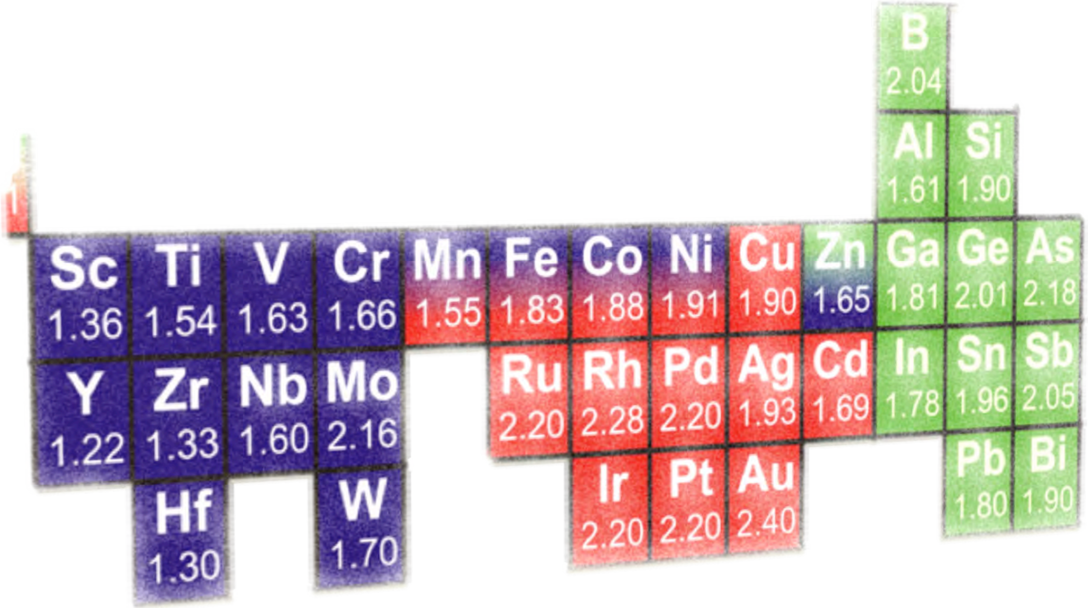
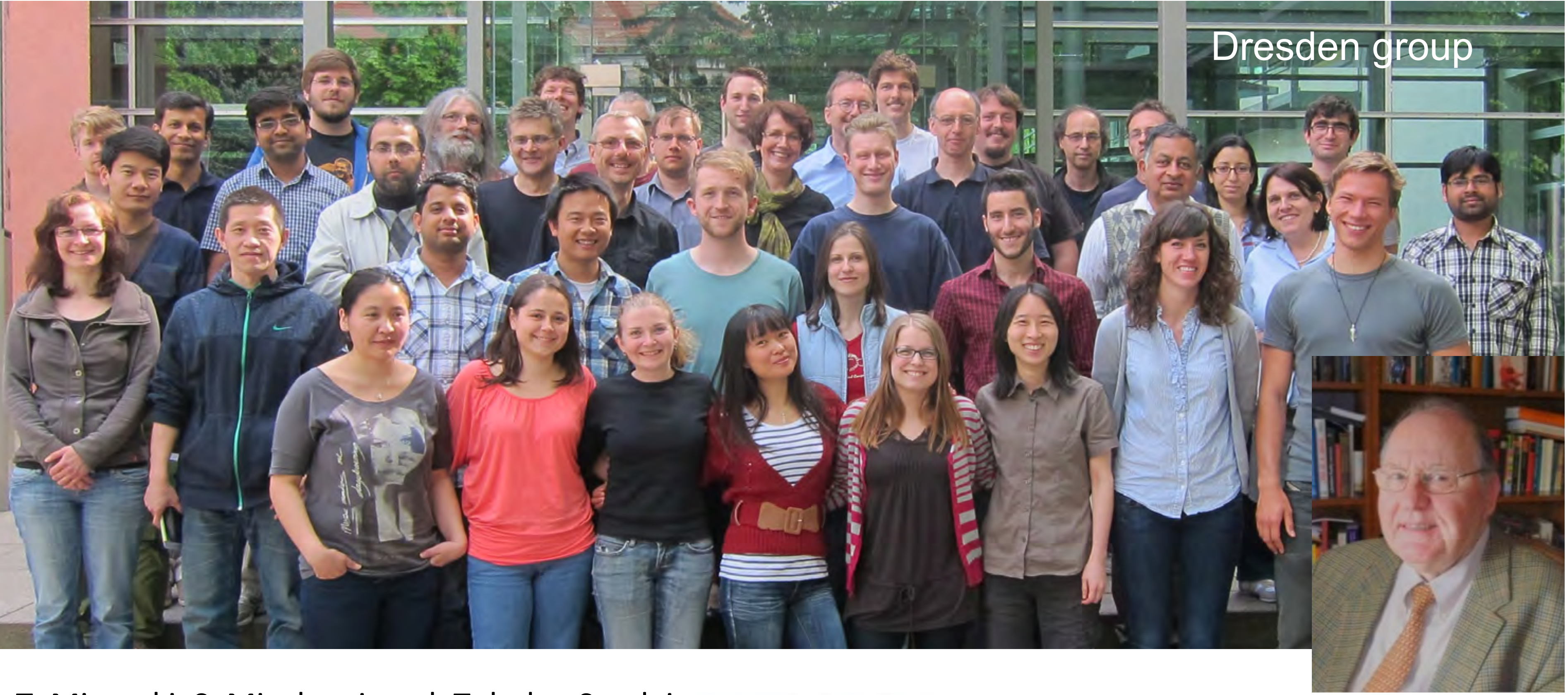
Magnetism in Mn-rich Heusler compounds



Claudia FELSER,

www.superconductivity.de

Co-workers in Dresden and elsewhere

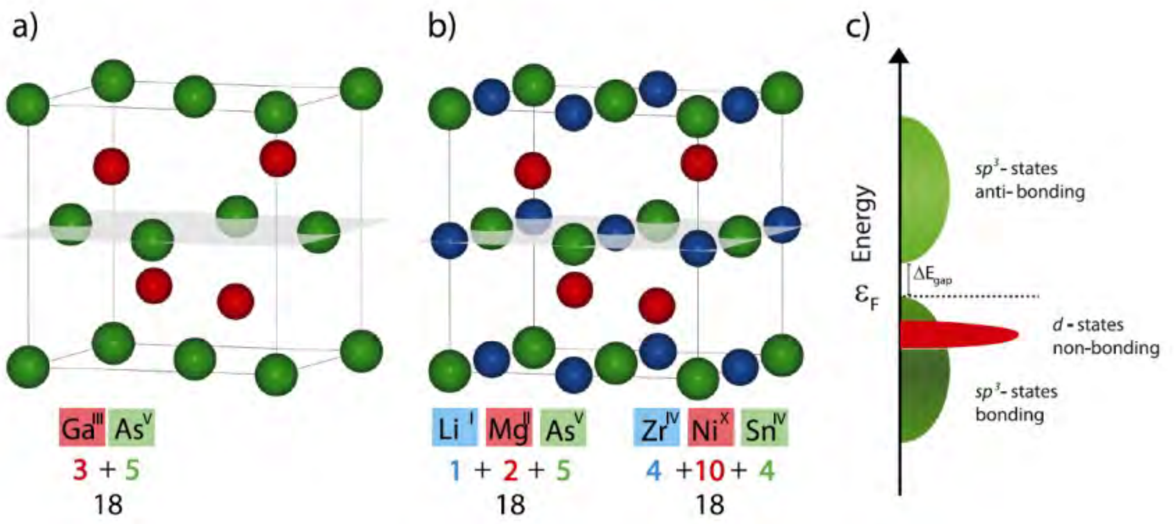


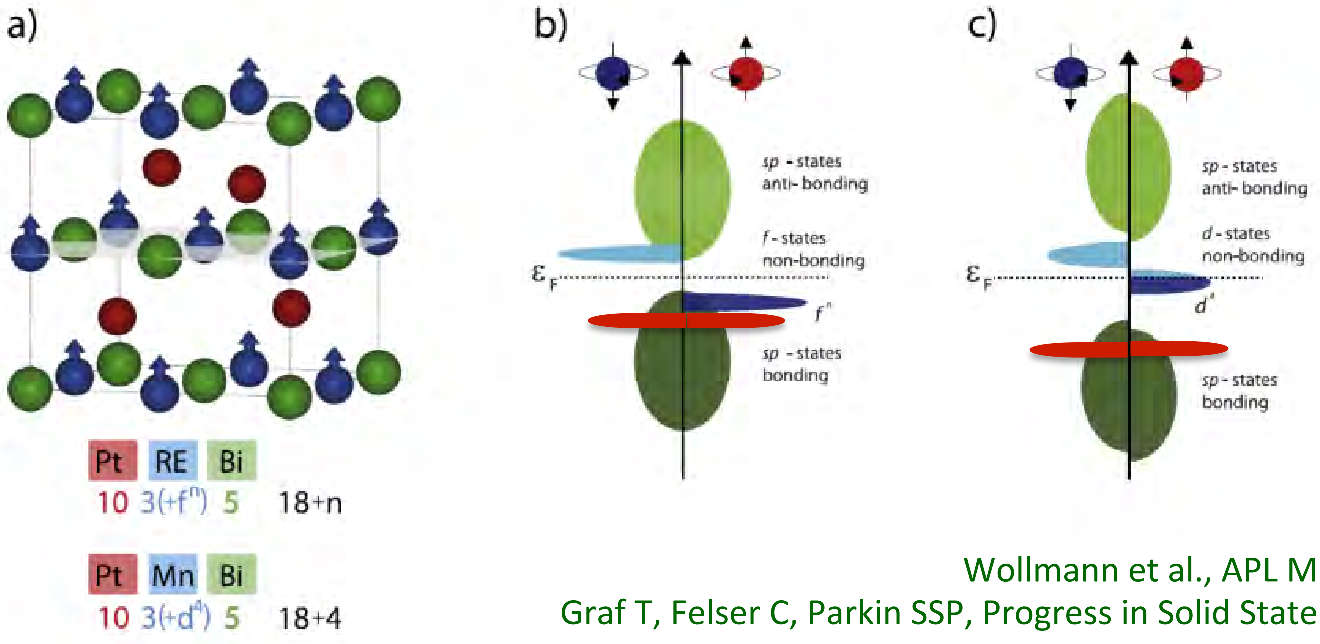
T. Miyazaki, S. Mizukami et al. Tohoku, Sendai

S. S. P. Parkin et al. IBM Almaden, MPI Halle

M. Coey, Dublin

Half metallic Ferromagnets



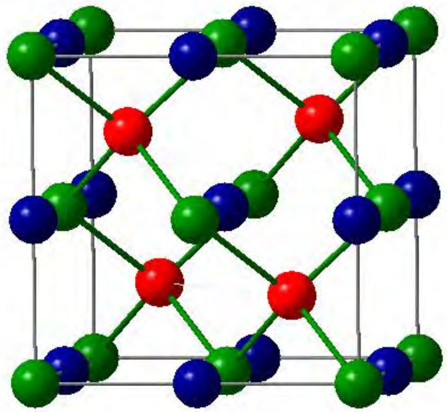


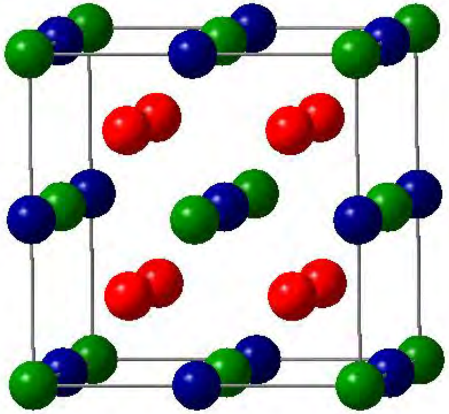
Wollmann et al., APL Mat. 3 (2015) 041518

Graf T, Felser C, Parkin SSP, Progress in Solid State Chemistry (2011) 1

Kandpal *et al.*, CF J. Phys. D **39** (2006) 776

Ternary Semiconductors …





Ga **As**

13 + 5 = 18

Co **Ti** **Sb**

9 + 4 + 5 = 18

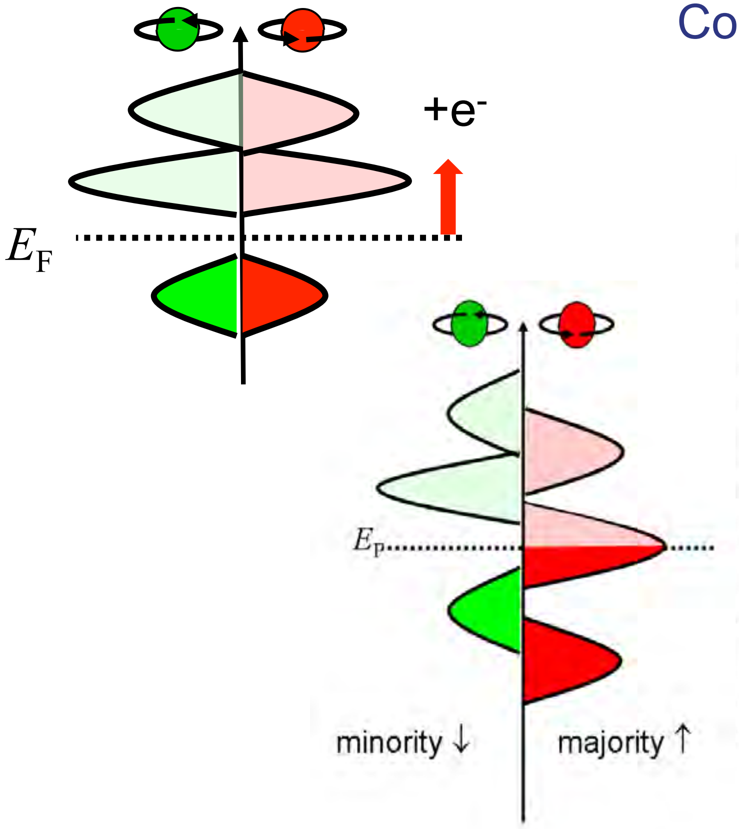
Fe_2 **Ti** **Sn**

2*8 + 4 + 4 = 24

additional t_2-levels

Materials: … to half metallic ferromagnets

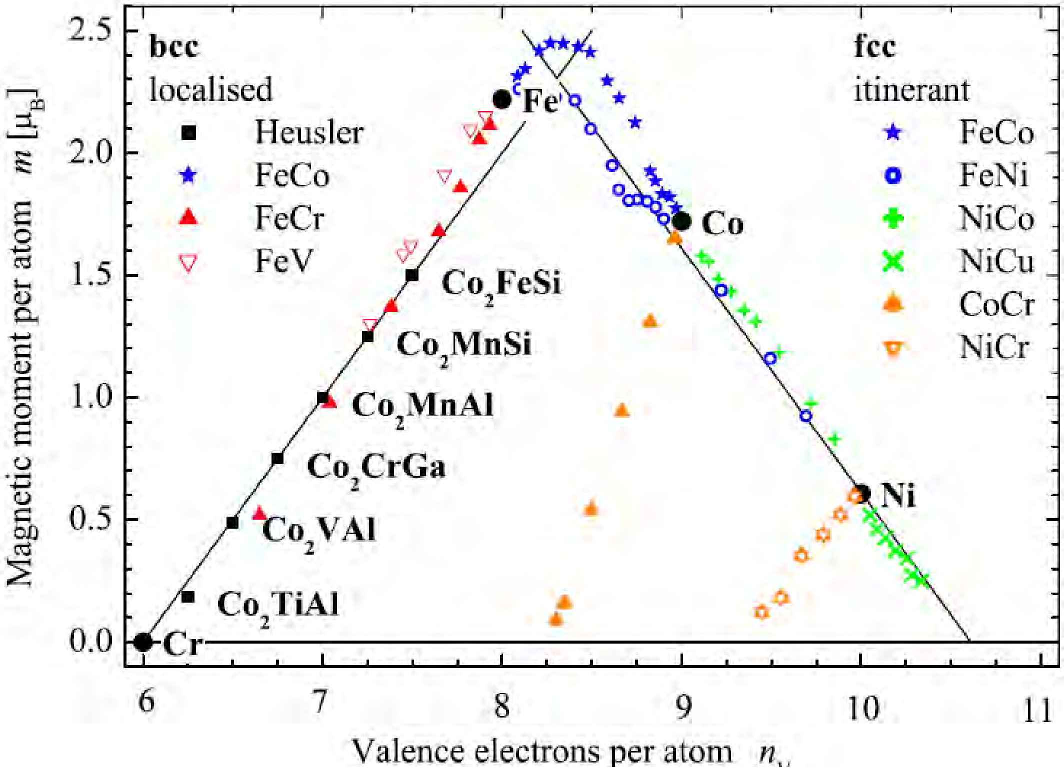
X_2YZ



Example: Co$_2$MnSi

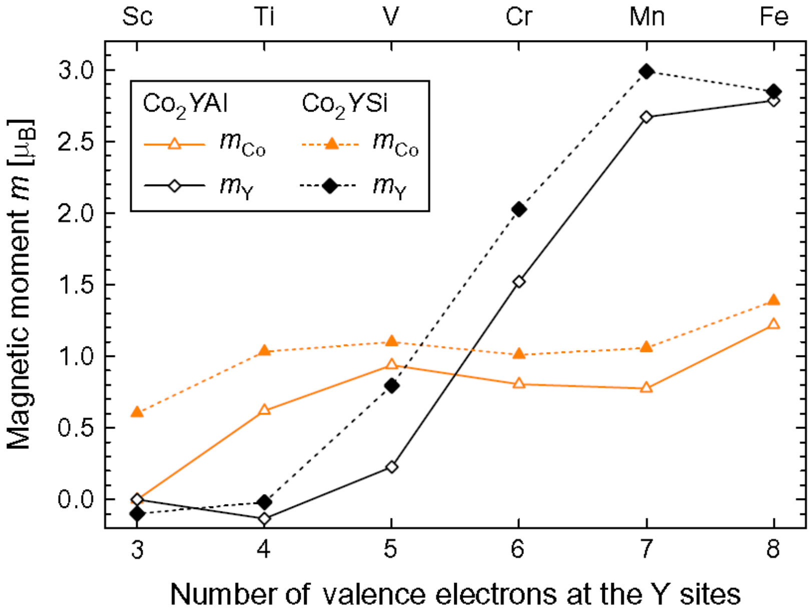
- magic valence electron number: 24
- valence electrons = 24 + magnetic moments

Co$_2$MnSi: 2×9 + 7 + 4 = 29 Ms = 5μ_B



Kübler *et al.*, PRB **28**, 1745 (1983)
Galanakis *et al.*, PRB **66**, 012406 (2002)

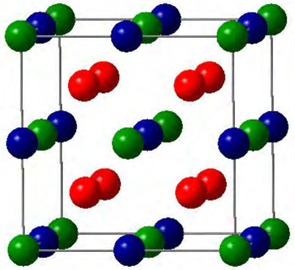
Tunability Co_2YZ

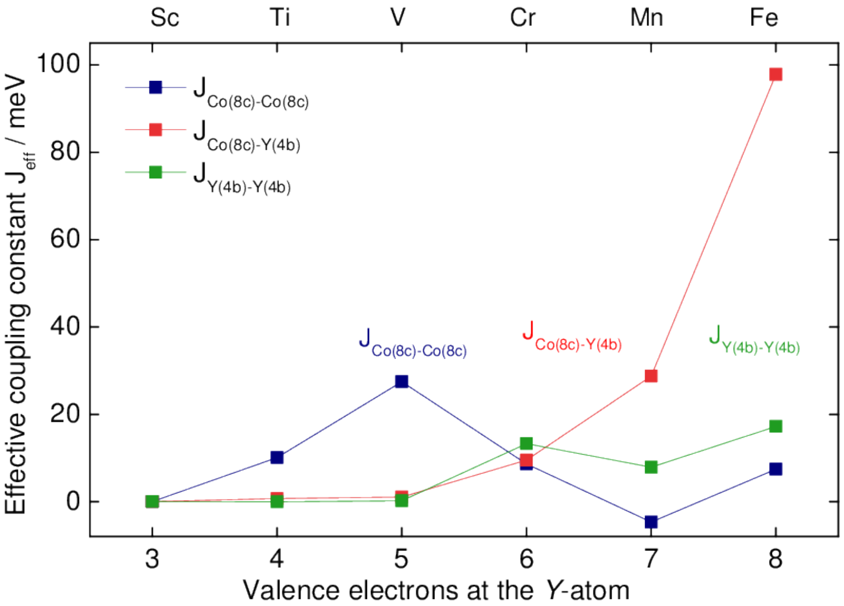


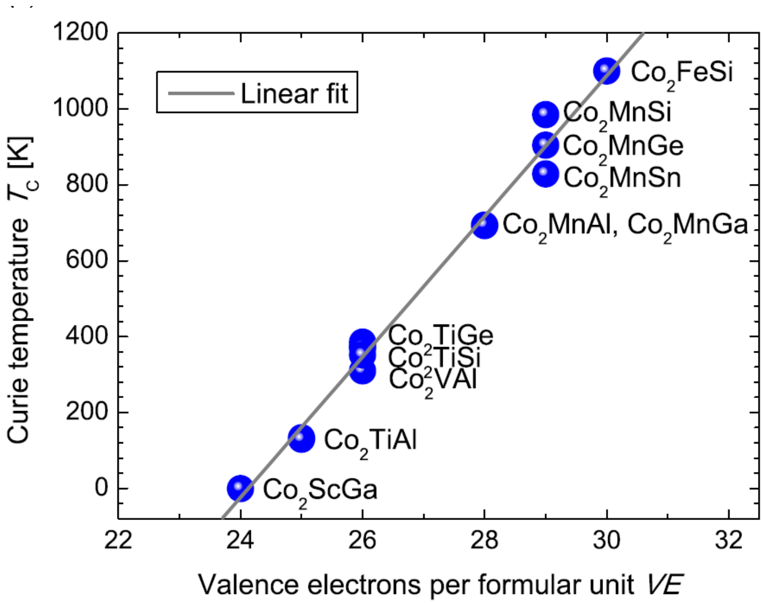
m (Co) ~ 1μ_B

m (Mn) ~ 3μ_B

Exchange coupling: ferro

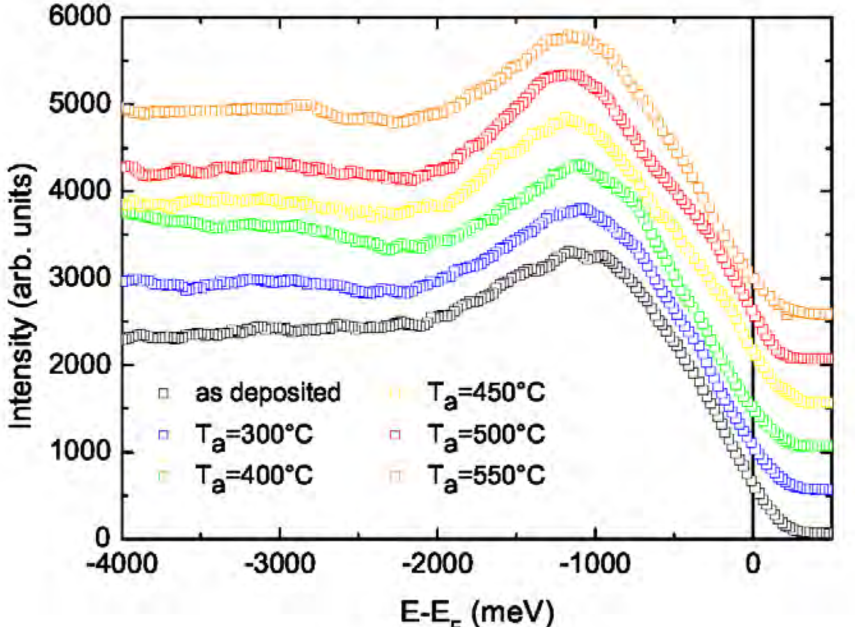


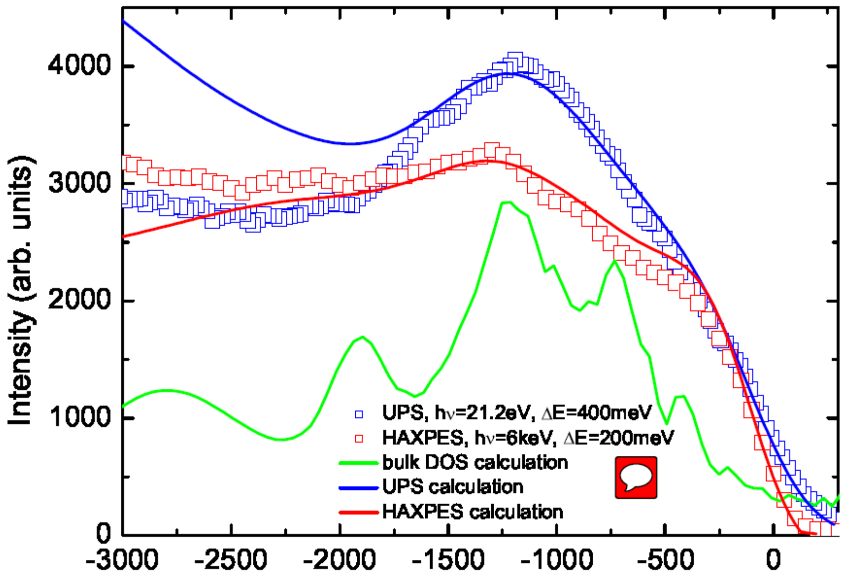


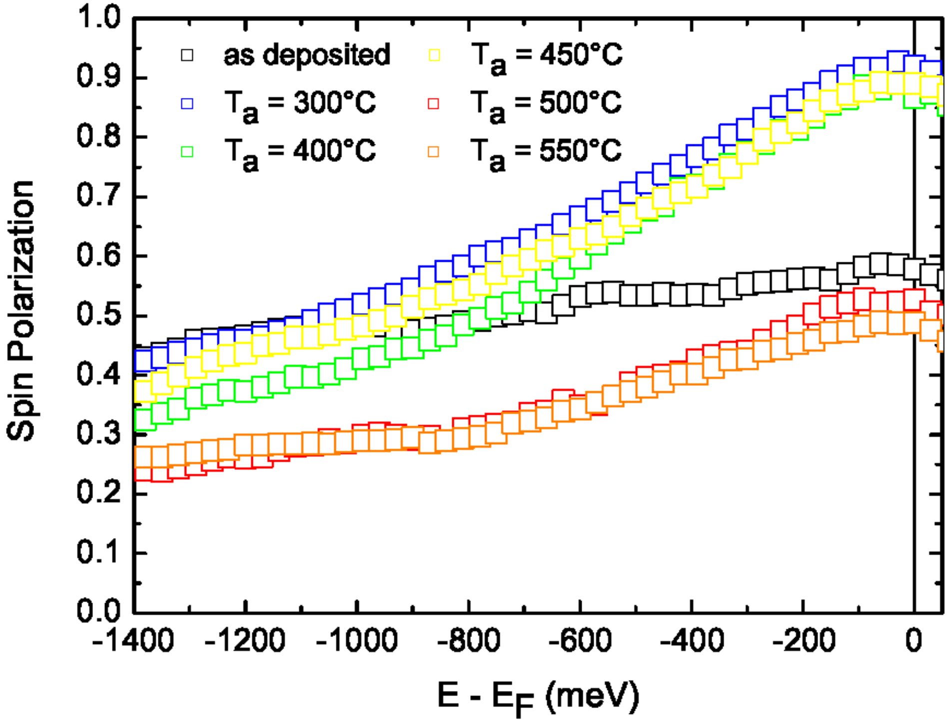


Kandpal et al., J. Phys. **D 40** (2007) 1507.
Balke *et al.* Solid State Com. **150** (2010) 529
Kübler *et al.*, Phys. Rev. B **76** (2007) 024414

100% spinpolarisation Co_2MnSi

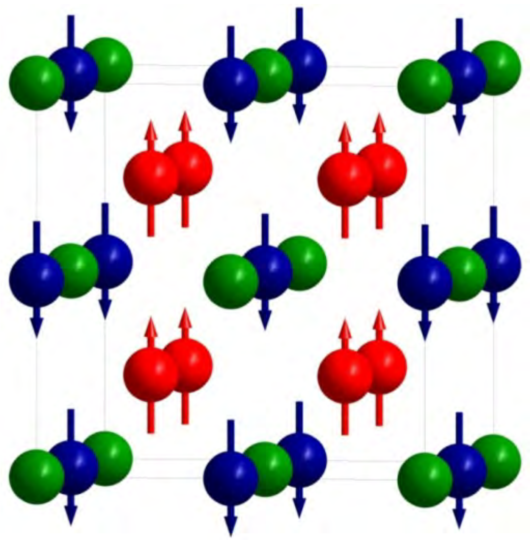


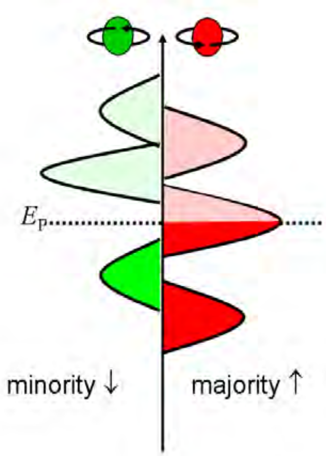


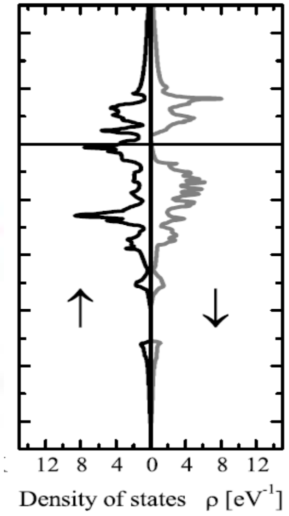


Jourdan et al. Nature Com. 5 (2014) 3974

Ferrimagnetic Heusler compounds







Kübler’s Rule
Slater Pauling Rule

X_2MnGa

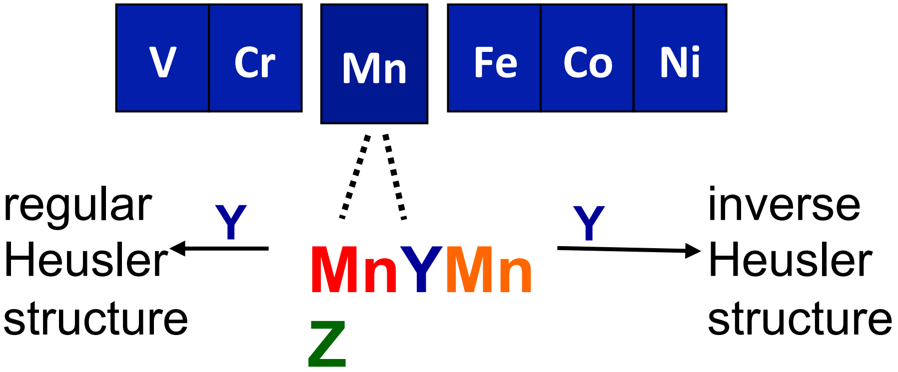
Two magnetic sublattices
24 Valence electrons – 0 μ_B
Mn^{3+} at octahedral site – 4 μ_B
Mn compensates

Mn_2MnGa
3*7 + 3 = 24
⇒ Compensated ferrimagnet

Wurmehl, *et al.*, J. Phys. Cond. Mat. **18** (2006) 6171
Balke *et al.* CF, APL **90** (2007) 152504

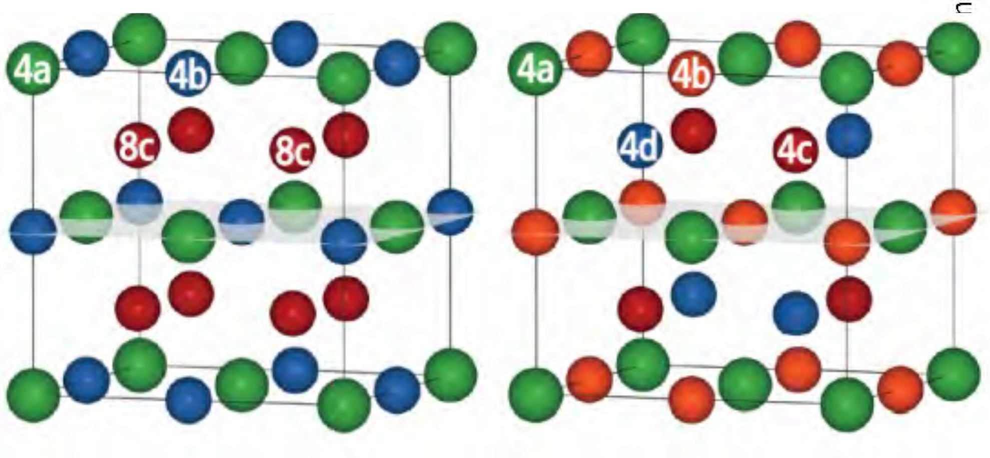
Kübler et al., Phys. Rev. **B** (1983)

Mn$_2$-Heusler compounds

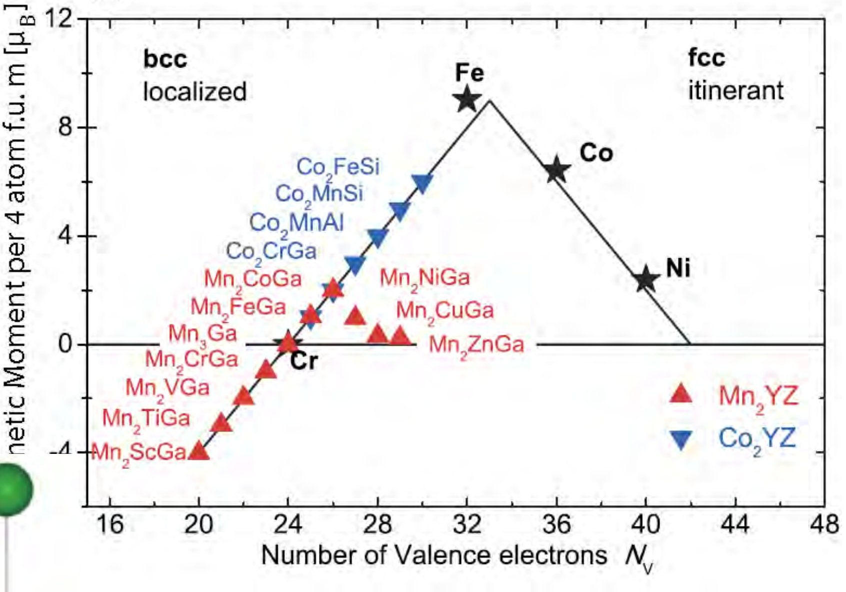


V Cr **Mn** Fe Co Ni

regular Heusler structure ← Y **MnYMn Z** Y → inverse Heusler structure



(a) $Mn_2^{(8c)}Y^{(4b)}Z^{(4a)}$ (b) $Mn^{(4d)}Y^{(4c)}Mn^{(4b)}Z^{(4a)}$

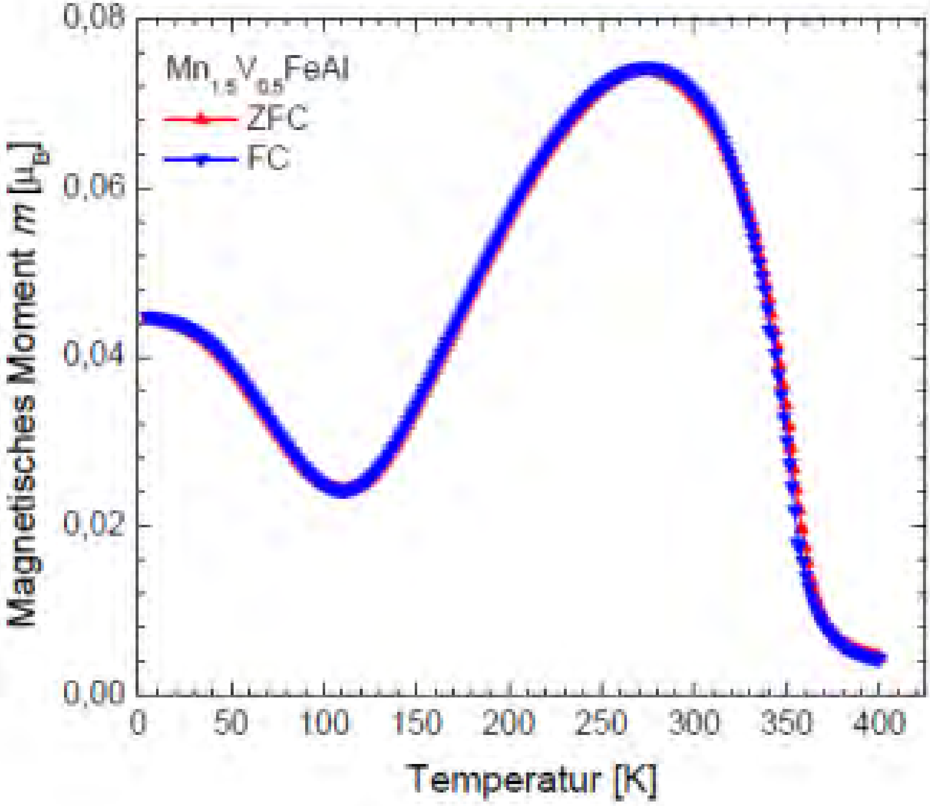


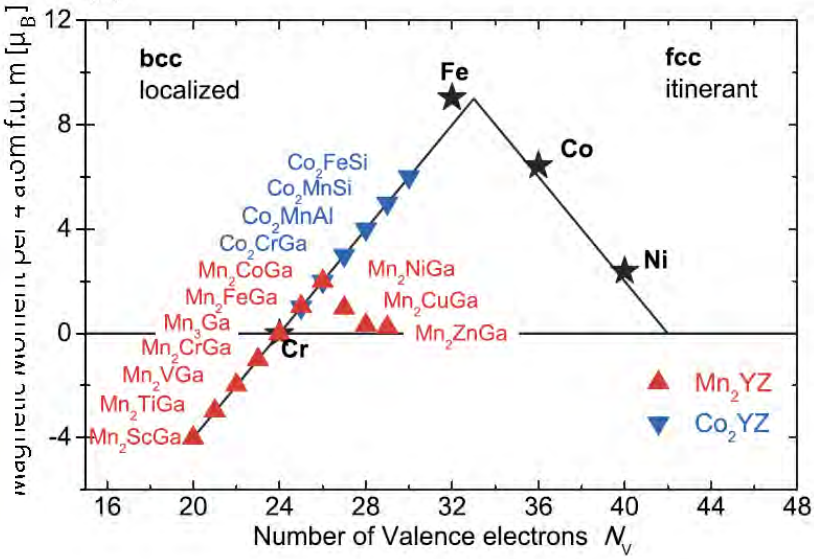
Wollmann et al., APL Mat. 3 (2015) 041518
Graf T, Felser C, Parkin SSP, Progress in Solid State Chemistry (2011),

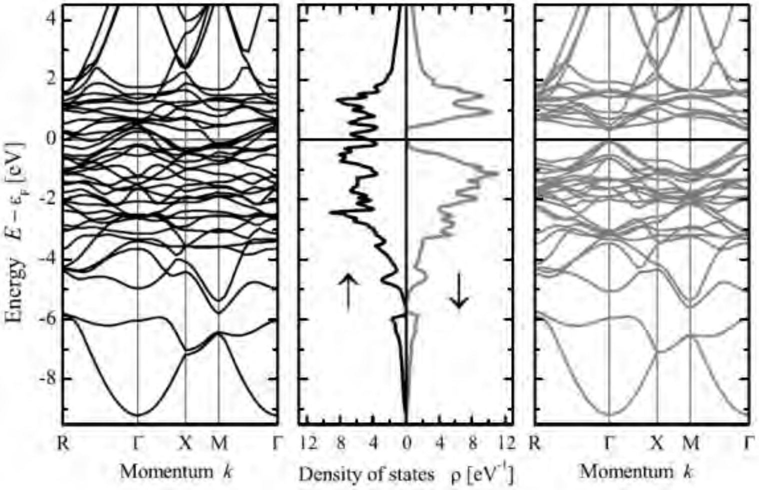
Mn$_2$VGa + Fe$_2$MnGa = compensated

Wurmehl, *et al.*, J. Phys. Cond. Mat. **18** (2006) 6171

Compensated ferrimagnet



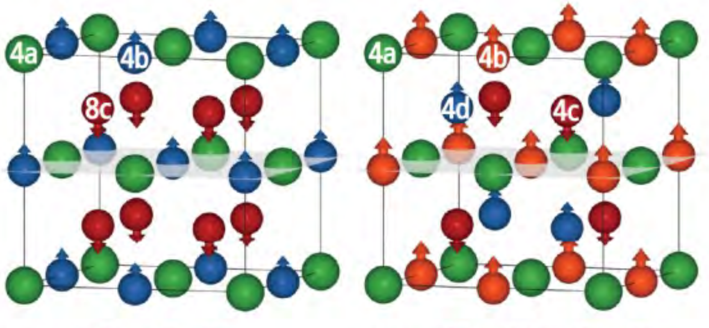




Mn_2VGa + Fe_2MnGa = compensated

Wurmehl, *et al.*, J. Phys. Cond. Mat. **18** (2006) 6171

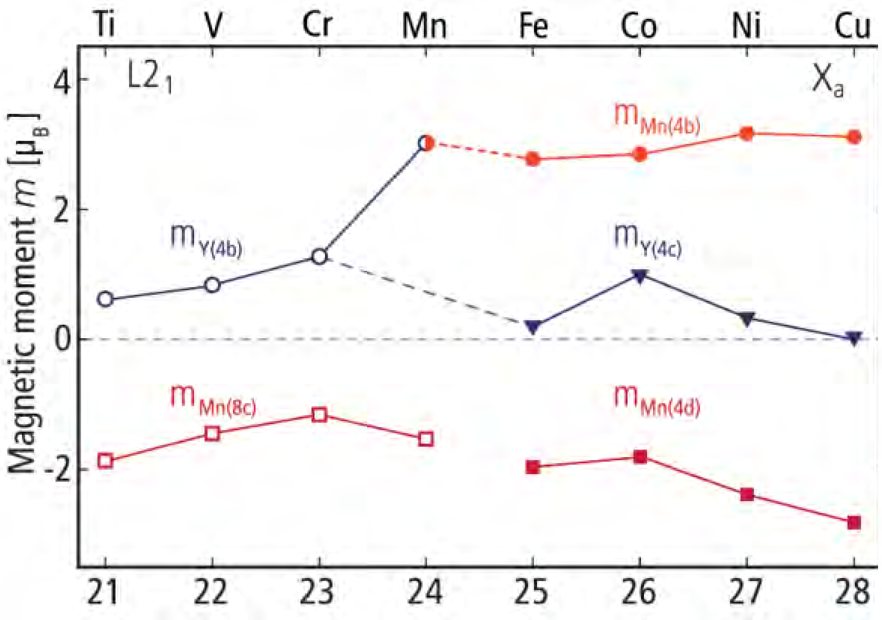
Tunability Mn_2YZ

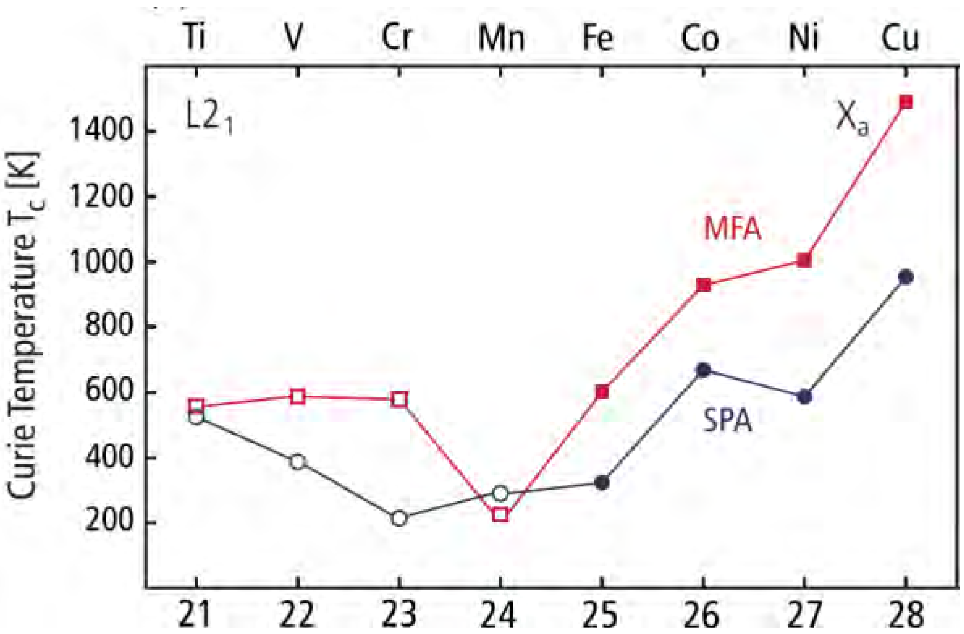


(a) $Mn_2^{(8c)}Y^{(4b)}Z^{(4a)}$ (b) $Mn^{(4d)}Y^{(4c)}Mn^{(4b)}Z^{(4a)}$

m (Mn) ~ 3μ_B
m (Mn) ~ 2μ_B

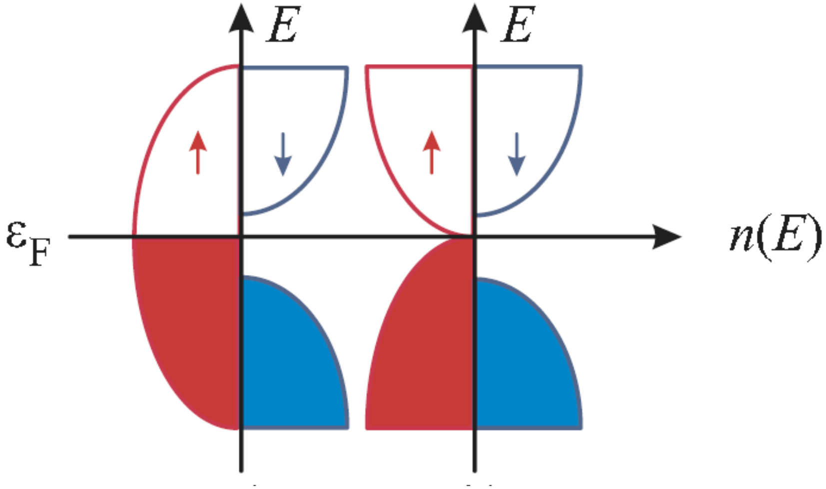
Exchange coupling: ferri

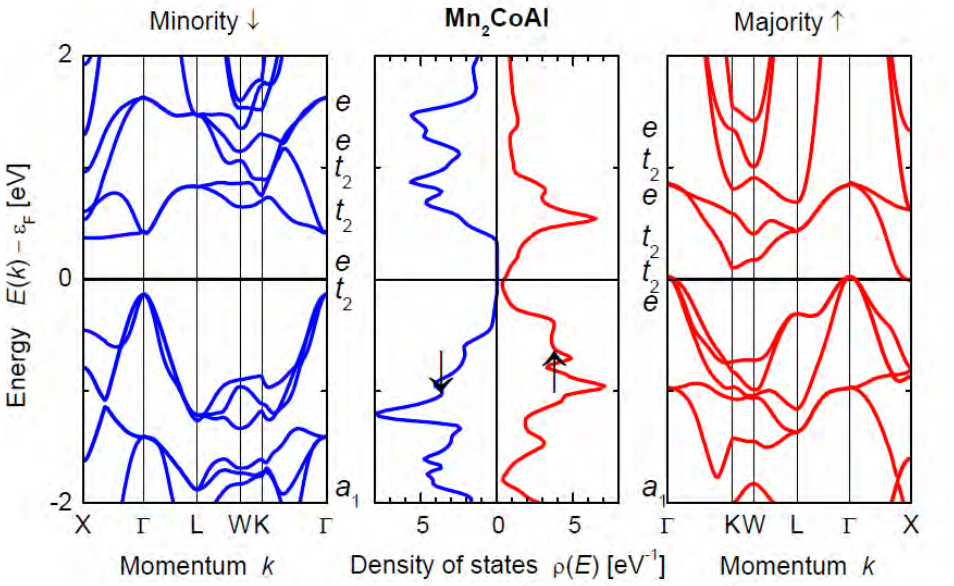




Wollmann et al., Phys. Rev. B 90 (2014) 214420 preprint arXiv:1409.6532

Spin gapless semiconductor Mn_2CoAl





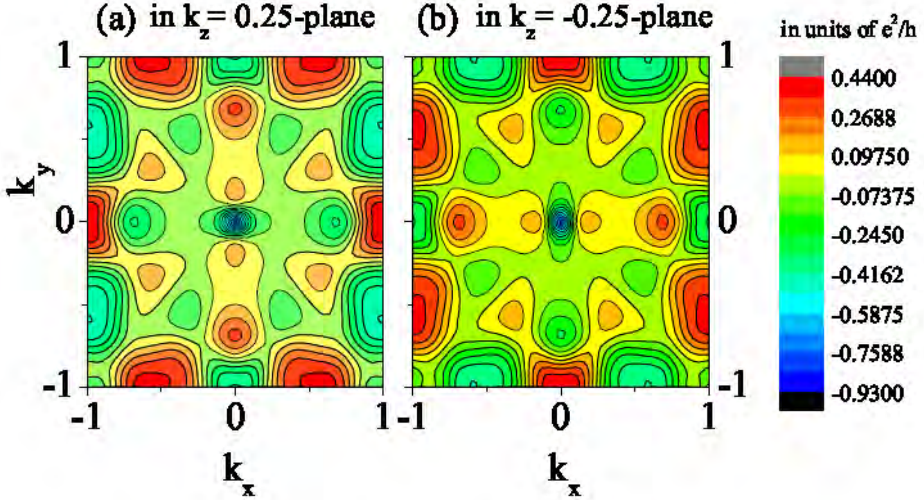
Expected properties

100% spin polarisation

Properties sensitive to pressure

… gating … electrolyte gating

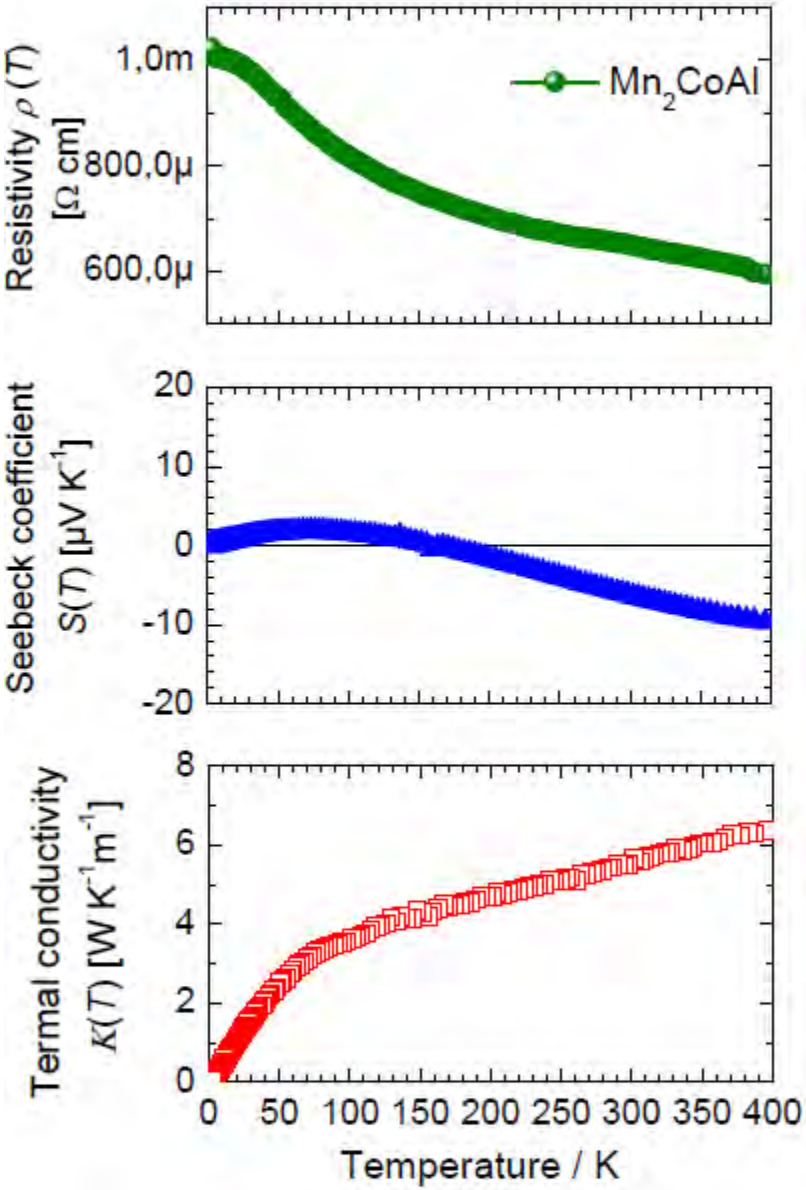
➔ new devices



Wang PRL **100,** 156404 (2008)

Ouardi et al., PRL 110 (2013) 100401

Mn_2CoAl a semiconducting ferromagnet

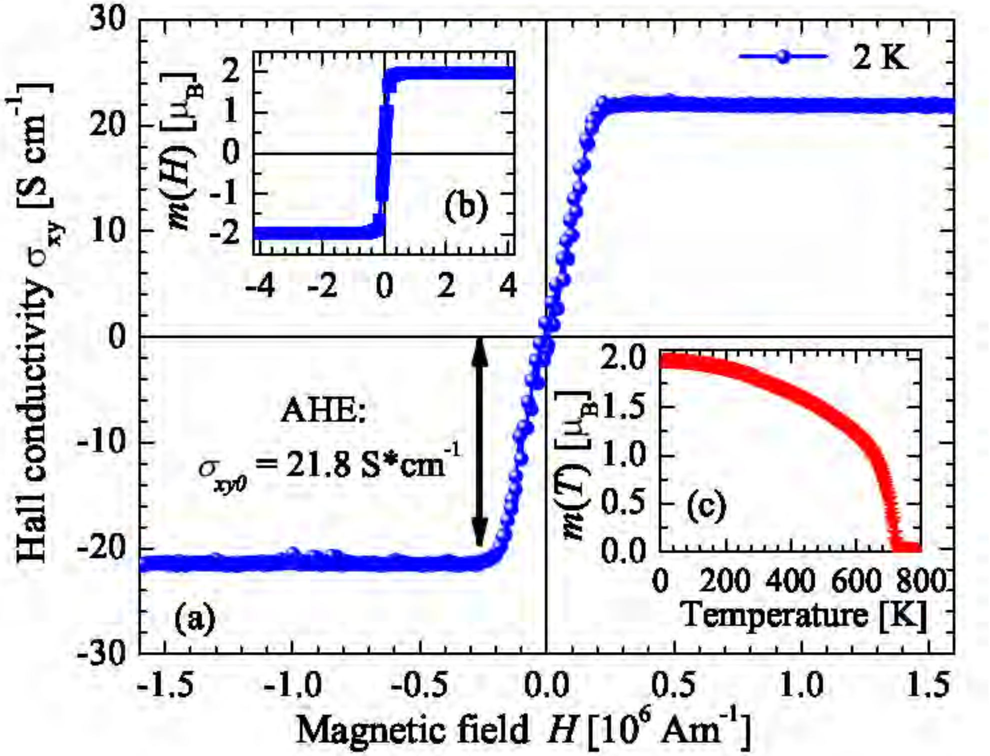


$2*7 + 9 + 3 = 26$

$m = 2\ \mu_B$

$T_C = 800$ K

Charge carrier ~ $10^{17} cm^{-3}$

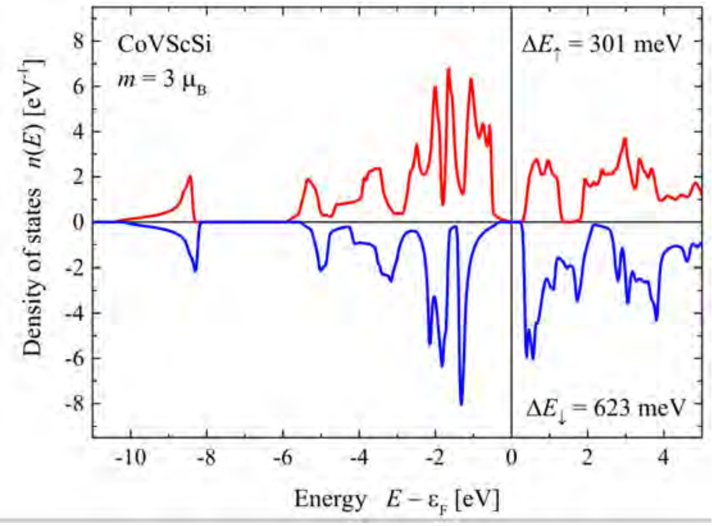


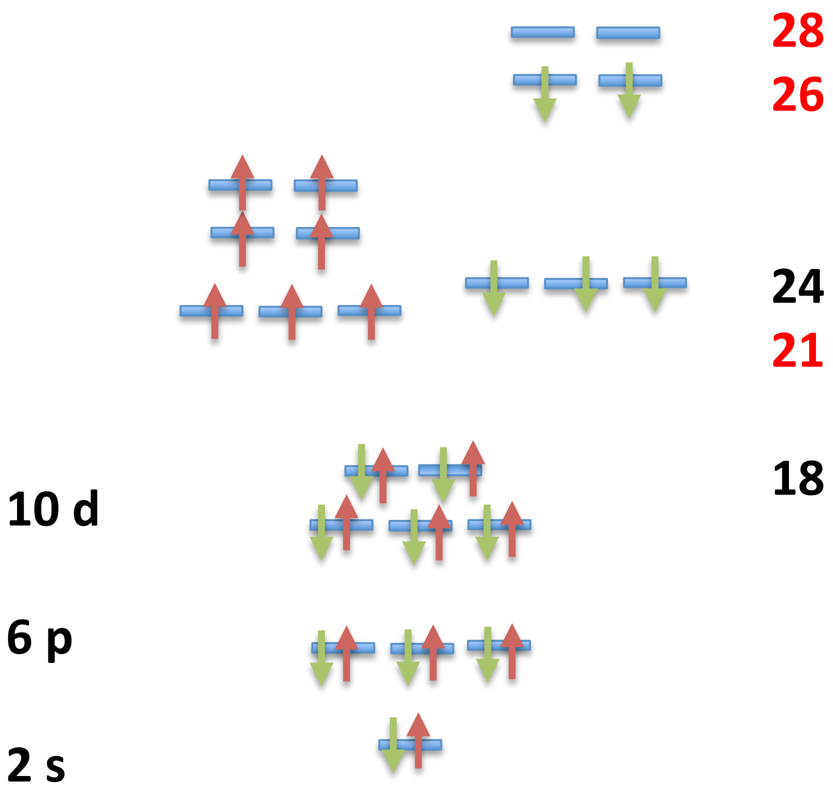
Ouardi et al., Phys. Rev. Lett. 110 (2013) 100401

More semiconductors

26	21
Mn_2CoAl	FeVTiSi
CoFeCrAl	CoVScSi
CoMnCrSi	FeCrScSi
CoFeVSi	FeVTiSi
FeMnCrSb	FeMnScAl

18	28
V_3Al	CoFeMnSi





28

26

24

21

18

10 d

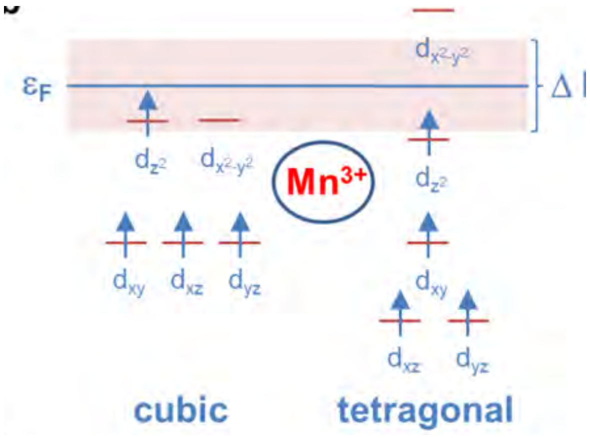
6 p

2 s

Özdogan et al., JAP 113, 193903 (2013)

Fecher et al.unpublished

Mn_3Ga tetragonal distortion

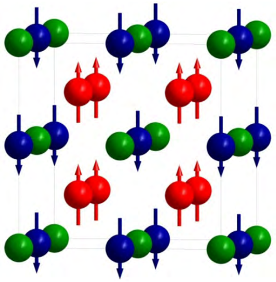


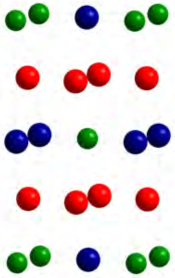
Designed Materials

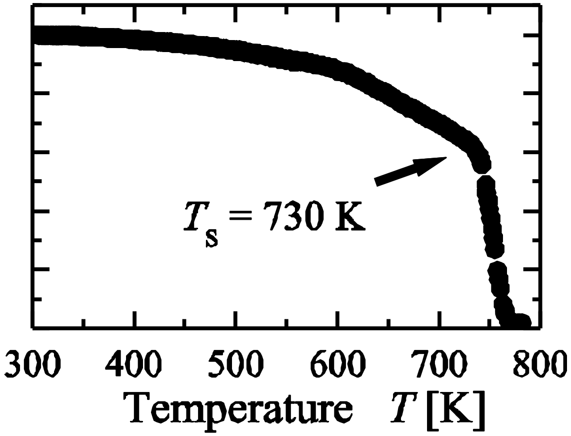
- Materials with low magnetic damping
- Materials with low magnetic moments
- **Materials with high perpendicular anisotrop**

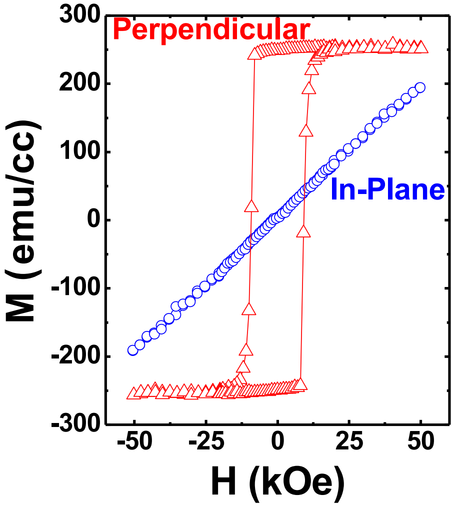
Tetragonal Heusler compounds: Mn_3Ga, $FeMn_2Ga$ …

theory → **bulk material** → **thin film and devices**







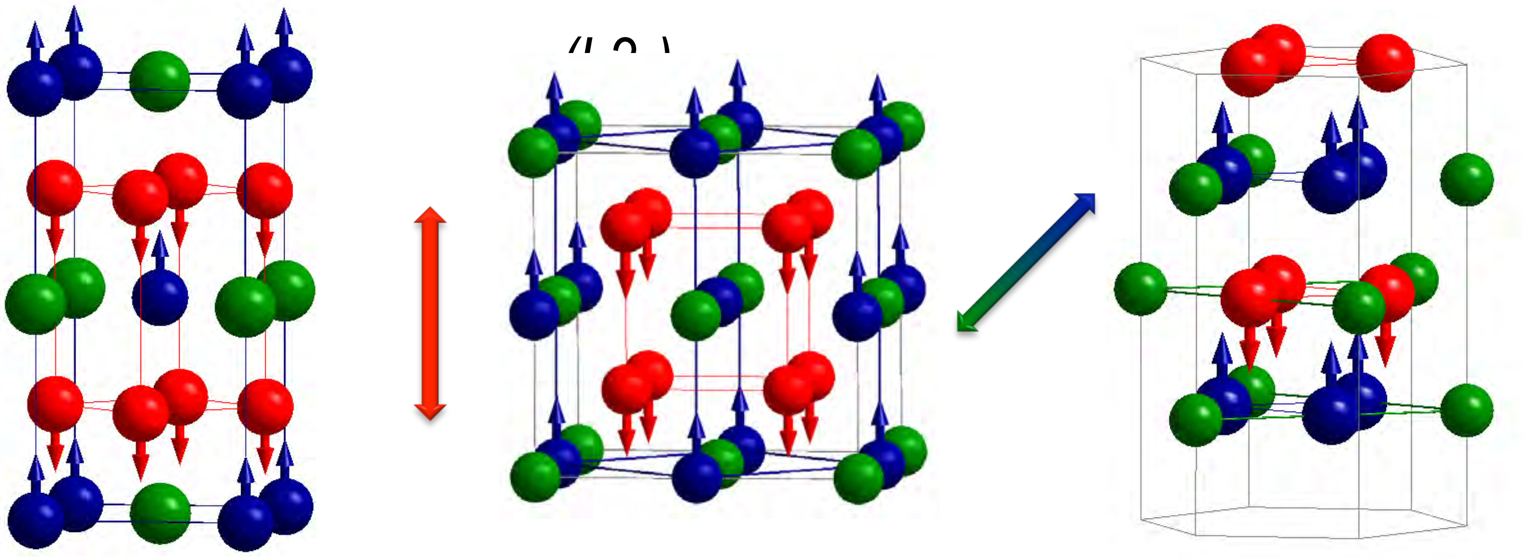


Balke *et al*. CF, APL **92**, 152504 (2007)

F. Wu *et al*., APL **94**, 122503 (2009)

Structural distortion

I4/mmm ($D0_{22}$) $Fm3\ m$ $P6_3/mmc$ ($D0_{19}$)



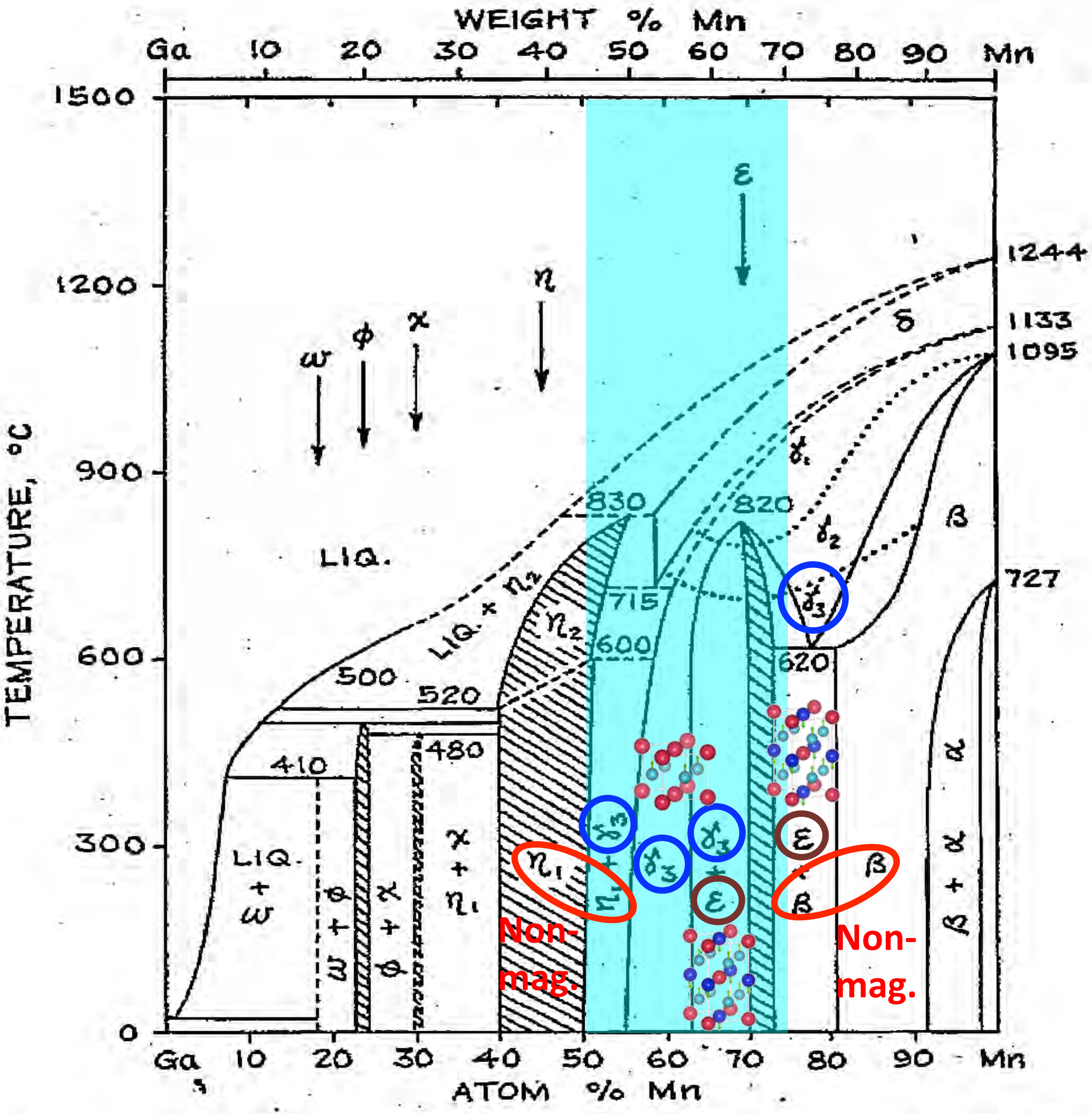
tetragonal ⟷ cubic ⟷ hexagonal

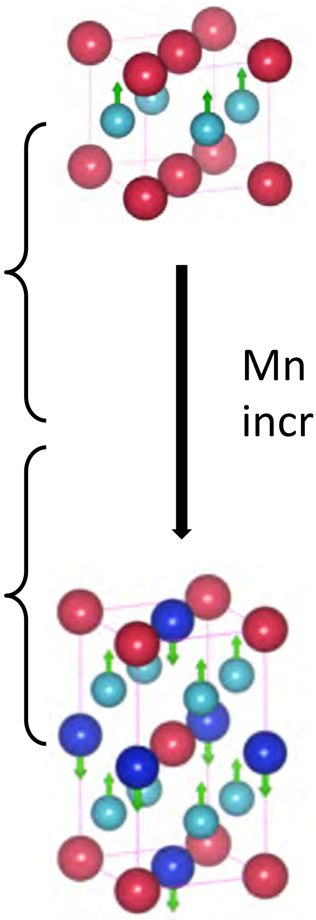
STT-RAM with out of plane
Compensated ferrimagnets
Permament magnets
Non-collinear magnetism
Topological Hall effect
Skyrmions

Half metallic ferro/i
Spin gapless
mag. semiconductors
compensated ferrim.
QAH

mag. shape memory
Magnetocalorics – CDW?

Out of plane magnets
Antiferromagnets: Mn_3Ge
Ferromagnets: Fe_3Sn
Anomalous Hall effect
Spin reorientation transition?





$L1_0$

γ_3 phase

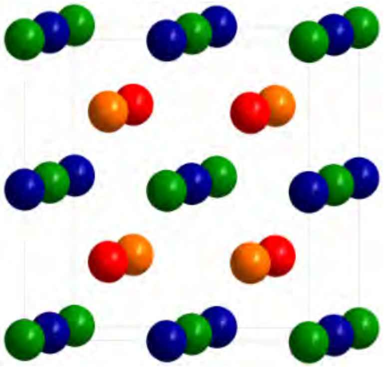
Mn increase

ε phase

$D0_{22}$

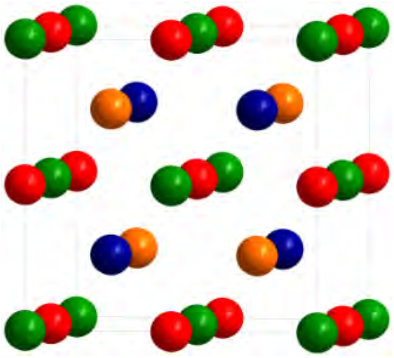
the Handbook of Binary Phase Diagrams (W.G.Moffatt ed.)

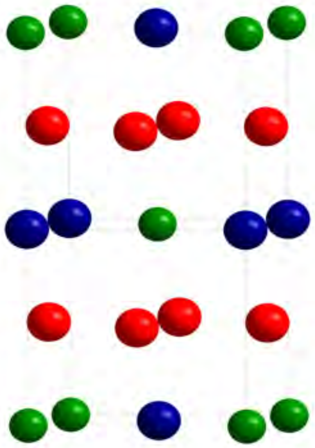
The tetragonal structure

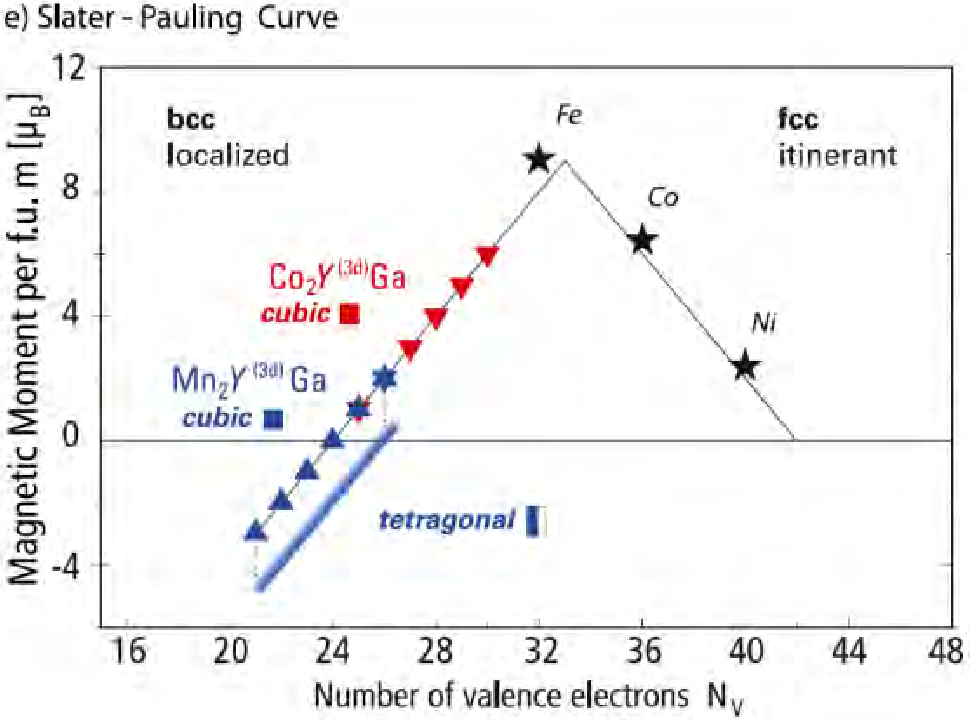


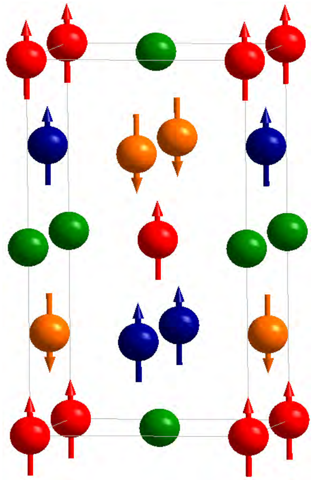
regular
Heusler
structure

inverse
Heusler
structure

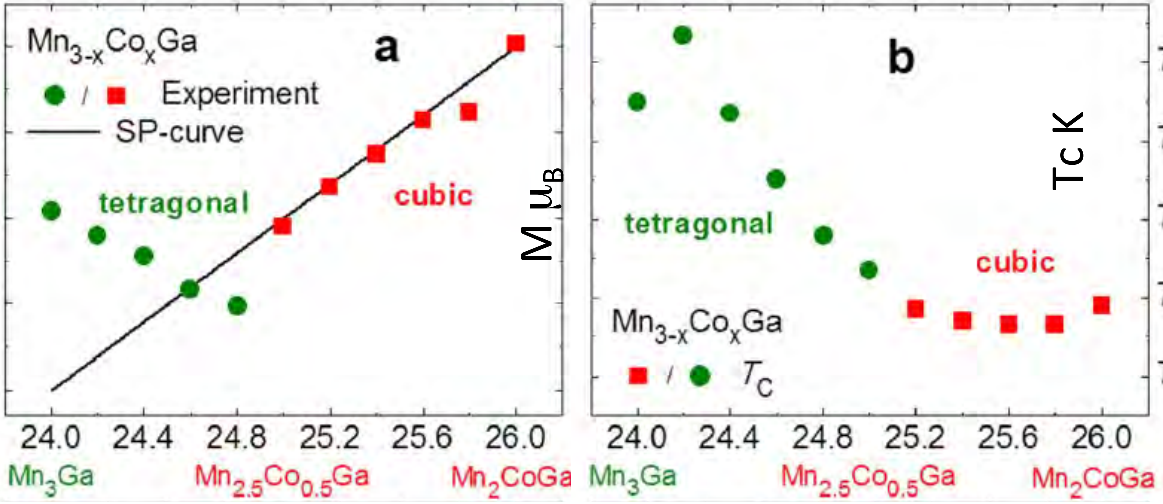


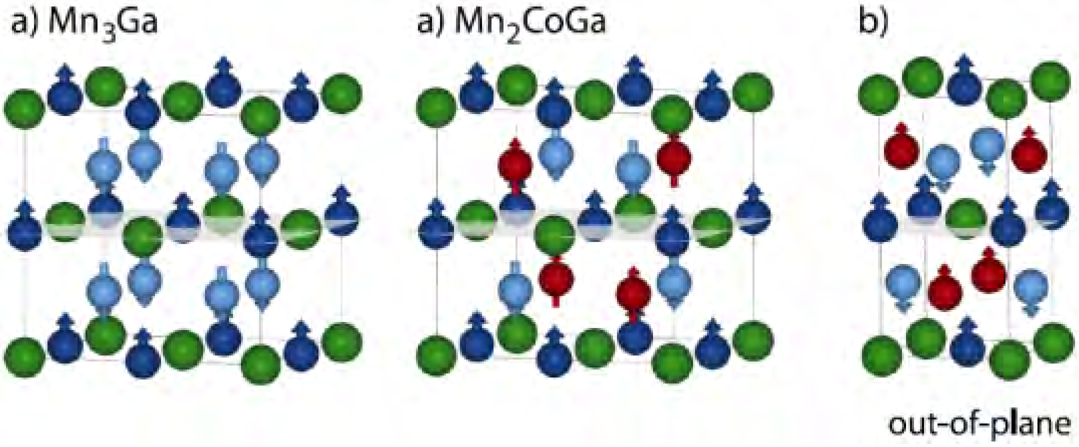


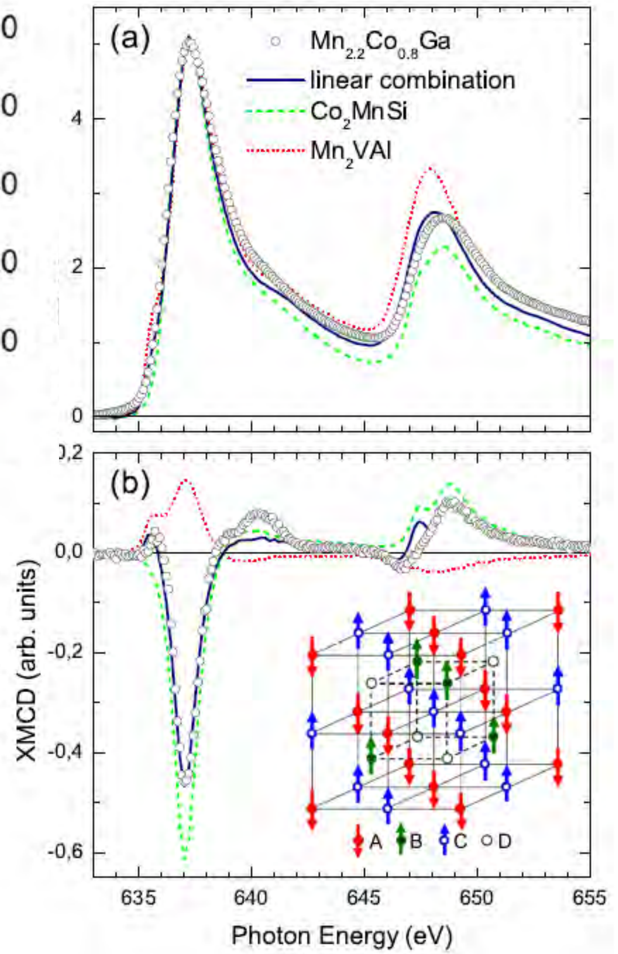




Mn_2CoGa – Mn_3Ga







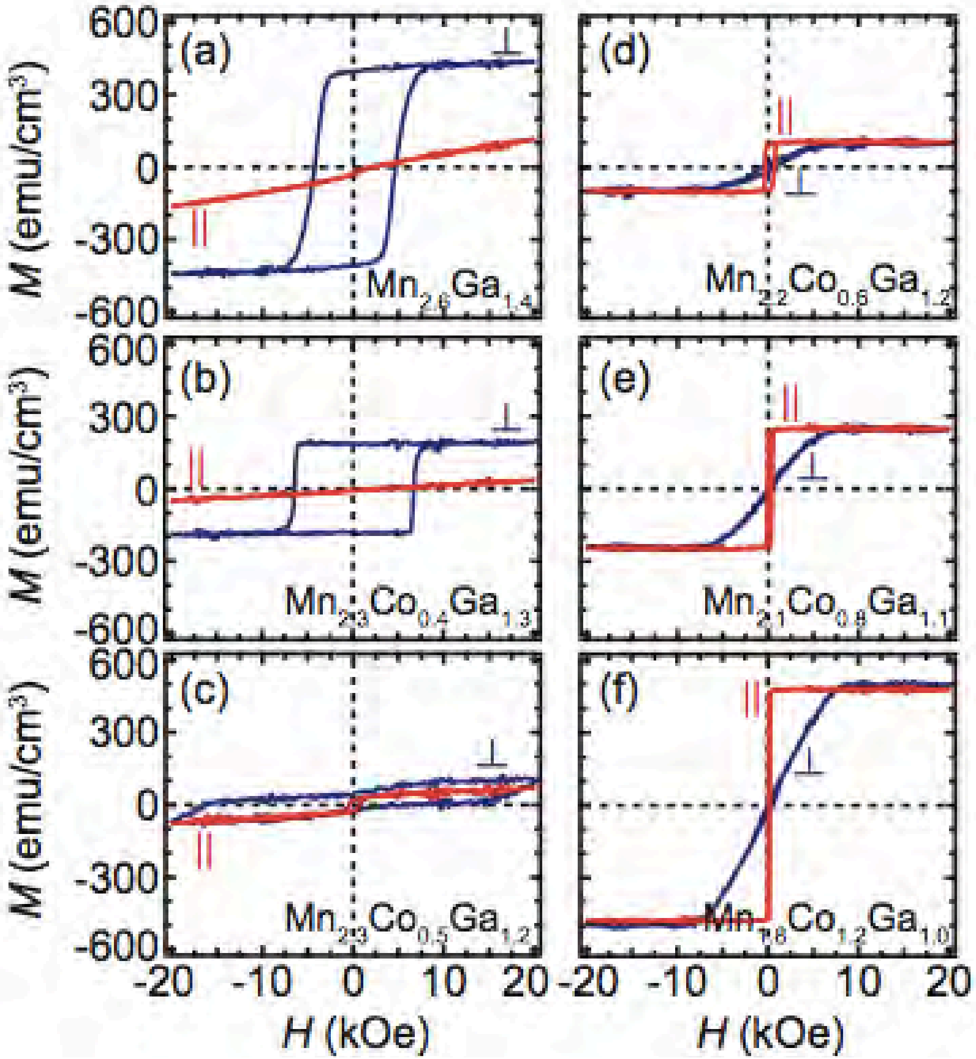
Winterlik, J et al, Advanced Materials 24 (2012) 6283

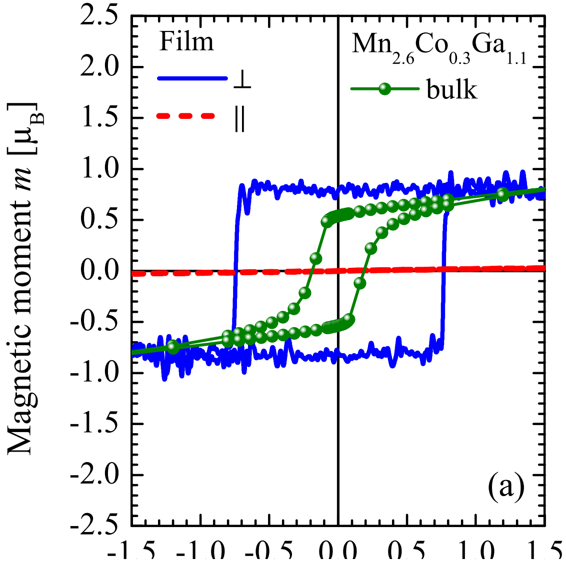
Klaer et al. Appl. Phys. Lett. 98 (2011) 212510.

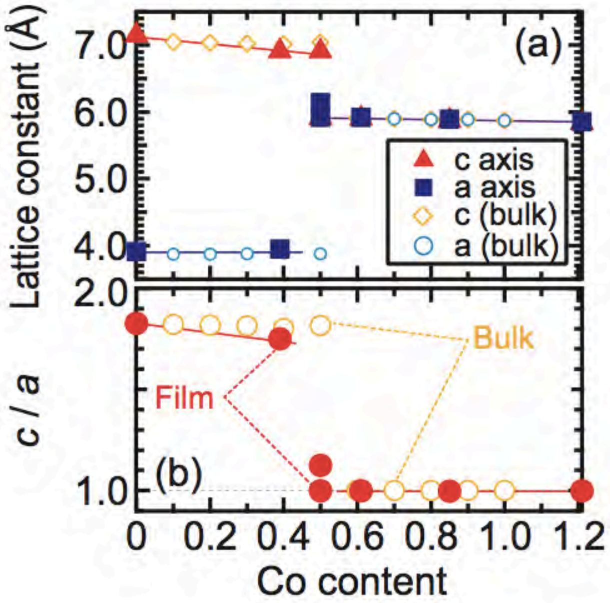
Graf T, Felser C, Parkin SSP, IEEE TRANSACTIONS ON MAGNETICS 47 (2011) 367

Graf T, Felser C, Parkin SSP, Progress in Solid State Chemistry (2011), doi:10.1016/j.progsolidstchem.2011.02.001

Compensated ferrimagnet





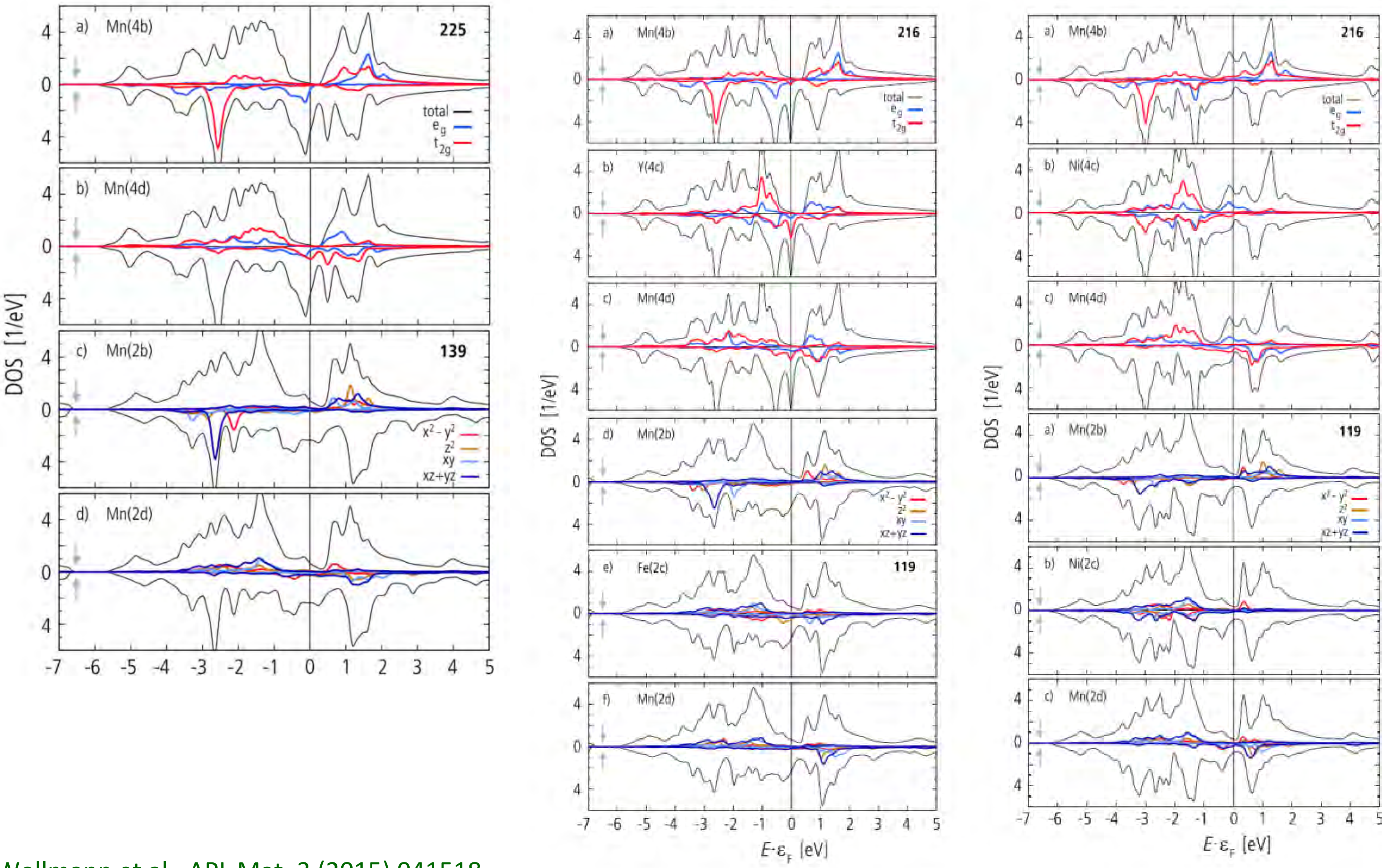


prepared in Mizukami lab

S. Ouardi, et. al , APL 101 (2012) 242406 arXiv:1211.2440

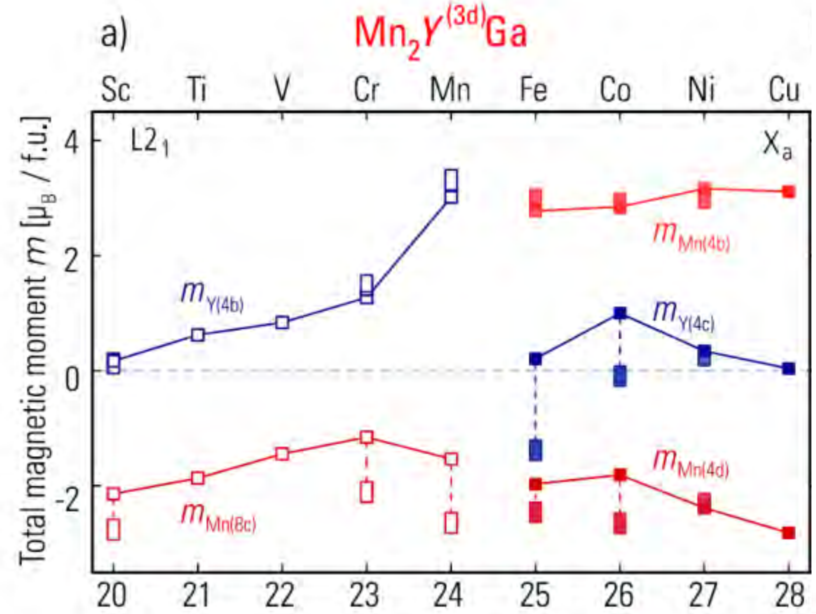
T. Kubota, S. Ouardi, arXiv:1211.2524

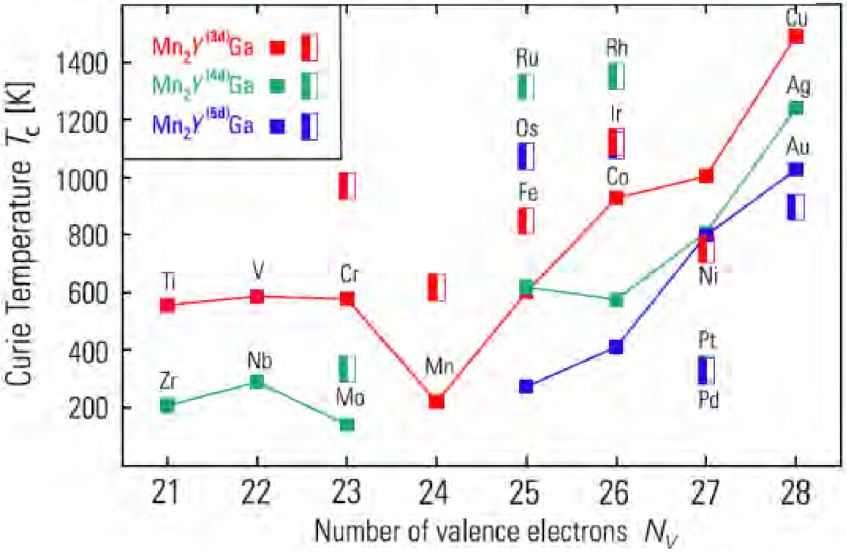
Tetragonal Heusler

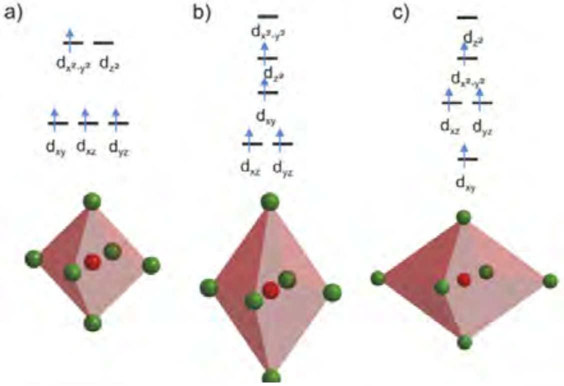


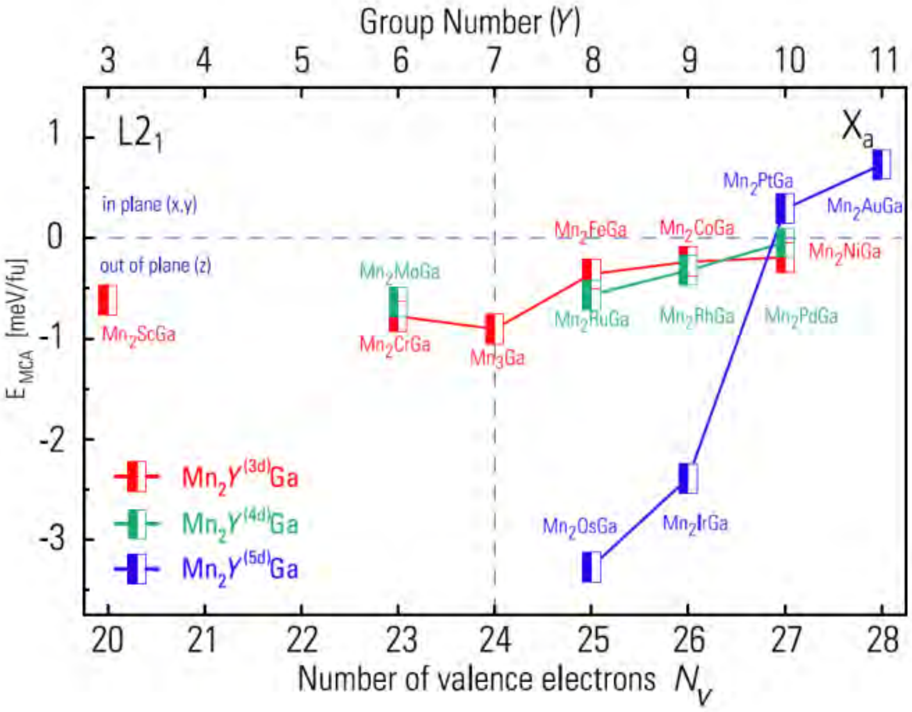
Wollmann et al., APL Mat. 3 (2015) 041518

Magnetocrystalline Anisotropy



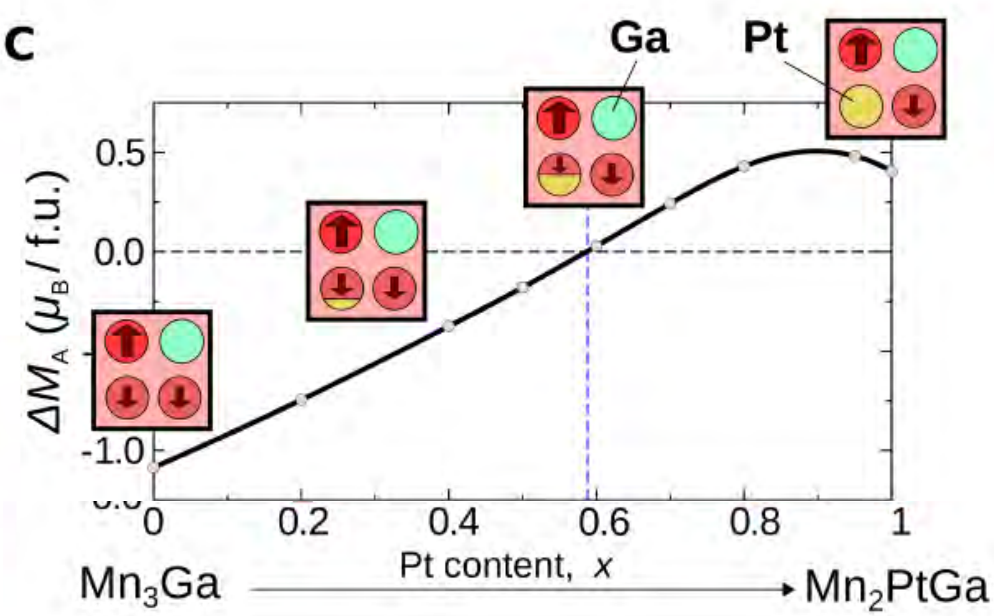


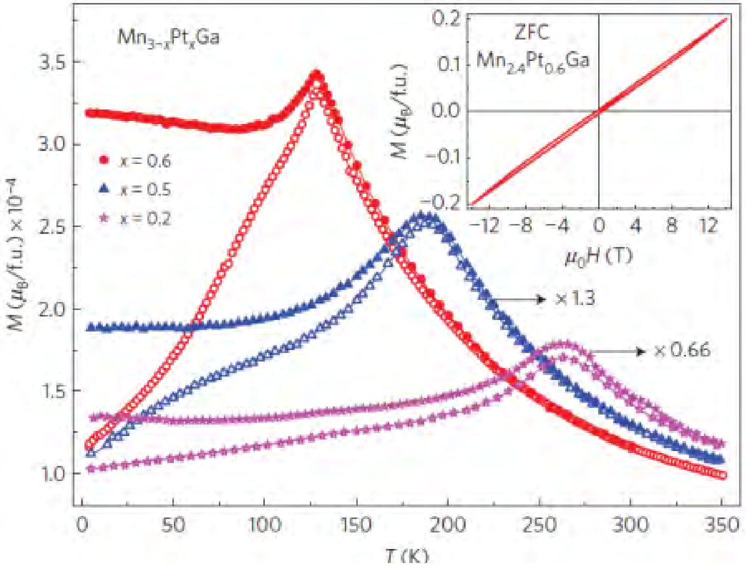


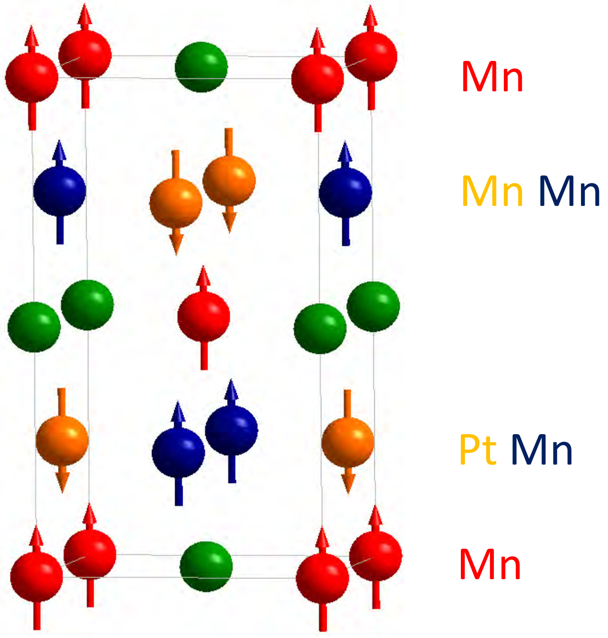


Wollmann et al. to be published

Artificial AFM or compensated ferrimagnet

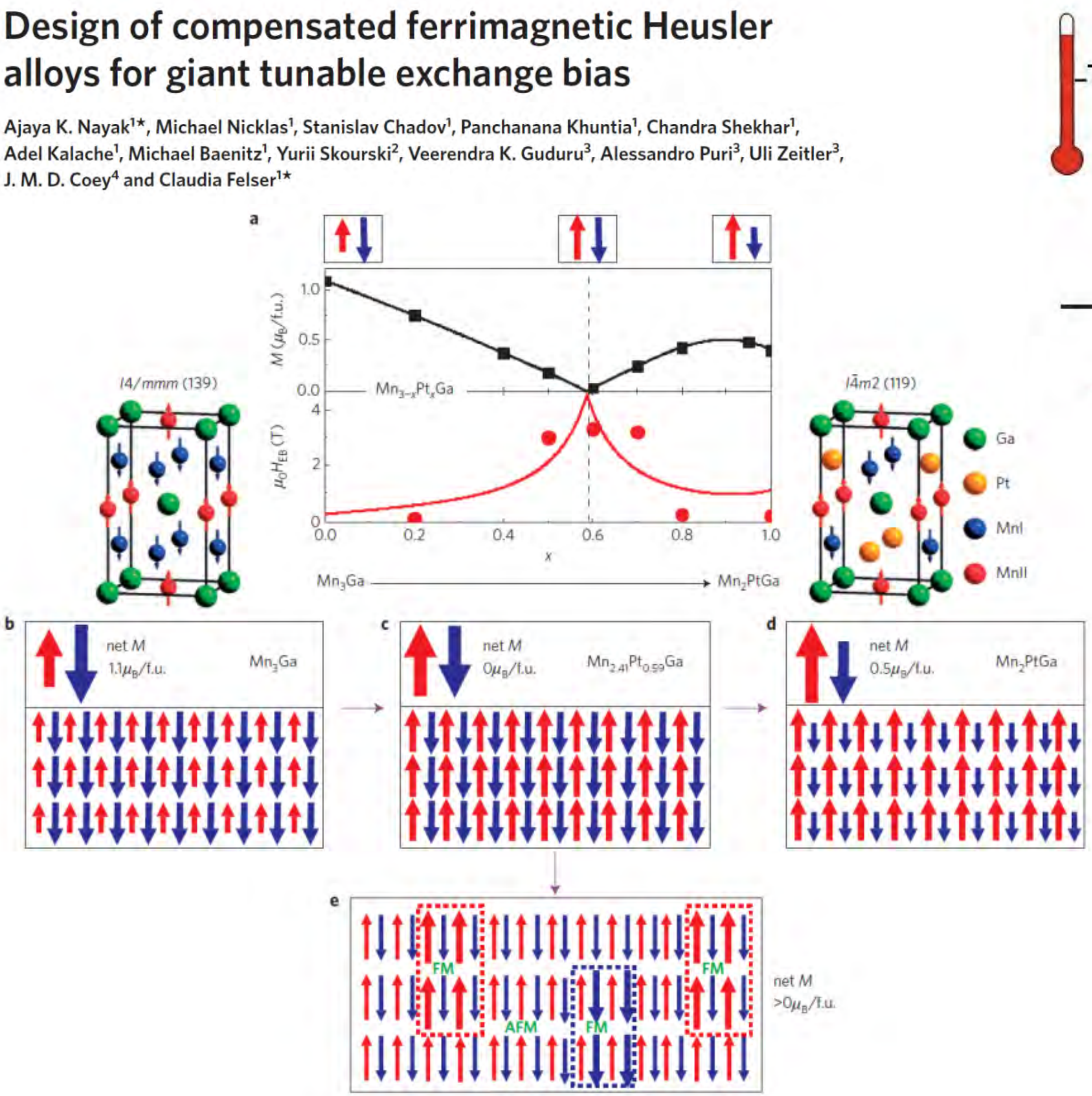






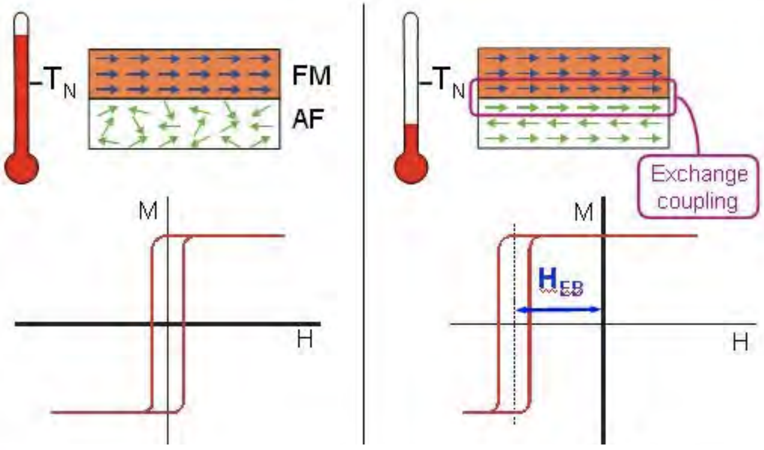
Ajaya K. Nayak, et al PRL 110 (2013) 127204

Ajaya K. Nayak, et Nature Materials (2015) doi:10.1038/nmat4248



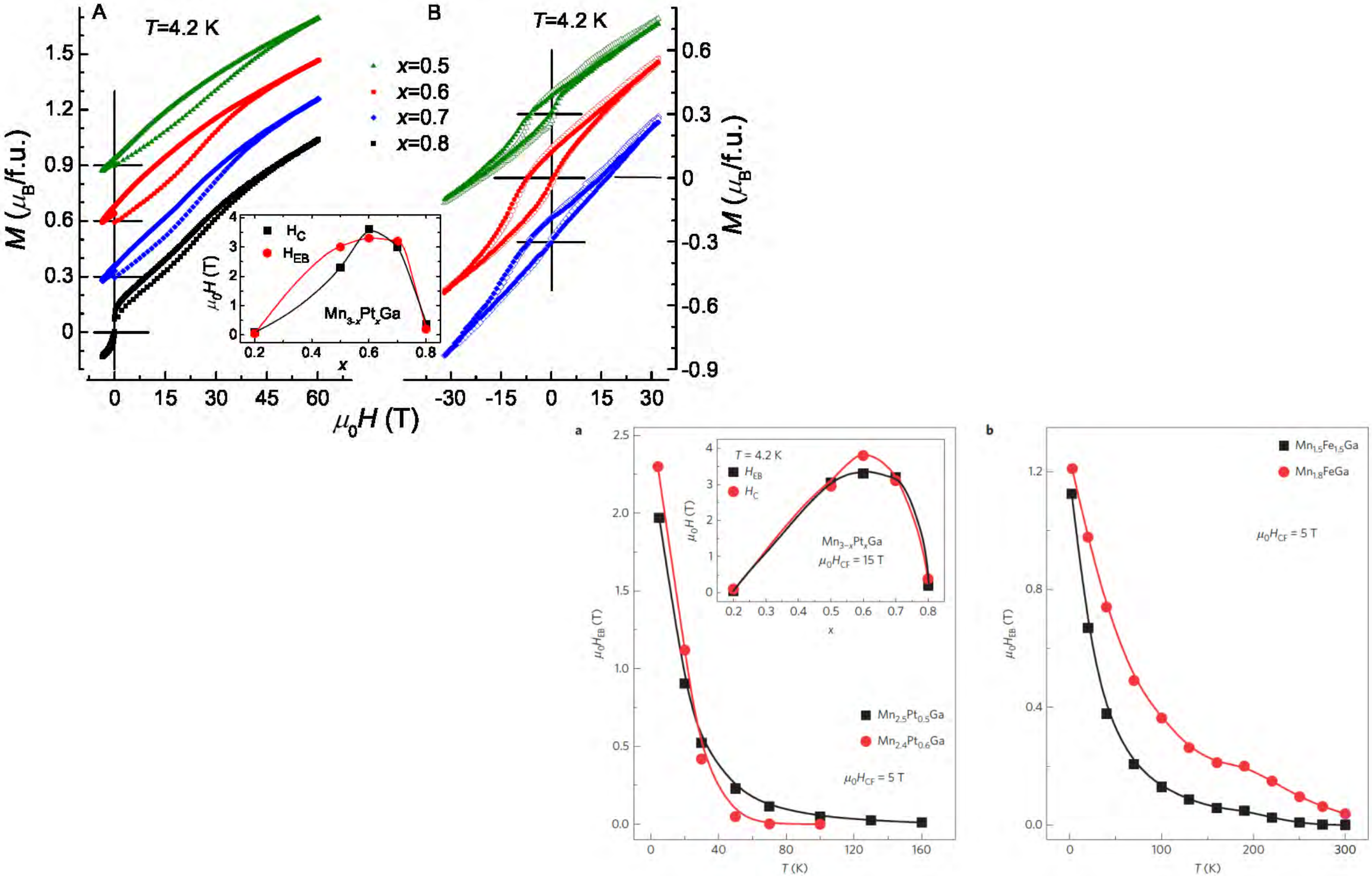
Design of compensated ferrimagnetic Heusler alloys for giant tunable exchange bias

Ajaya K. Nayak[1]*, Michael Nicklas[1], Stanislav Chadov[1], Panchanana Khuntia[1], Chandra Shekhar[1], Adel Kalache[1], Michael Baenitz[1], Yurii Skourski[2], Veerendra K. Guduru[3], Alessandro Puri[3], Uli Zeitler[3], J. M. D. Coey[4] and Claudia Felser[1]*



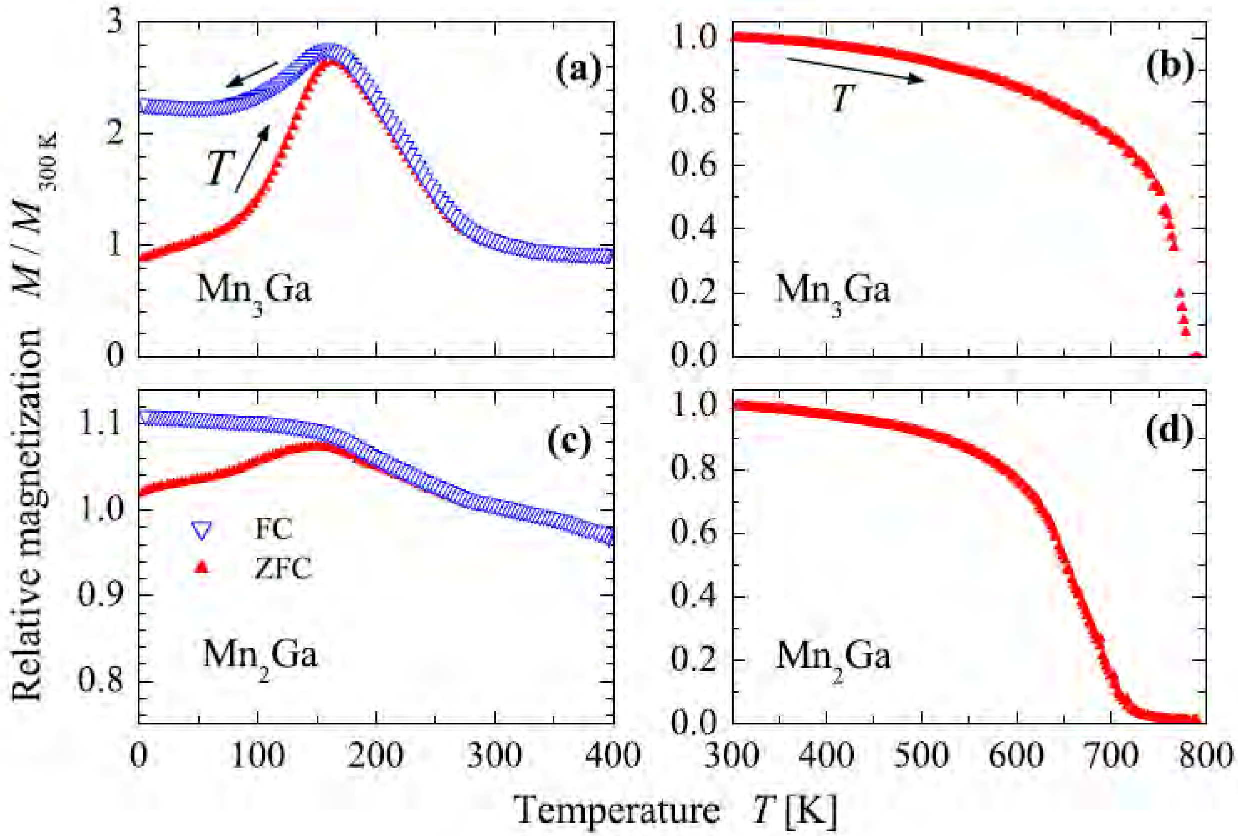
Ajaya K. Nayak, et. al, Nature Materials (2015) doi:10.1038/nmat4248

Artificial AFM or compensated ferrimagnet



Ajaya K. Nayak, et. al, Nature Materials (2015) doi:10.1038/nmat4248

$Mn_{3-x}Ga$: Tunability

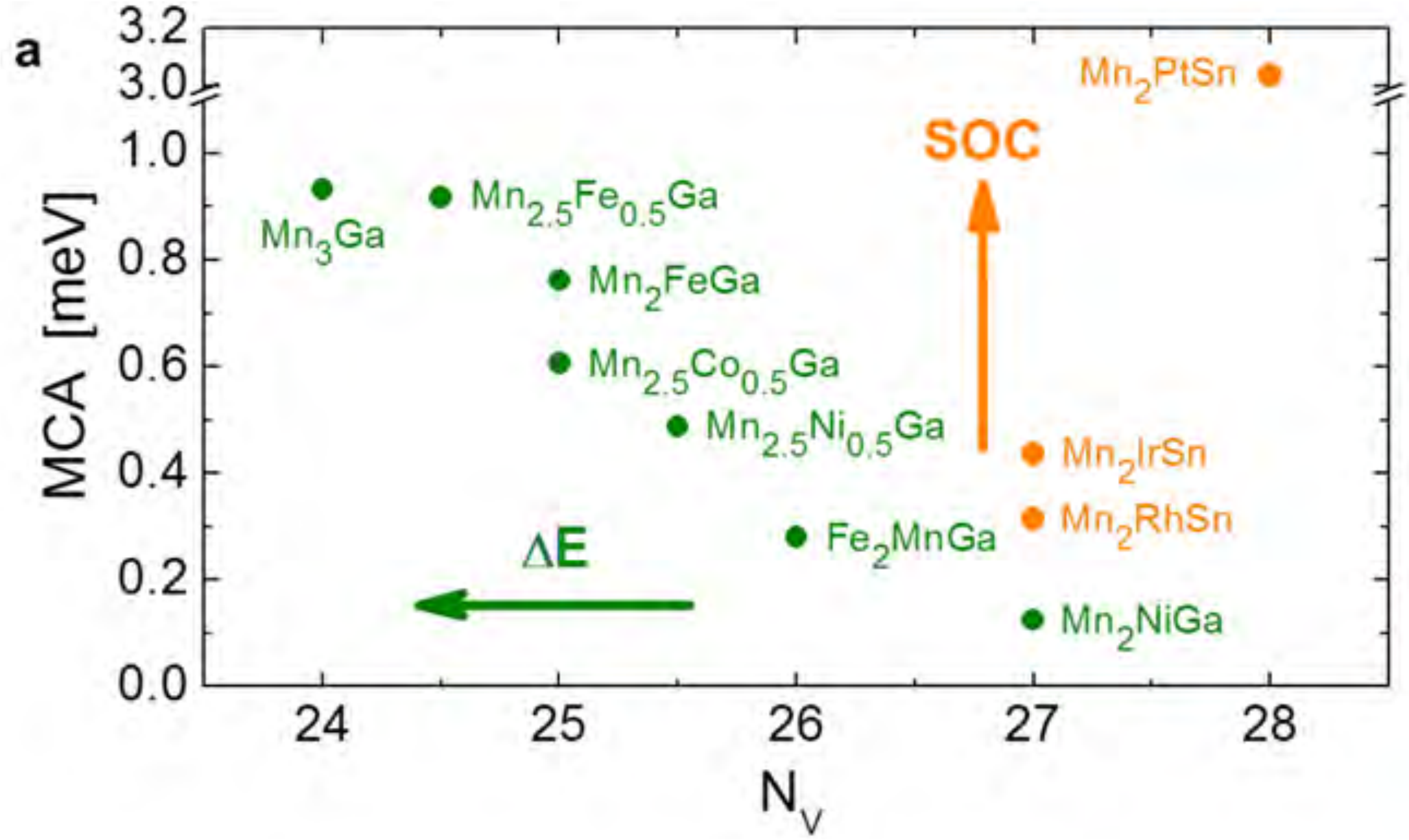


More complex magnetism at low T

Removing one sort of Mn (octahedral) leads to ferromagnetism

Winterlik *et al.* Phys. Rev. B **77** (2008) 054406

Heuslers with SOC

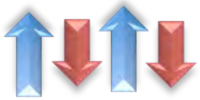


Winterlik et al. Advanced Materials 24 (2012) 6283

Magnetic orderings in Heusler compounds

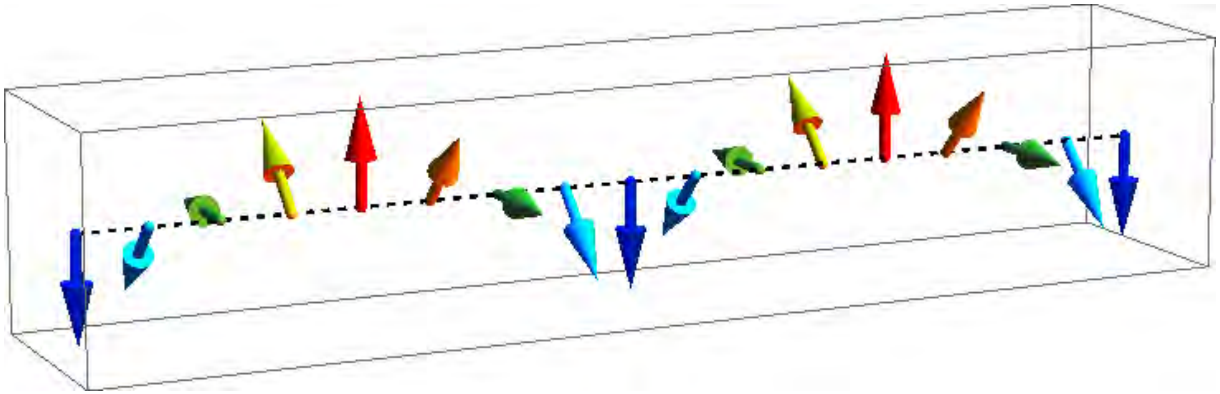
Half-metallic ferromagnetism: **Co_2MnZ…**

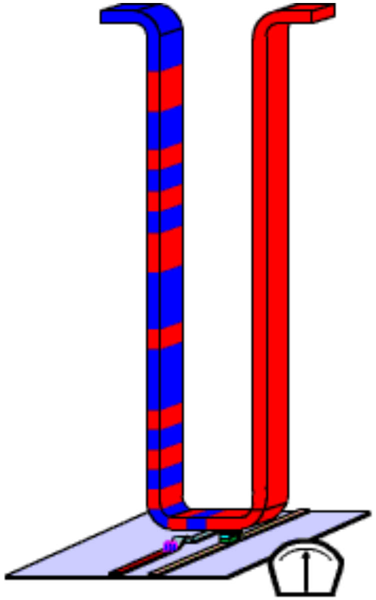
Half-metallic ferrimagnetic: **Mn_2YZ**



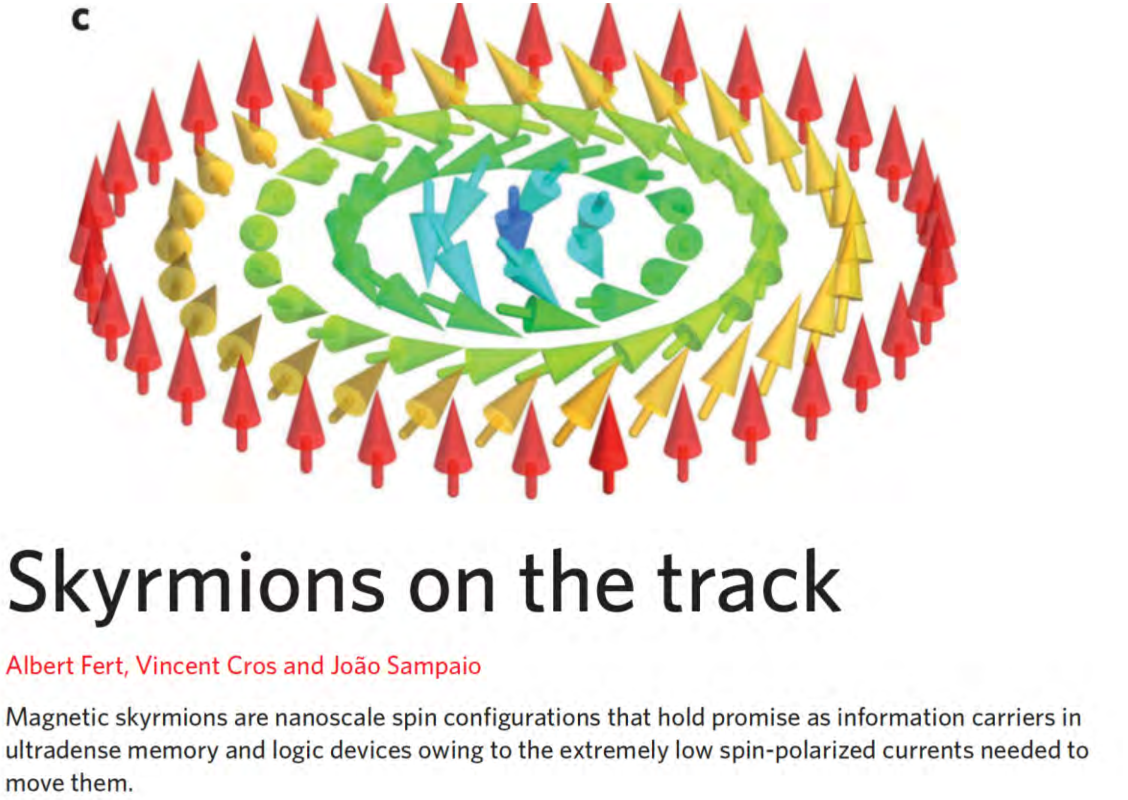
Antiferromagnetic: **Mn_3Si, Fe_2VSi, Ru_2MnGe,**

Compensated ferrimagnetic: **Mn-Pt-Ga, Mn-Co-Ga**





Stuart S. P. Parkin, et al.: *Magnetic Domain-Wall Racetrack Memory*, *Science* 320 (2008) 190–194



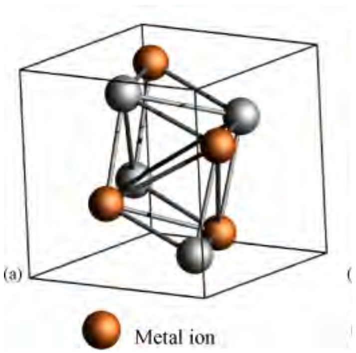
Skyrmions on the track

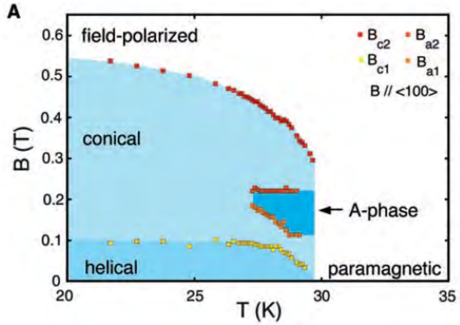
Albert Fert, Vincent Cros and João Sampaio

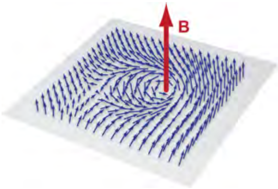
Magnetic skyrmions are nanoscale spin configurations that hold promise as information carriers in ultradense memory and logic devices owing to the extremely low spin-polarized currents needed to move them.

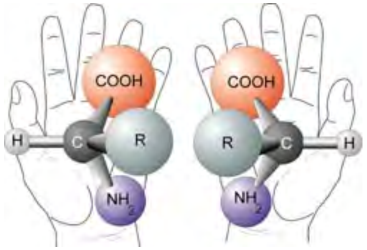
Recipe

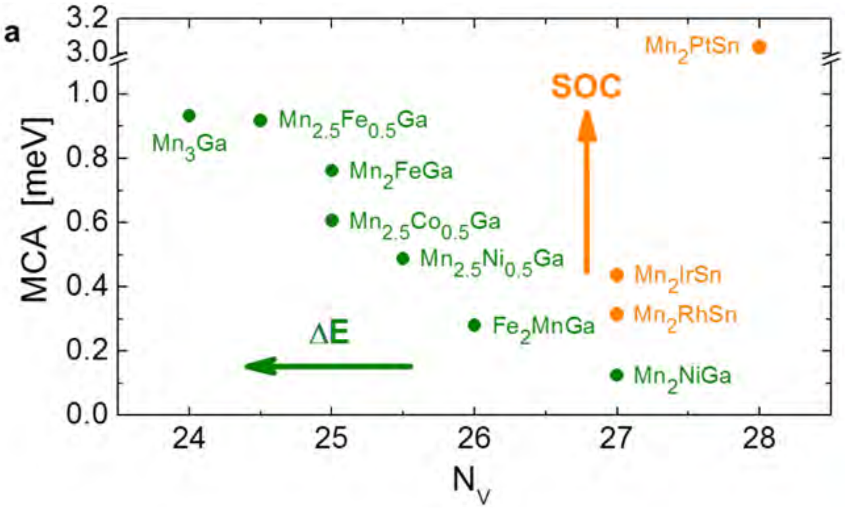
- Large spin orbit coupling
- Dzyaloshinsky–Moriya interaction
  - Non centro symmetric structure
  - Helical magnetism
- Topology: Berry phase in real space
- RT Skyrmions – high T_C
- Skyrmion in zero field via high magneto crystalline anisotropy
- For data storage: bulk materials





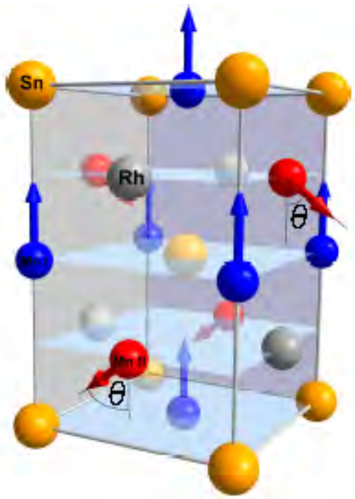


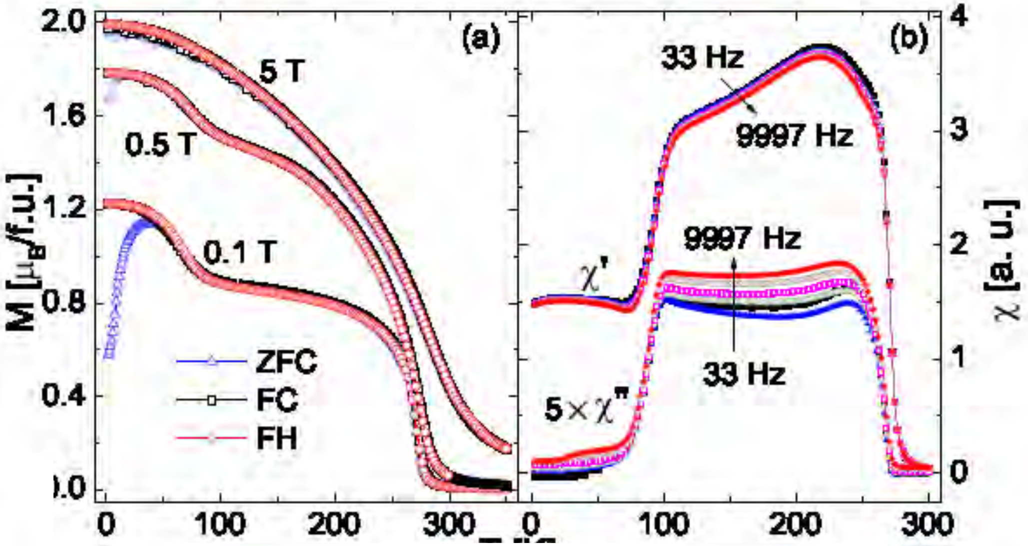


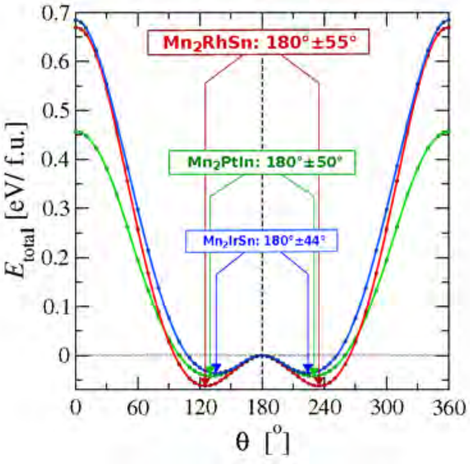


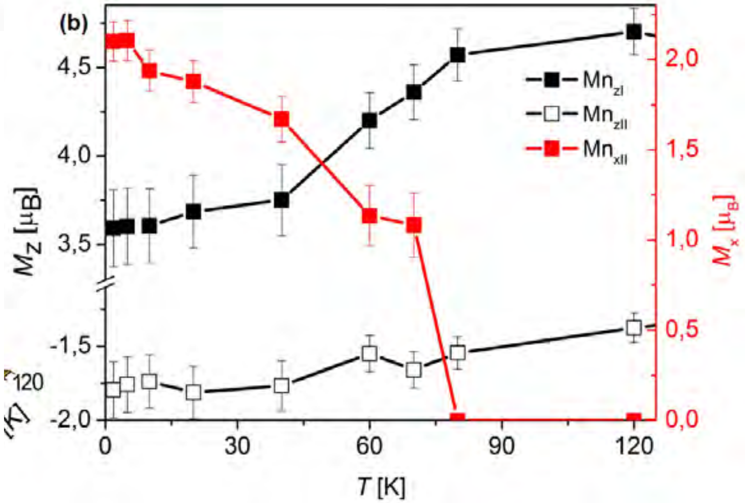
Skyrmions, C. Felser, Angewandte Chemie 125 (2013) 1673, Int. Ed. 52 (2013) 1631

Mn_2RhSn – non collinear magnet



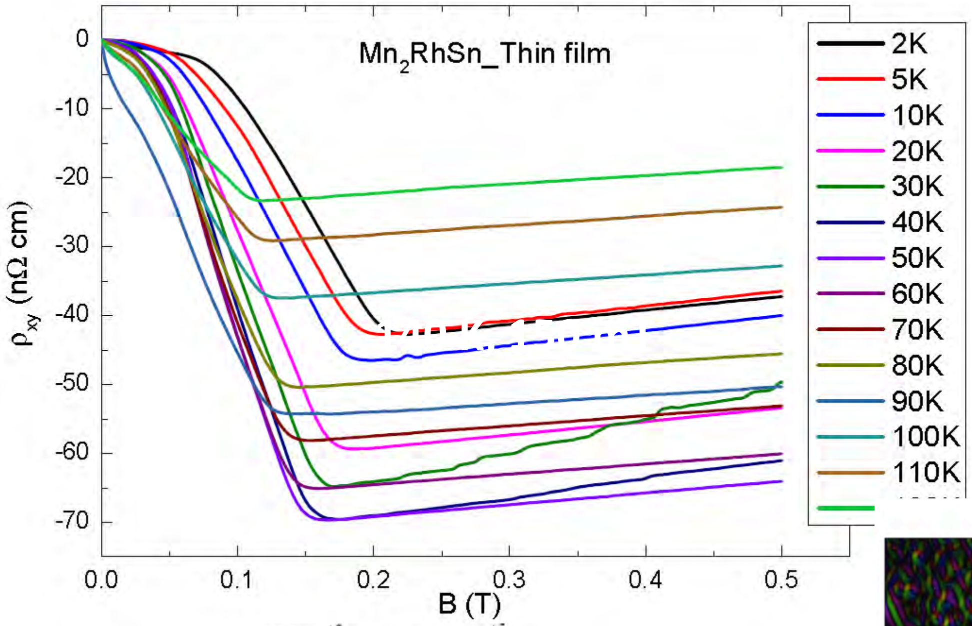


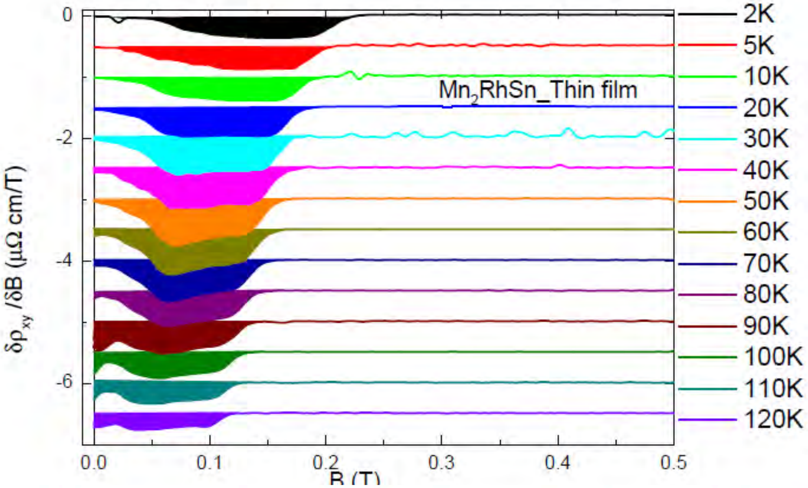


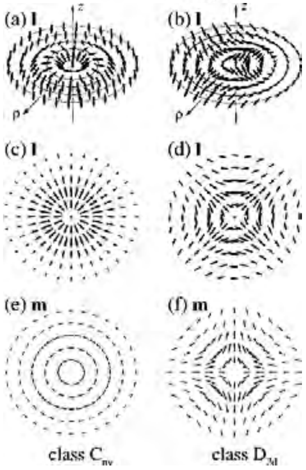


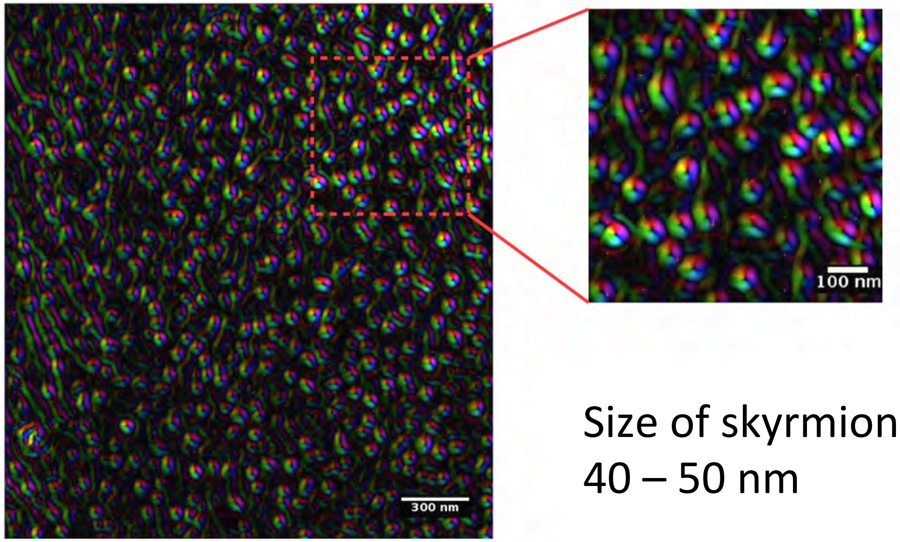
O. Meshcheriakova et al. Phys.Rev.Lett. 113 (2014) 087203, preprint arxiv:1404.4581

Skyrmions







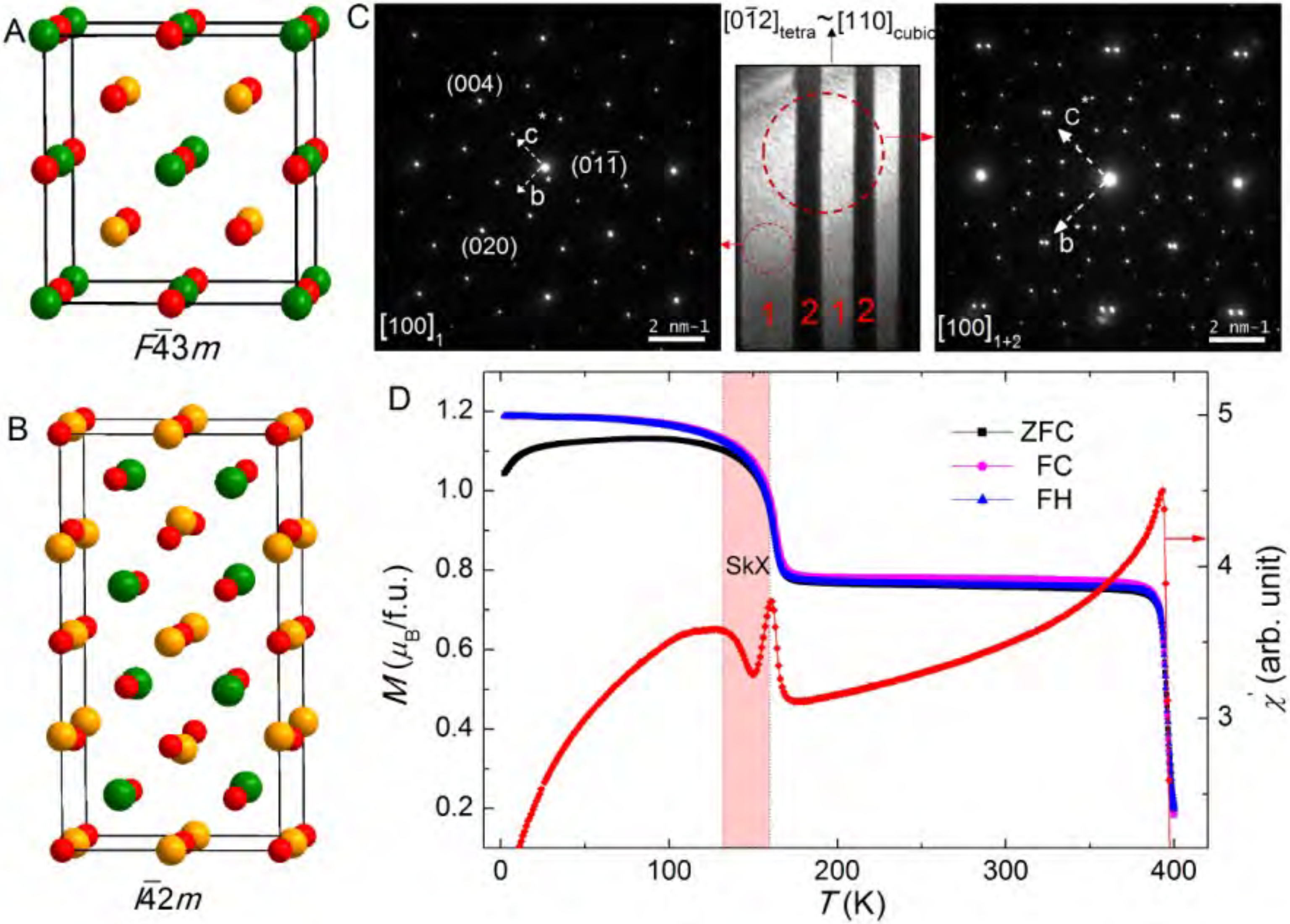


Size of skyrmion ~ 40 – 50 nm

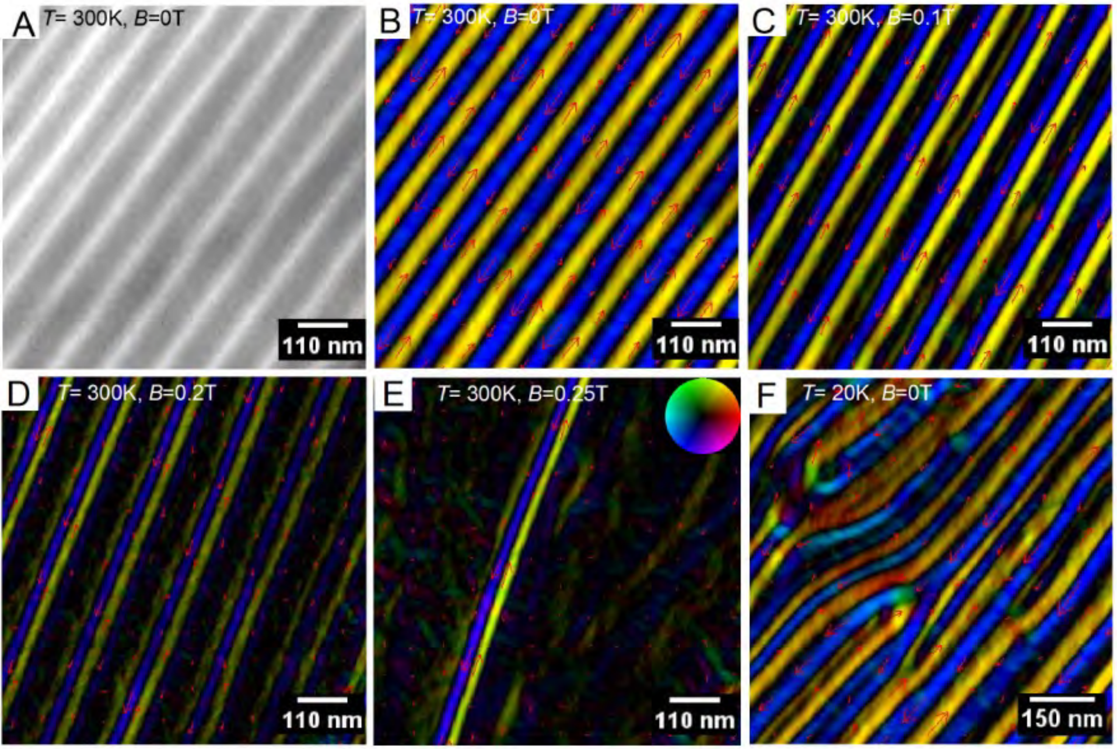
Bogdanov et al PRB **66**, 214410 (2002)

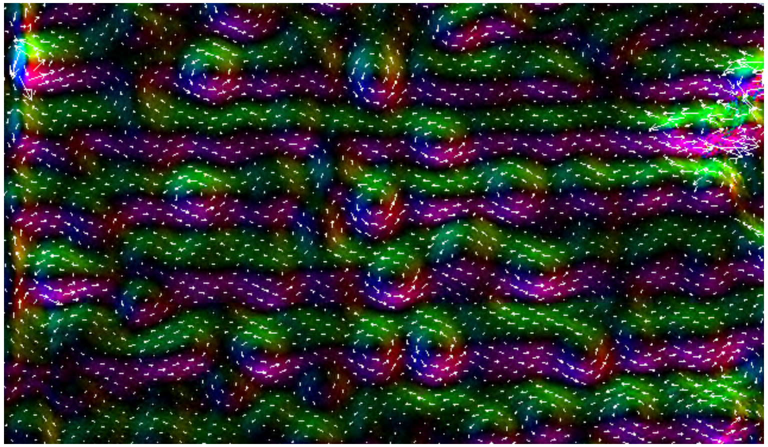
Ajaya K. Nayak and O. Meshcheriakova et al. unpublished (2015)

Mn-Pt-Sn – Skyrmions

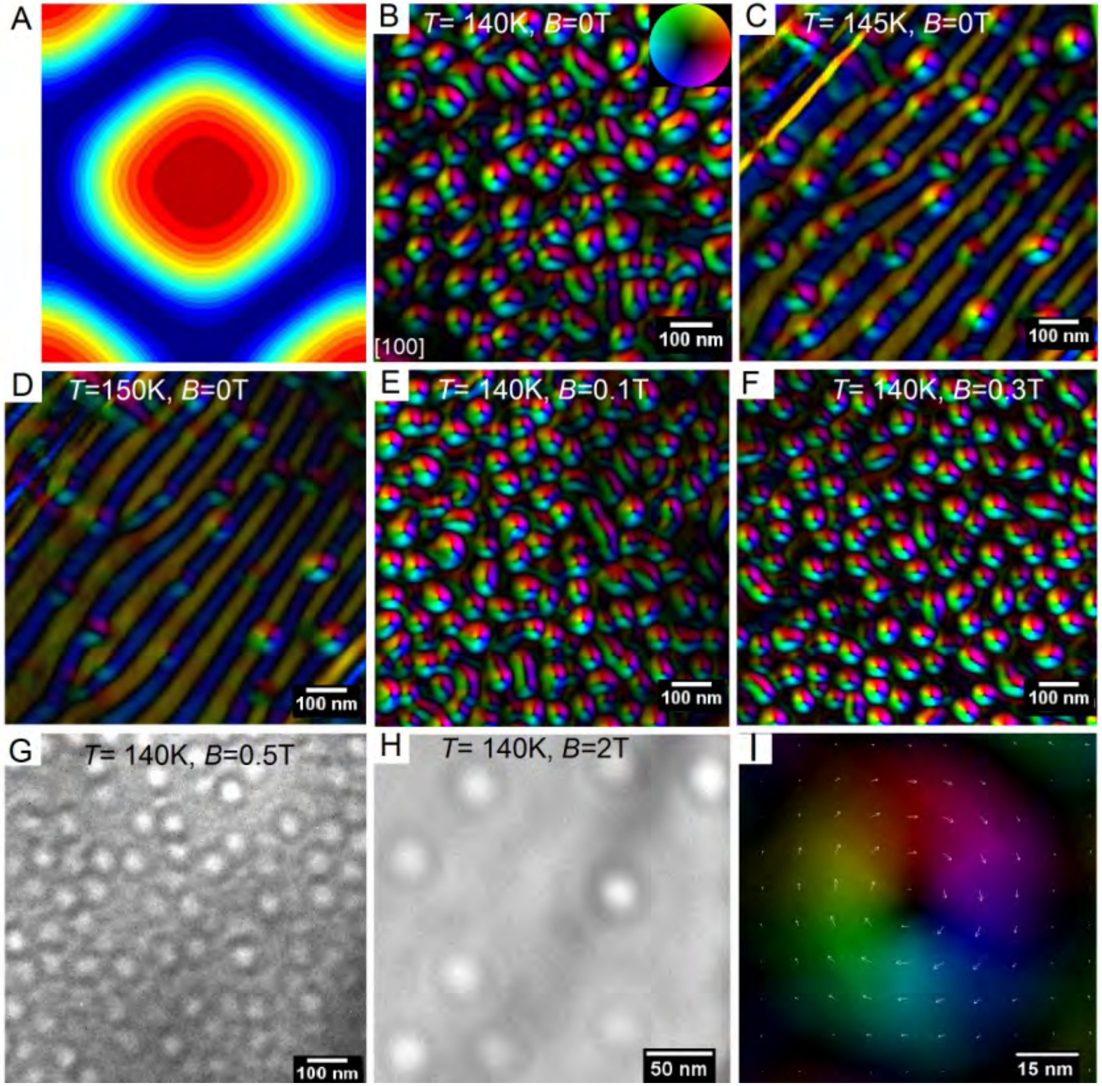


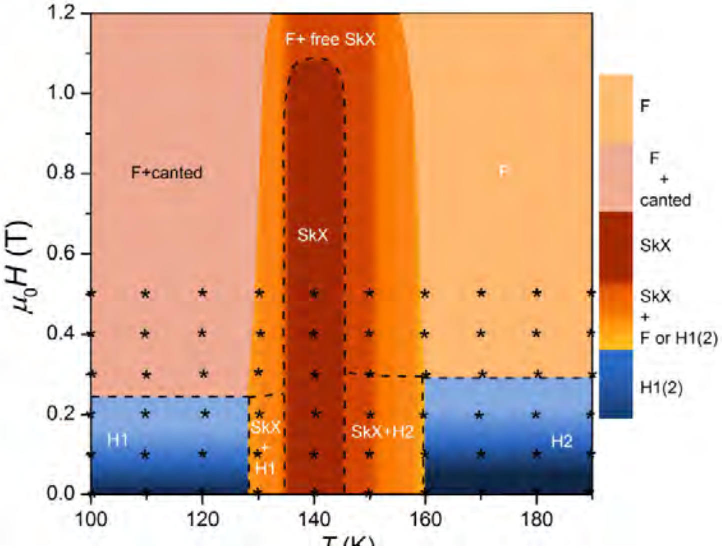
Ajaya K. Nayak et al. under review (2015)





- The infocus Lorentz TEM image shows the structural microstructure (martensitic like plates).
- The stripes in the out of focus images correspond to the helical magnetic structure.
- They disappear completely for fields > 0.3 T.
- The helix propagates along [110].


A
B
T= 140K, B=0T
[100]
100 nm
C
T= 145K, B=0T
100 nm
D
T=150K, B=0T
100 nm
E
T= 140K, B=0.1T
100 nm
F
T= 140K, B=0.3T
100 nm
G
T= 140K, B=0.5T
100 nm
H
T= 140K, B=2T
50 nm
I
15 nm


1.2
1.0
0.8
0.6
0.4
0.2
0.0
$\mu_0 H$ (T)
100
120
140
160
180
T (K)
F+canted
F+ free SkX
SkX
F
H1
SkX + H1
SkX+H2
H2
F
F + canted
SkX
SkX + F or H1(2)
H1(2)

spin injection
spin transfer torque

spin Seebeck effect

half-metallic &
compensated ferrimagnets

semiconductors

quantum spin & Hall effect
topological insultor

heavy fermions

GMR & TMR
spin & magneto-calorics

perpendicular
magnetic anisotropy

Kondo systems

thermoelectrics

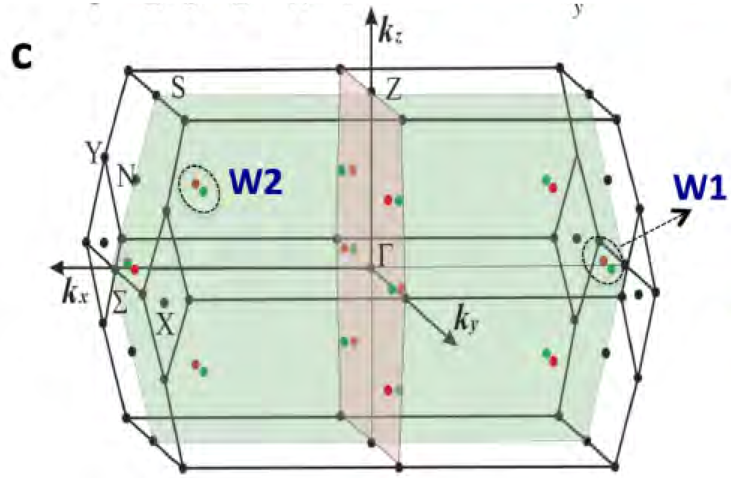
superconductors

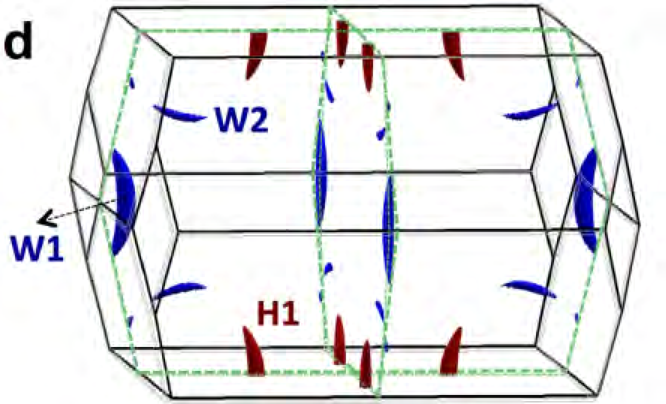
shape memory

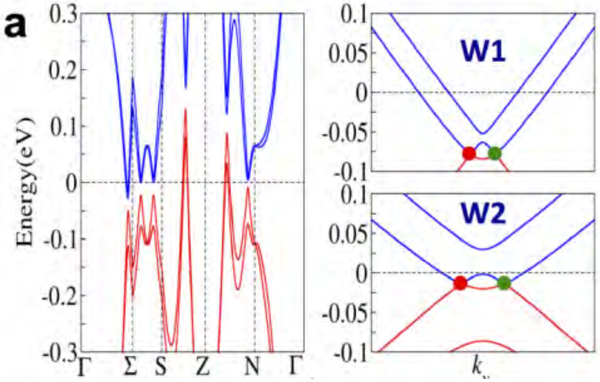
Heusler Compounds

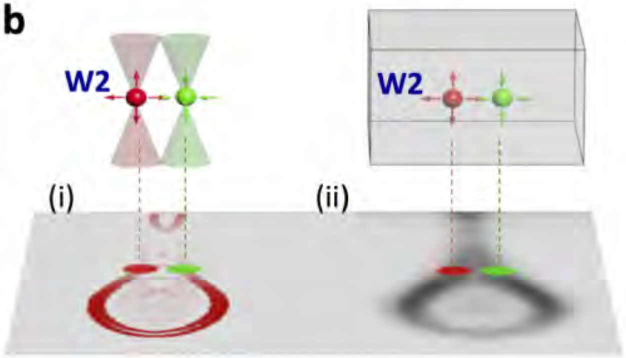
Graf, Felser, Parkin, IEEE TRANSACTIONS ON MAGNETICS 47 (2011) 367
Graf, Felser, Parkin, Progress in Solid State Chemistry 39 (2011) 1

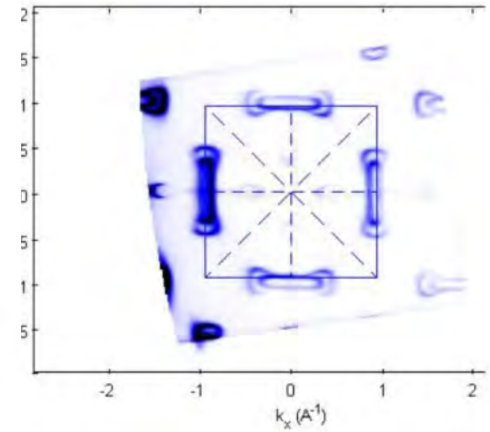
NbP combined Weyl semimetal







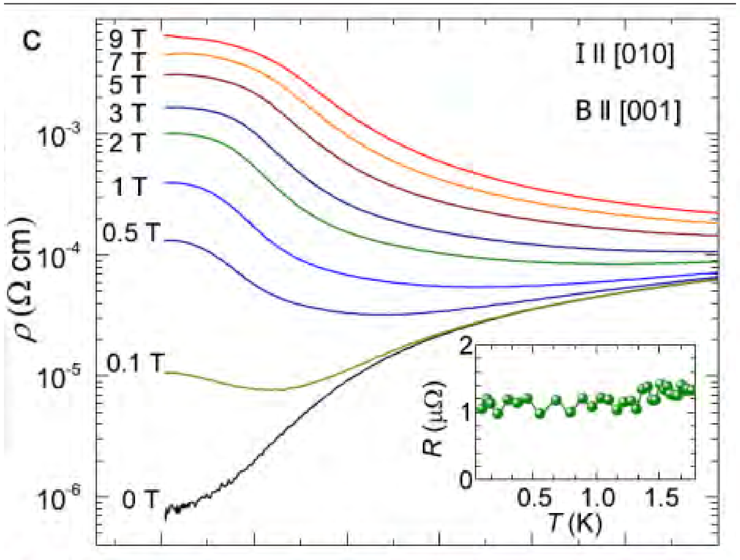


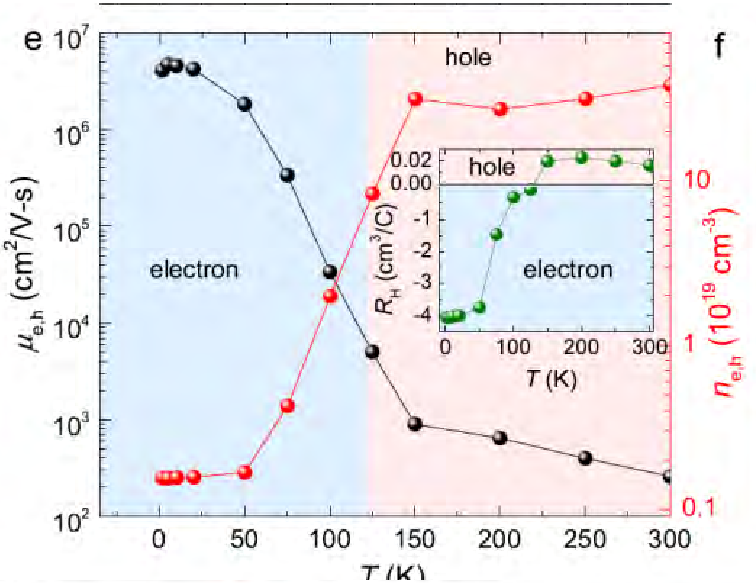


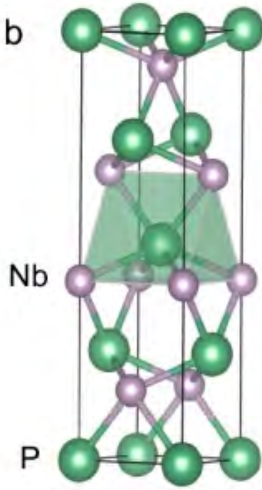
Chandra Shekhar, et al. Nature Physics accepted preprint arXiv:1502.04361

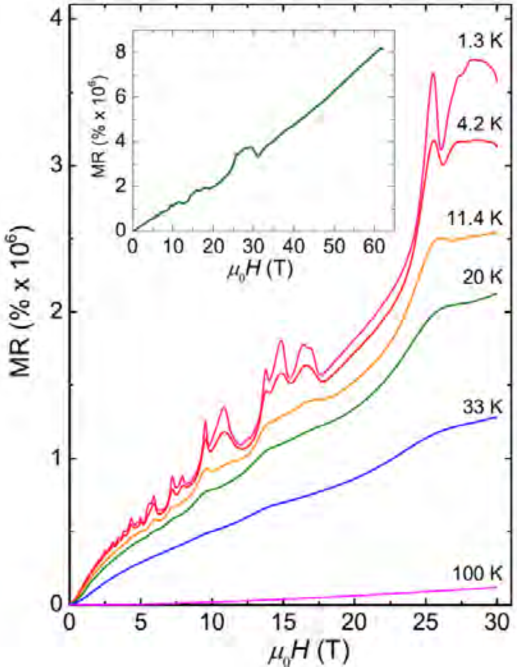
Yulin Chen et al. to be published

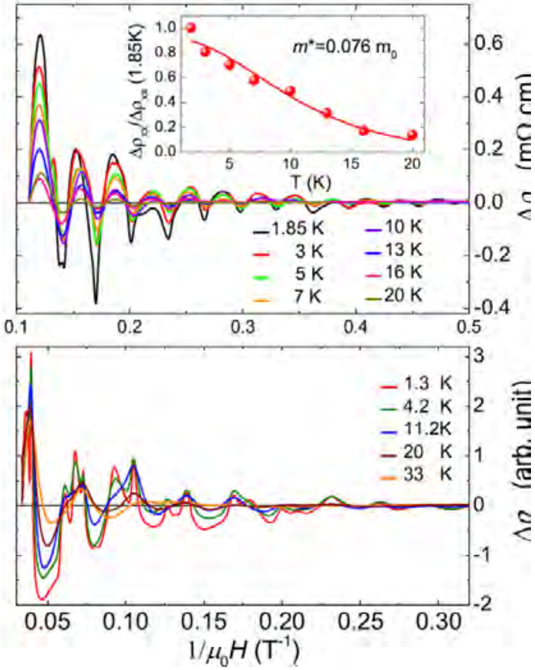
NbP combined Weyl semimetal



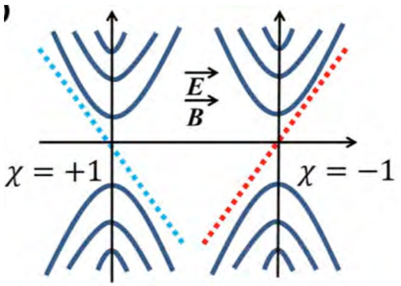








TaP proves the chiral anomaly

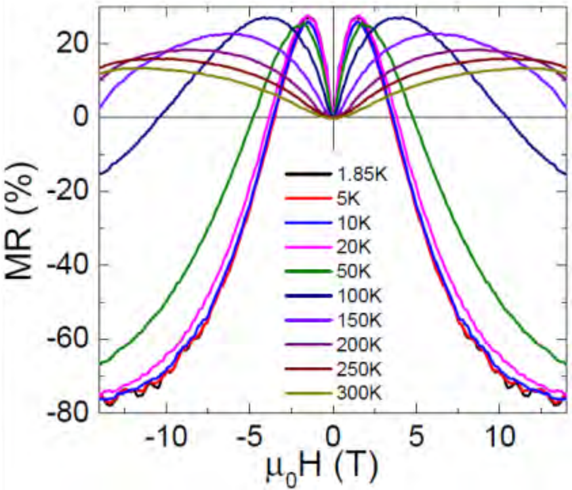


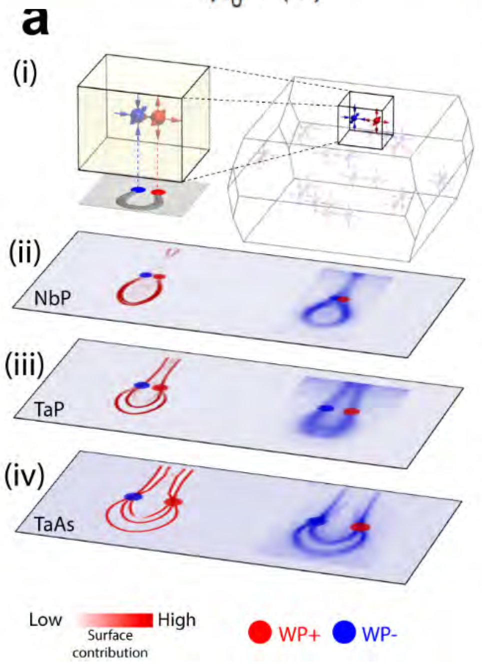
Topological effect

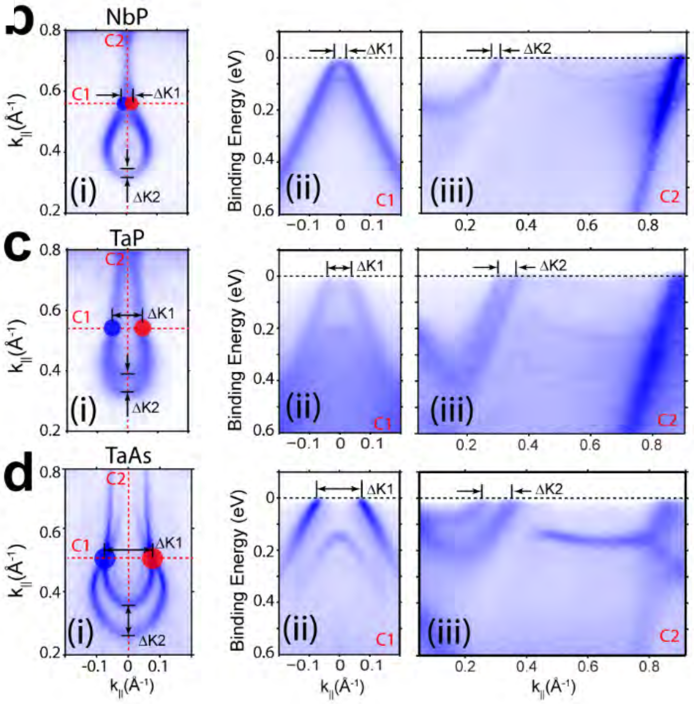
$$\partial_\mu j^\mu_\chi = -\chi \frac{e^3}{4\pi^2\hbar^2} \boldsymbol{E}\cdot\boldsymbol{B}$$

$$\sigma_a = \frac{e^3 v_f^3}{4\pi^2 \hbar \mu^2 c} B^2,$$

Experimental evidence:
Field enhanced conductivity or negative magnetoresistance







Chandra Shekhar, et al. to be published; Yulin Chen et al to be published