Modeling Transport in Heusler-based Spin Devices

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Electronic Structure

- Extended Hückel theory
- Application to Heusler alloys (Co_2FeAl)

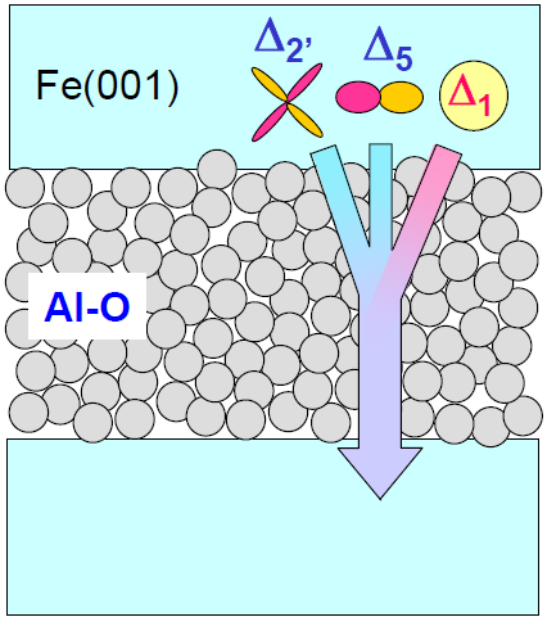
Transport

- Non-equilibrium Green's functions
- Transport calculations in CFA/MgO/CFA structures

Magnetic Tunnel Junctions

Amorphous Al-O barrier

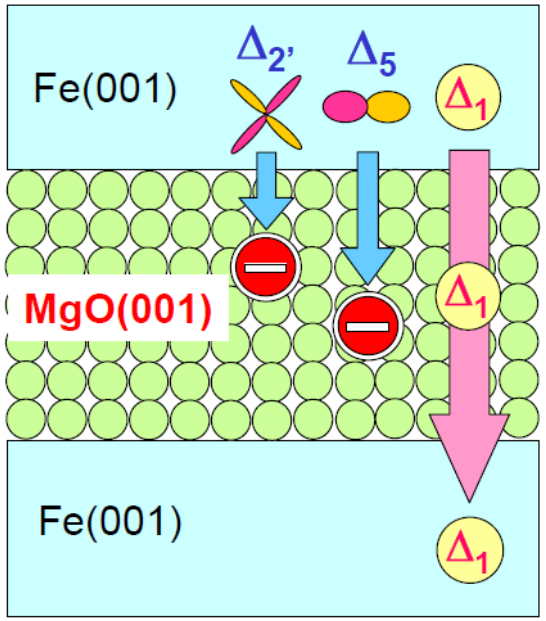
No symmetry



Various Bloch states tunnel incoherently.

Crystalline MgO(001) barrier

4-fold symmetry

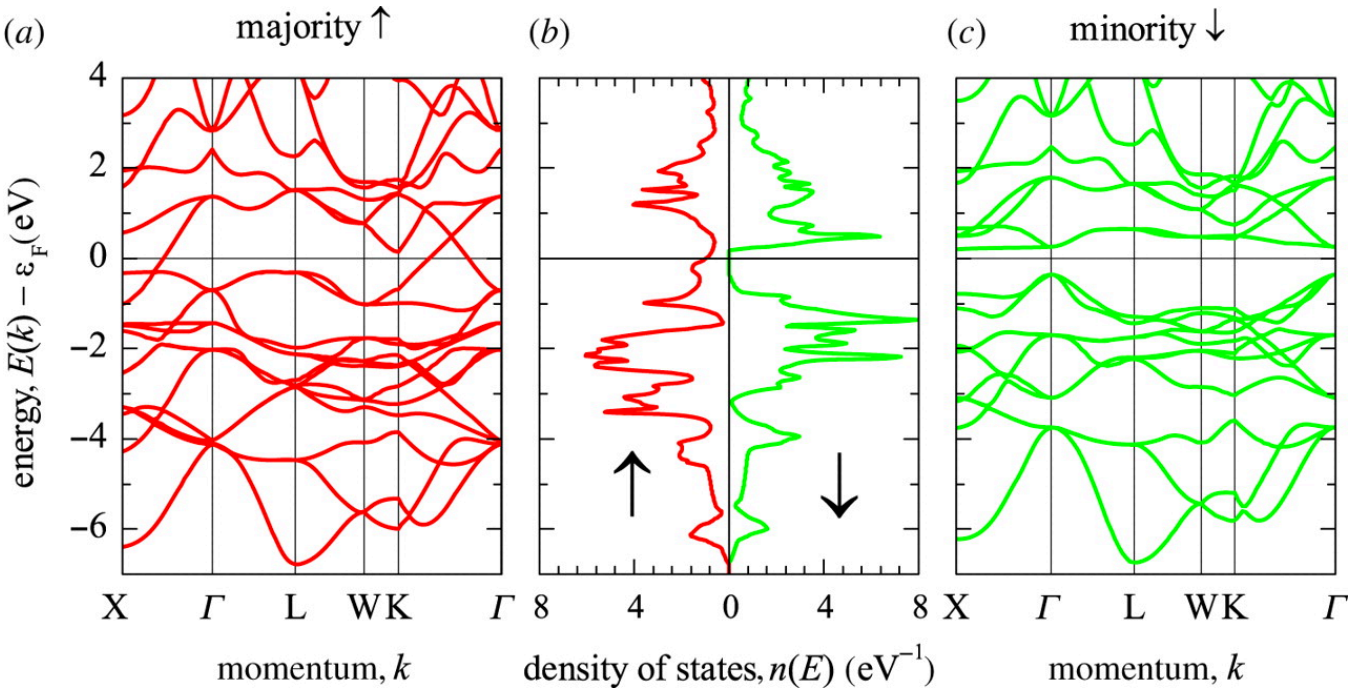


Only the Bloch states with Δ_1 symmetry tunnel dominantly.

S. Yuasa, J. Phys. D: Appl. Phys. 40 (2007)

Heusler Alloys

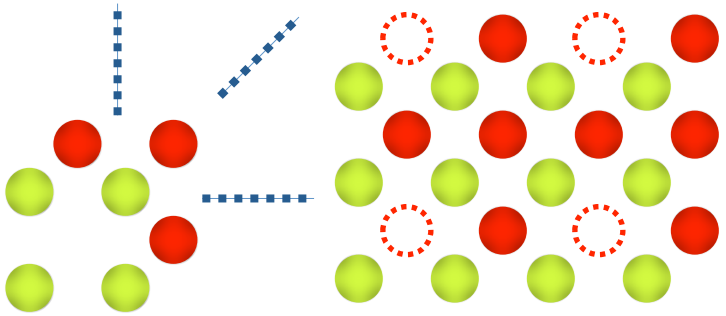
- Choice of electrode material represents an opportunity
- Several full Heusler alloys (X_2YZ) are half-metallic
- Our experience with a half-metal: Co_2FeAl (CFA)



Co_2TiGe from J. Barth et al., Phil. Trans. R. Soc. A, 369, 3588-3601 (2011)

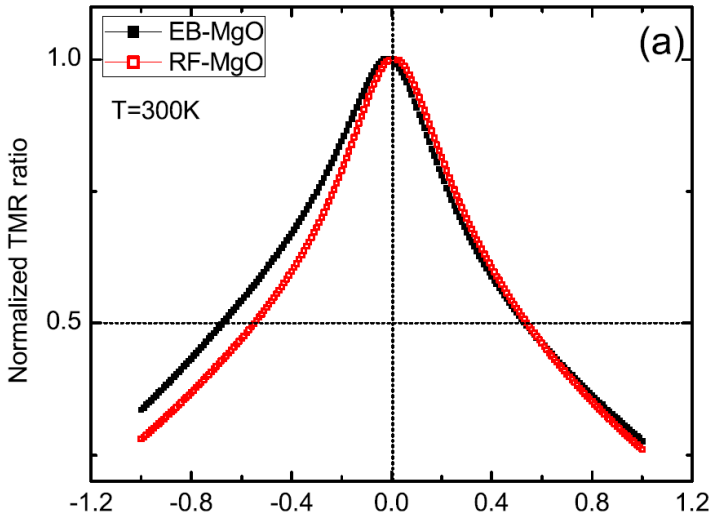
Project Goals

MTJ physics at equilibrium has been well-studied using *ab initio*



We hope to take it a step further by:

- Modeling non-equilibrium transport to study device behavior under bias
- Assessing the impact of defects on device performance



Hierarchy of Models

Effective Mass:
Parabolic
+ Corrections

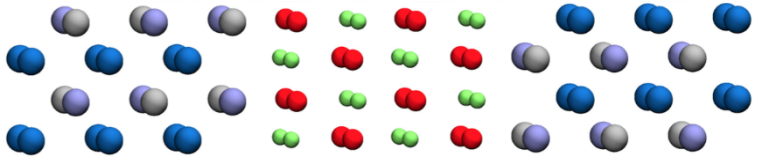
"Empirical" Tight-binding:
1st Nearest Neighbor
Multiple Neighbors

"Semi-empirical" Tight-binding:
EHT
DFTB

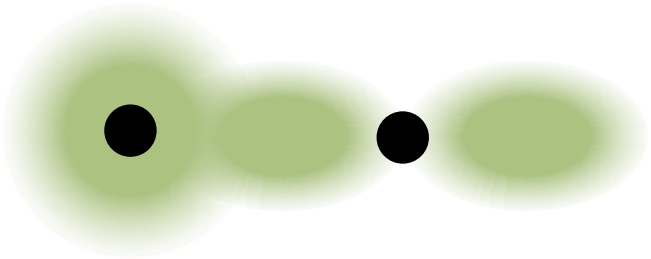
Ab Initio:
DFT, GW, DMFT, CI, CC, etc.

Extended Hückel Theory

Atomic Configuration → H, S Matrices



$$\psi_{n,l,m} = c_1 R_{n,\zeta_1} Y_{l,m} + c_2 R_{n,\zeta_2} Y_{l,m}$$



s-p_z orbital overlap

$$R(r,n,\zeta) = (2\zeta)^n \left(\frac{2\zeta}{(2n)!}\right)^{1/2} r^{n-1} e^{-\zeta r}$$

$$Y_l^m(\theta,\phi) = \left[\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(cos\theta) e^{im\phi}$$

EHT Hamiltonian

E_{11}	t_{12}	t_{13}
t_{21}	E_{22}	t_{23}
t_{31}	t_{32}	E_{33}

2nd nearest neighbor

Nearest neighbor

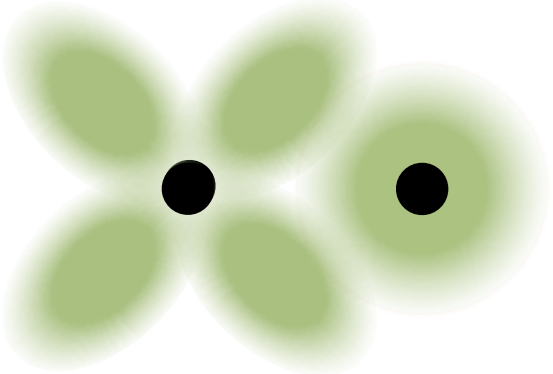
Orbital onsite

$$H_{ii} = E_{onsite}$$

$$H_{ij} = K \; S_{ij} \; (H_{ii} + H_{jj})/2$$

$$S_{ij} = \langle \psi_i \,|\, \psi_j \rangle$$

$$\psi_{n,l,m} = c_1 R_{n,\zeta_1} Y_{l,m} + c_2 R_{n,\zeta_2} Y_{l,m}$$

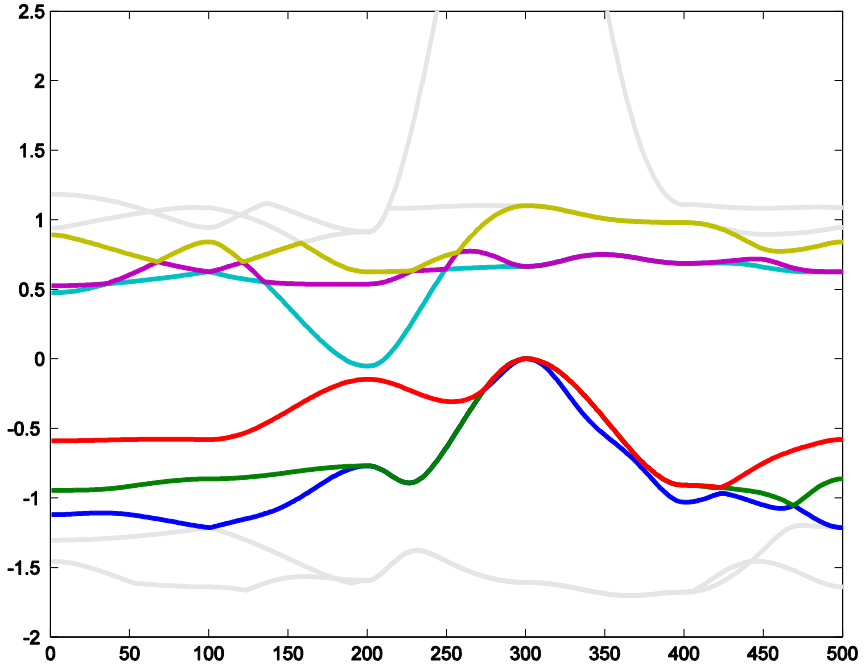


d-s overlap (vanishes)

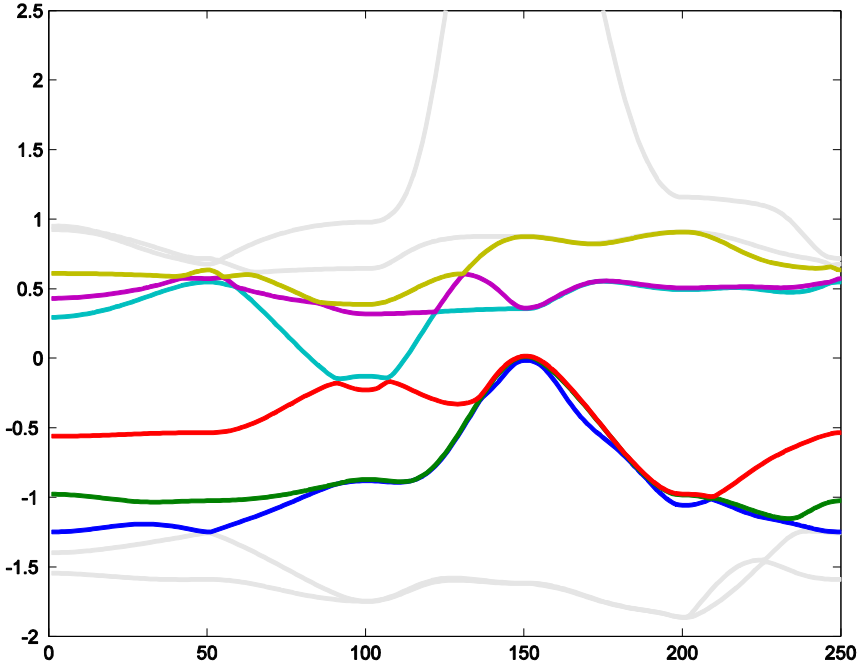
Transferability?

CFA minority spin E-k with elemental metal parameters – i.e. no attempt at fitting

DFT



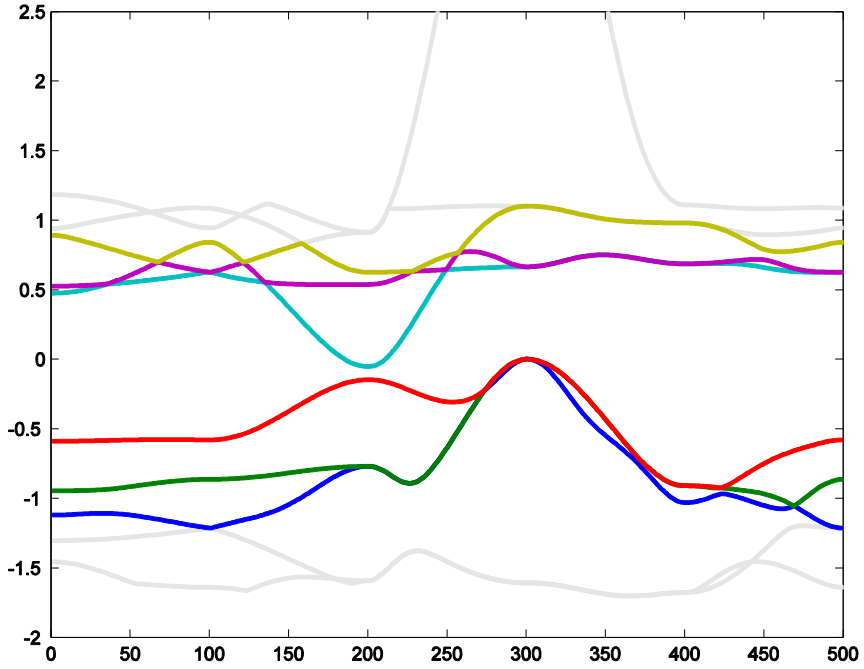
EHT



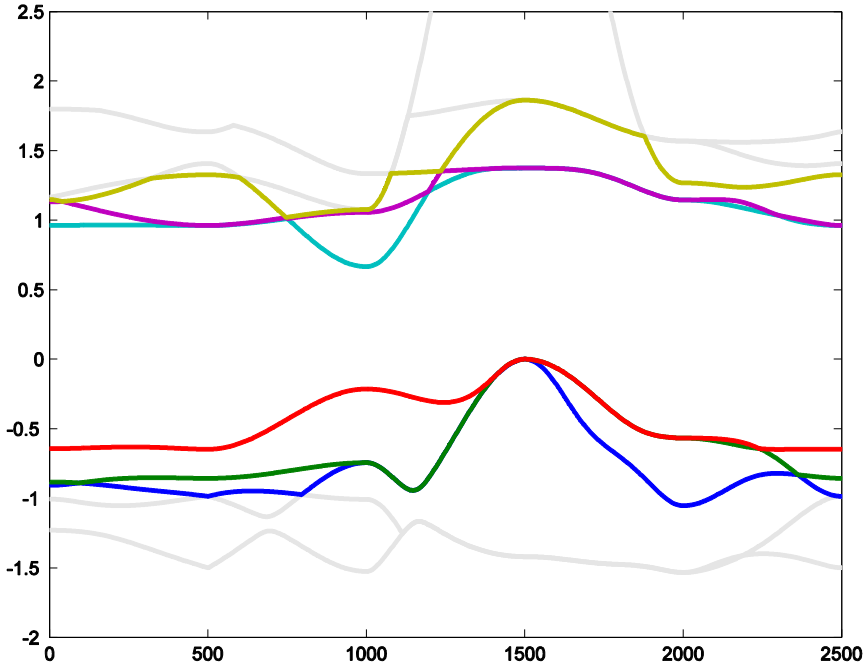
Band Gap Correction

DFT underestimates band gap as usual; need +U

DFT (standard)



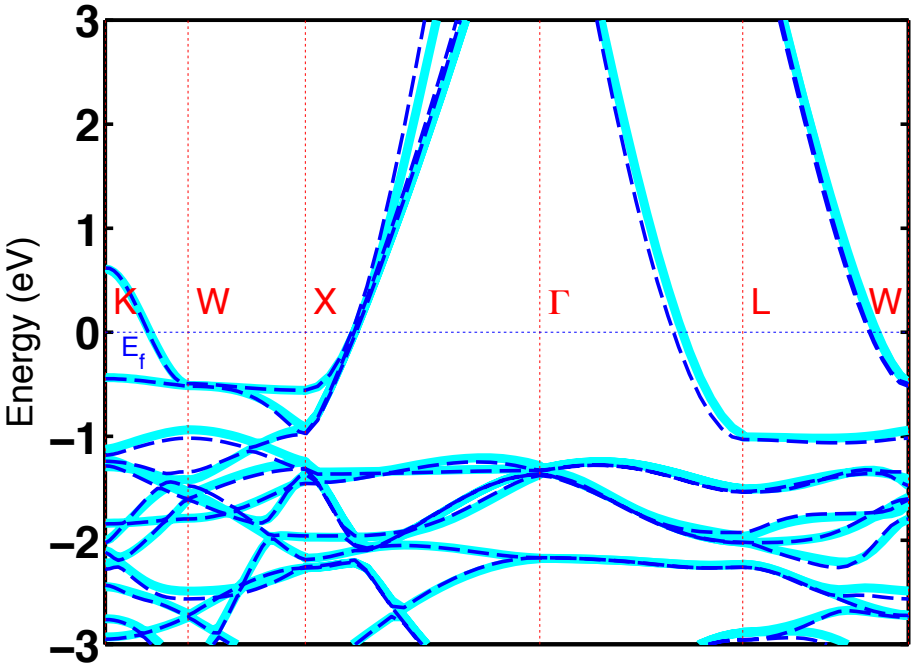
DFT (+U)



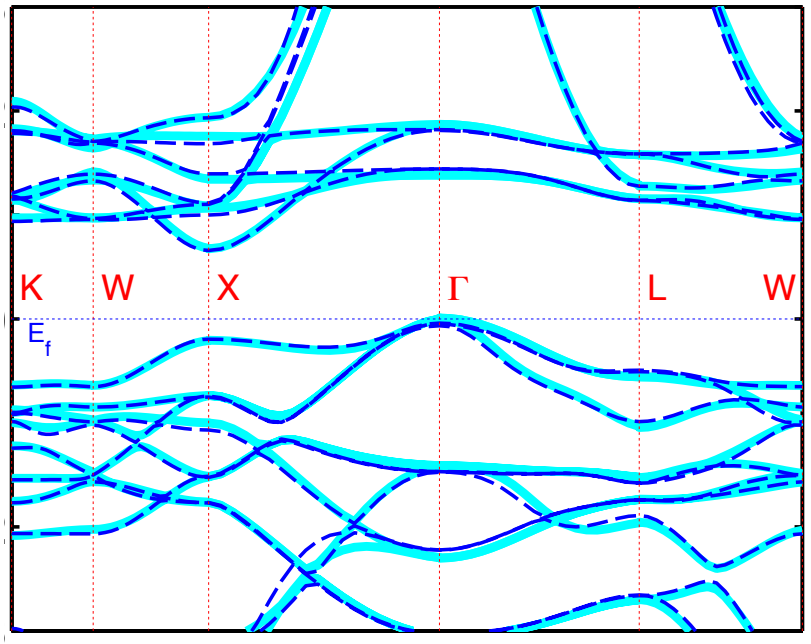
EHT v. DFT: Co_2FeAl

E-k fit is accurate over a very wide energy range

Majority Spin



Minority Spin



Crystal Field Splitting

Broken spherical symmetry

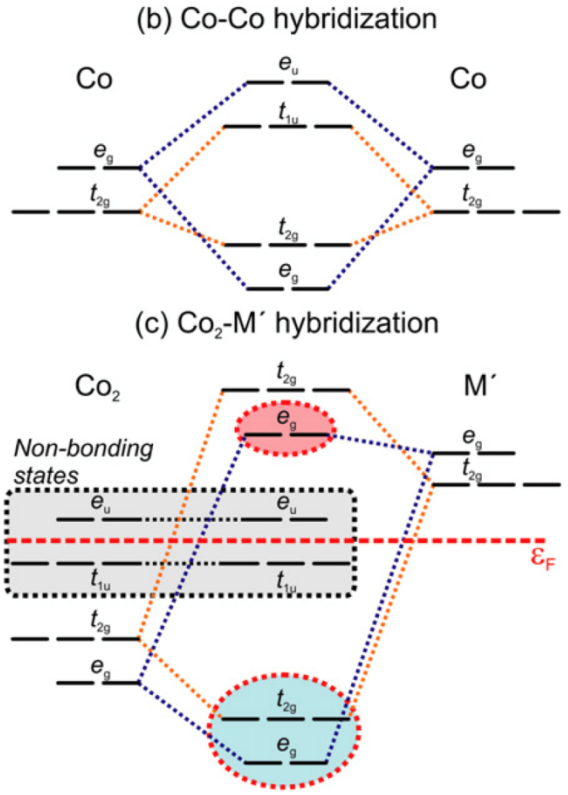
- Orbital degeneracy lifted
- e_g group: d_{x2-y2} d_{z2}
- t_{2g} group: d_{xy} d_{yz} d_{zx}

Adapting tight-binding

- Onsite energies must be resolved by the *m* quantum number
- 1-2 extra parameters in EHT

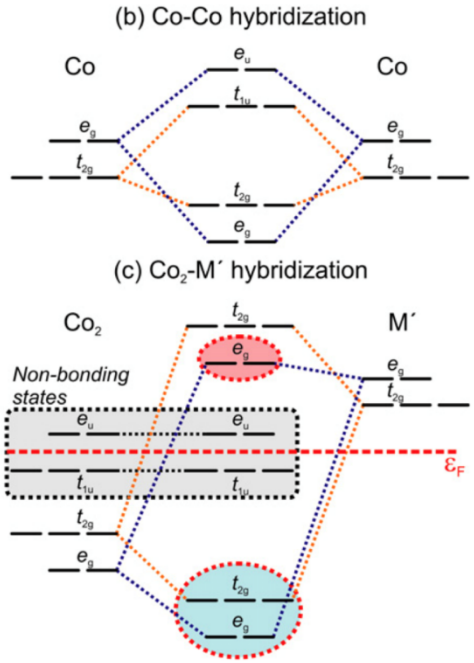
Case of full Heusler alloys

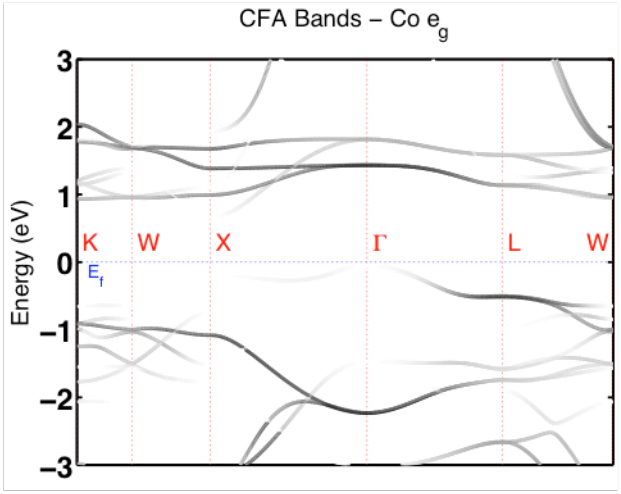
- X_2YZ has T_d symmetry
- But lattice of X atoms has the broader O_h symmetry

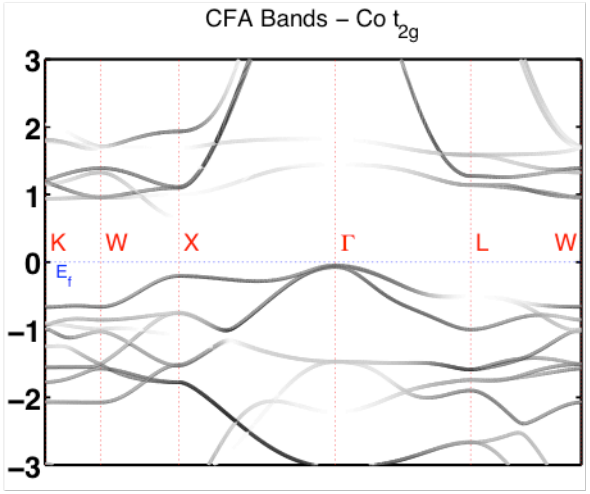


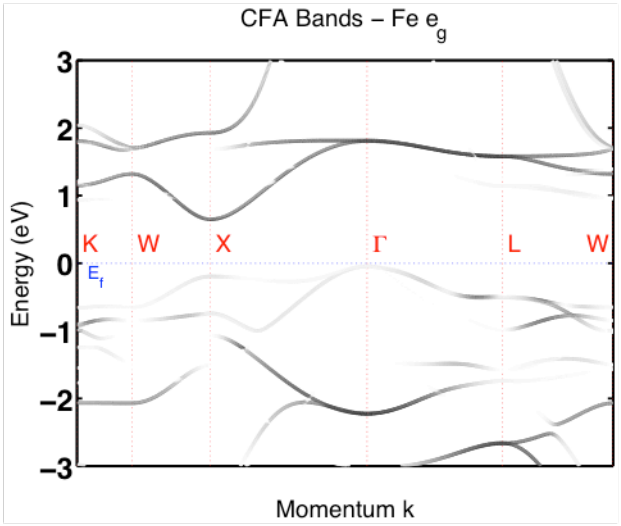
I. Galanakis et al., Phys. Rev. B **66**, 174429 (2002)

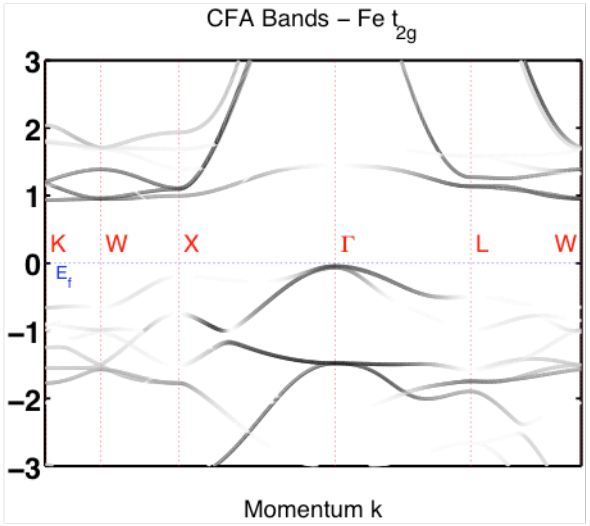
Orbital Projections











Non-equilibrium Green's Functions

NEGF consists of a set of integro-differential equations (in time) or matrix equations (in energy)

$$\boldsymbol{G}^{r/a}(t,t')\mathcal{G}'^{-1}(t')$$
$$= \boldsymbol{\delta}(t-t') + \int \mathrm{d}t_1 \boldsymbol{G}^{r/a}(t,t_1)\boldsymbol{\Sigma}^{r/a}(t_1,t'),$$

$$\boldsymbol{G}^{\lessgtr}(t,t')\mathcal{G}'^{-1}(t')$$
$$= \int \mathrm{d}t_1 \left[\boldsymbol{G}^{r}(t,t_1)\boldsymbol{\Sigma}^{\lessgtr}(t_1,t') + \boldsymbol{G}^{\lessgtr}(t,t_1)\boldsymbol{\Sigma}^{a}(t_1,t')\right]$$

$$\mathcal{G}^{-1}(E)\mathbf{G}^{r/a}(E) = \mathbf{I} + \Sigma^{r/a}(E)\mathbf{G}^{r/a}(E),$$

$$\mathcal{G}^{-1}(E)\mathbf{G}^{\lessgtr}(E) = \Sigma^{r}(E)\mathbf{G}^{\lessgtr}(E) + \Sigma^{\lessgtr}(E)\mathbf{G}^{a}(E)$$

Landauer Formalism

Landauer formalism with transmission computed using Green's functions:

$$J = \frac{q}{h} \int dE \; T(E) \; (f_1 - f_2)$$

$$T(E) = Tr[\Gamma_1 \; G \; \Gamma_2 \; G^{\dagger}]$$

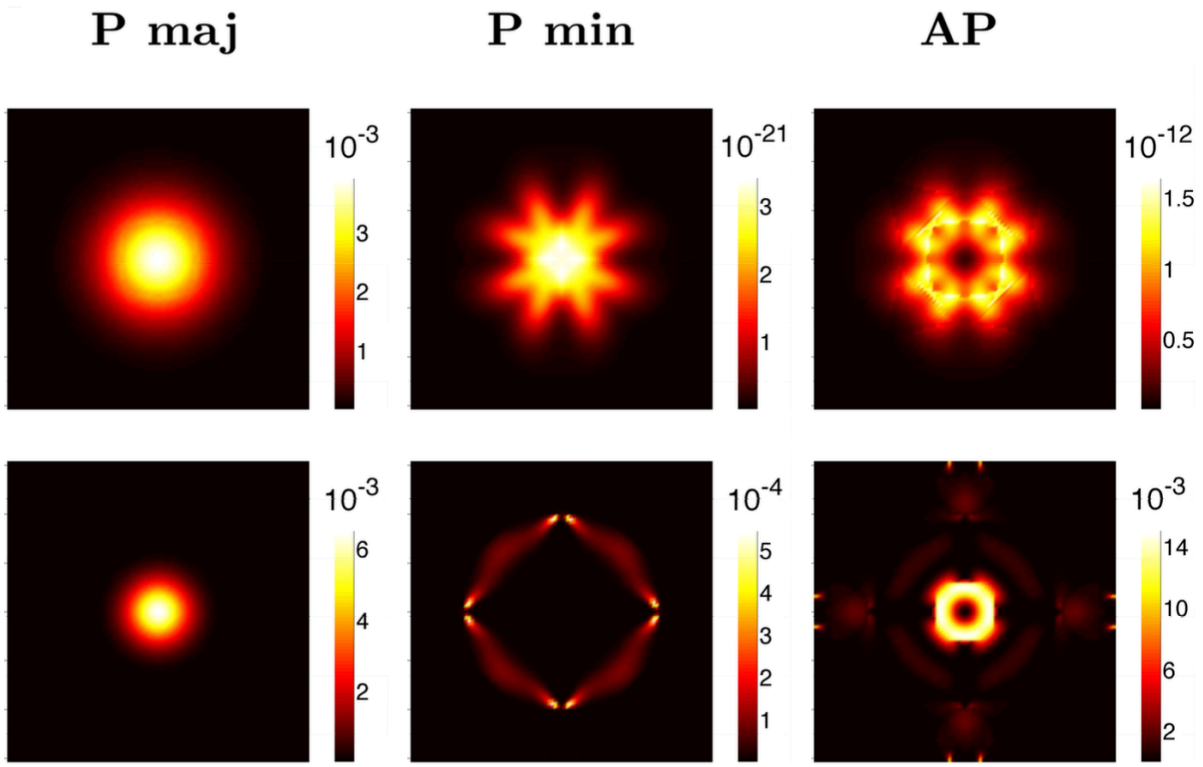
$$G(E) = [(E + i0^{+})S - H - U - \Sigma_1 - \Sigma_2]^{-1}$$

Periodicity permits working in k-space:

$$H(\vec{k_{\parallel}}) = \sum_{\vec{r}} H(\vec{r}) \; e^{i\vec{k_{\parallel}} \cdot \vec{r}}$$

CFA/MgO/CFA Transmission

Same broad Δ_1-like peak in parallel majority $T(E_F)$
Much lower minority and anti-parallel $T(E_F)$

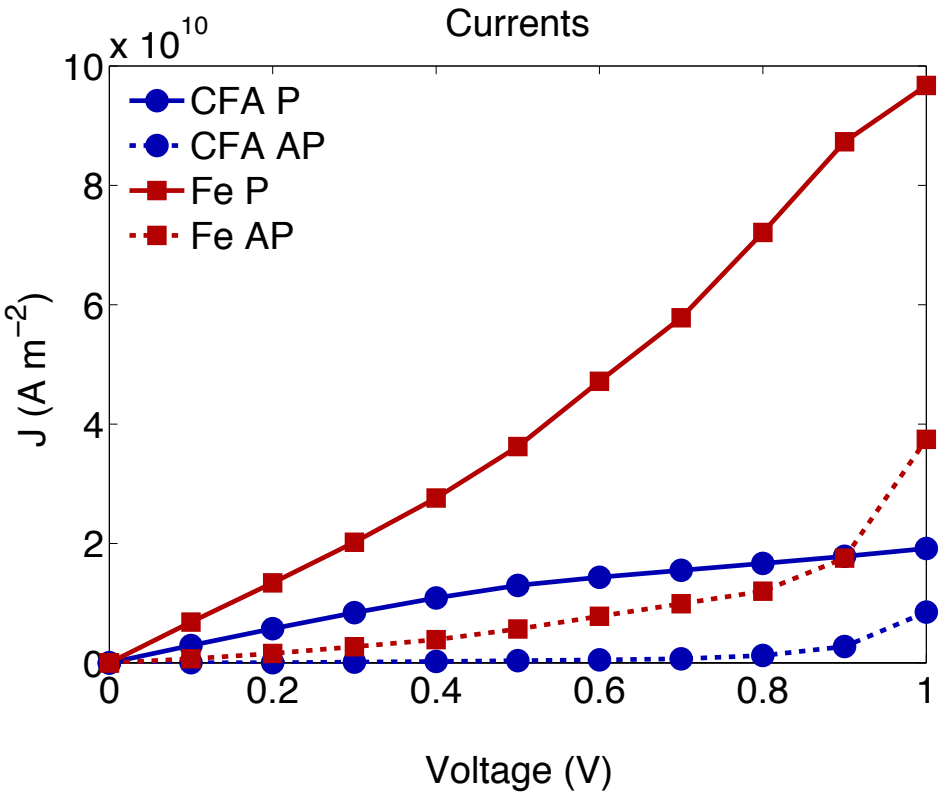


CFA and Fe MTJs: J-V

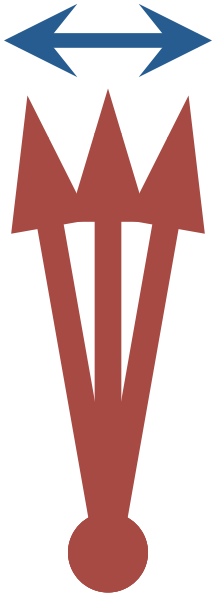
Anti-parallel current nicely suppressed up very high biases

We pay a price in resistance-area (RA)

1. Lower signal-to-noise ratio (SNR)
2. Bad for scaling!



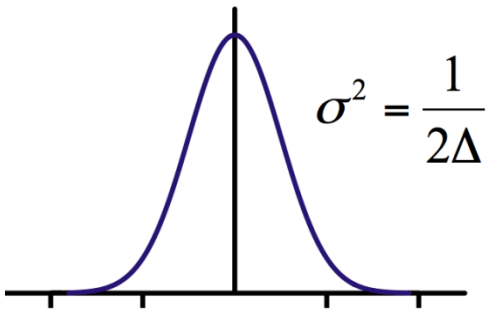
Fluctuation Spin Mixing



$$I = I_P + \left(I_{AP} - I_P\right)\sin^2\left(\theta/2\right)$$

$$f \propto \exp\left(-U_b \sin^2\theta / kT\right)$$

$$U_b / kT = \Delta \approx 30 - 60$$



$$\left\langle I_{AP}\right\rangle = I_{AP} + \frac{\left(I_P - I_{AP}\right)}{8\Delta} \qquad \left\langle I_P\right\rangle = I_P + \frac{\left(I_{AP} - I_P\right)}{8\Delta}$$

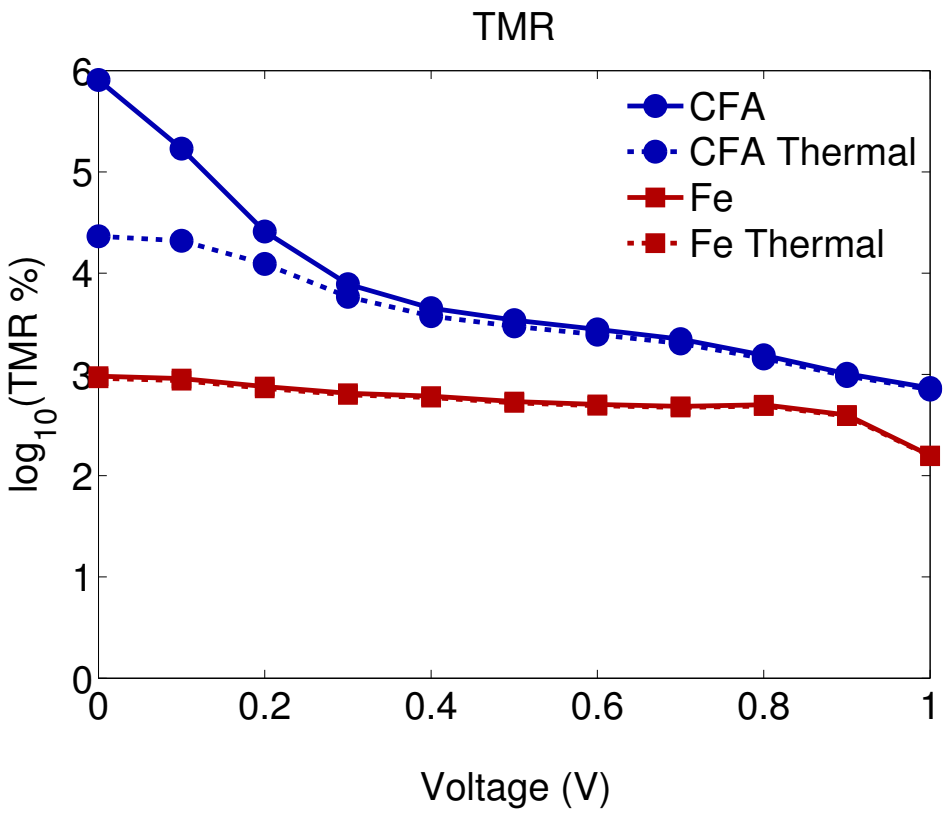
CFA and Fe MTJs: TMR

Half-metal benefits TMR across a wide bias range

- A consequence of the ~1 eV minority gap

Thermal spin flips lower TMR but not dramatically

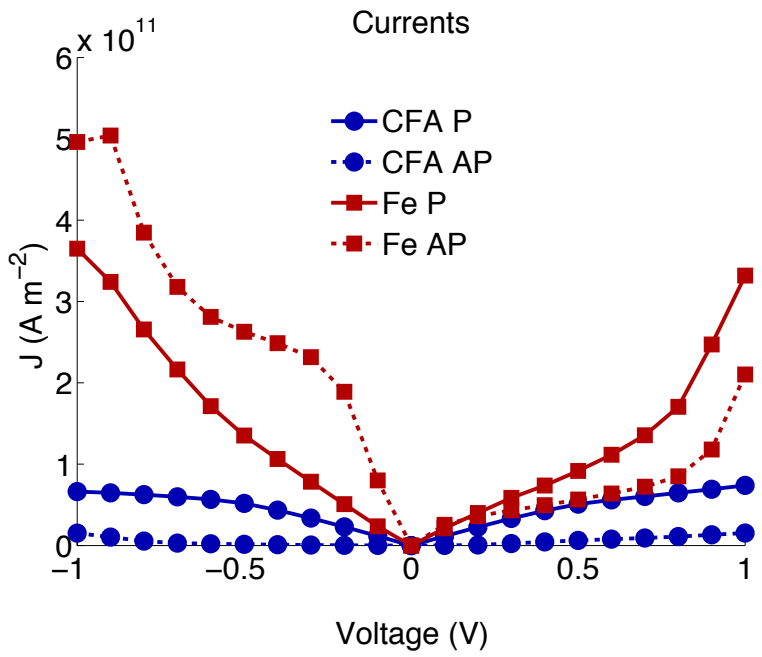
- i.e. we must have spin flipping processes besides thermal energy



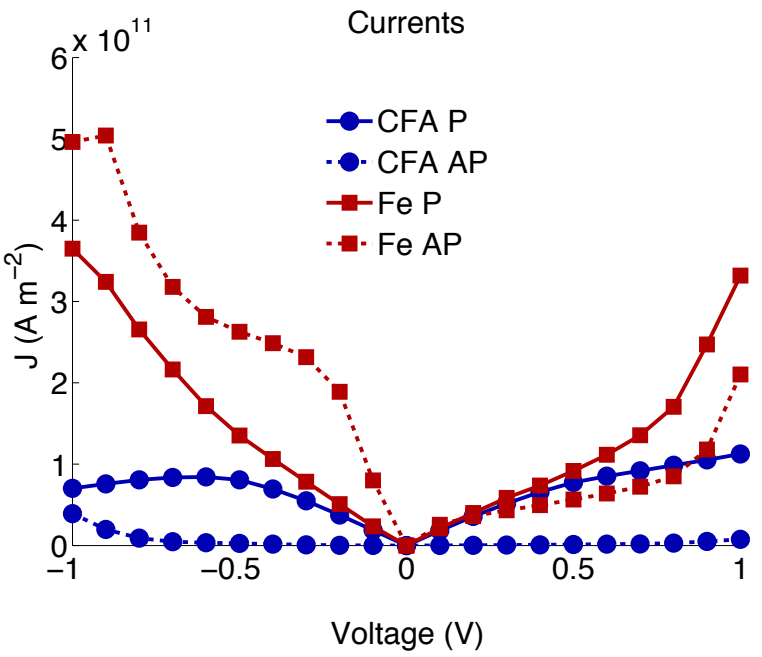
Vacancy Defects

Fe/MgO/Fe is known to be degraded by oxygen vacancies, borne out in experiments and theory

O Vacancy (Fe)



O Vacancy (Al)



Conclusions

- We find the E-k of Co_2FeAl to be well reproduced by extended Hückel theory
  - EHT proves to have high transferability
  - Crystal field splitting needs to be taken into account
  - Generalizable to other L21 Heusler alloys
  - Paves the way for engineering-scale modeling
- Ideal crystals show superior properties across a wide bias range, but far from reality
  - TMR much higher, but so is RA
  - Simple picture of temperature-induced spin flips do not account for experimental values
- Oxygen vacancies do not have the same effect as on Fe/MgO/Fe structures
  - The quality of the Heusler alloy films possibly plays a greater role than the oxide interfaces

Thank you.

Questions?

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Free Parameters

Parameter	Interpretation
E_{Onsite}	Ionization energy
c_1, c_2	LCAO coefficients
ζ_1, ζ_2	Radial decay strength
K_{EHT}	---
extra E_{Onsite}	Crystal field splitting

$$\psi_{n,l,m} = c_1 R_{n,\zeta_1} Y_{l,m} + c_2 R_{n,\zeta_2} Y_{l,m}$$

$$R(r,n,\zeta) = (2\zeta)^n \left(\frac{2\zeta}{(2n)!}\right)^{1/2} r^{n-1} e^{-\zeta r}$$

$$Y_l^m(\theta,\phi) = \left[\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(cos\theta) e^{im\phi}$$

TABLE I. Slater-type orbital parameters for EHT.

Atom	Orbital	E_{onsite}	ζ_1	c_1	ζ_2	c_2
Co	$4s$	−9.08194	1.55335	0.90903		
maj	$4p$	−6.47874	1.23006	0.76289		
	$3d$: e_g	−12.52229	1.79648	0.49542	3.15170	−0.29220
	$3d$: t_{2g}	−12.28094				
Co	$4s$	−9.06115	1.47081	1.00122		
min	$4p$	−5.69197	1.30977	0.75543		
	$3d$: e_g	−9.99179	2.23952	0.54039	2.54008	0.47420
	$3d$: t_{2g}	−10.94967				
Fe	$4s$	−9.32601	1.72377	0.64710		
maj	$4p$	−7.17093	1.21583	0.58874		
	$3d$: e_g	−13.79933	1.76803	0.19158	2.65159	0.55383
	$3d$: t_{2g}	−13.42214				
Fe	$4s$	−12.61727	1.36962	0.51054		
min	$4p$	−7.01363	1.31013	0.80327		
	$3d$: e_g	−9.70934	1.48670	0.52120	2.58892	−0.34367
	$3d$: t_{2g}	−10.50984				
Al	$3s$	−9.89636	1.83633	0.78624		
maj	$3p$	−7.67787	1.29712	0.80058		
	$3d$	−4.38275	0.95234	0.89036		
Al	$3s$	−10.02916	1.86711	0.99474		
min	$3p$	−7.39278	1.39211	0.91397		
	$3d$	−4.72923	0.89174	0.74137		
Mg	$3s$	−6.13538	1.19399	0.92777		
	$3p$	−5.35848	0.79858	0.62475		
O	$2s$	−22.99335	3.17712	1.00000		
	$2p$	−15.75406	1.85529	1.00000		

Fermi level set to -10 eV. e_g is $d_{z^2}, d_{x^2-y^2}$ and t_{2g} is d_{xy}, d_{yz}, d_{xz}.