Heusler Compounds: Multifunctional Materials for Spintronics

Claudia Felser
www.superconductivity.de

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Synchrotron: SPring8, Japan K. Kobayashi and team ; Chuck Fadley LBNL, USA
PETRAIII, Drube, Claessen, Würzburg

Concept

Goal: Directed Design of new functional Materials

Preconditions for a Designer Material

- Reliable structure type - Heusler structure type
- Tunable class of Materials (800 existing compounds)
- Compounds with different properties
- Understanding structure-property relationships
- Development of a properties-oriented recipe

- Multifunctional Materials → Ternary … Multinary Materials moment

Properties

Property	Example	Discovered	Rule
Ferromagnetism	Cu_2MnZ	Heusler	
Half metallic ferromagnetism	NiMnSb Co_2YZ	De Groot, Kübler Galanakis, Felser	Slater Pauling
Magneto optical application	MnPtSb	Vanengen	22 VE
Heavy Fermions	Fe_2VAl, YbPtBi	Lui, Fisk	24 VE 18 VE
Superconductivity	Ni_2ZrSn	Felser	27 VE
Multiferroics – Shape memory	Ni_2MnGa, Mn_2NiGa	Webster, Liu	Jahn Teller
Ferrimagnets and compensated ferrimagnets	Mn_2YZ Cr_2YZ,	Felser	Jahn Teller
Semiconductors for optoelectronics	LiZnP, LiCuS	Zunger, Felser	8 VE Wide gap
Topological Insulators	REPtBi	Felser	18VE and high Z

Concept

Goal: Directed Design of new functional Materials

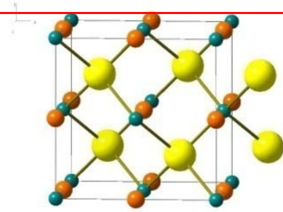
Computational Design
(LDA and beyond
Monte Carlo)

Advanced measurements
Hard Xray
Photoemission spectroscopy

Synthesis
Single crystals, thin films

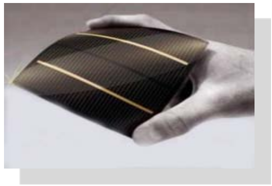
Properties

- Semiconductors

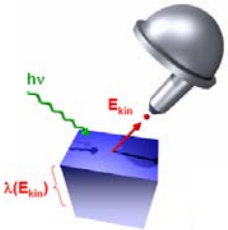


- Thermoelectrics

- Solar cells

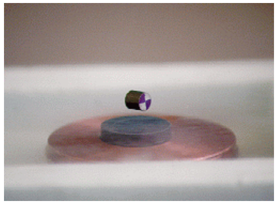


- Hard x-ray PES



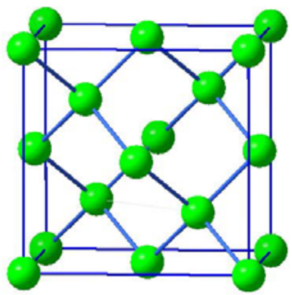
- Spintronics

- Superconductivity

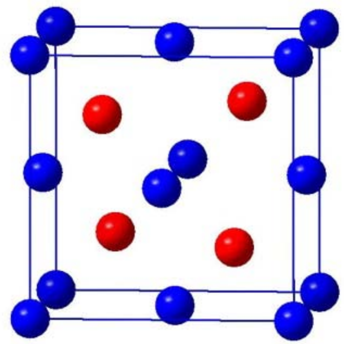


Half Heusler: Ternary Semiconductors

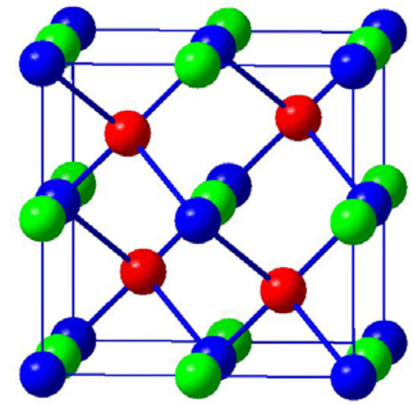
Diamond

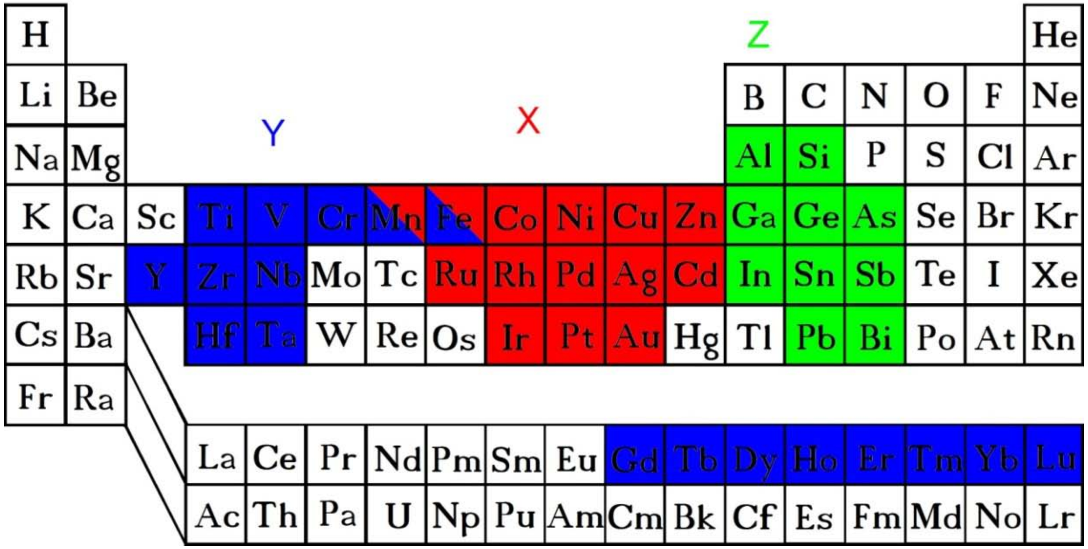


XY



XYZ

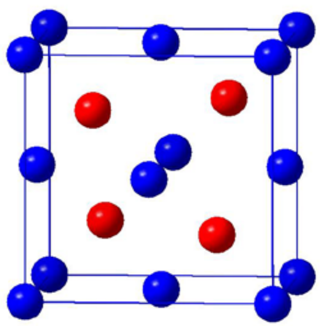


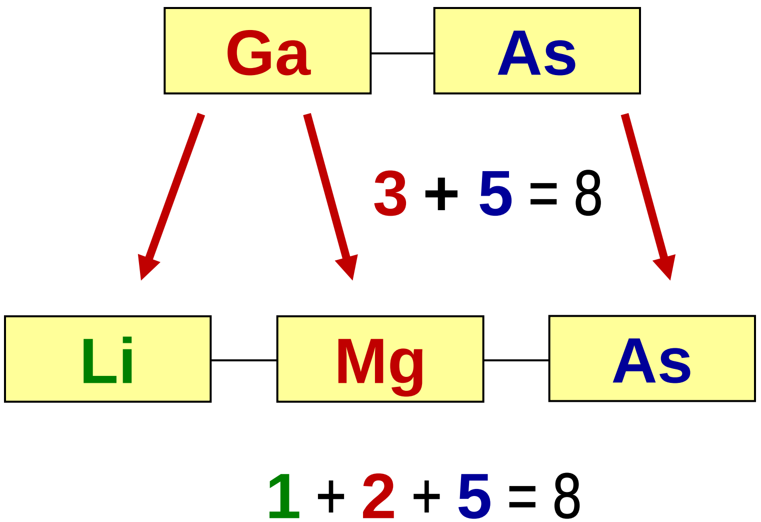


Materials: ternary semiconductors …

Zincblende structure

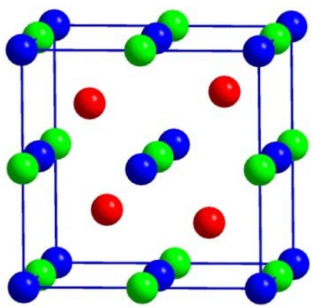
YZ





Half Heusler Structure

XYZ



Semiconductors

- with the magic electron number 8

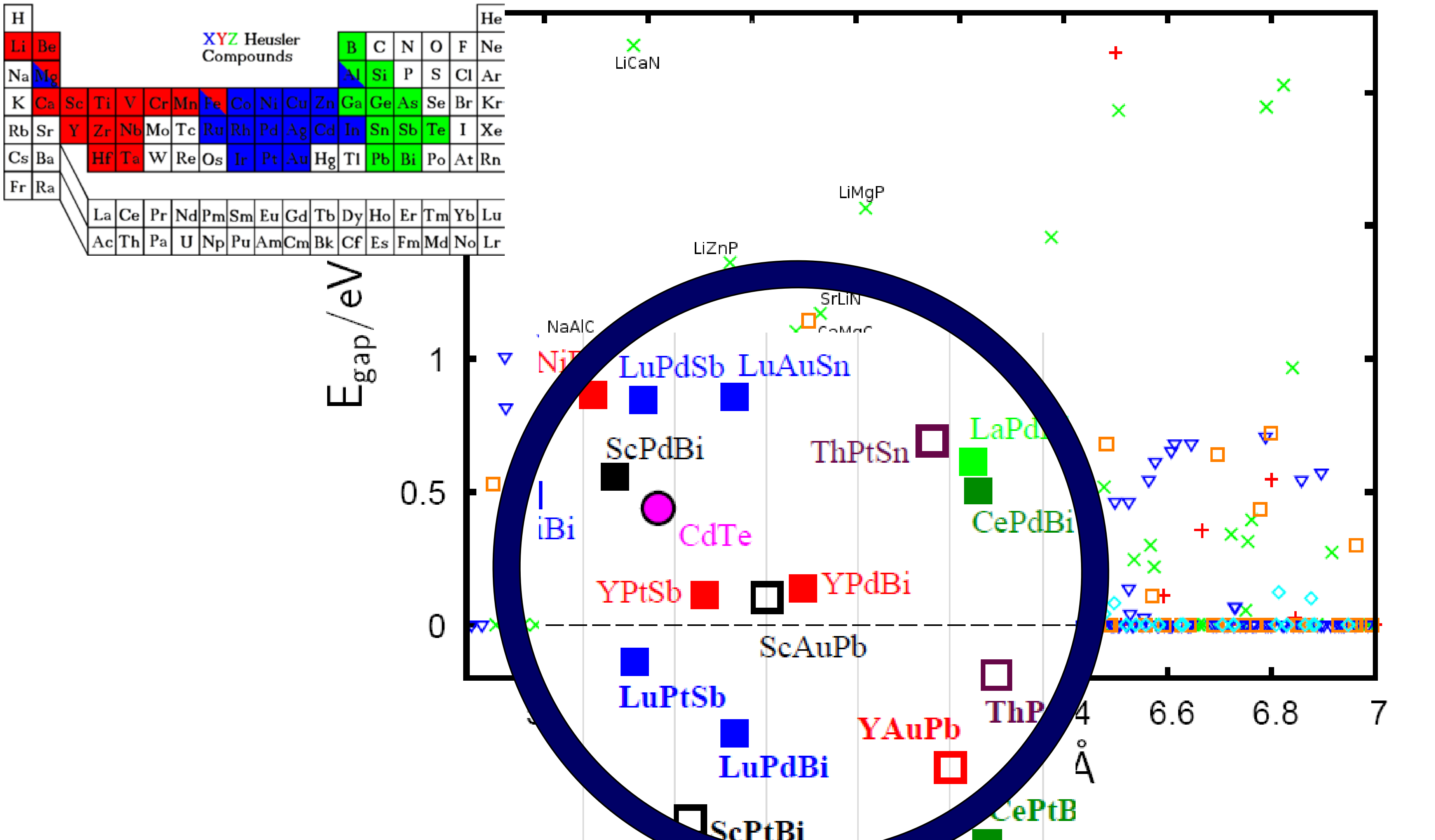
Half Heusler or Juza-Nowotny compounds

- Filled tetrahedral structures: Li^{+} $[MgAs]^{-}$ YZ
- NaCl Lattice between XZ

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

Ternary Semiconductors … zero gap

Half Heusler compounds XYZ with variable gaps



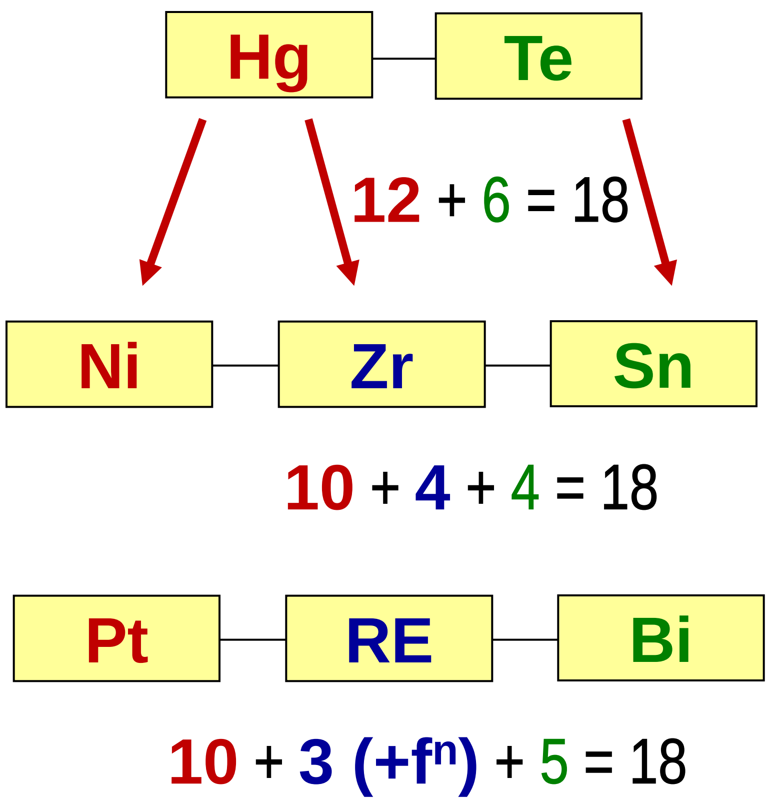
Kieven et … 81 (2010) 075208 , patent submitted

Ternary semiconductors … low band gap

Low band gap semiconductor for

- Thermoelectric materials
- Topological Insulators

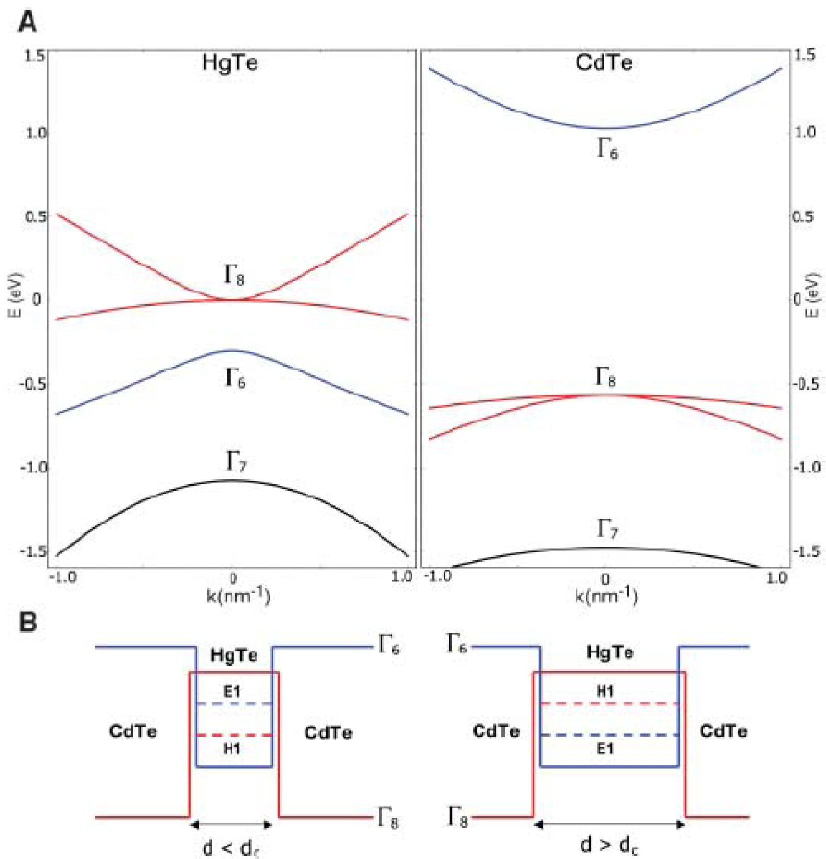
- the f-electrons are localized … the compounds stay semiconducting

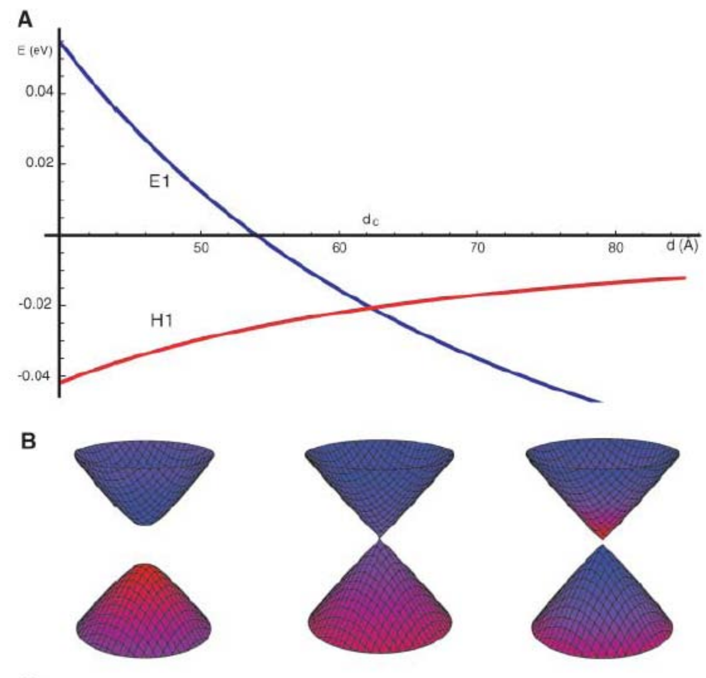


- ZnS lattice YZ
- NaCl Lattice between XZ

Zero gap

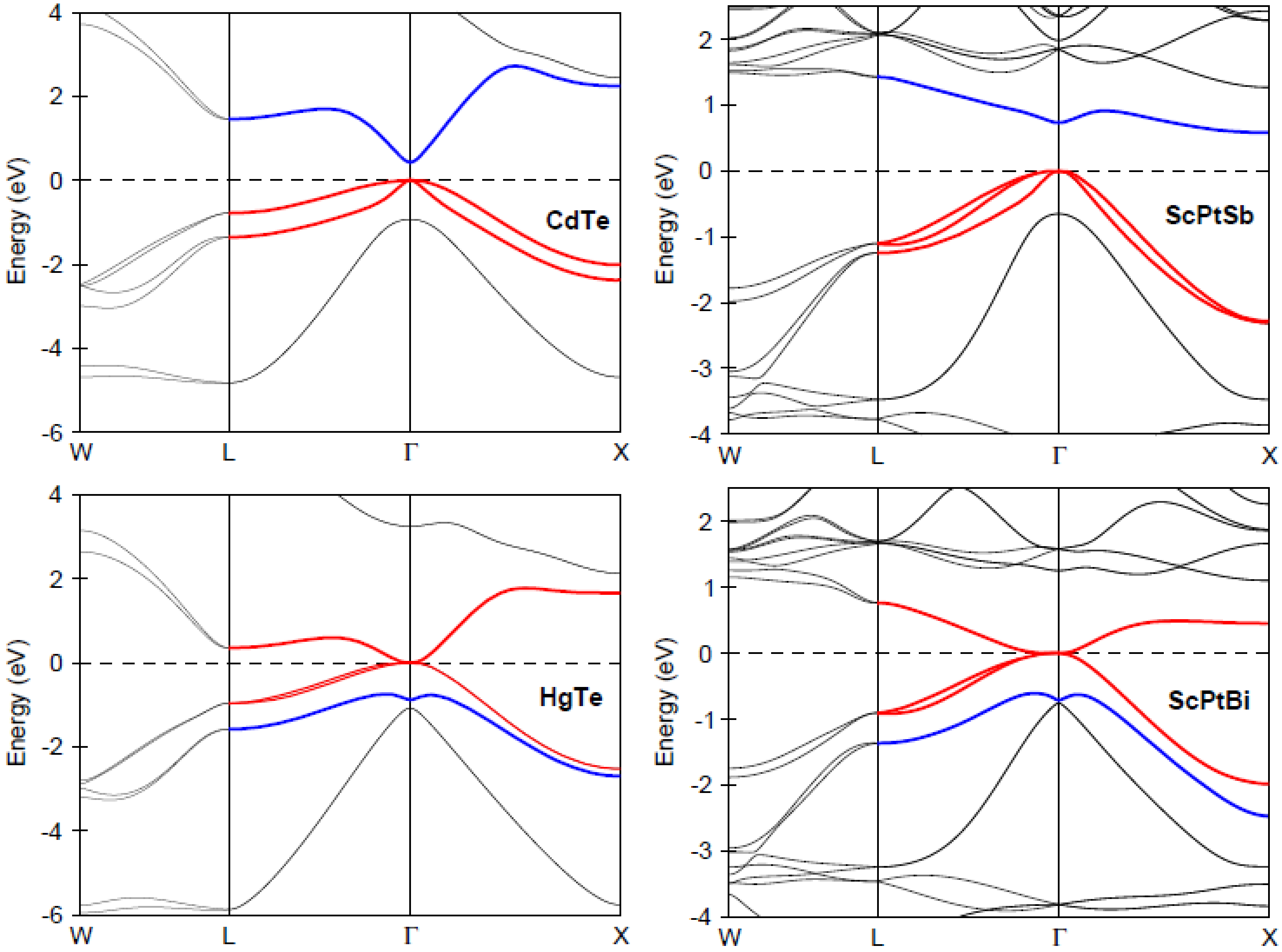
Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells
B. Andrei Bernevig, *et al.*
Science **314**, 1757 (2006);
DOI: 10.1126/science.1133734





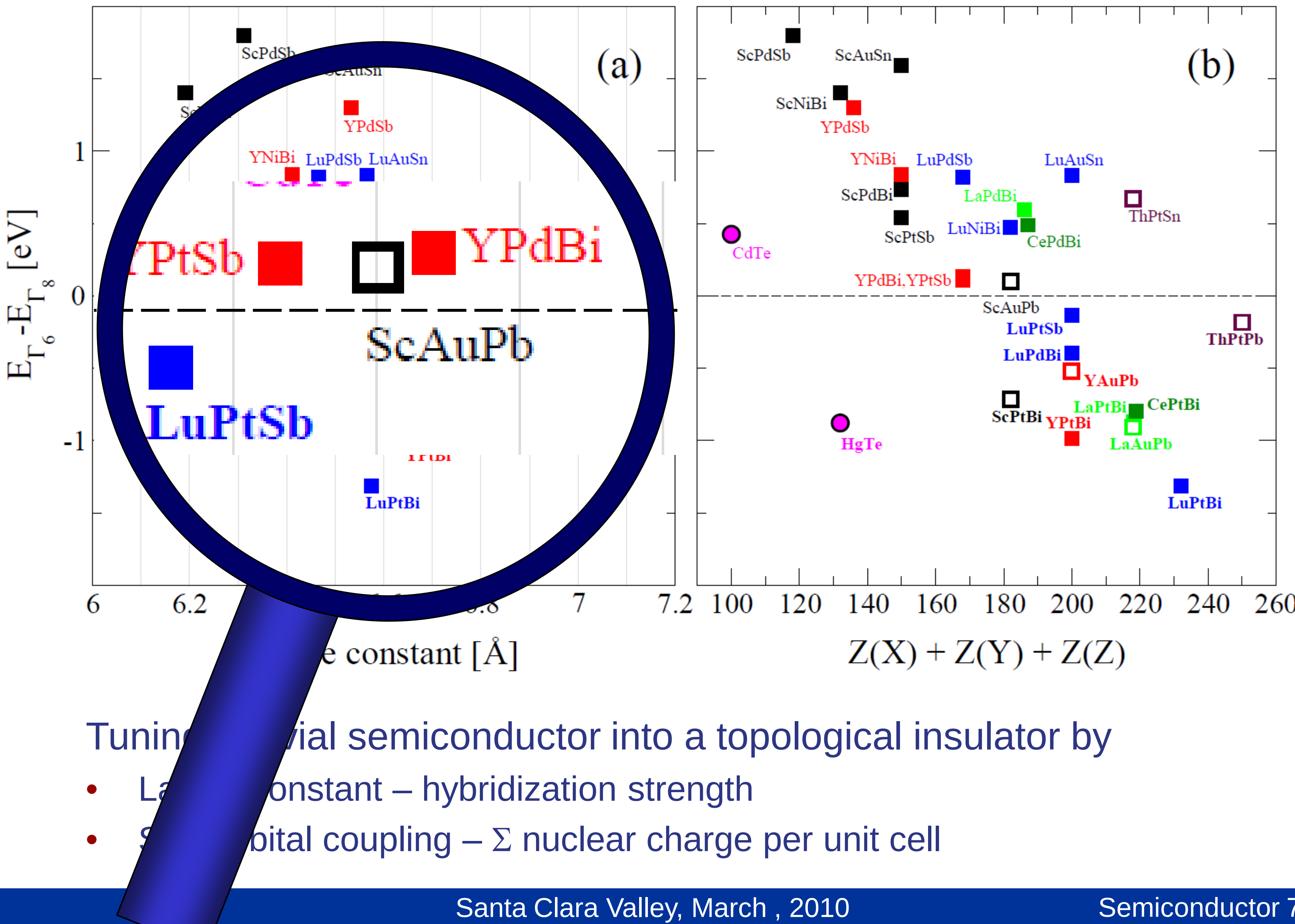
SC Zhang et al.

Zero gap: fingerprints, binaries→ternaries



Chadov, Qi, Kübler, Zhang, Felser arXiv:1003.0193

Zero gap: tunable ternary Heuslers



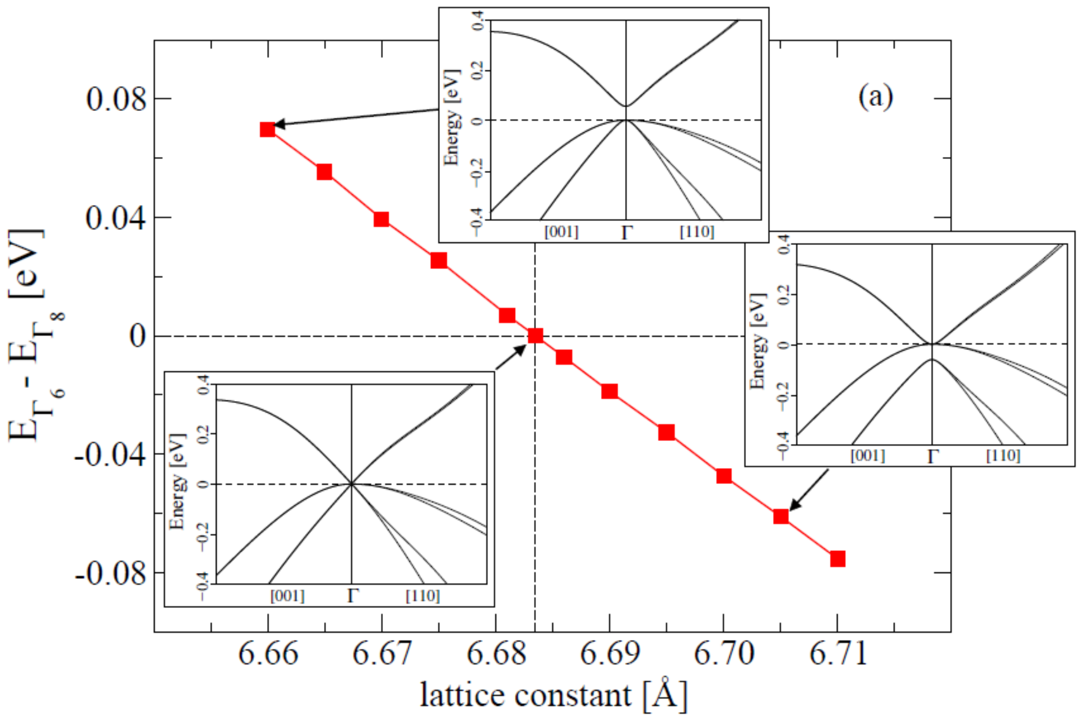
Tunin[...]vial semiconductor into a topological insulator by

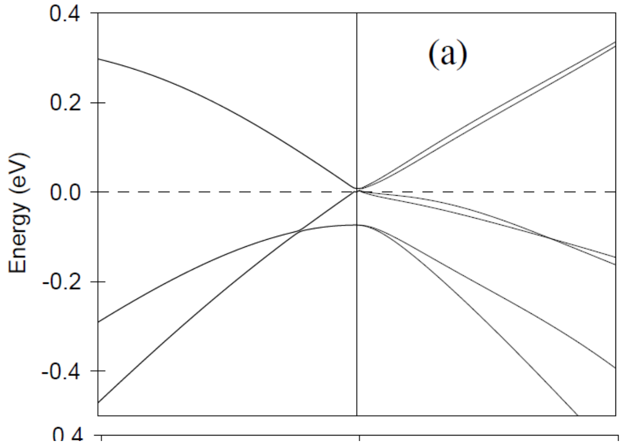
- La[...]onstant – hybridization strength
- S[...]bital coupling – Σ nuclear charge per unit cell

Zero gap: strain

Proof of the topological character

- Taking the borderline compound
- Applying strain
- A gap will be opened and the Dirac cone stays in the gap (a)





Chadov, Qi, Kübler, Zhang, Felser arXiv:1003.0193

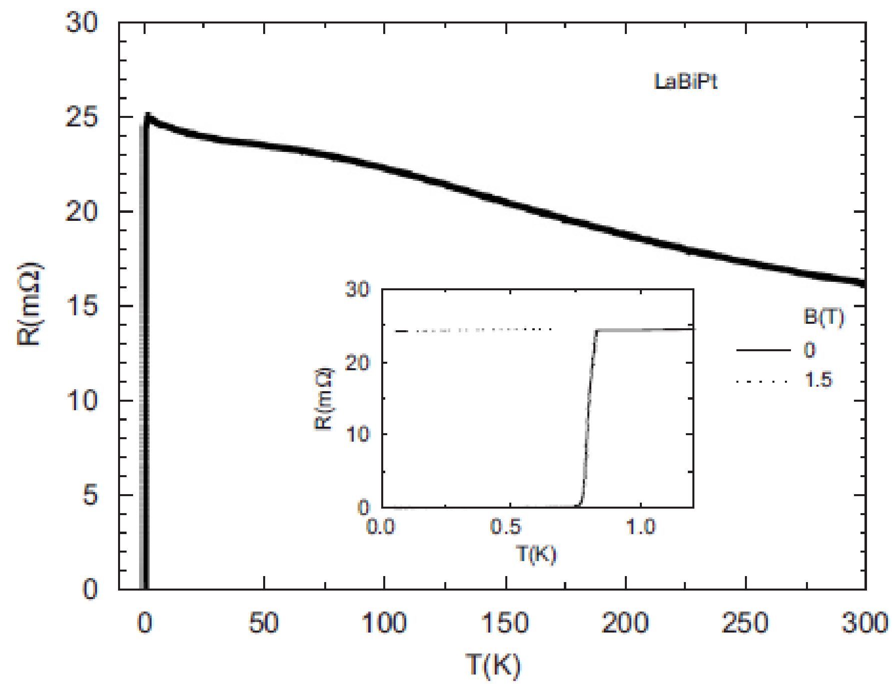
REPtBi … multifunctional topologic insulators

Tuning the propoerties with RE atom

Pt — RE — Bi

10 + 3 (+f^n) + 5 = 18

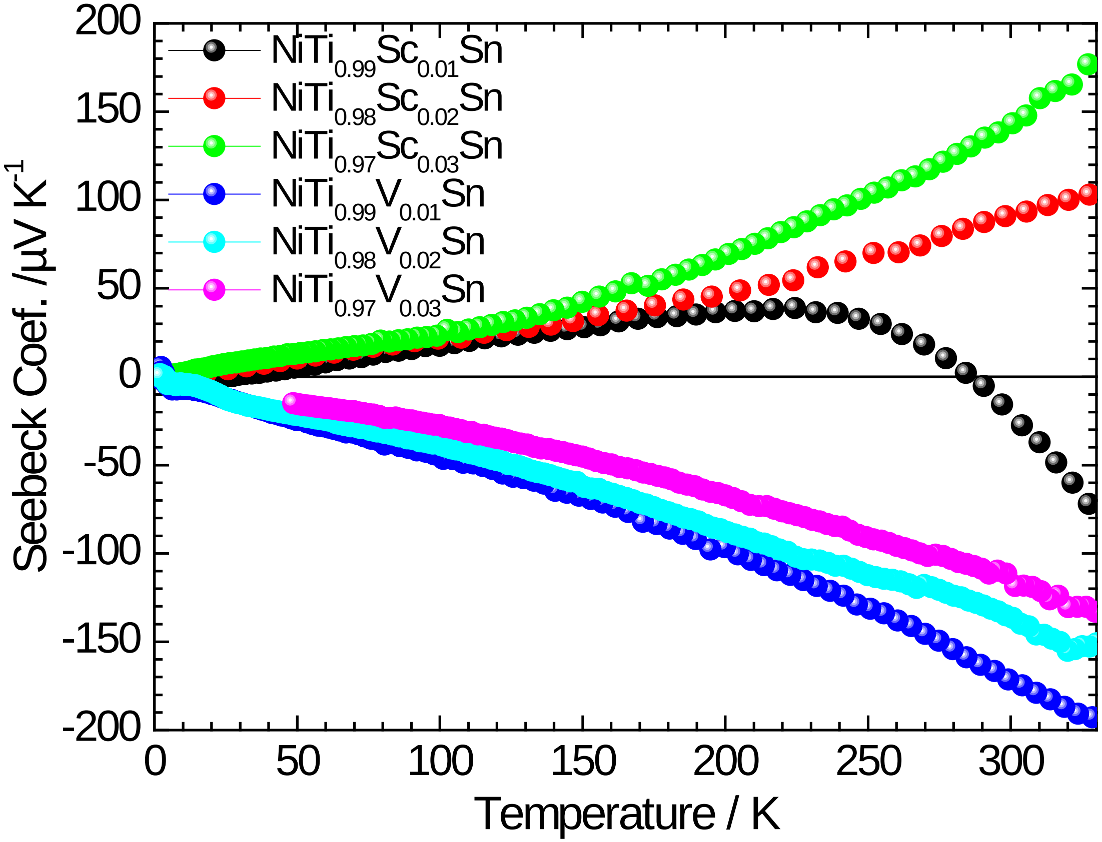
- LaPtBi is also a topological superconductor without inversion symmetry and low charge carrier concentration n = $6*10^{18}cm^{-3}$
- Antiferromagnetism with GdPtBi
- Ferromagnetism in MnPtBi
- YbPtBi is a super heavy fermion
- Fermi energy tunable with magnetic fields, e.g., CePtBi



All TI are good thermoelectrics

Goll *et al.* Physica B 403 1065 (2008)

One material … from p to n

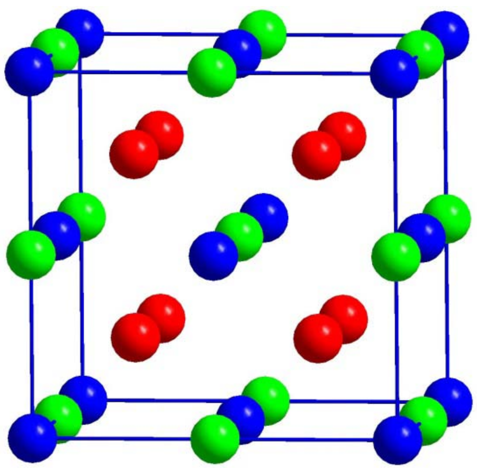


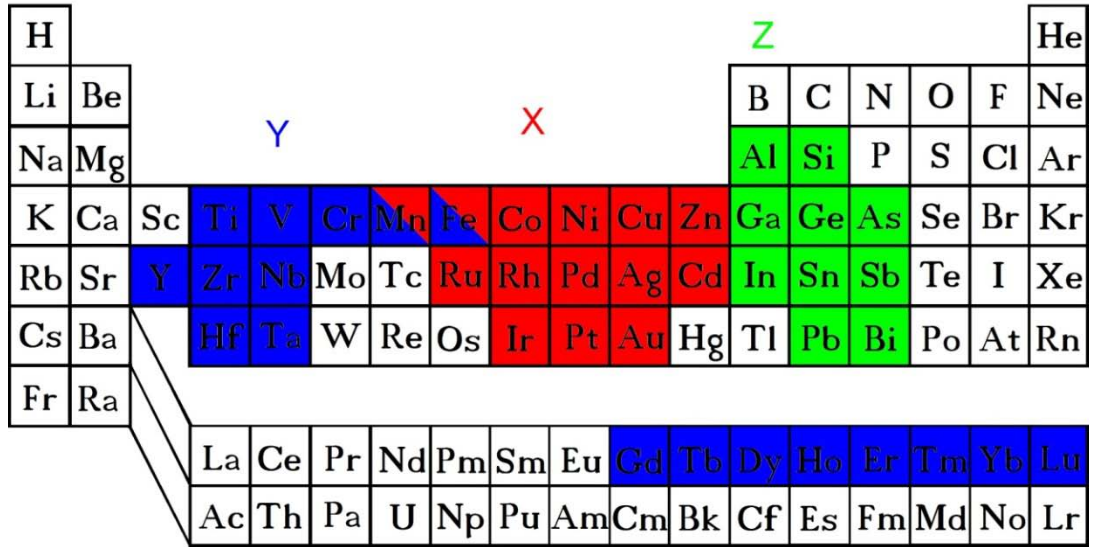
Important for manufacturing (same thermal expansion coefficient)

p- and n-doping in the same material NiTiSb

Starting point

Heusler compounds: X_2YZ





CCFA - $Co_2Cr_{0.6}Fe_{0.4}Al$

1903: First „Heusler“ compound Cu_2MnAl by Friedrich Heusler

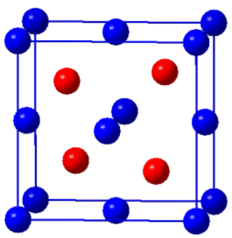
1983: De Groot and Kübler: Prediction of half metallicity

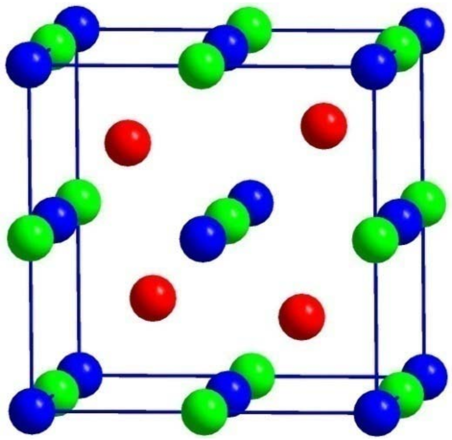
1999: Discovery of CCFA by us (patented with IBM)

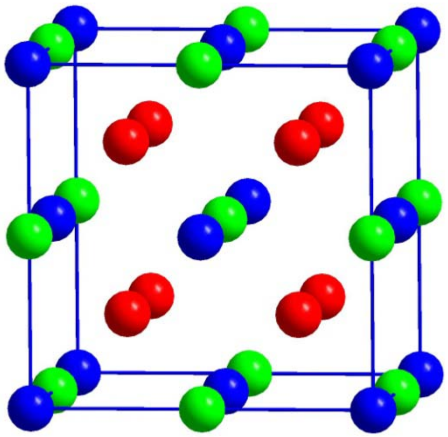
2003: First TMR device with 19% room temperature effect by K. Inomata

Materials: Ternary Semiconductors …

XYZ







X_2YZ

Ga — As

13 + 5 = 18

Co — Ti — Sb

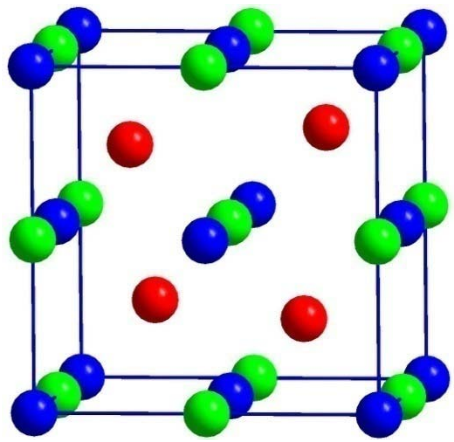
9 + 4 + 5 = 18

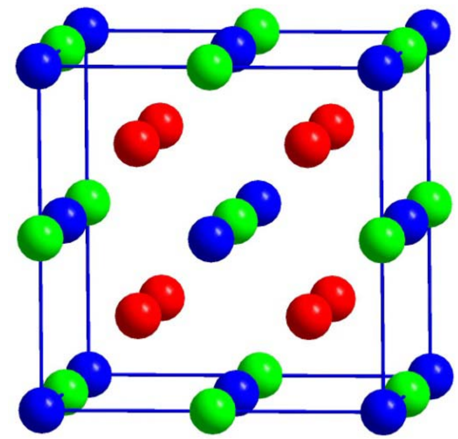
Fe_2 V Al

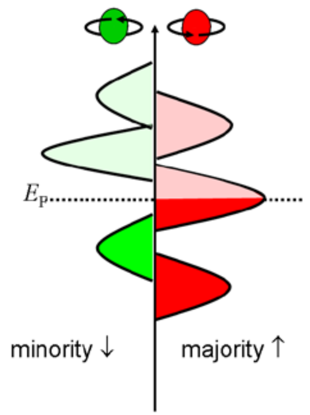
2*8 + 5 + 3 = 24

additional t_2-levels

Half metallic ferromagnets







Pt — **RE** — **Bi**

$10 + 3\ (+f^n) + 5 = 18$

Ni — **Mn** — **Sb**

$10 + 3\ (+d^4) + 4 = 18 + 4$

$4\mu_B$

Fe_2 **V** **Al**

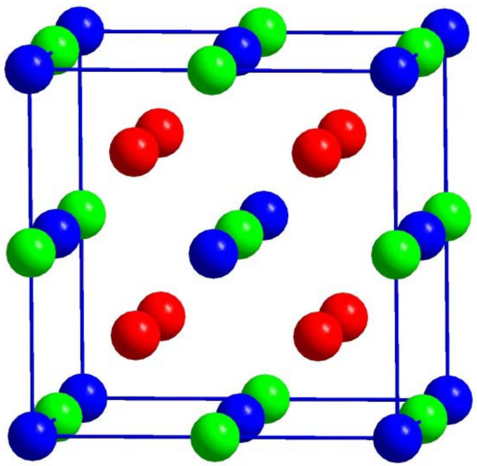
$2*8 + 5 + 3 = 24$

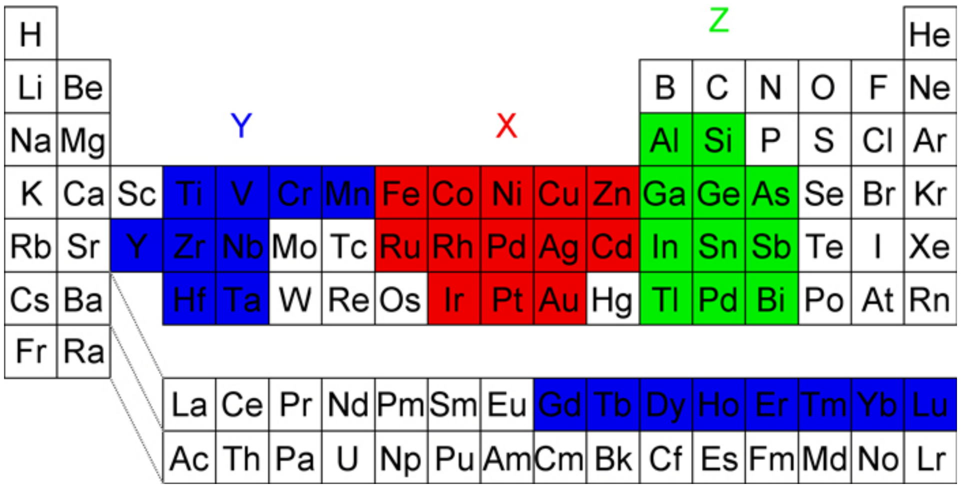
Co_2 — **Mn** — **Si**

$2*9 + 3\ (+d^4) + 4 = 29$

$29-24=5\ \mu_B$

Heusler compounds: X_2YZ





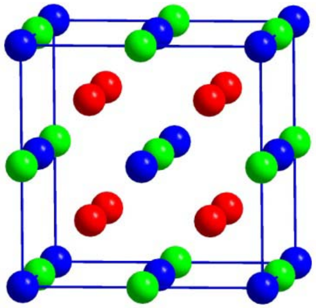
X_2YZ

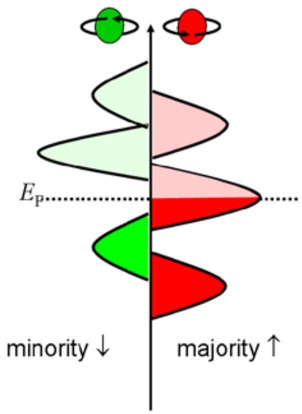
- Y=Mn^{3+} (d^4) (Kübler rule) or another transition element – provides a local magnetic moment $4\mu_B$
- Filled tetrahedral position X leads to a second magnetic sublattice – more delocalized electrons (cobalt can carry up to 1.5 μ_B)

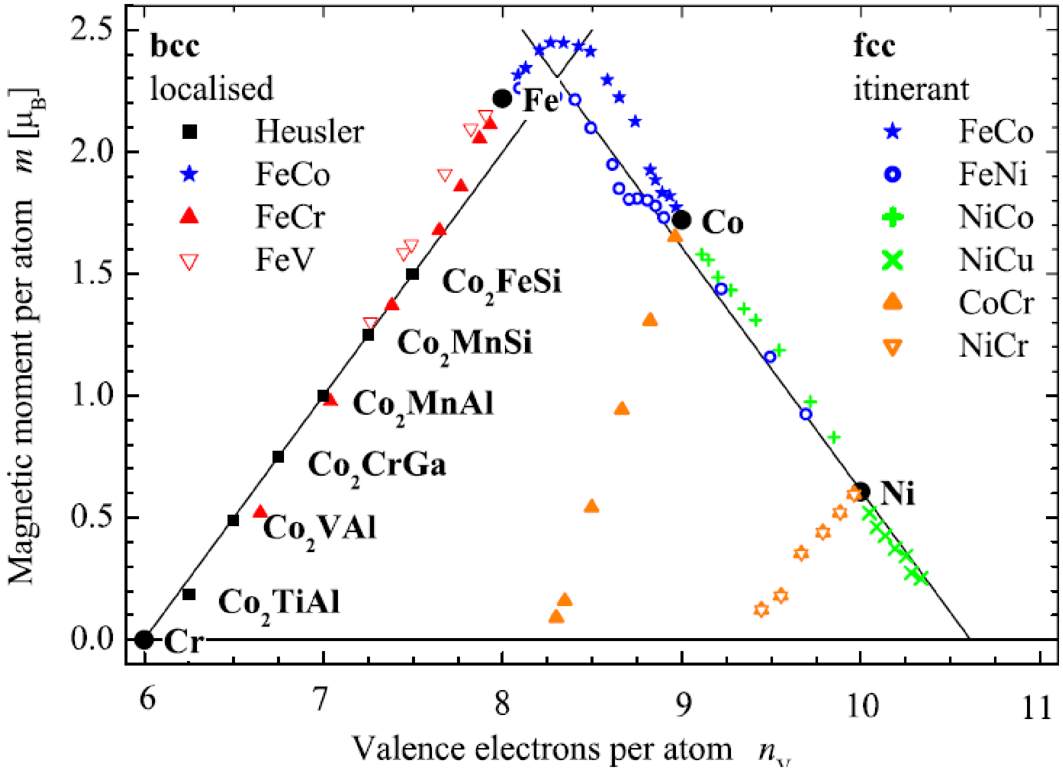
Materials: … to half metallic ferromagnets

Full Heusler compounds

X_2YZ



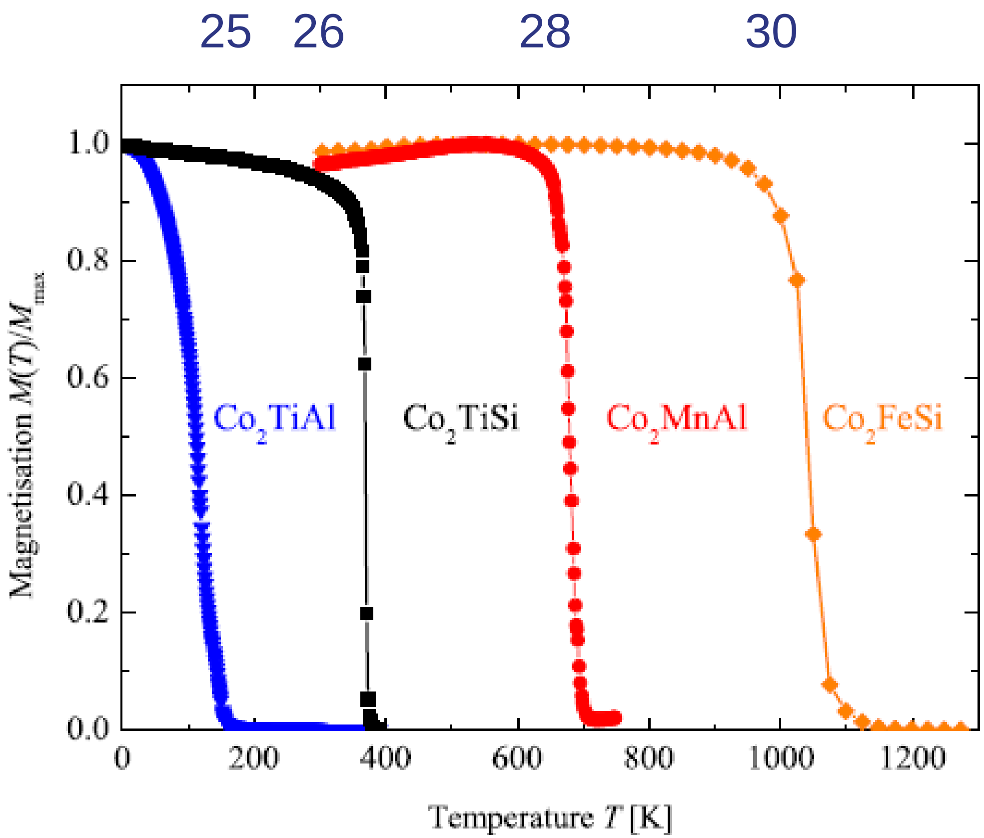




- magic valence electron number: 24
- valence electrons = 24 + magnetic moments
- Co_2FeAl: 2×9 + 8 + 3 = 29 Ms = $5\mu_B$

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

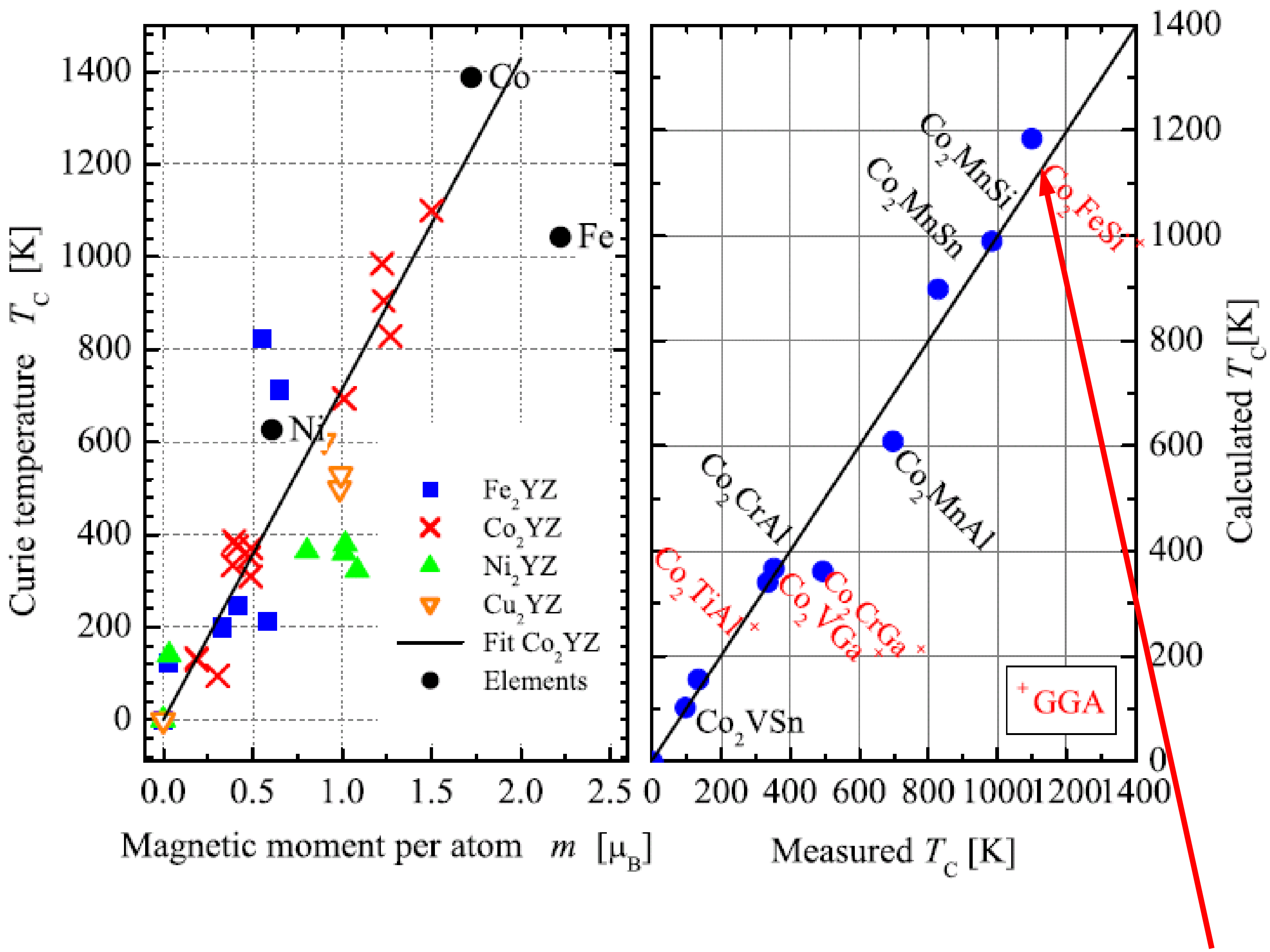
Curie Temperatures



VE	μ_B/atom	T_C [K]
24	0	0
25	0.25	~175
26	0.5	~350
27	0.75	~520
28	1	~700
29	1,25	~970
30	1.5	~1120

Balke *et al.* CF Solid State Com. accepted (2010)
Kübler *et al*. CF, Phys. Rev. B **76** (2007) 024414

High Curie Temperatures

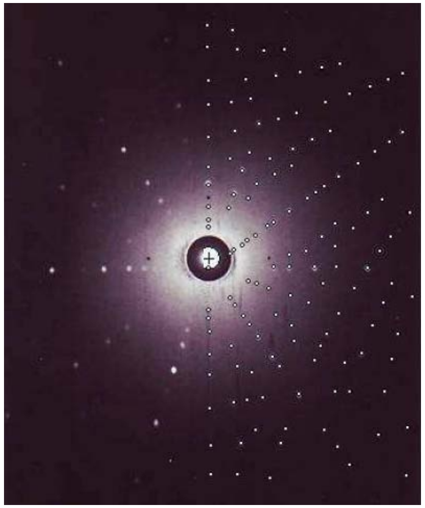


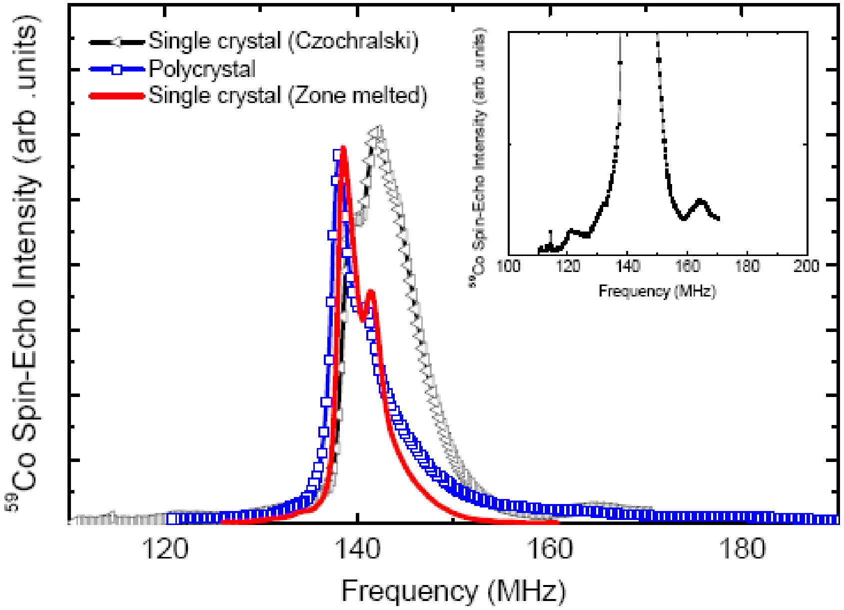
Expected Curie temperature for *Co_2FeSi* : > 1000K

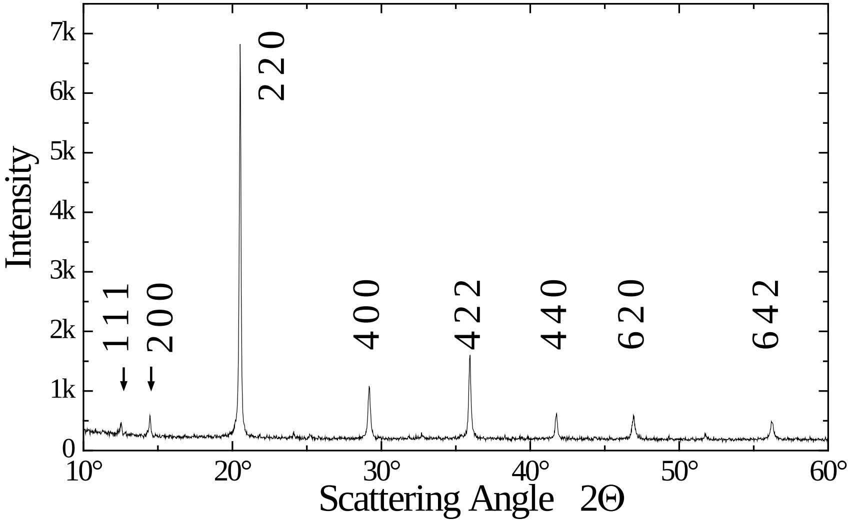
Fecher, J. Appl. Phys. 99 (2006) 08J106

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

Co_2FeSi







XRD – small super structure reflections

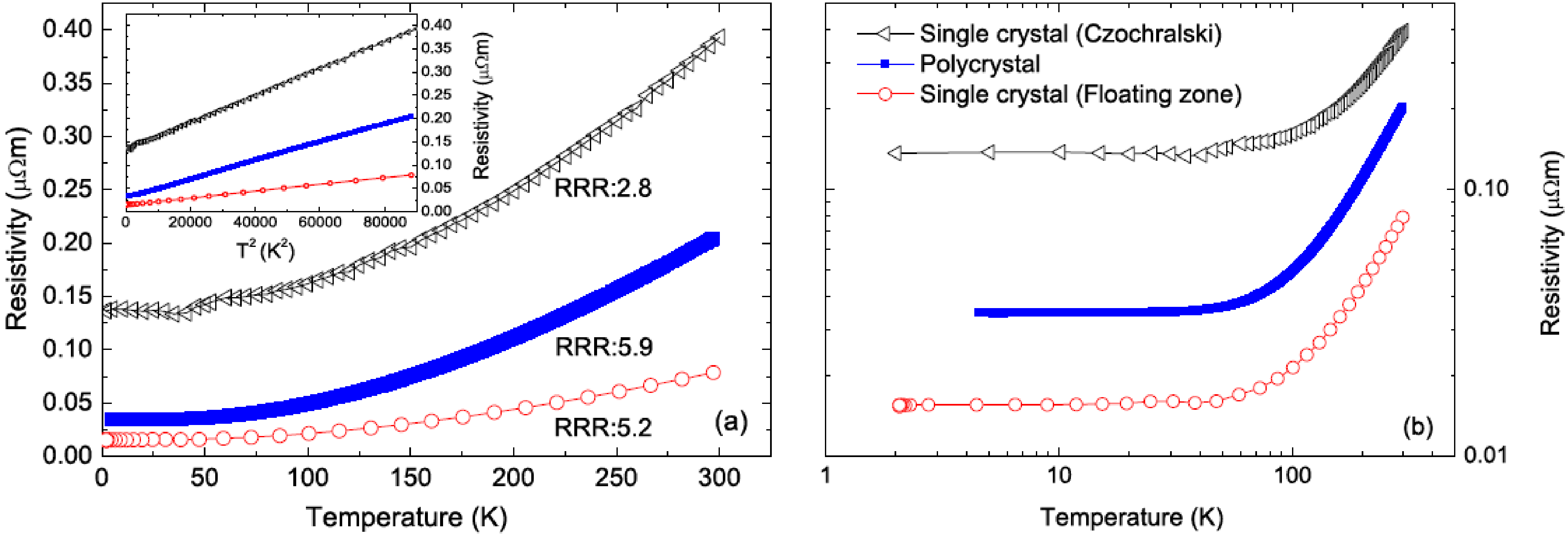
Co-NMR - local probe

Laue - confirms the single crystallinity of the floating zone single crystal

Blum *et al.*, APL 95 (2009) 161903

moment

Co_2FeSi



Floating zone crystal shows the lowest resistance

Polycrystalline and single crystal (floating zone) show the best residual resistance

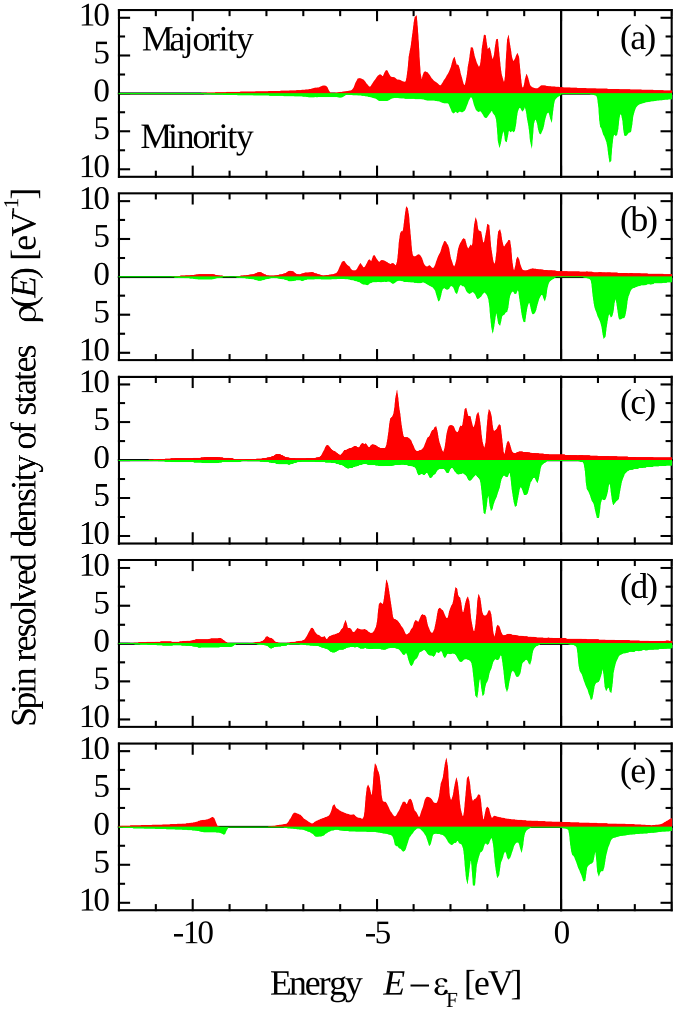
Resistivity above 50K shows a T^2 behavior: ferromagnetic metal with one magnon scattering

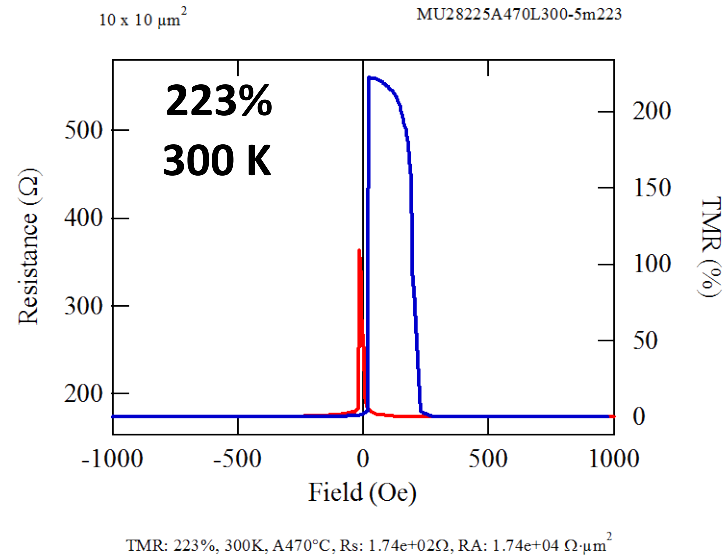
Resistivity below 50K is temperature independent

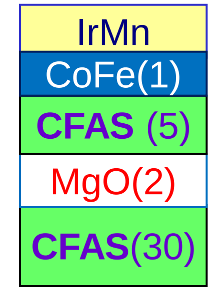
Blum et al., APL 95 (2009) 161903

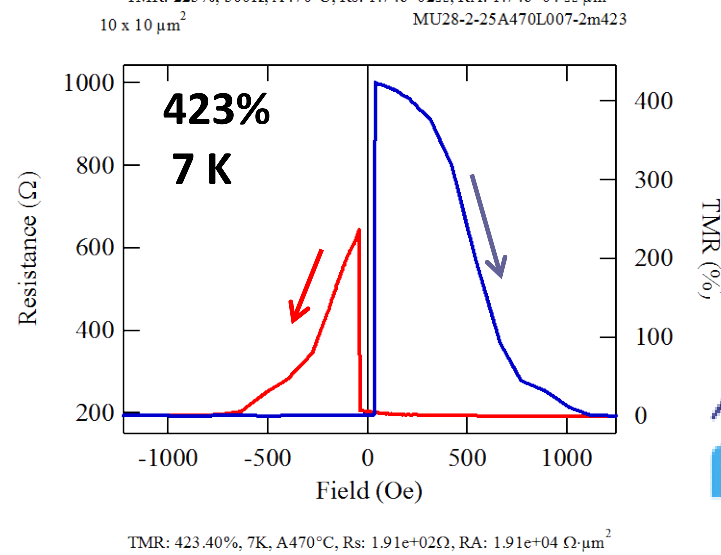
Tuning the Fermienergy

$Co_2FeAl_{1-x}Si_x$









Fecher, Felser J. Phys. D 40 1582 (2007)

N. Tezuka et al.,Jpn. J. Appl. Phys. **46**, L454 (2007)

Tunnel junctions and more …

$Co_2Cr_{0.6}Fe_{0.4}Al$: First Magneto resistance effect

Block, Felser, et al. J. Solid State Chem. 176 (2003) 646

Co_2FeSi: Halfmetallic ferromagnet with T_C 1120 K

Wurmehl, et al ., APL 88 (2006) 032502.

$Co_2Fe_{0.5}Mn_{0.5}Si$, $CoFeSi_{0.5}Al_{0.5}$: Tuning the Fermi energy

Fecher, Felser J. Phys. D 40 (2007) 1582

Mn_3Ga: Spin torque application

Balke et al. APL 90 (2007) 152504

Co_2MnSi/Al-O/Co_2MnSi-MTJ
TMR ratio = 67%@RT, 580%@2K
Sakuraba et al. APL 88 (2006) 192508

Co_2MnSi/Mg/Al-O/CoFe-MTJ
TMR ratio = 93%@RT, 203%@2K
Sakuraba et al. JMSJ (2006)

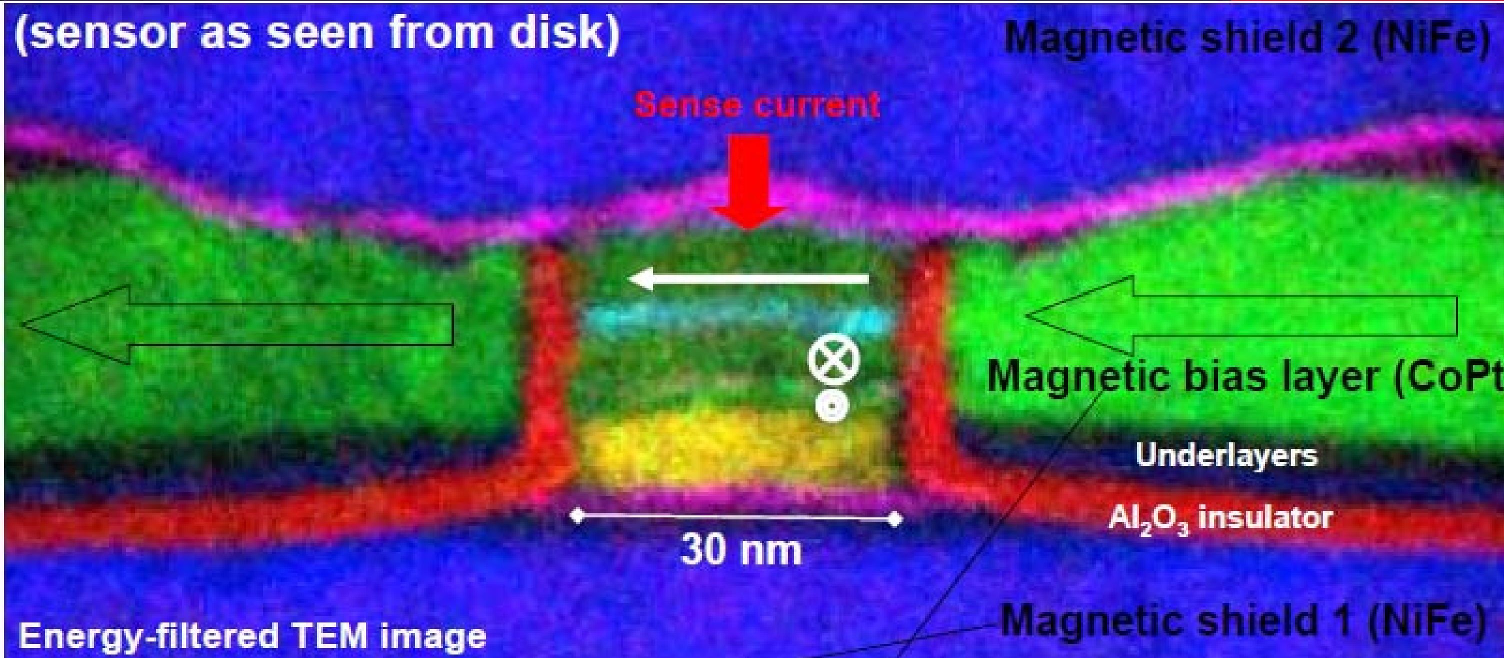
$Co_2FeAl_{0.5}Si_{0.5}$/MgO/$Co_2FeAl_{0.5}Si_{0.5}$-MTJ
TMR ratio = 386%@RT, 832%@2K
Tezuka et al. APL 94 (2009) 162504

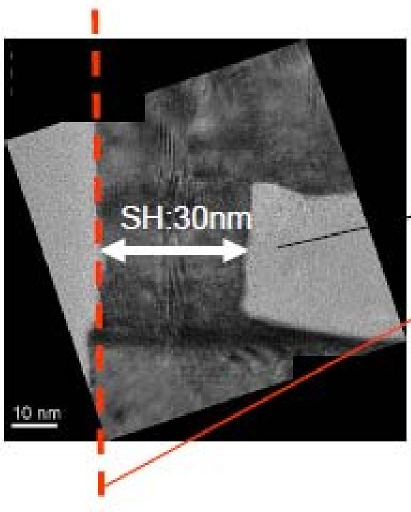
$Co_2FeAl_{0.5}Si_{0.5}$/Ag/$Co_2FeAl_{0.5}Si_{0.5}$
CPP-GMR = 12.4%@RT, 31%@12K
Tezuka et al. APL 94 (2009) 162504

Co_2MnSi/Ag/Co_2MnSi
CPP-GMR ratio = 28.8%@RT
Iwase et al., Appl. Phys. Exp. 2 (2009) 063003

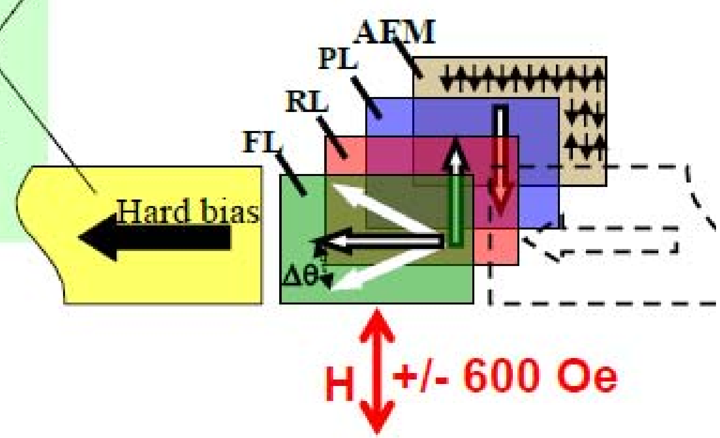
$Mn_{2.5}Ga$ with
Giant perpendicular anisotropy
Wu et al., APL 94, 122503 (2009)

Read-Head Fabrication w/Heusler alloy



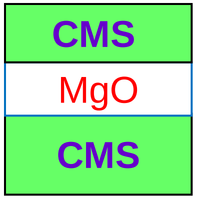


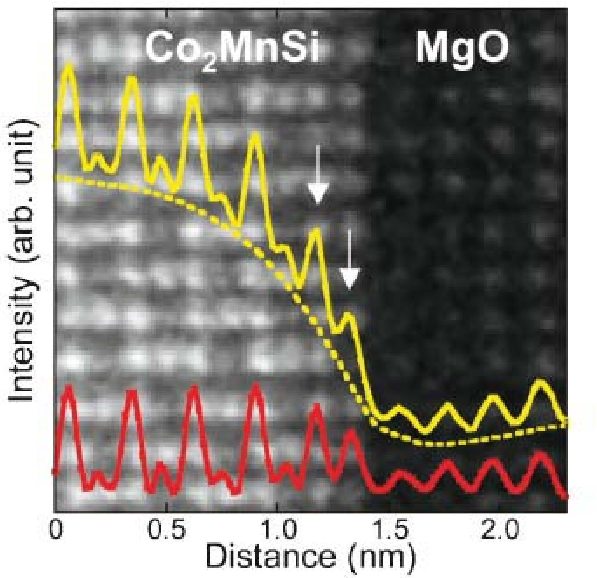
- Shielded sensor.
- Stabilized sensor through hard bias
- Stripe height defined through lapping.
- Air-bearing surface (ABS)

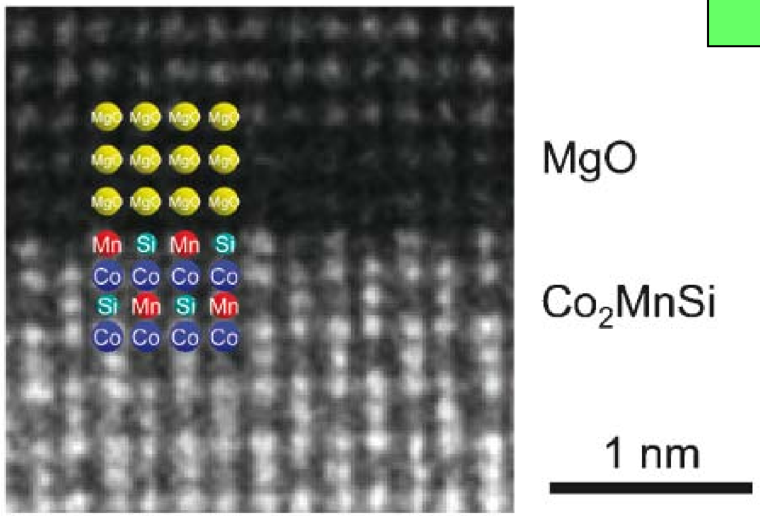


Interface

- Structure - Property – Relation

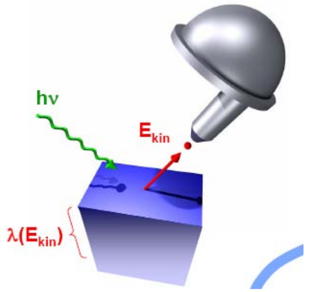


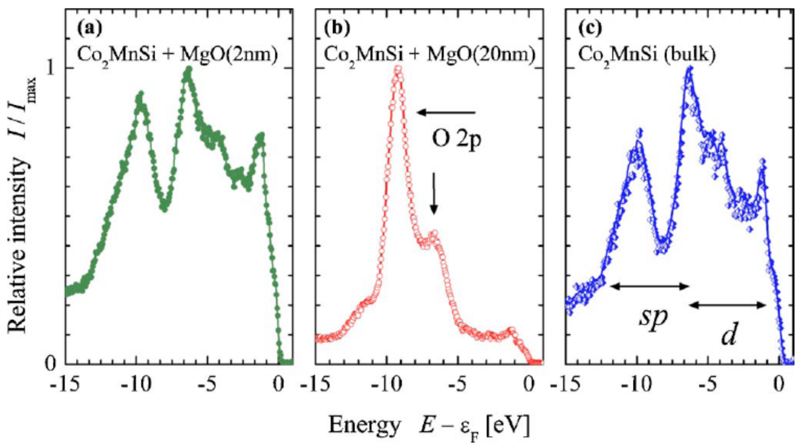


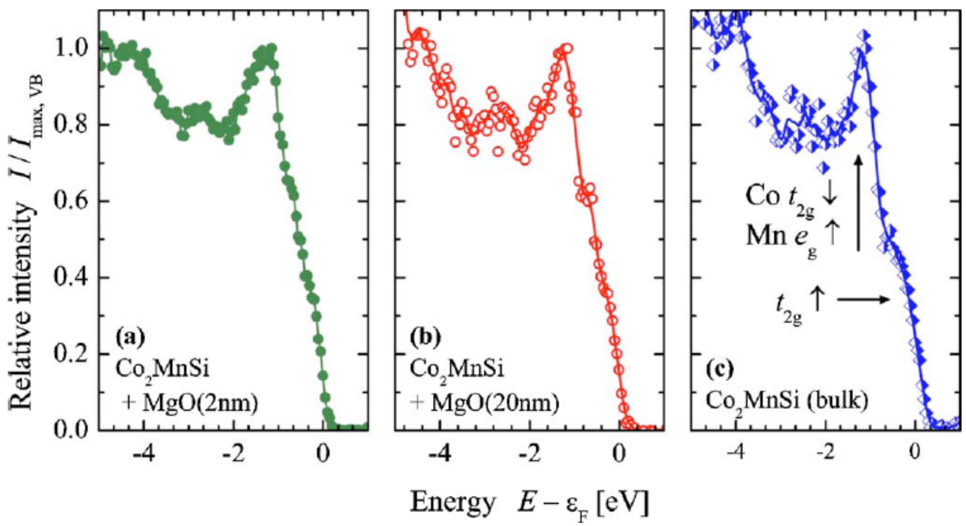


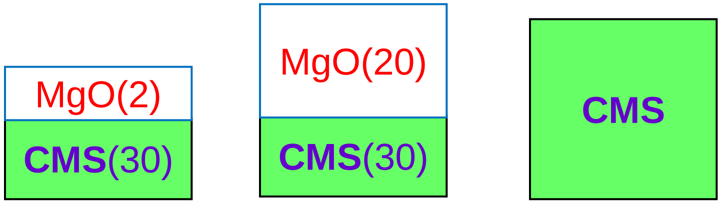
Miyajima *et al*., Appl. Phys. Expr. **2,** 093001 (2009)

- Structure - Property – Relation







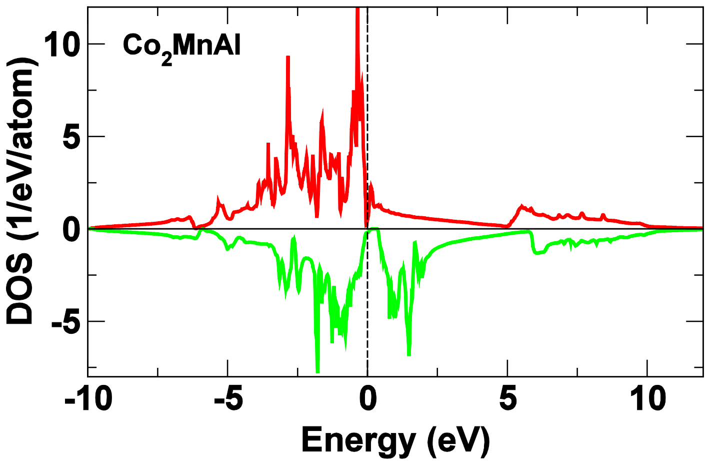


Fecher *et al*., APL **92,** 19351 (2008)

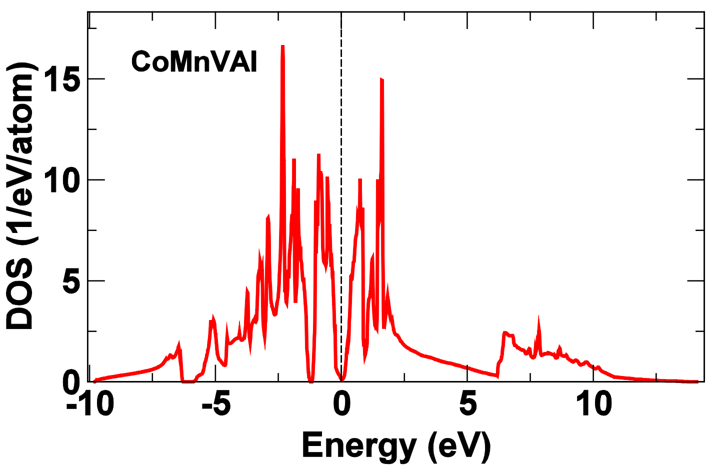
Interface Design

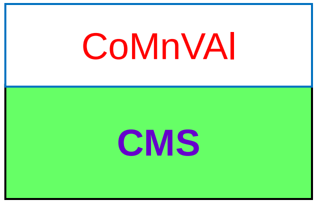
Tuning interfaces by adjusting combination

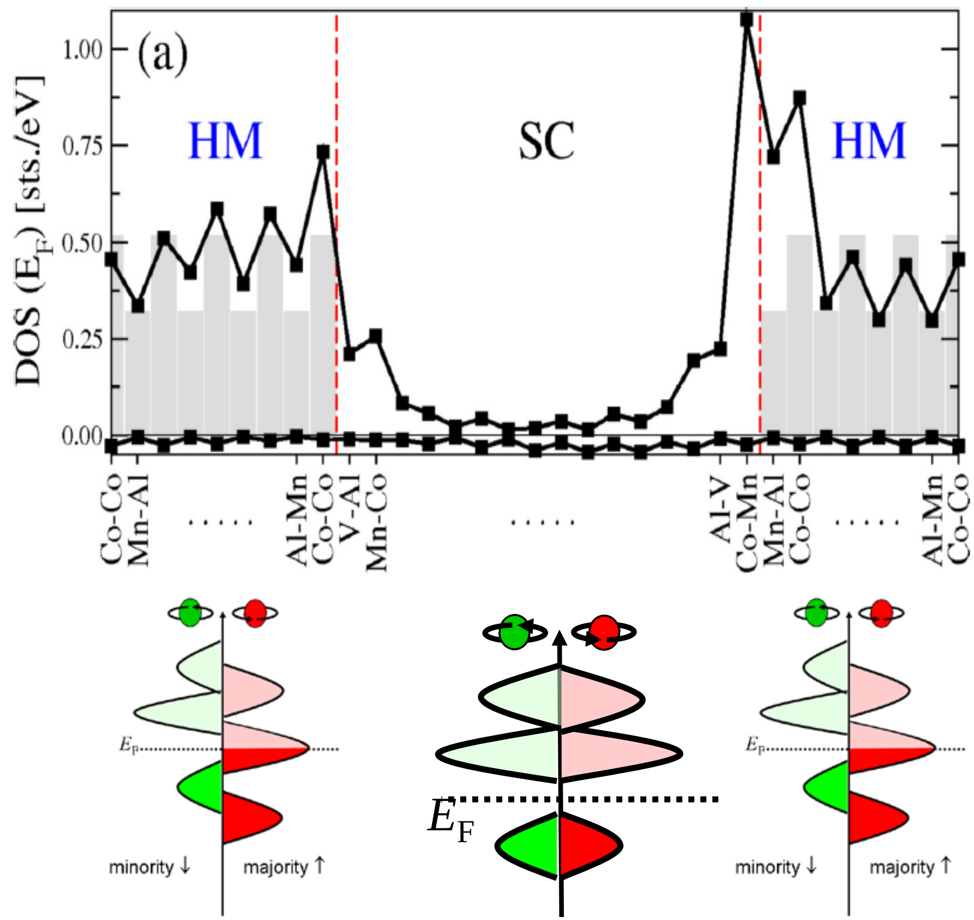
- of a half metal Co_2MnAl



- a semiconductor CoMnVAl

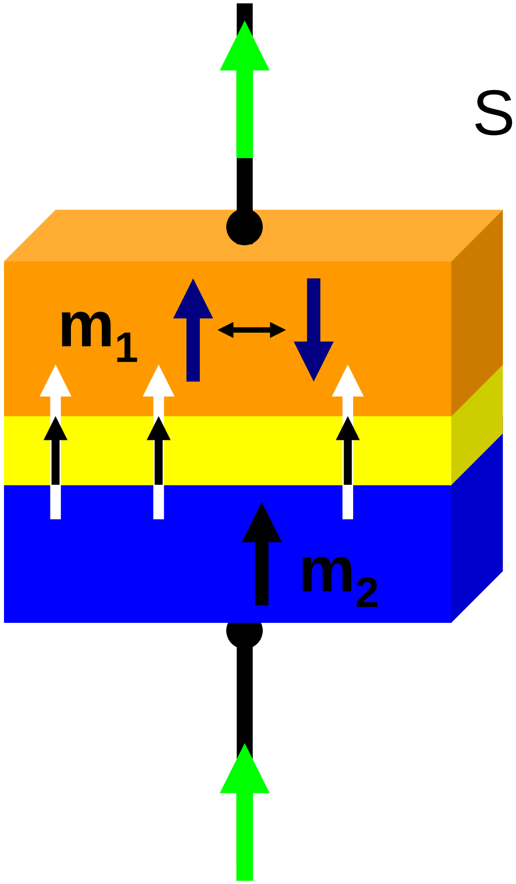






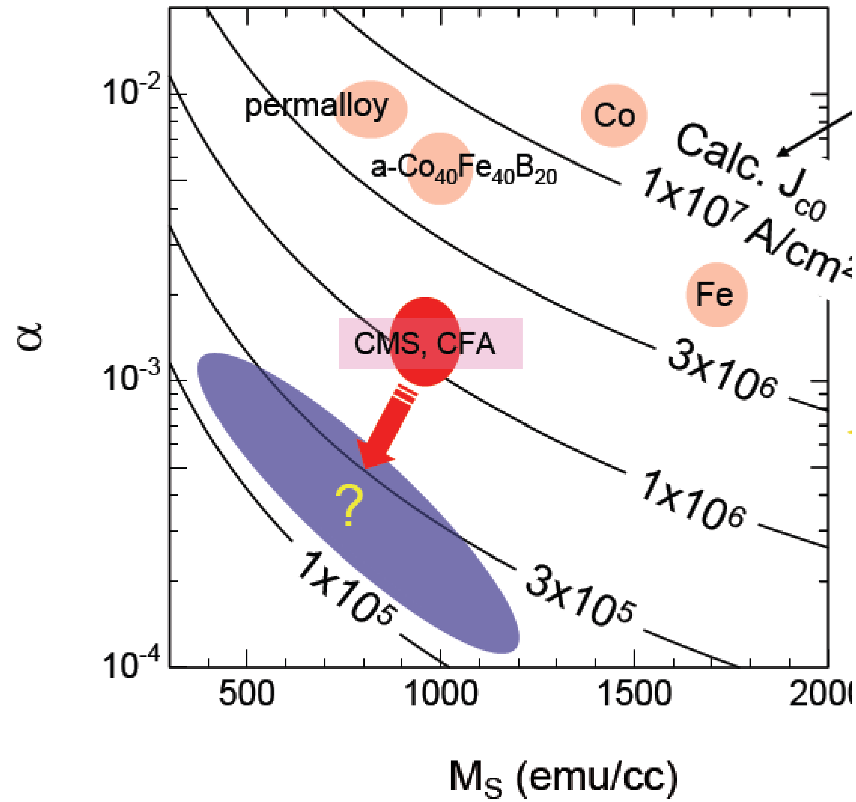
Spin transfer switching

Slonczewski 1996



$J \approx 1 - 100\ MA/cm^2$

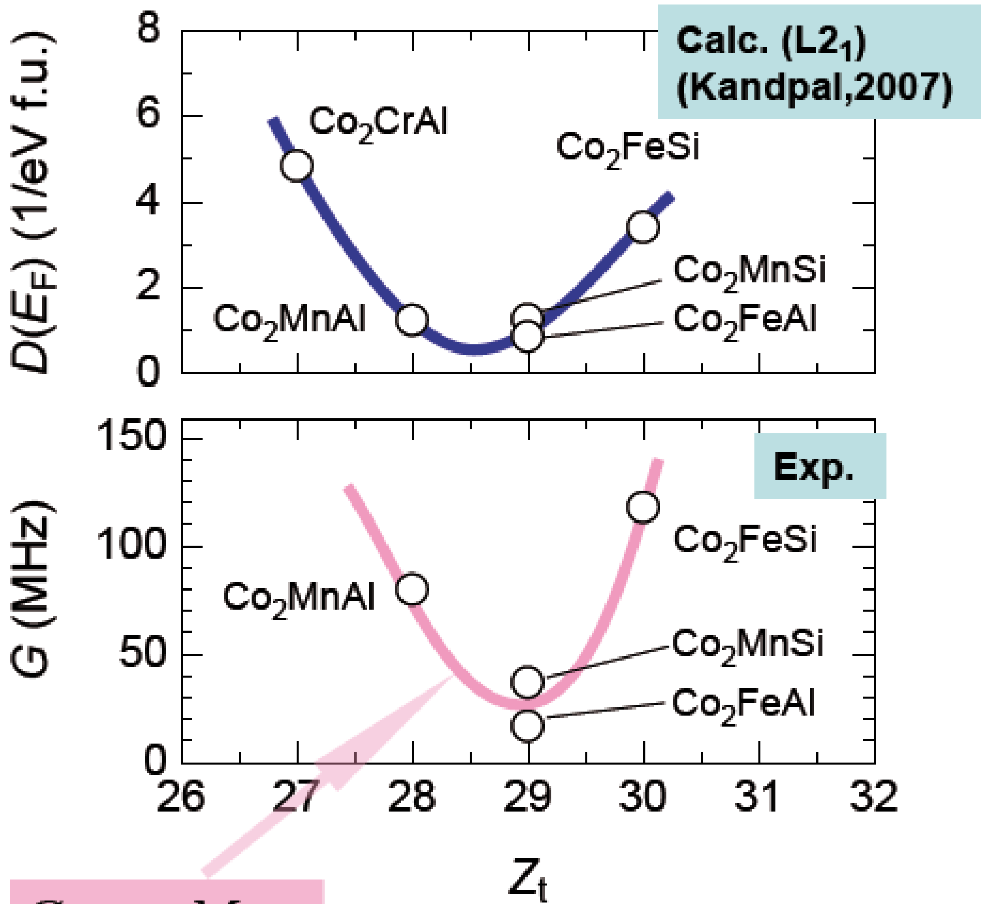
$$J \approx \frac{e}{\hbar g} \alpha M_s H_U d$$



reduction of α & M_S

Courtesy after Shigemi Mizukami

Gilbert damping



$$G = \gamma\alpha M_s$$
$$\propto D_\uparrow + D_\downarrow$$

Heinrich et al. (JAP2004)

Yilgin et al. (IEEE2005)

Yilgin et al. (JJAP2007)

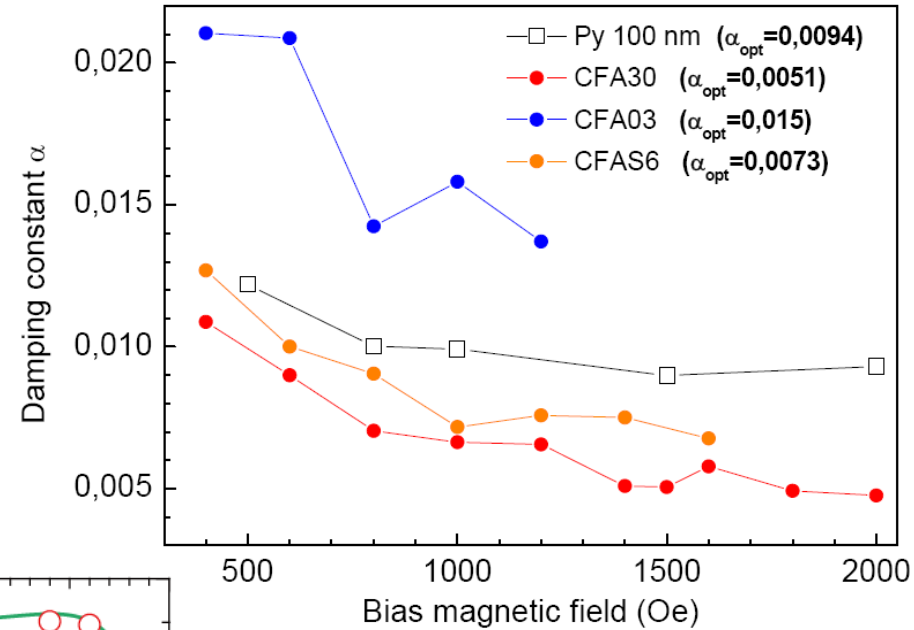
Oogane et al. (JAP2007)

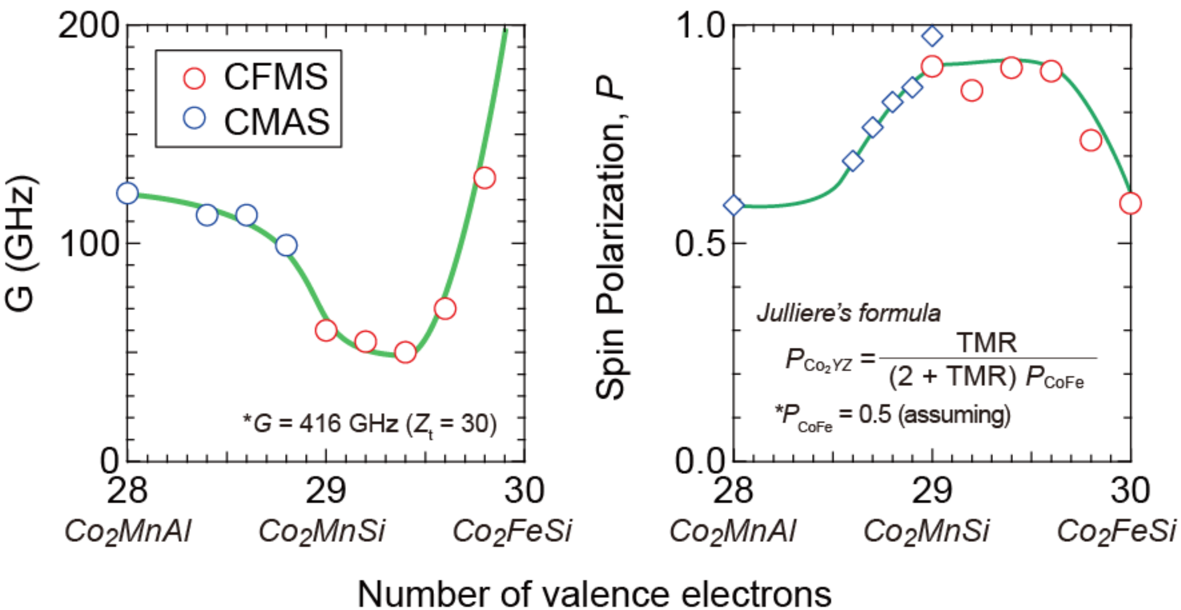
Kandpal, *et al* ., J. Phys. D 40 1507 (2007)

Gilbert damping

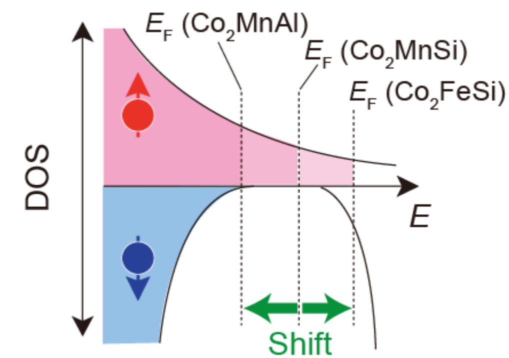
Low Gilbert damping
Brillouin Light scattering (Hillebrand et al.)
Co_2FeAl

Co_2MnSi – Co_2FeSi
lower than permalloy !





Possible shape of DOS of Co_2-Heuslers

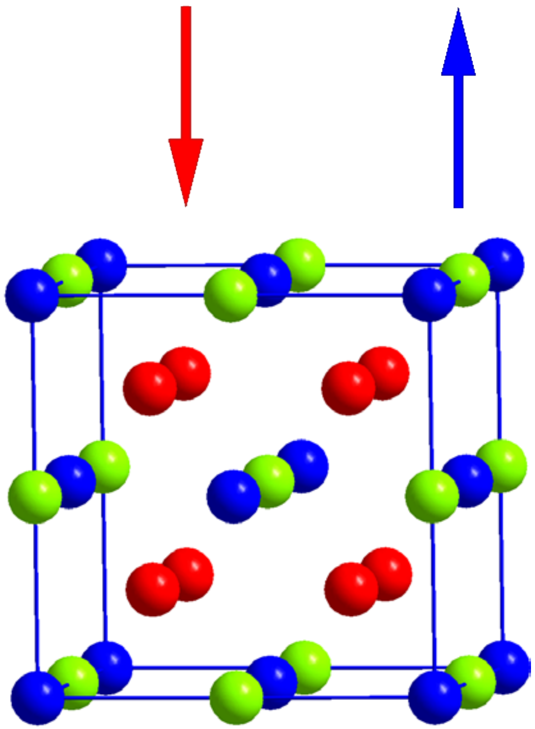


$$G = \alpha \gamma M_s \propto \xi_{SO}^2 (D_\uparrow + D_\downarrow)$$

Kambersky, Can. J. Phys. (1974)

Mizukami, *et al.*, J. Appl. Phys., 105, 07D306 (2009).

Halfmetallic Ferrimagnet



Kübler's Rule
Slater Pauling Rule

X_2MnGa

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

Mn_2MnGa
$3*7 + 3 = 24$
$\Rightarrow$ Compensated ferrimagnet

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

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

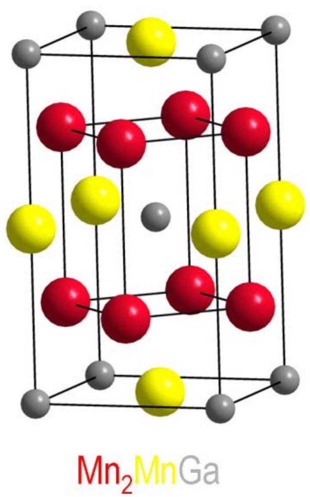
Spin Torque Application

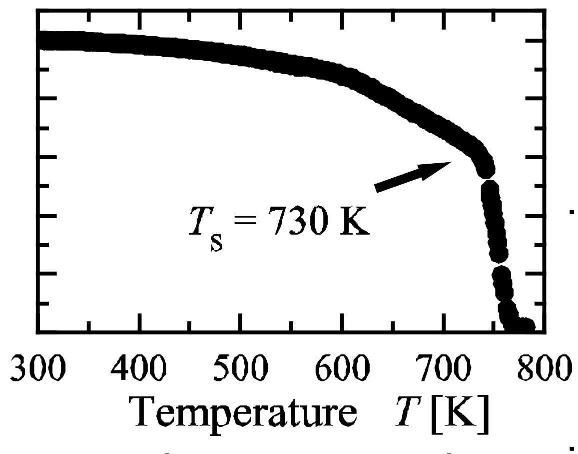
For spin torque application

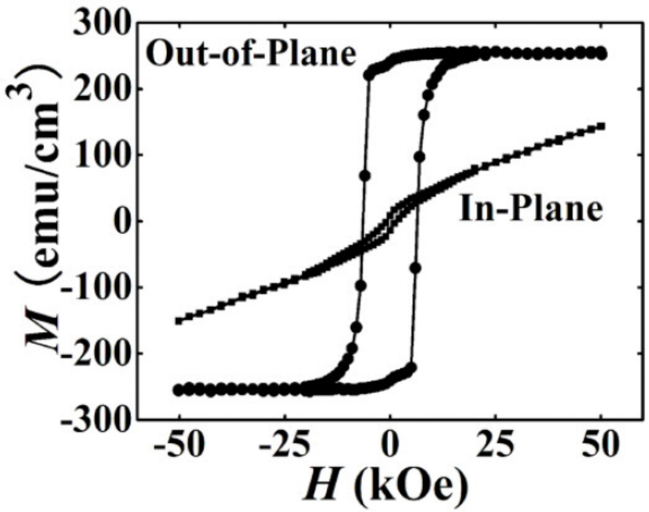
- low magnetic moment, High T_C
- low damping
- **out of plane magnetization**

tetragonal Heusler compounds: Mn_3Ga, $FeMn_2Ga$

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



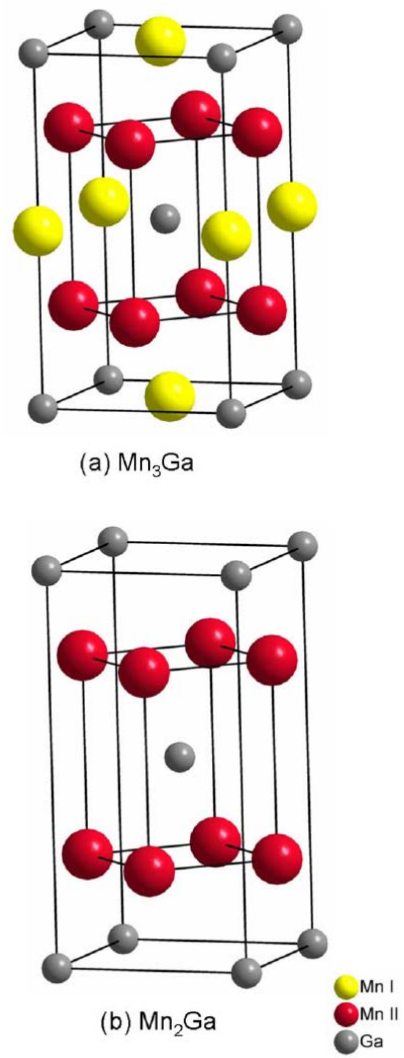


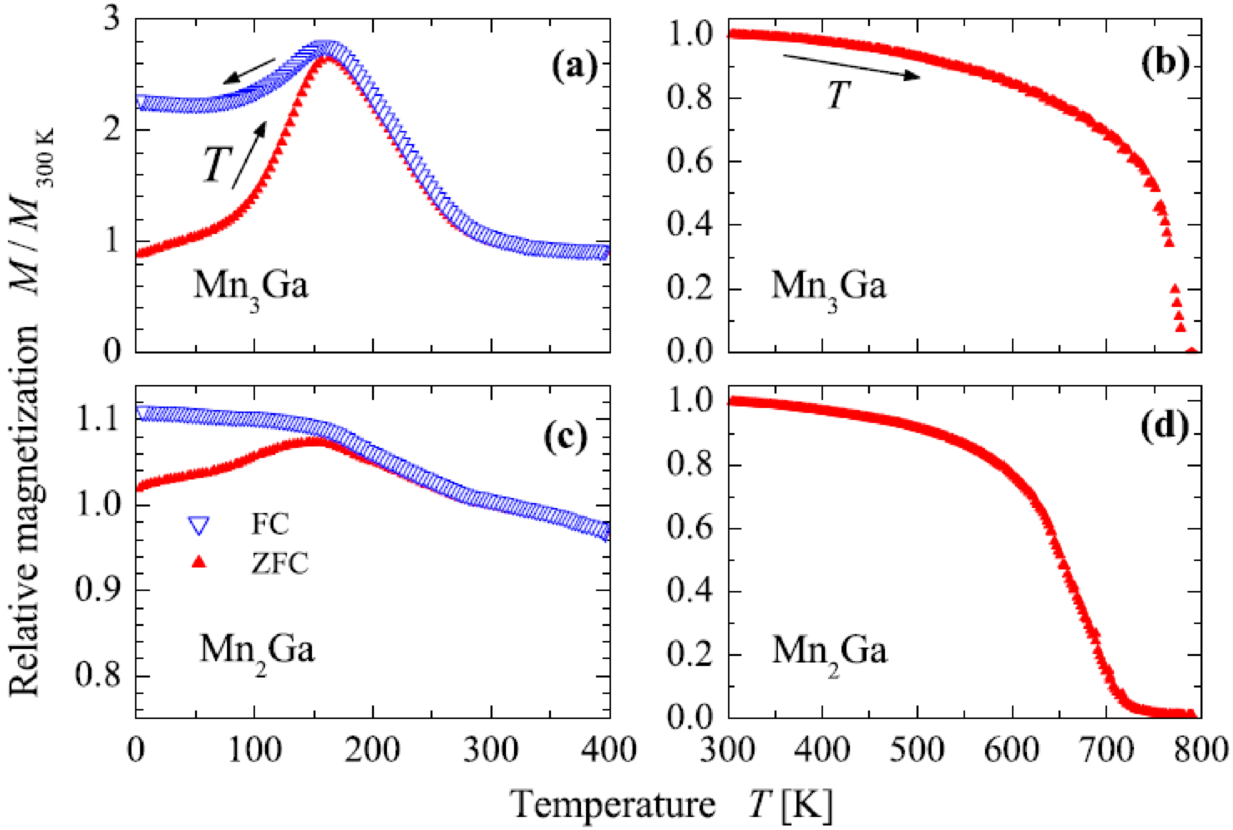


Balke *et al*.CF, APL **92**, 152504 (2007)

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

$Mn_{3-x}Ga$: Tunability



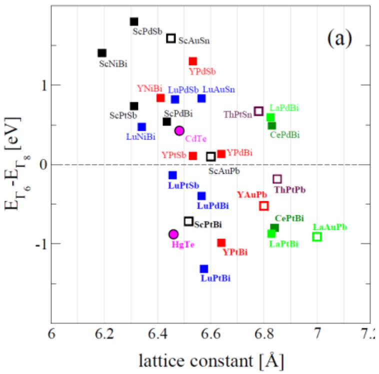


Winterlik *et al.* CF, Phys. Rev. B **77** (2008) 054406

Summary

More than 200 semiconducting Heusler compounds

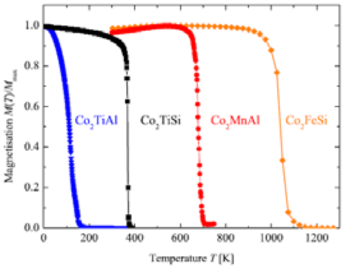
- Tunable – gaps and charge carriers
- Multifunctional topological insulators
- Thermoelectric devices with high ZT and nano structuring



Spintronics

- Materials with high spin polarization at high Curie temperature

  ➔ TMR devices

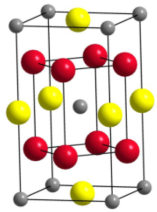


- Materials with low magnetic damping
- Materials with low magnetic moments
- Materials with high perpendicular anisotropy

  ➔ spin torque oscillators – STTRAM, MAMR

- Combination of adjusted Materials as Hybrid materials

  ➔ spin injection into semiconductors,



Mn_2MnGa

- Multifunctional materials

  ➔ new effects