

# Superconductivity and Magnetism in Topological Half-Heusler Semimetals

Yasuyuki Nakajima<sup>1</sup>, Rongwei Hu<sup>1</sup>, Kevin Kirshenbaum<sup>1</sup>, Alex Hughes<sup>1</sup>, Paul Syers<sup>1</sup>, Xiangfeng Wang<sup>1</sup>, Kefeng Wang<sup>1</sup>, Renxiong Wang<sup>1</sup>, Shanta Saha<sup>1</sup>, Daniel Pratt<sup>2</sup>, Jeffrey W Lynn<sup>2</sup>, Johnpierre Paglione<sup>1</sup>

<sup>1</sup>University of Maryland, College Park

<sup>2</sup>NIST, Center for Neutron research

Sci. Adv. **1**, e1500242



*Center for Nanophysics & Advanced Materials*

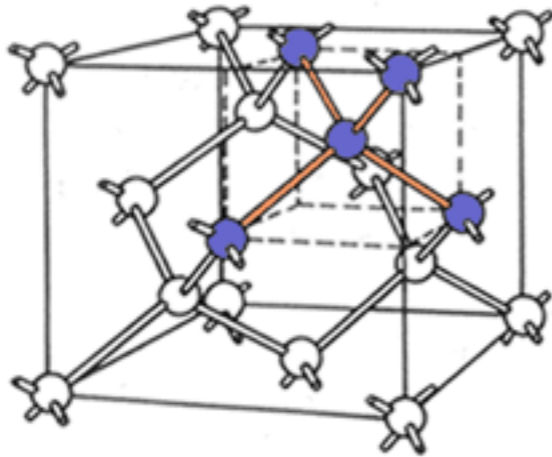
# Outline

- Introduction:
  - Topological insulator: a new quantum state of matter
  - Half Heusler semimetal RPdBi:  
promising candidate for a topological material
- Experimental Results for RPdBi:
  - Magnetic susceptibility: Localized f electrons
  - Neutron diffraction: Antiferromagnetism
  - Charge transport and magnetic measurements:  
Superconductivity
- Discussion:
  - Realization of peculiar superconductivity:  
Singlet-triplet mixing, Magnetic SC, BCS-BEC crossover
- Summary

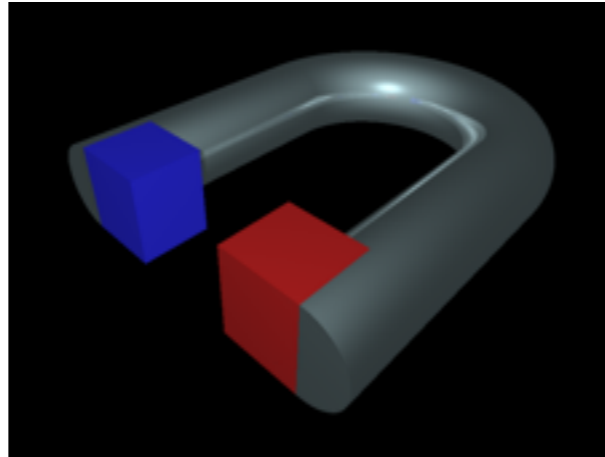
# Topological Insulator

**Phase transition**

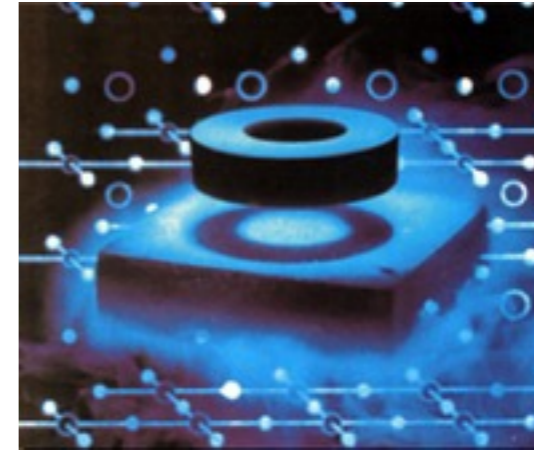
**Breaking symmetry**



Crystal: Broken translational symmetry



Magnet: Broken rotational symmetry



Superconductor: Broken gauge symmetry

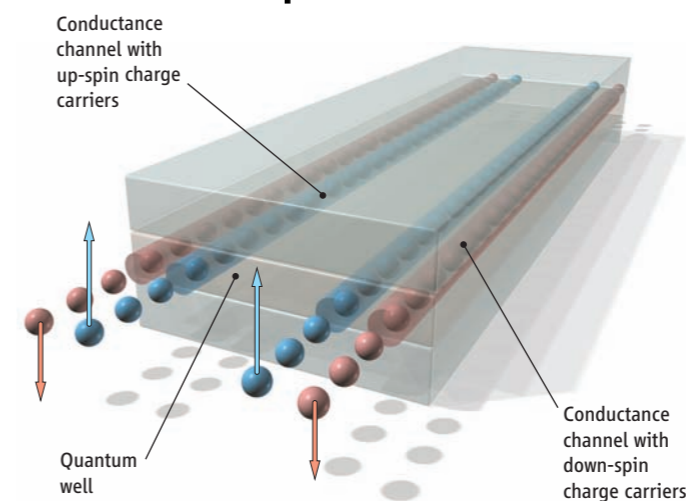
**Topological insulator**

New quantum phase of matter

**absence of symmetry breaking**

e.g. Quantum spin Hall state  
2D topological insulator

**chiral boundary state**



Schematic of the spin-polarized edge channels in a quantum spin Hall insulator.

M. Konig *et al.* Science (2007)

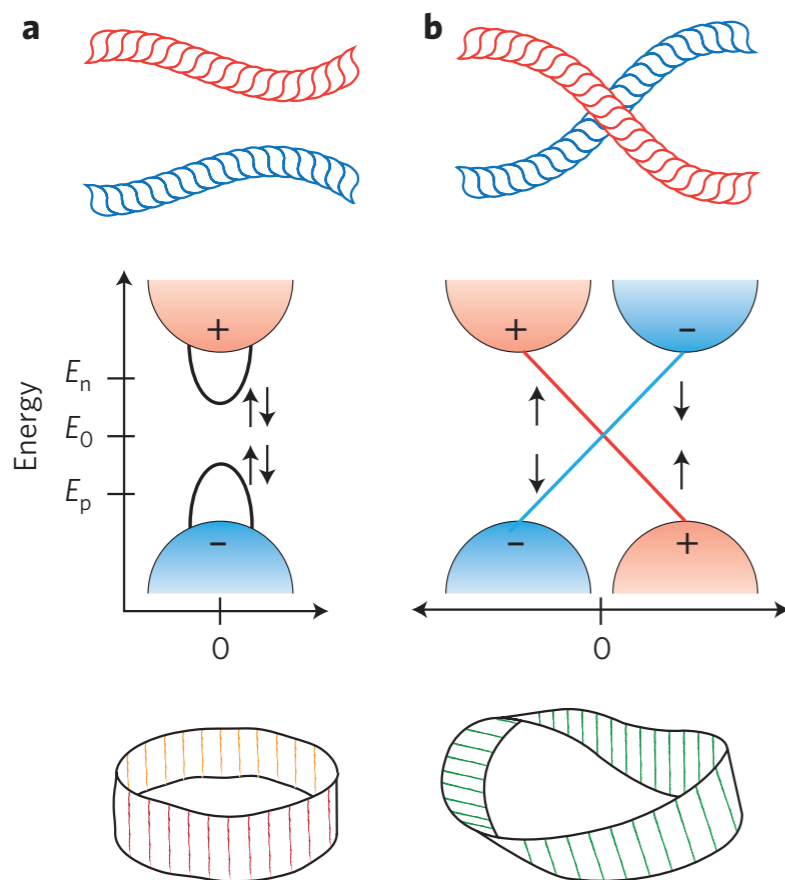
# Topological Insulator

## 3D Topological insulator

L. Fu *et al.* Phys. Rev. Lett. (2007)

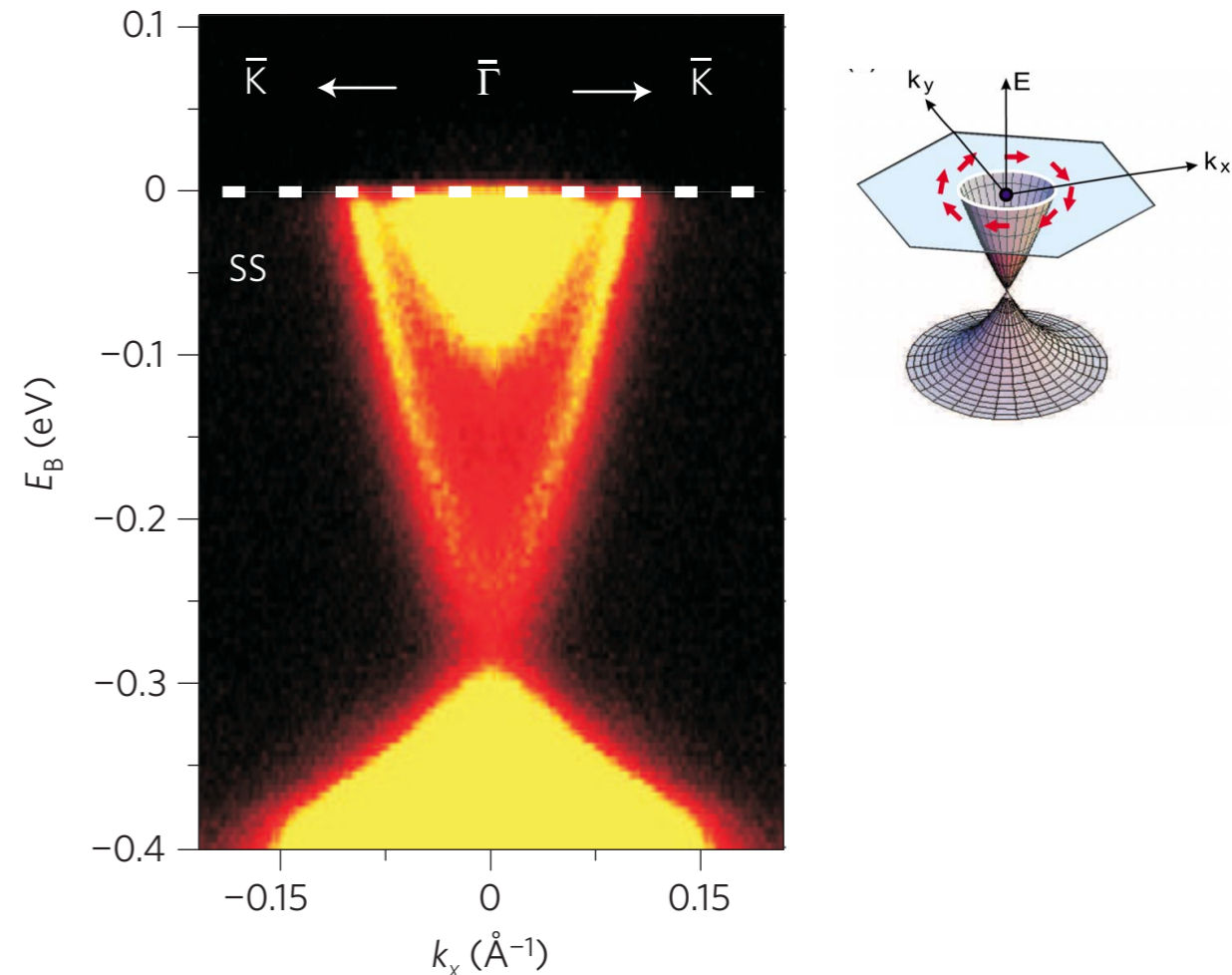
Metallic surface state protected against time reversal invariant perturbations

### Trivial Topological



H.C. Manoharan *et al.* Nat. Nano (2010)

### Bi<sub>2</sub>Se<sub>3</sub>



Y. Xia *et al.* Nat. Phys. (2009)

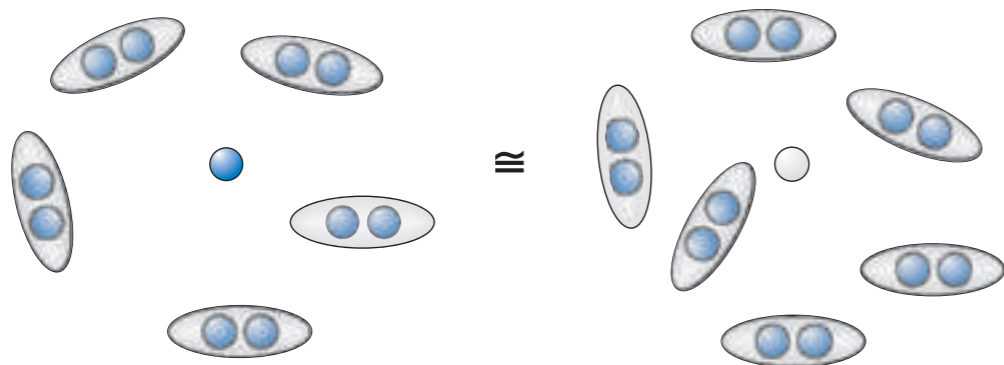
# Topological order with symmetry breaking

Unusual collective modes predicted in particle physics

Majorana fermion

Charge neutral

$$\hat{c}^\dagger = \hat{c}$$



F. Wilczek *et al.* Nat. Phys. (2009)

Topological order

+

Superconductivity

Axion

Anomalous magnetoelectric effect

$$\mathbf{M} = -(e^2/4\pi\hbar c)\theta\mathbf{E}$$

$\theta$  : axion field

R. Li *et al.* Nat. Phys. (2010)

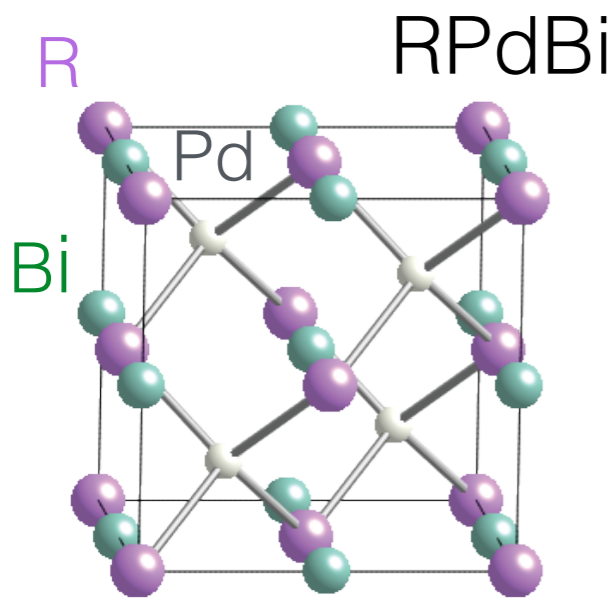
Topological order

+

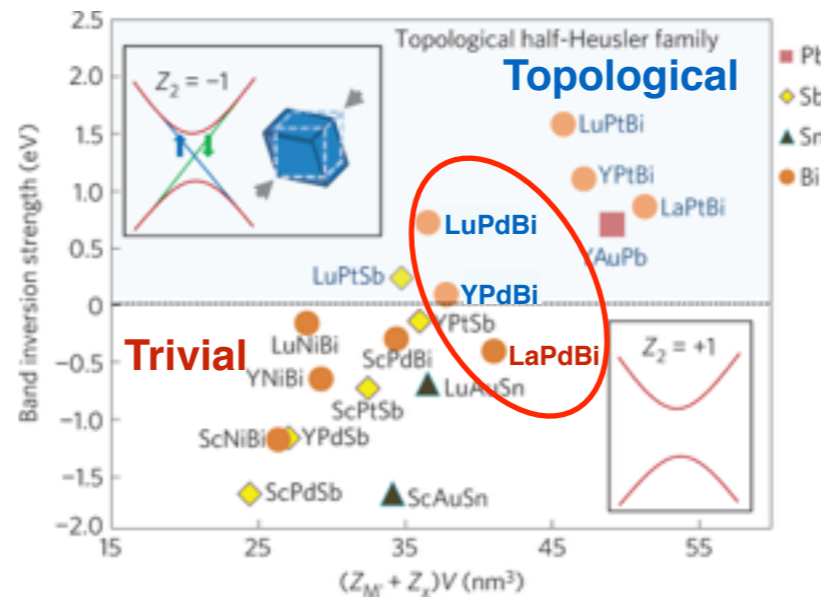
Magnetism

# Half Heulser semimetals

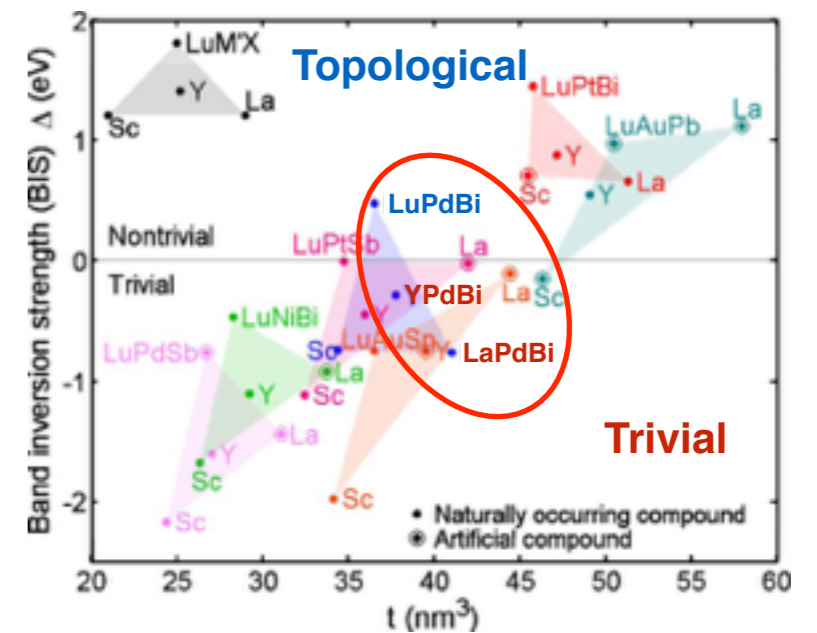
Cubic MgAgAs type



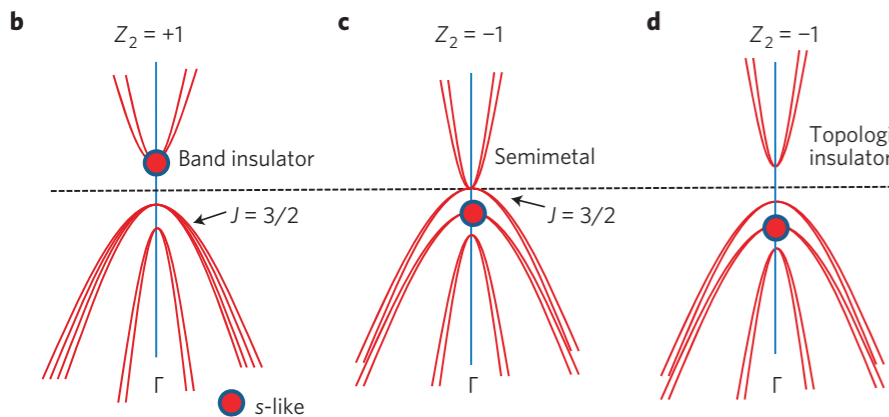
Lack of inversion symmetry



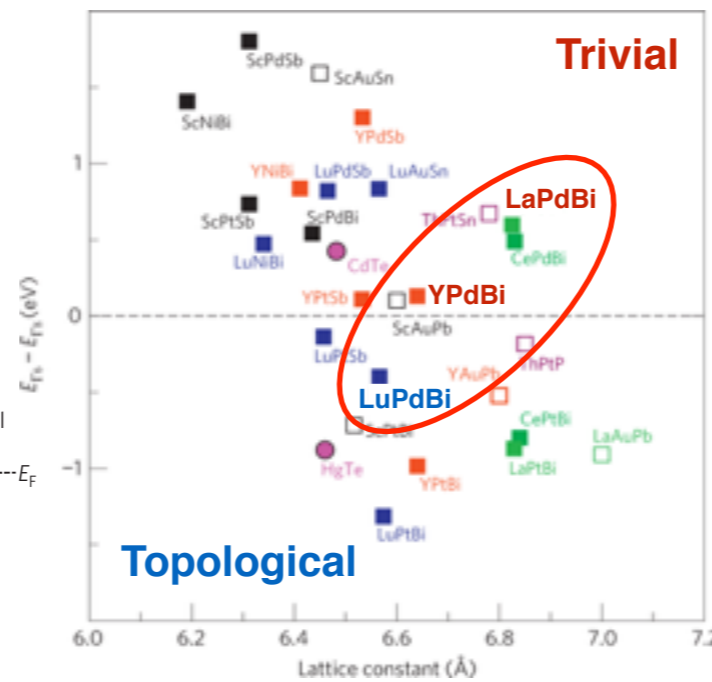
Lin et al. Nat. Mat. (2010)



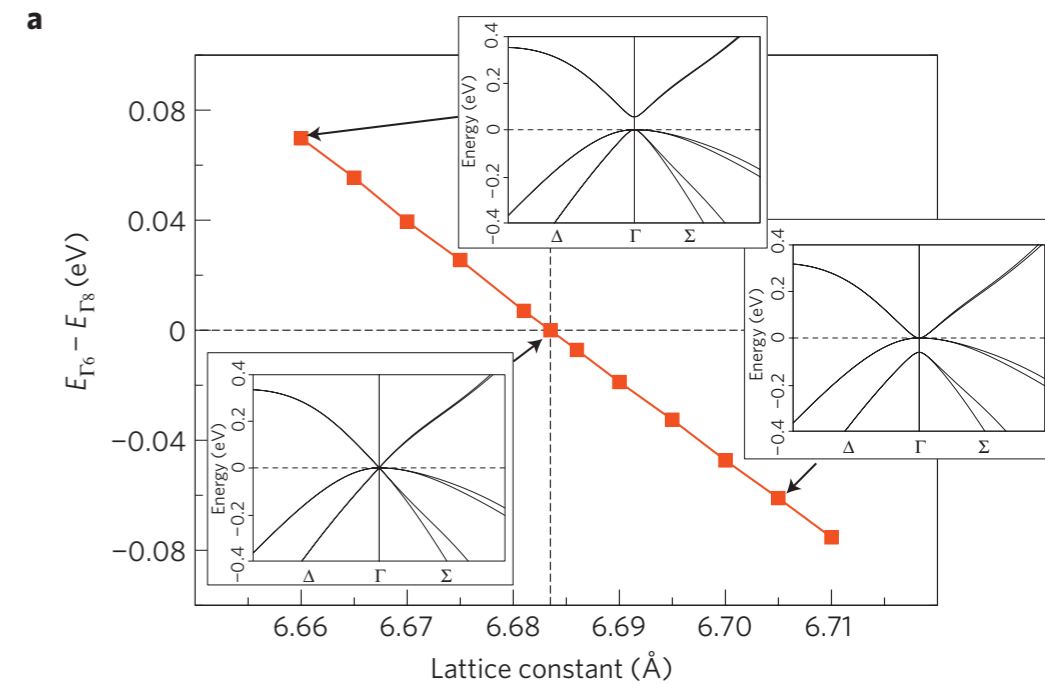
Al-Sawai et al. PRB (2010)



Lin et al. Nature material (2010)



S. Chadov et al. Nature Material (2010)

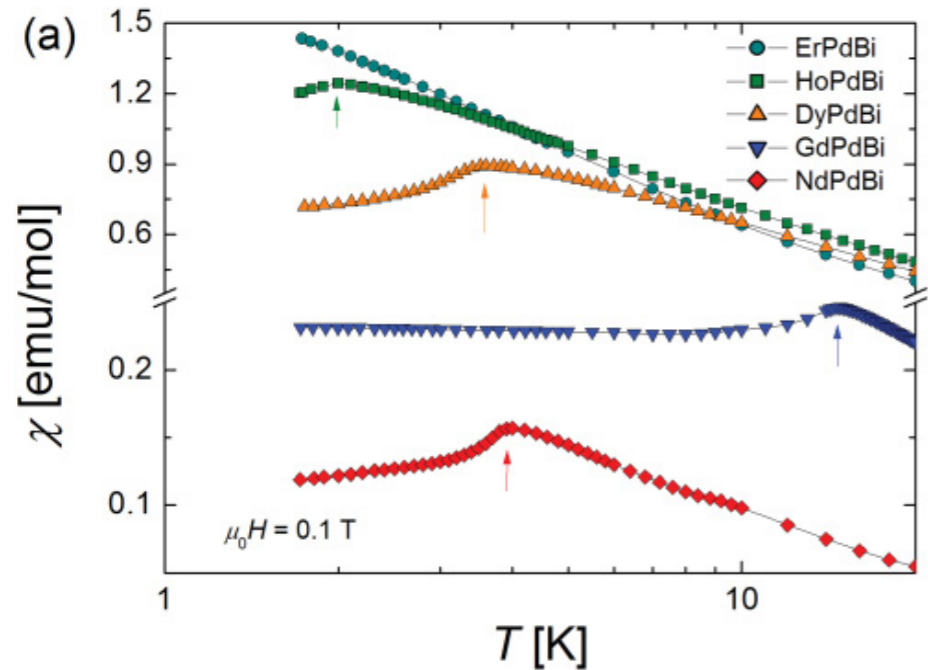


At the border between trivial and topological states

# Rare earth based RPdBi

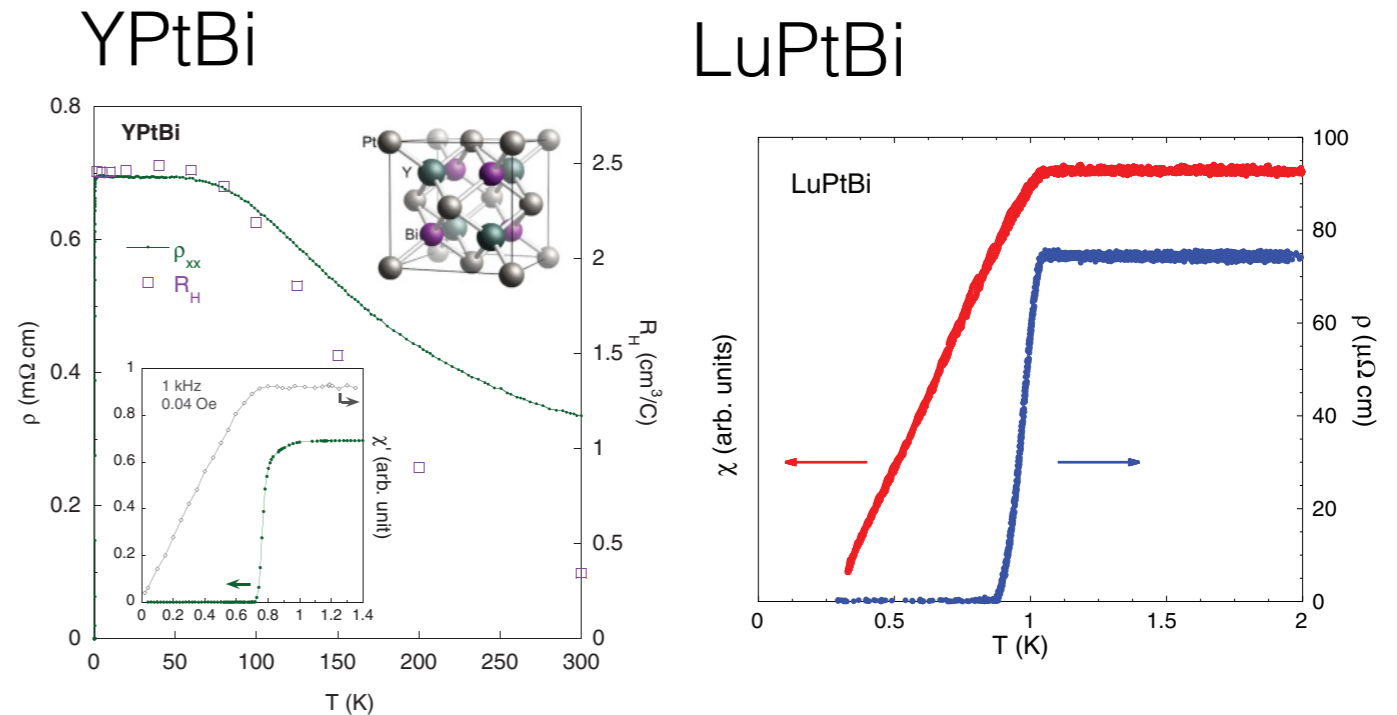
**RPdBi**: Promising tunable topological materials with (multi-)symmetry breaking

Antiferromagnetism



K. Gofryk *et al.* PRB (2011)

Superconductivity



N. Butch *et al.* PRB (2011)

F. Tafti *et al.* PRB (2013)

RPdBi

polycrystalline samples

RPtBi

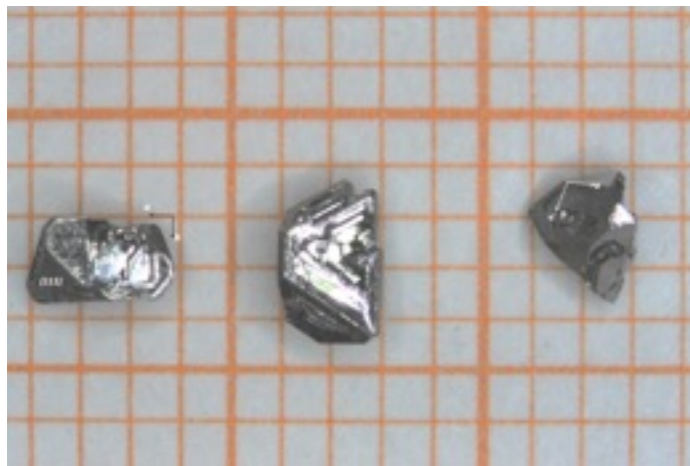
single crystal

# Sample preparation

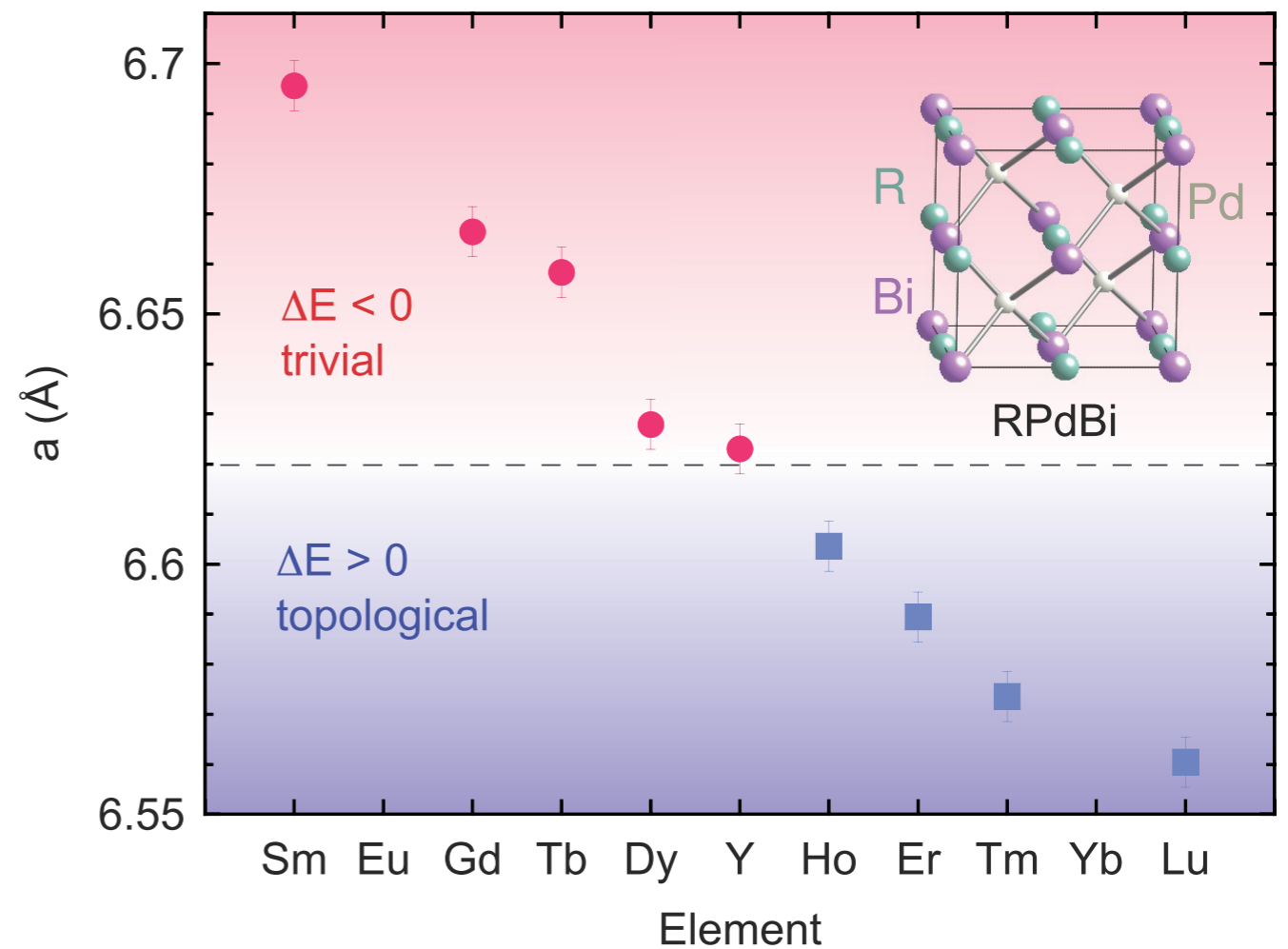
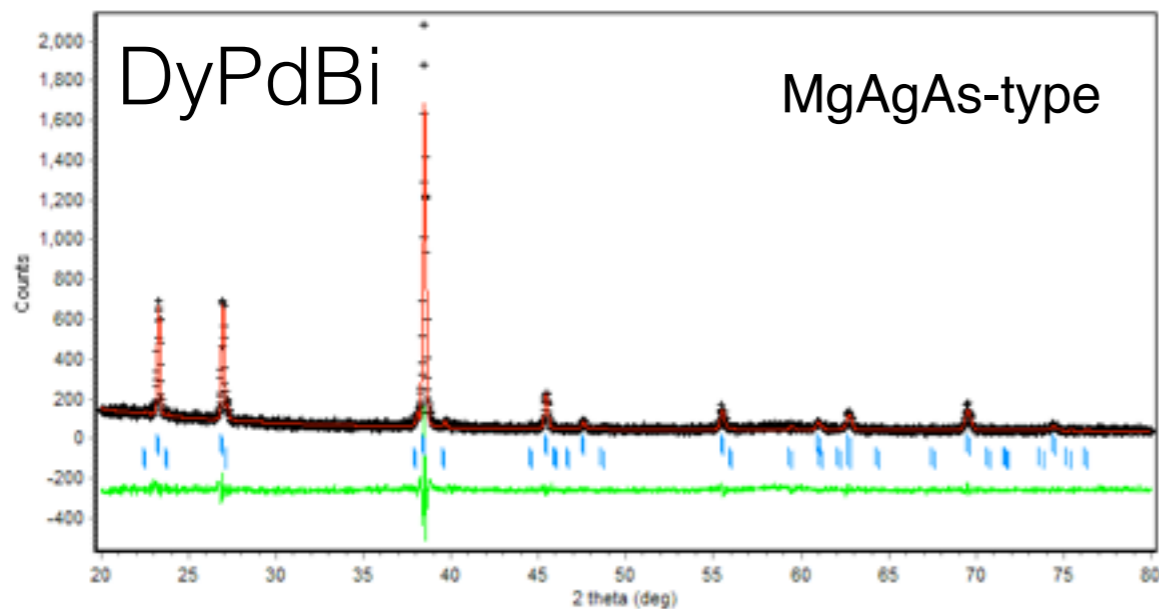
Single crystal

Self-flux method

R : Pd : Bi = 1 : 1 : 5 -10



1 mm

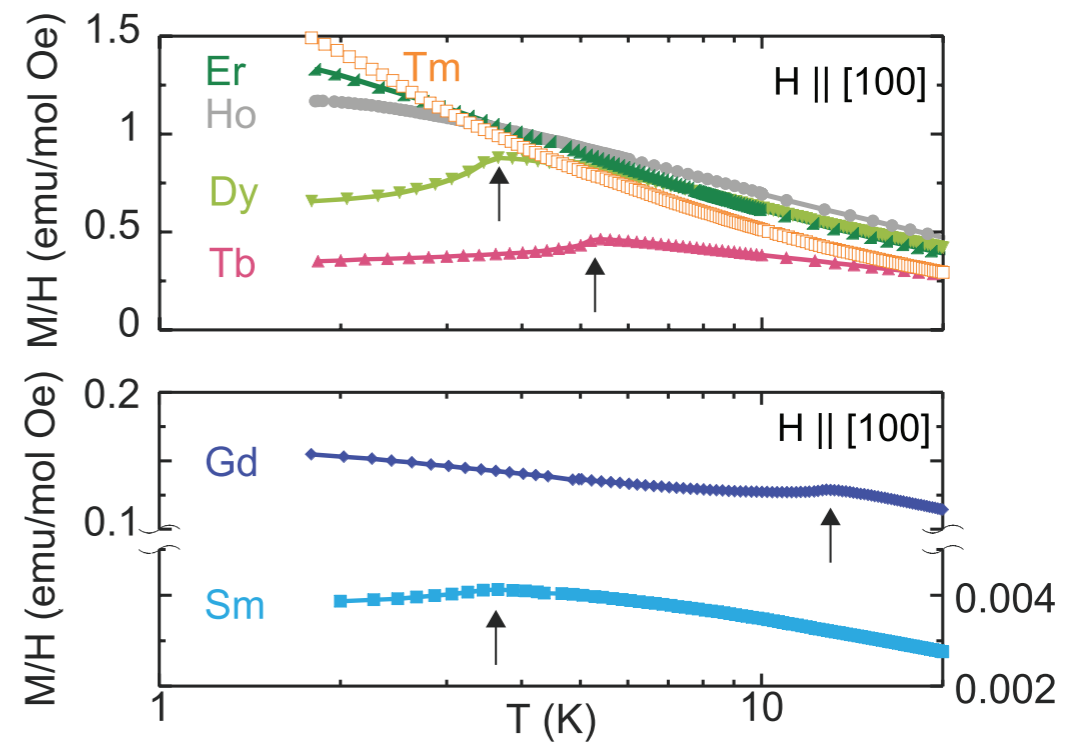
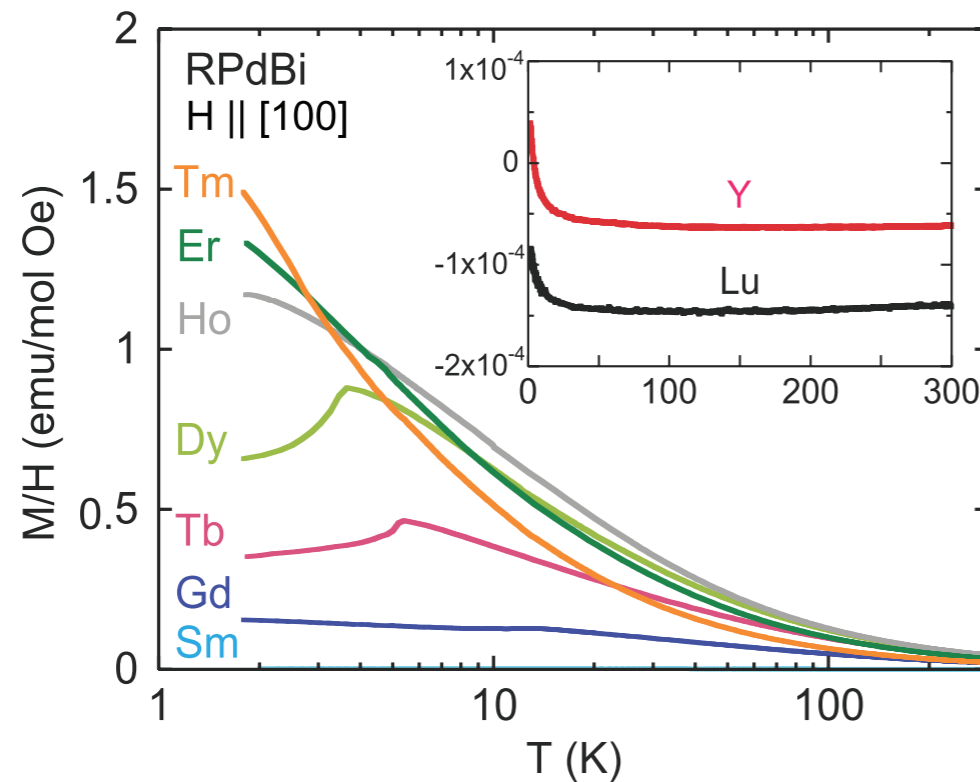


$$a_c = 6.62 \text{ \AA}$$

S. Chadov *et al.* Nat. Mat. (2010)



# Magnetic susceptibility



$R$	$T_N$ (K)	$\Theta_W$ (K)	$\mu_{eff}$ ( $\mu_B$ )	$\mu_{free}$ ( $\mu_B$ )
Sm	3.4	-258	1.9	0.85
Gd	13.2	-49.6	7.66	7.94
Tb	5.1	-28.9	9.79	9.72
Dy	2.7	-14.3	10.58	10.65
Ho	1.9	-9.4	10.6	10.6
Er	1.0	-4.8	9.18	9.58
Tm	<0.4	-1.7	7.32	7.56

Currie-Weiss behavior  $\frac{M}{H} = \frac{C}{T - \Theta_W}$

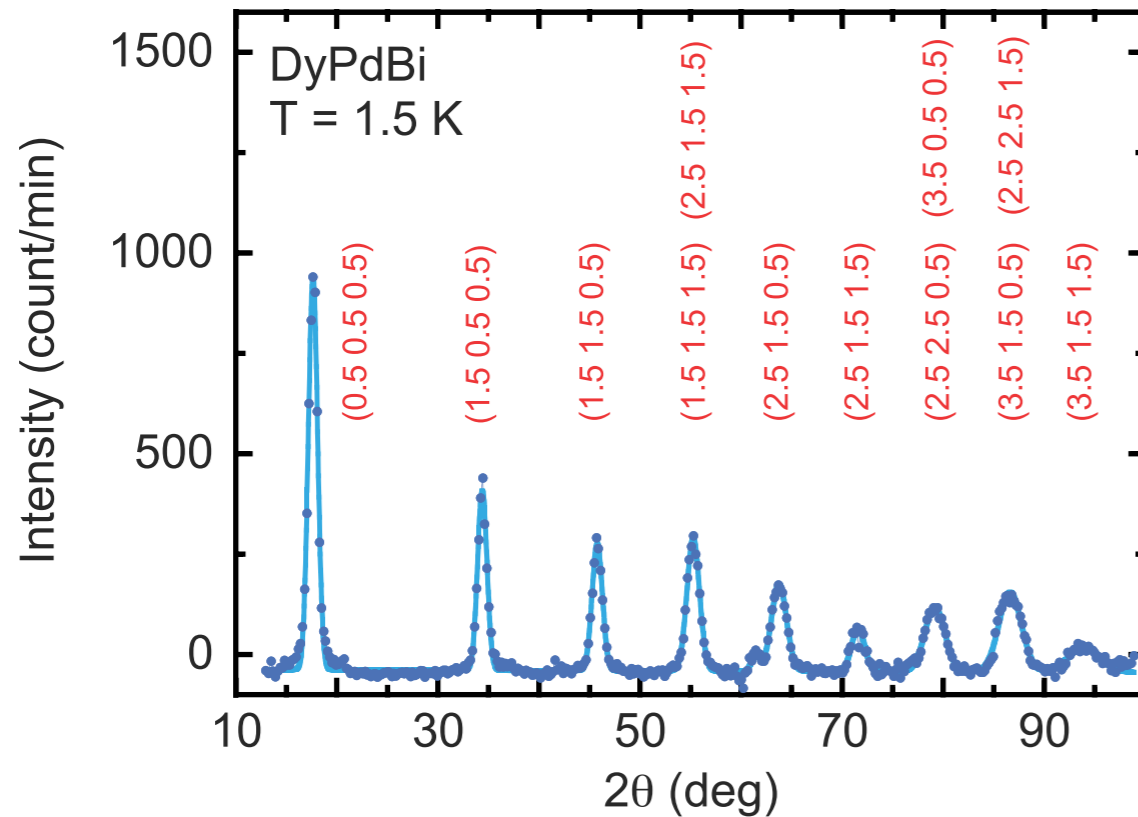
$\Theta_W$ : Weiss temperature

$f$  electrons: well-localized

Low temperature anomaly associated with AFM

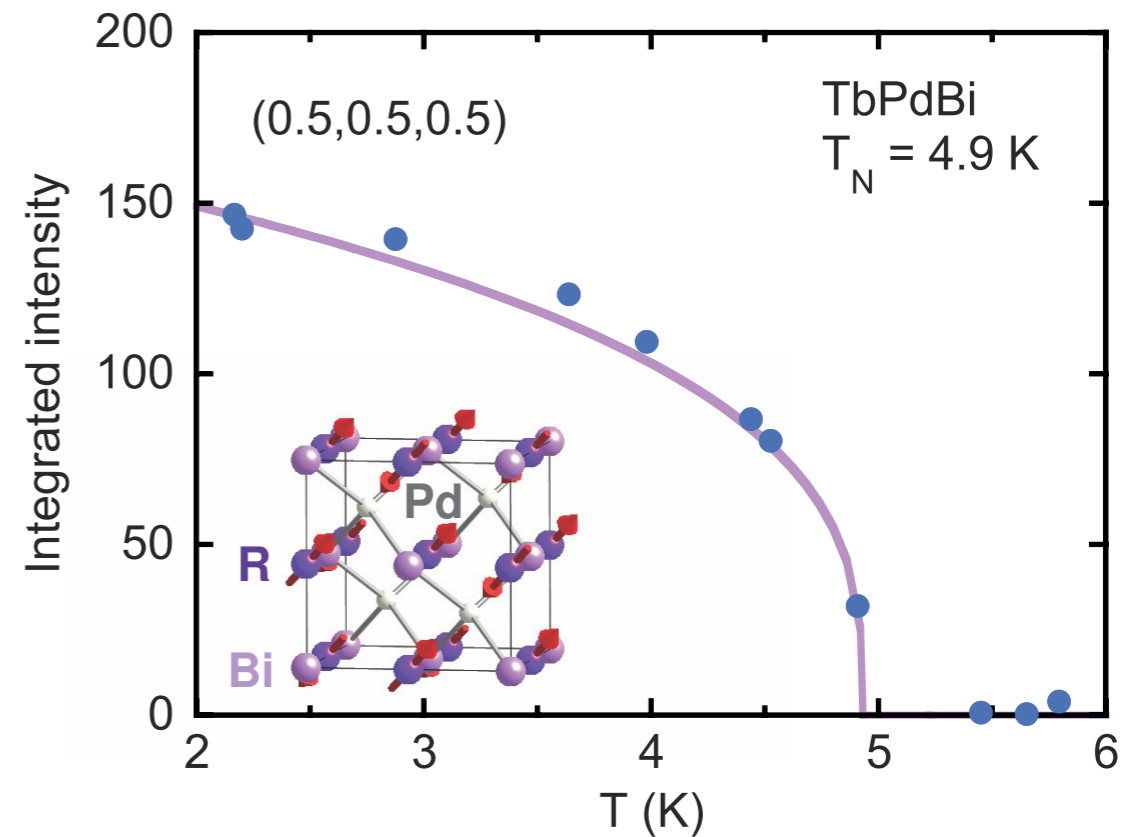
# Neutron diffraction

## Magnetic Bragg peak



fcc type-II AFM

## Order parameter

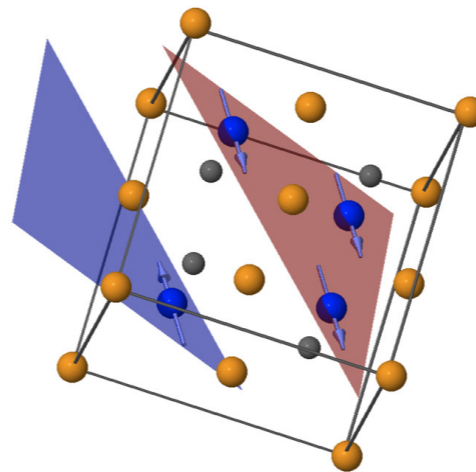


$$Q = (1/2, 1/2, 1/2)$$

## Topological AF insulator?

R. Mong *et al.* PRB (2010)

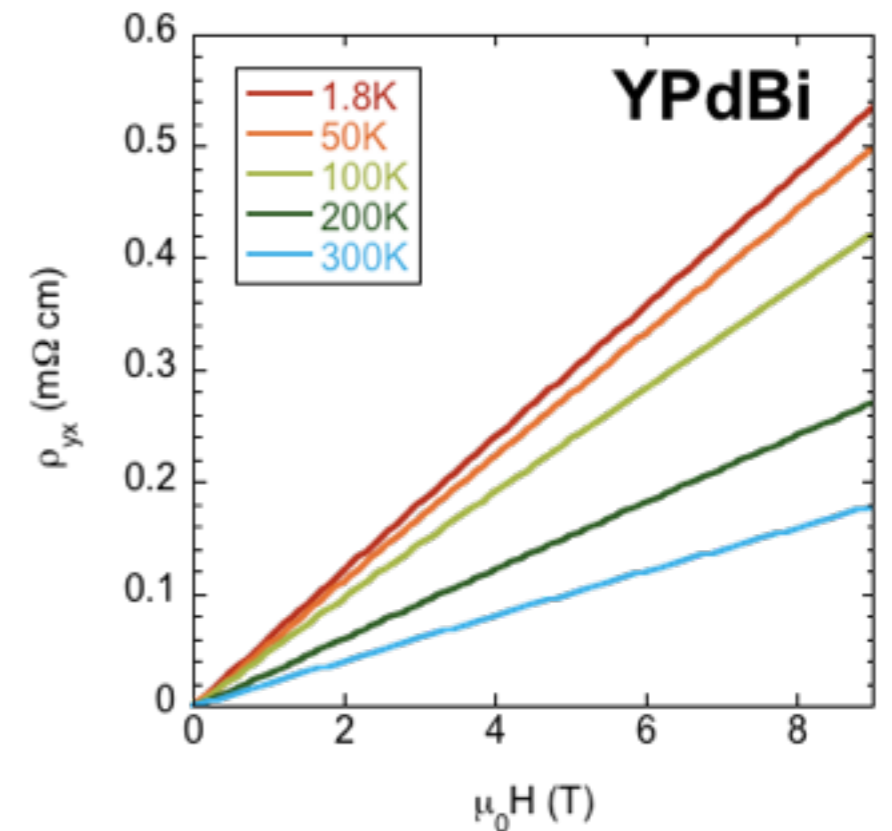
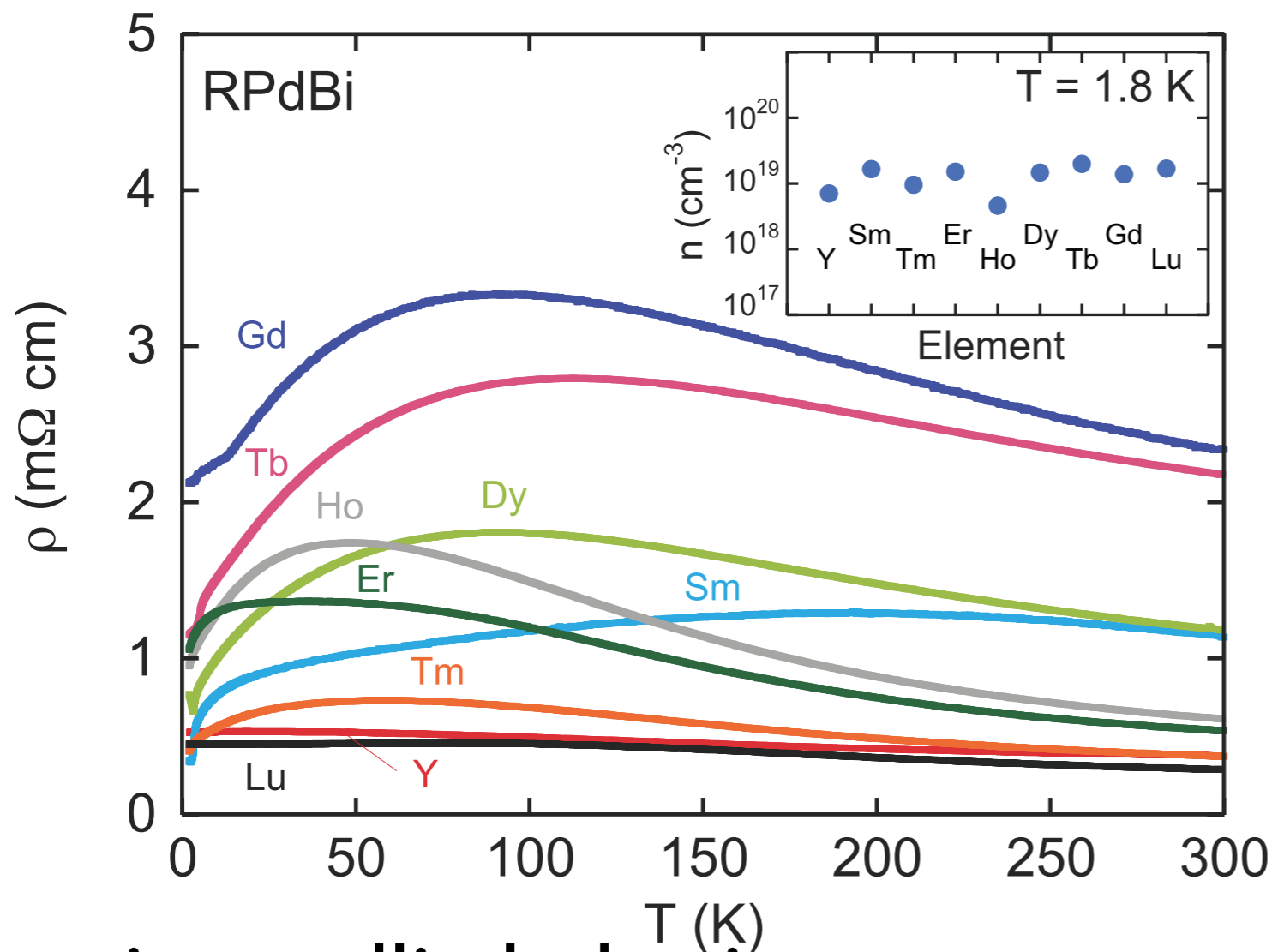
R. Muller *et al.* PRB (2014)



Ho, Tb

the same magnetic structure

# Charge transport

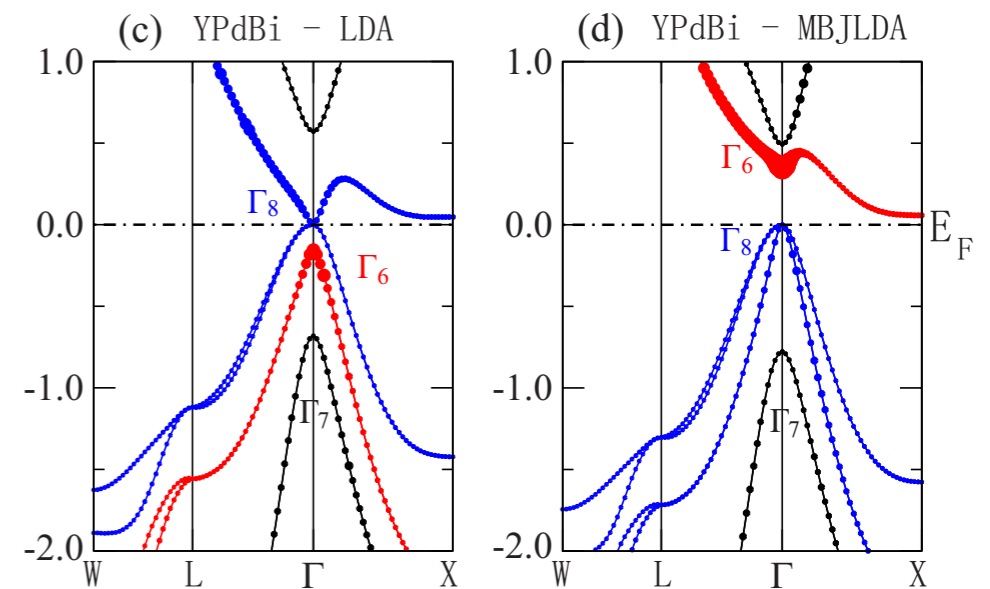


Carrier: Hole

Semi-metallic behavior

$n \sim 10^{19} \text{ cm}^{-3}$

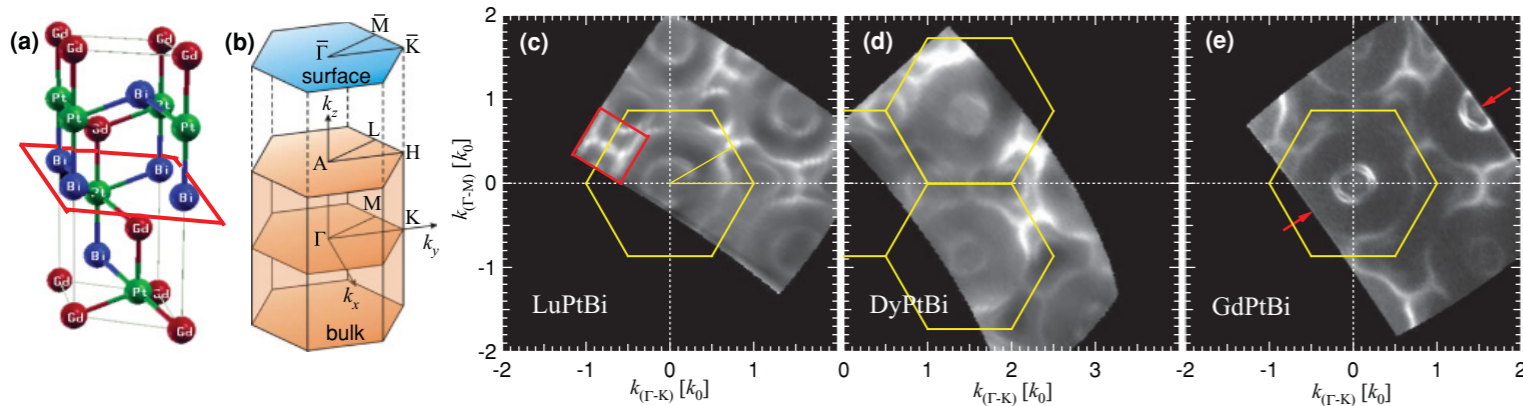
Consistent with band calculations



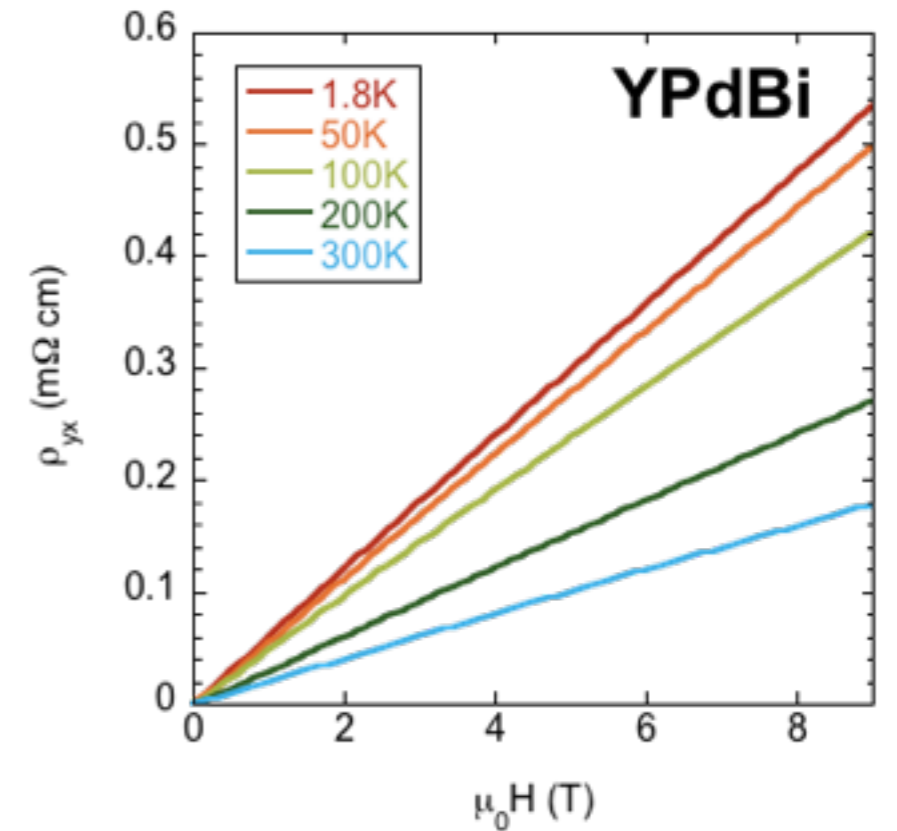
Feng et al. PRB (2010)

# Charge transport

## Surface Fermi surface in RPtBi



C. Liu *et al.* PRB (2011)



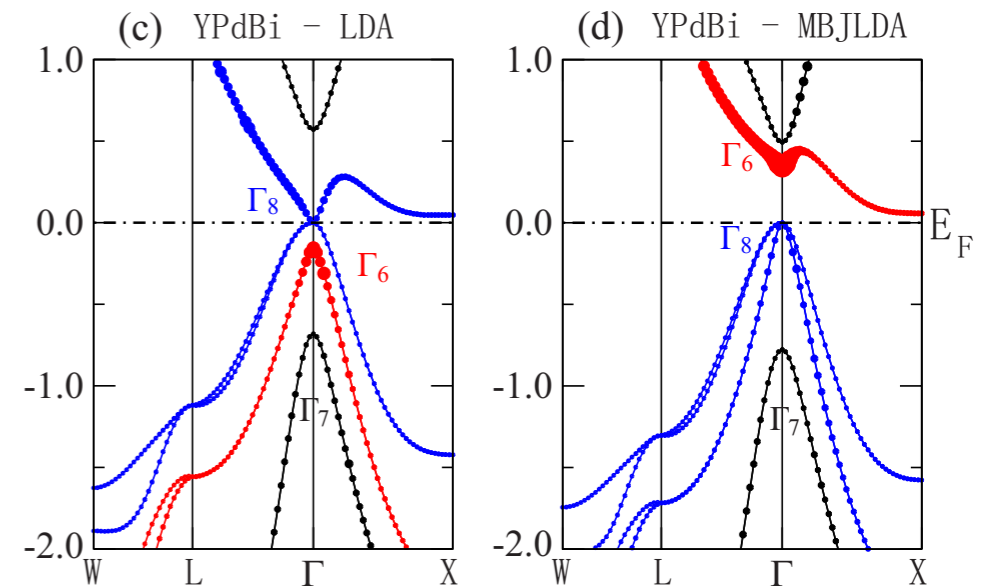
Carrier: Hole

not inconsistent with TI properties

Semi-metallic behavior

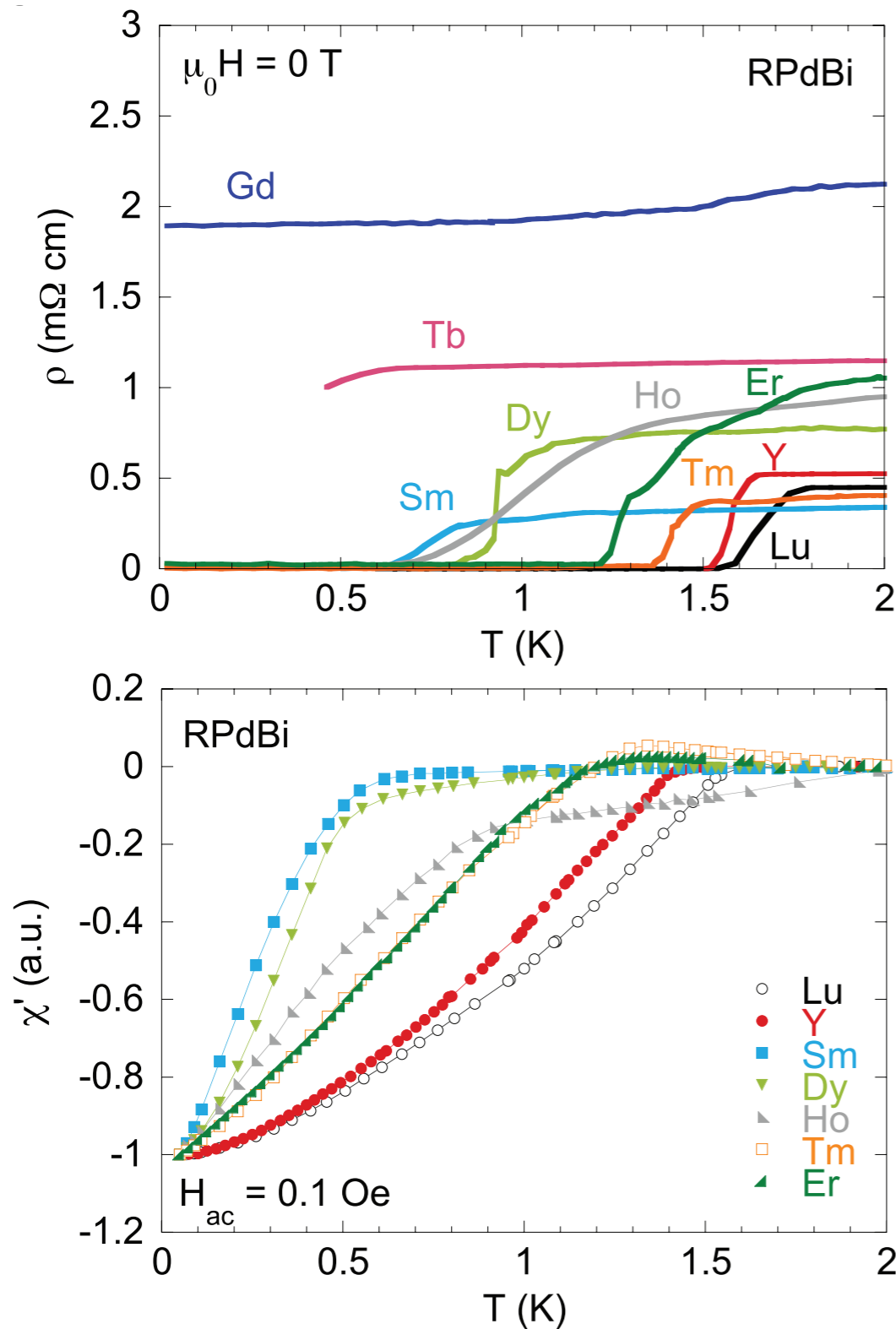
$$n \sim 10^{19} \text{ cm}^{-3}$$

Consistent with band calculations



Feng *et al.* PRB (2010)

# Superconductivity



Low temperature  
Superconductivity  
except for Gd

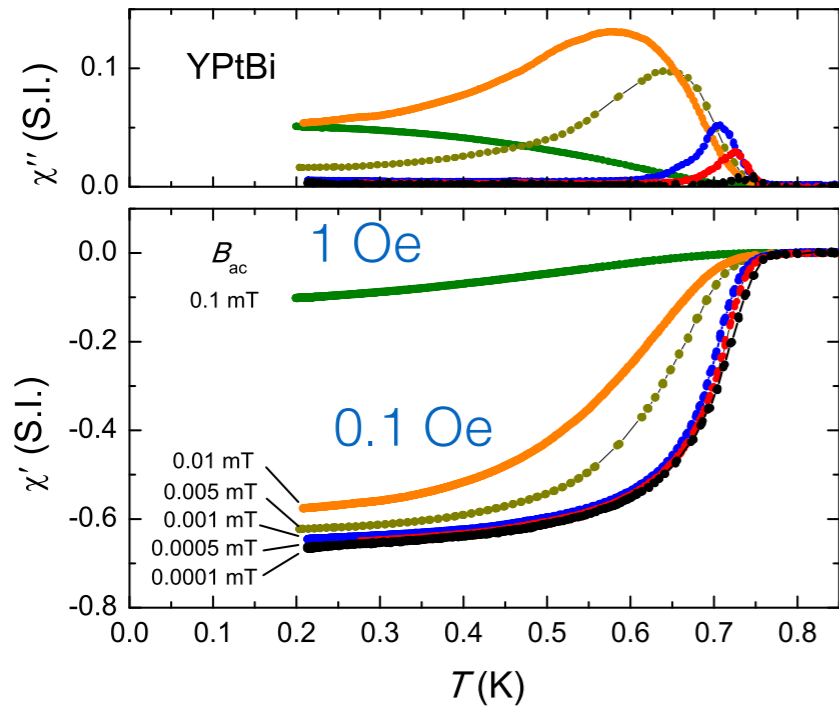
Large but non-saturating  
screening

Extremely small  $H_{c1}$

Extremely long  
penetration depth due  
to low carrier density

$$H_{c1} \propto \lambda^{-2} \quad \lambda \propto \sqrt{\frac{m}{n}}$$

# Superconductivity



Huge field dependence of magnetic susceptibility

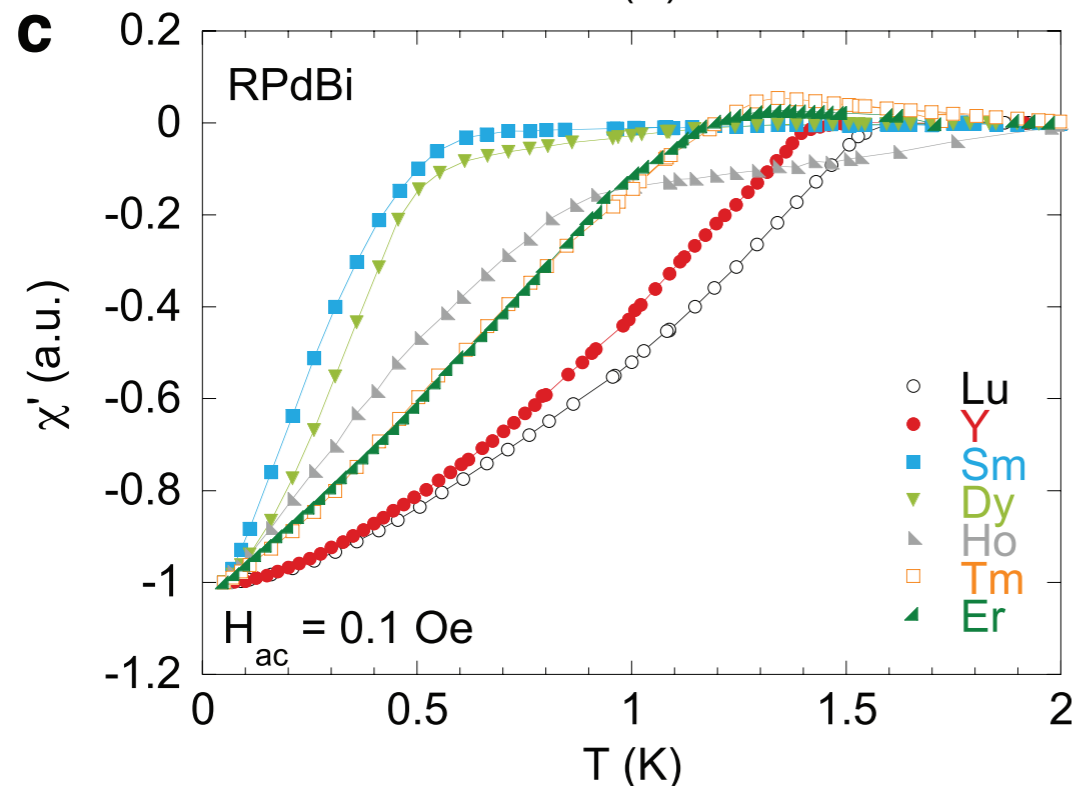
T.V. Bay *et al.* Solid State Commun. (2014)

Large but non-saturating screening

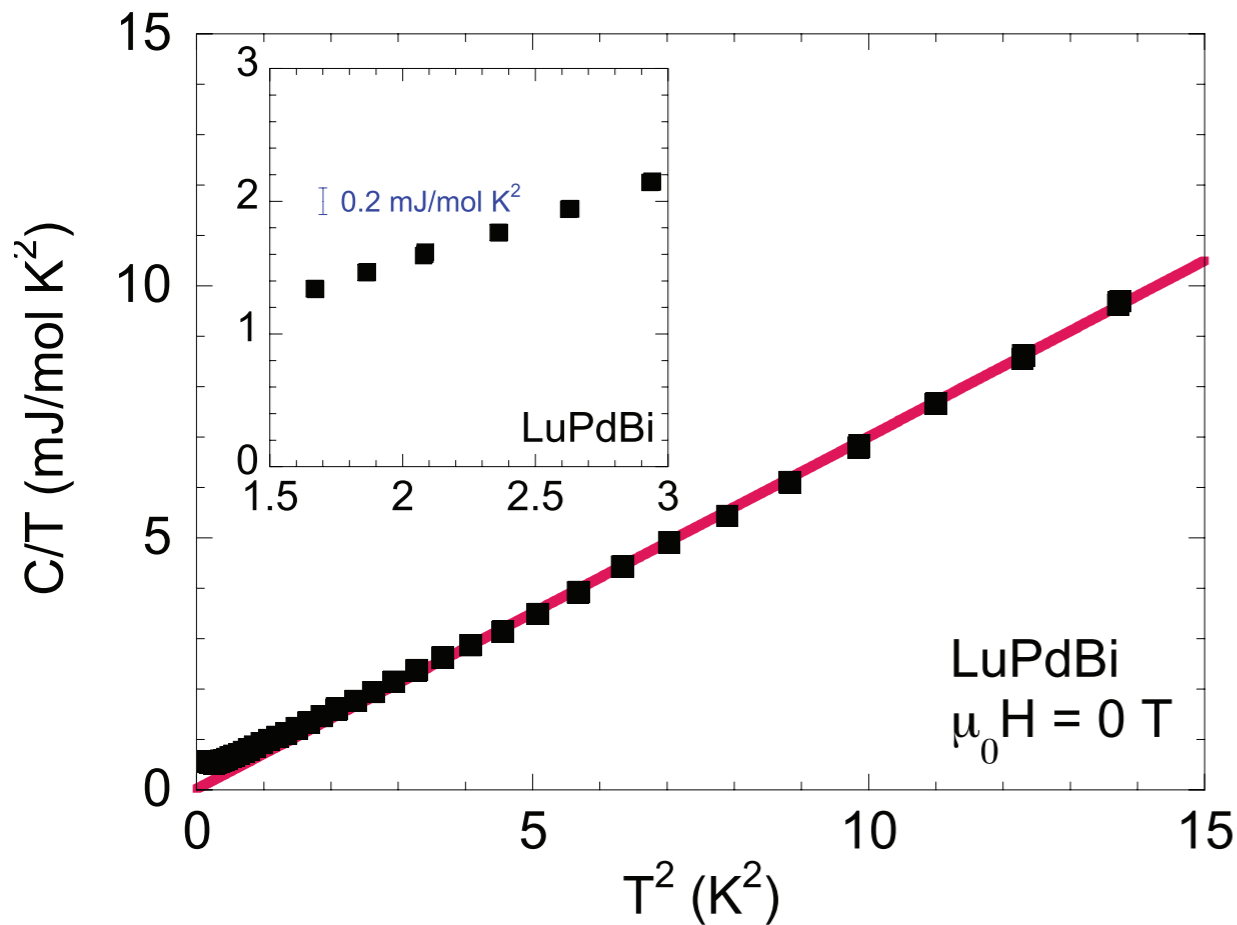
Extremely small  $H_{c1}$

Extremely long penetration depth due to the low carrier density

$$H_{c1} \propto \lambda^{-2} \quad \lambda \propto \sqrt{\frac{m}{n}}$$



# Lack of heat capacity jump



$$C/T = \gamma_n + \beta T^2$$

$$\gamma_n = 0.0 \pm 0.5 \text{ mJ/mol K}^2$$

Low carrier density

$$n \sim 10^{19} \text{ cm}^{-3}$$

$$m^* \sim 0.09 m_e$$

W. Wang *et al.* Sci. Rep. (2013)

$$\Delta C / \gamma_n T_c = 1.43$$

$$\Delta C / T < 0.2 \text{ mJ/mol K}^2$$

beyond the resolution

Dominant triplet pairing?

A<sub>1</sub> phase of superfluid <sup>3</sup>He

D.Vollhardt and P.Wolfle,  
The Super fluid Phases of Helium 3 (1990)

# Non-centrosymmetric SC

Superconducting pairing function

$$\Psi_{\sigma\sigma'}(\mathbf{k}) = \underbrace{g(\mathbf{k})}_{\text{orbital}} \underbrace{\chi(\sigma, \sigma')}_{\text{spin}}$$

orbital spin

exchange electrons

$$\Psi_{\sigma'\sigma}(-\mathbf{k}) = -\Psi_{\sigma\sigma'}(\mathbf{k})$$

antisymmetric

Singlet :  $g(-\mathbf{k}) = g(\mathbf{k}), \chi(\sigma', \sigma) = -\chi(\sigma, \sigma')$

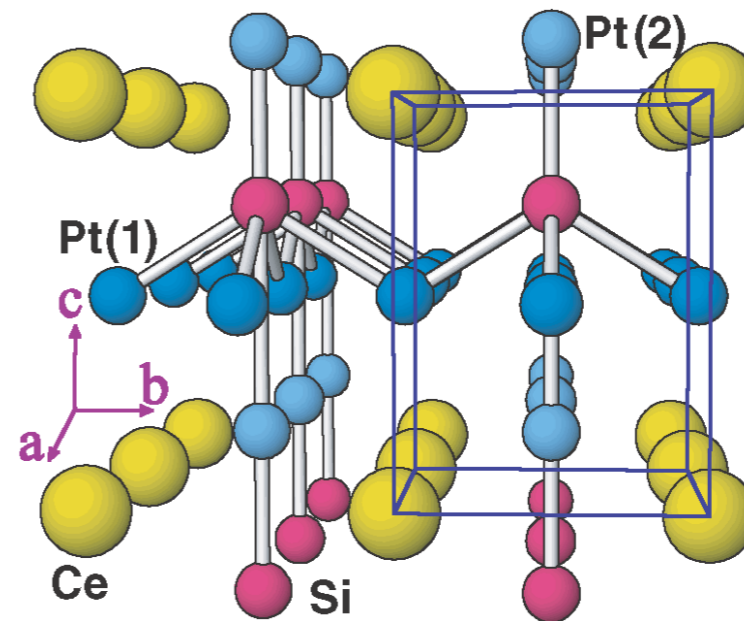
Triplet :  $g(-\mathbf{k}) = -g(\mathbf{k}), \chi(\sigma', \sigma) = \chi(\sigma, \sigma')$

Lack of inversion symmetry

No restriction of spin parity

**Admixture of singlet and triplet**

c.f. heavy fermion SC CePt<sub>3</sub>Si

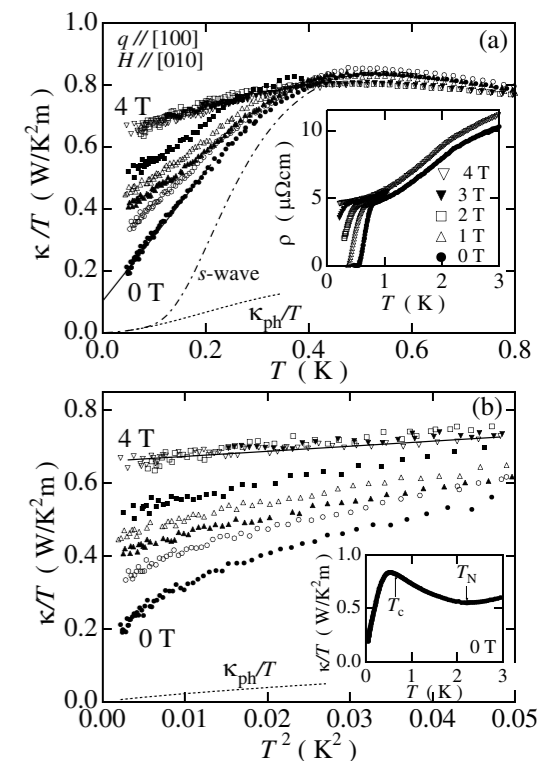


E. Bauer et al. PRL (2004)

$$\kappa/T \sim N(E_F)v_F\ell$$

$$\kappa/T \propto T$$

Nodal SC



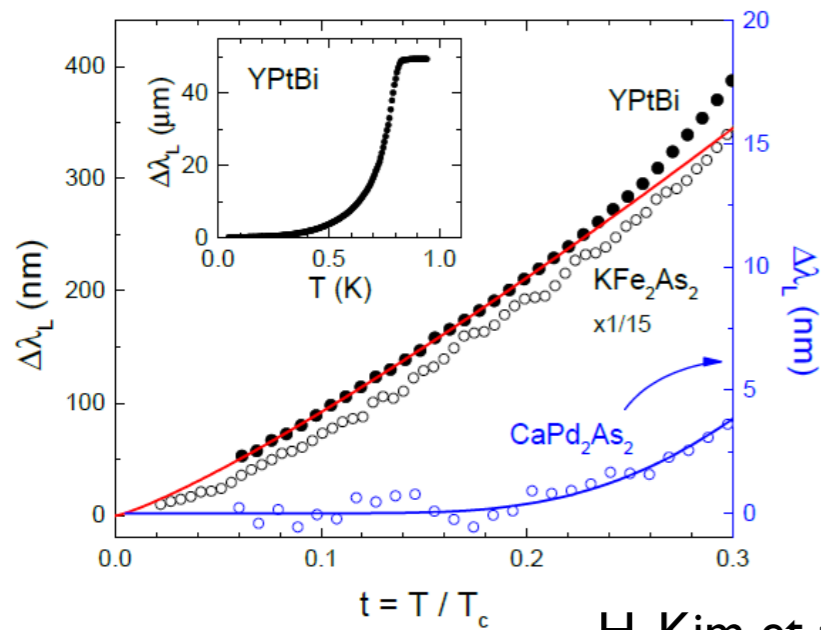
K. Izawa et al. PRL (2005)



# Nodal SC in half Heusler

Penetration depth

Nodal SC



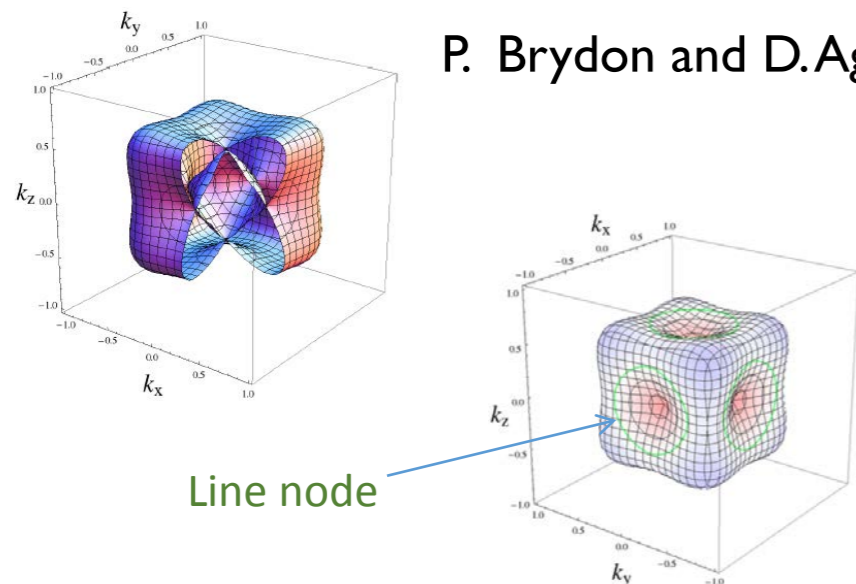
YPtBi

Tuning dominant contribution of singlet/triplet pairing states

H. Kim et al., unpublished

$$\Delta\lambda_L \propto T^{1.2}$$

Theoretical Fermi surface

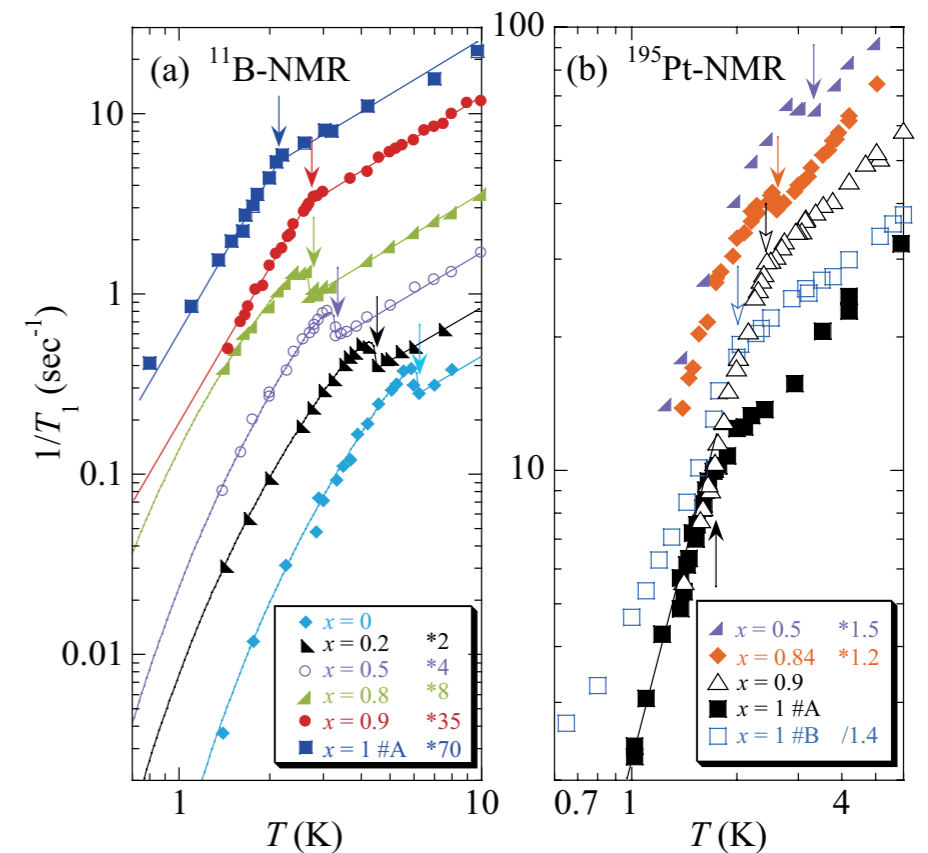


P. Brydon and D. Agterberg, unpublished

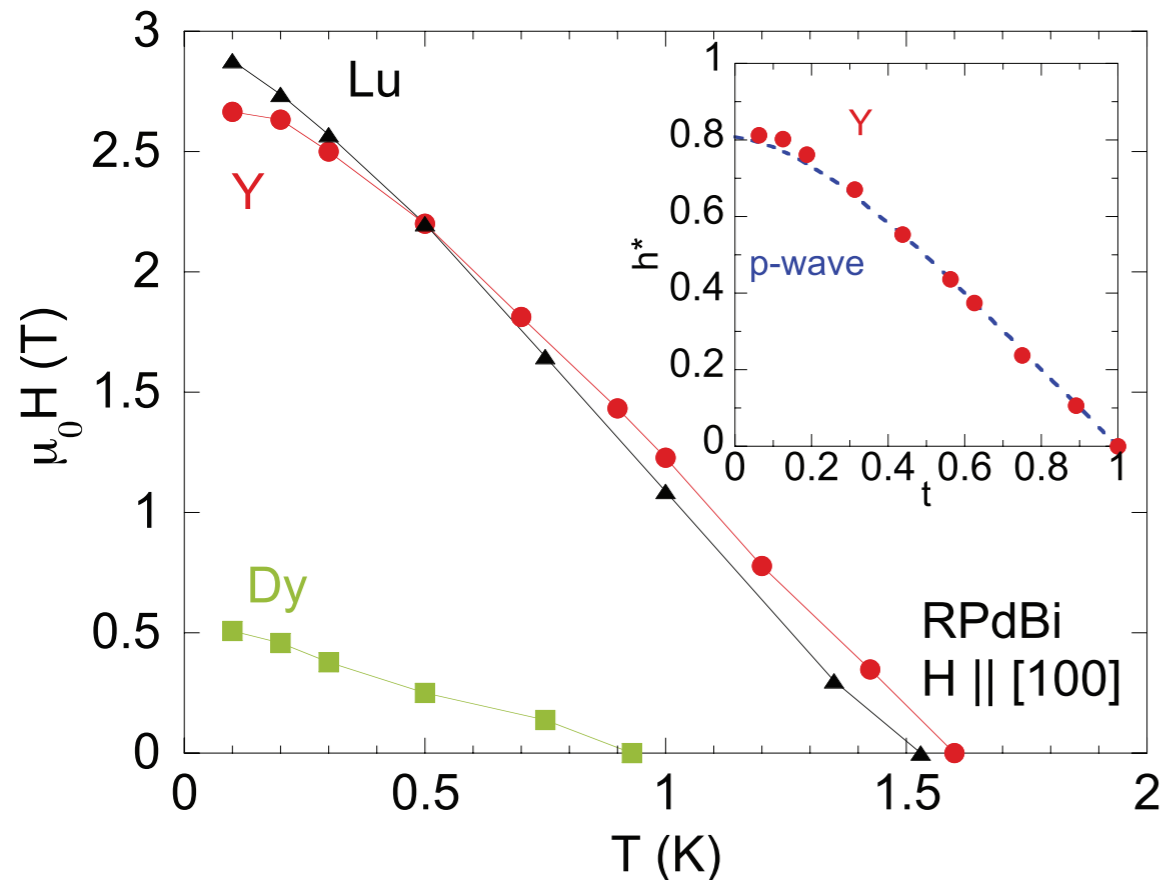
Line node

c.f. Li(Pd,Pt)<sub>2</sub>B<sub>3</sub>

S. Harada et al. PRB (2012)



# Finite triplet component



WHH theory

N.Werthamer *et al.* PR (1966)

$$H_{c2}(0) = -\alpha T_c \left. \frac{dH_{c2}}{dT} \right|_{T=T_c}$$

$$\alpha = 0.69 \quad \text{dirty SC}$$

$$\alpha = 0.74 \quad \text{clean SC}$$

exceeding of orbital  
depairing field

$$\text{YPdBi: } \mu_0 H_{c2}(0) = 2.7 \text{ T, } \alpha = 0.82$$

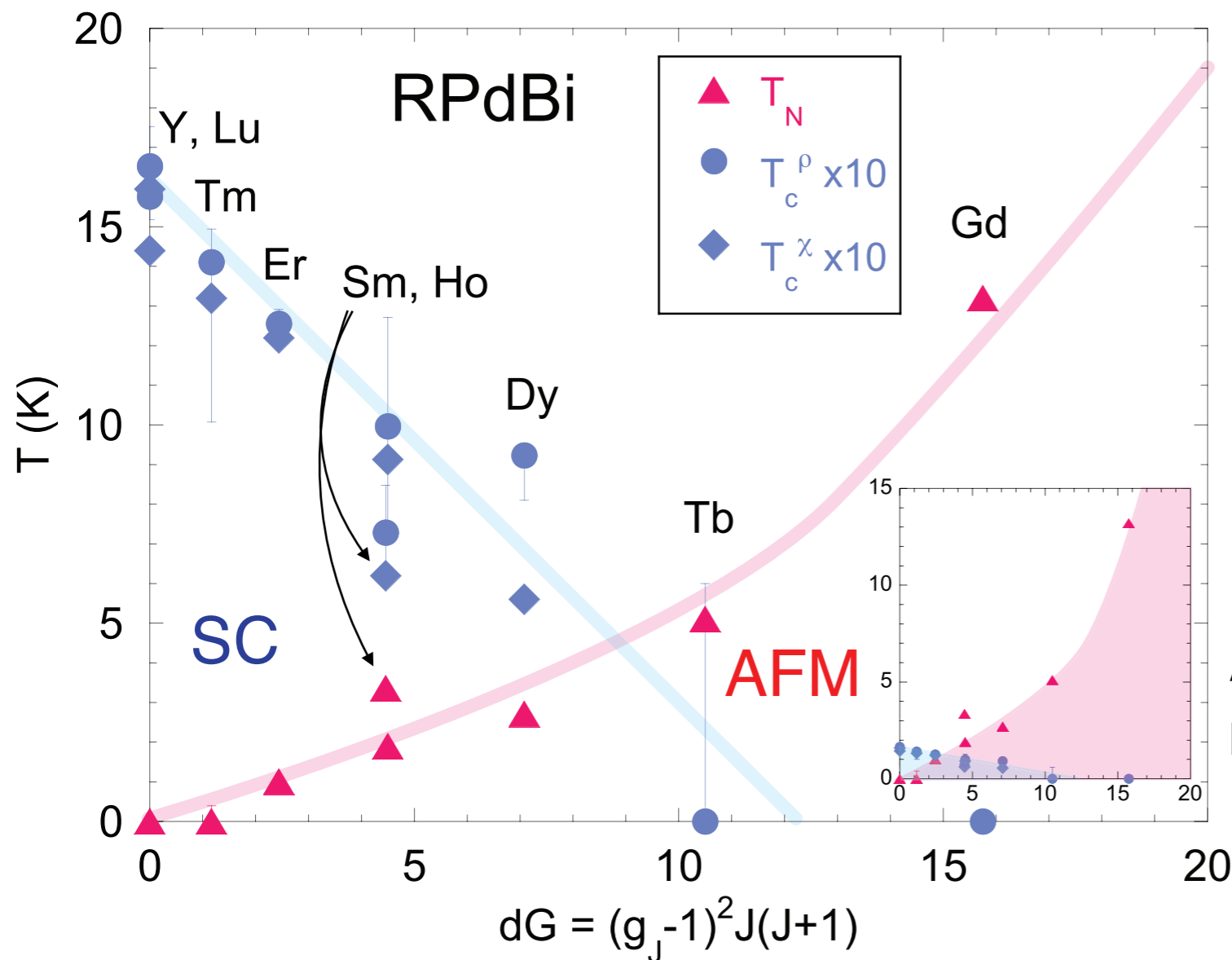
$$\text{LuPdBi: } = 2.9 \text{ T, } \alpha = 0.91$$

$$\text{DyPdBi: } = 0.7 \text{ T, } \alpha = 0.93$$

Finite triplet component?

# Magnetic superconductivity

Anticorrelation between  $T_c$  and  $T_N$ , well-scaled by de Gennes factor



SC is suppressed by magnetic scattering due to local moments of f electrons

AFM is induced by RKKY interaction

**Another canonical material for magnetic superconductor**

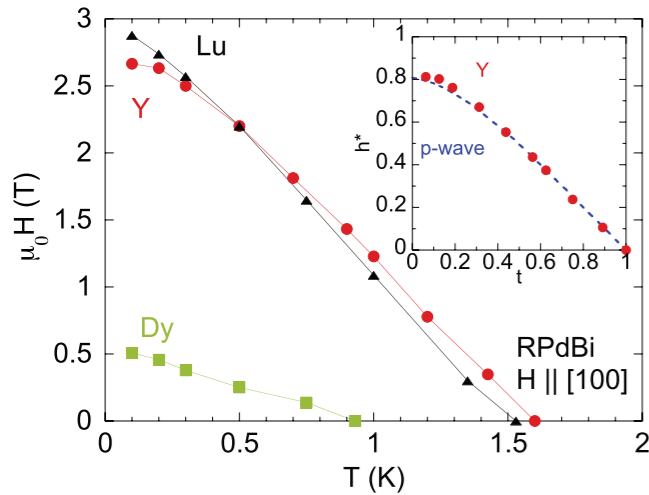
c.f. Borocarbide

H. Müller *et al.* Rep. Prog. Phys. (2001)

Chevrel phases

Φ. Fischer *et al.* Appl. Phys. (1978)

# BCS-BEC crossover?



$$H_{c2}(0) = \frac{\phi_0}{2\pi\xi^2}$$

$\phi_0$ : flux quantum

$$\xi \gg d_{e-e}$$

$$\xi \ll d_{e-e}$$

Coherence length

$$\xi \sim 10 \text{ nm} \quad \text{YPdBi}$$

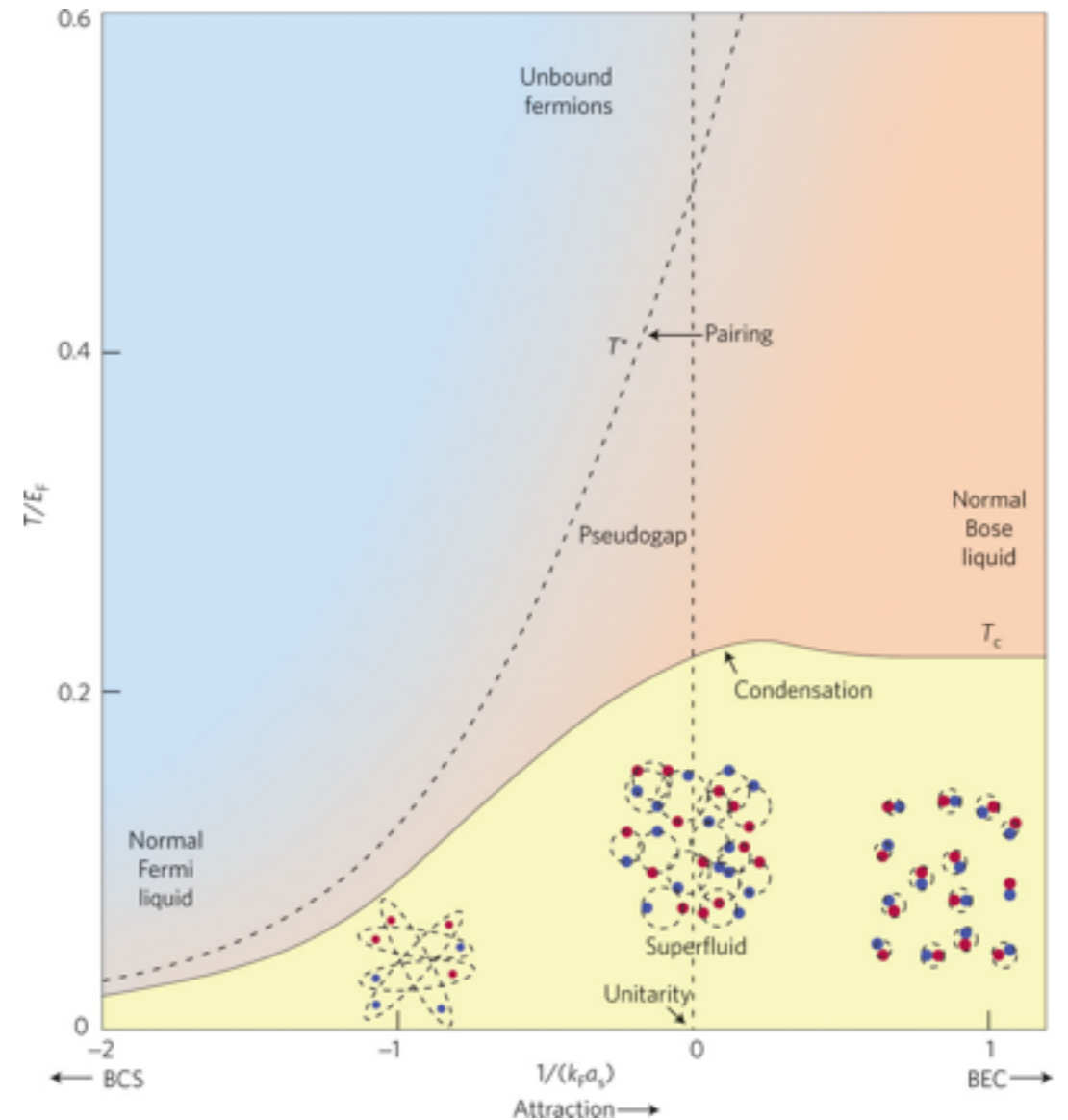
Average inter-electron distance

$$d_{e-e} \sim n^{-1/3} \sim 5 \text{ nm}$$

$$n \sim 10^{19} \text{ cm}^{-3}$$

$$\xi \sim d_{e-e}$$

Exotic superconducting state?



M. Randeria et al. Nature Physics (2010)

# Summary

We have studied superconductivity and magnetism in the topological half semimetal RPdBi.

- fcc type II AFM with  $Q = (1/2, 1/2, 1/2)$
- Anticorrelation between  $T_c$  and  $T_N$ , well-scaled by de Gennes factor
- Anomalous SC: Triplet dominant? BCS-BEC crossover?

**Strong candidate for tunable topological materials with multi-symmetry breaking**



# Combination of topological and symmetry-breaking order

	SC	AFM	Topo
Y	✓	✗	✗
Lu	✓	✗	✓
Tm	✓	✓(?)	✓
Er	✓	✓	✓
Sm	✓	✓	✗
Ho	✓	✓	✓
Dy	✓	✓	✗
Tb	✓(?)	✓	✗
Gd	✗	✓	✗