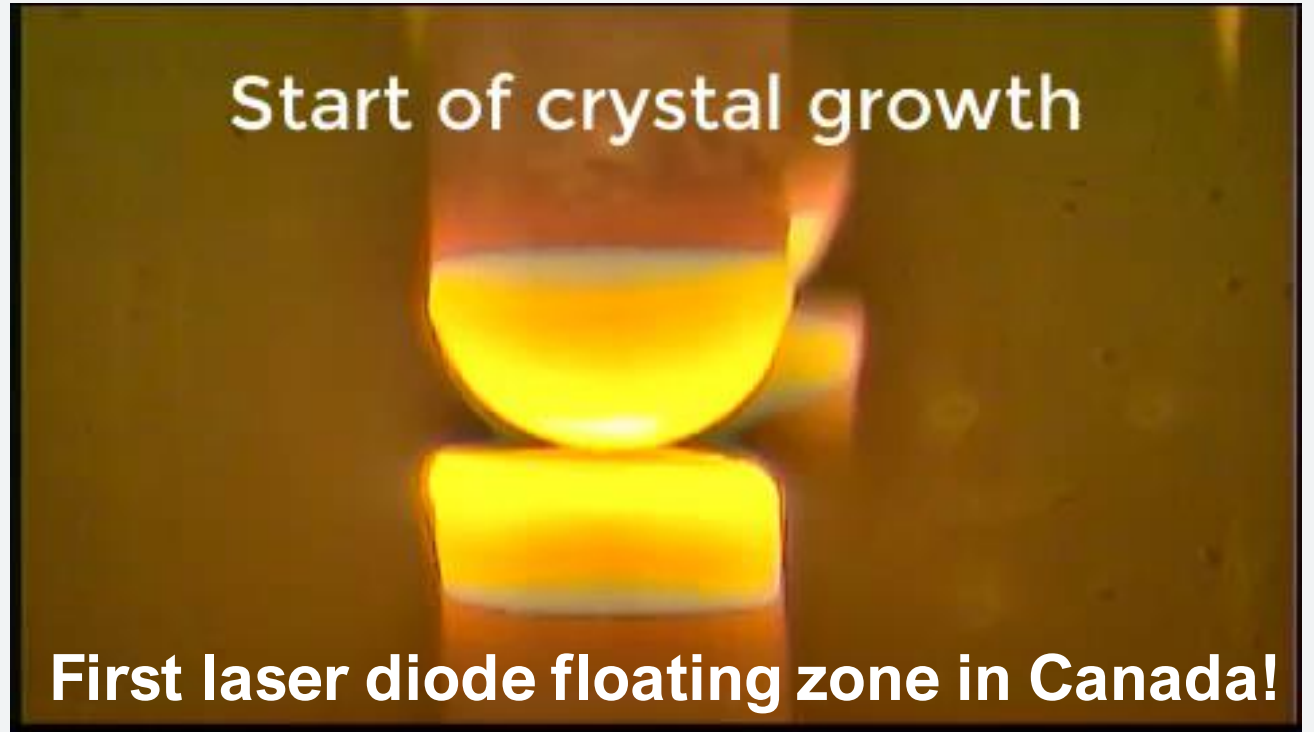
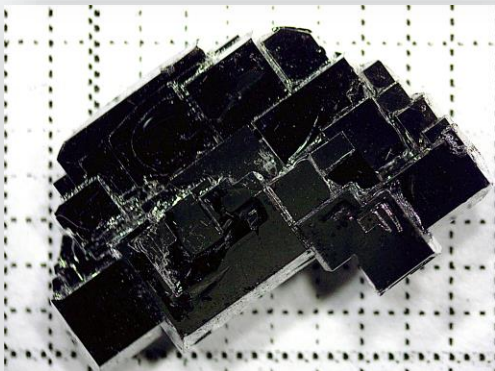
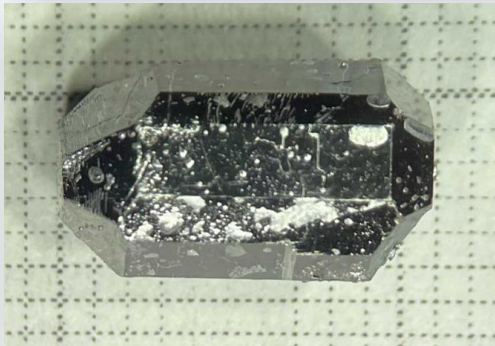
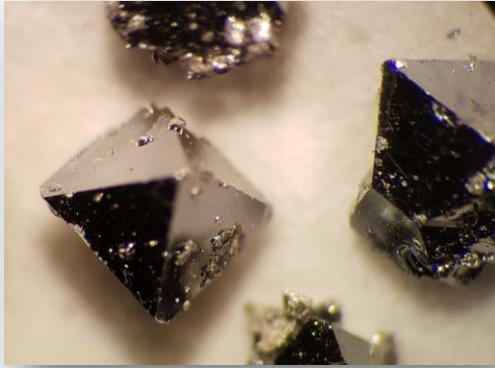




Discovery of itinerant antiferromagnetism in Ti_3Cu_4

Alannah Hallas

Crystal growth of quantum materials in the Hallas group at UBC



Website: hallas.phas.ubc.ca

Twitter: @AlannahHallas
for crystal photos



Itinerant Magnet Collaborators



Jaime Moya



Kyle Bayliff



Chien-Lung Huang



Emilia Morosan



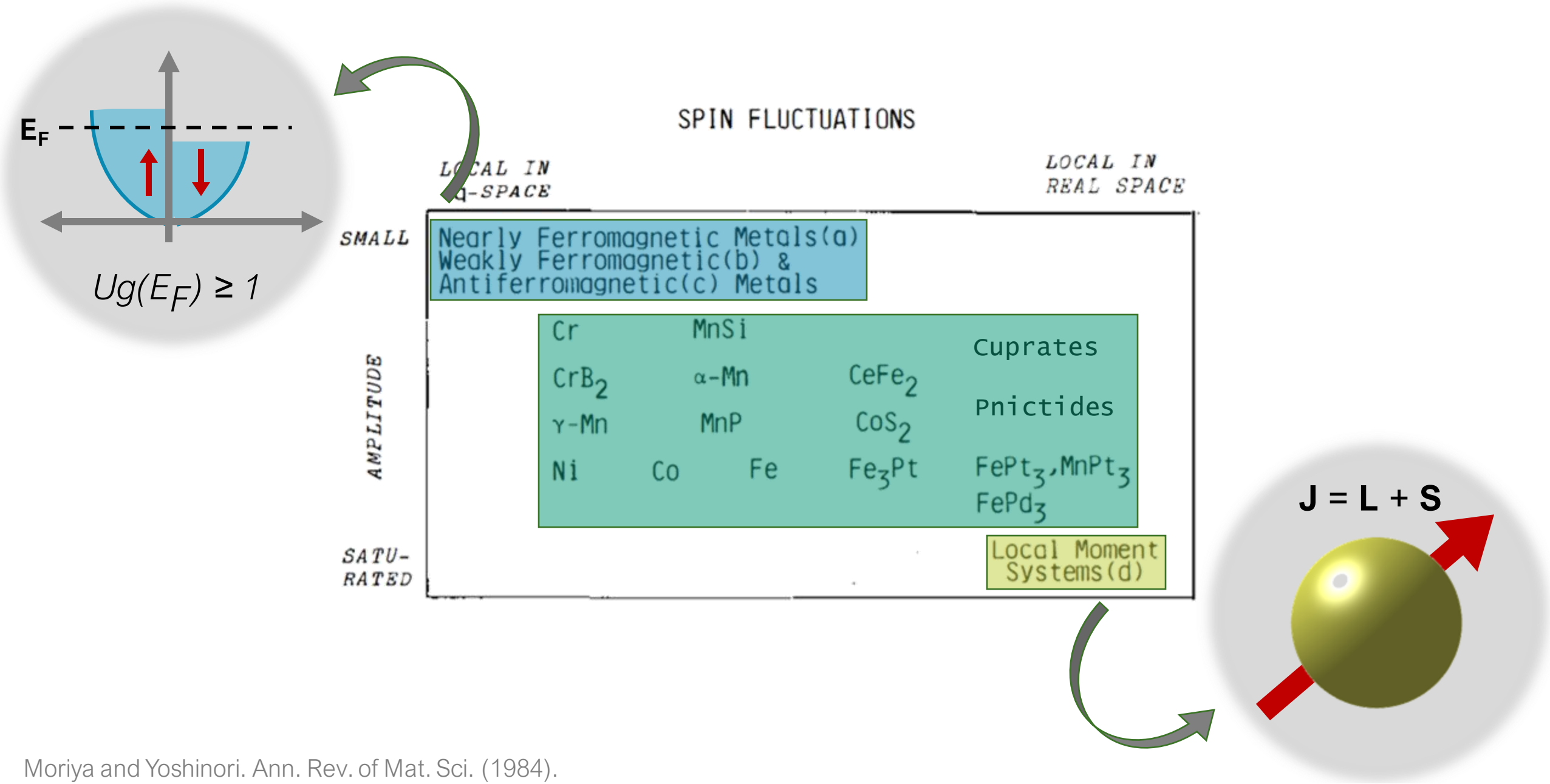
Emilia Morosan
Jaime Moya
Kyle Bayliff
Chien-Lung Huang
Vaideesh Loganathan

Graeme Luke
James Beare
Yipeng Cai

Yaohua Liu

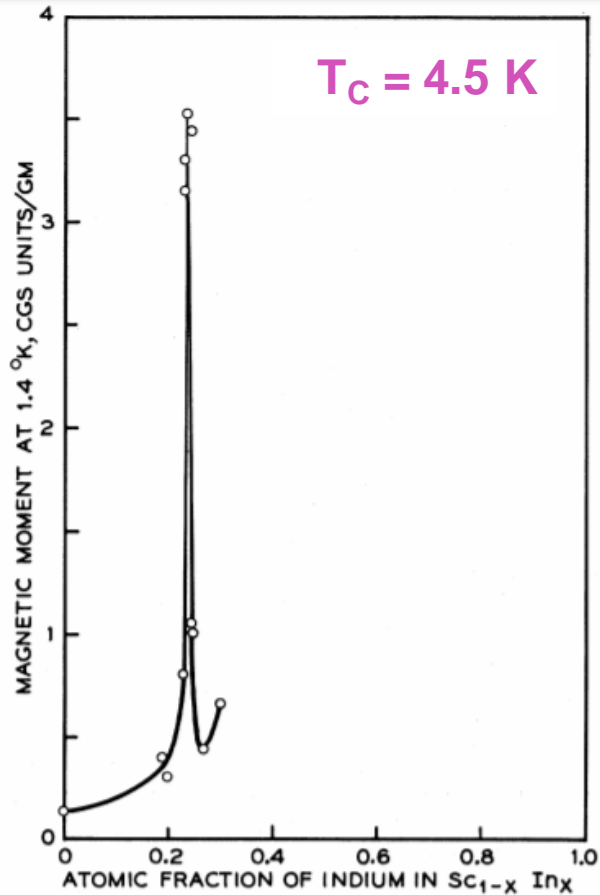


The Magnetic Spectrum – from Local to Itinerant

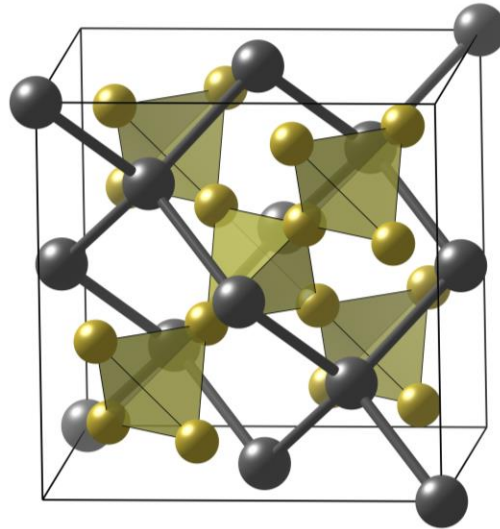


There are two known ferromagnetic metals without magnetic elements

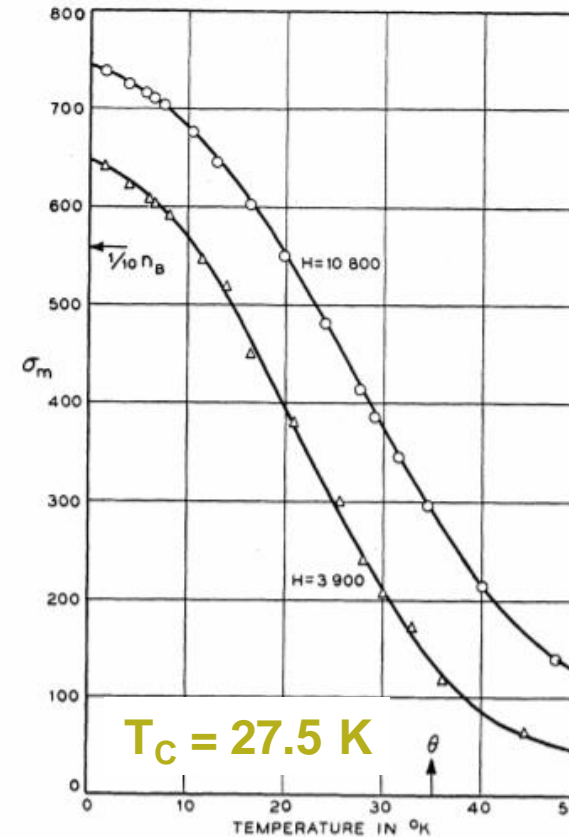
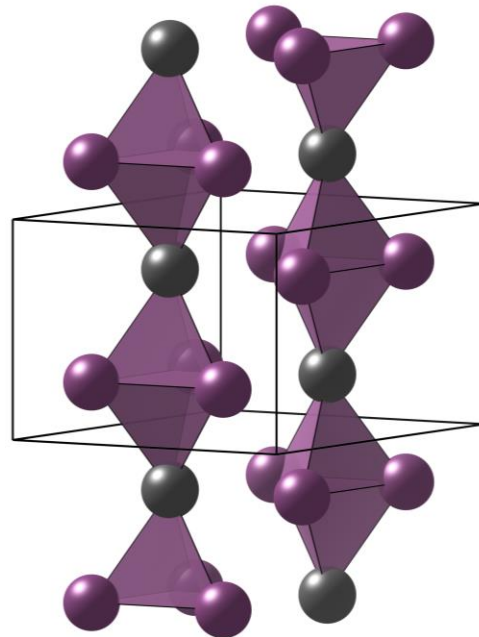
B. T. Matthias, *et al.* PRL (1961)



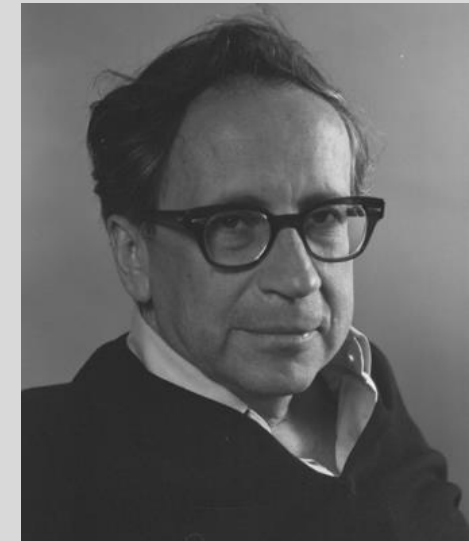
$Sc_{3.1}In$



$ZrZn_2$

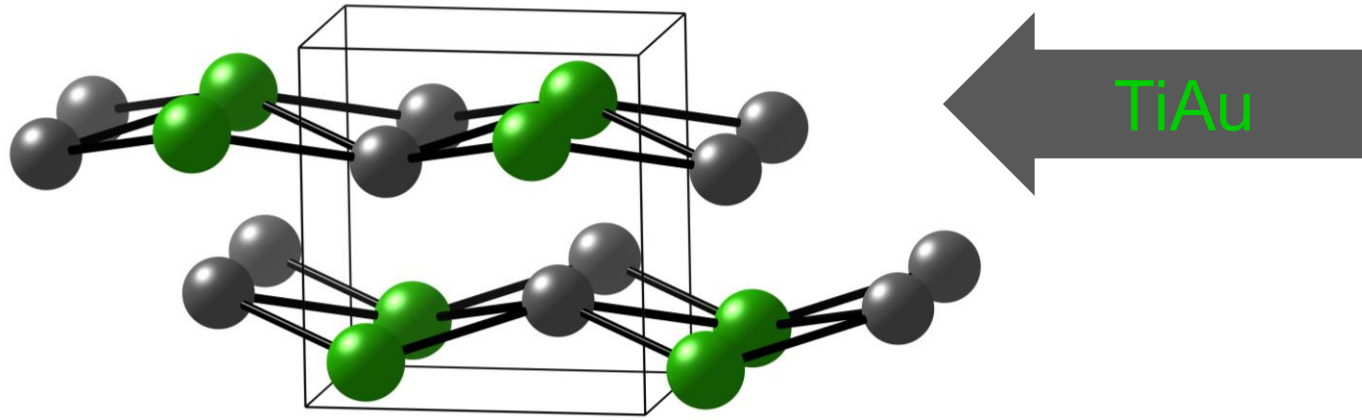


B. T. Matthias, *et al.* Phys. Rev. (1958)

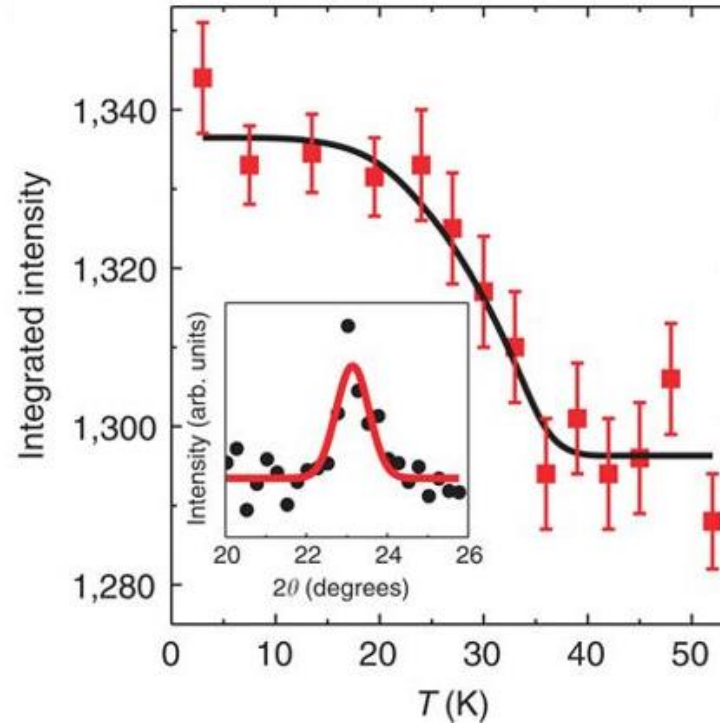
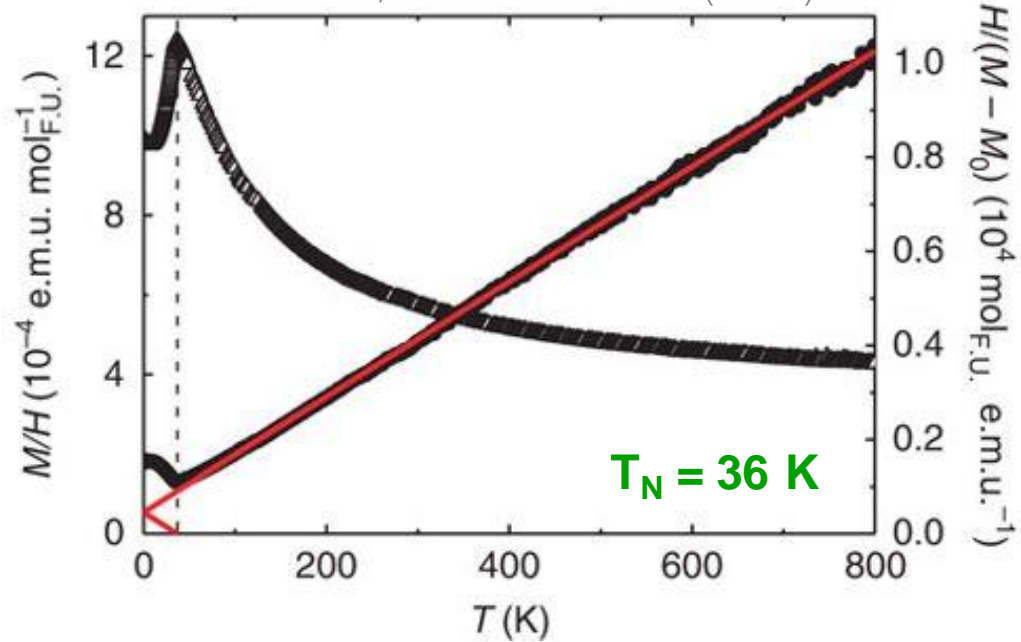


Discovered by
Bernd Matthias
around 1960

TiAu is the first itinerant antiferromagnet without magnetic elements

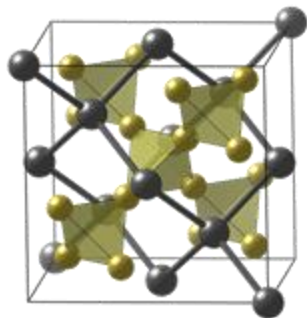


E. Svanidze, *et al.* Nat. Comm. (2015)

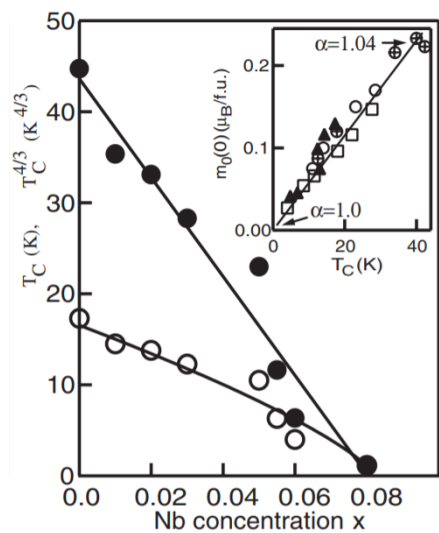


Discovered by
Emilia Morosan
in 2015

ZrZn₂

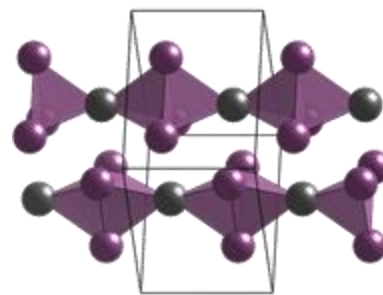


- 3D crystal structure
- Mean field ferromagnet
- Small single crystals
- Nb-doping induced QCP

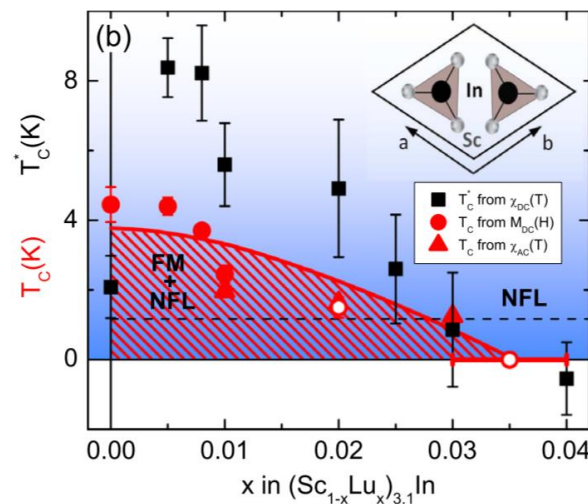


D.A. Sokolov *et al.*, PRL (2006)

Sc_{3.1}In

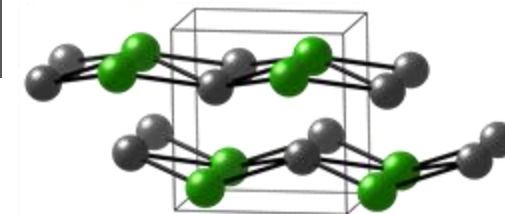


- Quasi-1D crystal structure
- Non-mean field ferromagnet
- No single crystals
- Lu-doping induced QCP

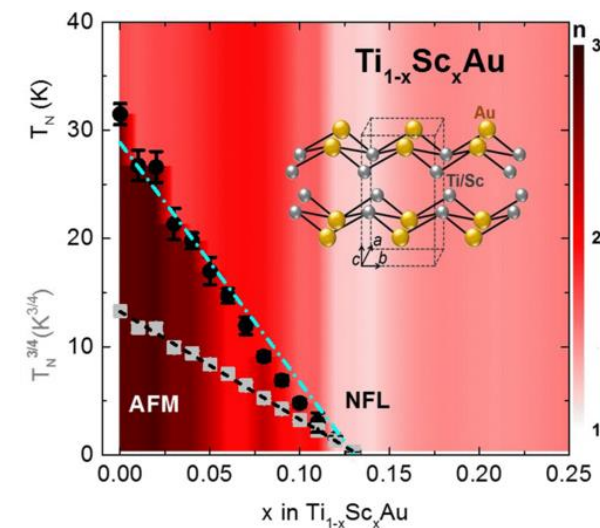


E. Svanidze *et al.* PRX (2015)

TiAu



- Quasi-2D crystal structure
- Antiferromagnetic
- No single crystals
- Sc-doping induced QCP



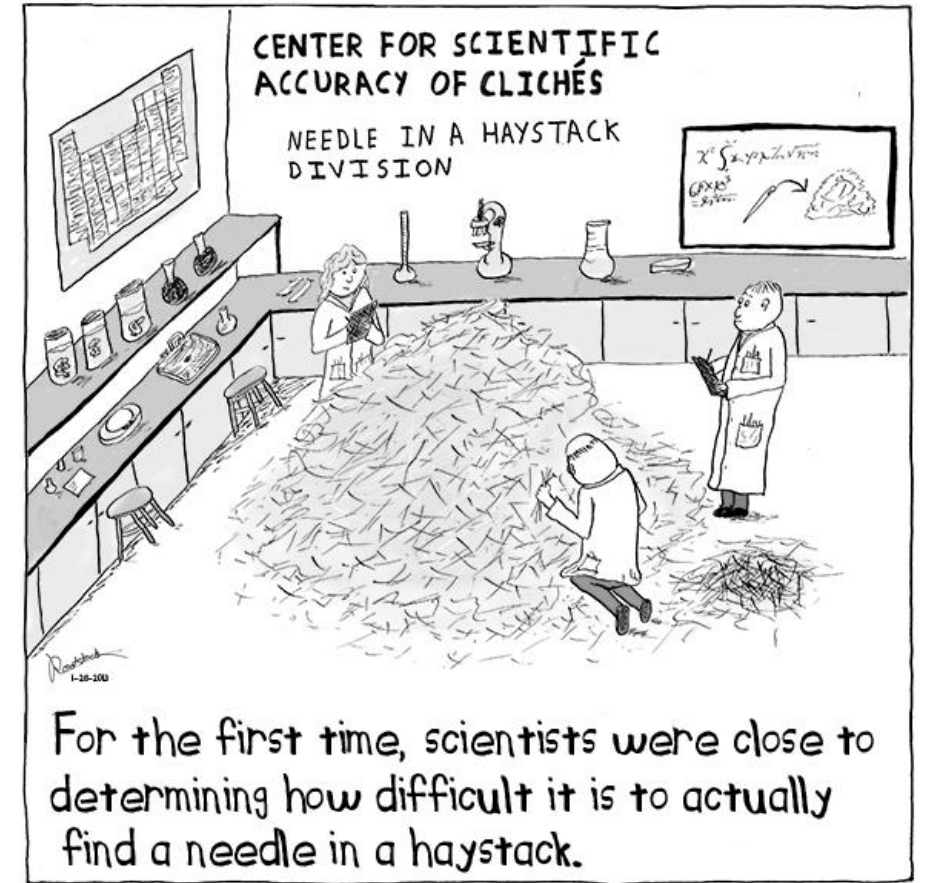
E. Svanidze *et al.* PRB(R) (2017)

How to design a purely itinerant magnet *ie.* How to search for a needle in a haystack

1 H Hydrogen 1.008																	2 He Helium 4.003						
3 Li Lithium 6.941	4 Be Beryllium 9.012																	5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305																	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 84.798						
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294						
55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71 Lanthanides	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018						
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103 Actinides	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [293]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown						

$$\binom{29}{2} = 406 \text{ combinations}$$

57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.243	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967
89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]



How to design a purely itinerant magnet *ie.* How to search for a needle in a haystack

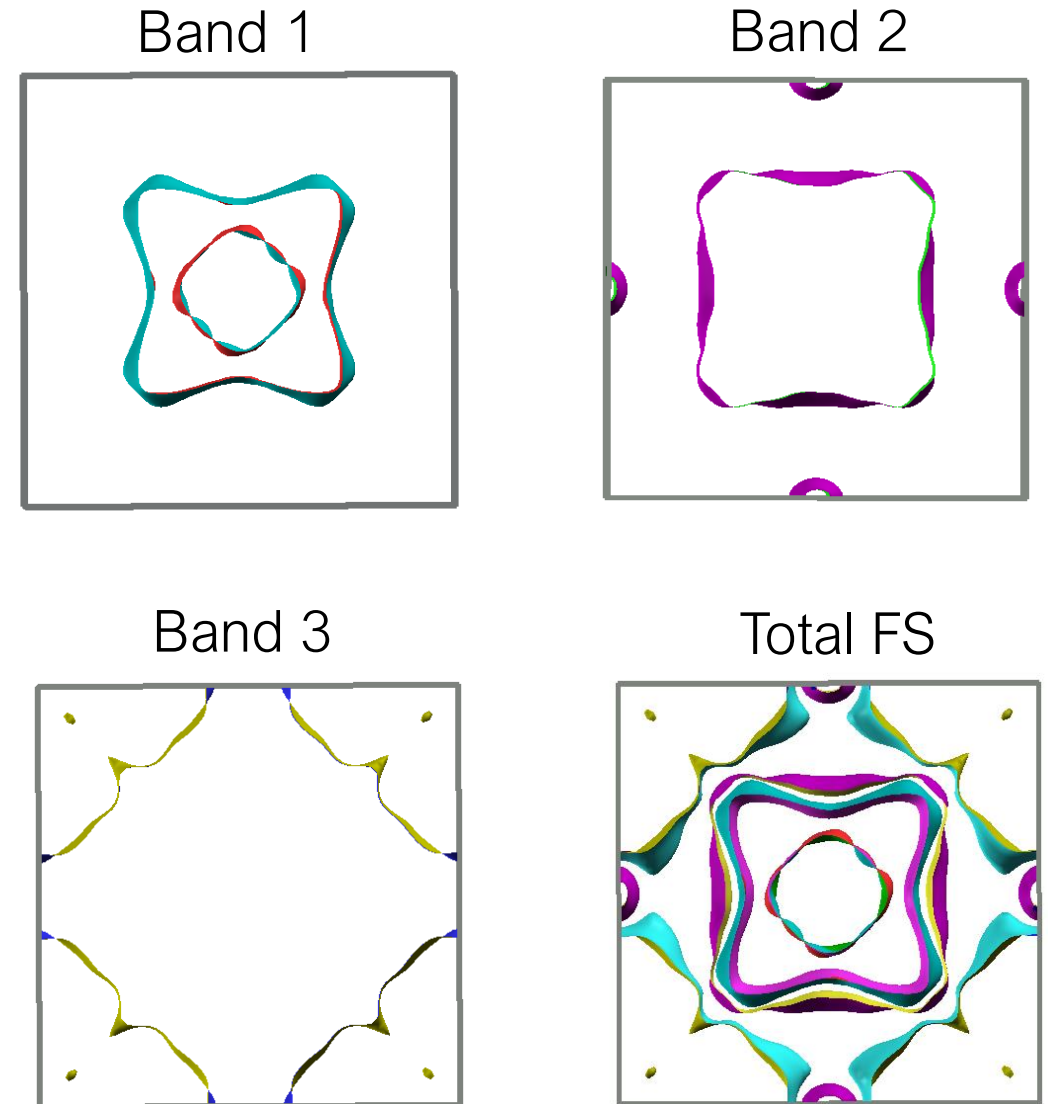
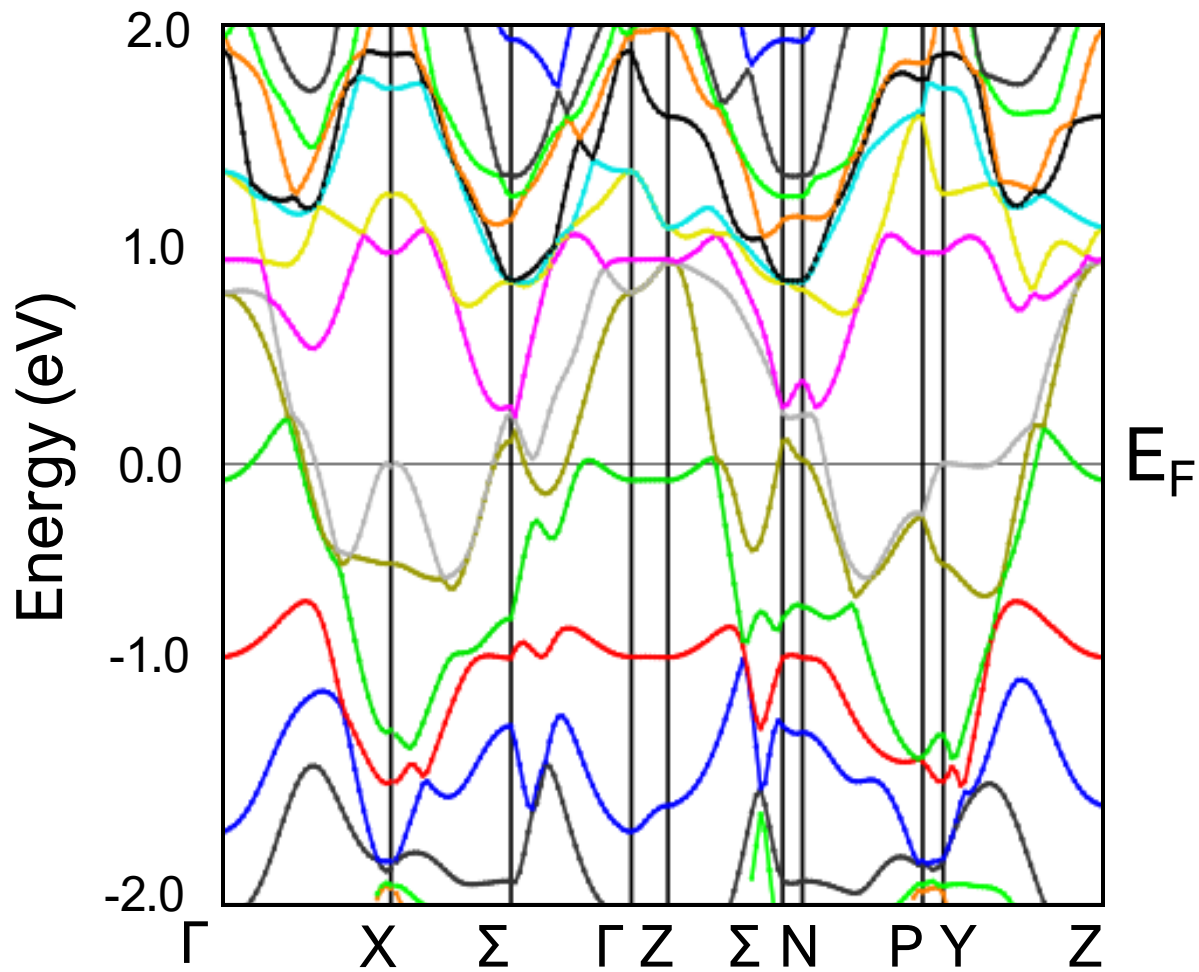
<50 compounds!

1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 84.798
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294
55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71 Lanthanides	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103 Actinides	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown
57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.243	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967			
89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]			

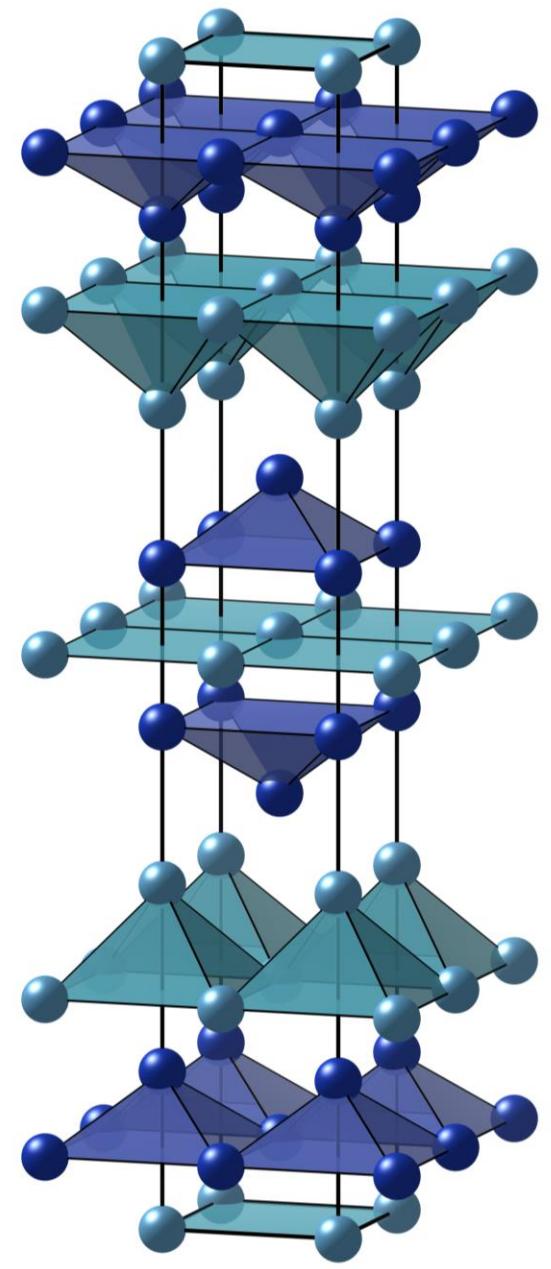
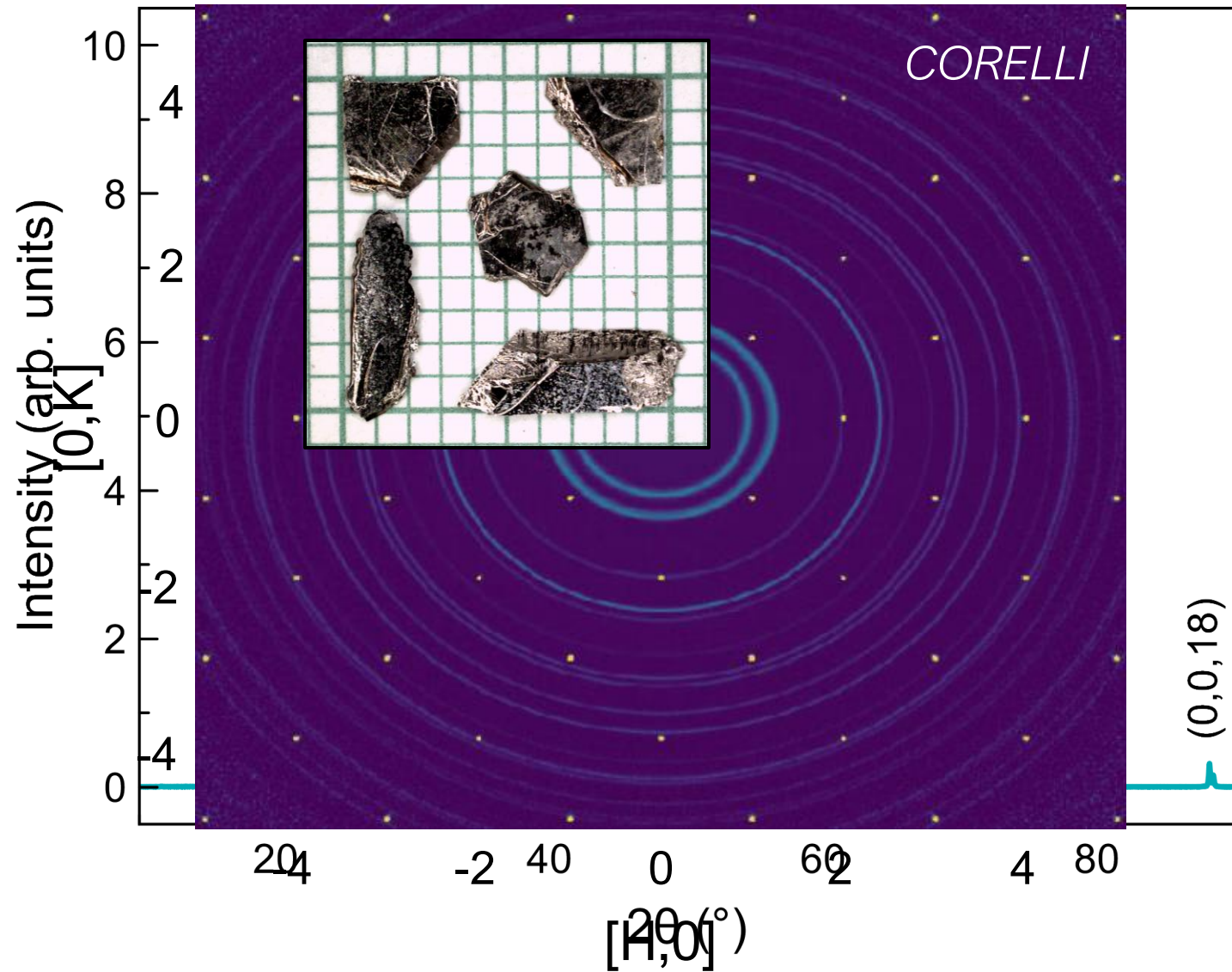
Let's Build a Binary Intermetallic

1. No unstable, radioactive, inert, or deadly elements
2. Exclude non-metals and metalloids
3. Exclude elements that are commonly magnetic in intermetallics ^{*semi-empirical}

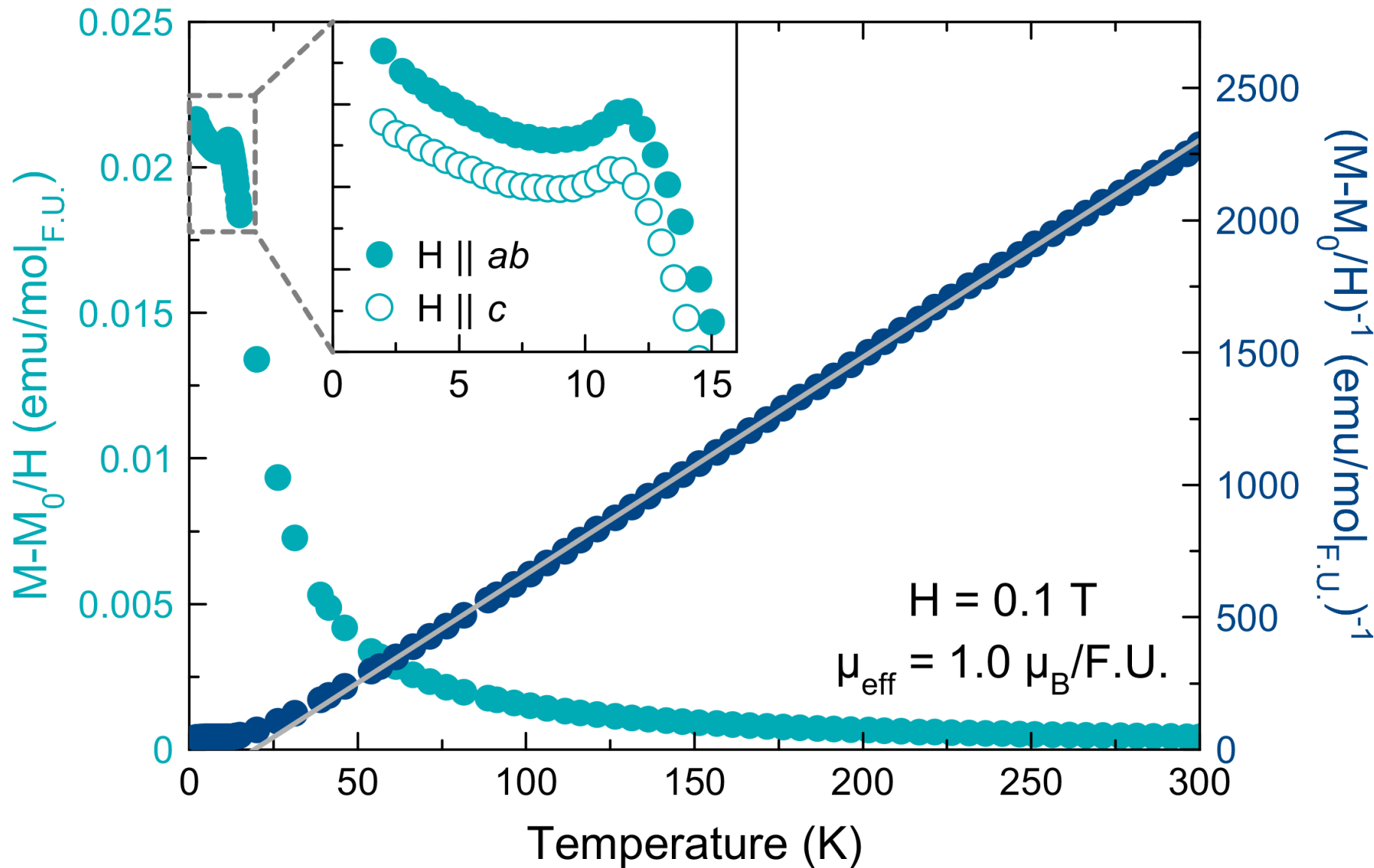
The Fermi surface of Ti_3Cu_4 is heavily nested



We were able to grow large single crystals of Ti_3Cu_4



Ti₃Cu₄ orders antiferromagnetically at T_N = 11 K



Ferromagnets:

ZrZn₂:

T_C = 27.5 K

μ_{eff} = 1.8 μ_B

Sc_{3.1}In:

T_C = 4.5 K

μ_{eff} = 1.3 μ_B

Antiferromagnets:

TiAu:

T_N = 36 K

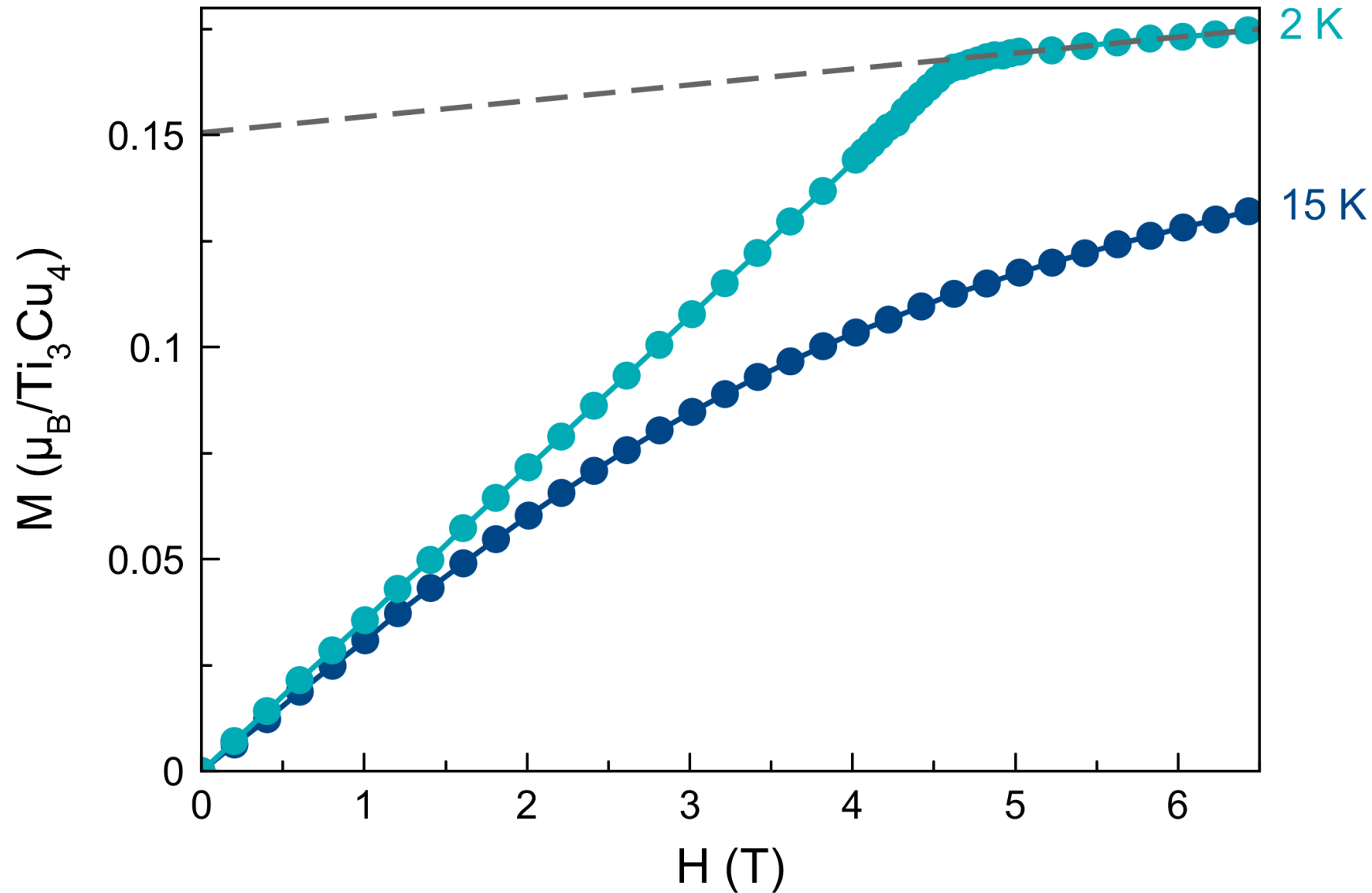
μ_{eff} = 0.8 μ_B

Ti₃Cu₄:

T_N = 11 K

μ_{eff} = 1.0 μ_B

Ti_3Cu_4 has a saturated magnetic moment of $0.15 \mu_B$



Ferromagnets:

ZrZn_2 :

$\mu_{\text{sat}} = 0.17 \mu_B/\text{f.u.}$

$\text{Sc}_{3.1}\text{In}$:

$\mu_{\text{sat}} = 0.2 \mu_B/\text{f.u.}$

Antiferromagnets:

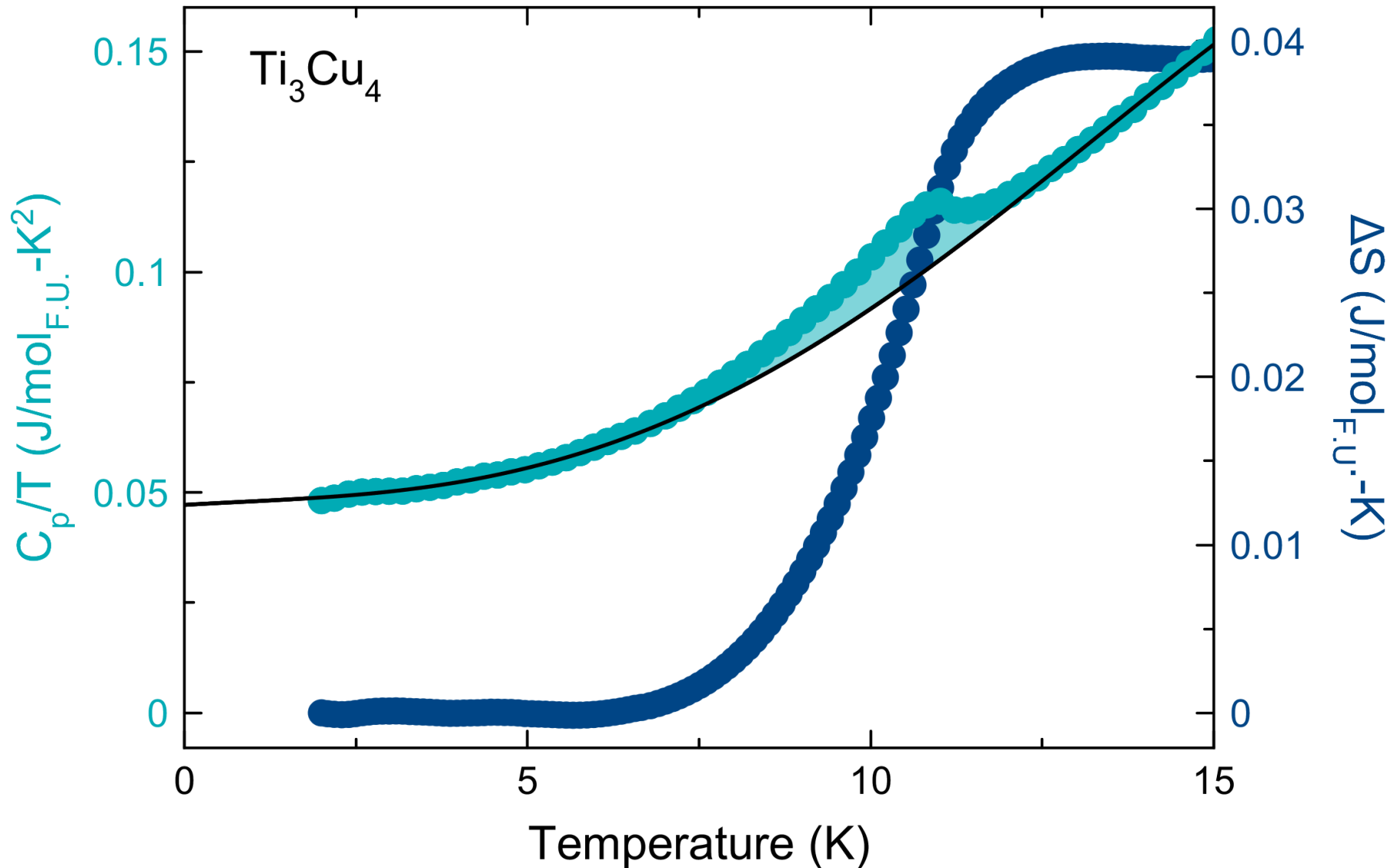
TiAu :

$\mu_{\text{sat}} = 0.13 \mu_B/\text{f.u.}$

Ti_3Cu_4 :

$\mu_{\text{sat}} = 0.15 \mu_B/\text{f.u.}$

The entropy release in Ti_3Cu_4 at $T_N = 11$ K is very small



Ferromagnets:

ZrZn_2 :

$\Delta S = 3\% R \ln 2$

$\text{Sc}_{3.1}\text{In}$:

$\Delta S = 2\% R \ln 2$

Antiferromagnets:

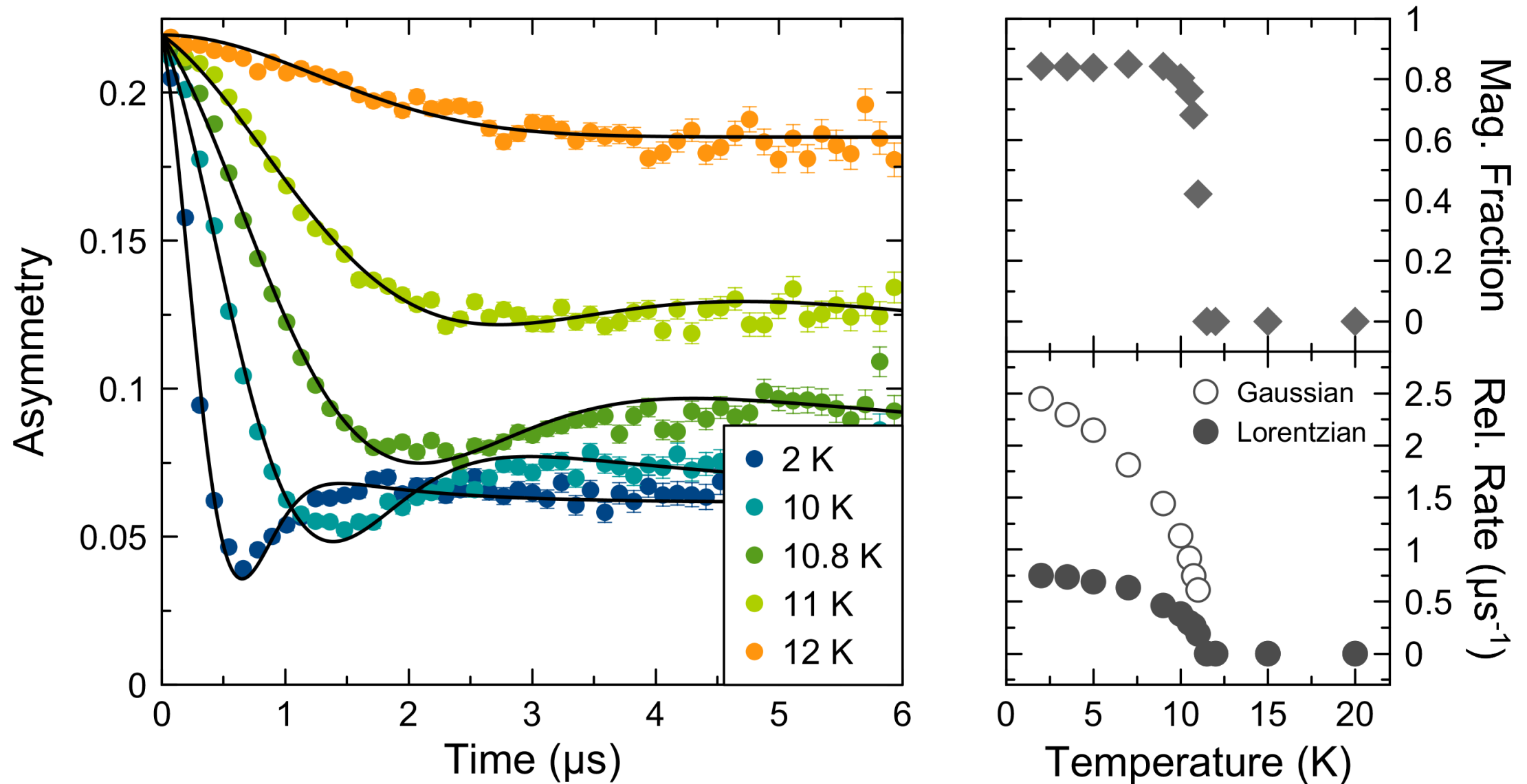
TiAu :

$\Delta S = 3\% R \ln 2$

Ti_3Cu_4 :

$\Delta S = 0.7\% R \ln 2$

Muon spin relaxation confirms that the magnetic order in Ti_3Cu_4 is bulk



Summary: Ti_3Cu_4 is the second known purely itinerant antiferromagnet and the first such compound in single crystal form.

communications physics












ARTICLE

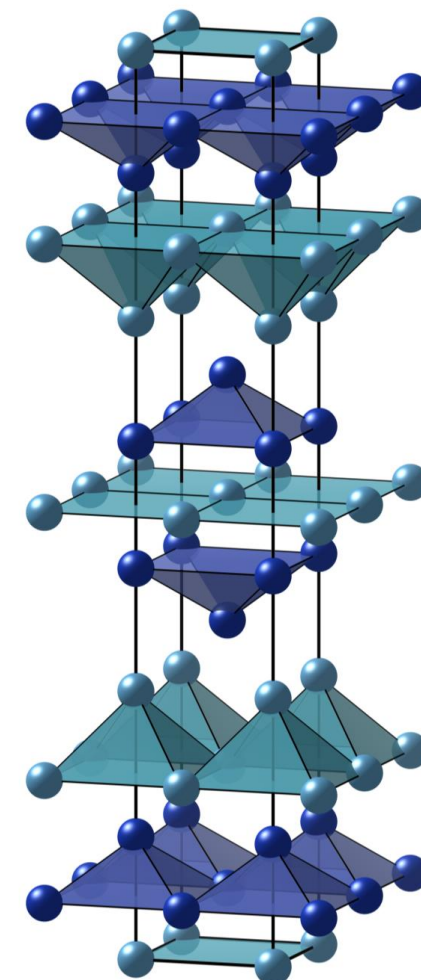
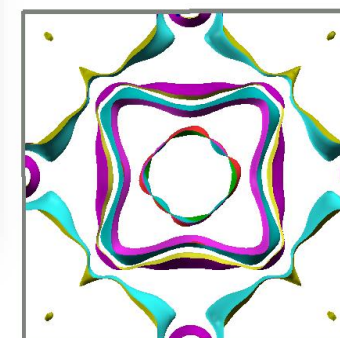
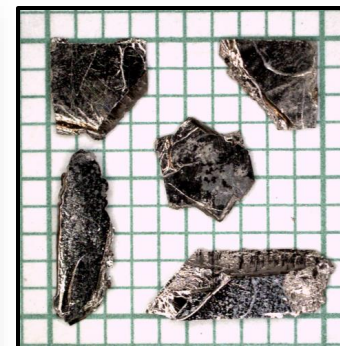
 Check for updates

<https://doi.org/10.1038/s42005-022-00901-7>

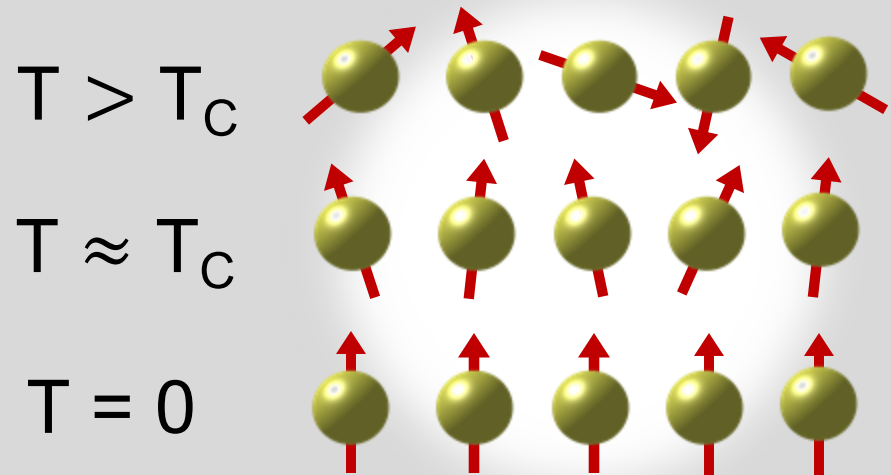
OPEN

Field-induced quantum critical point in the itinerant antiferromagnet Ti_3Cu_4

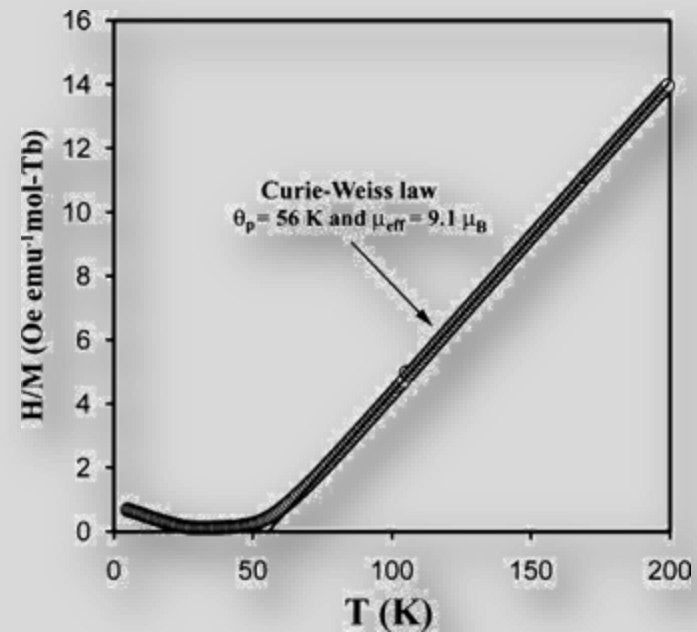
Jaime M. Moya ^{1,2}, Alannah M. Hallas ^{2,3}, Vaideesh Loganathan², C.-L. Huang^{2,4}, Lazar L. Kish ⁵, Adam A. Aczel ⁶, J. Beare ⁷, Y. Cai⁷, G. M. Luke ^{7,8}, Franziska Weickert ⁹, Andriy H. Nevidomskyy ², Christos D. Malliakas ¹⁰, Mercuri G. Kanatzidis ¹⁰, Shiming Lei², Kyle Bayliff¹¹ & E. Morosan ²✉



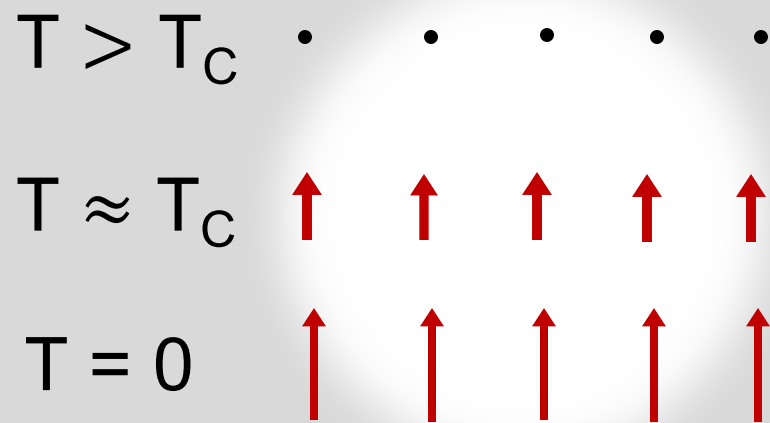
The Local Limit



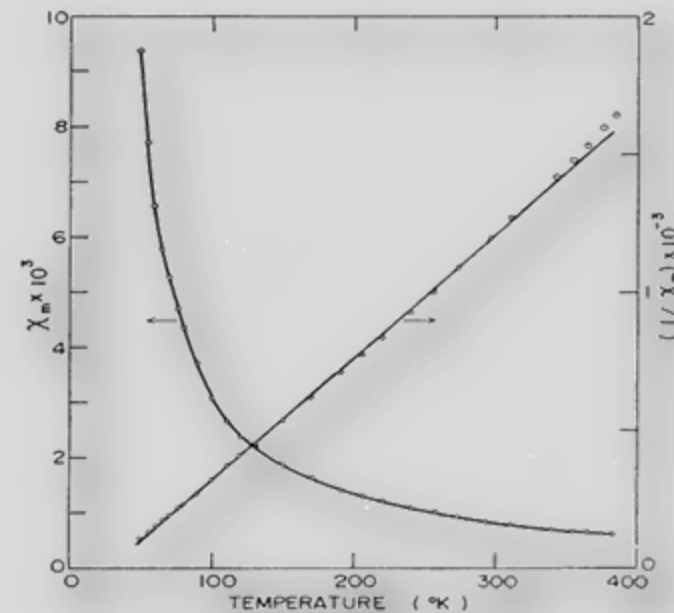
Mean-field Curie-Weiss law gives $\chi \propto 1/T$ for temperatures above T_C/T_N

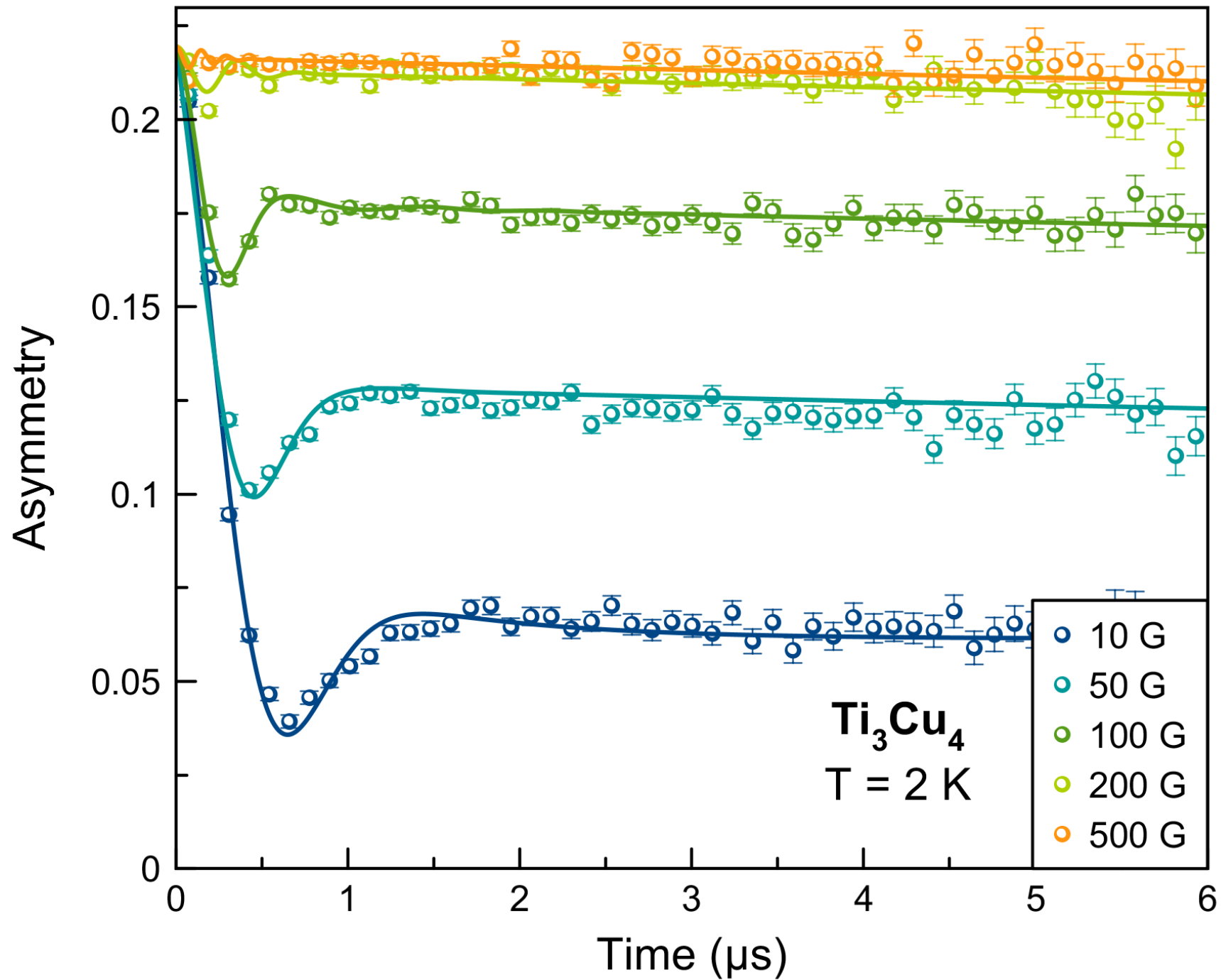


The Itinerant Limit

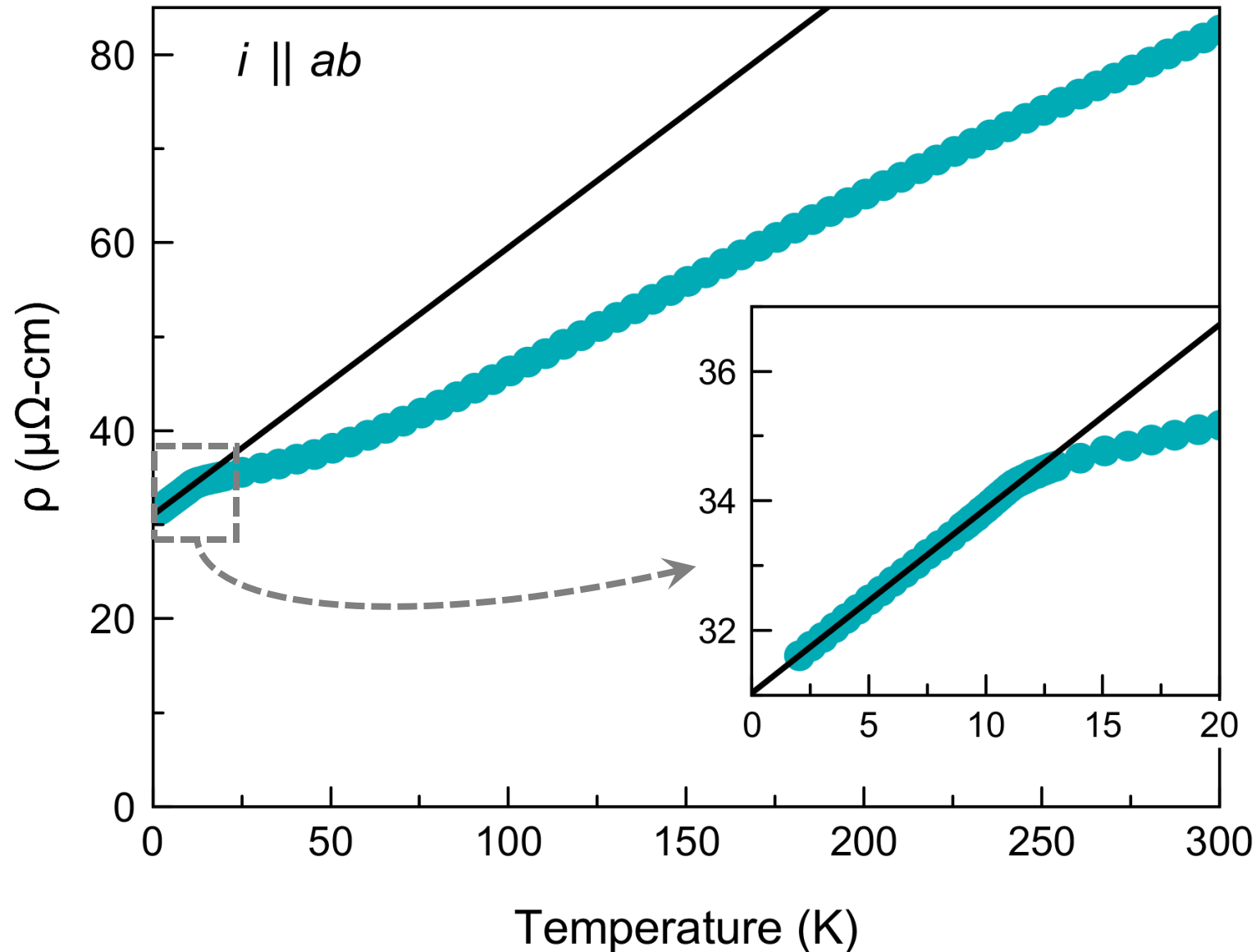


SCR theory of spin fluctuations gives $\chi \propto 1/T$ for temperatures above T_C/T_N





Ti₃Cu₄ has T -linear resistivity below $T_N = 11$ K



Ferromagnets:

ZrZn₂:

$$\rho(T) \propto T^{5/3}$$

Sc_{3.1}In:

$$\rho(T) \propto T$$

Antiferromagnets:

TiAu:

$$\rho(T) \propto T^3$$

Ti₃Cu₄:

$$\rho(T) \propto T$$