



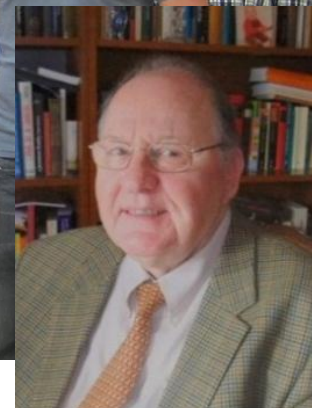
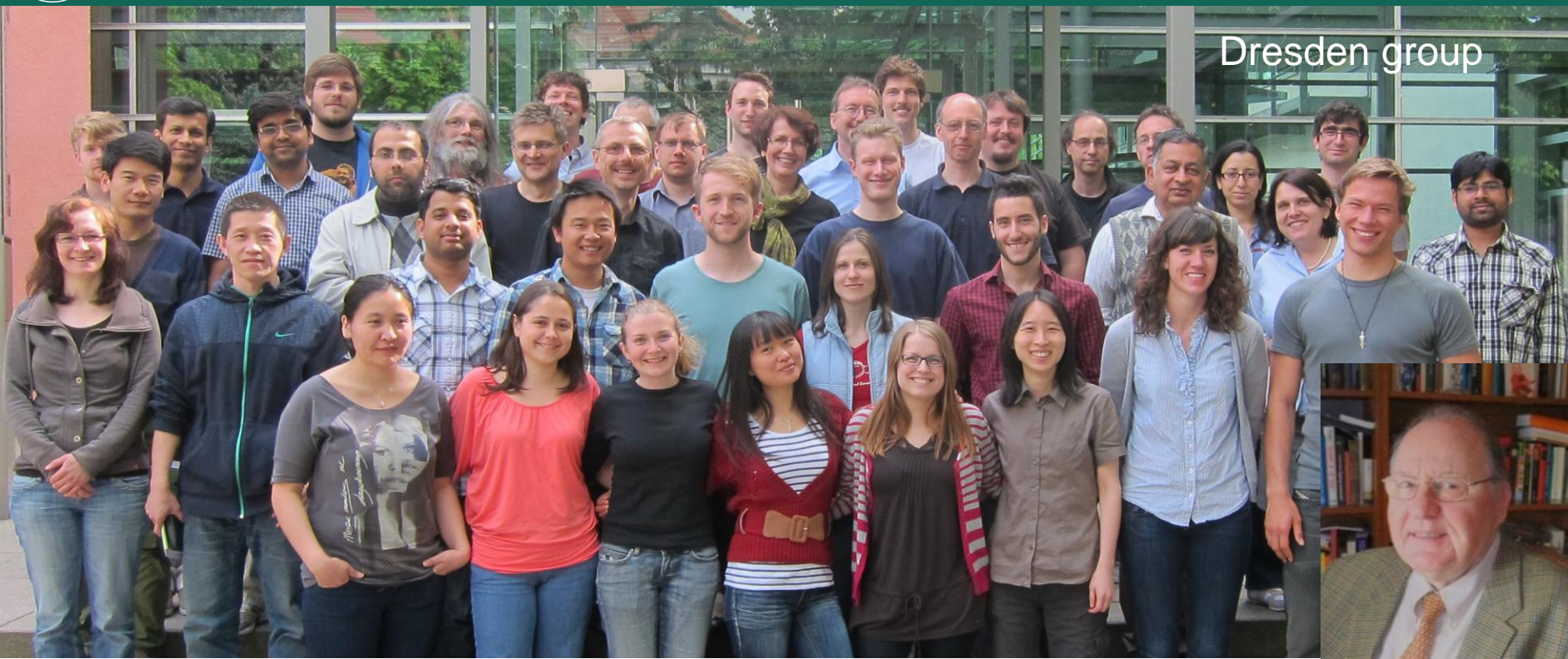
# Magnetism in Mn-rich Heusler compounds

									B 2.04				
									Al 1.61	Si 1.90			
	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18
	Y 1.22	Zr 1.33	Nb 1.60	Mo 2.16		Ru 2.20	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05
		Hf 1.30		W 1.70		Ir 2.20	Pt 2.20	Au 2.40				Pb 1.80	Bi 1.90

Claudia FELSER, Ajaya K. NAYAK, Daniel EBKE, Gerhard H.  
FECHER, Lukas WOLLMANN, Jürgen KÜBLER, Olga  
MESHCHERIAKOVA, Stas CHADOV  
[www.superconductivity.de](http://www.superconductivity.de)



# Co-workers in Dresden and elsewhere



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

G. Reiss et al. Bielefeld, G. Jakob, M. Jourdan Mainz

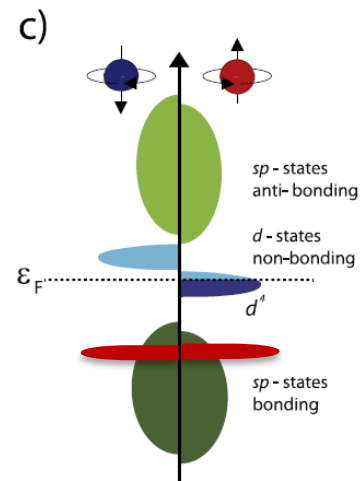
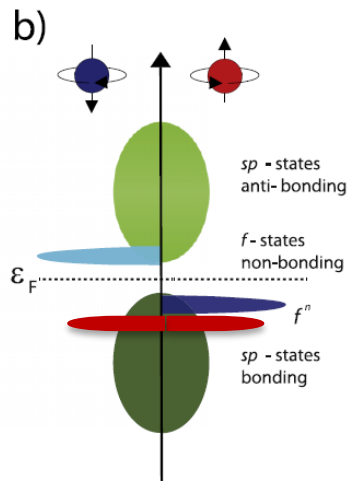
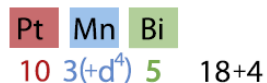
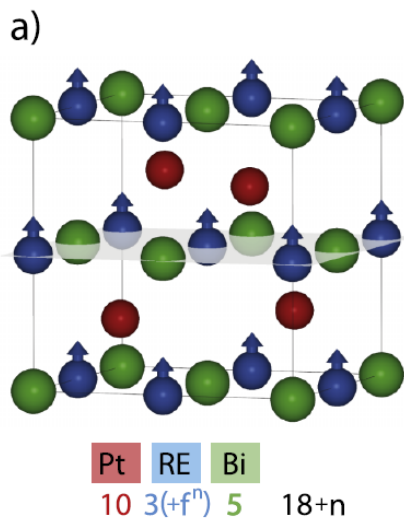
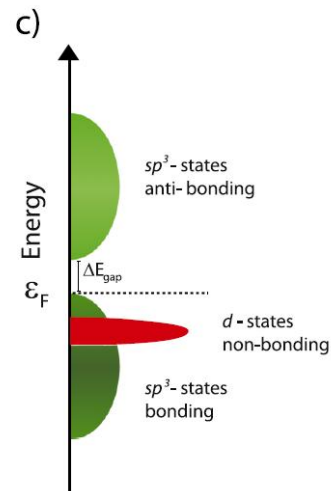
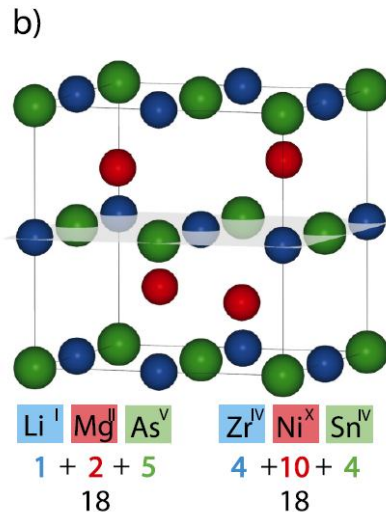
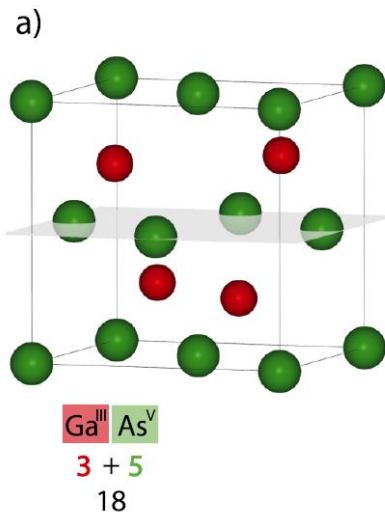
S. S. P. Parkin et al. IBM Almaden, MPI Halle

M. Coey, Dublin





# Half metallic Ferromagnets



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

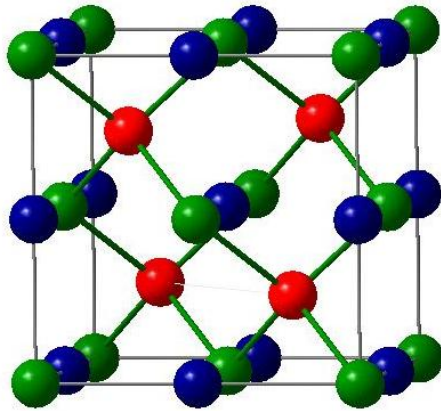
Graf T, Felser C, Parkin SSP, Progress in Solid State Chemistry (2011) 1

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





# Ternary Semiconductors ...



Ga

As

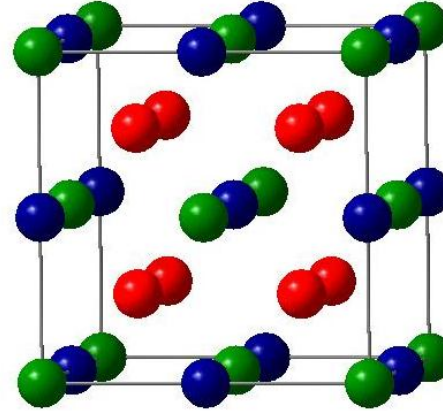
$$13 + 5 = 18$$

Co

Ti

Sb

$$9 + 4 + 5 = 18$$



Fe<sub>2</sub>

Ti

Sn

$$2 \cdot 8 + 4 + 4 = 24$$

additional  $t_2$ -levels



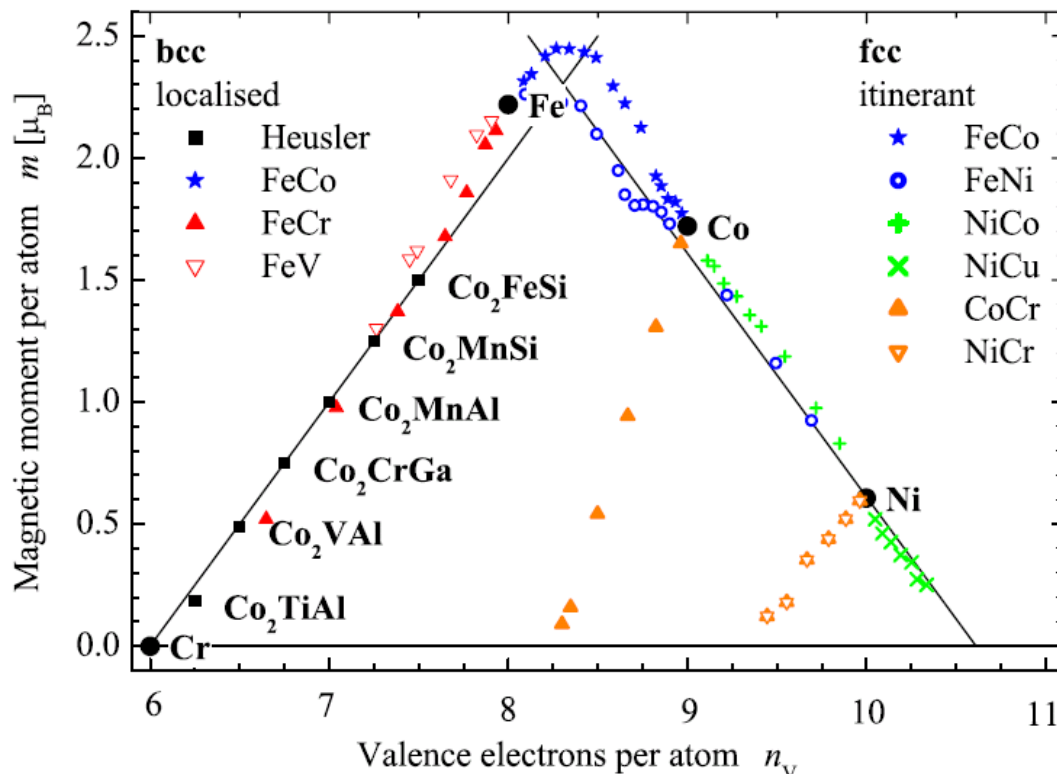
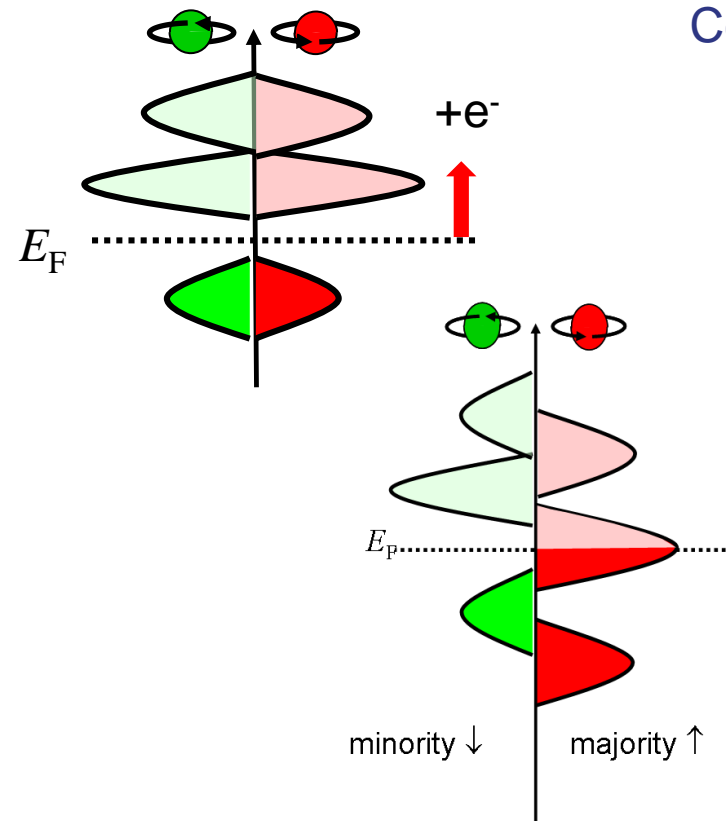
# Materials: ... to half metallic ferromagnets



Example:  $\text{Co}_2\text{MnSi}$

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

$$\text{Co}_2\text{MnSi}: 2 \times 9 + 7 + 4 = 29 \quad M_s = 5\mu_B$$

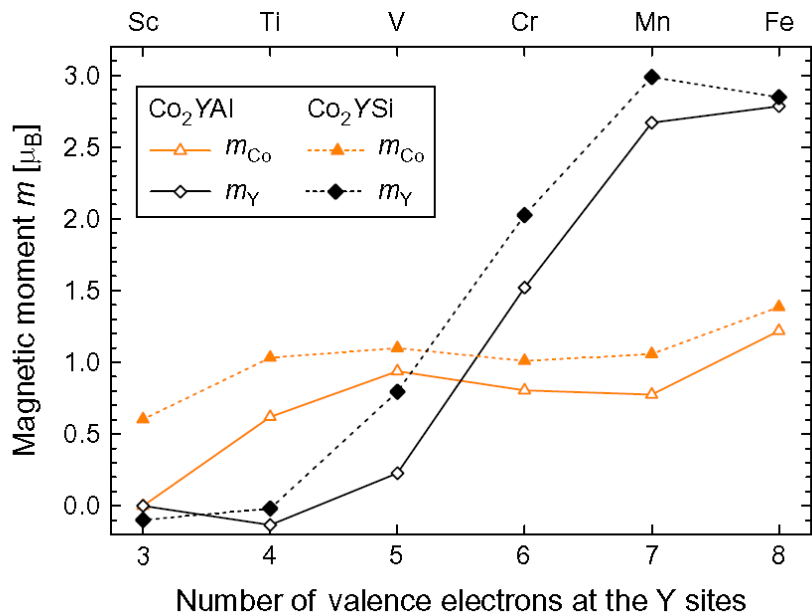


Kübler *et al.*, PRB **28**, 1745 (1983)

Galanakis *et al.*, PRB **66**, 012406 (2002)



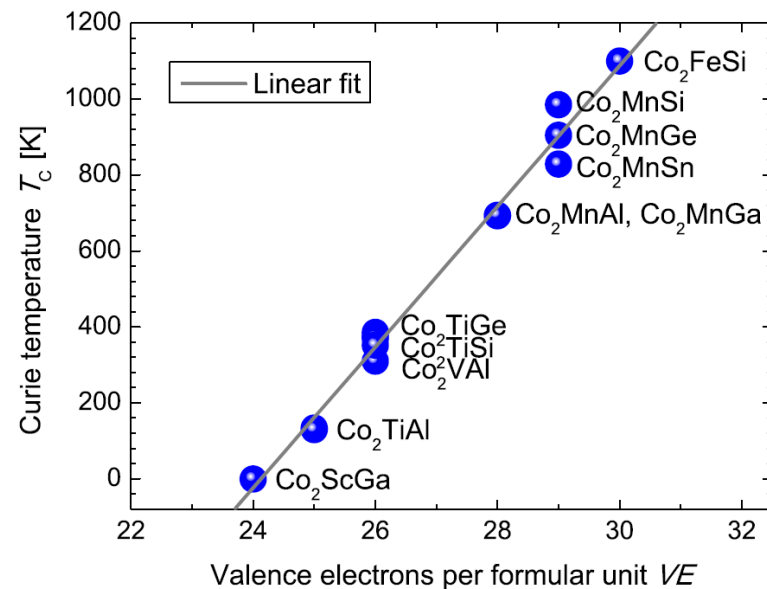
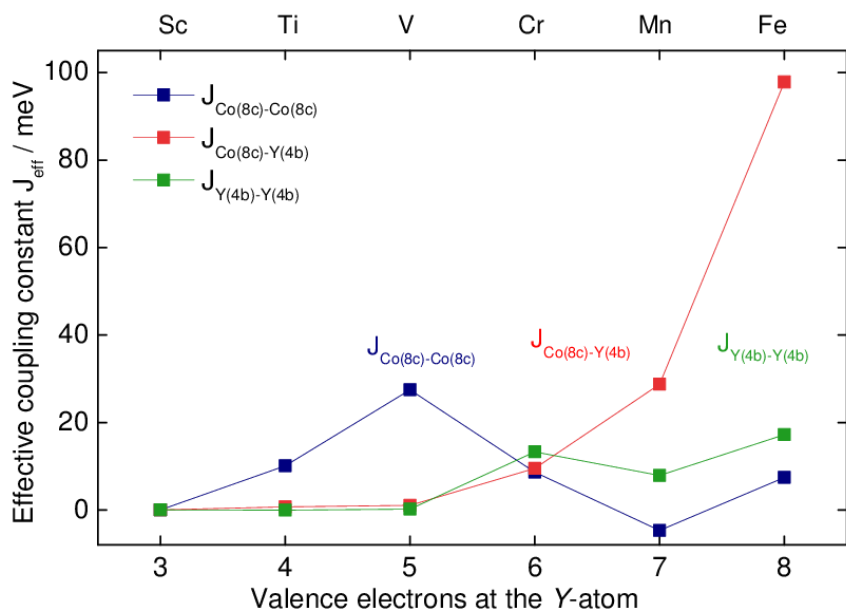
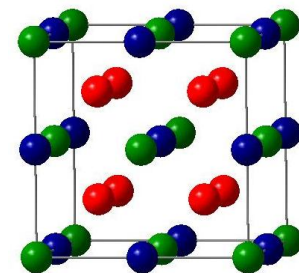
# Tunability Co<sub>2</sub>YZ



$$m(\text{Co}) \sim 1\mu_B$$

$$m(\text{Mn}) \sim 3\mu_B$$

Exchange coupling: ferro



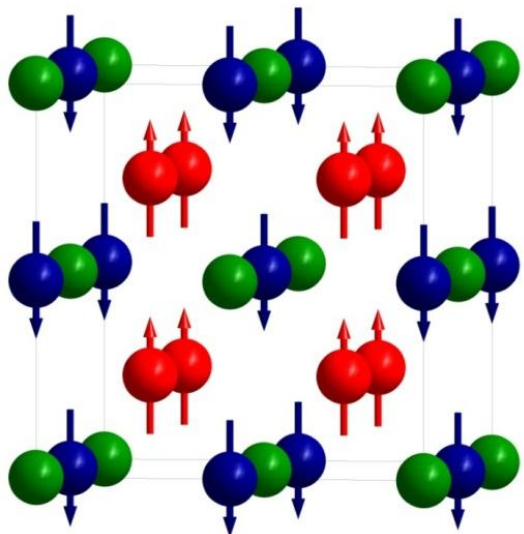
Kandpal et al., J. Phys. D **40** (2007) 1507.

Balke et al. Solid State Com. **150** (2010) 529

Kübler et al., Phys. Rev. B **76** (2007) 024414



# Ferrimagnetic Heusler compounds



Kübler's Rule  
Slater Pauling Rule

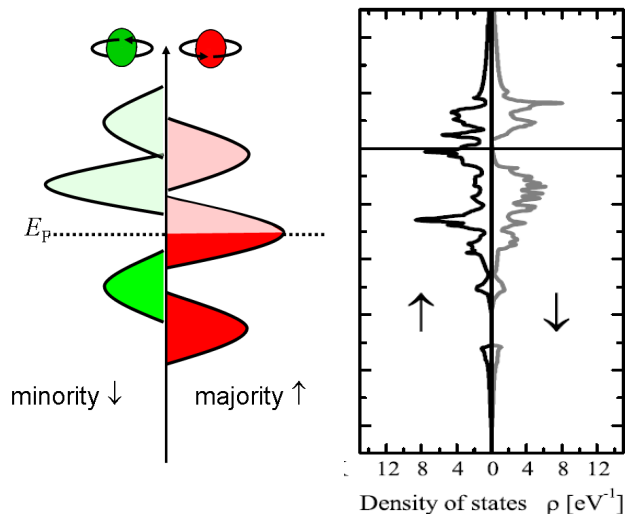


Two magnetic sublattices  
24 Valence electrons –  $0 \mu_B$   
 $Mn^{3+}$  at octahedral site –  $4 \mu_B$   
**Mn** compensates



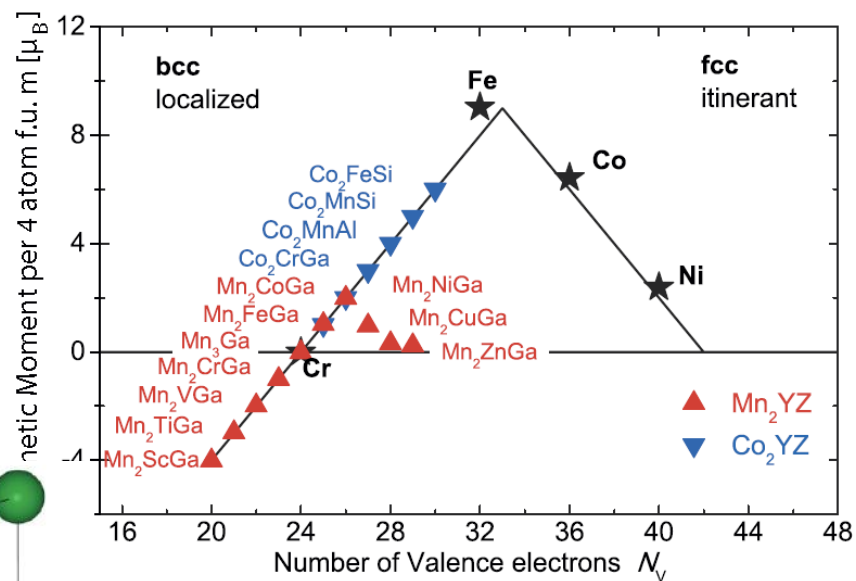
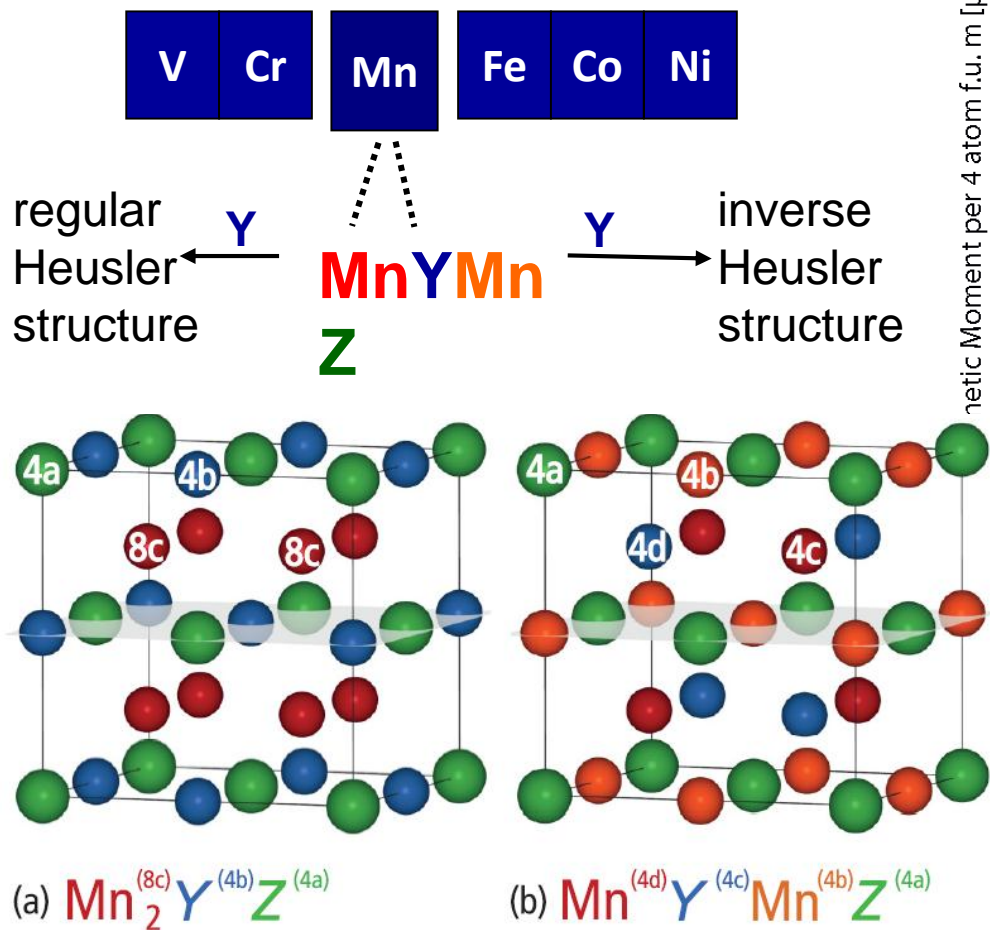
$3 \cdot 7 + 3 = 24$

$\Rightarrow$  **Compensated ferrimagnet**





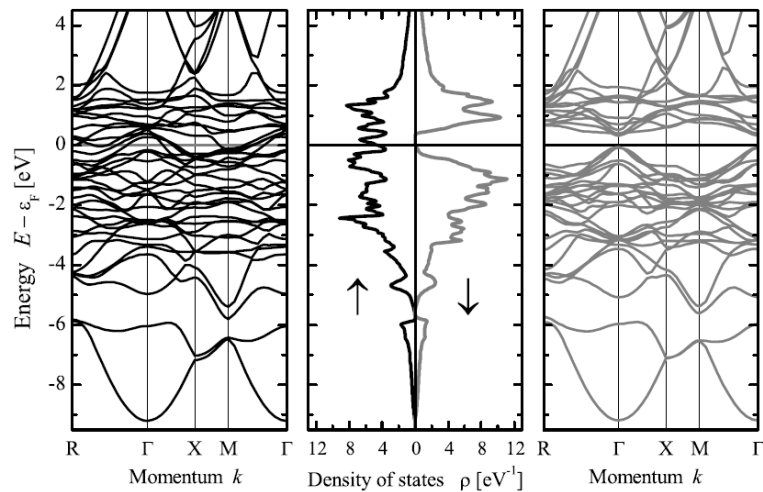
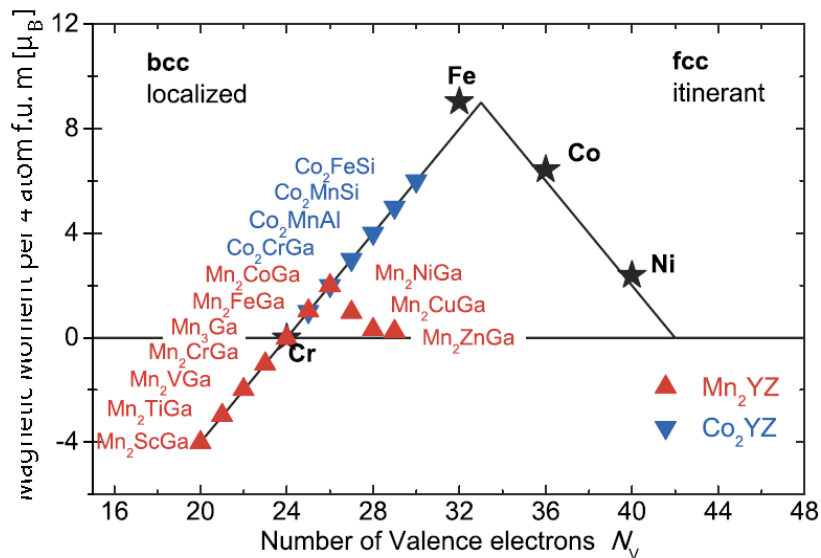
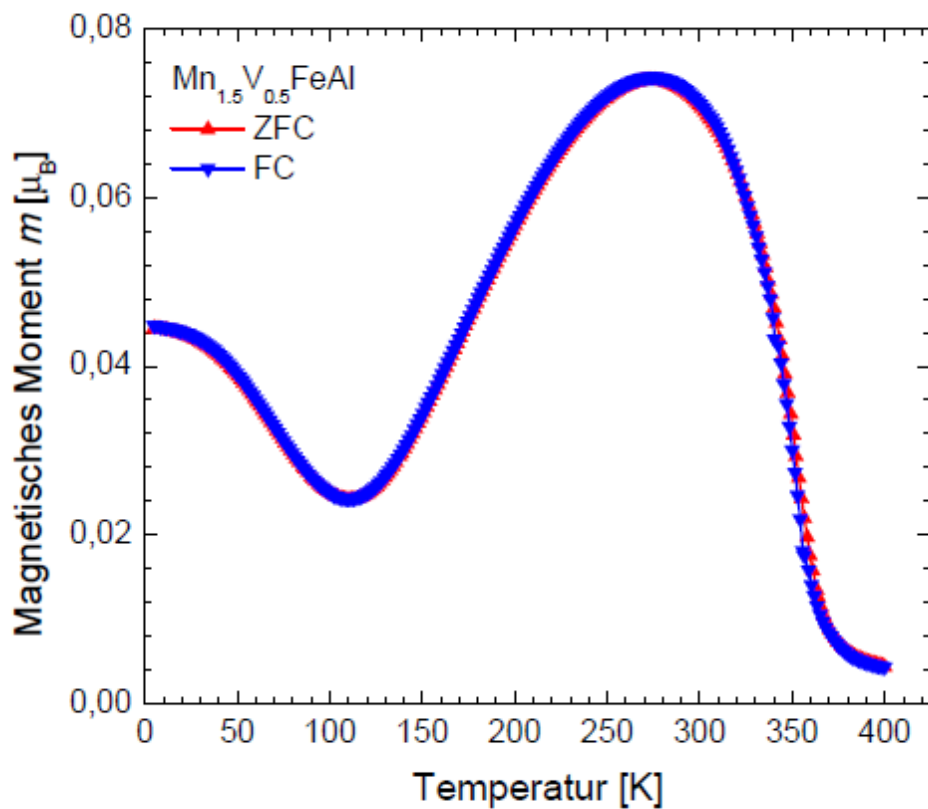
# Mn<sub>2</sub>-Heusler compounds







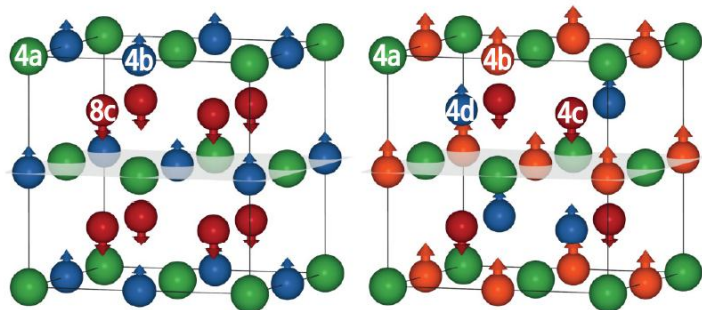
# Compensated ferrimagnet



**$Mn_2VGa + Fe_2MnGa =$  compensated**



# Tunability $\text{Mn}_2\text{YZ}$



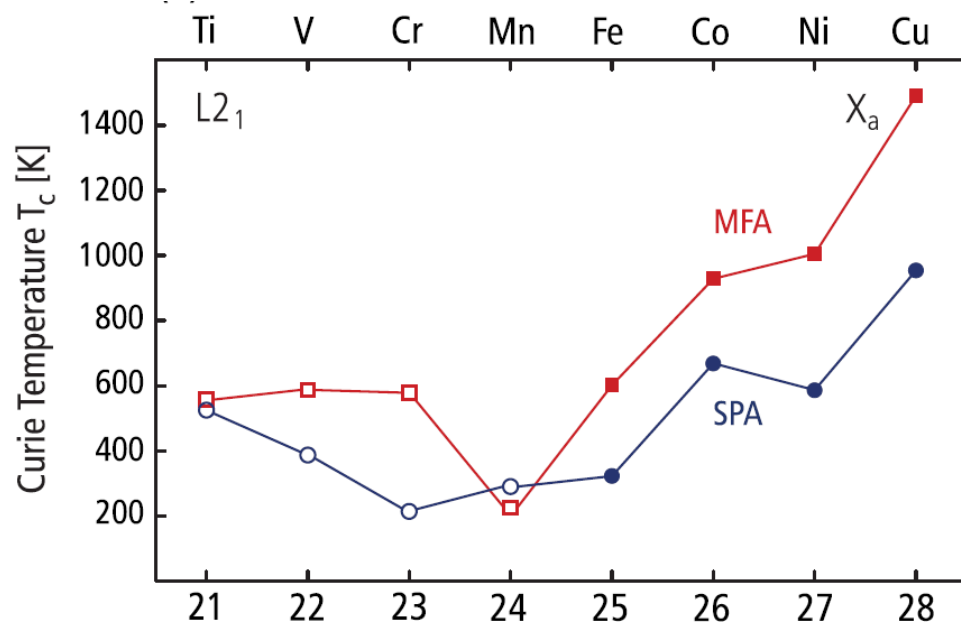
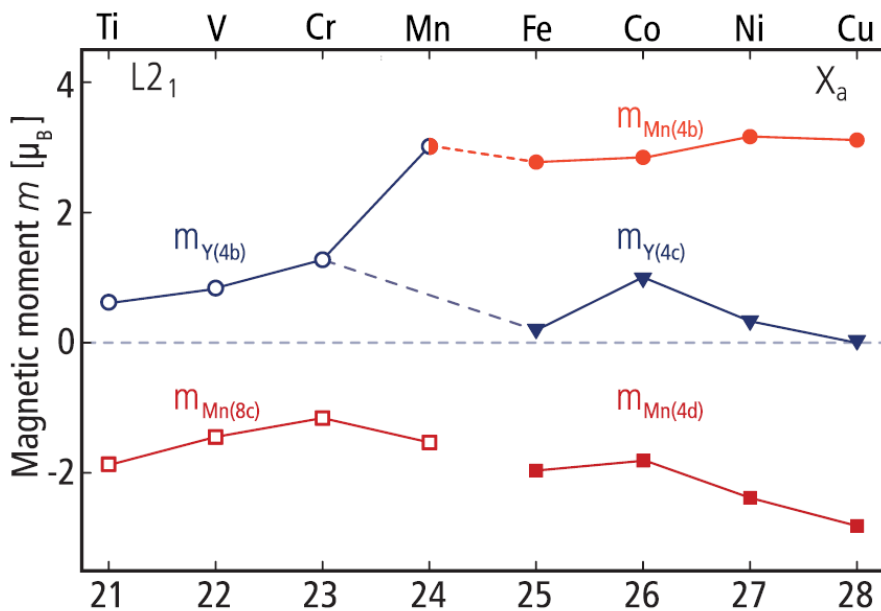
(a)  $\text{Mn}_2^{(8c)}\text{Y}^{(4b)}\text{Z}^{(4a)}$

(b)  $\text{Mn}^{(4d)}\text{Y}^{(4c)}\text{Mn}^{(4b)}\text{Z}^{(4a)}$

$m(\text{Mn}) \sim 3\mu_B$

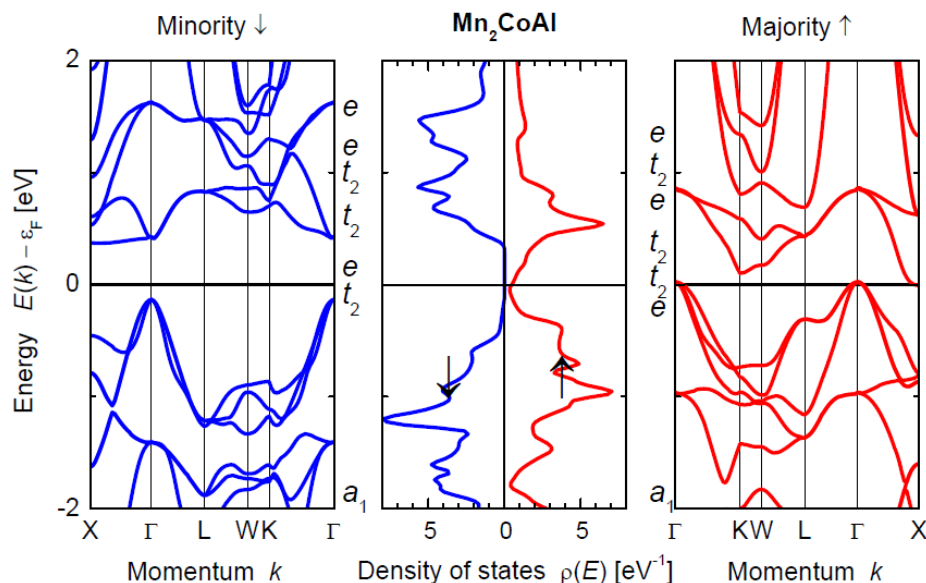
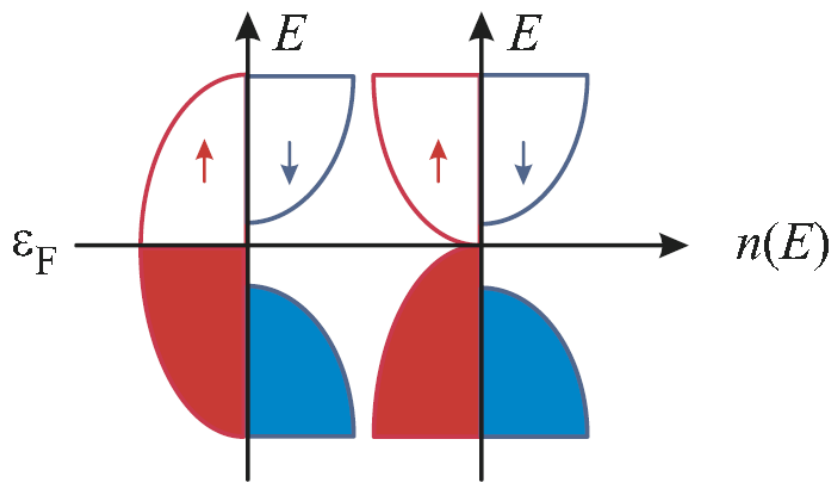
$m(\text{Mn}) \sim 2\mu_B$

Exchange coupling: ferri





# Spin gapless semiconductor $\text{Mn}_2\text{CoAl}$



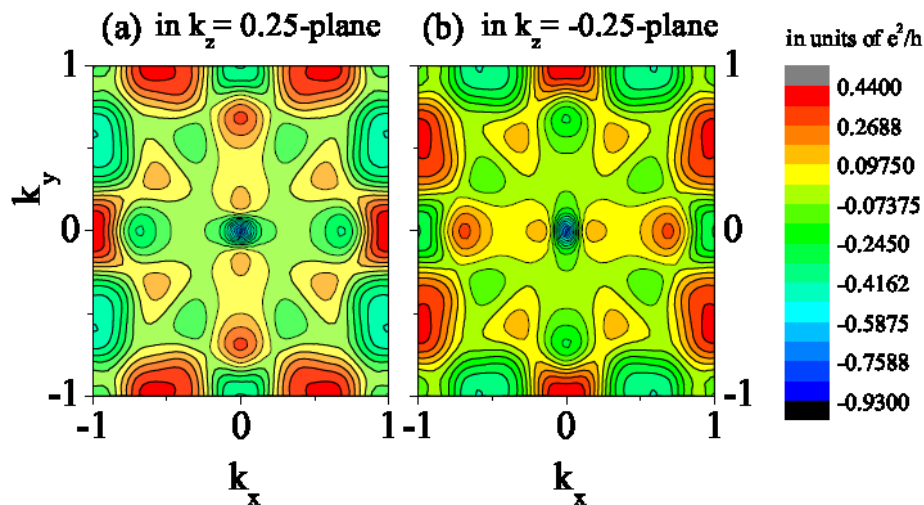
## Expected properties

100% spin polarisation

Properties sensitive to pressure

... gating ... electrolyte gating

→ new devices



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

Guardi et al., PRL **110** (2013) 100401



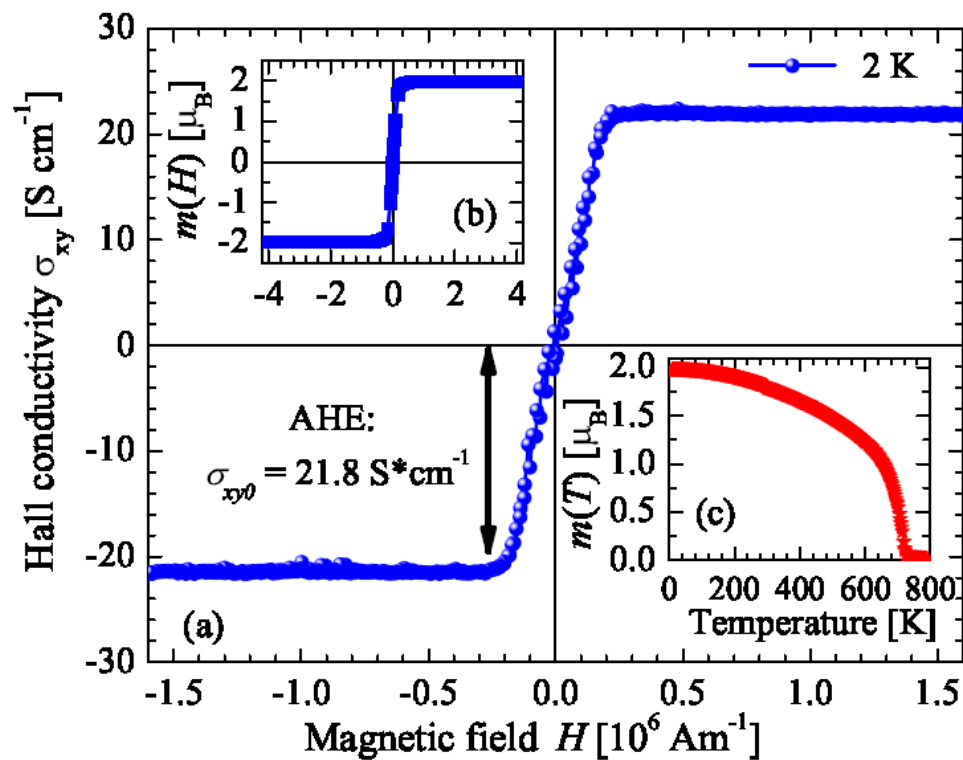
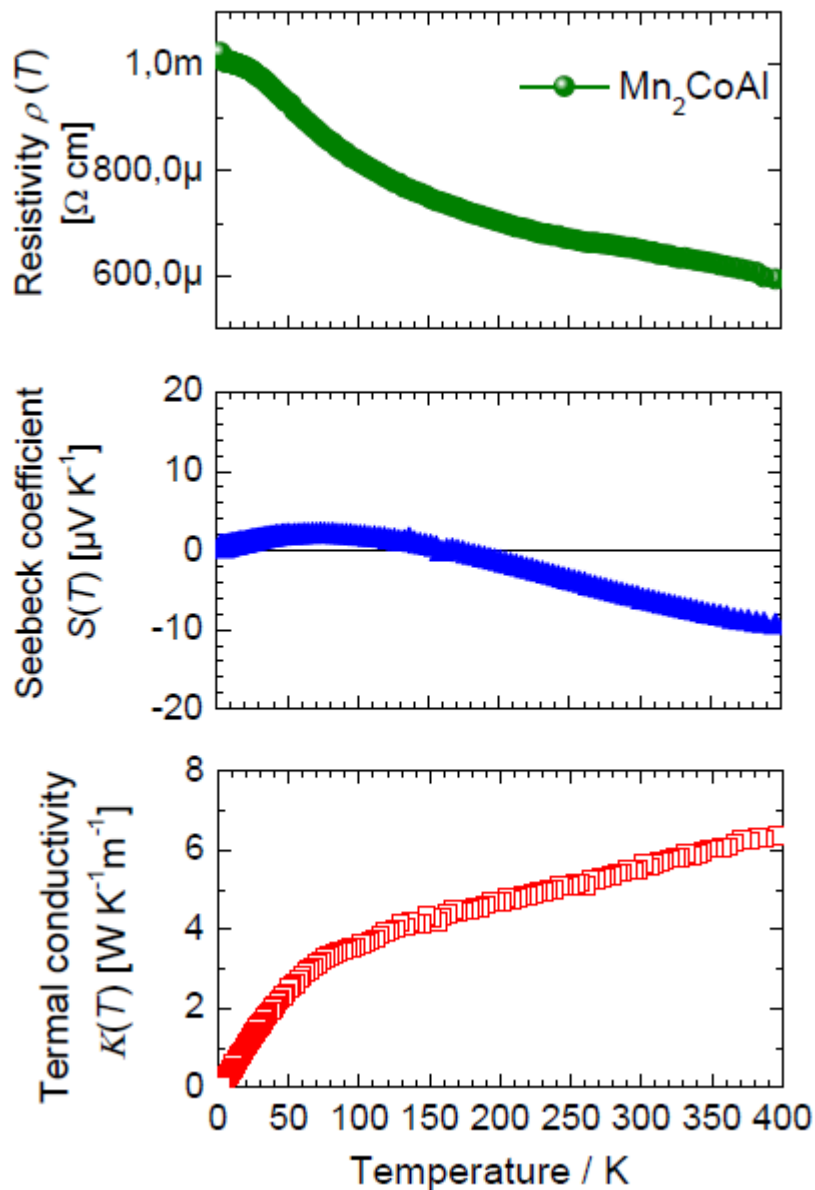
# Mn<sub>2</sub>CoAl a semiconducting ferromagnet

$$2 \cdot 7 + 9 + 3 = 26$$

$$m = 2 \mu_B$$

$$T_C = 800 \text{ K}$$

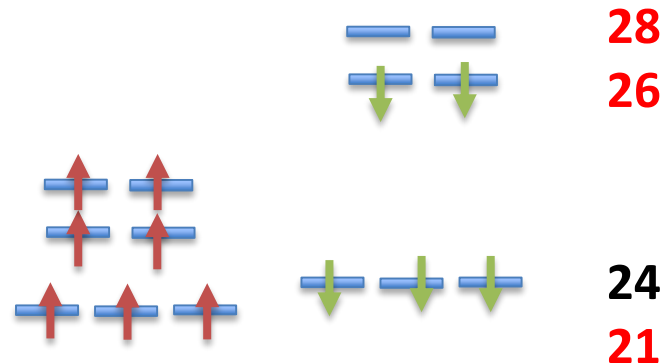
$$\text{Charge carrier} \sim 10^{17} \text{ cm}^{-3}$$



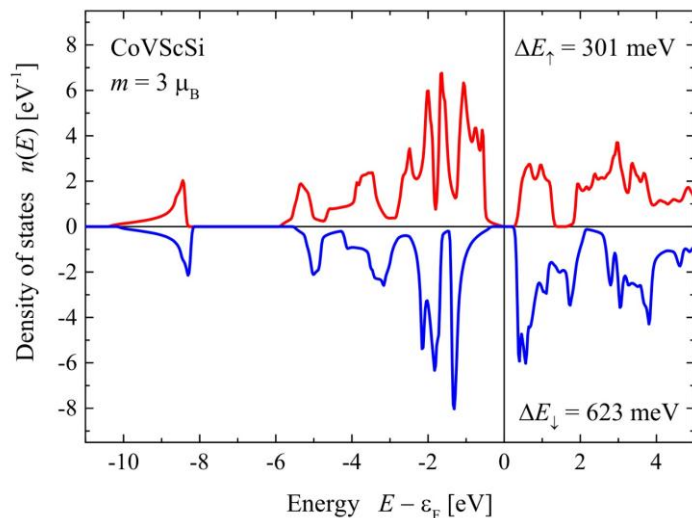
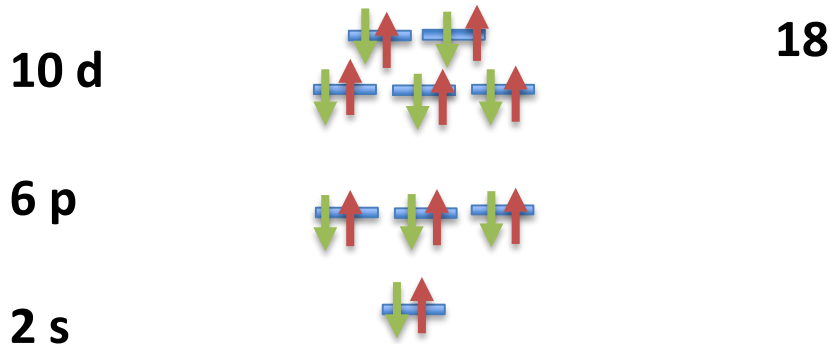


# More semiconductors

26	21
Mn <sub>2</sub> CoAl	FeVTiSi
CoFeCrAl	CoVScSi
CoMnCrSi	FeCrScSi
CoFeVSi	FeVTiSi
FeMnCrSb	FeMnScAl



18	28
V <sub>3</sub> Al	CoFeMnSi







$$J \approx \frac{e}{\hbar g} \alpha M_s H_U d$$

J.C. Slonczewski: "Current-driven excitation of magnetic multilayers(1996)",  
Journal of Magnetism and Magnetic Materials Volume 159 (1996) L1-L7

### Spin torque devices

- High Spin polarization
- Materials with High  $T_C$
- High perpendicular anisotropy
- Low magnetic damping
- Low saturation magnetization

### Problems:

- Better lattice match new Mn<sub>2</sub>-Heuslers
- Higher spinpolarization
- Resonant tunneling
- interface engineering - smooth
  - atomic structure - disorder
  - magnetic structure – non collinear



# Mn<sub>3</sub>Ga tetragonal distortion

## Designed Materials

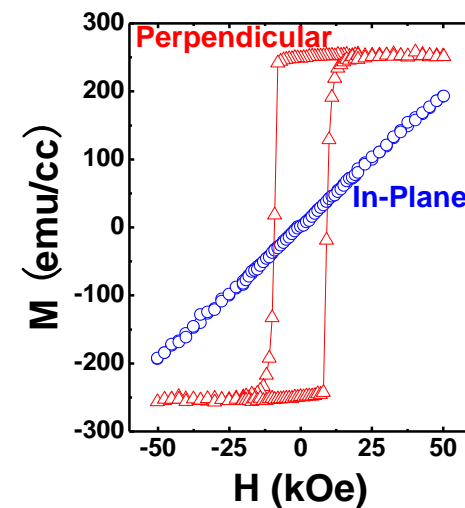
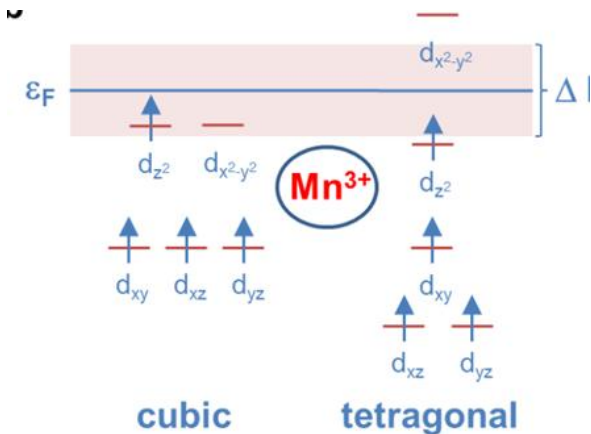
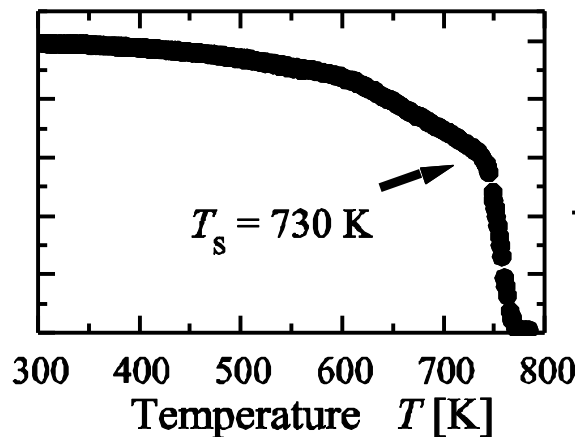
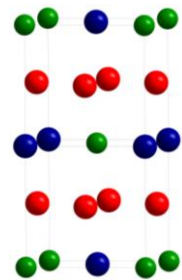
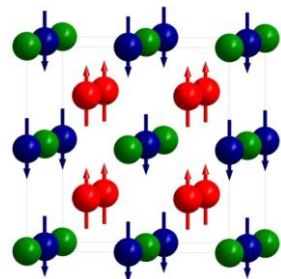
- Materials with low magnetic damping
- Materials with low magnetic moments
- Materials with high perpendicular anisotropy

Tetragonal Heusler compounds: Mn<sub>3</sub>Ga, FeMn<sub>2</sub>Ga ...

theory

bulk material

thin film and devices





$$J \approx \frac{e}{\hbar g} \alpha M_s H_U d$$

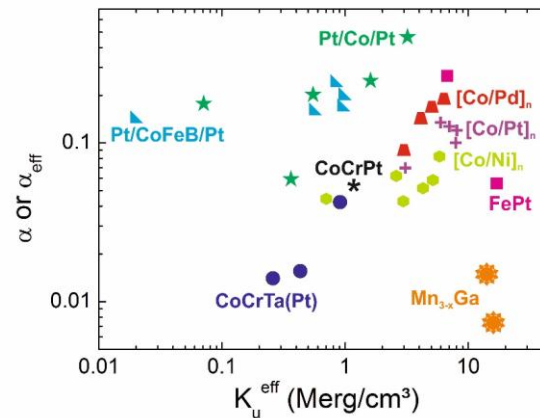
J.C. Slonczewski: "Current-driven excitation of magnetic multilayers(1996)",  
Journal of Magnetism and Magnetic Materials Volume 159 (1996) L1-L7

## Spin torque devices

- High Spin polarization
- Materials with High  $T_C$
- High perpendicular anisotropy
- Low magnetic damping
- Low saturation magnetization

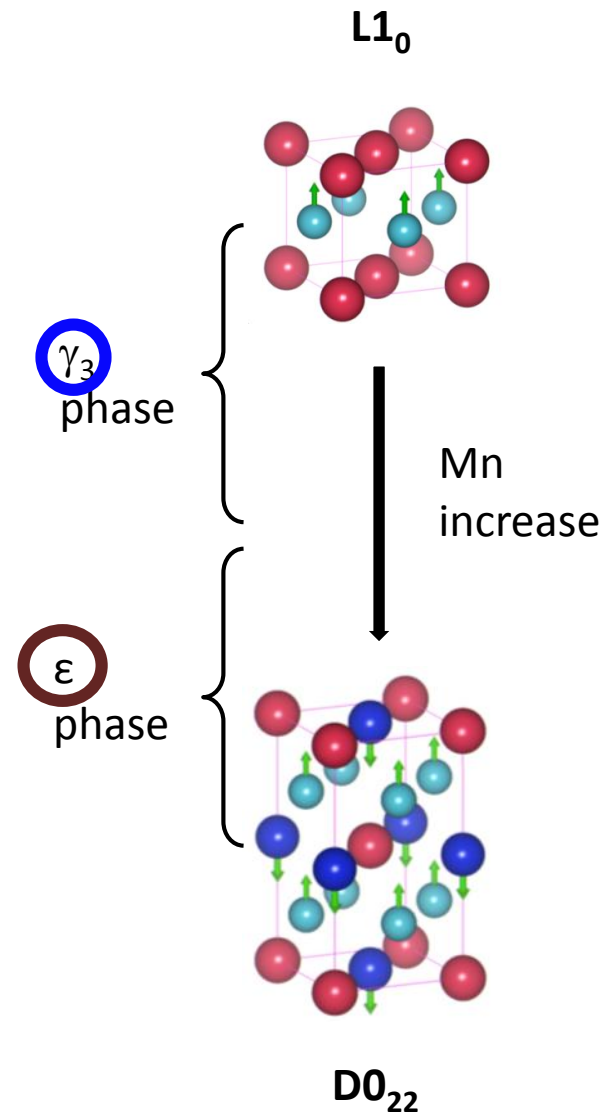
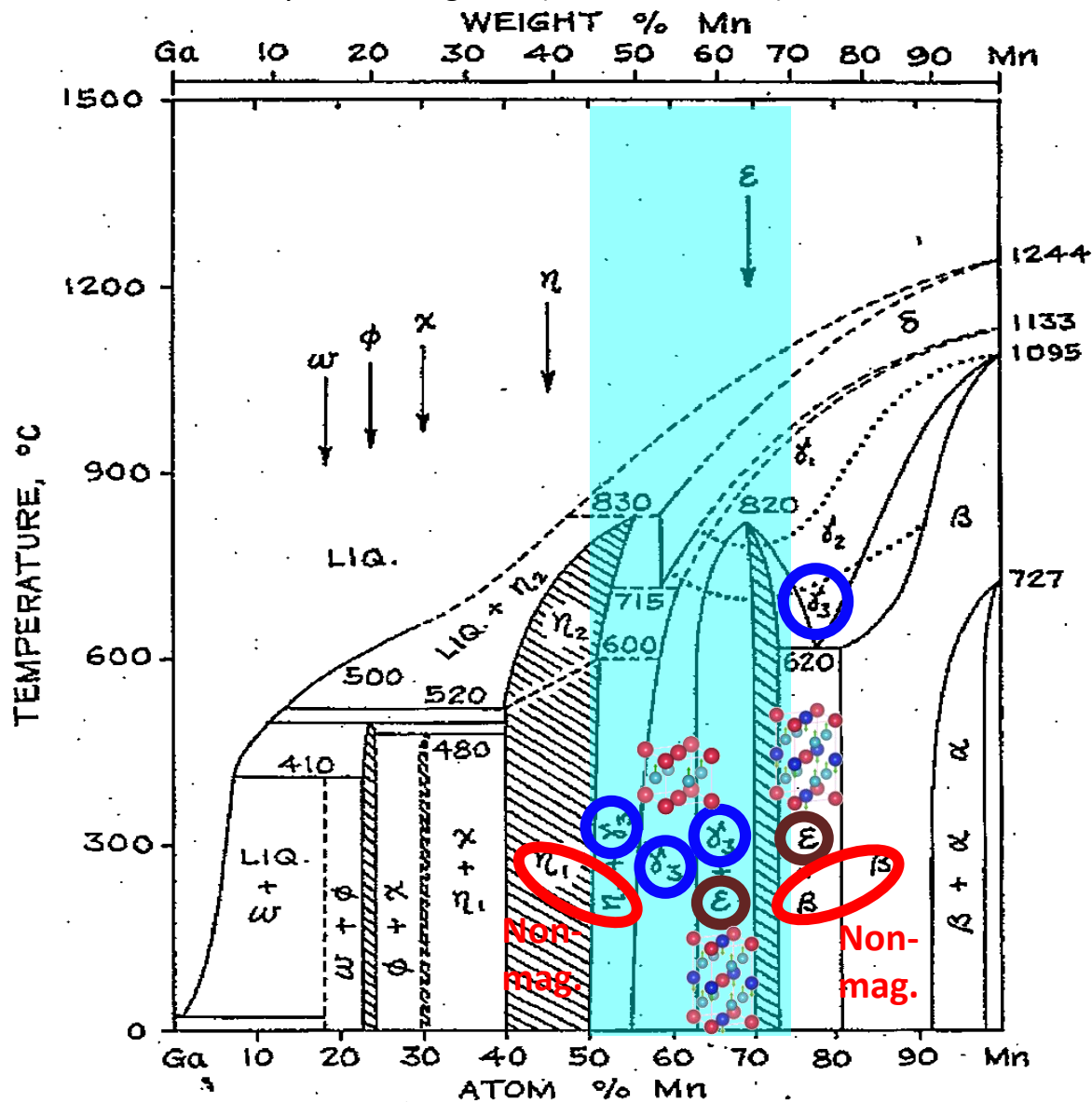
## Problems:

- Better lattice match new Mn2-Heuslers
- Higher spinpolarization
- Resonant tunneling
- interface engineering - smooth
  - atomic structure - disorder
  - magnetic structure – non collinear



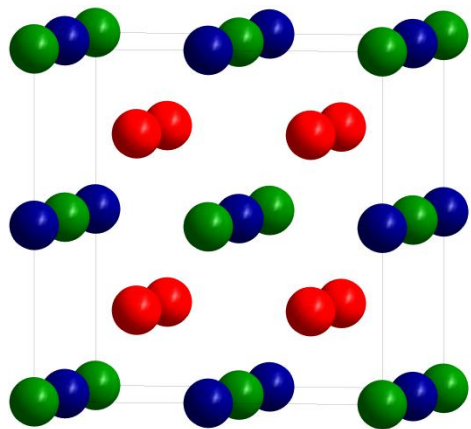


the Handbook of Binary Phase Diagrams (W.G.Moffatt ed.)

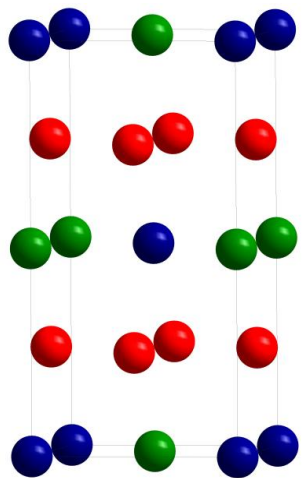
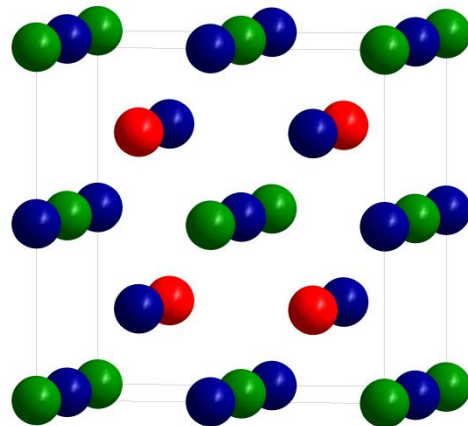




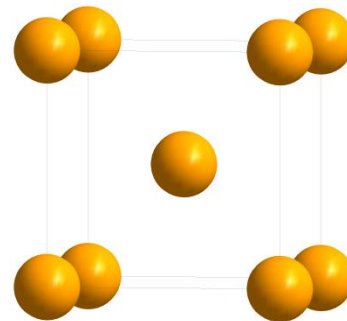
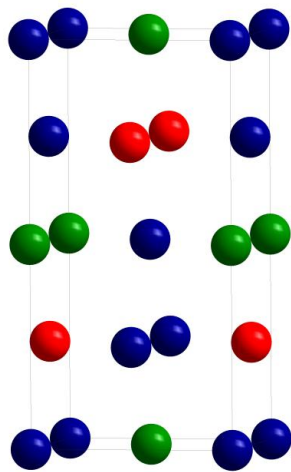
# Disorder and Design recipe



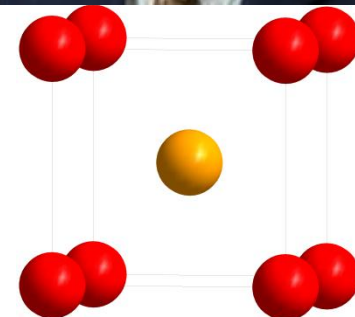
L<sub>2</sub><sub>1</sub> structure



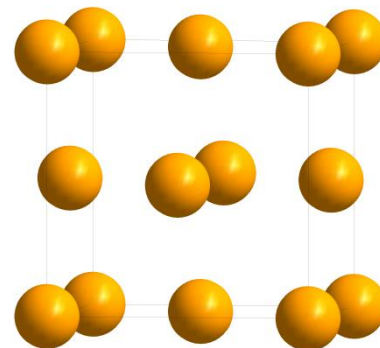
DO<sub>22</sub> structure



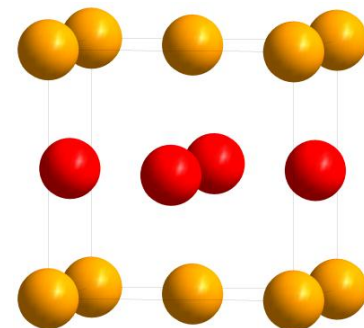
A2 structure



B2 structure



A1 structure



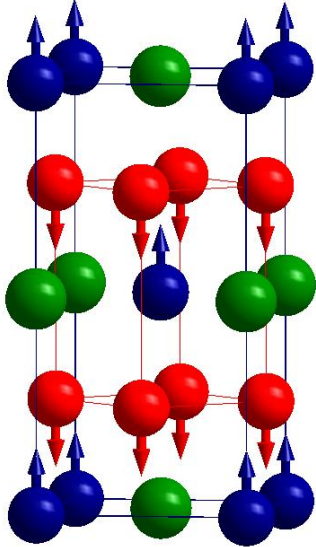
L<sub>1</sub><sub>0</sub> structure





# Structural distortion

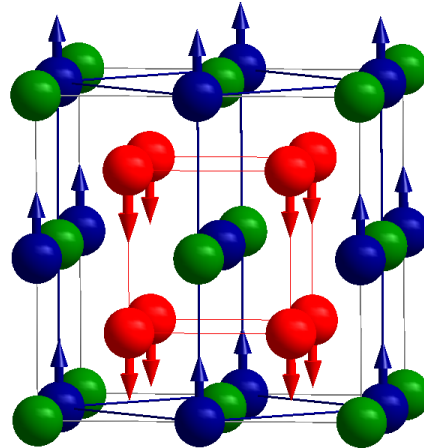
$I4/mmm$  ( $D0_{22}$ )



tetragonal

STT-RAM with out of plane  
Compensated ferrimagnets  
Permanent magnets  
Non-collinear magnetism  
Topological Hall effect  
Skyrmions  
mag. shape memory  
Magnetocalorics – CDW?

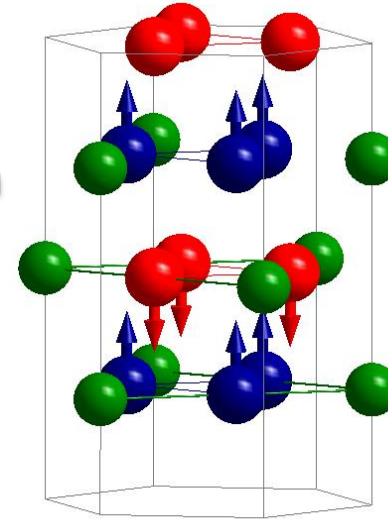
$Fm\bar{3}m$  ( $L2_1$ )



cubic

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

$P6_3/mmc$  ( $D0_{19}$ )



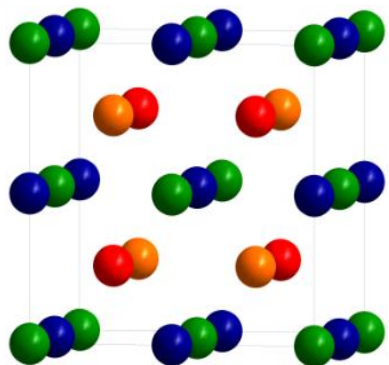
hexagonal

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

J. F. Qian, et al., *J. Phys. Cond. Mat.* 47 (2014)  
J. Kübler and C. Felser *EPL* 108 (2014) 67001

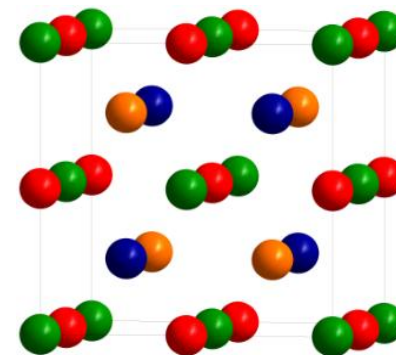


# The tetragonal structure

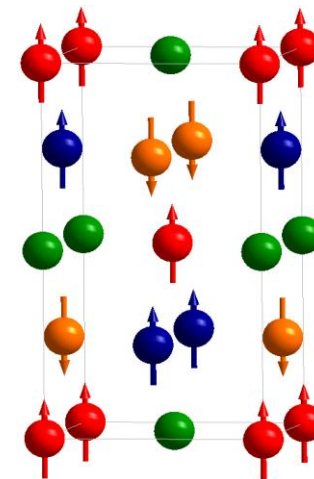
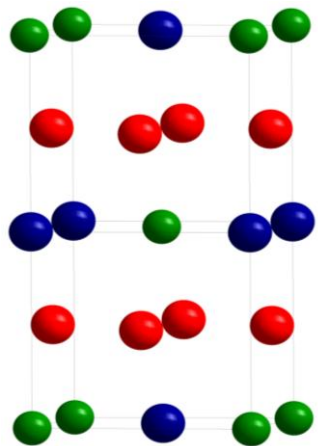
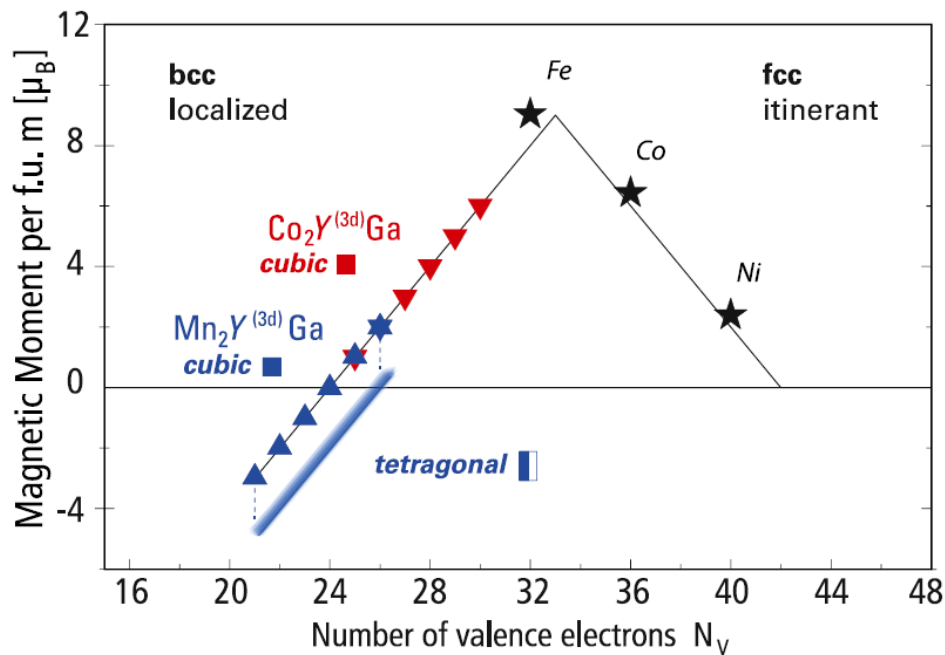


regular  
Heusler  
structure

inverse  
Heusler  
structure



e) Slater - Pauling Curve

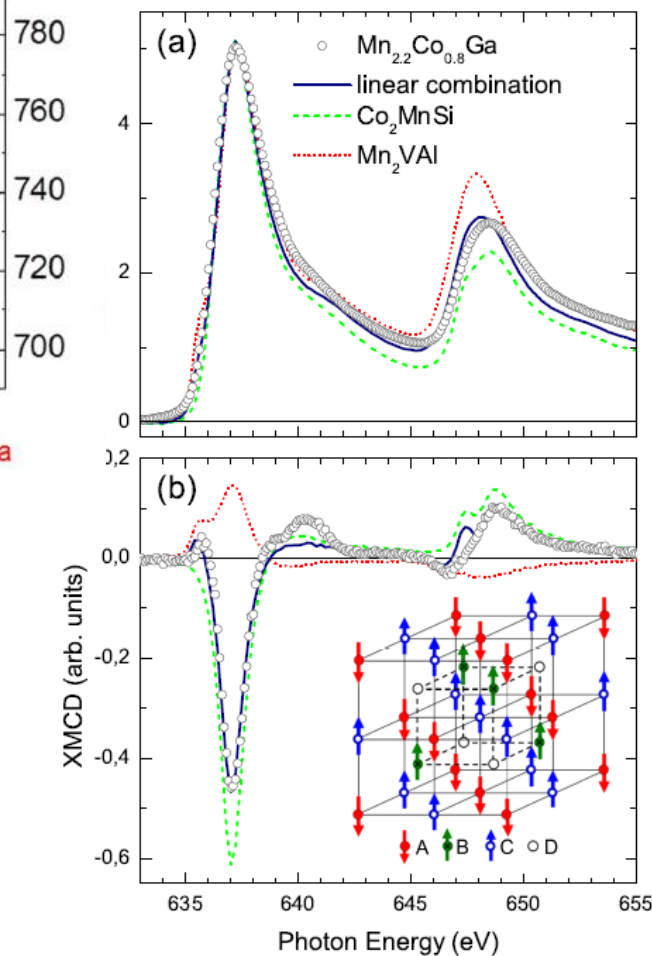
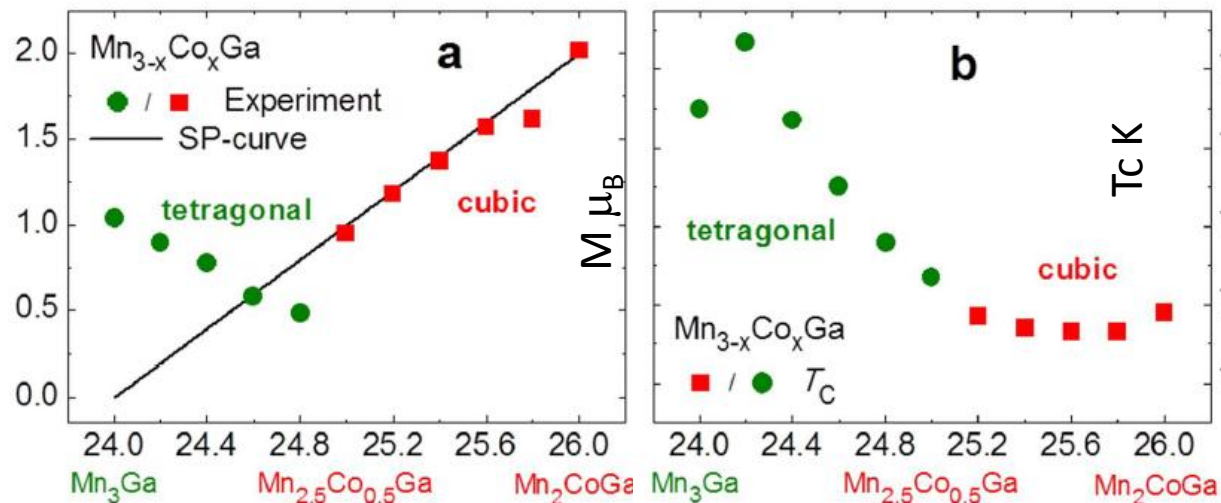


Wollmann et al., APL Mat. 3 (2015) 041518

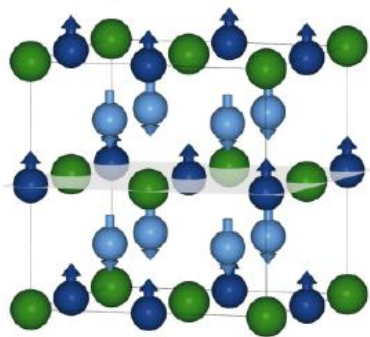
Wollmann et al. Phys. Rev. B accepted arXiv:1506.03735



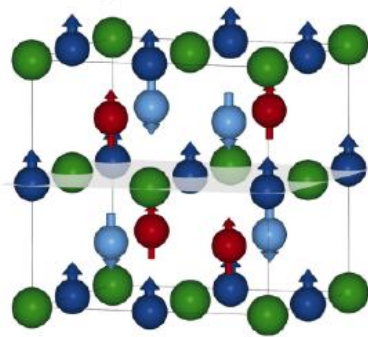
# Mn<sub>2</sub>CoGa – Mn<sub>3</sub>Ga



a) Mn<sub>3</sub>Ga



a) Mn<sub>2</sub>CoGa



b)



out-of-plane

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

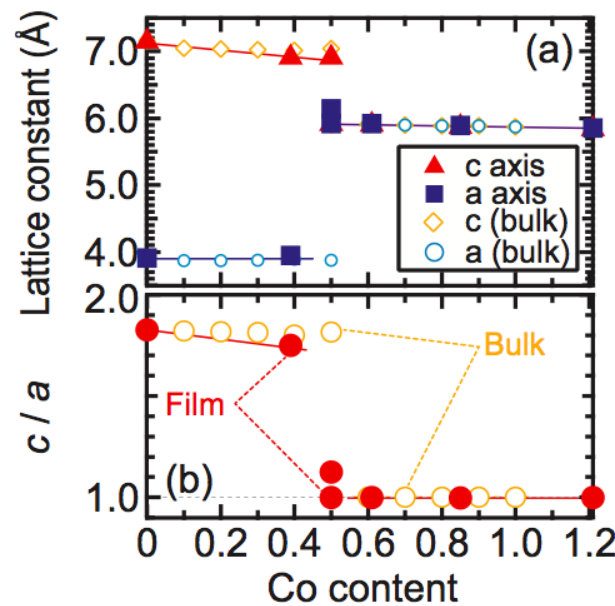
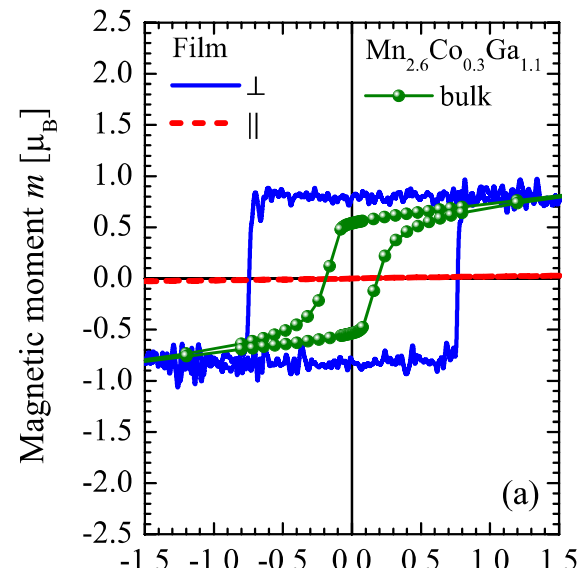
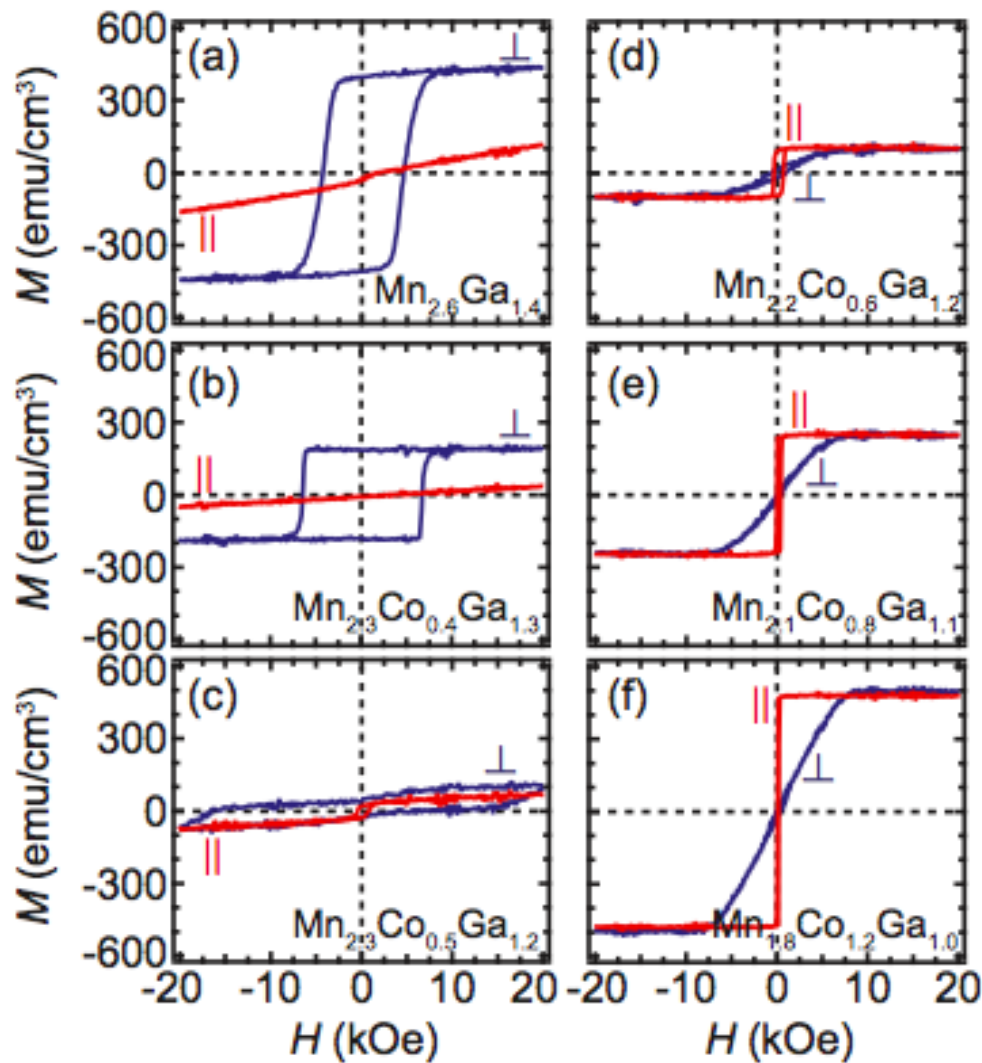
Klaer et al. *Appl. Phys. Lett.* 98 (2011) 212510.

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



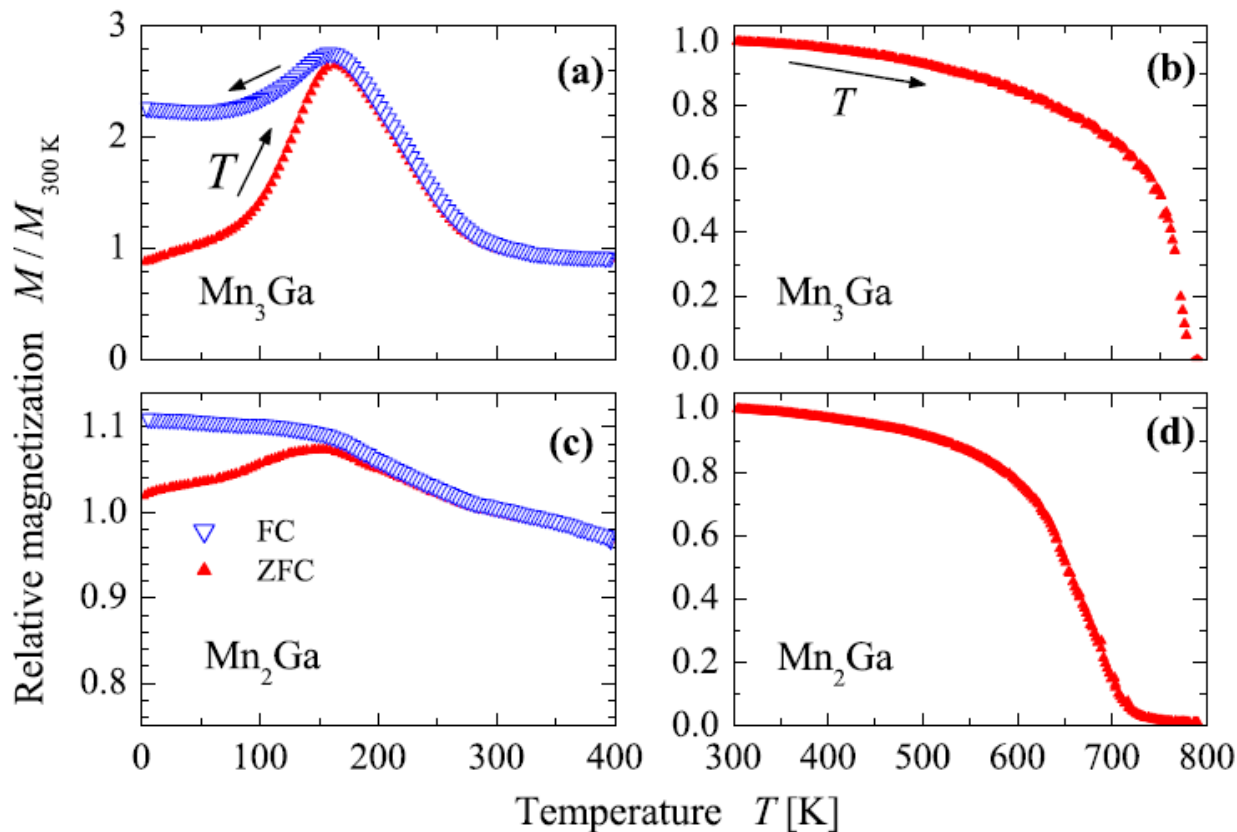
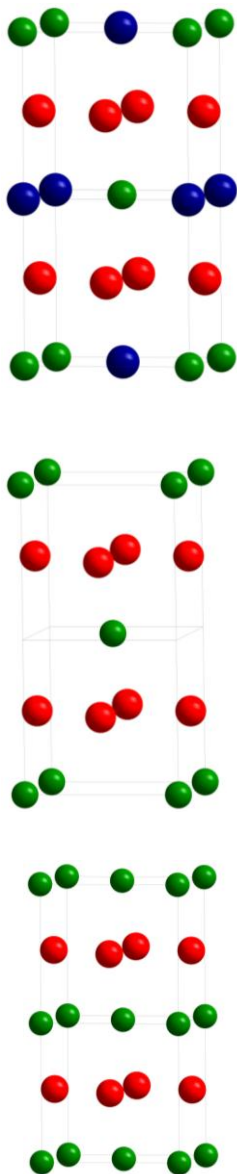
prepared in Mizukami lab

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

T. Kubota, S. Ouardi, arXiv:1211.2524



# Mn<sub>3-x</sub>Ga: Tunability

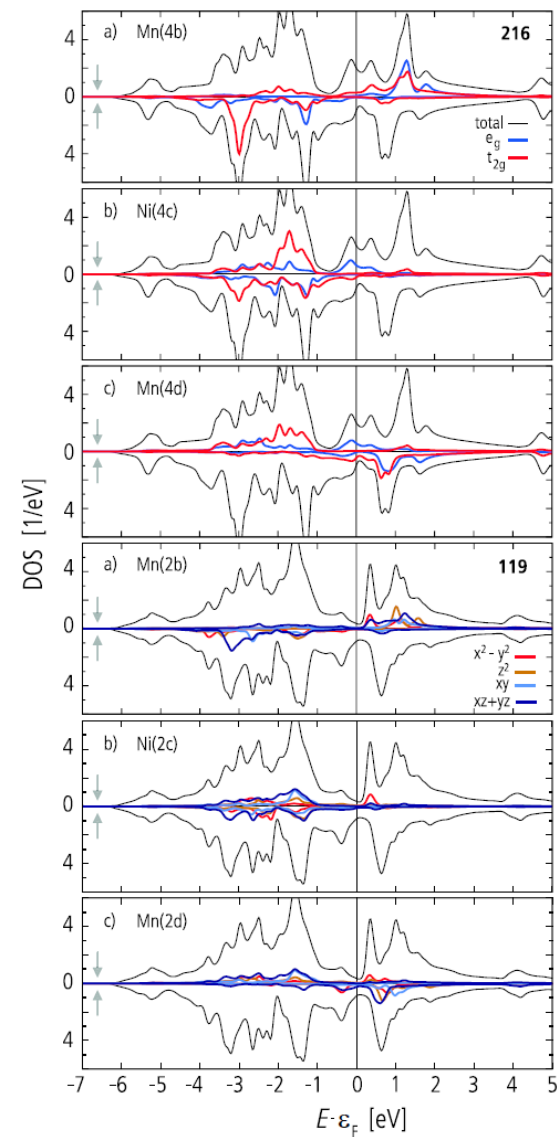
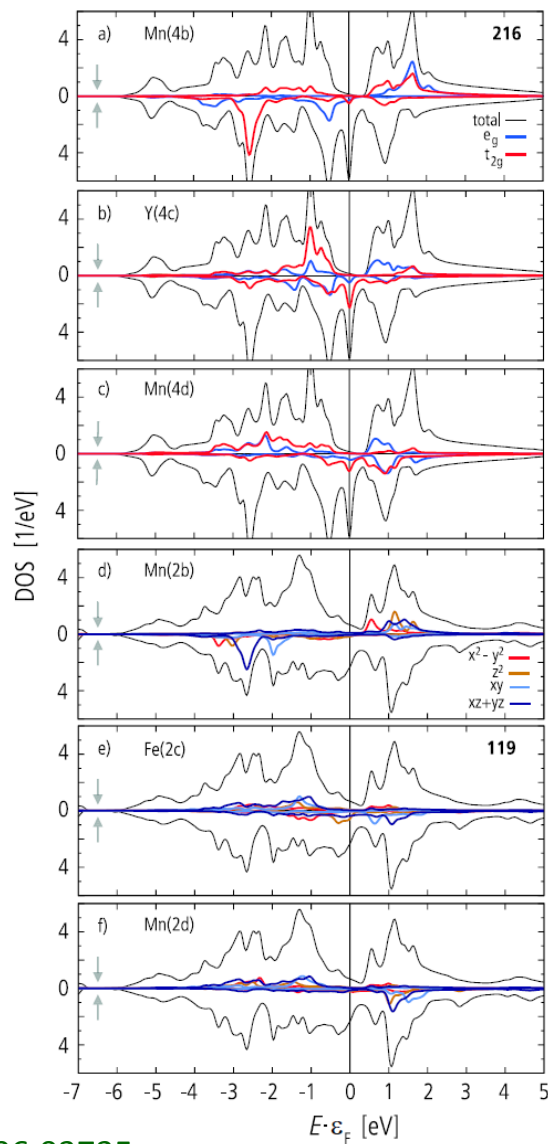
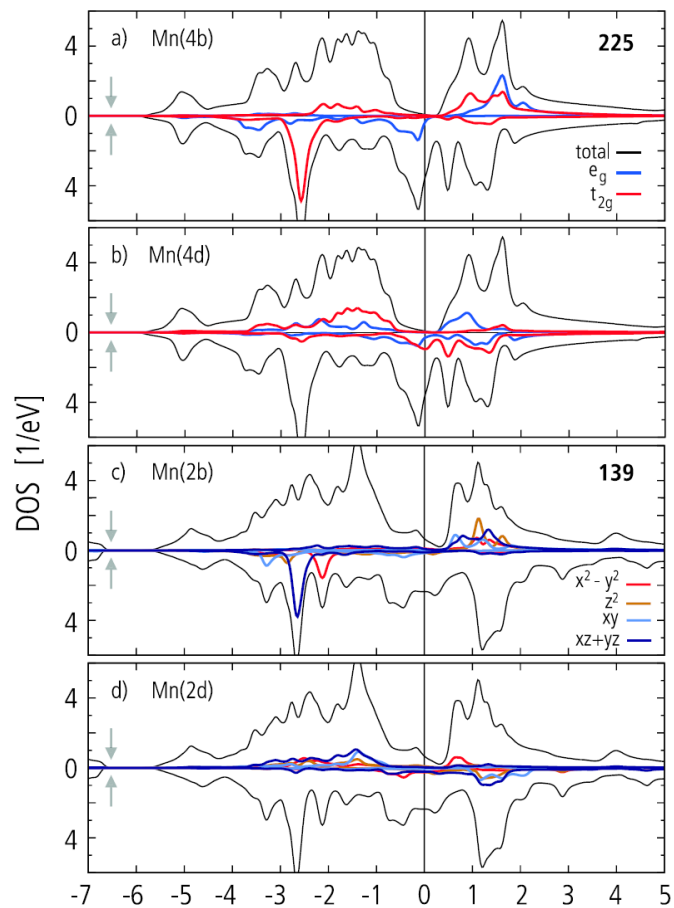


More complex magnetism at low T  
Removing one sort of Mn (octahedral) leads to ferromagnetism



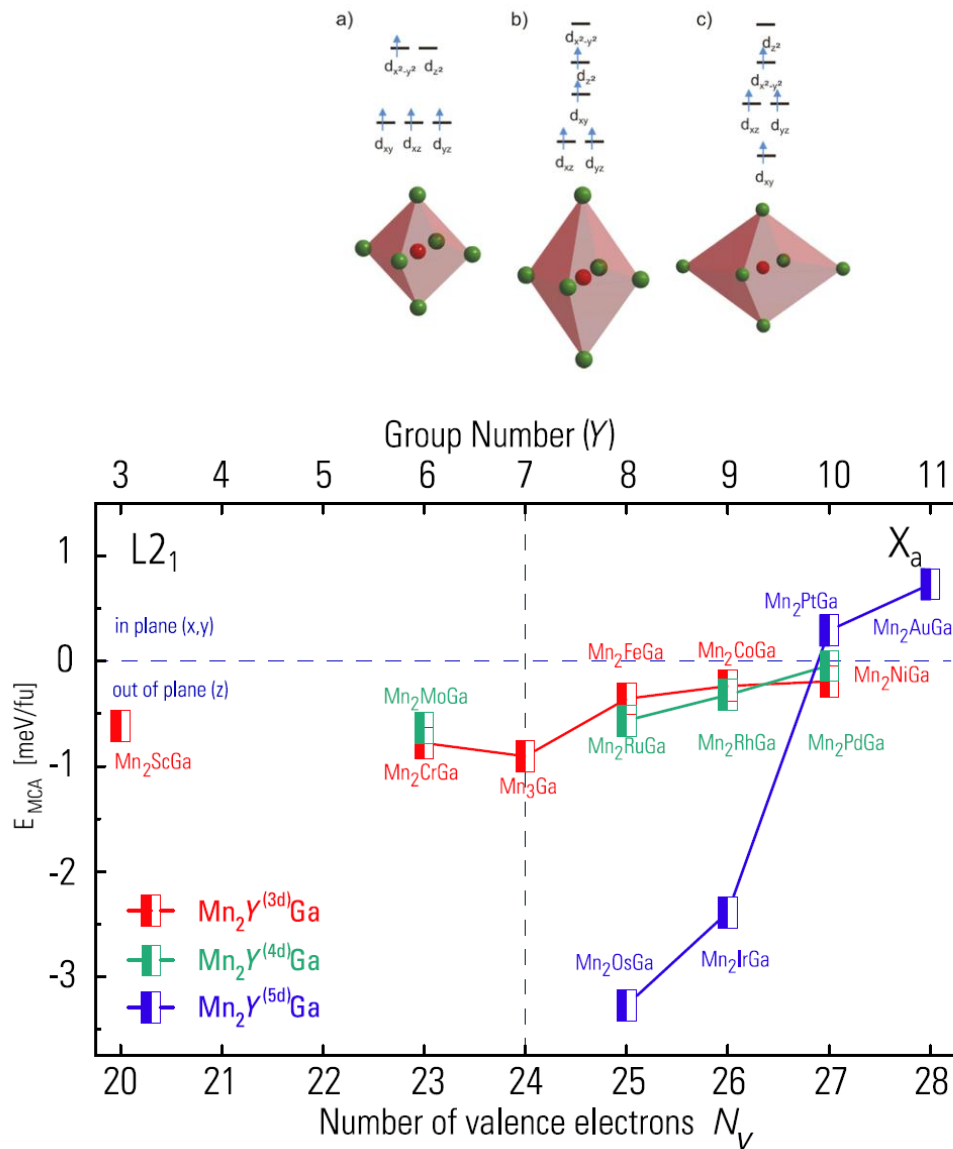
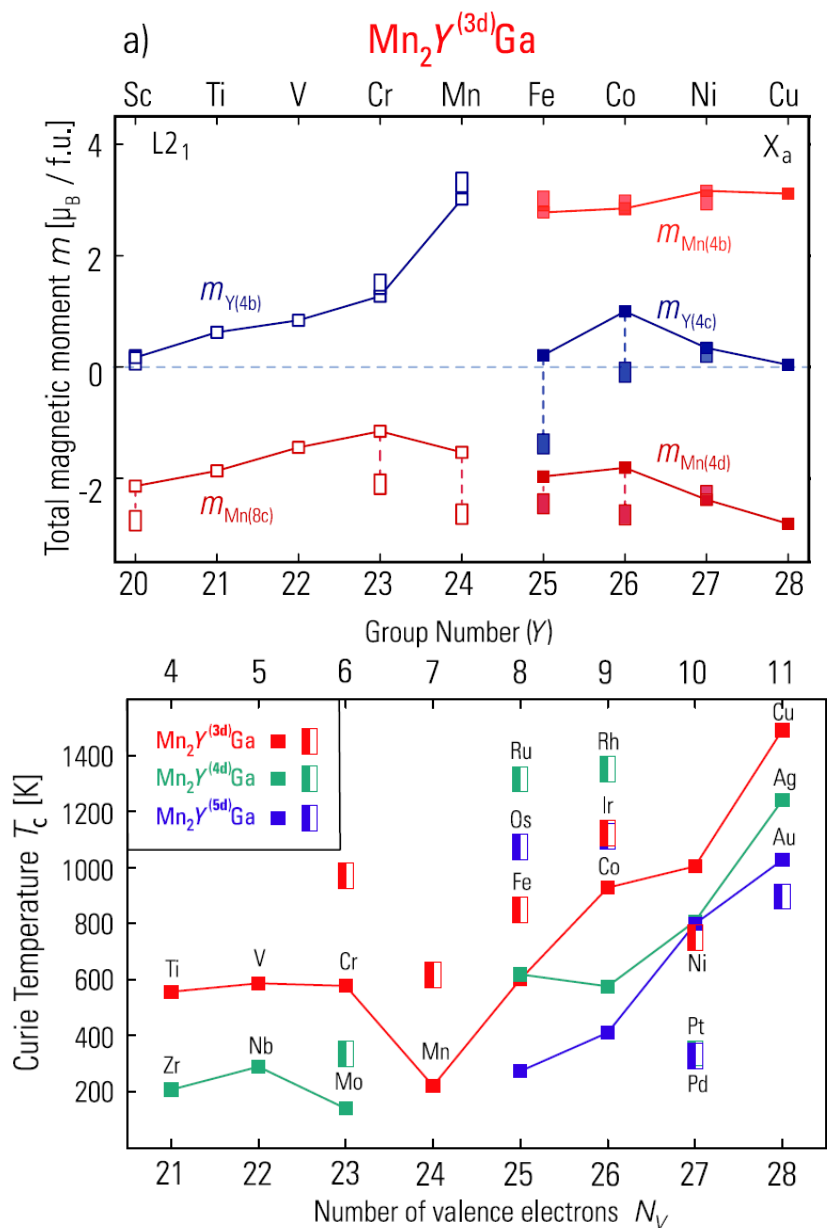


# Tetragonal Heusler



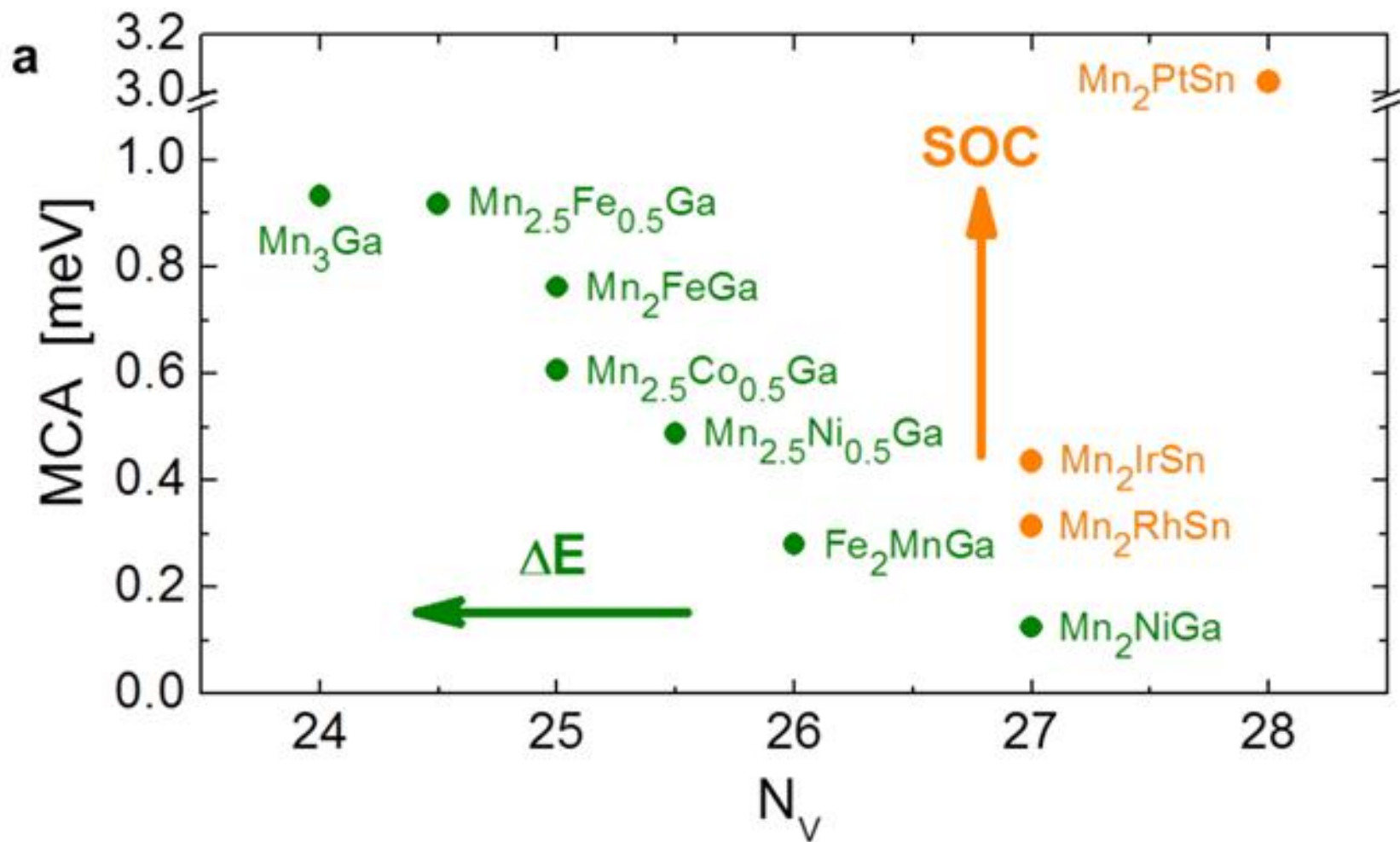


# Magnetocrystalline Anisotropy





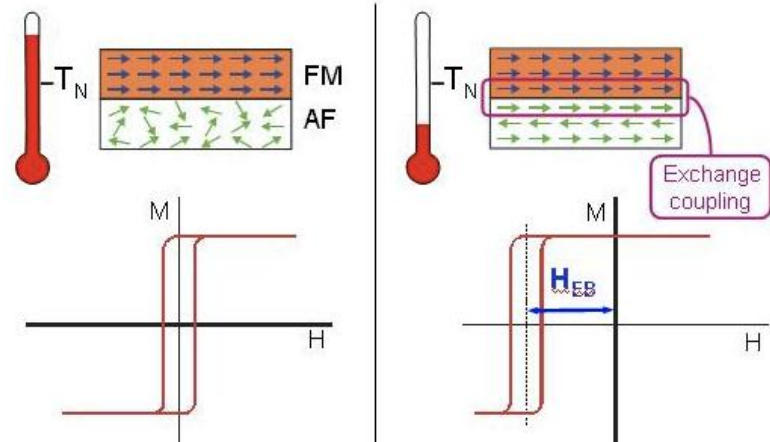
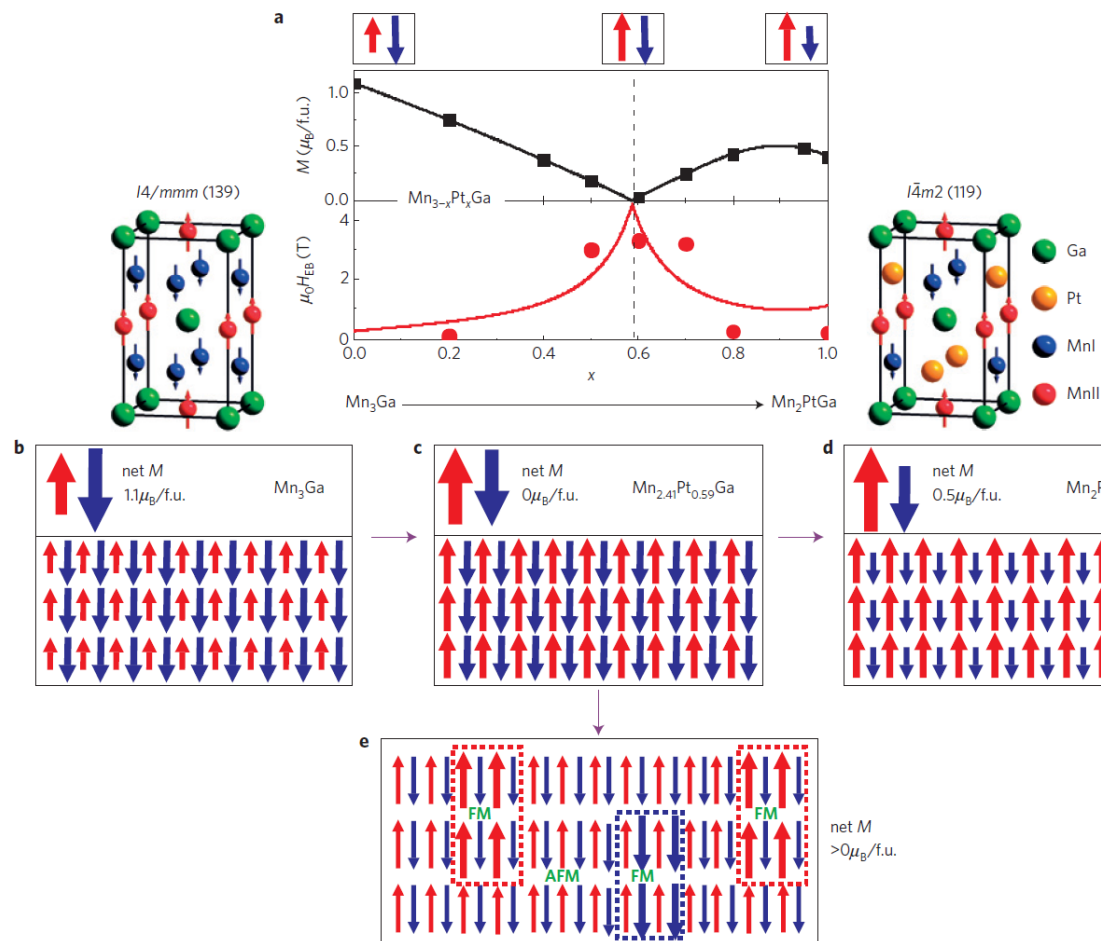
# Heuslers with SOC – DM interaction





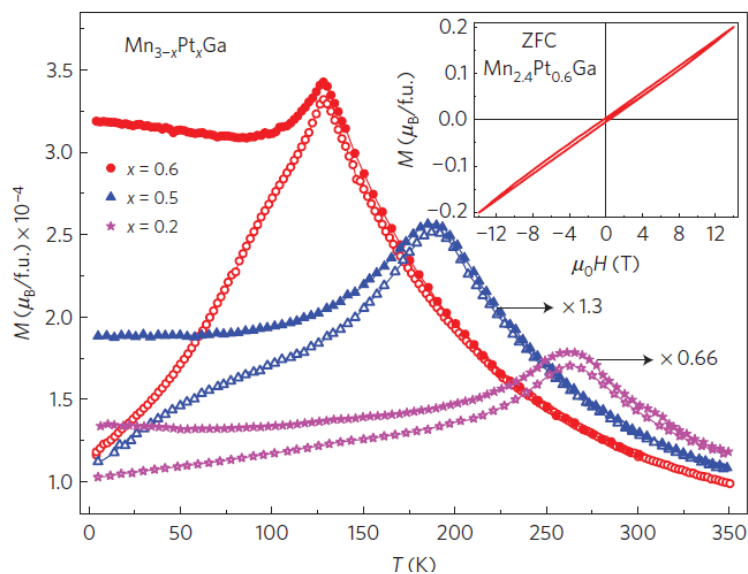
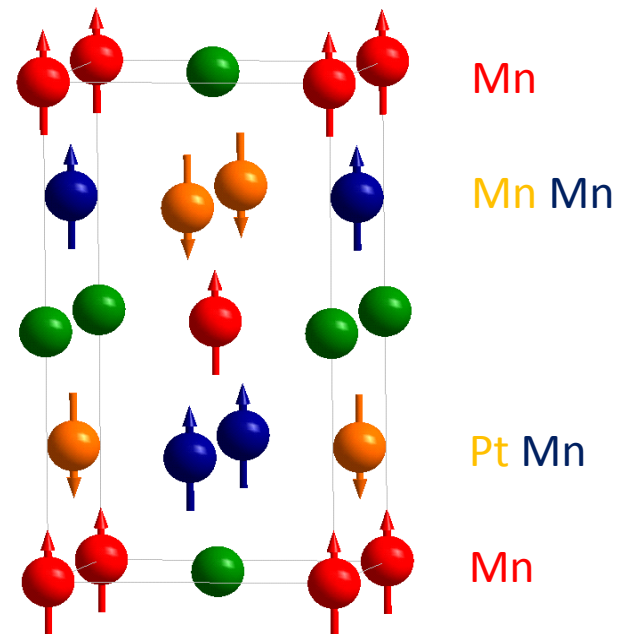
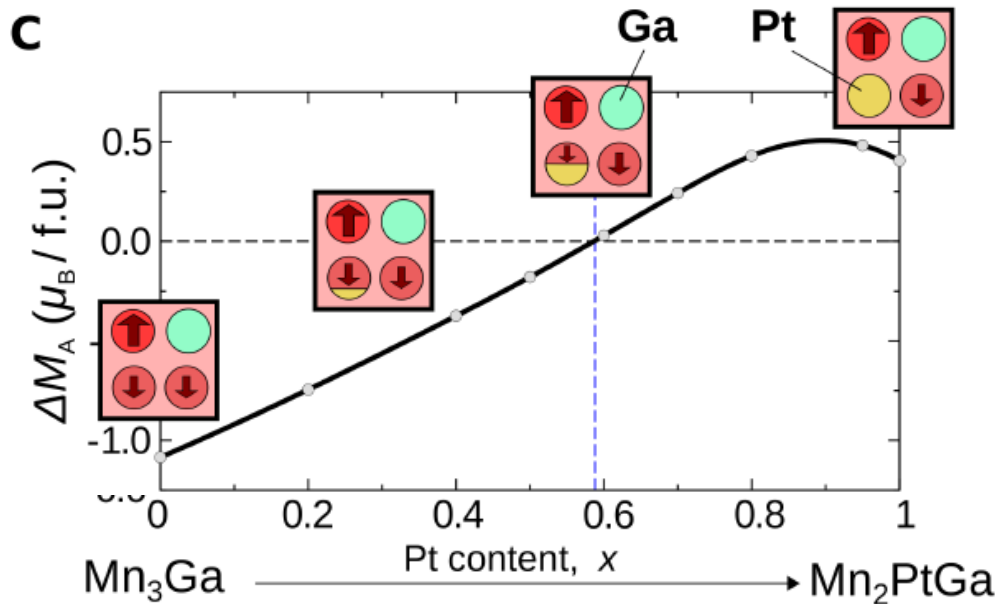
# Design of compensated ferrimagnetic Heusler alloys for giant tunable exchange bias

Ajaya K. Nayak<sup>1\*</sup>, Michael Nicklas<sup>1</sup>, Stanislav Chadov<sup>1</sup>, Panchanana Khuntia<sup>1</sup>, Chandra Shekhar<sup>1</sup>, Adel Kalache<sup>1</sup>, Michael Baenitz<sup>1</sup>, Yuri Skourski<sup>2</sup>, Veerendra K. Gudur<sup>3</sup>, Alessandro Puri<sup>3</sup>, Uli Zeitler<sup>3</sup>, J. M. D. Coey<sup>4</sup> and Claudia Felser<sup>1\*</sup>





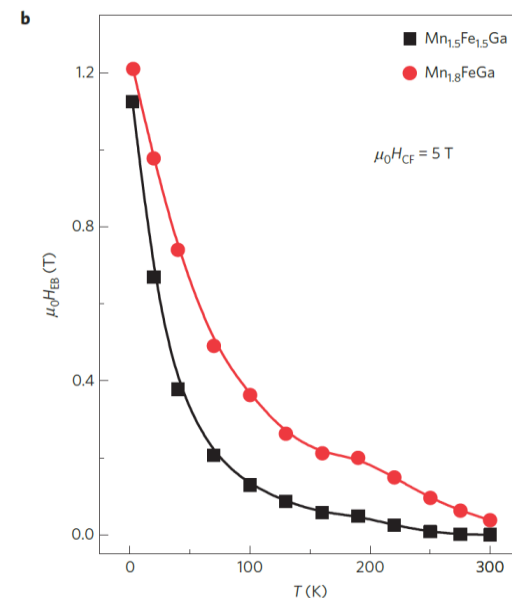
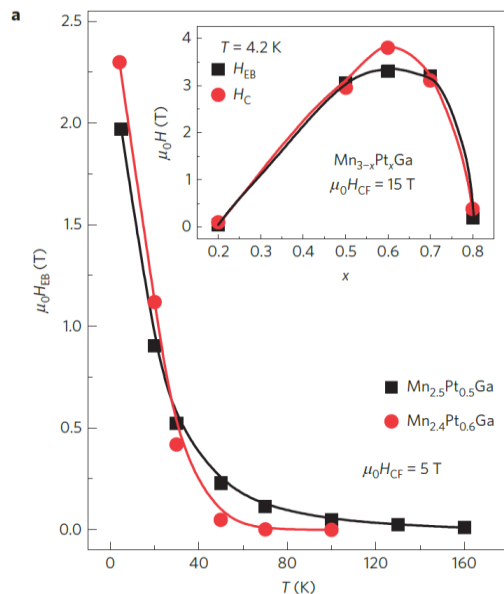
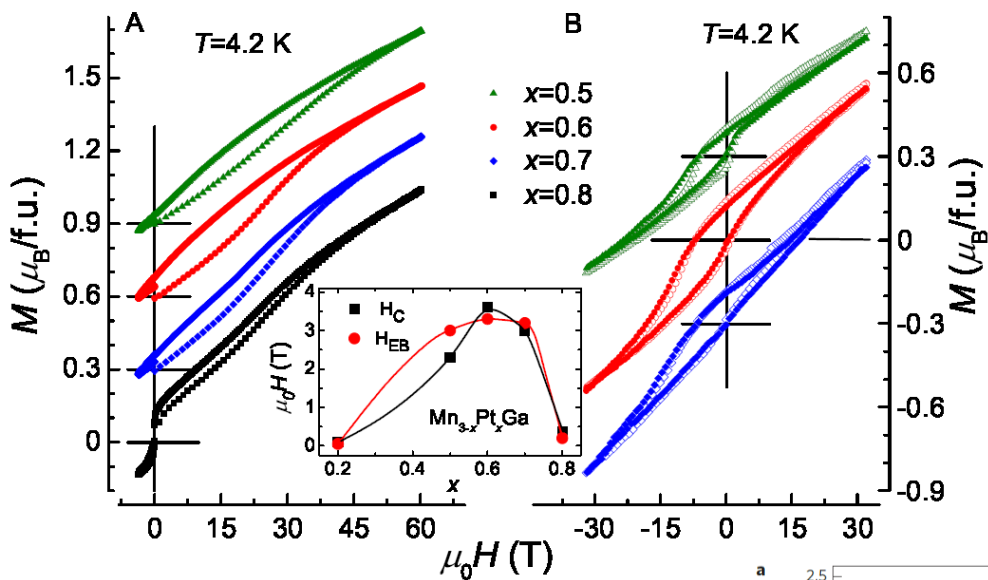
# Artificial AFM or compensated ferrimagnet



Ajaya K. Nayak, et al PRL 110 (2013) 127204  
Ajaya K. Nayak, et Nature Materials (2015) doi:10.1038/nmat4248



# Artificial AFM or compensated ferrimagnet







# Magnetic orderings in Heusler compounds

Half-metallic ferromagnetism:  $\text{Co}_2\text{MnZ}\dots$



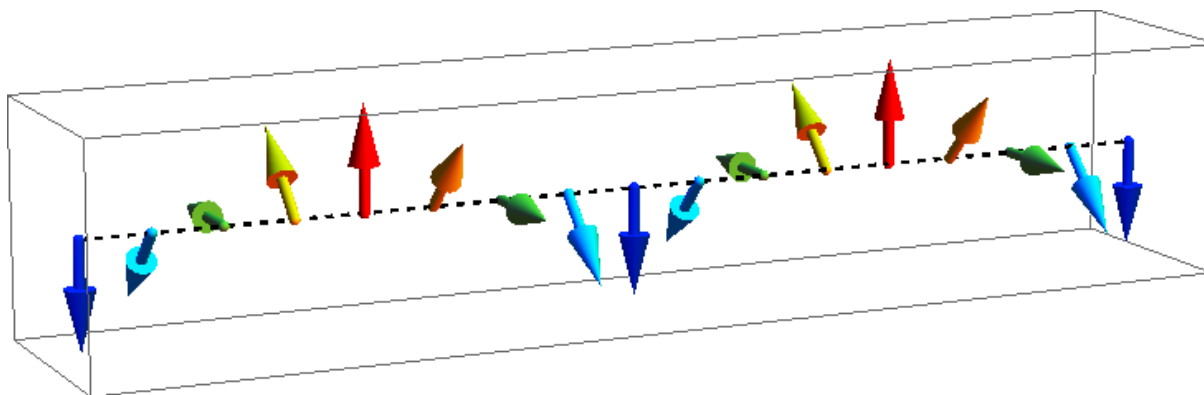
Half-metallic ferrimagnetic:  $\text{Mn}_2\text{YZ}$

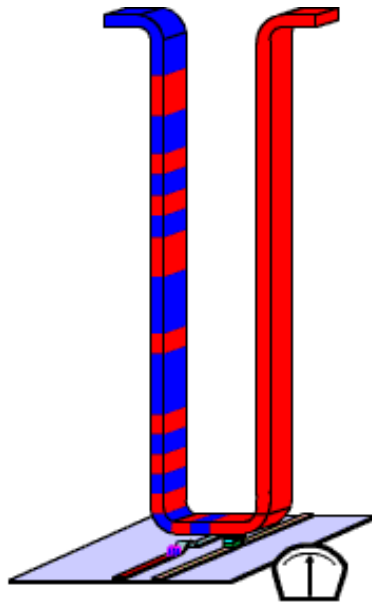


Antiferromagnetic:  $\text{Mn}_3\text{Si}$ ,  $\text{Fe}_2\text{VSi}$ ,  $\text{Ru}_2\text{MnGe}$ ,

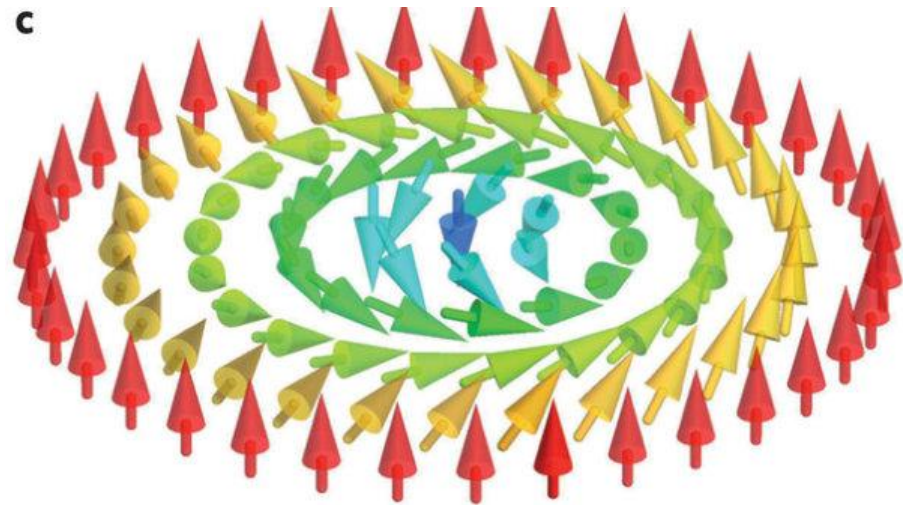


Compensated ferrimagnetic:  $\text{Mn-Pt-Ga}$ ,  $\text{Mn-Co-Ga}$





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



## Skyrmions on the track

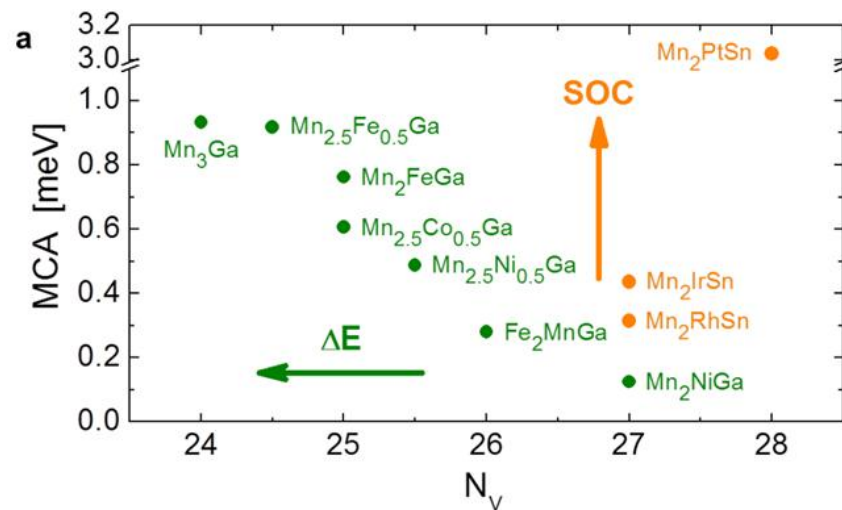
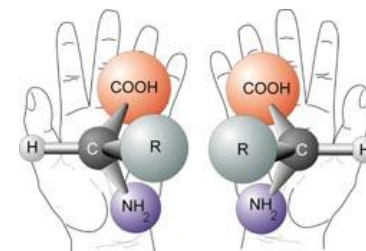
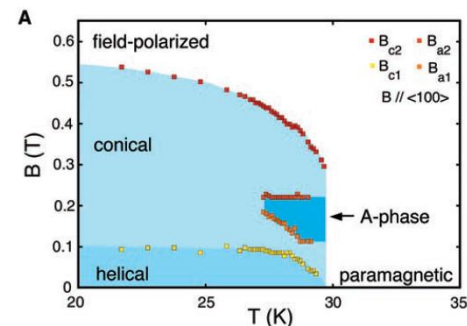
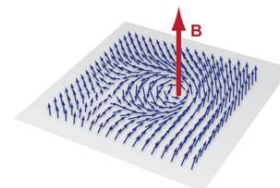
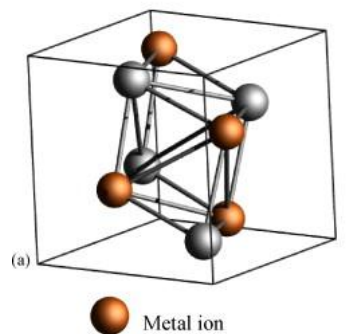
Albert Fert, Vincent Cros and João Sampaio

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.



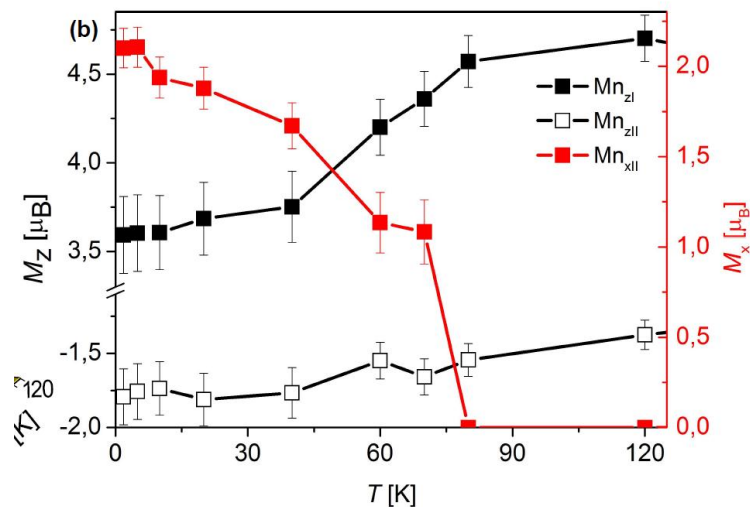
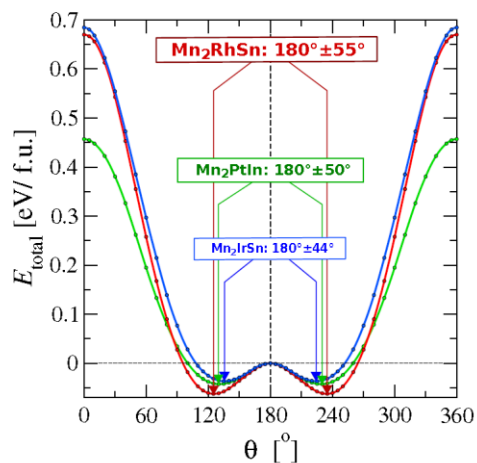
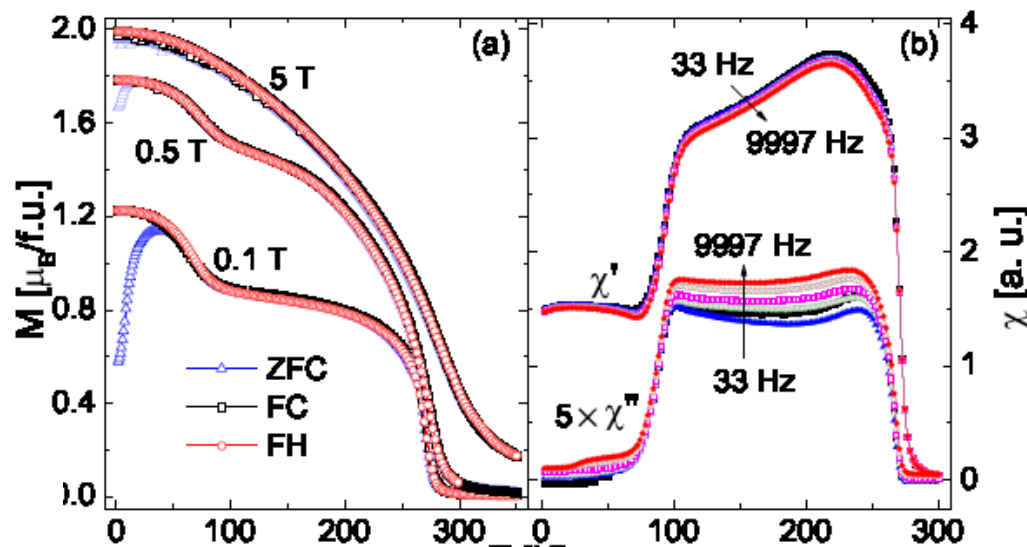
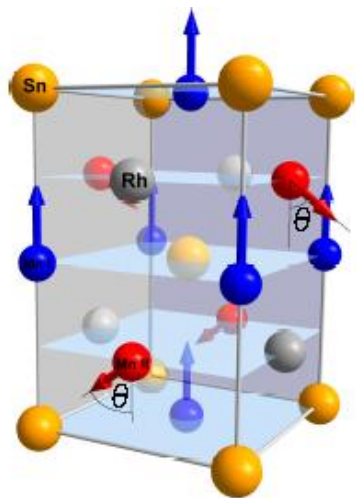
# Recipe

- 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



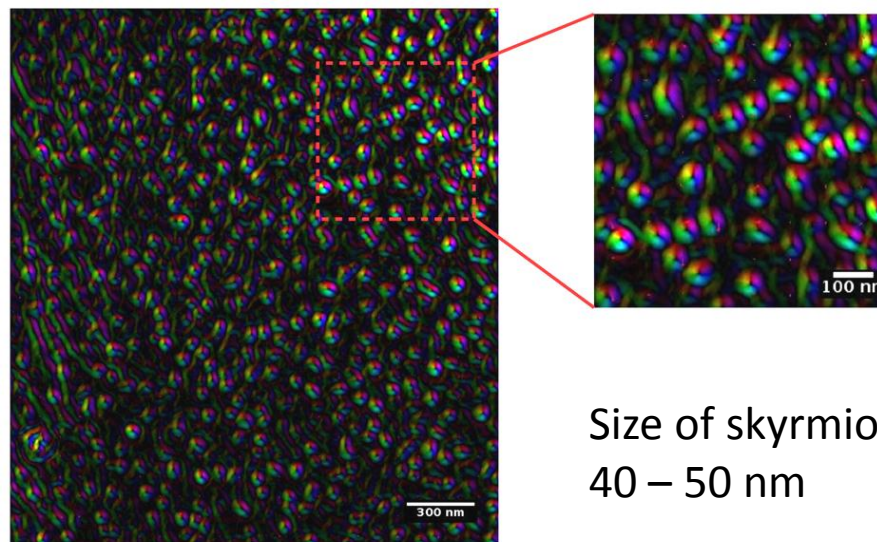
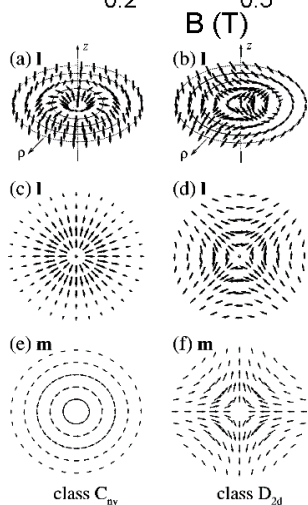
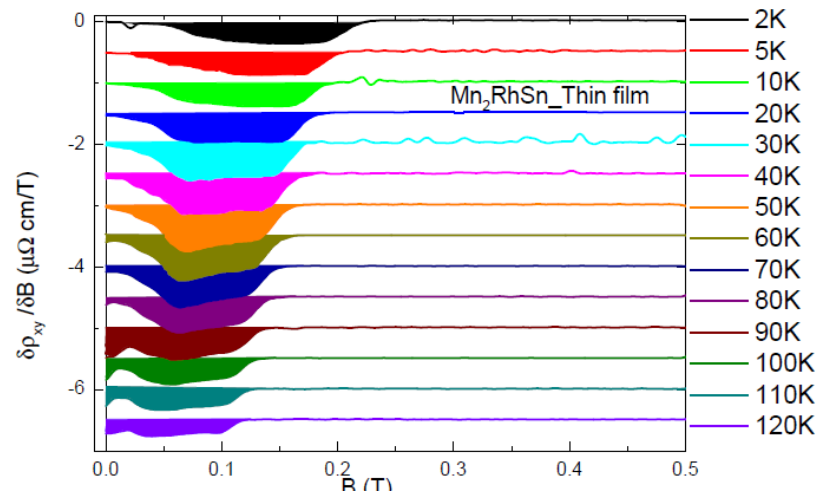
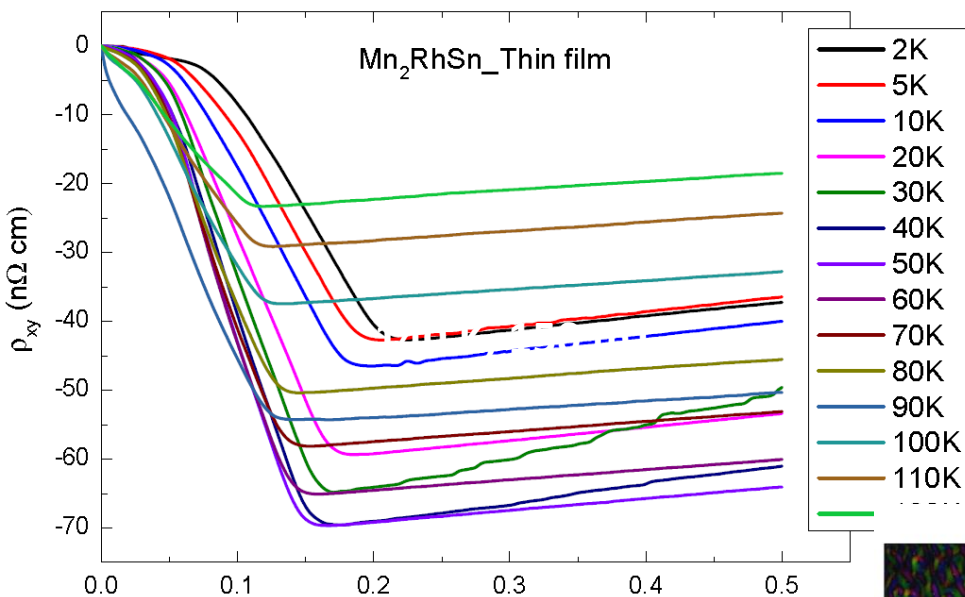


# Mn<sub>2</sub>RhSn – non collinear magnet





# Skyrmions

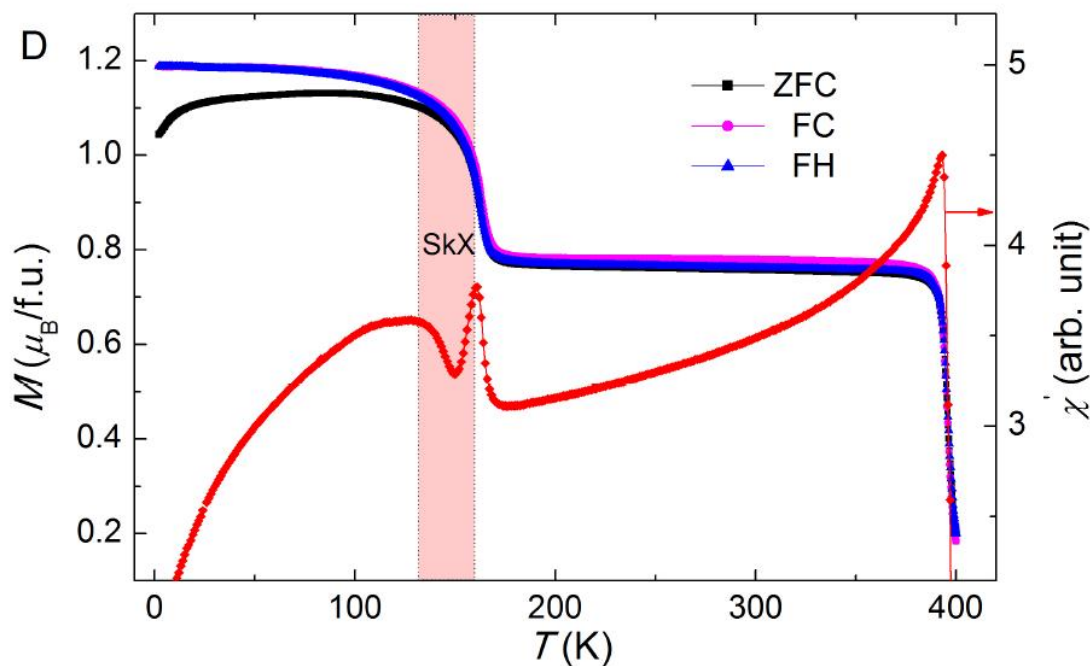
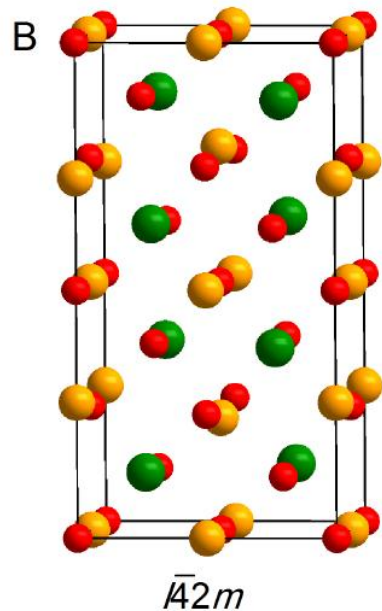
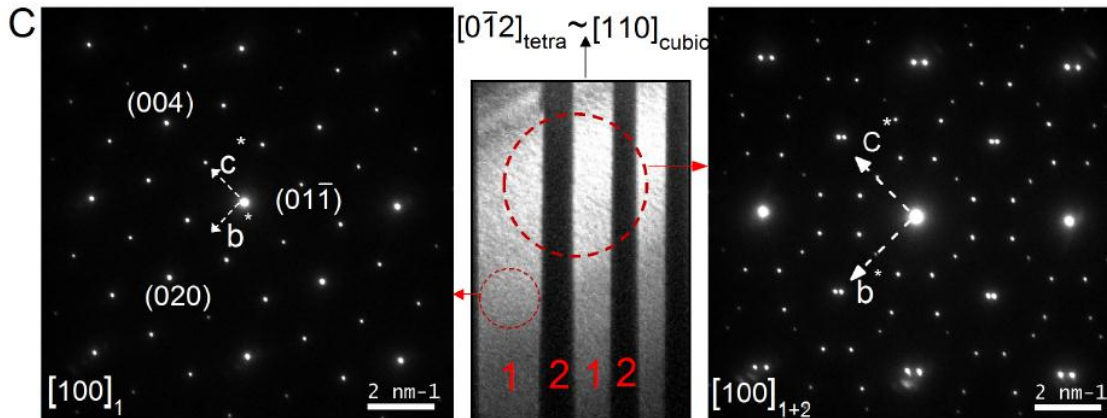
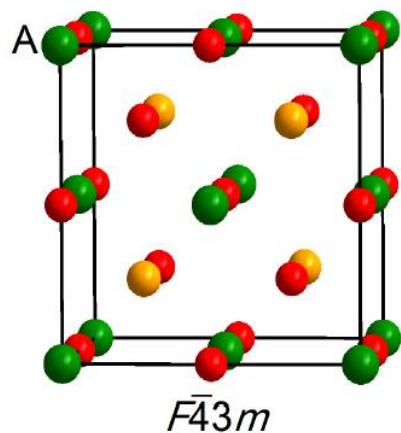


Size of skyrmion ~  
40 – 50 nm

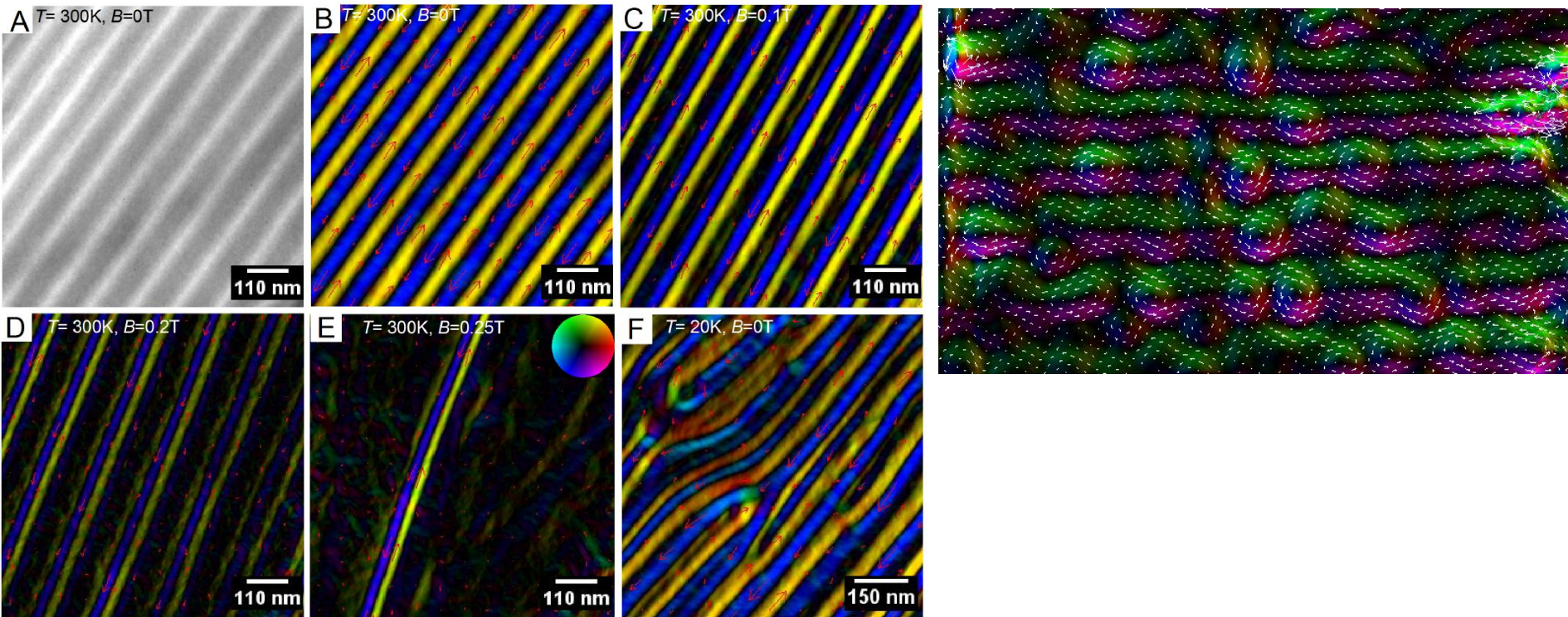




# Mn-Pt-Sn – Skyrmions







- 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  $[110]$ .



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