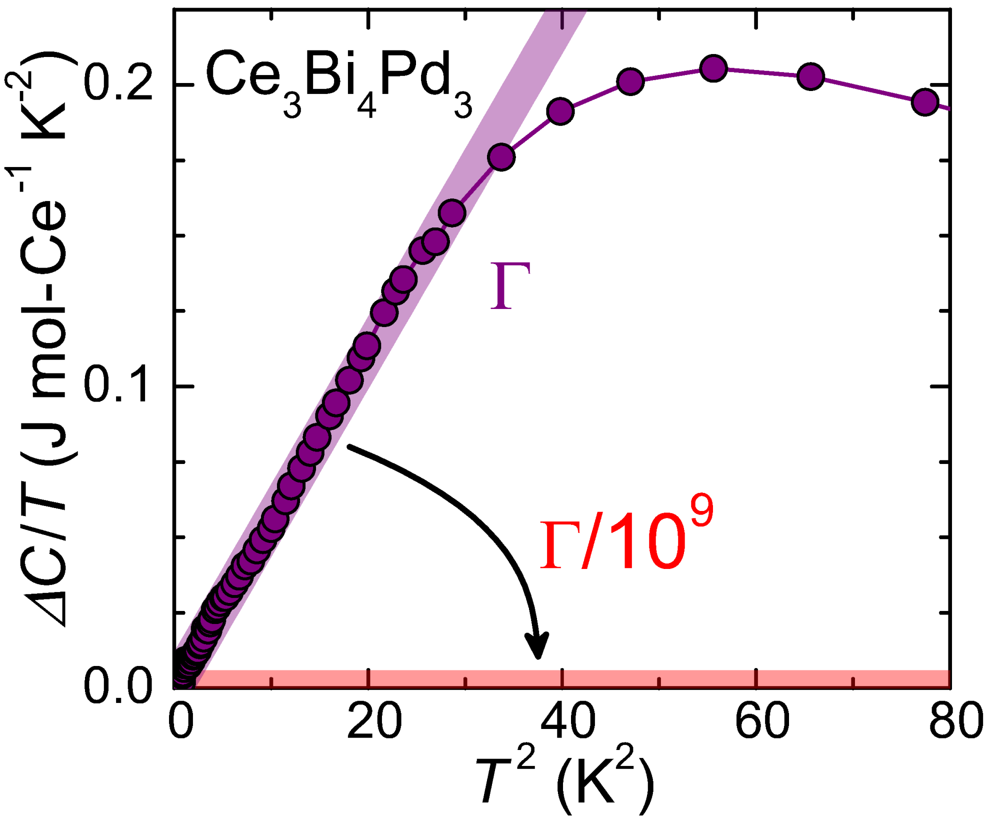
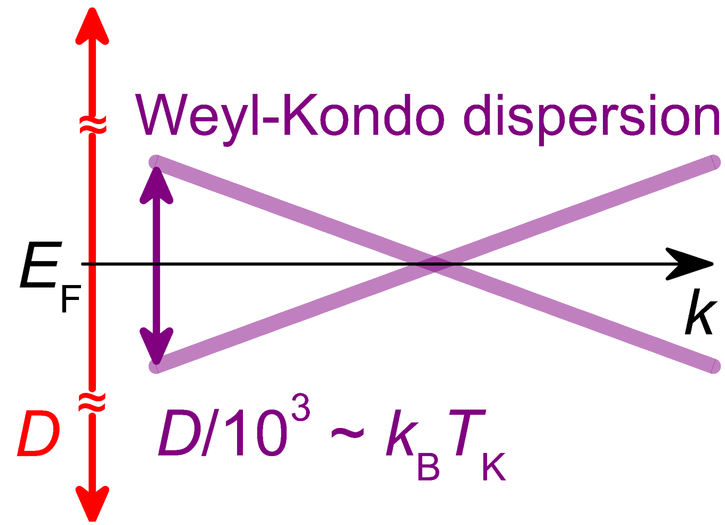
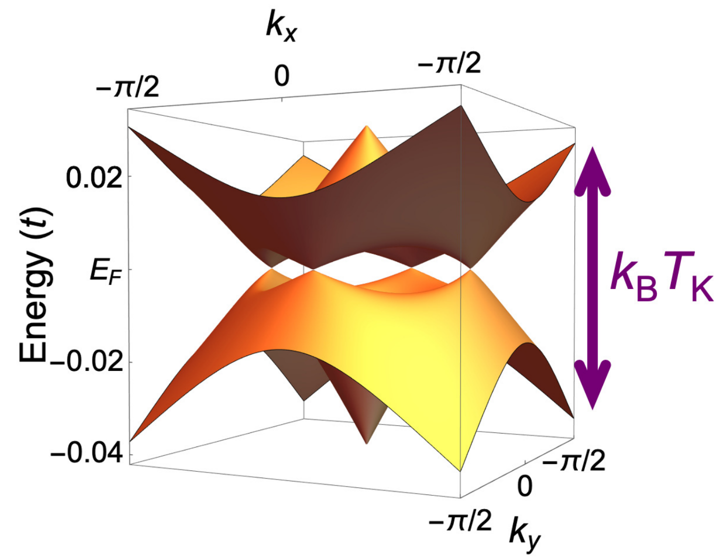






$C/T = \Gamma T^2$ with $\Gamma \sim 1/v^3$

$v = 886\,\text{m/s} \approx v_F/10^3$

noninteracting Weyl fermions with v_F
give nondetectable contribution ($\Gamma/10^9$)

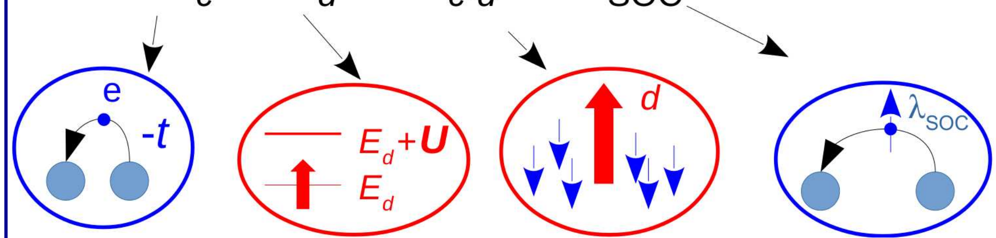
(Lai et al., PNAS 115 (2018) 93)

(Dzsaber et al., Phys. Rev. Lett. 118 (2017) 246601)

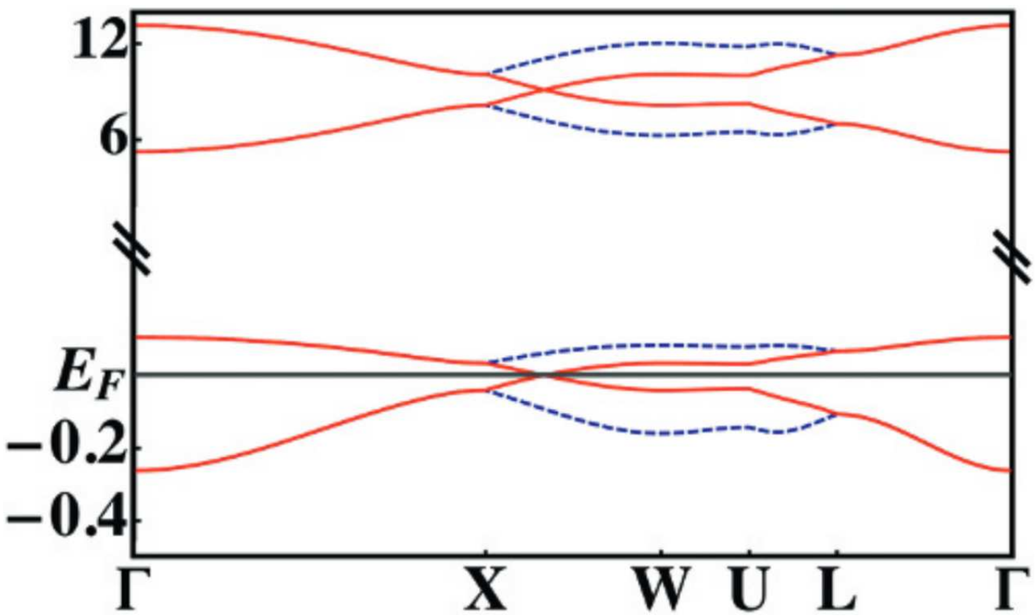
The Weyl-Kondo semimetal

Microscopic model

$$H = H_c + H_d + H_{c\text{-}d} + H_{\mathrm{SOC}}$$



(sketches: Dzsaber)



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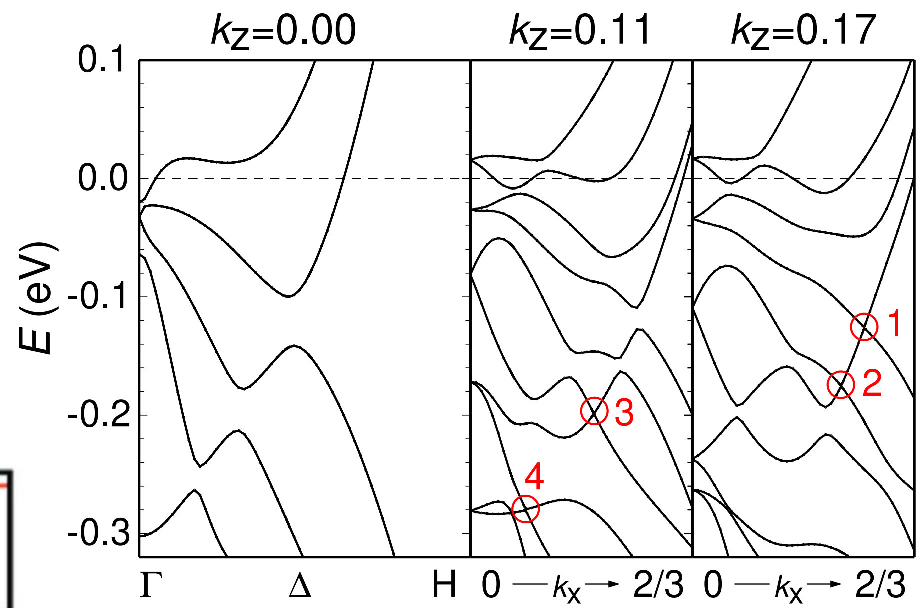
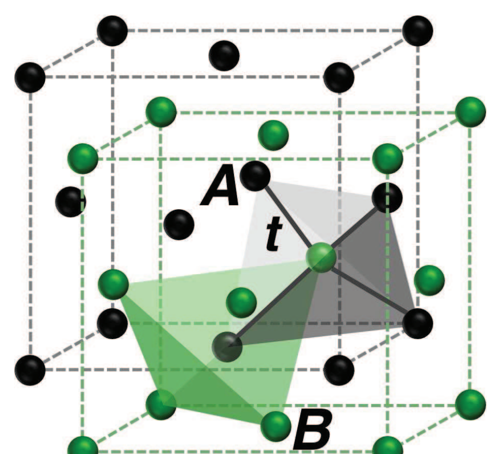
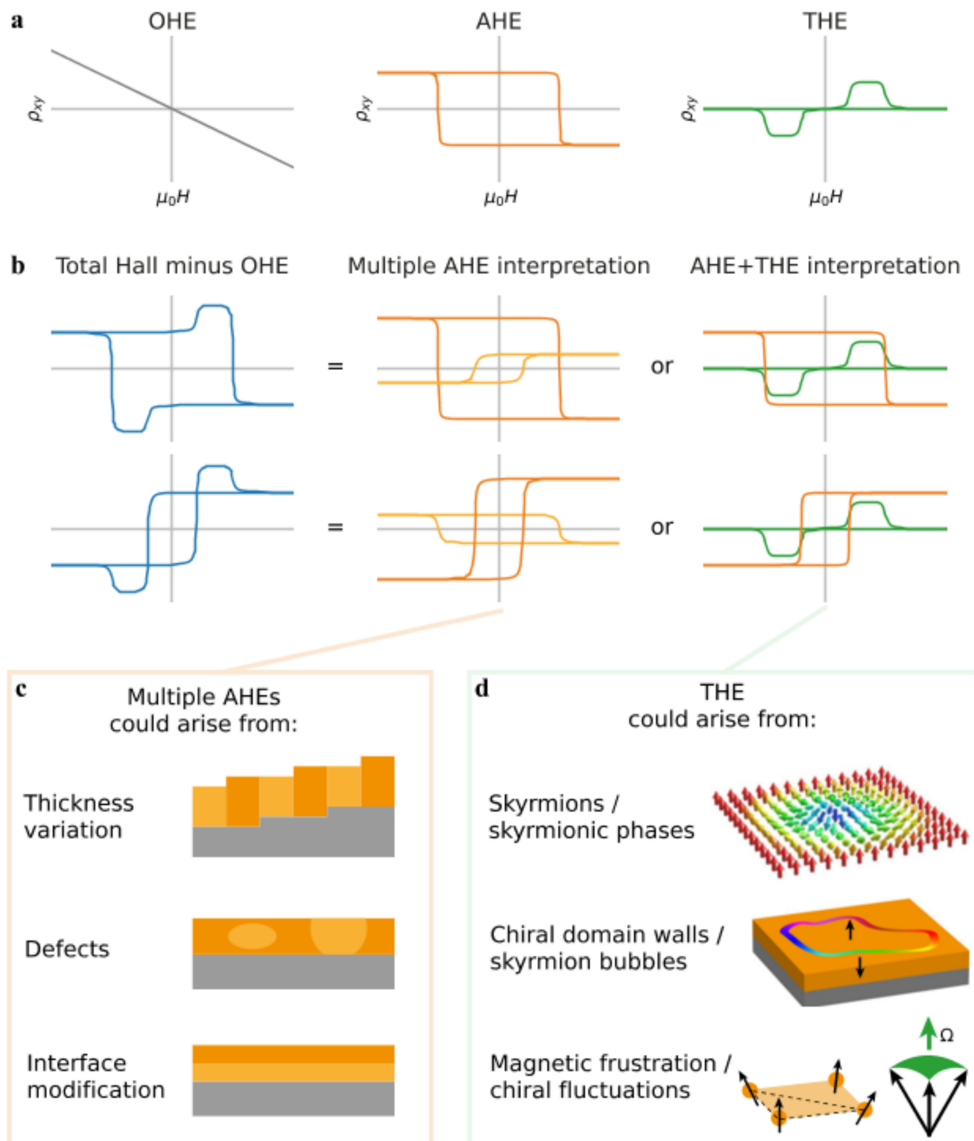
DFT bandstructure



(Dzsaber et al., PNAS 118 (2021) e2013386118)



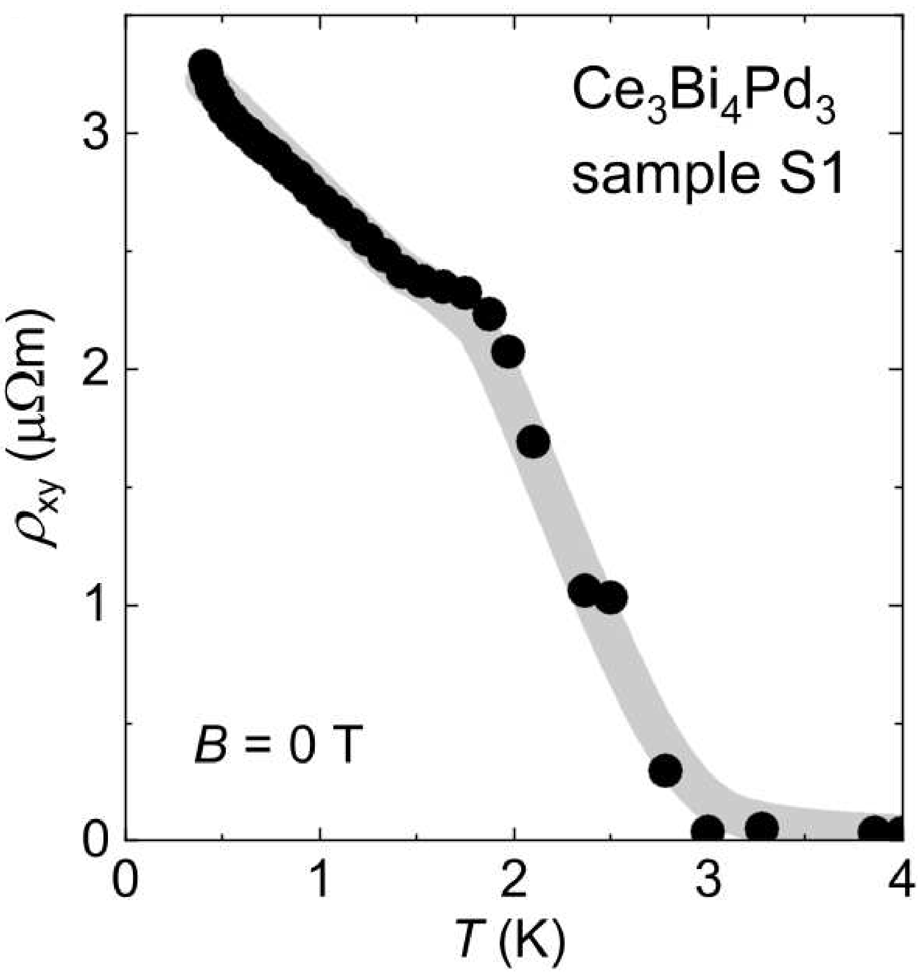
Hall effect in noninteracting (magnetic) Weyl semimetals



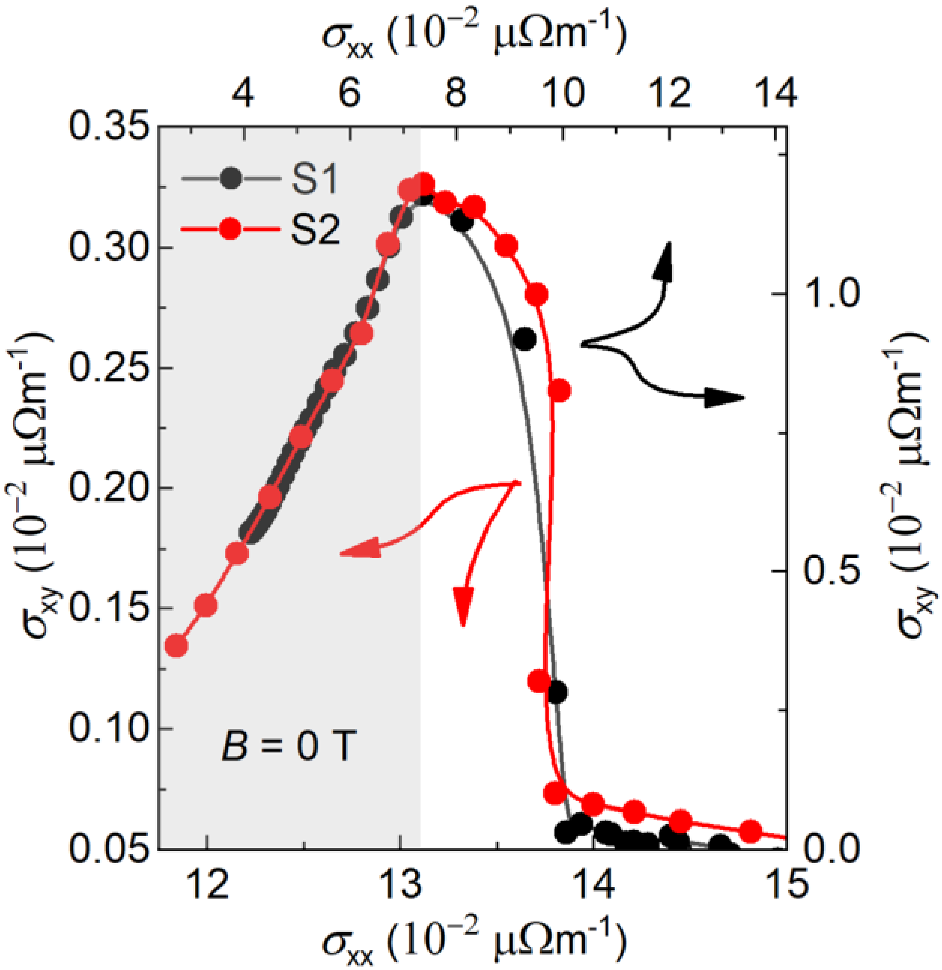
(Kimbell et al., Commun. Mater. 3 (2022) 19)

Extreme topological response 2: Spontaneous Hall effect

Spontaneous Hall resistivity



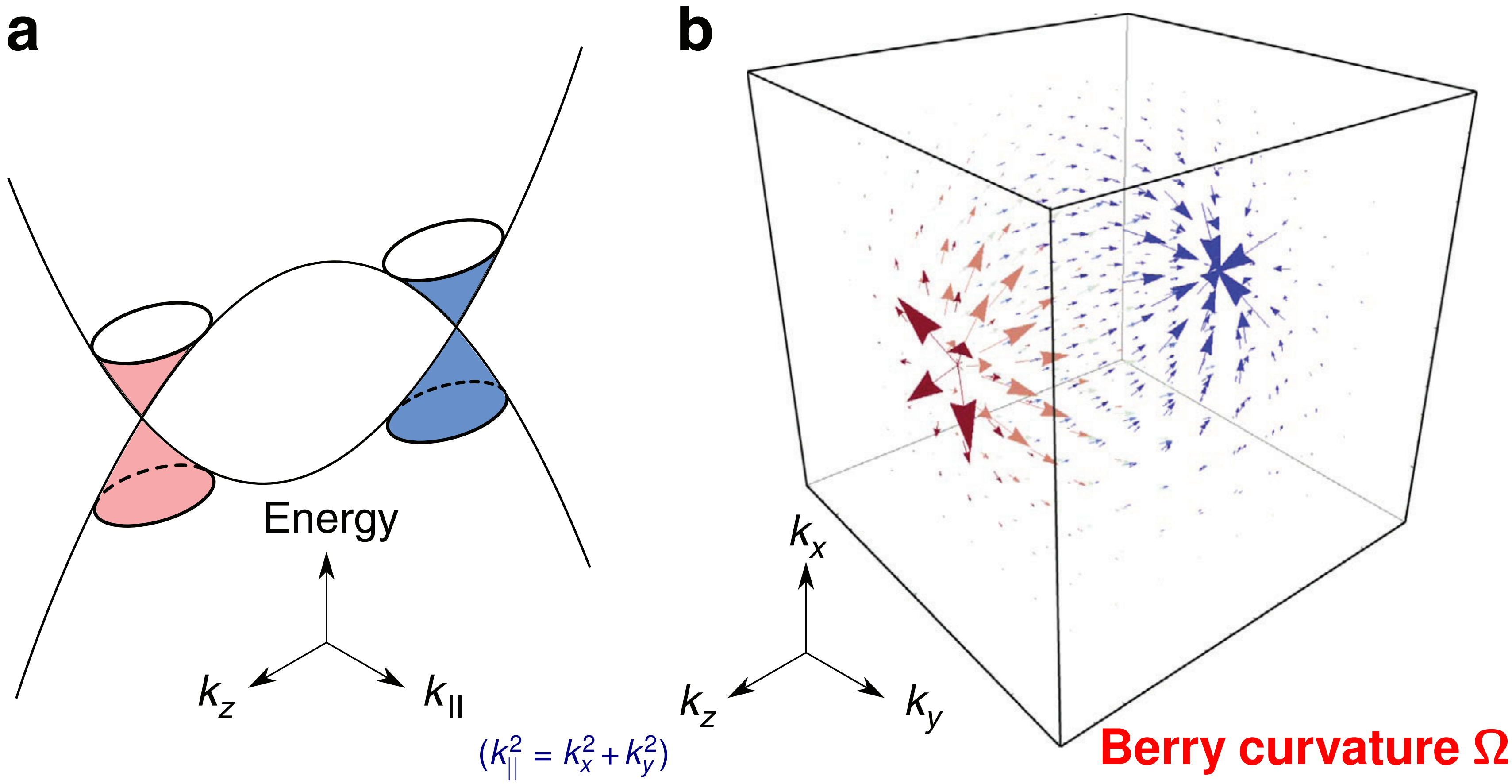
Spontaneous Hall conductivity



$\sigma_{xy} \approx 0.3 \frac{e^2}{h \cdot a}$; $\tan(\Theta) \approx 0.5$ Giant effect!

(Dzsaber et al., PNAS 118 (2021) e2013386118)

Berry curvature-driven Hall response (broken IS, preserved TRS)



(H. Li et al., Nat. Commun. 7 (2016) 10301)

$$j_y = \sigma_{xy} E_x = \frac{e^2}{\hbar} \int \frac{d^3k}{(2\pi)^3} g(\boldsymbol{k}, E_x, \tau) \Omega_z(\boldsymbol{k}) E_x$$

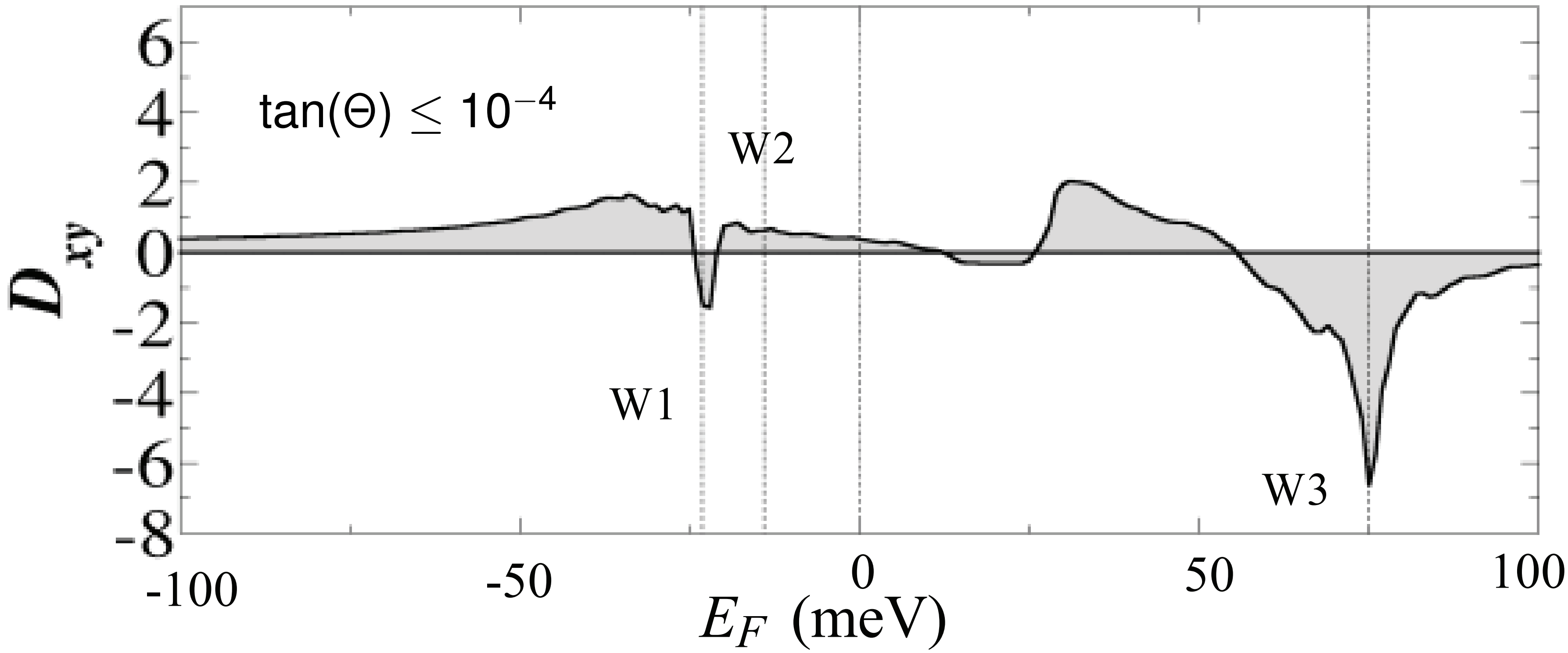
(Sodemann & Fu, Phys. Rev. Lett. 115 (2015) 216806)

Berry curvature-driven Hall response: Perturbative regime

$$\sigma_{xy} = \frac{e^3\tau}{2\hbar^2}\mathcal{E}_x D_{xz} \quad \text{with} \quad D_{xz} = \int \frac{d^3k}{(2\pi)^3} f_0(k) \frac{\partial \Omega_z^{\text{odd}}}{\partial k_x} \quad \text{Berry curvature dipole}$$

$\rightarrow 0\omega, 2\omega$ (Sodemann & Fu, Phys. Rev. Lett. 115 (2015) 216806)

Ab initio (DFT) calculation for TaAs



(Zhang et al., Phys. Rev. B, 97 (2018) 041101R)

Berry curvature-driven Hall response: Perturbative regime

$\sigma_{xy} = \frac{e^3\tau}{2\hbar^2}\mathcal{E}_x D_{xz}$ with $D_{xz} = \int \frac{d^3k}{(2\pi)^3} f_0(k) \frac{\partial \Omega_z^{odd}}{\partial k_x}$ Berry curvature dipole

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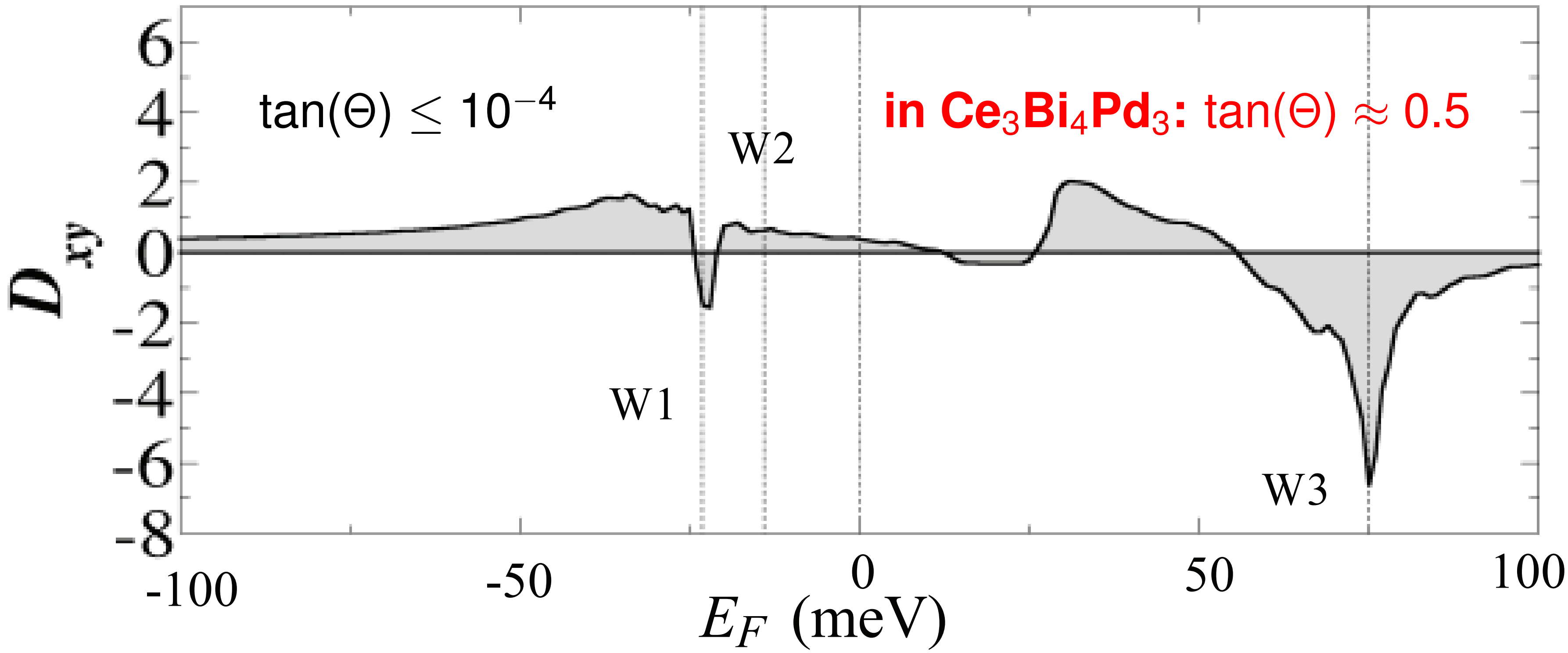

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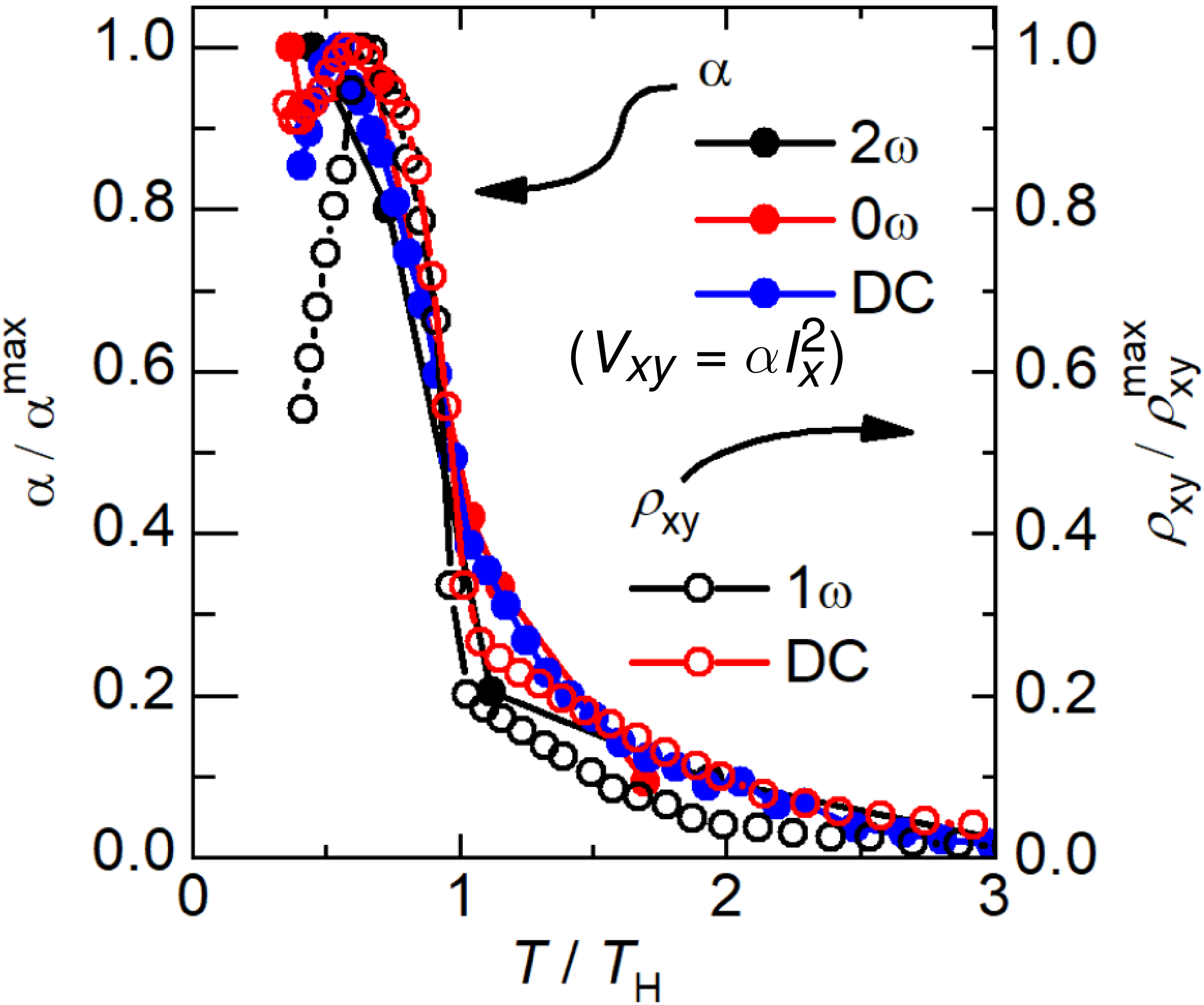
Extreme topological response 2: Beyond perturbative regime



(Dzsaber et al., PNAS 118 (2021) e2013386118)

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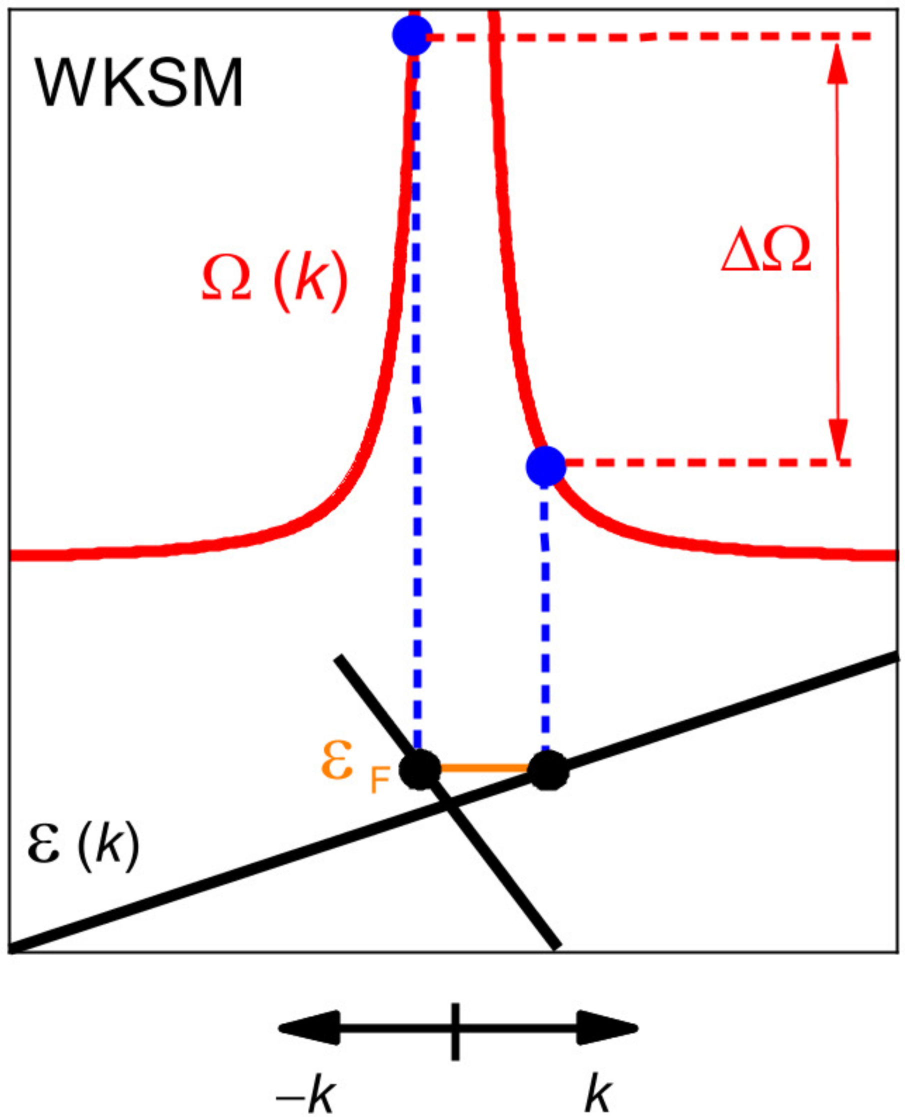

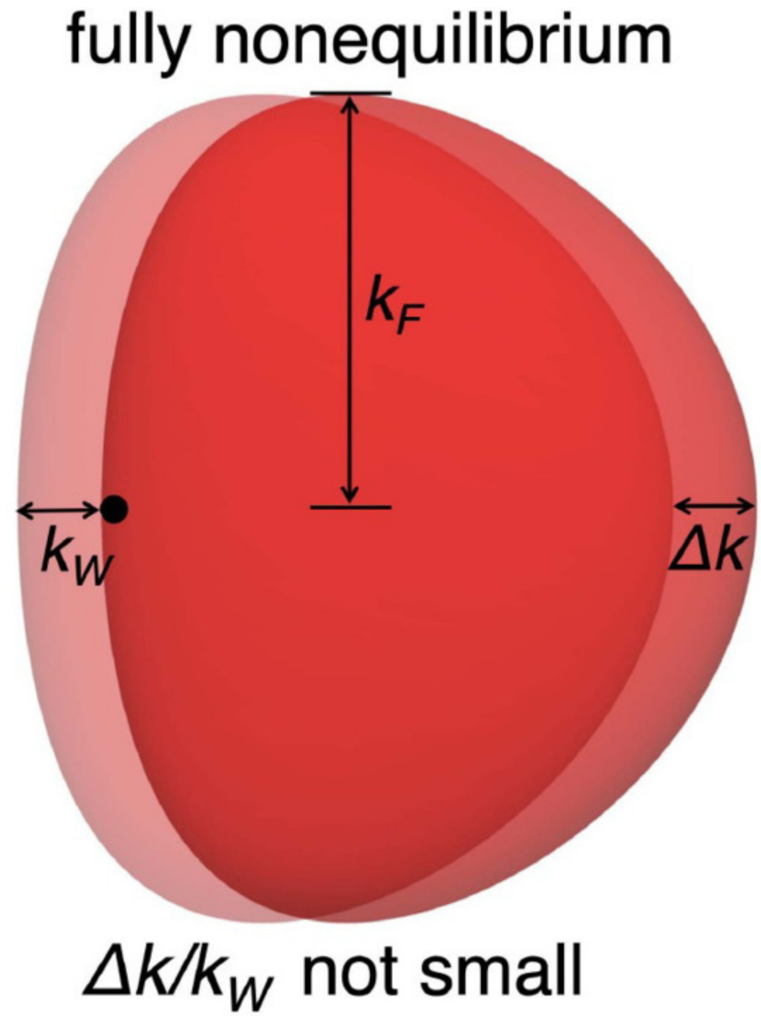

(Dzsaber, PhD thesis, 2020) (Dzsaber et al., PNAS 118 (2021) e2013386118)

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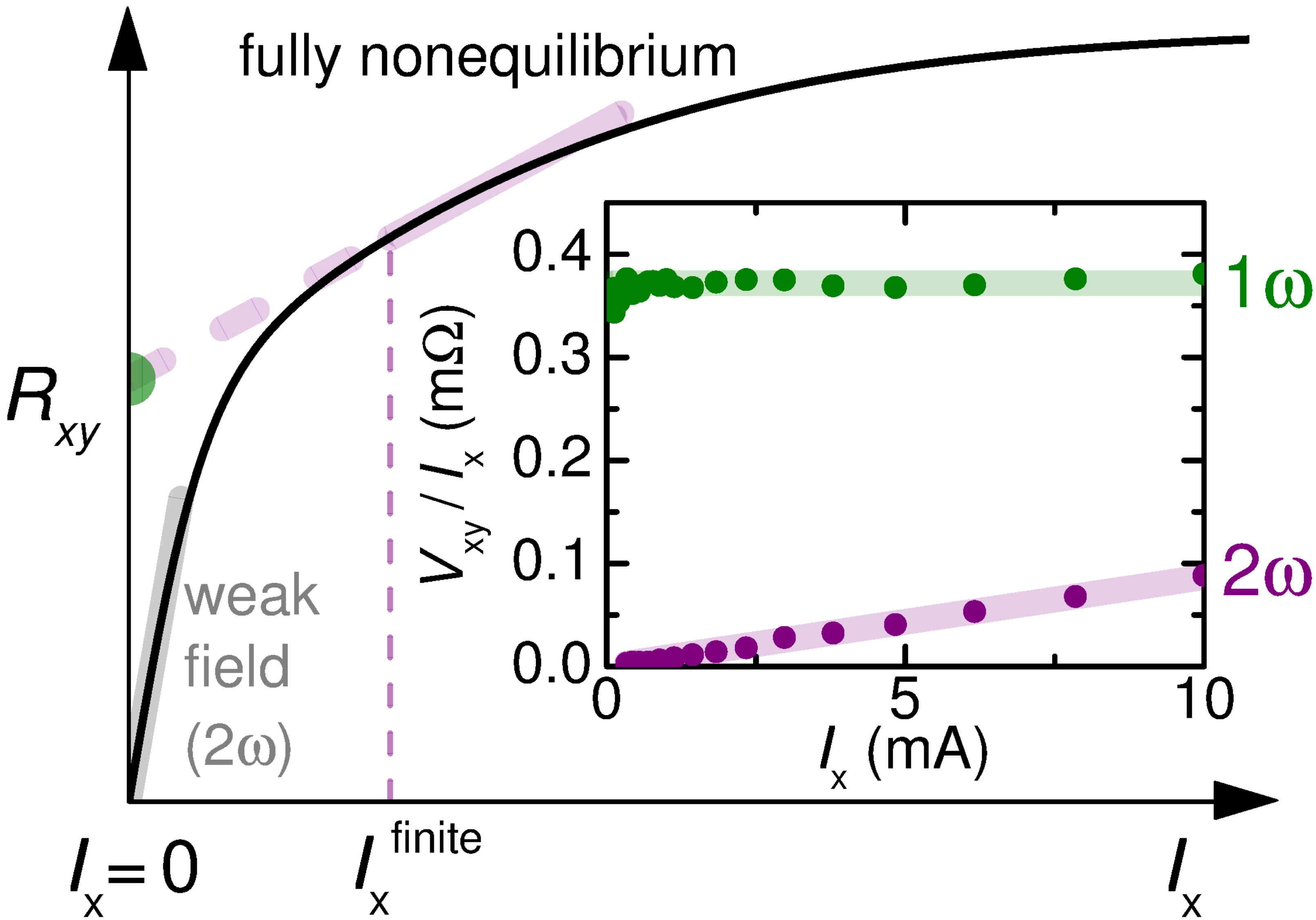

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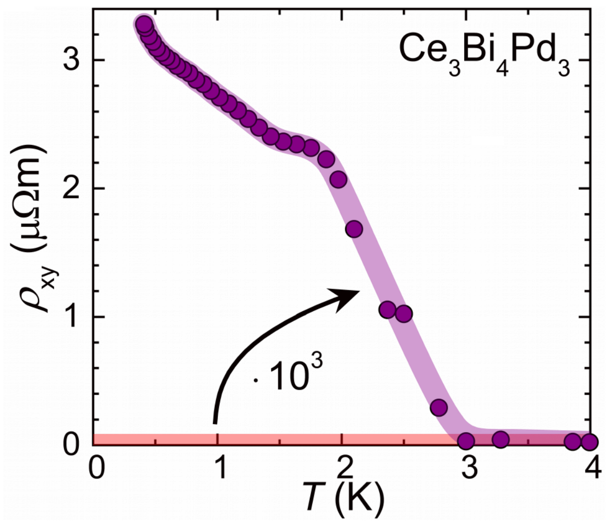

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Noninteracting Weyl semimetals

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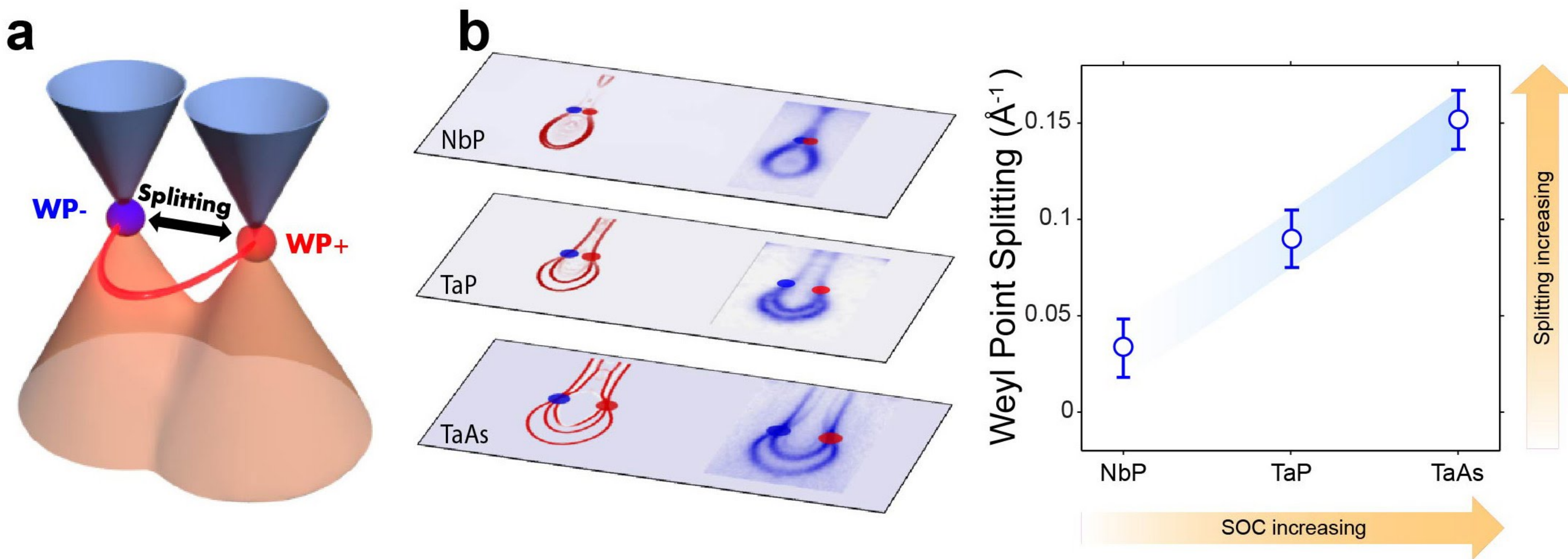
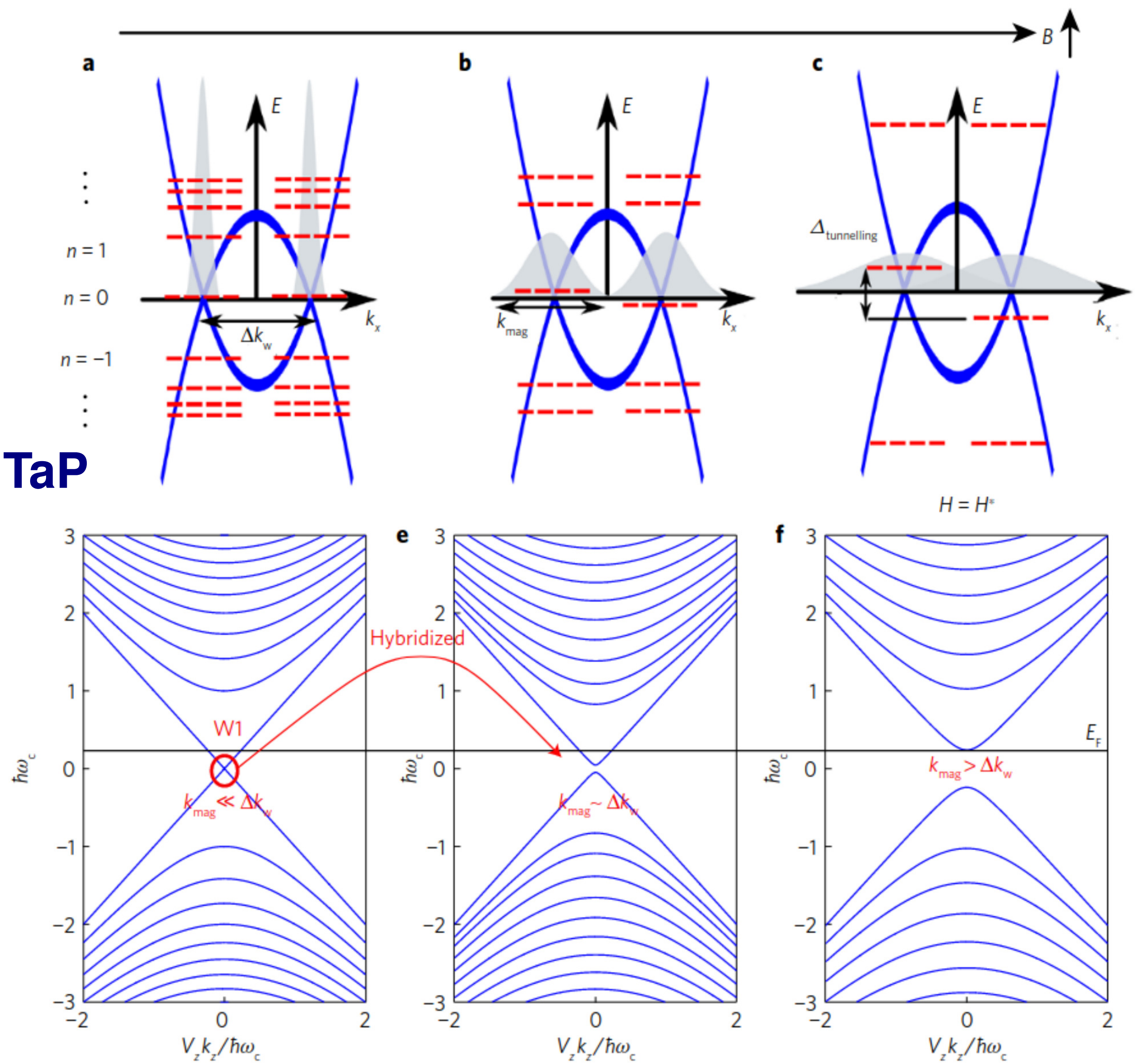


(Yang et al., Nat. Phys. 11 (2015) 728; Liu et al., Nat. Mater. 15 (2016) 27; Xu et al., Science 349 (2015) 613)

- **Control** of topology **difficult**:
  Limited tunability in momentum space;
  ***B* field tuning dominated by orbital effects (Zeeman effect $\ll$)**

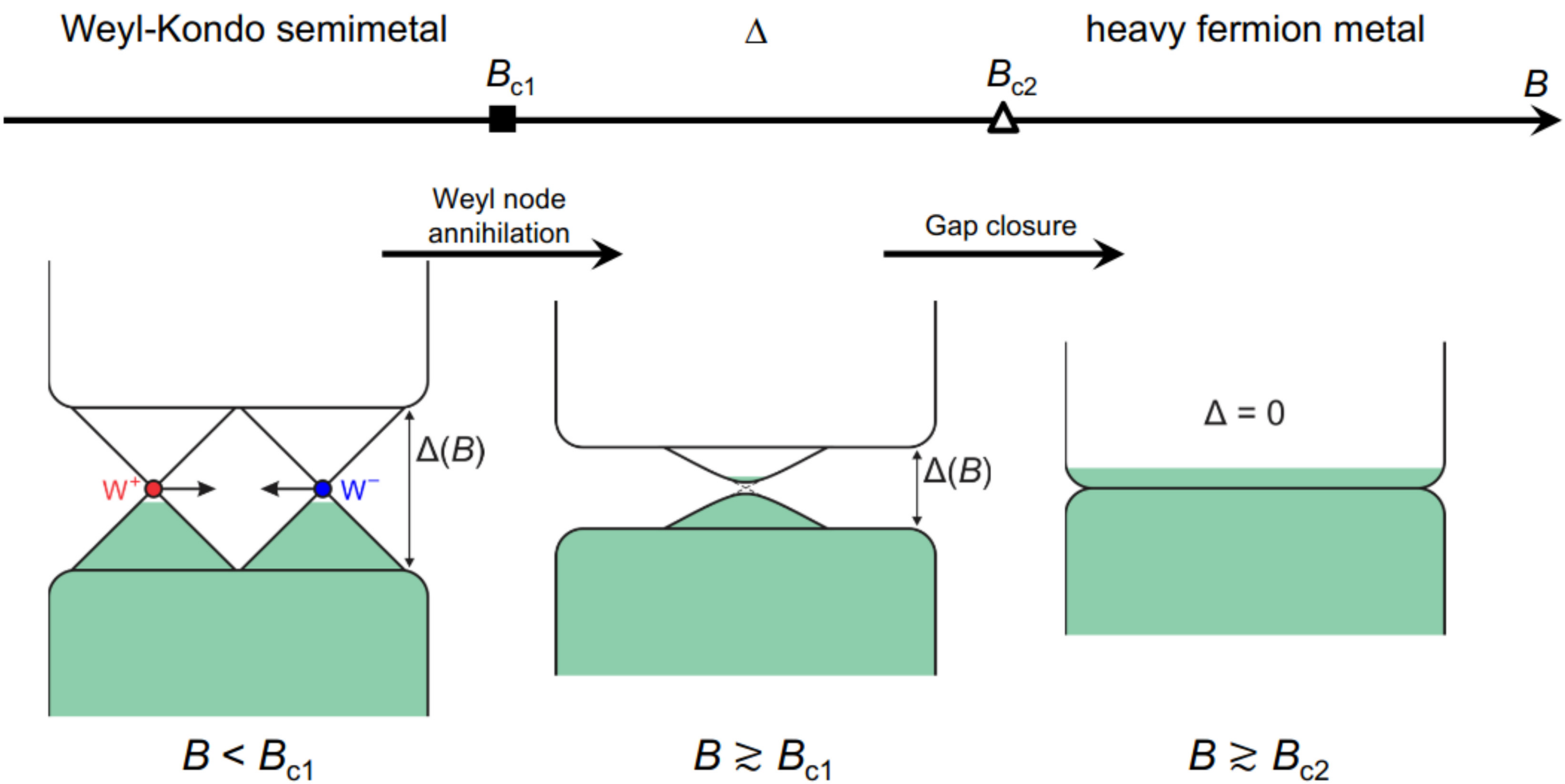
Noninteracting Weyl semimetals: Orbital effects of B

TaP



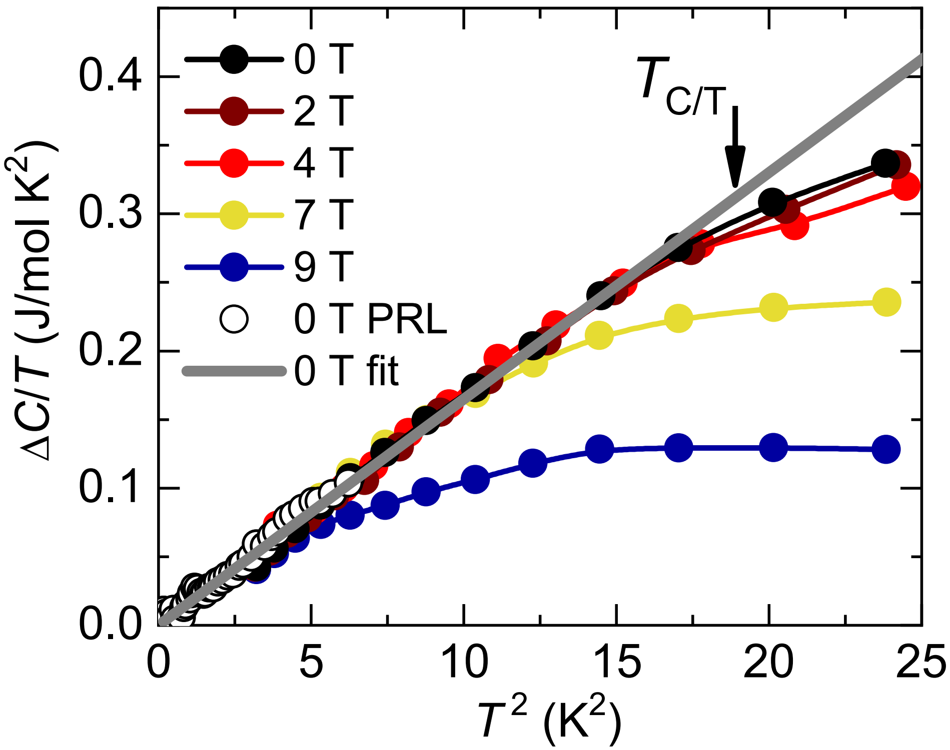
(Zhang et al., Nat. Phys. 13 (2017) 979)

Weyl node annihilation in Weyl-Kondo semimetal

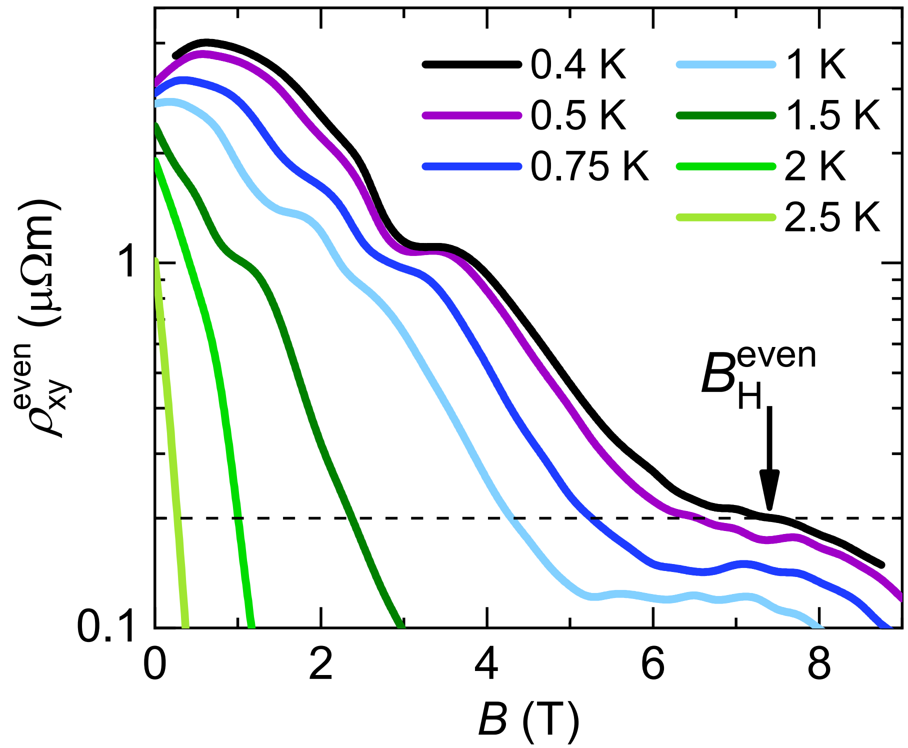


Suppression of topology signatures at B_{c1}

Specific heat



Even-in-B Hall resistivity

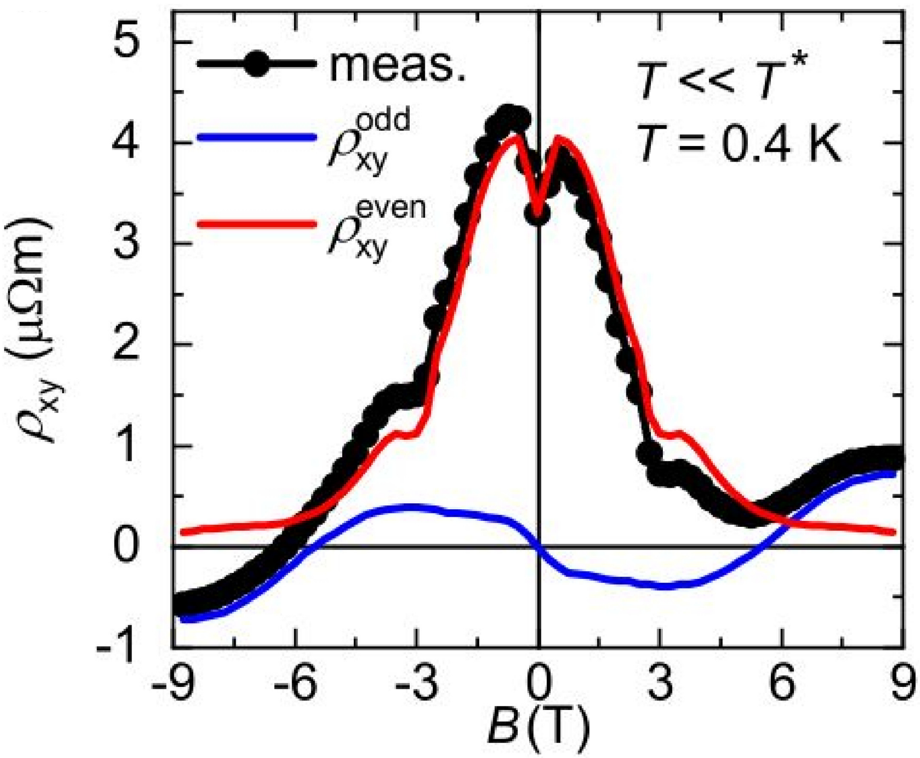


(Dzsaber et al., arXiv:1906.01182)

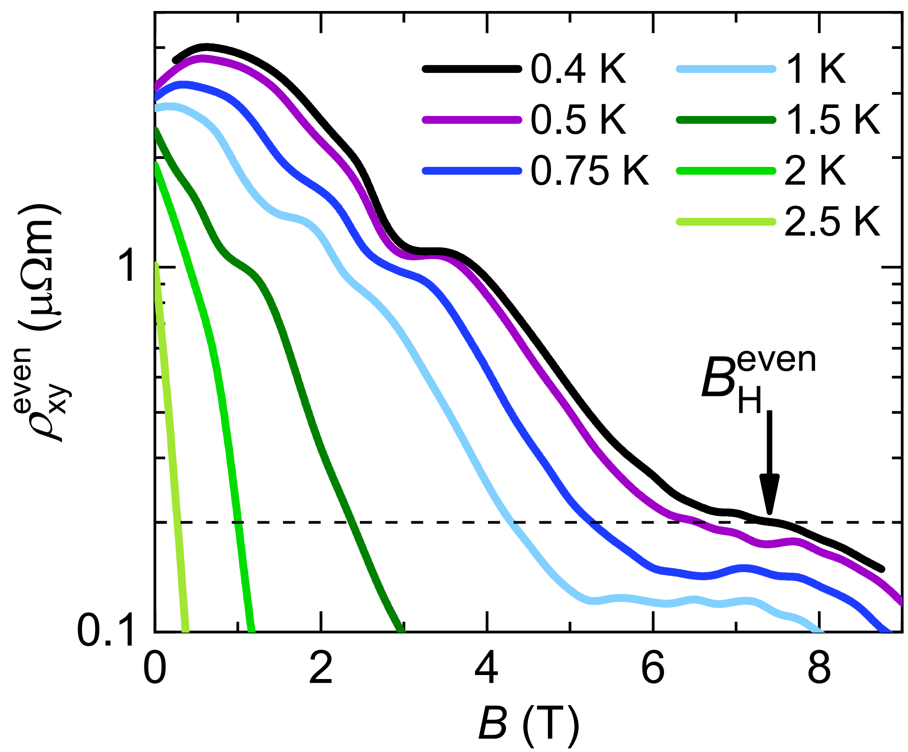
Theory on magnetic field effect in Weyl-Kondo semimetal model:
(Grefe et al., arXiv:2012.15841)

Suppression of topology signatures at B_{c1}

Hall data deconvolution



Even-in-B Hall resistivity

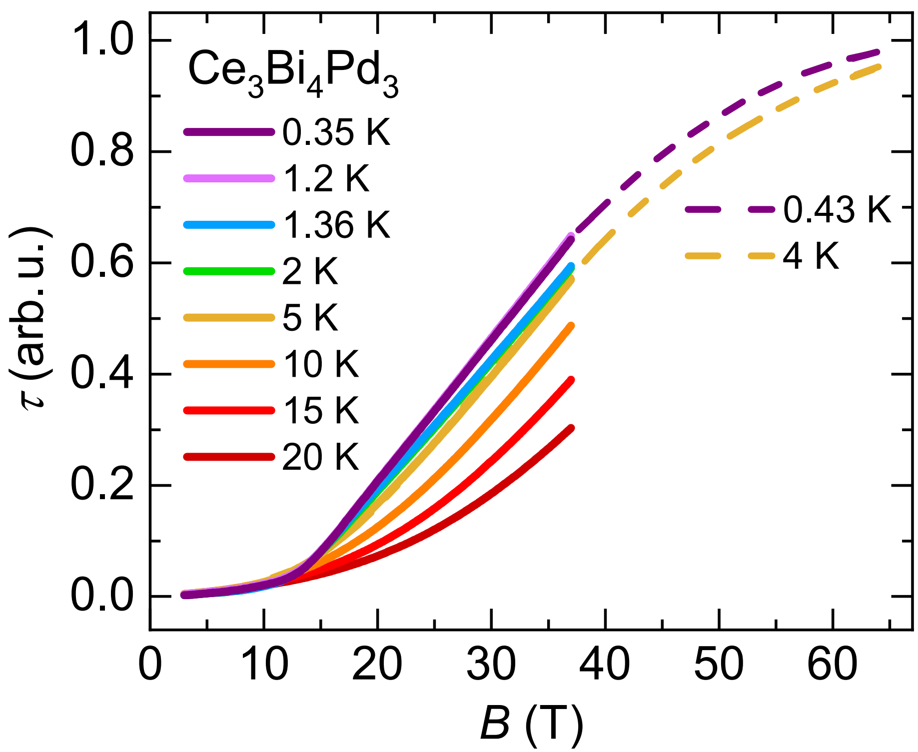


(Dzsaber et al., arXiv:1906.01182)

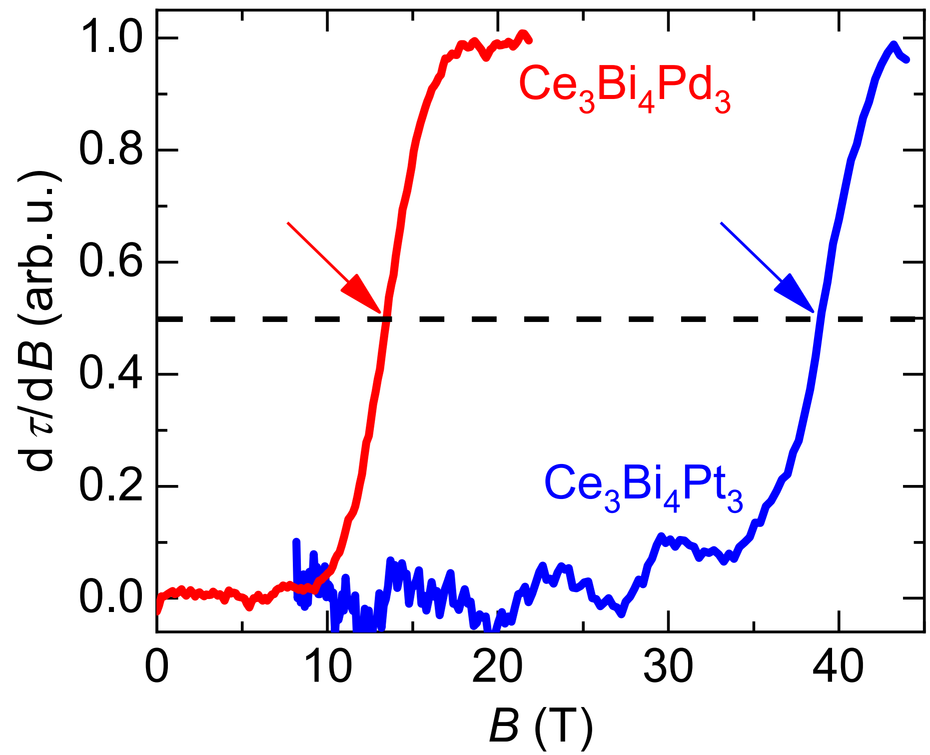
Theory on magnetic field effect in Weyl-Kondo semimetal model:
(Grefe et al., arXiv:2012.15841)

Suppression of (background) Kondo insulator gap at B_{c2}

Magnetic torque



Magnetic torque derivative

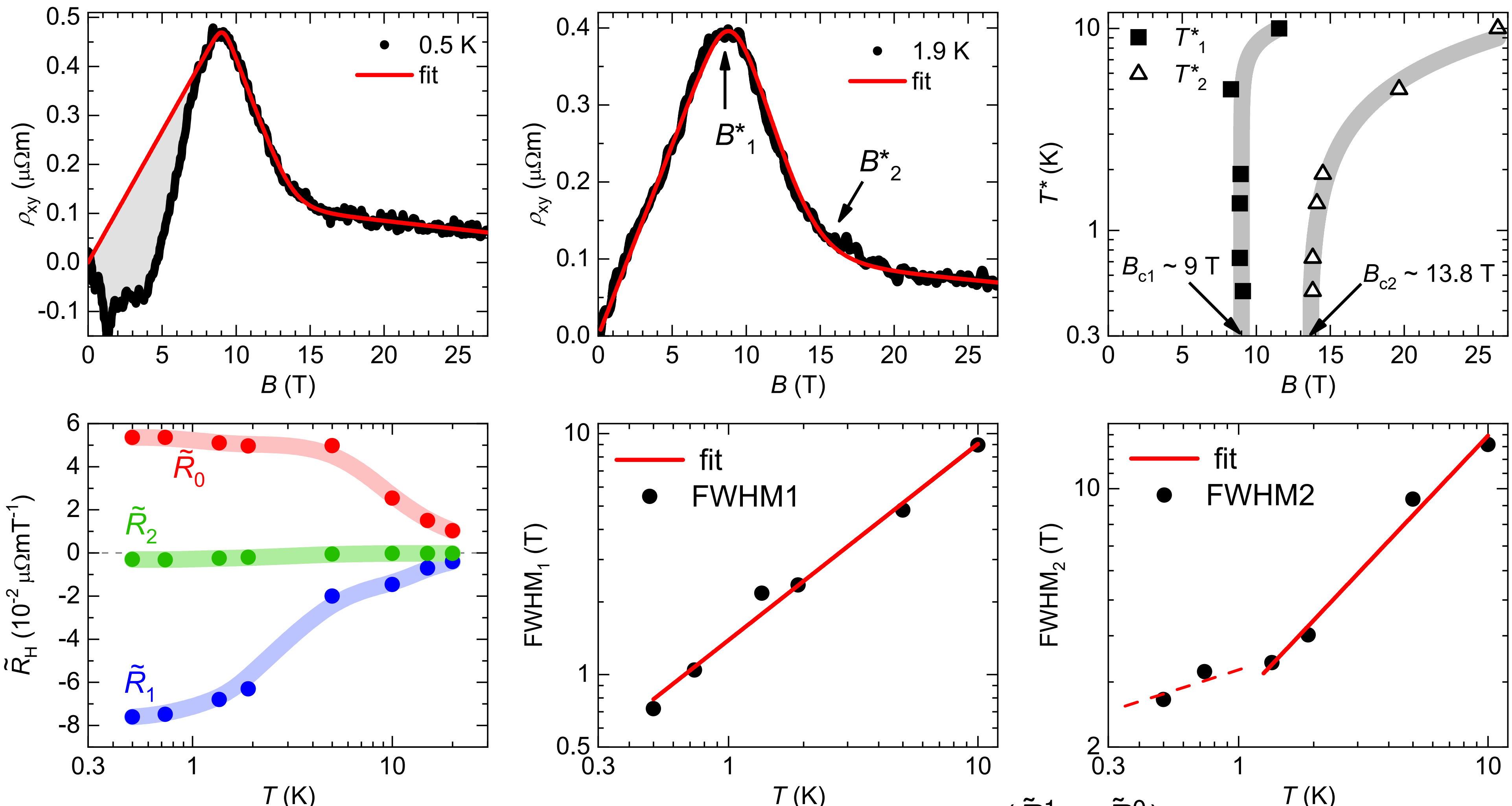


(Dzsaber et al., arXiv:1906.01182)

KI to metal transition seen from $c_p(B)$ in $Ce_3Bi_4Pt_3$:
(Jaime et al., Nature 405 (2000) 160)

Fermi surface reconstrutions at both B_{c1} and B_{c2}

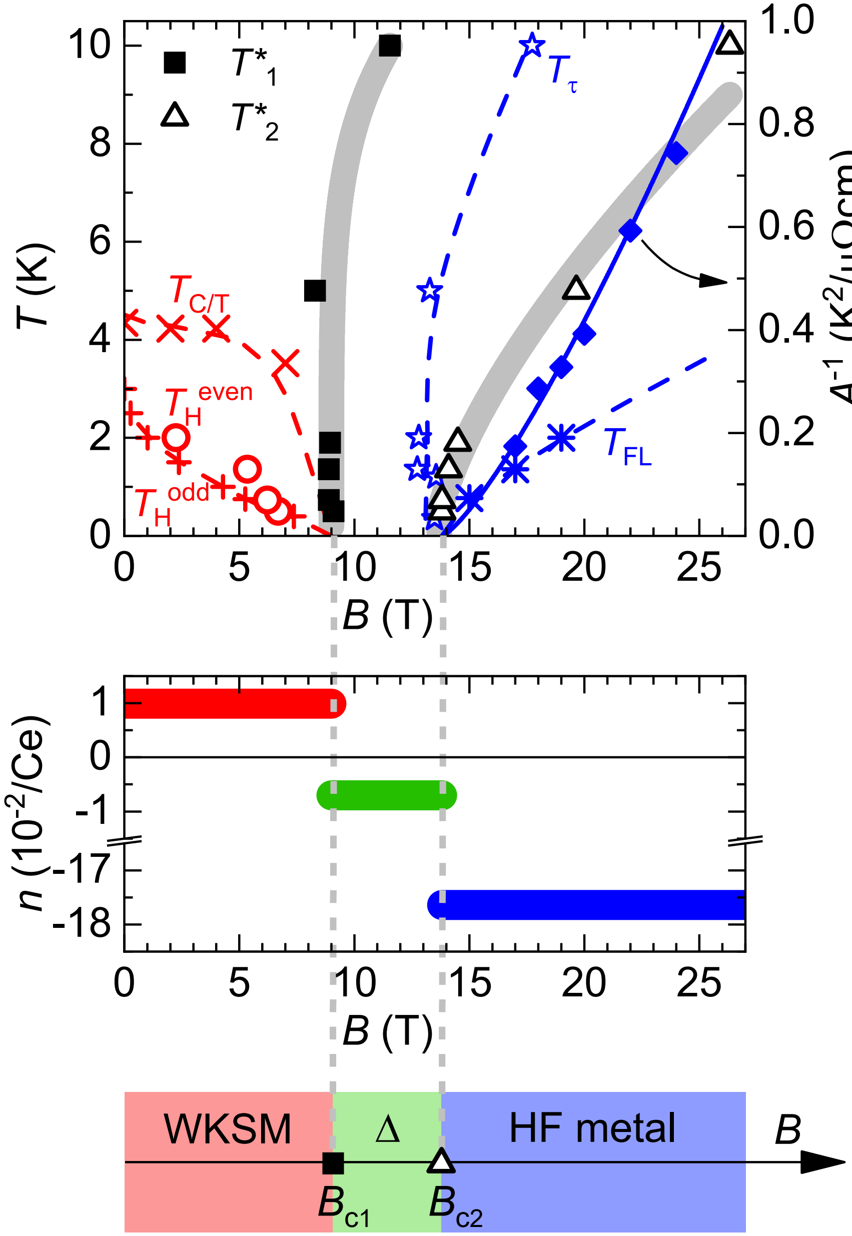
Quantitative analysis of “normal” (odd-in-B) Hall effect



$$\tilde{R}_{\mathrm{H}} = \tilde{R}_{\mathrm{H}}^{1} - \frac{(\tilde{R}_{\mathrm{H}}^{1} - \tilde{R}_{\mathrm{H}}^{0})}{\left[1 + \left(B/B_{1}^{*}\right)^{p}\right]}$$

(Dzsaber et al., arXiv:1906.01182)

Magnetic field-tuned phase diagram of $Ce_3Bi_4Pd_3$



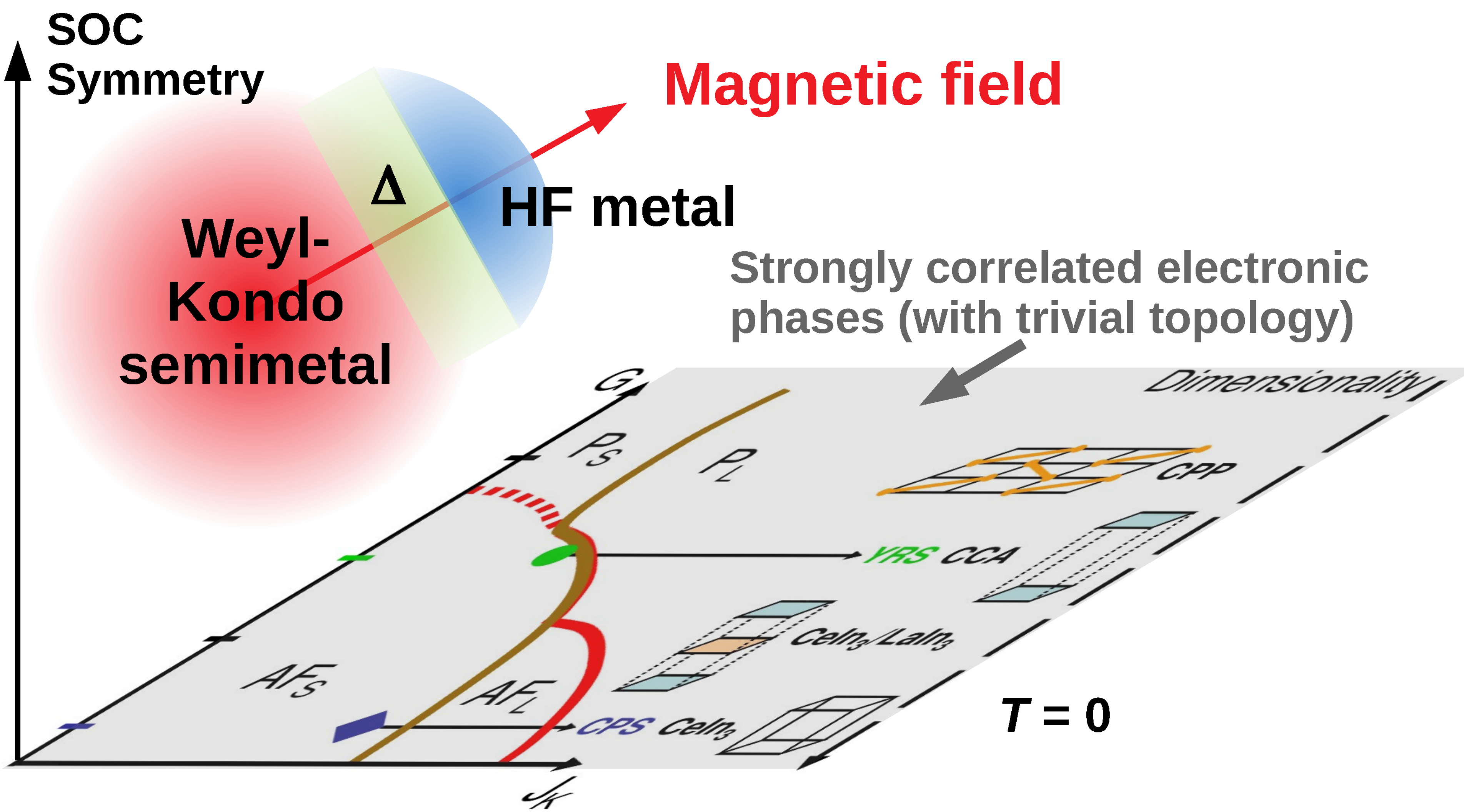
- **WKSM signatures suppressed at B_{c1}**
- **KI gap closed at B_{c2}**
- **Quantum phase transitions at B_{c1} and B_{c2}, with FS change**
- **Quantum criticality at B_{c2}**
- **Kondo interaction present across entire B range**

→ **Kondo-driven Weyl nodes annihilate in topological QPT**

→ **Genuine control of correlation-driven topology**

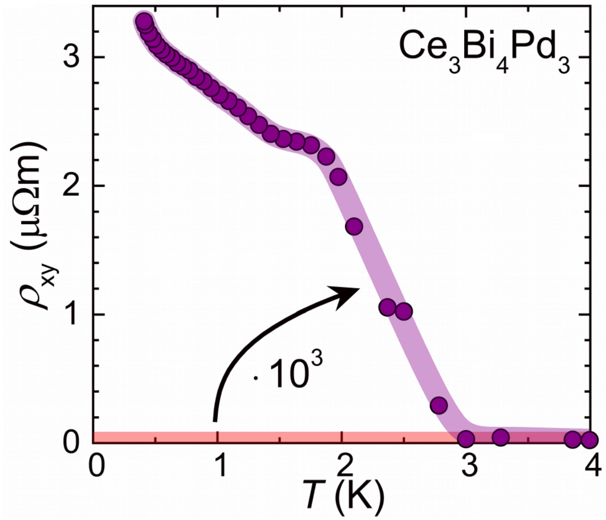
(Dzsaber et al., arXiv:1906.01182)

Genuine topology control by magnetic field



Heavy fermion systems

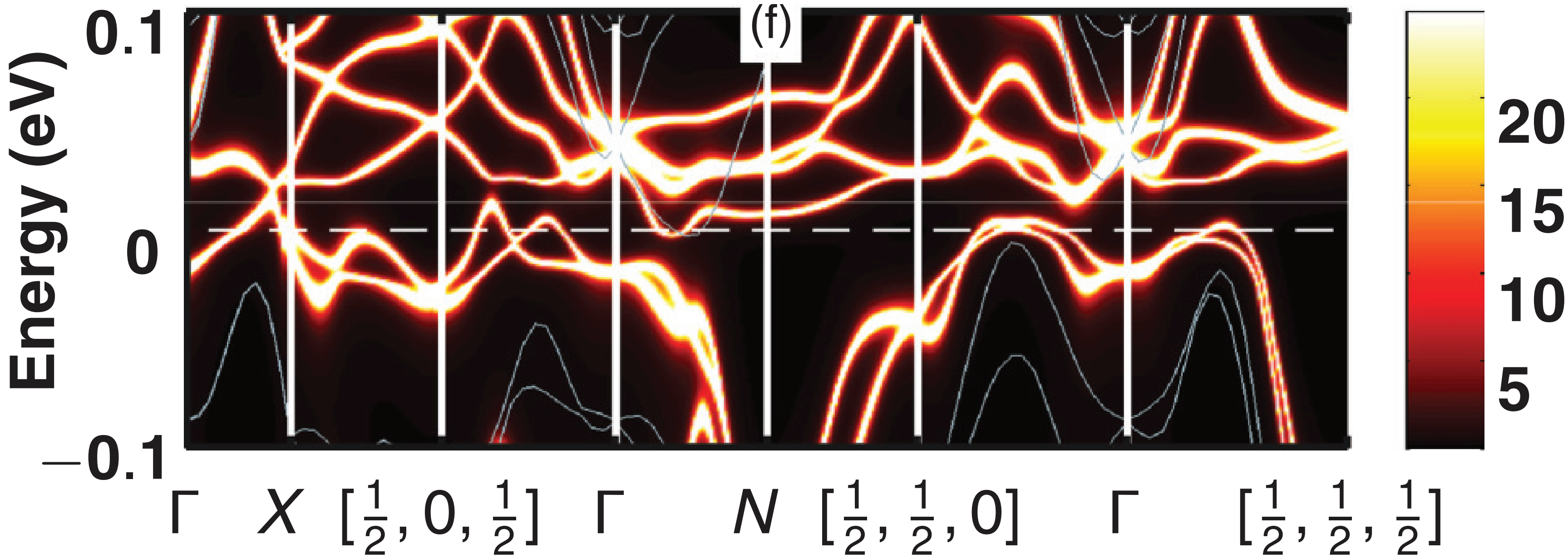
From quantum criticality to electronic topology



- Electronic topology: Noninteracting Weyl semimetals
- Discovery of the Weyl-Kondo semimetal
- Can strongly correlated topology be tuned?
- **New strongly correlated topological materials**
- Correlation-driven topology as emergent phase?

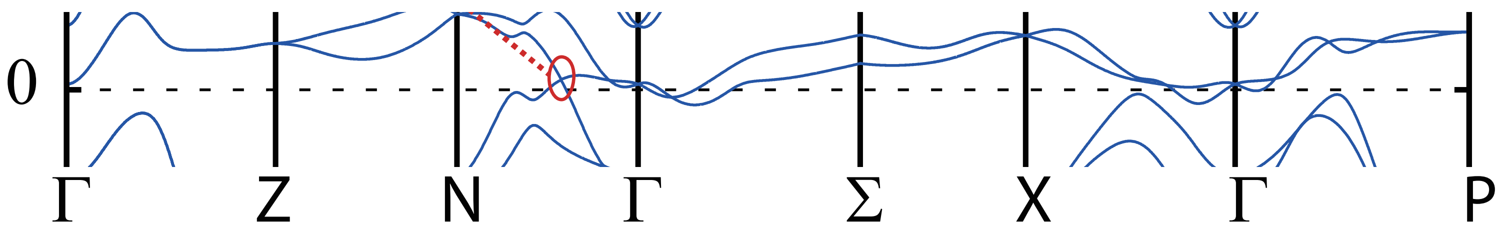
Noncentrosymmetric semimetal $CeRu_4Sn_6$

LDA + DMFT (290 K)



(Guritanu et al., Phys. Rev. B 87 (2013) 115129)

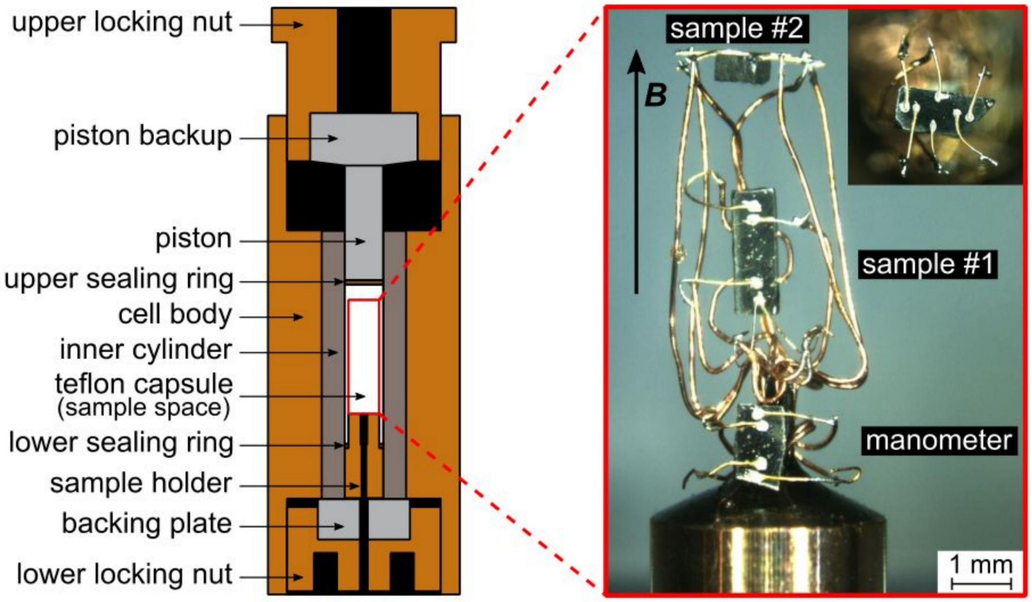
LDA + Gutzwiller (0 K)



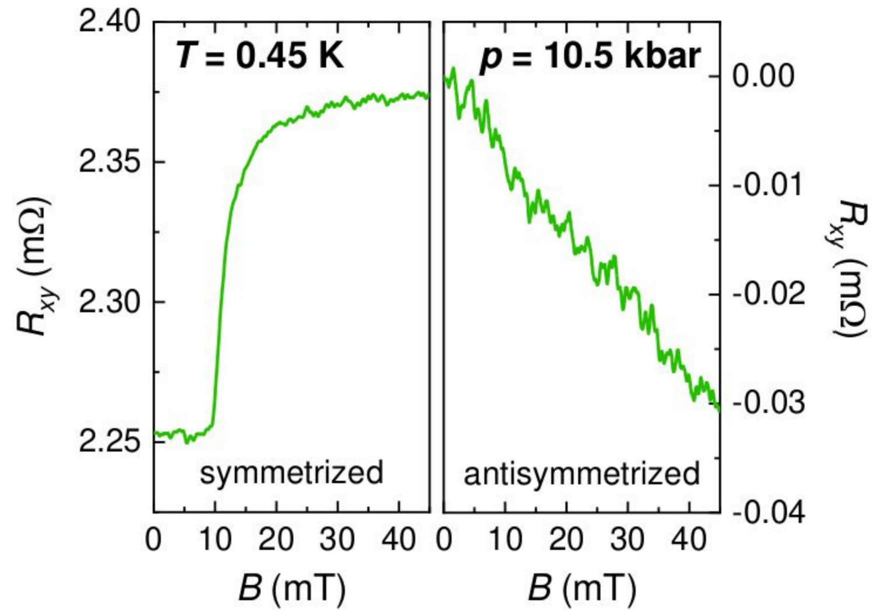
(Xu et al., Phys. Rev. X 7 (2016) 011027)

$CeRu_4Sn_6$: A Weyl-Kondo semimetal?

Pressure cell



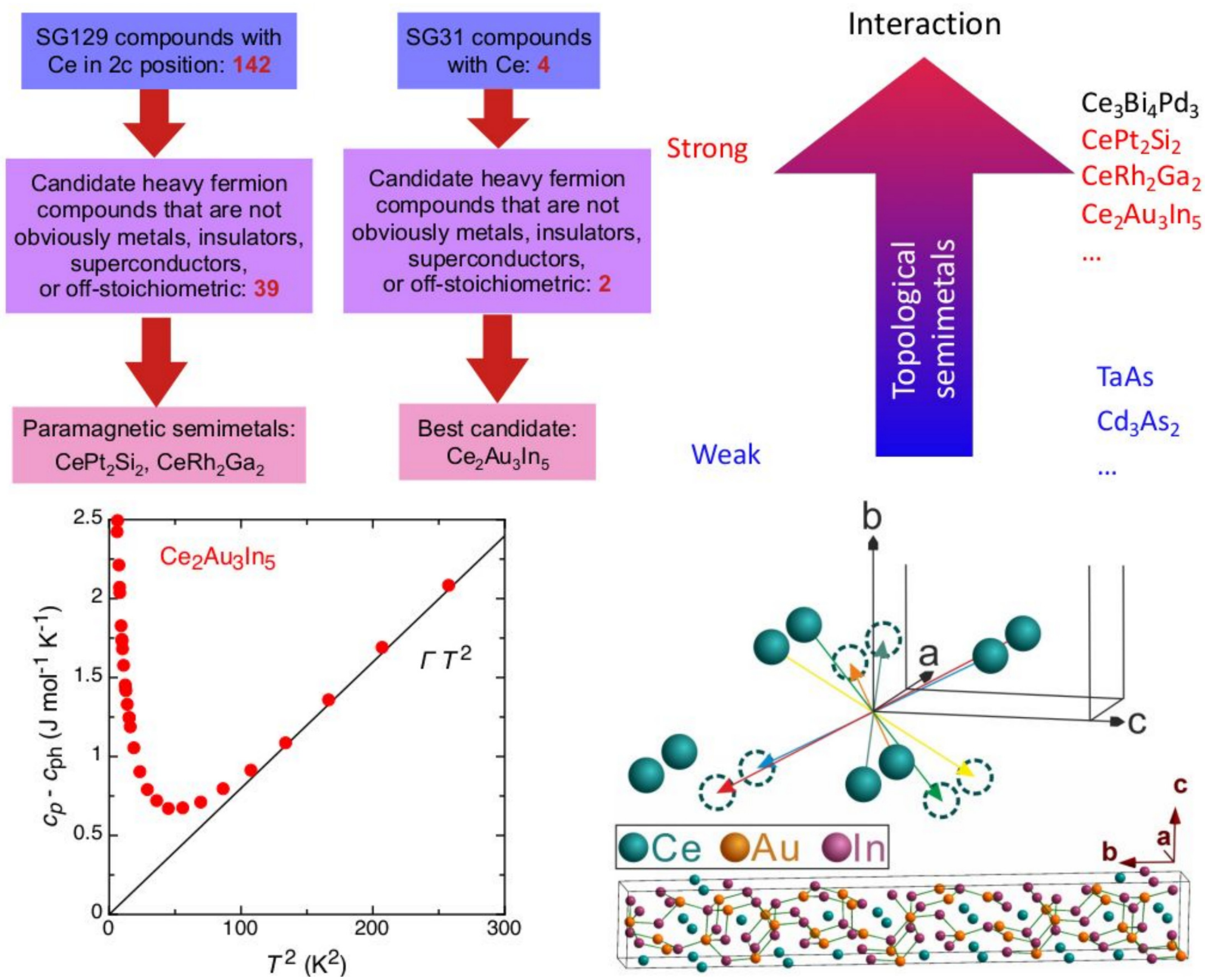
Even-in-field Hall response



→ Poster Diana Kirschbaum

Search strategy: Strong correlations & crystalline symmetry

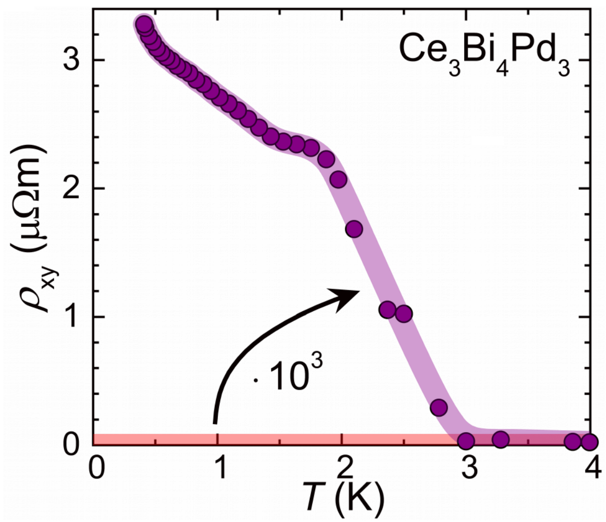
Kondo square net lattices + space group symmetries → Weyl-Kondo nodal-line semimetals



(Chen et al., arXiv:2107.10837)

Heavy fermion systems

From quantum criticality to electronic topology



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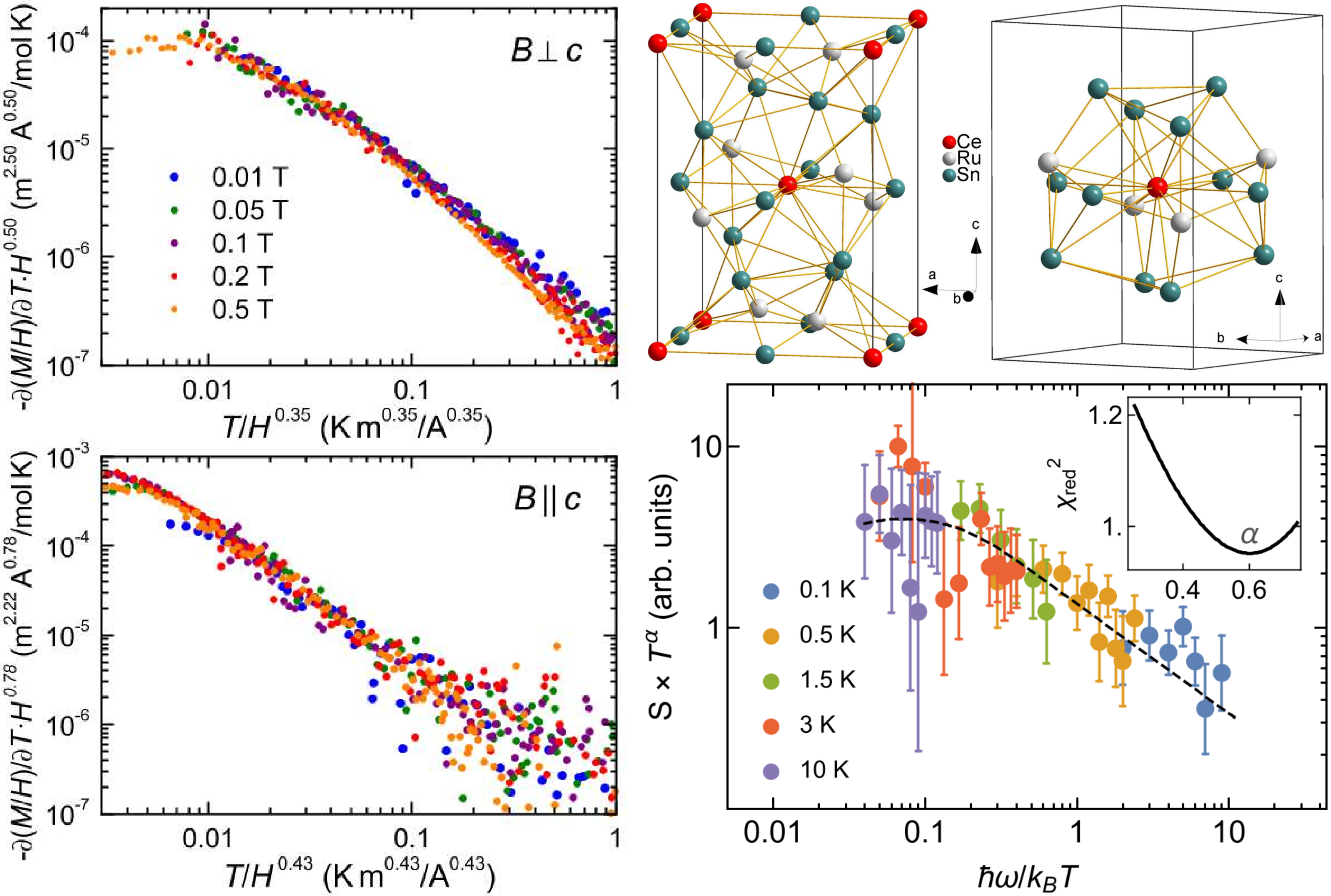
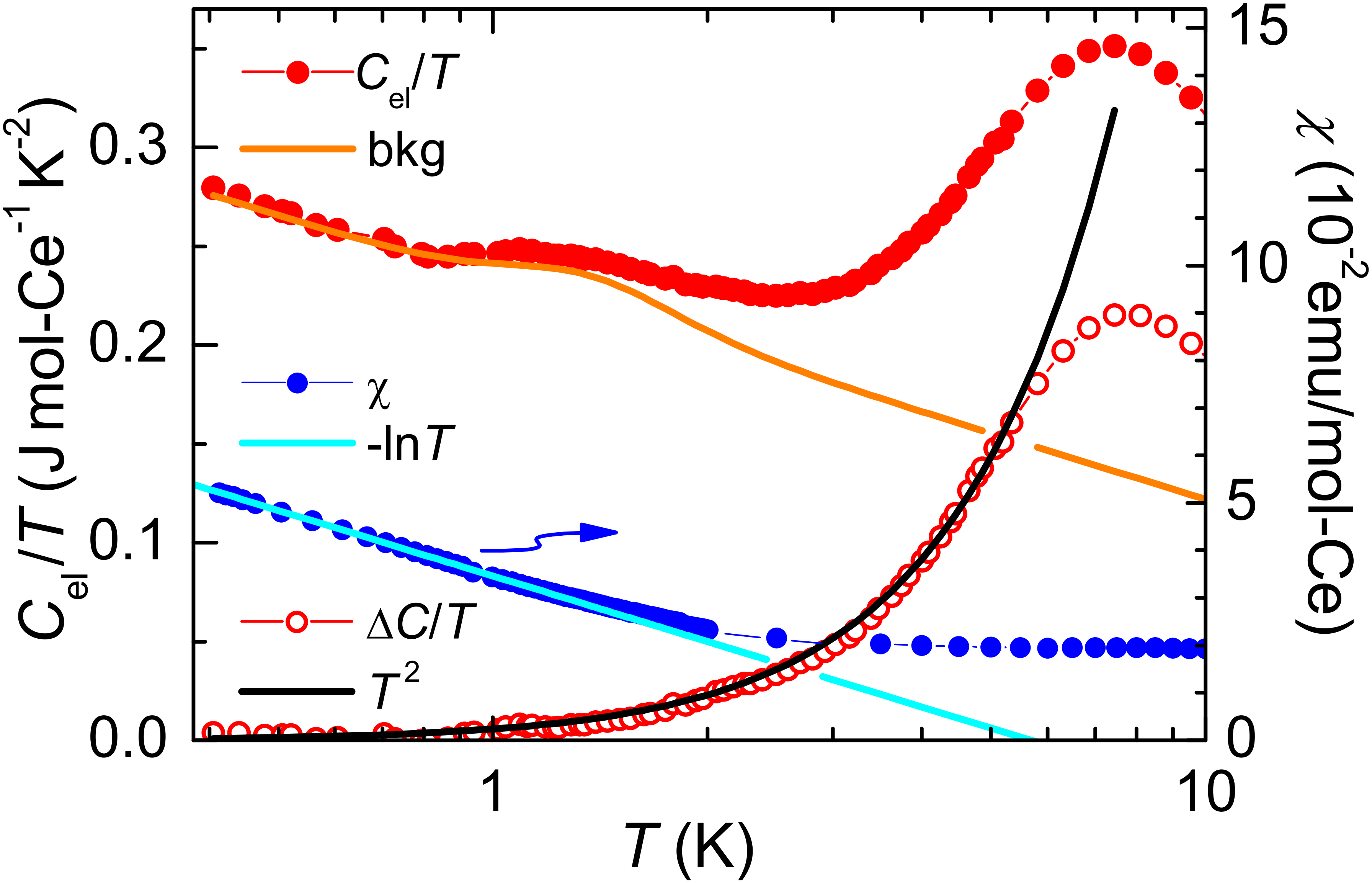
- **Correlation-driven topology as emergent phase?**

Quantum criticality in Kondo semimetal $CeRu_4Sn_6$



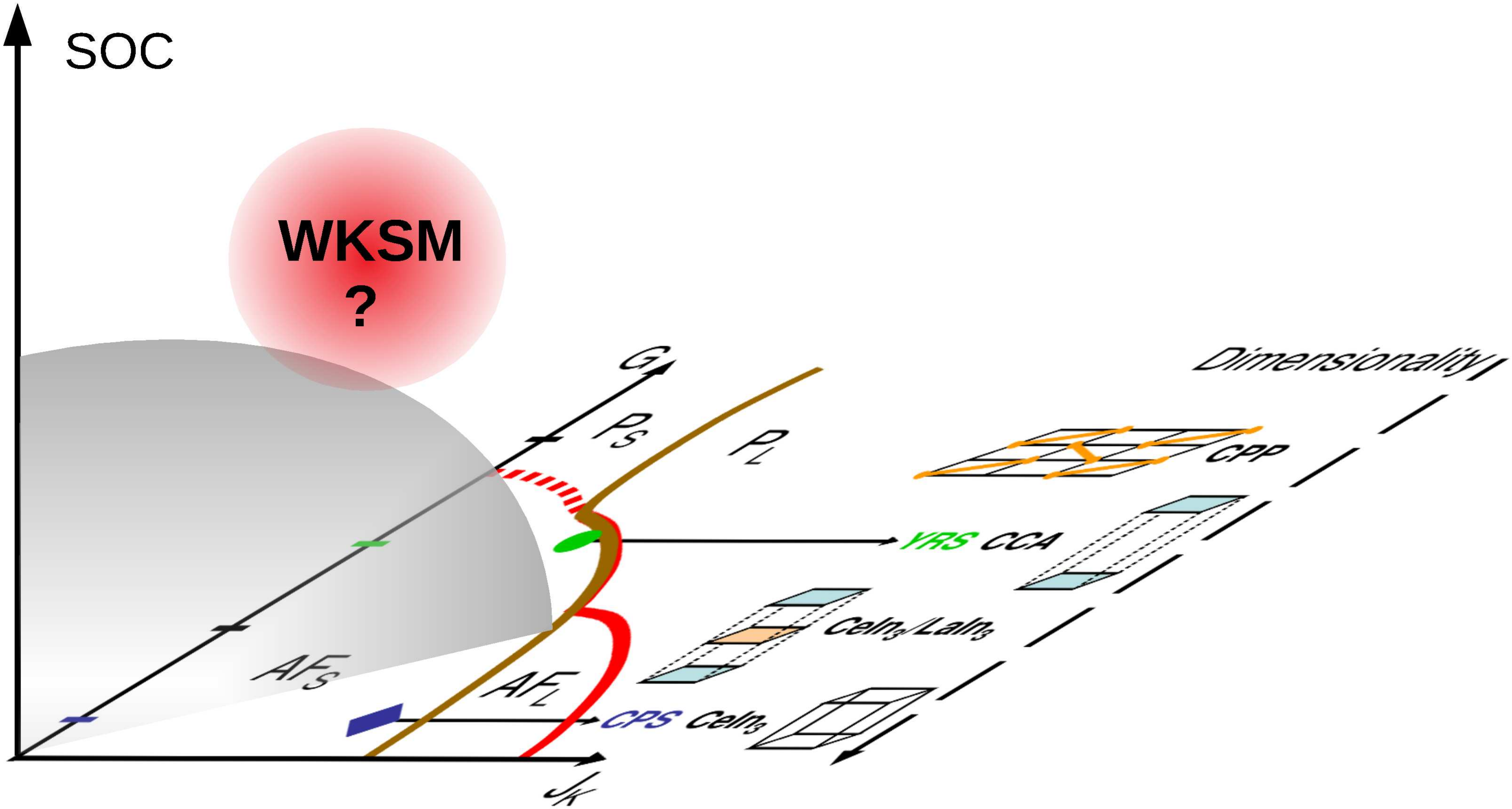
(Fuhrman et al., Sci. Adv. 7 (2021) eabf9134)

Tentative evidence for quantum criticality in $Ce_3Bi_4Pd_3$



(Dzsaber et al., Phys. Rev. Lett. 118 (2017) 246601)

Correlation-driven topology through quantum fluctuations?



S. Dzsaber, G. Eguchi, L. Fischer, L. Prochaska, A. Prokofiev, A. Sidorenko, R. Svagera, M. Taupin, M. Waas, X. Yan, D. A. Zocco

Institute of Solid State Physics, Vienna University of Technology

T. Shiroka

Paul Scherrer Institut, Villigen

A. McCollam, L. M. K. Tang, B. Vlaar

High Field Magnet Laboratory Nijmegen

F. Weickert, R. McDonald, L. Stritzinger, M. Jaime

Los Alamos National Laboratory

L. Chen, H.-H. Lai, S. E. Grefe, C. Setty, Q. Si

Rice University, Houston

P. Blaha; O. Rubel; M. G. Vergniory

Institute of Materials Chemistry, Vienna University of Technology; Department of Materials Science and Engineering, McMaster University; Max Planck Institute for Chemical Physics of Solids, Dresden & Donostia International Physics Center, San Sebastian

J. Cano

Department of Physics and Astronomy, Stony Brook University, Stony Brook & Center for Computational Quantum Physics, Flatiron Institute, New York

Summary

- Heavy fermion compounds can host robust gapless topological bands
- A new phase, the Weyl-Kondo semimetal, is established
- It has giant topological signatures
- Genuine topology control with magnetic field is realized
- New candidate materials are identified
- Are correlated topological phases emergent phases?