Electronic structure, spin transport and magnetic anisotropy of selected cubic Heusler and hexagonal Heusler like alloys

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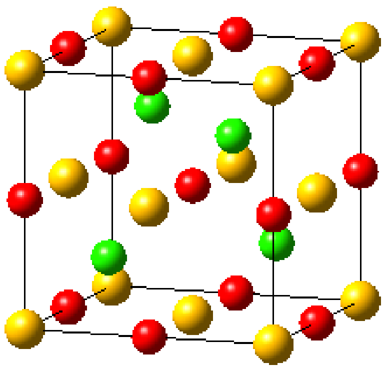
07.30.15 : UMN –Keller-Hall-3-176 : 3:10 pm

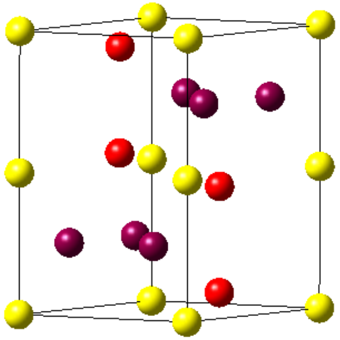
SCOPE : Combination of Properties

- Structure and composition X_2YZ, XYZ:



  - Variety of material
  - Mutli-functional properties

- Combination of Properties:



  - High spin polarization
  - Relatively high Curie point
  - Spin dependent transport
  - Magnetic anisotropy : bulk or interface

O U T L I N E

- **Tc : Comments on Disorder : spin disorder**

- spin mixing - Curie point calculations
- quaternary alloys strategy

- **Eg : Electronic structure: minority band gap**

- fundamental gap theory - alloys design

- ρ_{up}/ρ_{dn} **:Spin Dependent Transport : GMR**

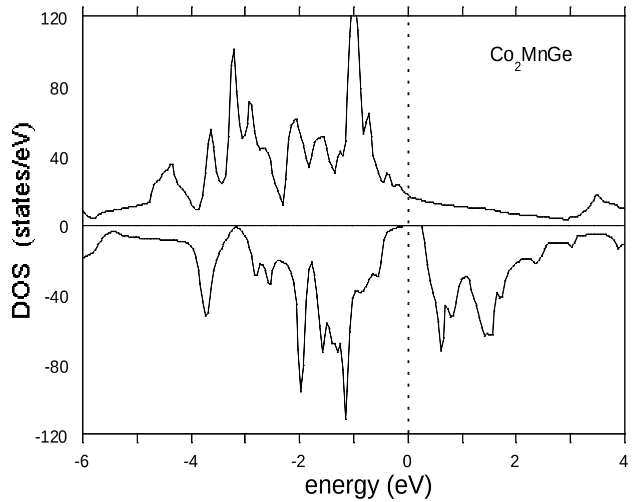
- Band matching - Q-alloy effects

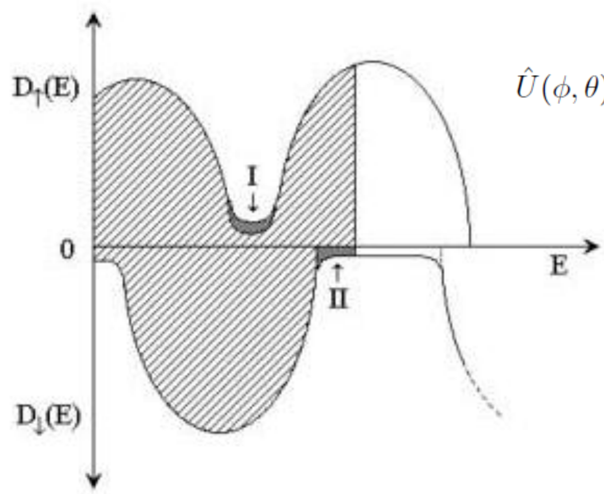
- **K1 : Hexagonal Heusler like alloys :**

- Magnetic Anisotropy

- Summary and Conclusions

Minority Band gap and Tc factor

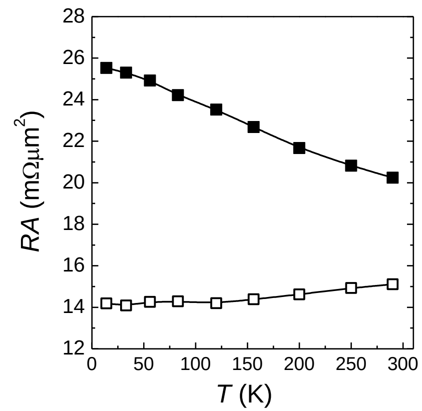


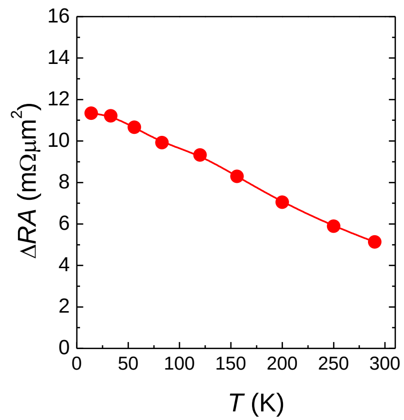


$$\hat{U}(\phi,\theta) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right)e^{i\theta/2} & \sin\left(\frac{\theta}{2}\right)e^{-i\phi/2} \\ -\sin\left(\frac{\theta}{2}\right)e^{i\phi/2} & \cos\left(\frac{\theta}{2}\right)e^{-i\phi/2} \end{pmatrix},$$

Prof. Hono

- Increase Minority Gap





CFGG = $Co_2Fe(Ge_{0.5}Ga_{0.5})$
CMGG = $Co_2Mn(Ge_{0.75}Ga_{0.25})$
CFAS = $Co_2Fe(Al_{0.5}Si_{0.5})$
CMFS = Co_2(Mn-Fe)Si
CMFG= Co_2(Mn-Fe)Ge

- Increase Tc

- Co2FeGe
- Co2FeGa larger Tc

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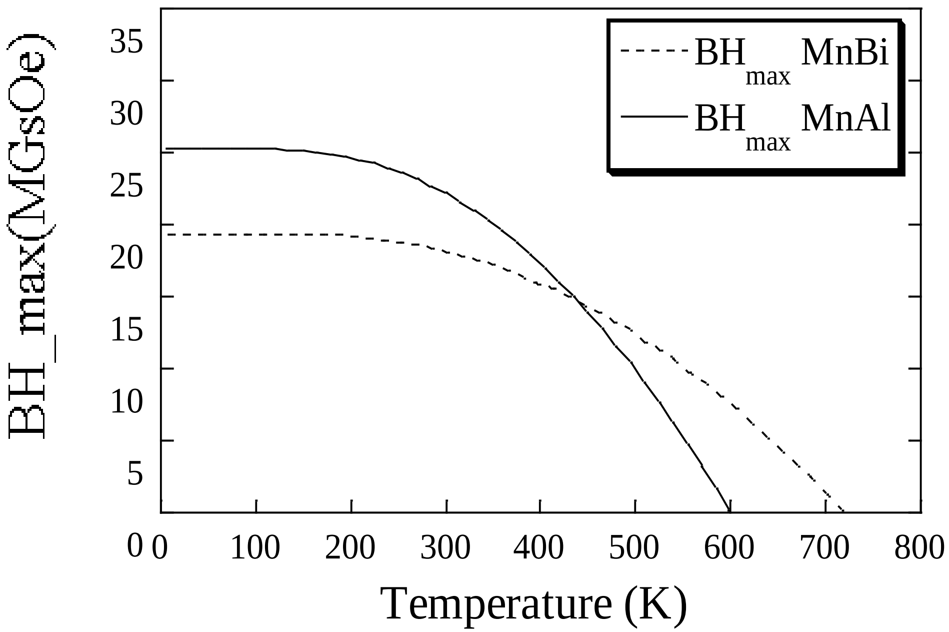
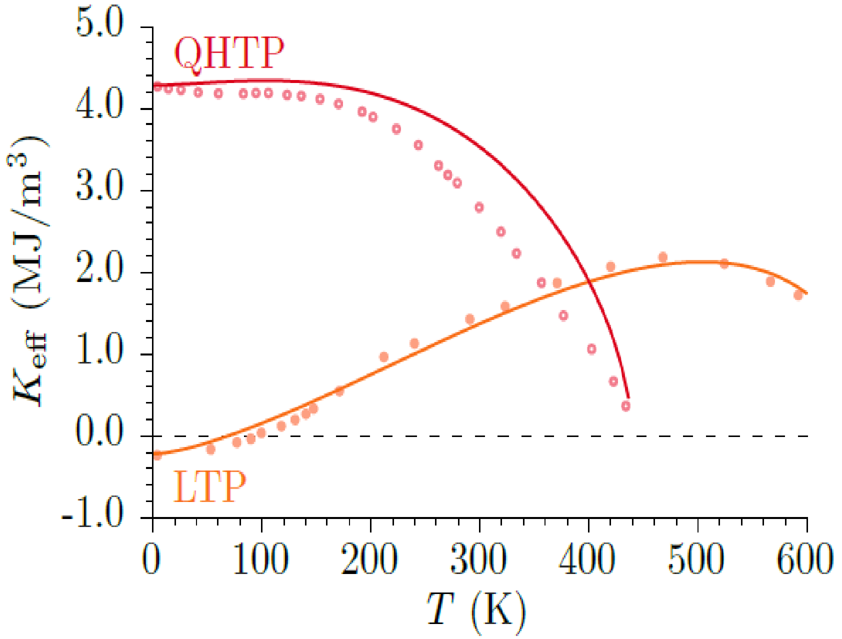
How to calculate M(T), K(T), P(T) ?





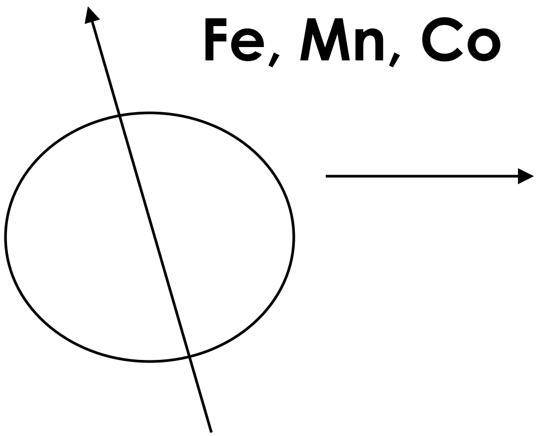
- Effective Spin Hamiltonian approach

*O. N. Mryasv et.al., EuroPhysics Letters, **69**(5), p.805 (2005)*

- statistical simulations/theory
- material specific parameterization

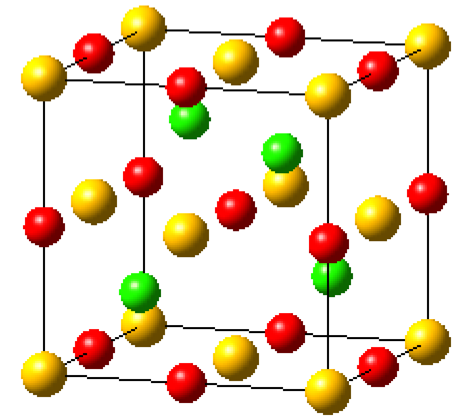
Spin Hamiltonian: Microscopic Definition

- Two terms in the effective potential variation:



$$\Delta V_i^{ex} = B_i \delta \vec{e}_i \vec{\sigma}$$

$$\Delta V_i^{so} = \frac{1}{2} \sum_l \xi_l^i \vec{L} \delta \vec{e} \vec{\sigma}$$



- Contributions to the total energy: $\delta E = \delta E^{EX} + \delta E^{DM} + \delta E^{MAE}$

$$E^{EX} = -\sum J_{ij} \vec{e}_i \vec{e}_j \qquad E_{DM} = \sum D_{ij} [\vec{e}_i \times \vec{e}_j] \qquad E^{MAE} = \sum \varepsilon_{ij}$$

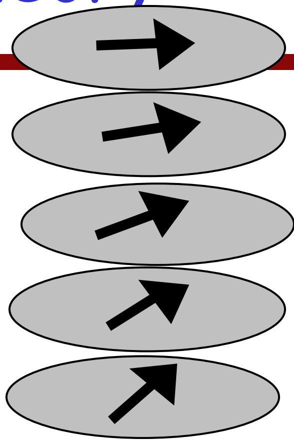
$$E^{EX} = -\sum J_{ij} \mathbf{e_i e_j}$$

$$E^{MAE} = -\sum k_{ii}^{(0)} \mathbf{e_i^z e_i^z} - \sum k_{ij}^{(2)} \mathbf{e_i^z e_j^z}$$

Generalized constrained density functional theory

$$E_{ex} = AVq^2$$

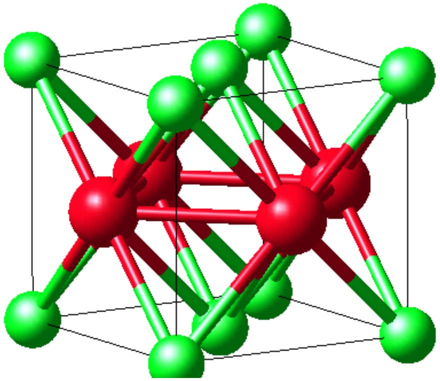
- *Spin spiral excitations*



$$A(x,T) = A(0,T)[1 - \lim_{q\to 0} << \Delta E_{ss}(x,q) >_x >_T / < E_{ss}(0,q) >_T]$$

O. Mryasov et.al Phys. Rev. B. 45, 12330 (1992)

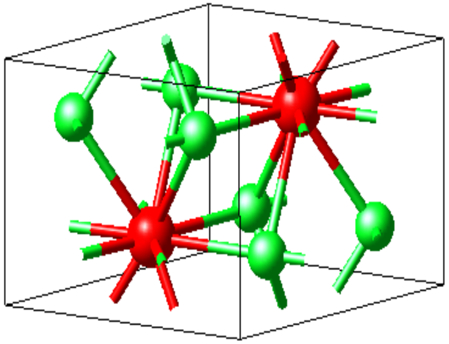
- *Constrained DFT calculations*



$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{eff}(\vec{r})\right]\varphi_i(\vec{r}) = \varepsilon_i \varphi_i(\vec{r})$$

$$\vec{B} = \left(\frac{\partial E_{xc}[\rho, m]}{\partial m}\frac{\vec{m}}{m}\right)$$

$$H_{so} = -\xi LS$$



$$E_{CLDA}[\rho, B, h_\perp] = E_{LDA}[\rho, B] + E_{Const}[\rho, h_\perp]$$

Multi-sub-lattice mean field

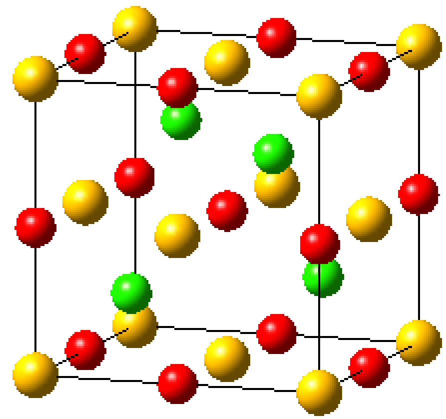
	Tc (Experiment)	Tc (Theory)
	(K)	(K)
Fe (bcc)	1040	1080
Co (fcc)	1400	1533
Co2FeGe	1000	1062
Co2MnGe	905	867
Co2FeSi	1120	1047
Co2MnSi	985	963
Co2FeAl	1000	1298
Co2MnAl	693	590

- Y = Fe vs. Mn – approach to increase Tc

Q: How this changes band gaps

Tc calculations beyond mean field

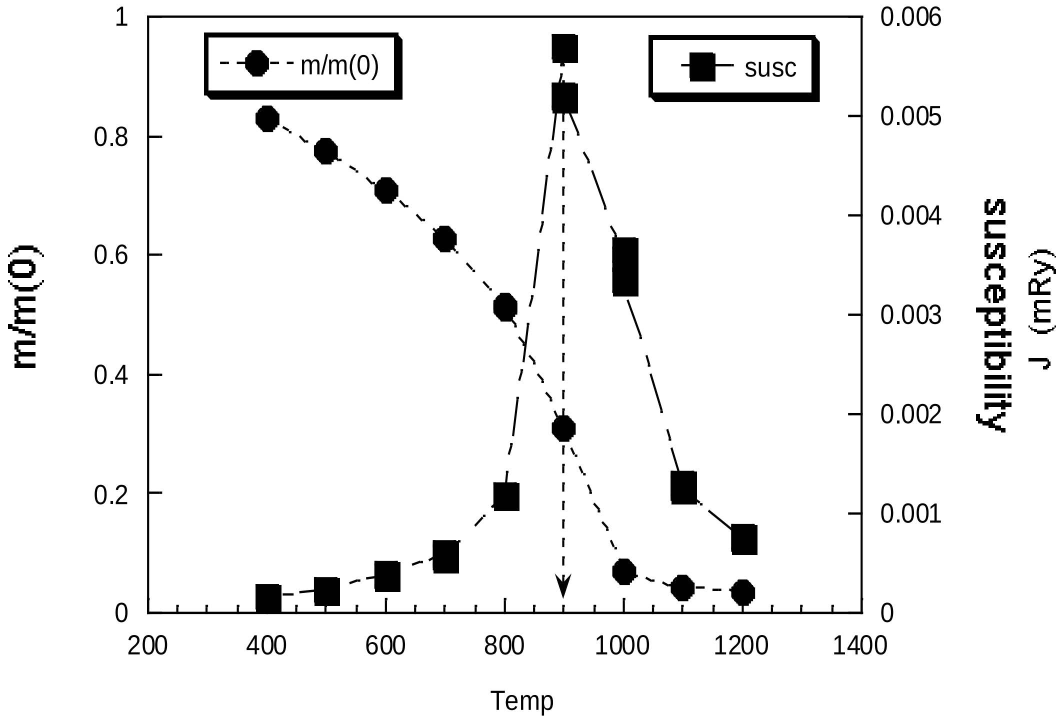
Mean field theory for Two sub-lattice magnets:

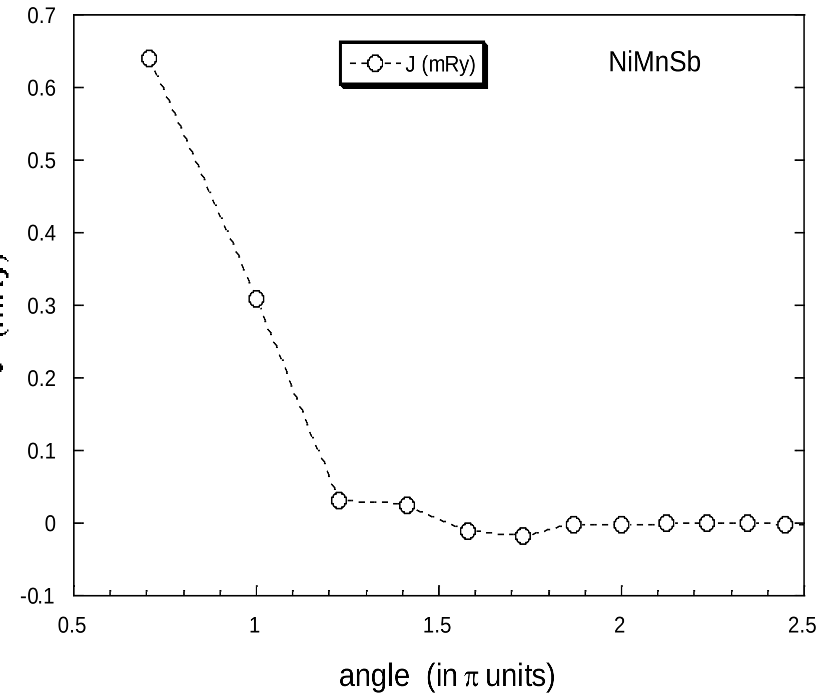


$$T_C = \frac{1}{2}(T_{TT} + T_{RR}) + \sqrt{\frac{1}{4}(T_{TT} - T_{RR})^2 + T_{RT}^2}$$

NiMnSb alloy test

Experimental Tc about 780 K





O.N. Mryasov, A.J. Freeman, A.I. Liechtenstein JAP. **79** (8): 4805-4807 (1996).

OUTLINE

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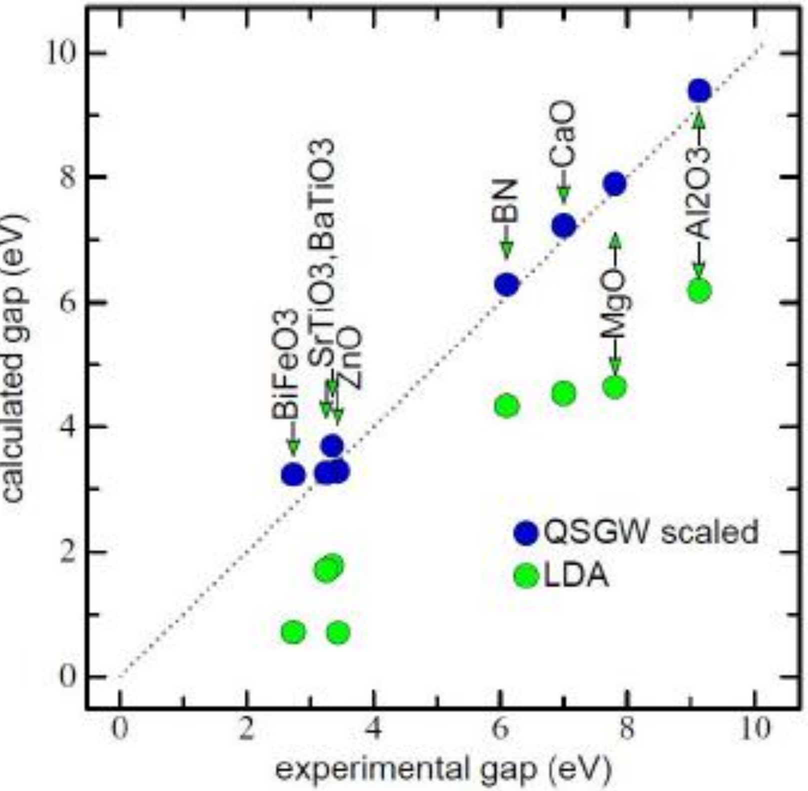
Challenaes : MF vs. RPA or LDA vs. QSGW



Schilfgaarde, Kotani, Faleev PRL 96, 26402 (2006)

LDA is a mean field type of approach

$$\left(-\frac{\nabla^2}{2m}+V_{nuc}(r)+V_H(r)+V_{xc}^{LDA}(\rho(r))\right)\Psi_{\mathbf{k}n}(r)=\varepsilon_{\mathbf{k}n}\Psi_{\mathbf{k}n}(r$$

GW approach is based on many-body theory

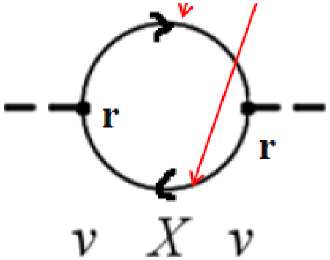
Typical error:

$$\left(-\frac{\nabla^2}{2m}+V_{nuc}(r)+V_H(r)\right)\Psi_{\mathbf{k}n}(r)+\int dr\,\Sigma(r,r',\varepsilon_{\mathbf{k}n})\Psi_{\mathbf{k}n}(r')=\varepsilon_{\mathbf{k}n}\Psi_{\mathbf{k}n}(r)$$

LDA 1-2 eV

G_0W_0 0.5 eV

QSGW 0.1-0.2 eV



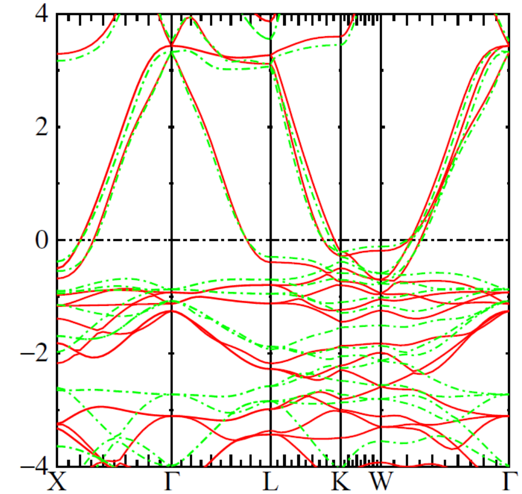
Polarizability (screening) !!!! RPA

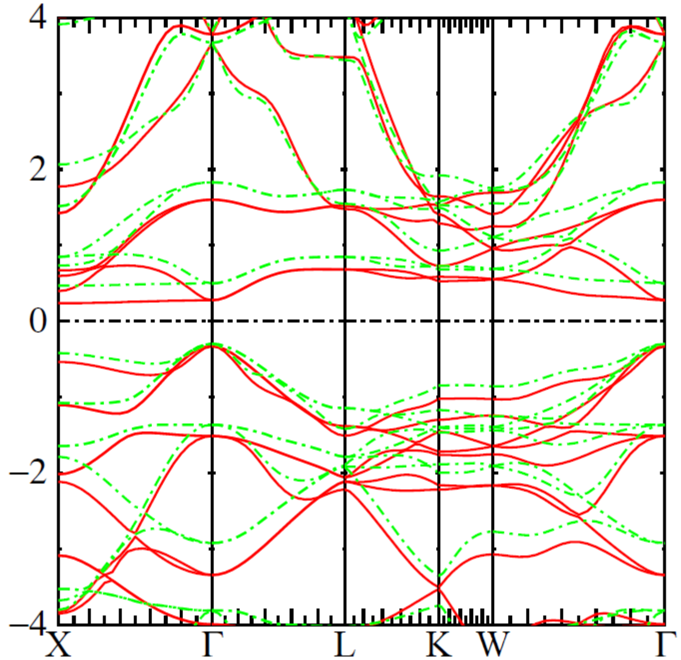
Systematic band "gap" analysis

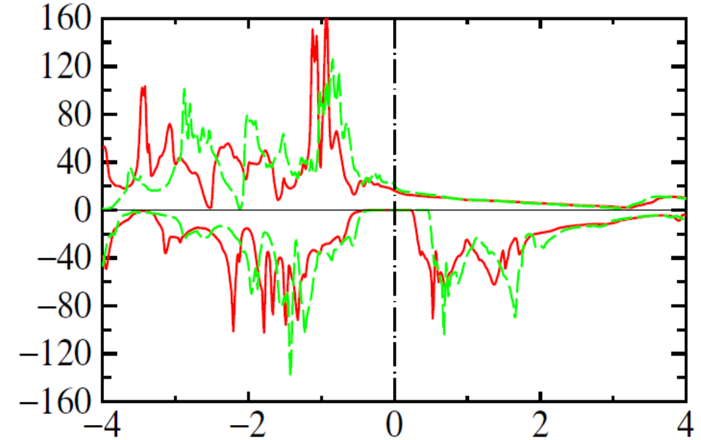
Co_2FeSi, Co_2FeGe, Co_2FeGa, Co_2FeAl
Co_2MnSi, Co_2MnGe, Co_2MnGa, Co_2MnAl

Electronic structure : minority band gap

$Co_2(Mn)Si$



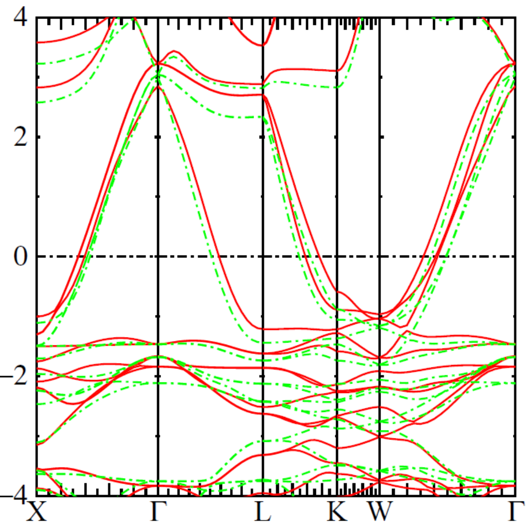


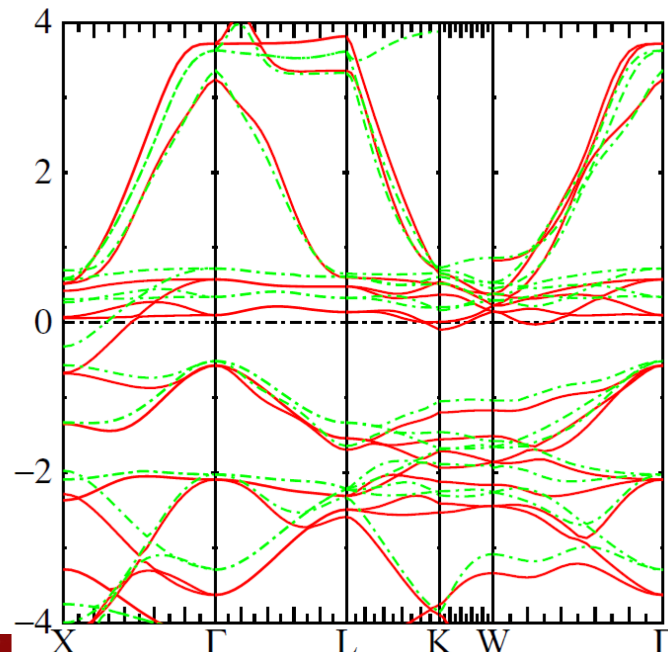


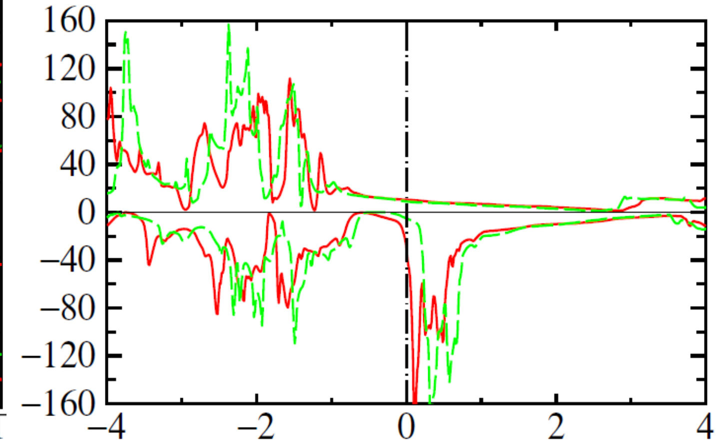
Co2MnSi : -LDA : 0.55 eV
-GW : 0.7 eV

Co2FeSi : -LDA : 0.7 eV
-GW : 1.33 eV

$Co_2(Fe)Si$

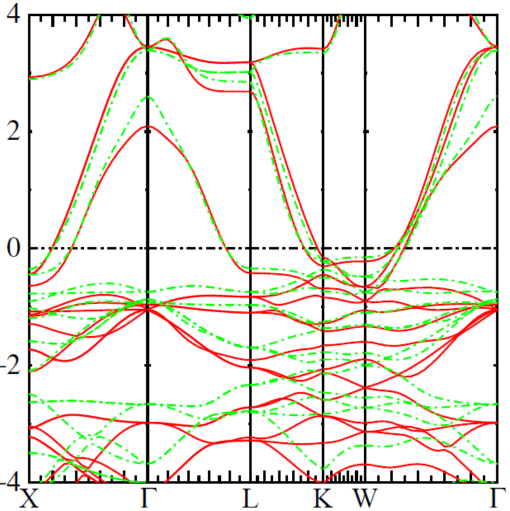


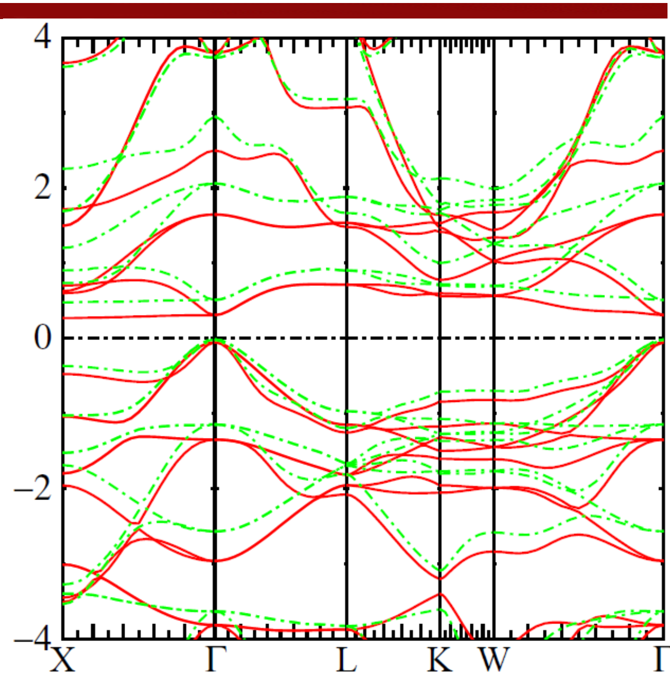


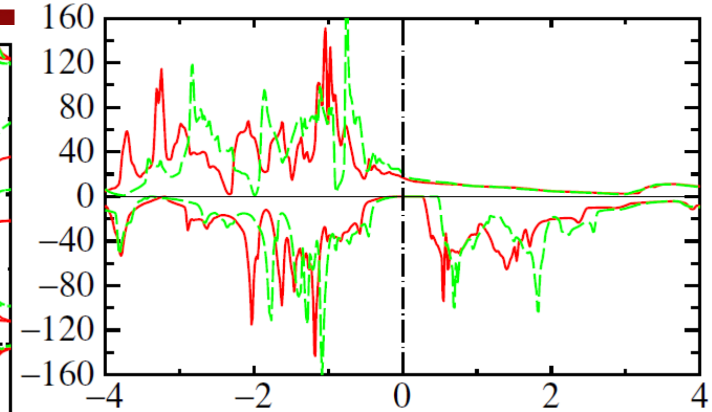


Electronic structure : minority band gap

$Co_2(Mn)Ge$







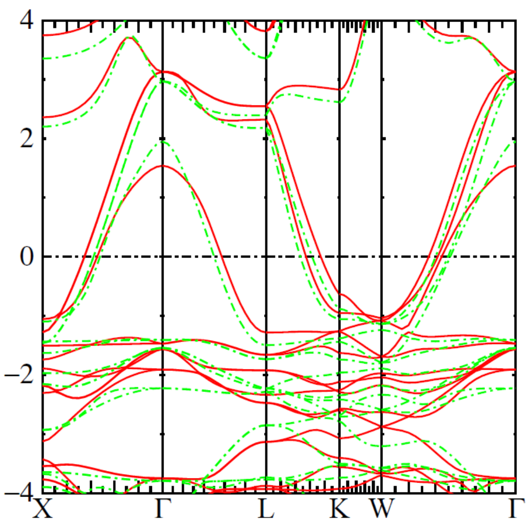
Co2MnGe : -LDA : 0.3 eV

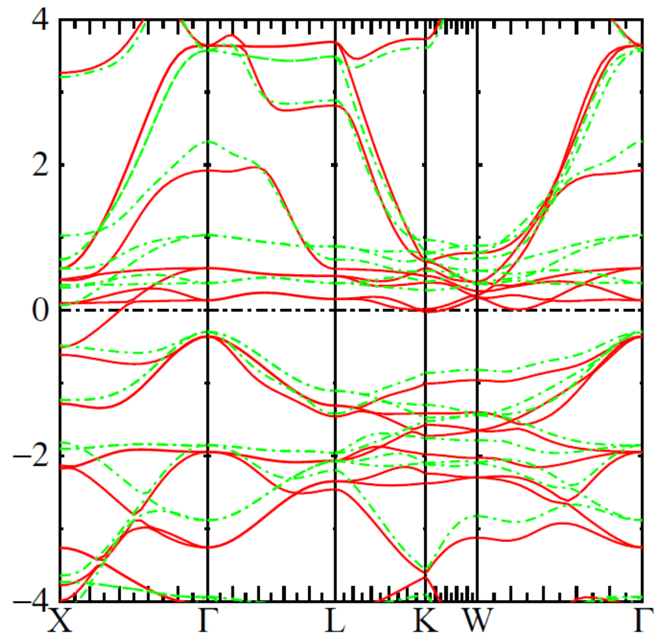
-GW : 0.45 eV

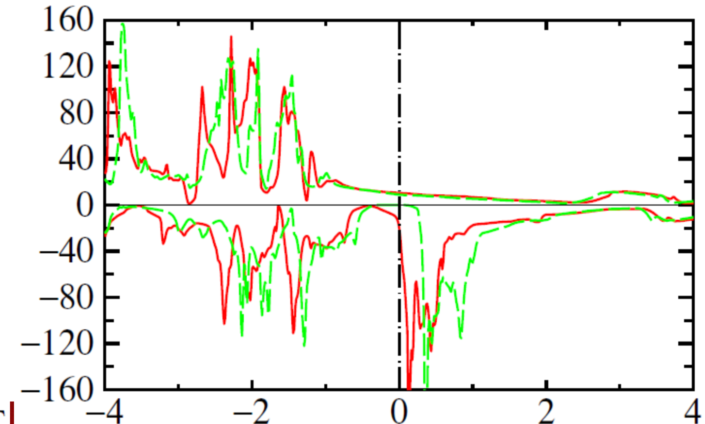
Co2FeGe : -LDA : 0.4 eV

-GW : 0.6 eV

$Co_2(Fe)Ge$

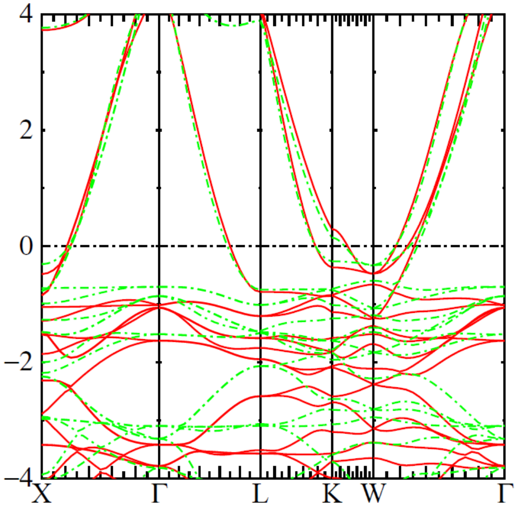


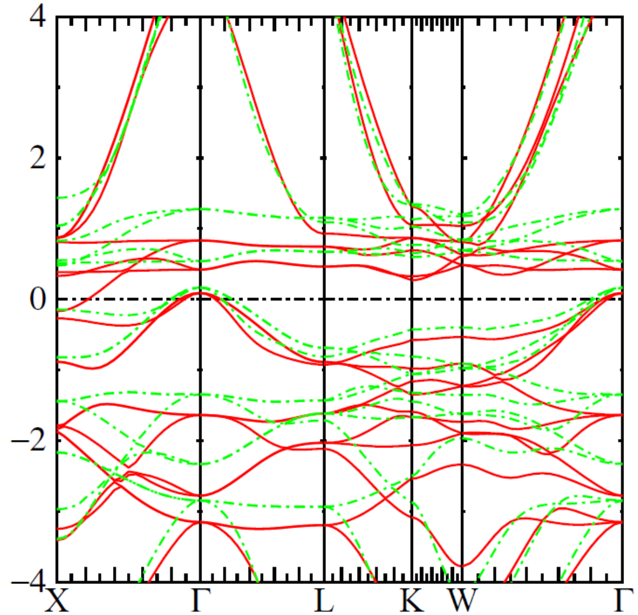


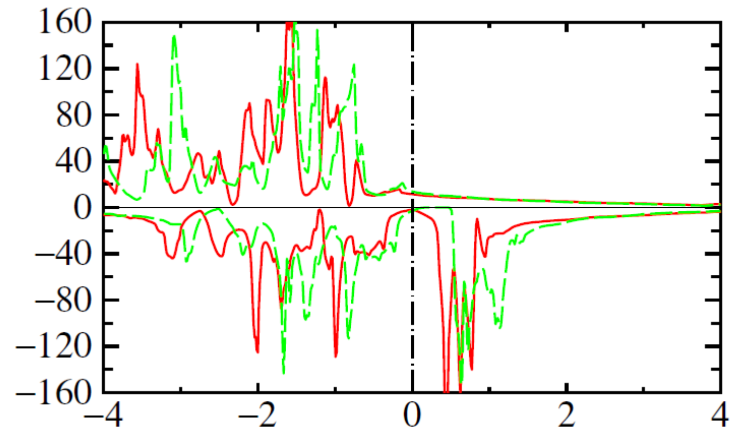


Electronic structure : minority band gap

$Co_2(Fe)Ga$







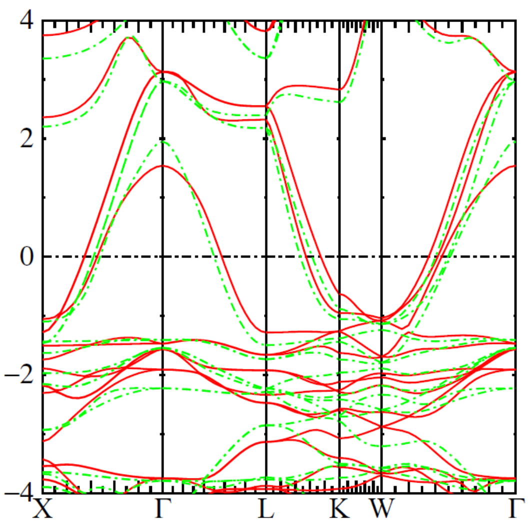
Co2FeGa : -LDA : 0.3 eV

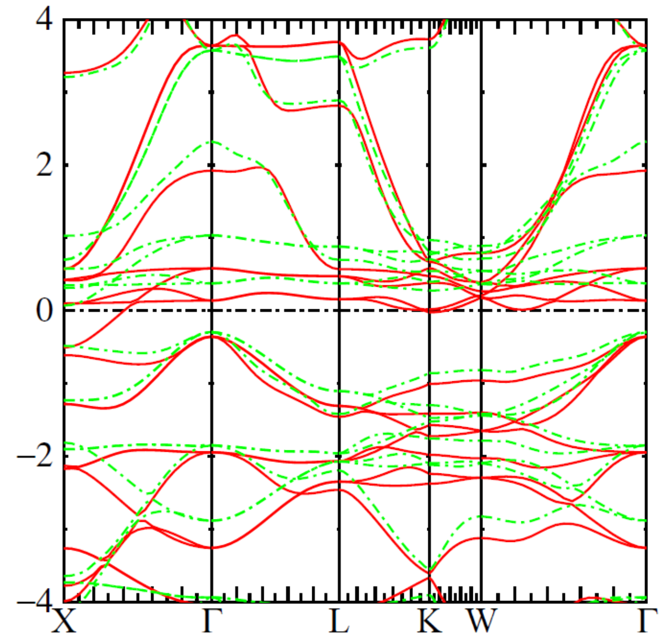
-GW : 0.3 eV

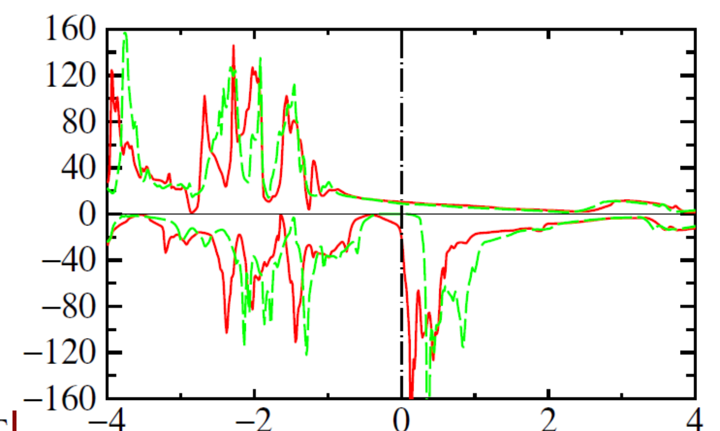
Co2FeGe : -LDA : 0.4 eV

-GW : 0.6 eV

$Co_2(Fe)Ge$







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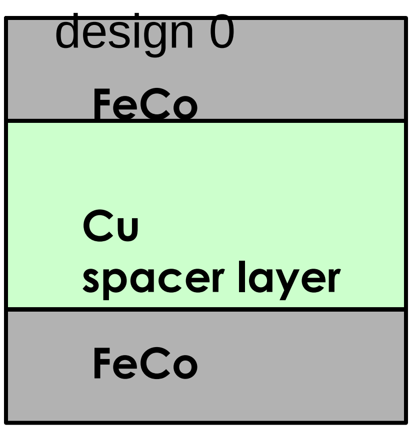
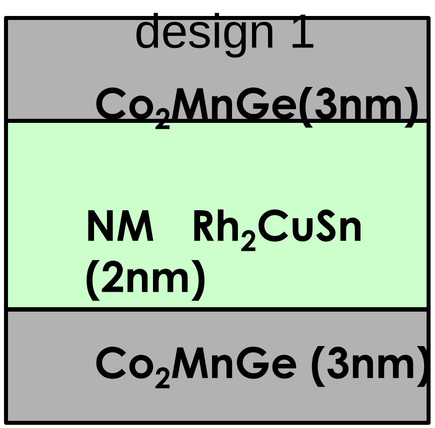
GMR SVs with Heusler alloys

K. Nikolaev, P. Kolbo, T. Pokhil, X. Peng, Y. Chen, T. Ambrose, and O. Mryasov, *Appl. Phys. Lett.* **94**, (09);



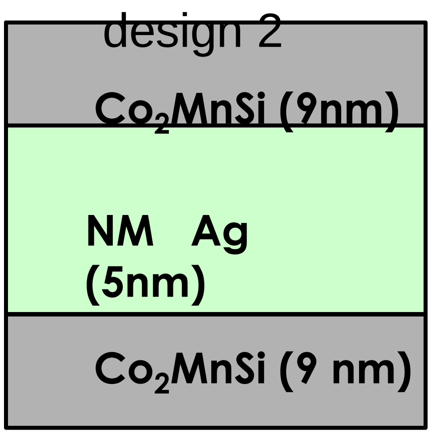
(111)

- ***Co/Cu GMR (111) texture***
- Low-bias MR~3.5%;
- RA= 45mΩ-μm^2
- ΔRA~ 1.6mΩ-μm^2



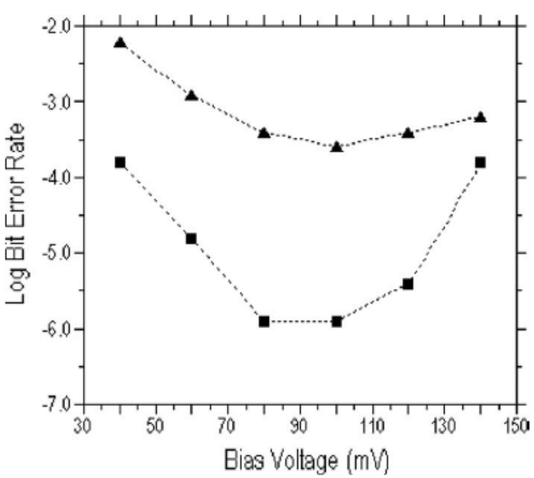
(110)

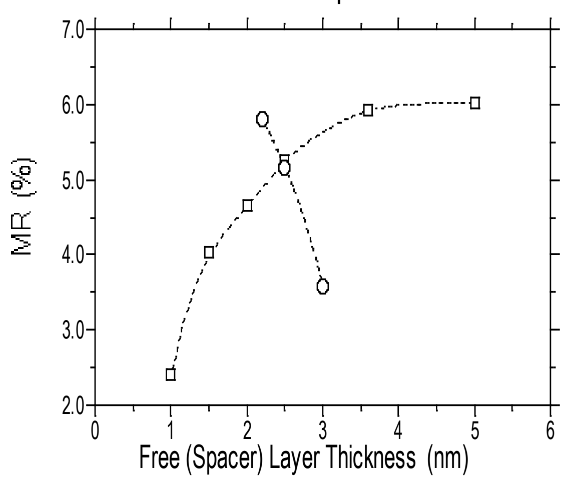
- ***Ambrose, Mryasov US 6,876, 522 B2***
- ***Nikolaev et.al. 2009,Seagate***
- Low-bias MR~6.8%;
- RA= 60mΩ-μm^2
- ΔRA~ 4.0mΩ-μm^2



(100)

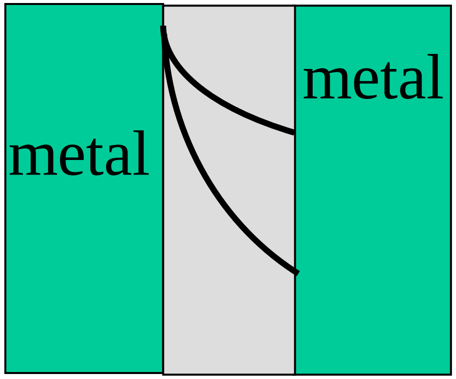
- ***Iwase et.al. 2009,***
- Low-bias MR~28.8%;
- RA= 66mΩ-μm^2
- ΔRA~8.9mΩ-μm^2



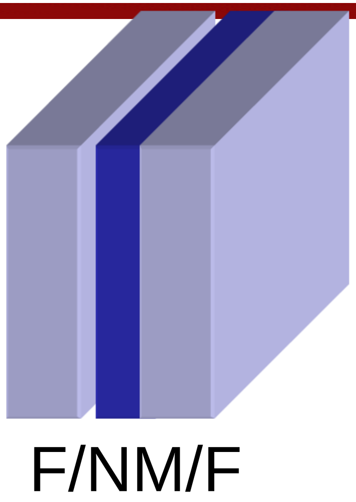


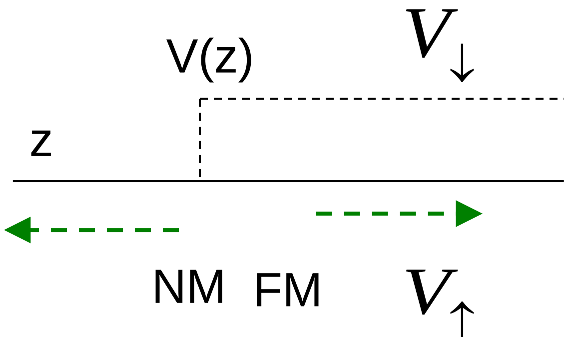
- Design 1:
  - anneal 200 C
  - test read heads
  - spacer short MFP
- Design 2:
  - problematic (100) texture
  - oxidation of spacer (Ag)
  - anneal seed 700 C/ CMS 350 C

BACKGROUND : spin dependent transport



TMR

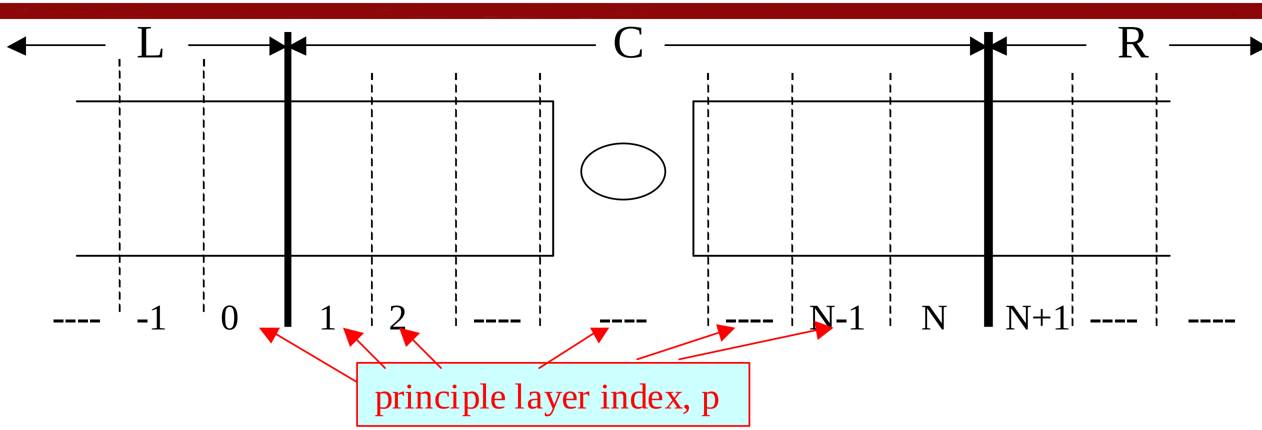


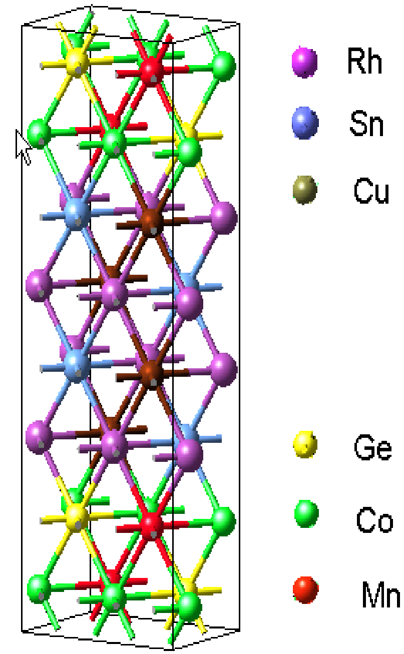


CPP-GMR

- if Modify materials set what RA and MR trends to expect
- Challenge is to improve spin dependent scattering :
  - β and γ bulk and interface spin asymmetry
  - Curie point or spin mixing stability
- Compare with available experiment

Direct transport simulations : model





$$\sigma \equiv \left.\frac{dI}{dV}\right|_{V=0} = -\frac{2e^2}{h} Tr[(\Sigma_{11} - \Sigma_{11}^{+}) g_{1N} (\Sigma_{NN} - \Sigma_{NN}^{+}) g_{N1}^{+}]_{E=E_F}$$

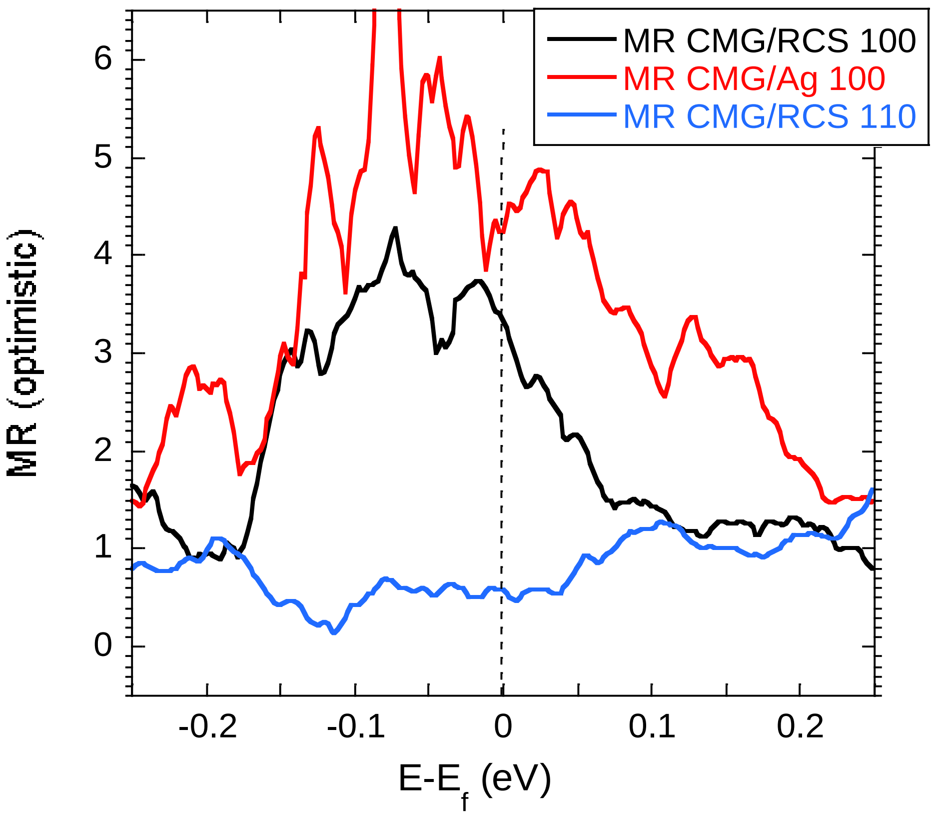
- All charge and potential relaxation takes place in central (C) region. Right (R) and left (L) regions assumed to have bulk charge density and potentials.
- Only adjacent layers interact, so the "Hamiltonian" $h \equiv P(E) - S^{\alpha}$ of auxiliary Green's function $g(E) = (P(E) - S^{\alpha})^{-1}$ has nonzero matrix elements only for adjacent principle layers and takes tridiagonal form in principal layer index:

Model 1: L = Ag ; C = CMG|RCS|CMG ; R = Ag (110) and (100)
Ag|Co2MnGe(3)|Rh2CuSn(3)|Co2MnGe(3)|Ag

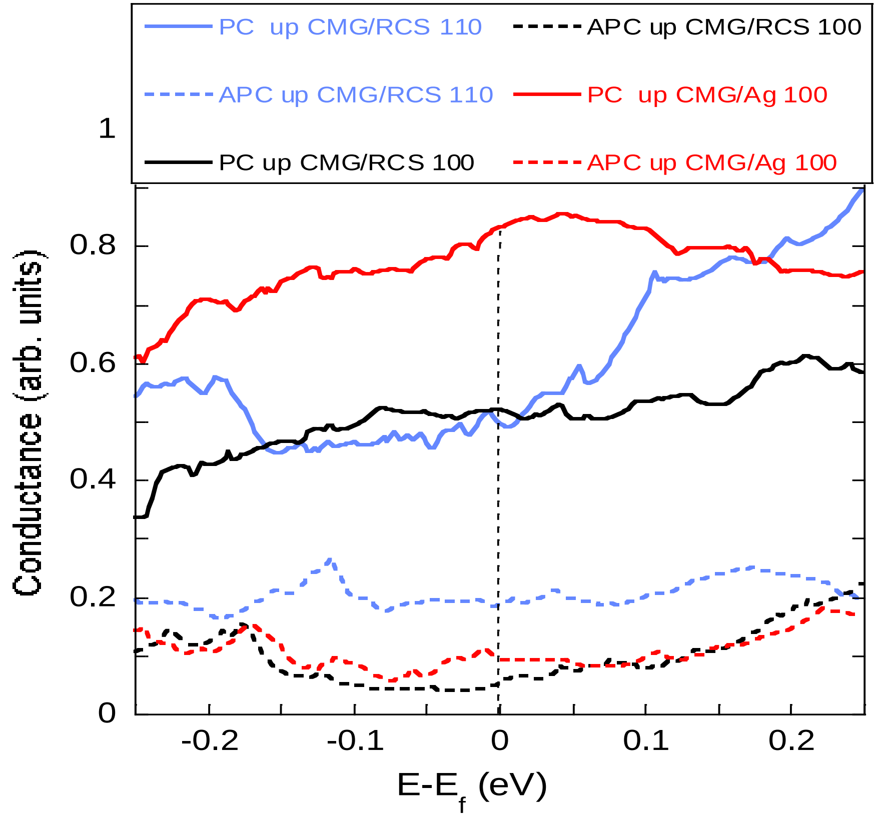
Model 2: L = Ag ; C = CMG|Ag|CMG ; R = Ag (100)
Ag|Co2MnGe(3)|Ag|Co2MnGe(3)|Ag

Direct transport simulations : Design 1 vs. Design 2

Model 1:
Ag|CMG(3)|RCS(3)|CMG(3)|Ag



Model 2:
Ag|CMG(3)|Ag|CMG(3)|Ag

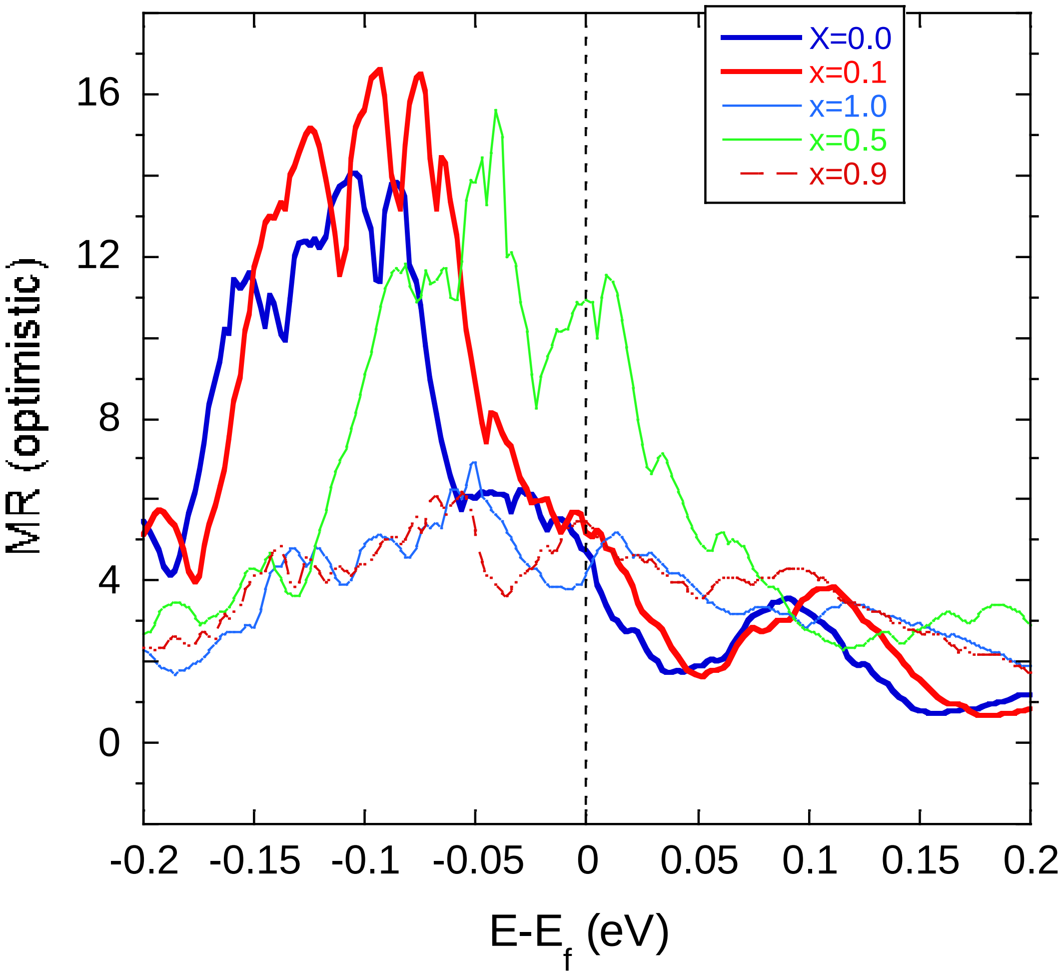


Direct transport simulations findings:

- better conductance for majority in the case of CMG/Ag spacer that CMR/RCS
- > than 4x higher conductance in the minority channel for 110 texture than in 100

Full transport simulations: Co_2(Mn-Fe)Ge

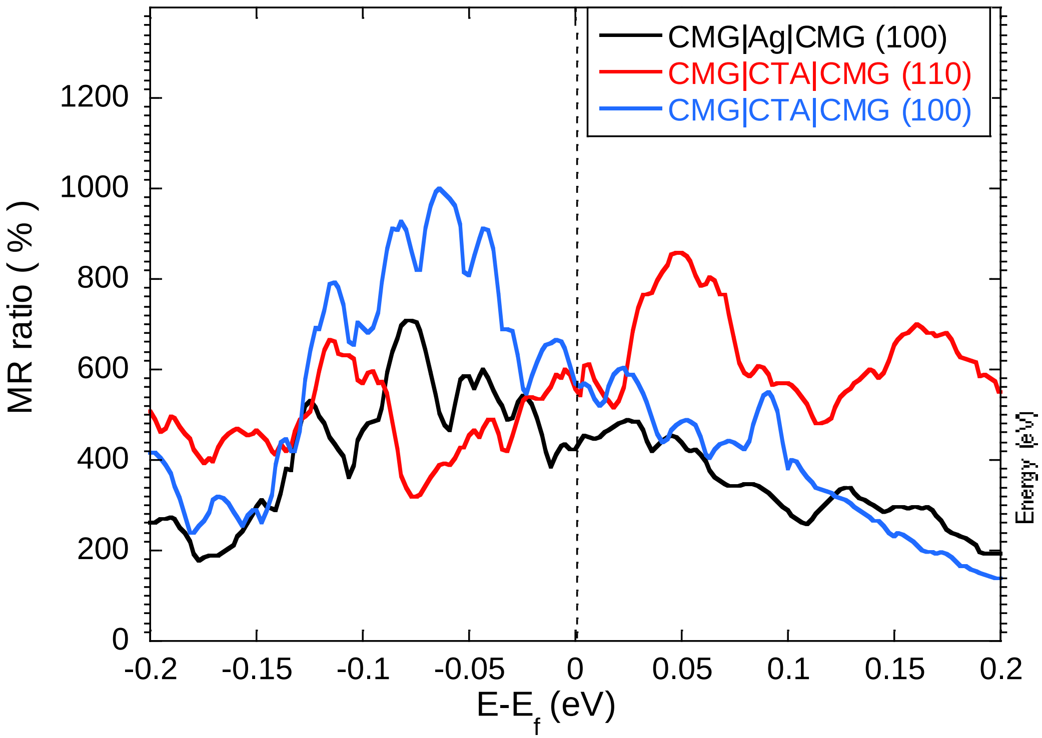
Co2(Fe-Mn)Ge/Ag/Co2(F-M)Ge (001)



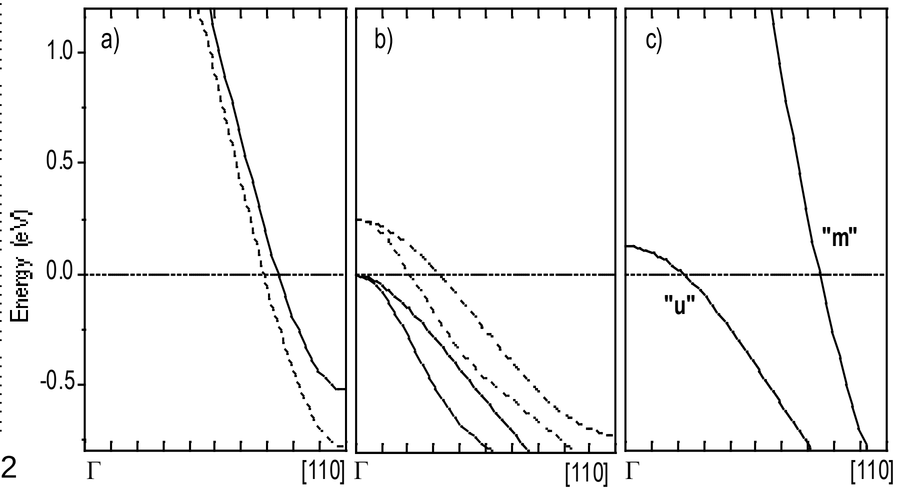
- **Co2(Fe-Mn)Ge**

-Preferable gaps
-Peferable Tc
-Transport result support advantages of
-Co2(Fe-Mn)Ge

Other Heusler alloys for all Heusler CPP-GMR



K. Nikolaev, P. Kolbo, T. Pokhil, X. Peng, Y. Chen, T. Ambrose, and O. Mryasov,
Appl. Phys. Lett. **94**, (09);



- within the ballistic transport limit all-Heusler junctions may outperform Ag based junction limited to (100) texture readily support more practical (110)
- experimental result in Prof. Hono's talk

OUTLINE

- Tc : Comments on Disorder : spin disorder
- spin mixing - Curie point calculations
- quaternary alloys strategy

- Eg : Electronic structure: minority band gap
- fundamental gap theory - alloys design

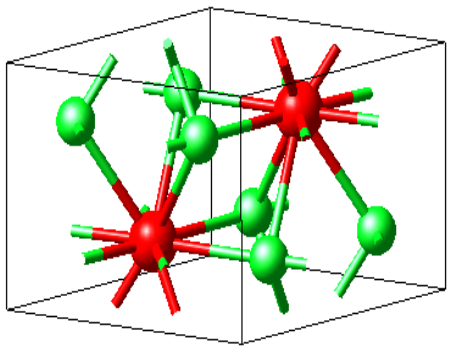
- ρ_{up}/ρ_{dn} :Spin Dependent Transport : GMR
- Band matching - Q-alloy effects

- **K1 : Hexagonal Heusler like alloys :**
- Magnetic Anisotropy

- Summary and Conclusions

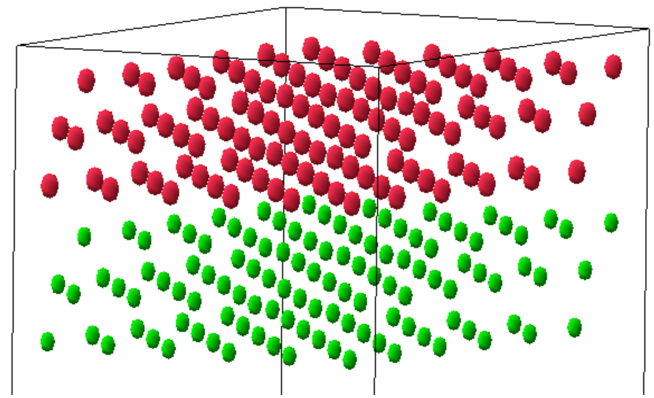
Materials landscape : 3d-5d vs. 3d-metalloid

$Co_{1-x}Pt_x$

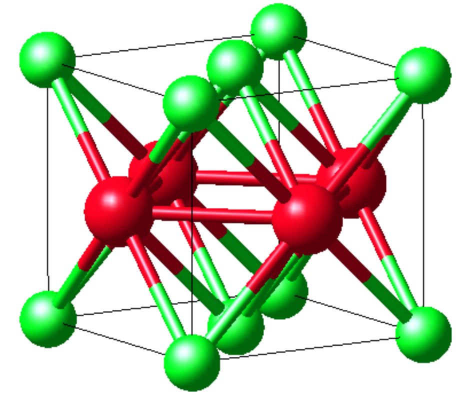


DO19

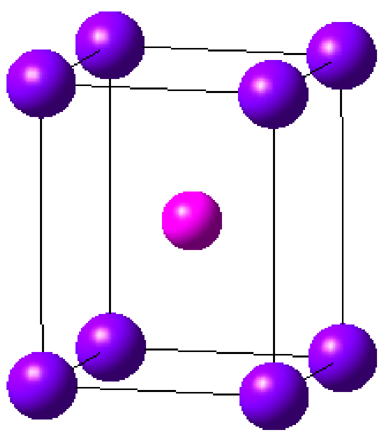
Co_n/Pt_m MLs



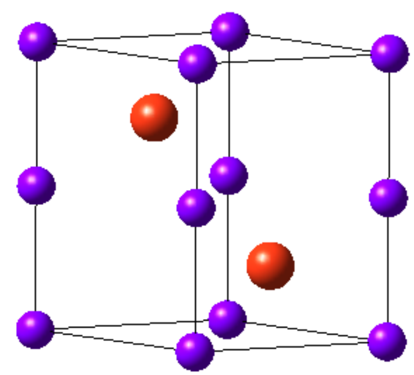
Fe/Co-Pt



L10



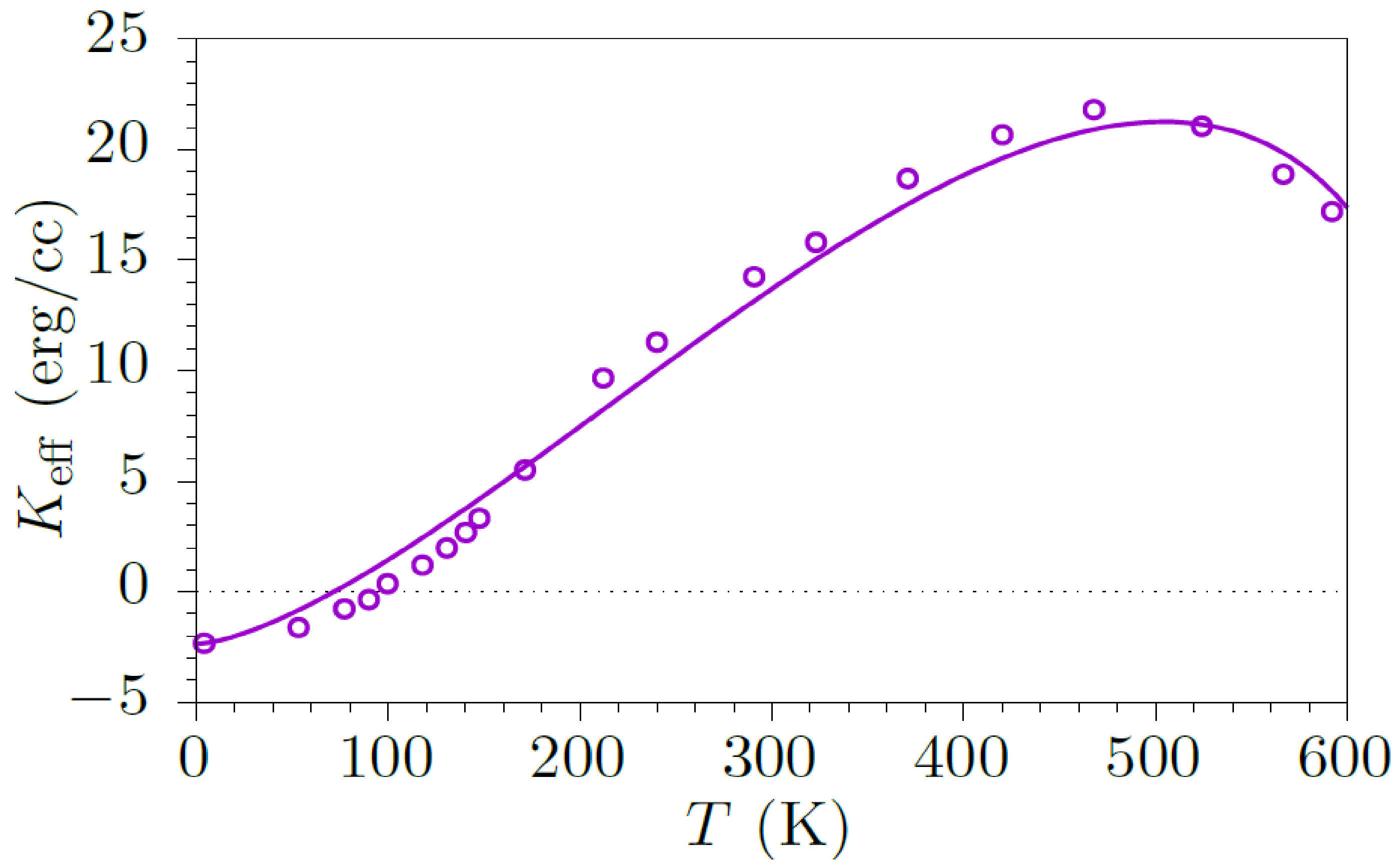
								B	C	N
								Al	Si	P
V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As
Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb
Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi
Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm



Two types of anisotropy:

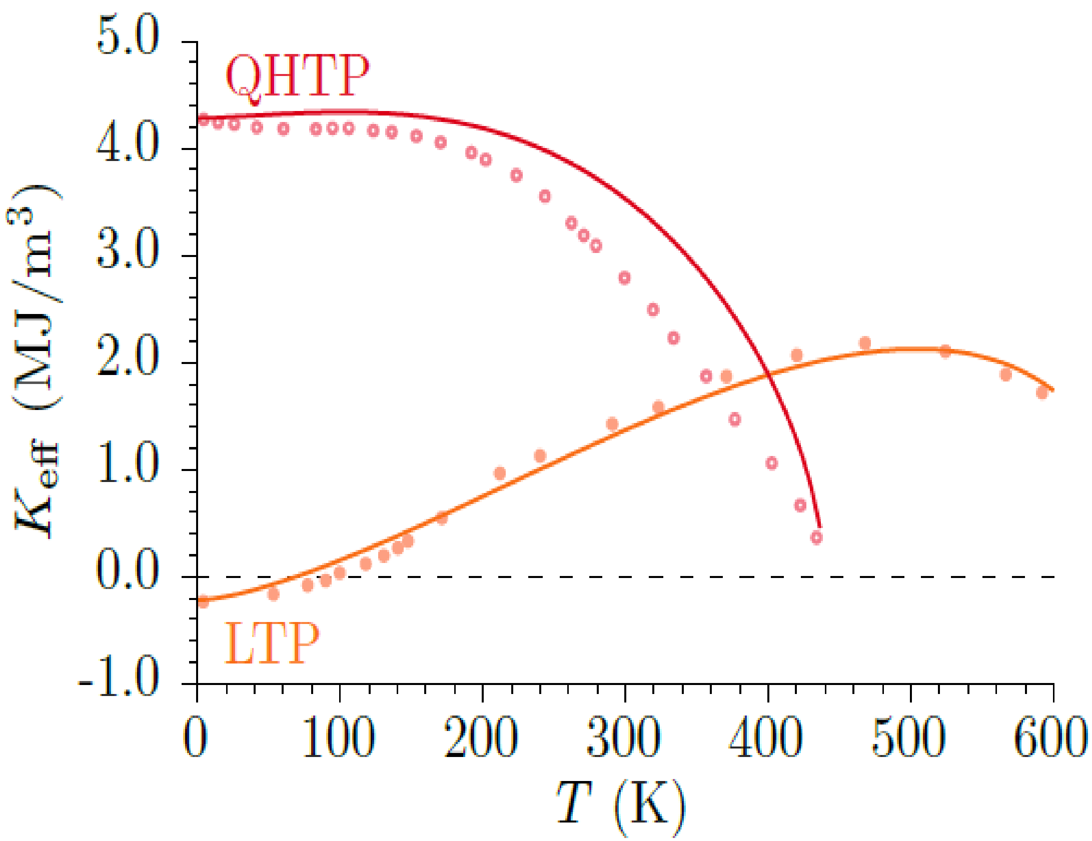
- Bulk (FePt, Fe16N2, Mn-Bi)
- Interface (Fe/MgO)

K(T) properties : the MnBi challenge



- Reorientation can be understood partially with lattice temperature
- Still hard to reconcile with large pick

Our approach to the problem : Keff(T)



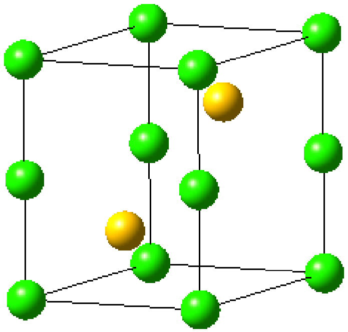
W. E. Stutius, T. Chen, and T. R. Sandin, AIP Conference Proceedings 18, 1222 (1974).

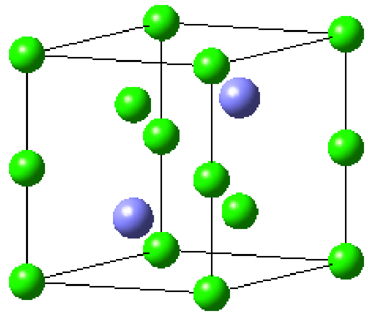
- K1(5K, K2(5K) , K3(5K) experimental
- determine k2 and d(2)
- m(T) from experiment

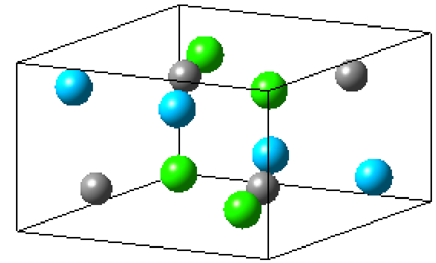
$$K_1 = \frac{3}{2}\kappa_2 + \delta_2 + \Delta_2$$

- Analysis indicate huge anisotropy of two-ion type d(2) of about + 8 MJ/mc compensated by large negative d(0) to give small in-plane K_eff

NiAs vs. Ni_2In vs. TiNiSi : CE technique XYZ (Z=Ge)

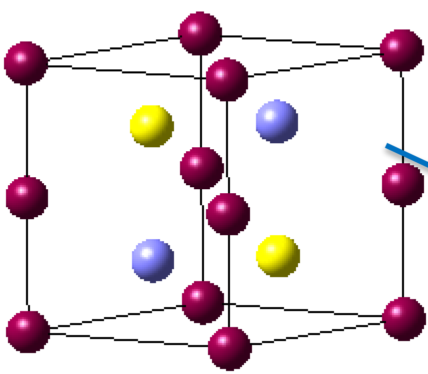


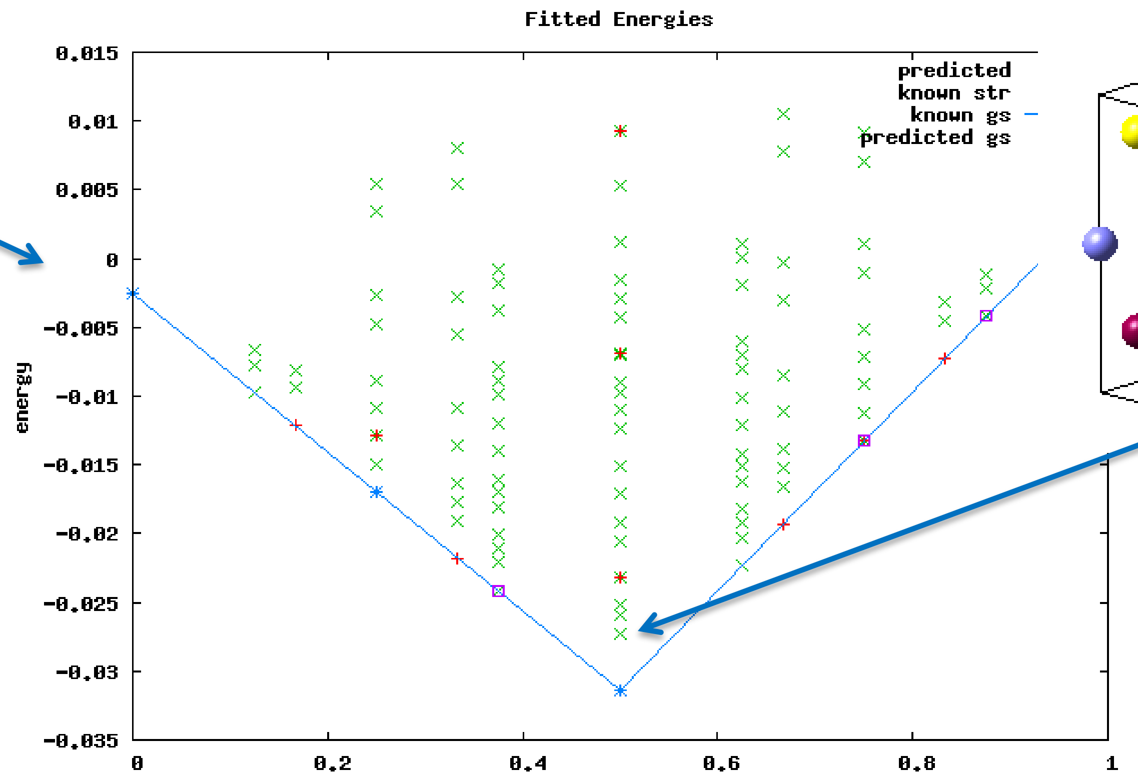


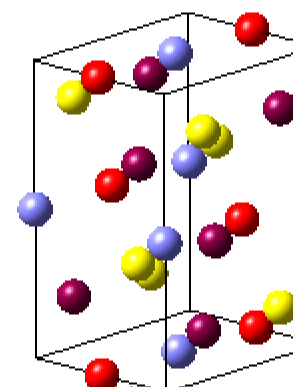


- Materials search : structure/phase generators: using generalized cluster expansion algorithms

-A. van de Walle, Nature Materials 7, 455 - 458 (2008)







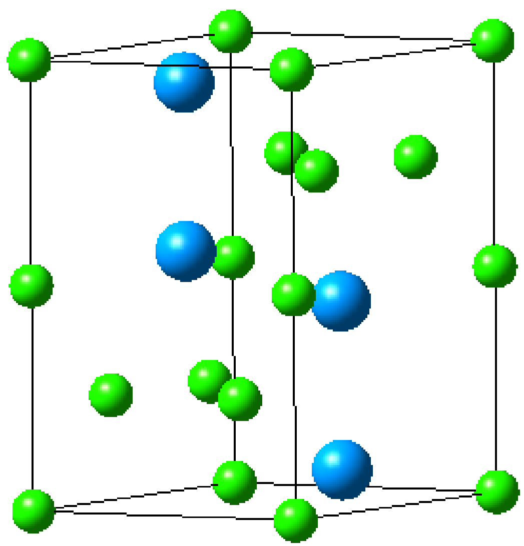
- Tuning Ms and Tc

$CoFe_{(1-x)}Mn_xGe$

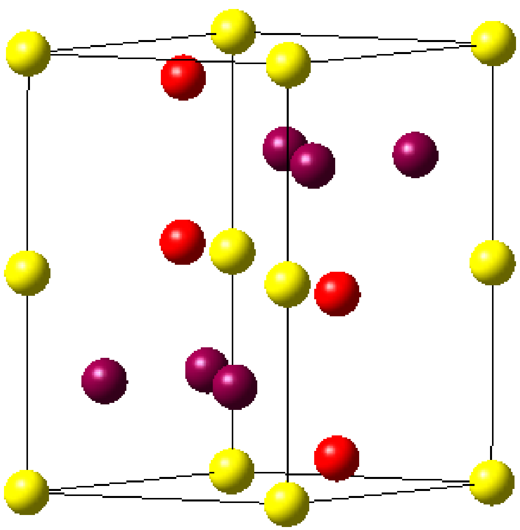
- Too Low Tc
- K<0

NiAs vs. Ni_2In vs. TiNiSi vs. Ni2U

Ni2U



XYZ , XY=MnFeCo, Z= Ge



- Keff = +0.45 MJ/m^3
- Ms = 1310 emu/cc
- Tc = 820 K

Decent performance , further enhancement of K might be needed

Summary and Conclusions

- Addressed some of the material physics challenges:
  (I) Tc, spin mixing ; (II) Band gap beyond DFT ;
  (III) spin dependent transport ;
  (IV) MAE
- 3d-3d hybridization nature of minority gap need to be addressed by the way of going beyond DFT
- Exchange coupling - MAE affected
- QSGW bands structure calculations enable accurate evaluation of HM features
  - Co2FeGe true HF (GW not LDA) with 0.6 eV gap
  - Co2FeSi X (GW) with 1.33 eV (0.7 eV) LDA gap unlike
- Co2(Fe-Mn)Ge alloy shows favorable spin transport trend
- GMR CMG/CTA(RCS)/CMG(100) and (110) evaluated

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Prof. Jian Ping Wang : UMN, $Fe_{16}N_2$, other PMA, C-SPIN director

Prof. K. Hono : CTA based all Heusler spacer

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Joseph Barker [2]

now AIMR Tohoku
Assistant Prof.

Sergey Faleev[2]
now IBM Almaden, SJ, CA

- ARPA-E ; DARPA-SRC- C-SPIN ;

early stage MnBi

C-SPIN

STARnet

Strategic Partnership Funding
Émergence/Partenariat
Stratégique

spintec
SPIN IN ELECTRONICS

Alan Kalitsov[1]
now WD

BACK UP SLIDES