

# Computational Spin Caloritronics

Ke Xia(Beijing Normal University)

Shizhou Wang, Lei Wang, HongKang Song (BNU)

X.T.Jia(Henan Polytechnic University)

G.E.W. Bauer(TU Delft)

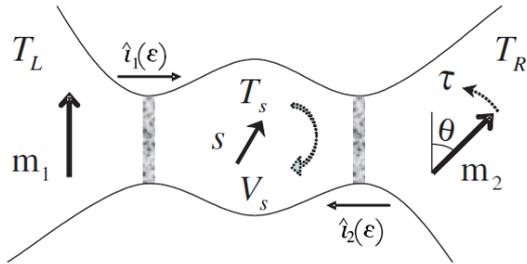
Thanks to

Y.Q. Ke, H. Guo(McGill)

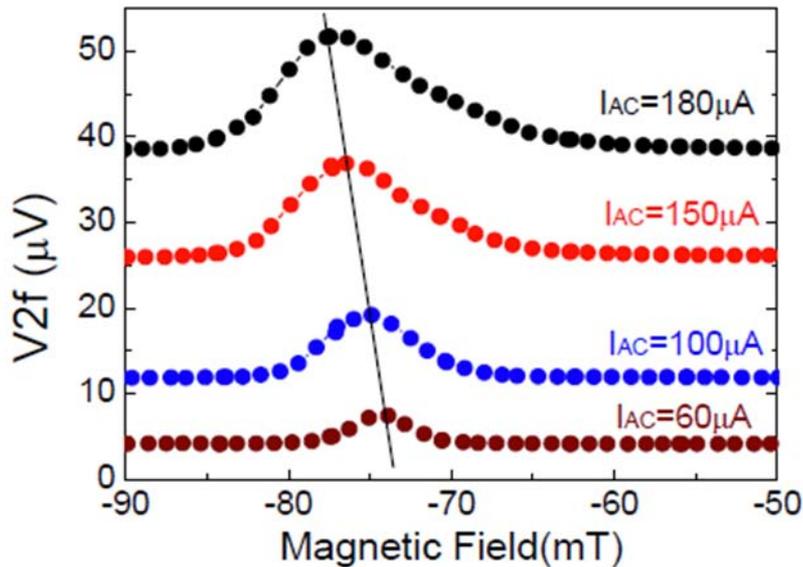
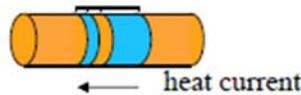
# Outline

- Transport through CoFe based MTJ
  - 1) Fe|MgO|Fe : TST & Shot Noise
  - 2) CoFe|MgO|CoFe: GMR comparison to experiment
  - 3) How to enlarge the thermo-electric effects
  - 4) Thermo-STT under bias
- Spin Mixing conductance at metal-FI interface
  - 1) Spin mixing conductance
  - 2) Local magnetic moment picture (Ag-YIG)
  - 3) CoFeO-Au interface
  - 4) Pt and Au surfaces with magnetic coating
- Summary

# Thermal induced STT in metallic spin valves

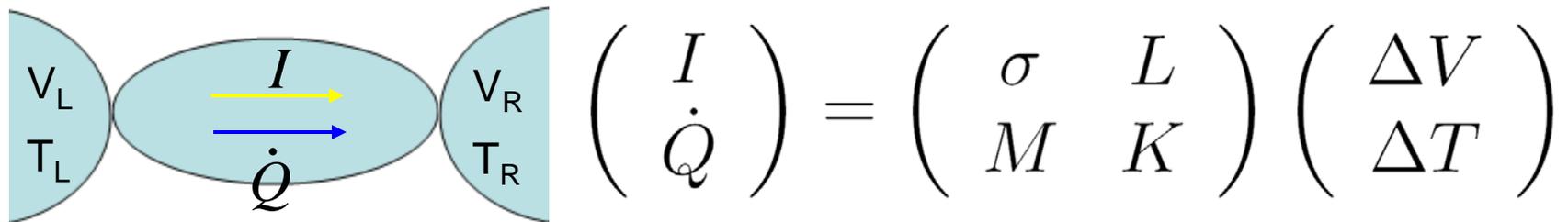


Hatami , Bauer, Zhang and Kelly,  
PRL **99**, 066603 (2007)



Haiming Yu, et al.,  
Phys. Rev. Lett. **104**, 146601 (2010)

# Thermal and electric transport



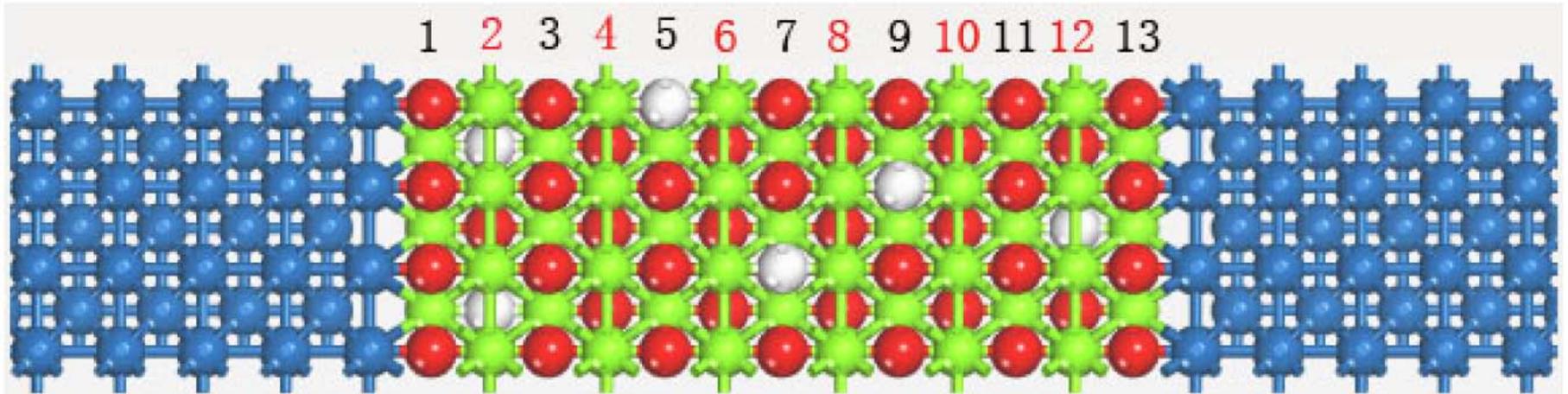
Landauer-Büttiker formalism

$$\sigma = -\frac{2e^2}{h} \int d\epsilon \frac{\partial f(\epsilon)}{\partial \epsilon} t(\epsilon) \qquad L = -\sigma S$$

$$K = \frac{2e^2}{h} \left( \frac{k_B}{e} \right)^2 T \int d\epsilon \frac{\partial f(\epsilon)}{\partial \epsilon} \left( \frac{\epsilon - \epsilon_F}{k_B T} \right)^2 t(\epsilon) \qquad M = \sigma S T$$

$$S = -\frac{1}{\sigma} \frac{2e^2 k_B}{h e} \int d\epsilon \frac{\partial f(\epsilon)}{\partial \epsilon} \left( \frac{\epsilon - \epsilon_F}{k_B T} \right) t(\epsilon) \qquad \text{Thermopower}$$

# Fe/MgO/Fe junction



$$\rho \sim \int G^< dE = \int G^R \Sigma^< G^A dE$$

Average over random disorder:

$$\bar{\rho} \sim \int G^< dE = \int \overline{G^R \Sigma^< G^A} dE$$

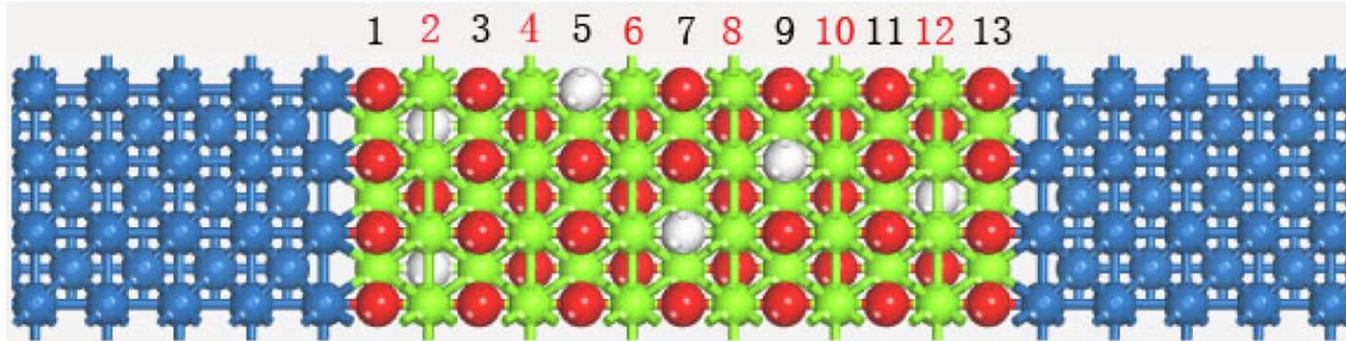
$$\bar{T} = \text{Tr} \left( \overline{G^R \Gamma_l G^A \Gamma_r} \right)$$

Nonequilibrium Vertex Correction (NVC)

$$\begin{aligned} \bar{g}^{\alpha, <} &= \overline{g^{\alpha, R} \Sigma^{\alpha, <} g^{\alpha, A}} \\ &= \bar{g}^{\alpha, R} (\Sigma^{\alpha, <} + \Omega_{NVC}) \bar{g}^{\alpha, A} \end{aligned}$$

Youqi Ke, Ke Xia and Hong Guo, PRL (2010).

# First principles approach to spin transfer torques



$$\tau \propto \langle \vec{s} \rangle \times \vec{M}$$

Spin current:

$$\hat{\mathcal{J}} \equiv \frac{1}{2} \left[ \hat{\sigma} \otimes \hat{V} + \hat{V} \otimes \hat{\sigma} \right]$$

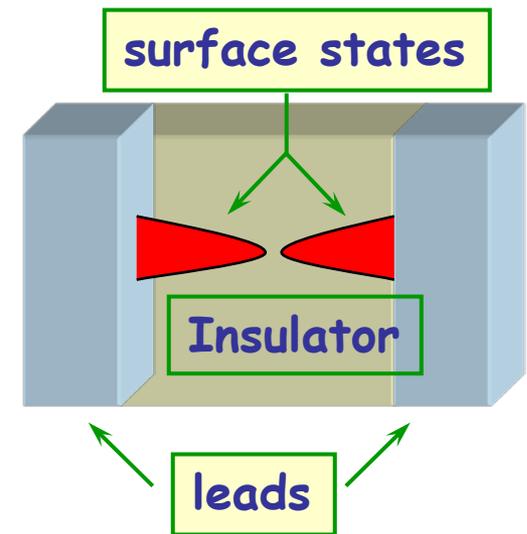
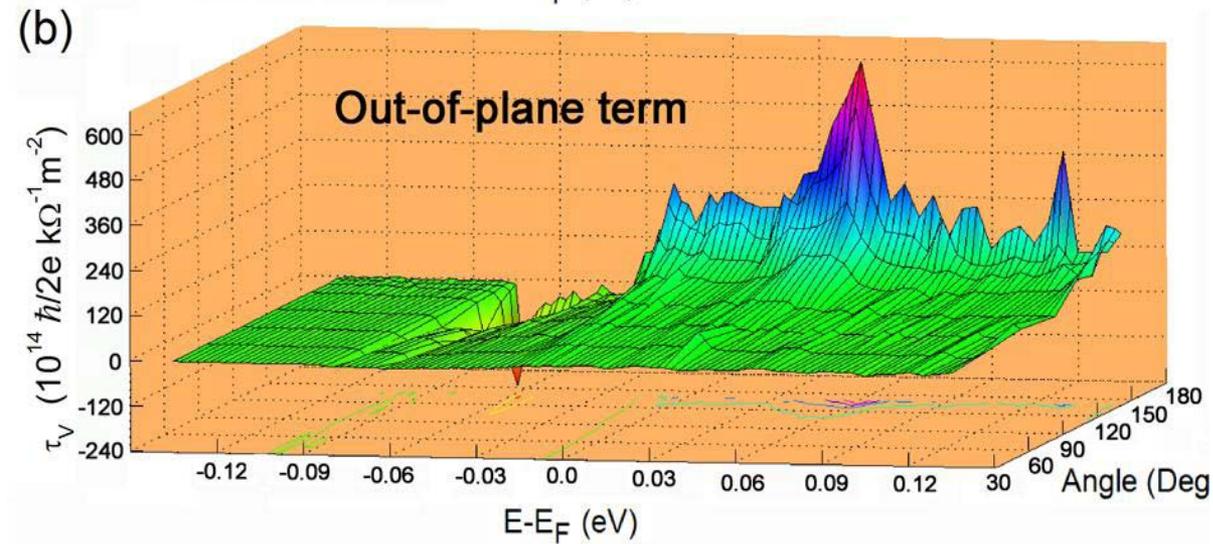
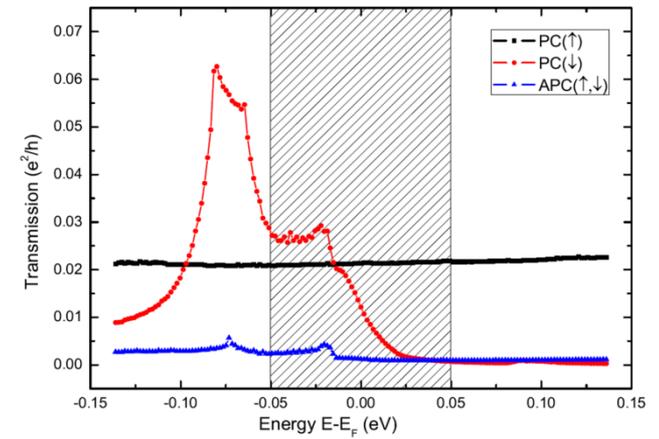
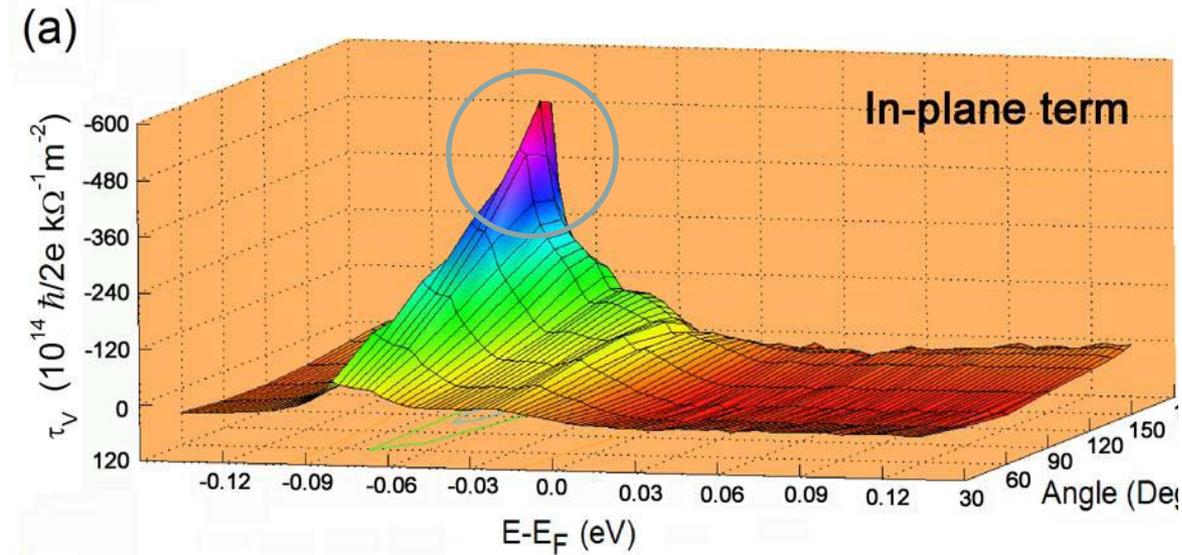
Spin torque from one lead:

$$\langle \hat{\mathbf{T}}_{\mathbf{R}}^s(\mathbf{k}_{\parallel}) \rangle = \sum_{\mathbf{R}' \in I-1, I} \langle \hat{\mathcal{J}}_{\mathbf{R}', \mathbf{R}}^s(\mathbf{k}_{\parallel}) \rangle - \sum_{\mathbf{R}' \in I, I+1} \langle \hat{\mathcal{J}}_{\mathbf{R}, \mathbf{R}'}^s(\mathbf{k}_{\parallel}) \rangle$$

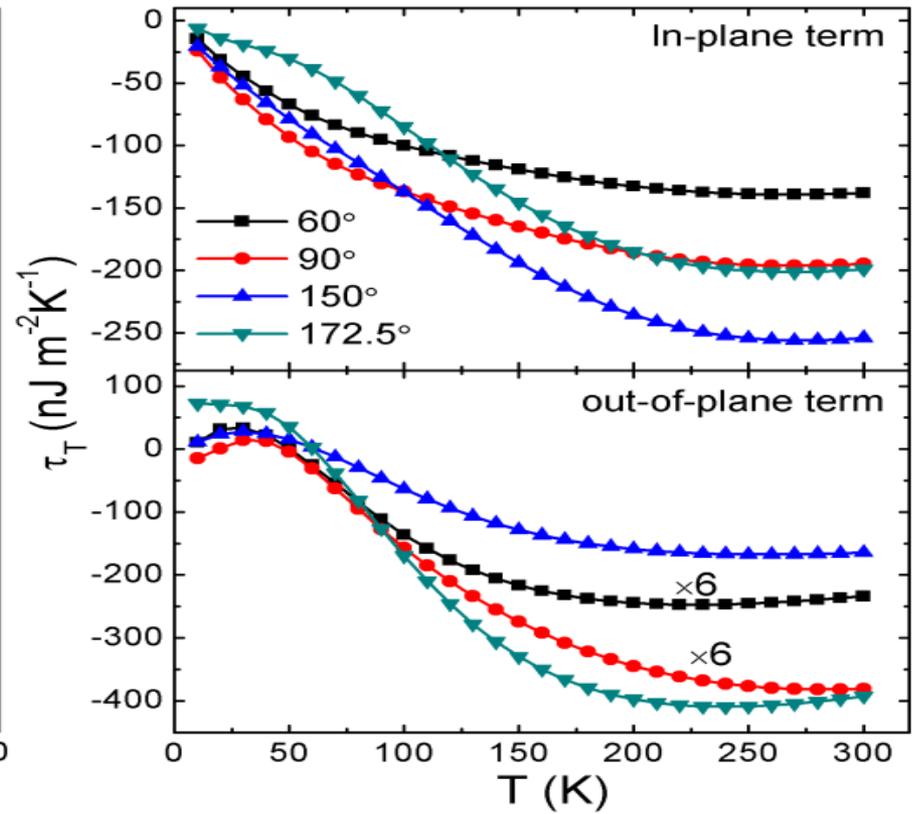
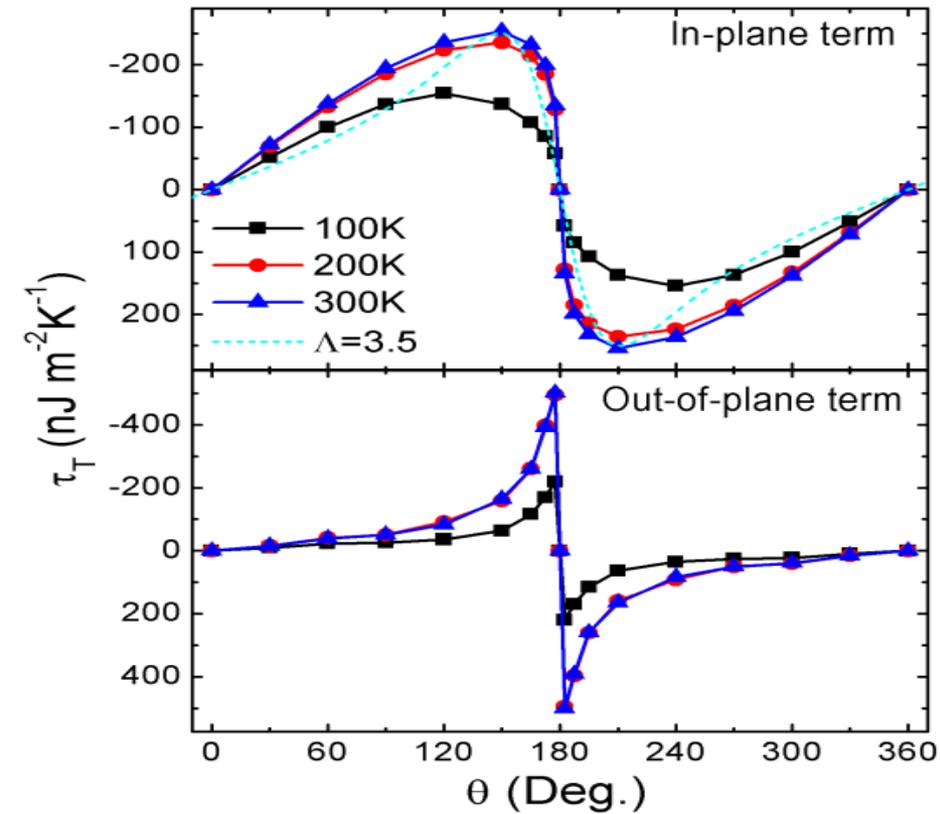
Spin torque on atom R:

$$\mathbf{T}_{\mathbf{R}} = \left( \frac{\hbar}{2} \right) \frac{e}{2h} \frac{1}{N_{\parallel}} \sum_{s, \mathbf{k}_{\parallel}} \left[ \langle \hat{\mathbf{T}}_{\mathbf{R}}^s(\mathbf{k}_{\parallel}) \rangle_{\mathcal{L}} - \langle \hat{\mathbf{T}}_{\mathbf{R}}^s(\mathbf{k}_{\parallel}) \rangle_{\mathcal{R}} \right] V_b$$

# Clean Fe/MgO(3L)/Fe



# Thermal torkance $\tau_T$



# Shot Noise[Kai Liu PRB B 86, 020408(R) (2012)]

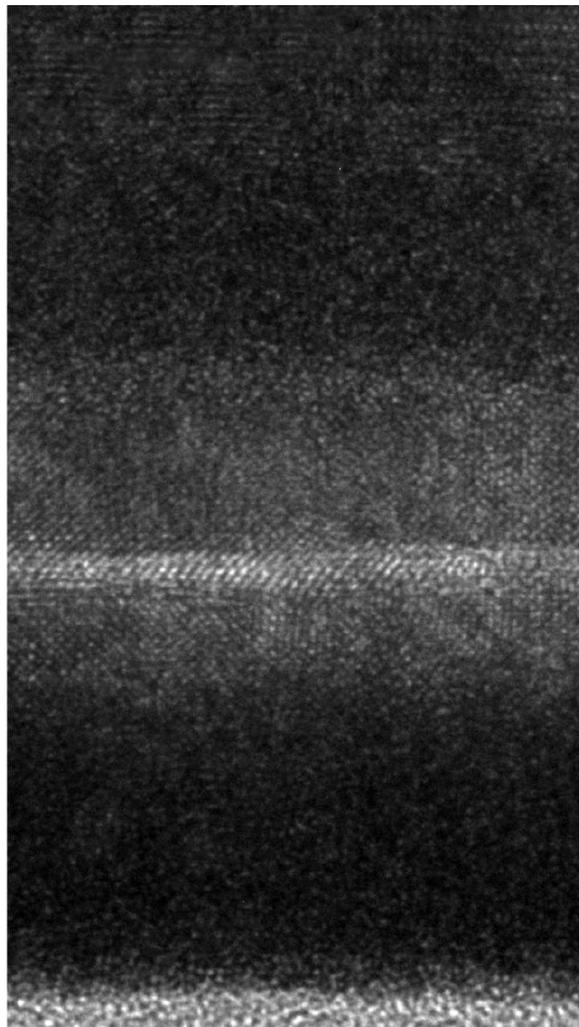
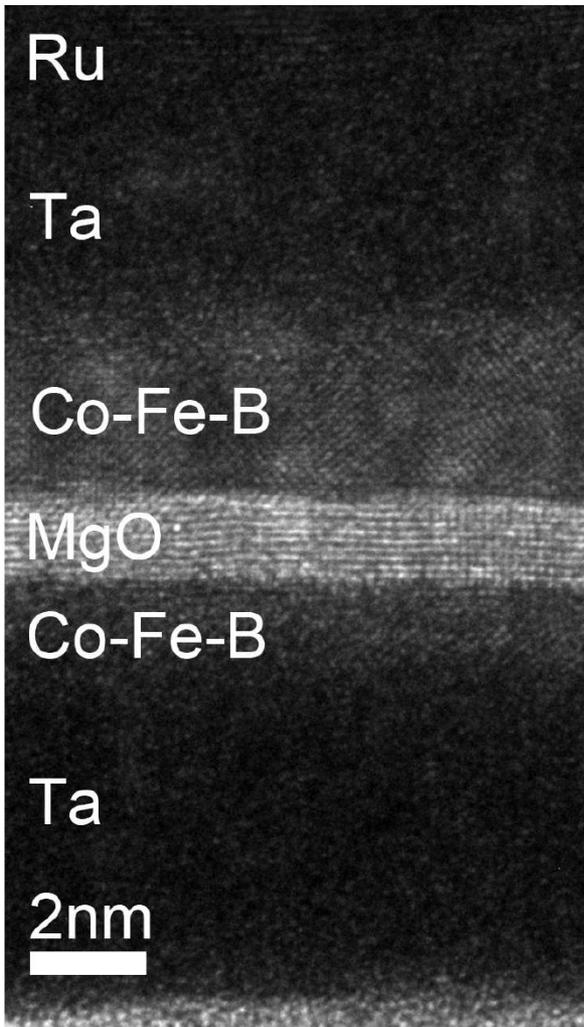
## ---Curial Check of the band structure

$$F = \frac{\sum_{\mathbf{k}_{||}} \sum_n T_n(\mathbf{k}_{||}) [1 - T_n(\mathbf{k}_{||})]}{\sum_{\mathbf{k}_{||}} \sum_n T_n(\mathbf{k}_{||})}$$

Fano factor	3MgO	4MgO	5MgO	7MgO
P	0.64[0.65(2)]	0.91[0.69(4)]	0.97[0.87(4)]	1.00[0.99(1)]
AP	0.94[0.77(2)]	1.00[0.94(1)]	1.00[0.98(1)]	1.00[0.99(1)]
TMR	1320%[165%]	2400%[288%]	3580%[250%]	5600%[107%]

at 3 K

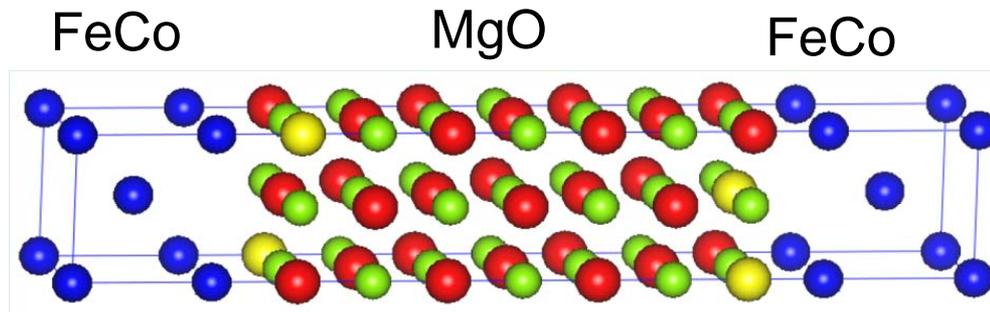
sample	Fano factor		MR ratio (%)	RA ( $\Omega \cdot \mu\text{m}^2$ )
	Parallel	Anti-parallel		
# 1	0.91±0.01	0.97±0.01	202.0	3.2
# 2	0.89±0.01	0.97±0.01	191.3	3.2
# 3	0.93±0.01	0.99±0.01	214.0	2.9
# 4	0.92±0.01	0.98±0.01	206.2	2.7



TMR  
55% to 64%

We have to treat  
CoFe alloy

# FeCo|MgO|FeCo (001) MTJs



## CPA--LMTO+CPA: Turek

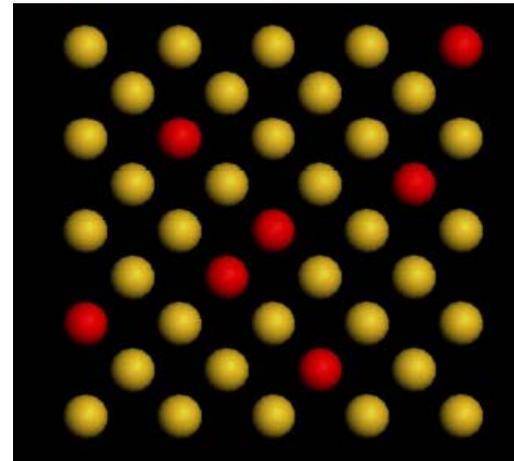
$$\rho \rightarrow \int G^< dE = \int G^R \Sigma^< G^A dE$$

Average over random disorder:

$$\overline{\rho} \rightarrow \int G^< dE = \int \overline{G^R \Sigma^< G^A} dE$$

$$\overline{T} = \text{Tr} \left( \overline{G^R \Gamma_l G^A \Gamma_r} \right)$$

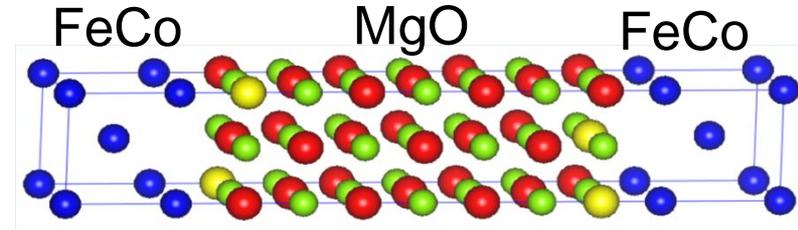
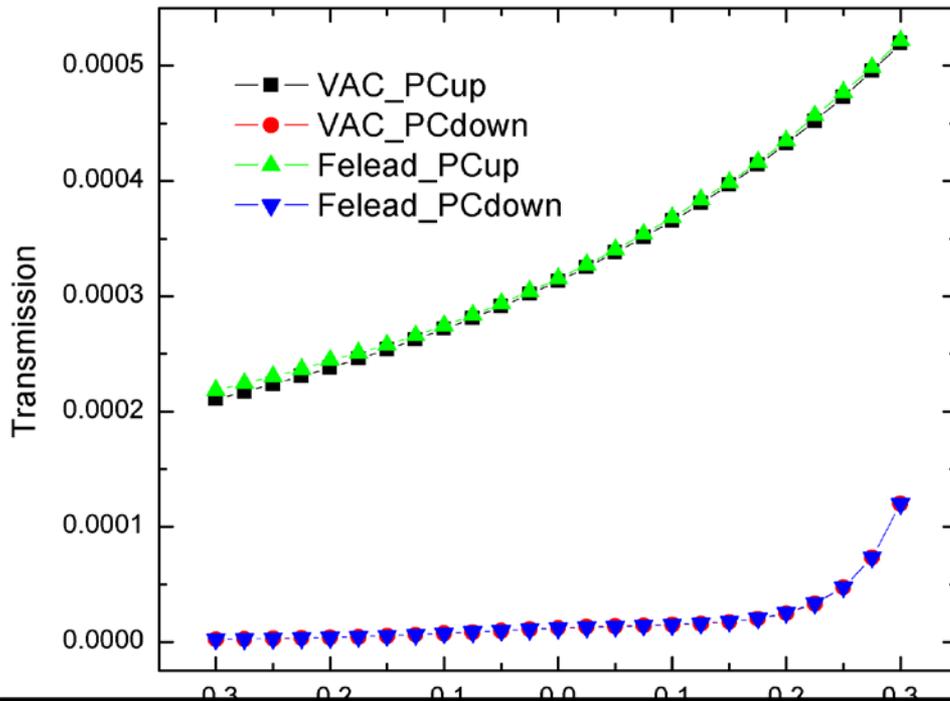
$$A_x B_{1-x}$$



$$\langle G^R(E) \rangle \rightarrow \rho$$

# VCA for alloy leads

VCA method :  $P_{vac}^{-1} = C_A P_A^{-1} + C_B P_B^{-1}$ .  $C_{A/B}$  concentration of element A/B



$\text{Co}_{0.75}\text{Fe}_{0.25}$	902%
$\text{Co}_{0.50}\text{Fe}_{0.50}$	957%
	(5% OV ~ 90%)
$\text{Co}_{0.25}\text{Fe}_{0.75}$	1061%
$\text{Co}_{0.20}\text{Fe}_{0.80}$	<b>1178%</b>

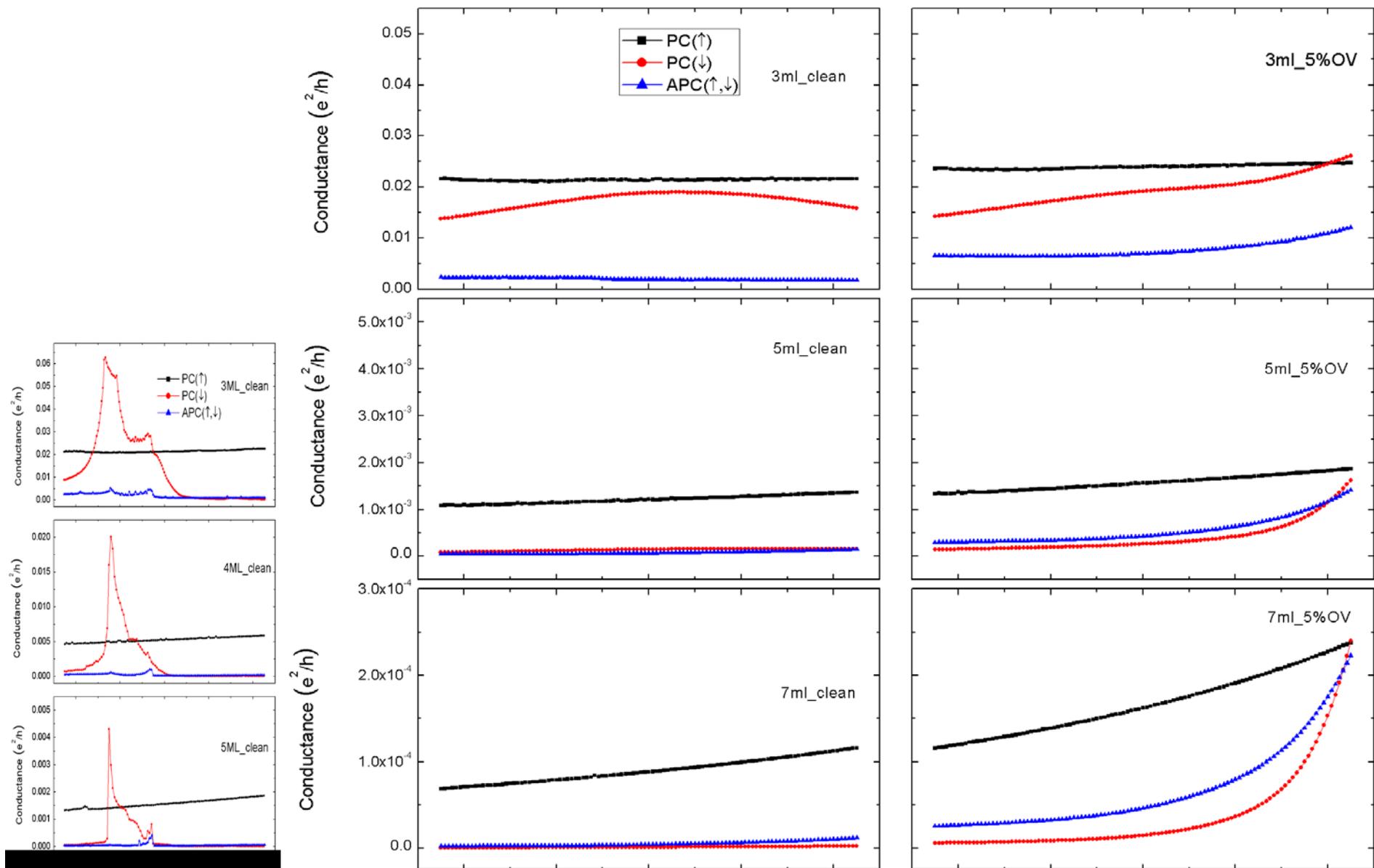
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$\text{Co}_{0.2}\text{Fe}_{0.6}\text{B}_{0.2}$	604(RT),
	<b>1144(5K)</b>

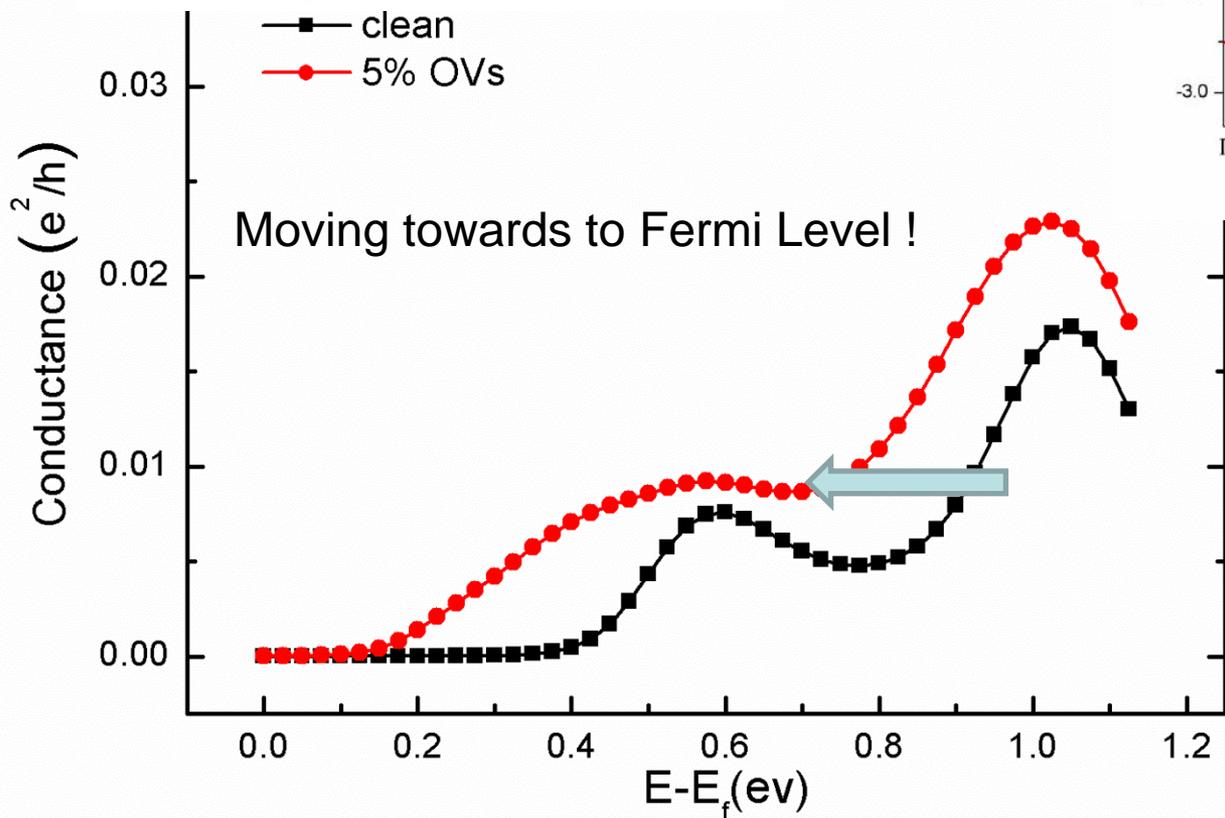
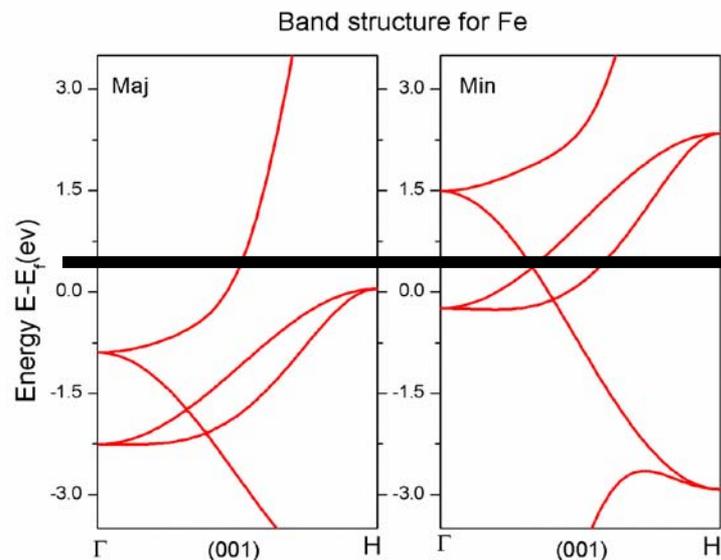
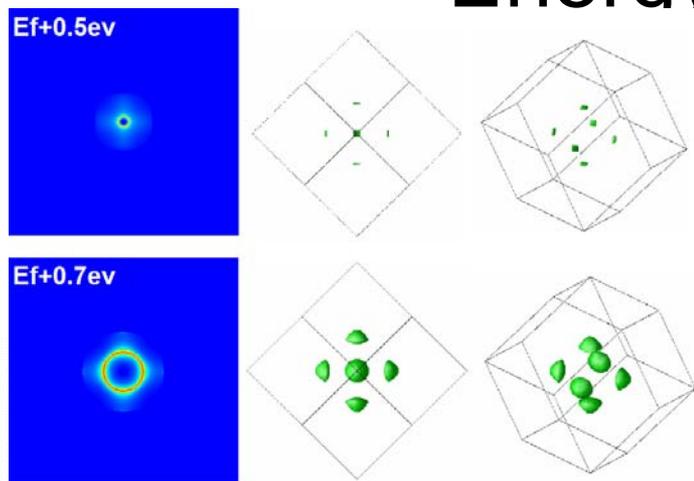
**S. Ikeda et al., APL 93, 082508 (2008)**

FeCo/MgO/FeCo

# Energy Dependent Conductance for $\text{Fe}_{0.5}\text{Co}_{0.5}\text{-MgO-Fe}_{0.5}\text{Co}_{0.5}$



# Energy dependent conductance



# Seebeck coefficient (in unit of $\mu\text{V}/\text{K}$ )

n	Roughness(OVs)	P	AP	$S_m$ %
5	Clean	-6.75	-31.2	362.2
	5%	-15.5	-38.8	150.3
	7.5%	-45.6	-58.2	27.6
	10%	-69.9	-67.7	-3.2
7	Clean	-12.8	-42.8	234.4
	5%	-26.7	-55.6	108.2
	7.5%	-78.2	-82.8	5.9
	10%	-107.9	-84.7	-27.4
9	Clean	-19.7	-52.2	165
	5%	-39.7	-71.0	78.8
	7.5%	-112.5	-105.2	-7.0
	10%	-140.5	-108.5	-29.5
Exp.		-107.9	-99.2	-8.8

Exp. M.Walter et al., Nature Mater. 10, 742 (2011).

# TMR and T- STT for FeCo-MgO-FeCo with different roughness

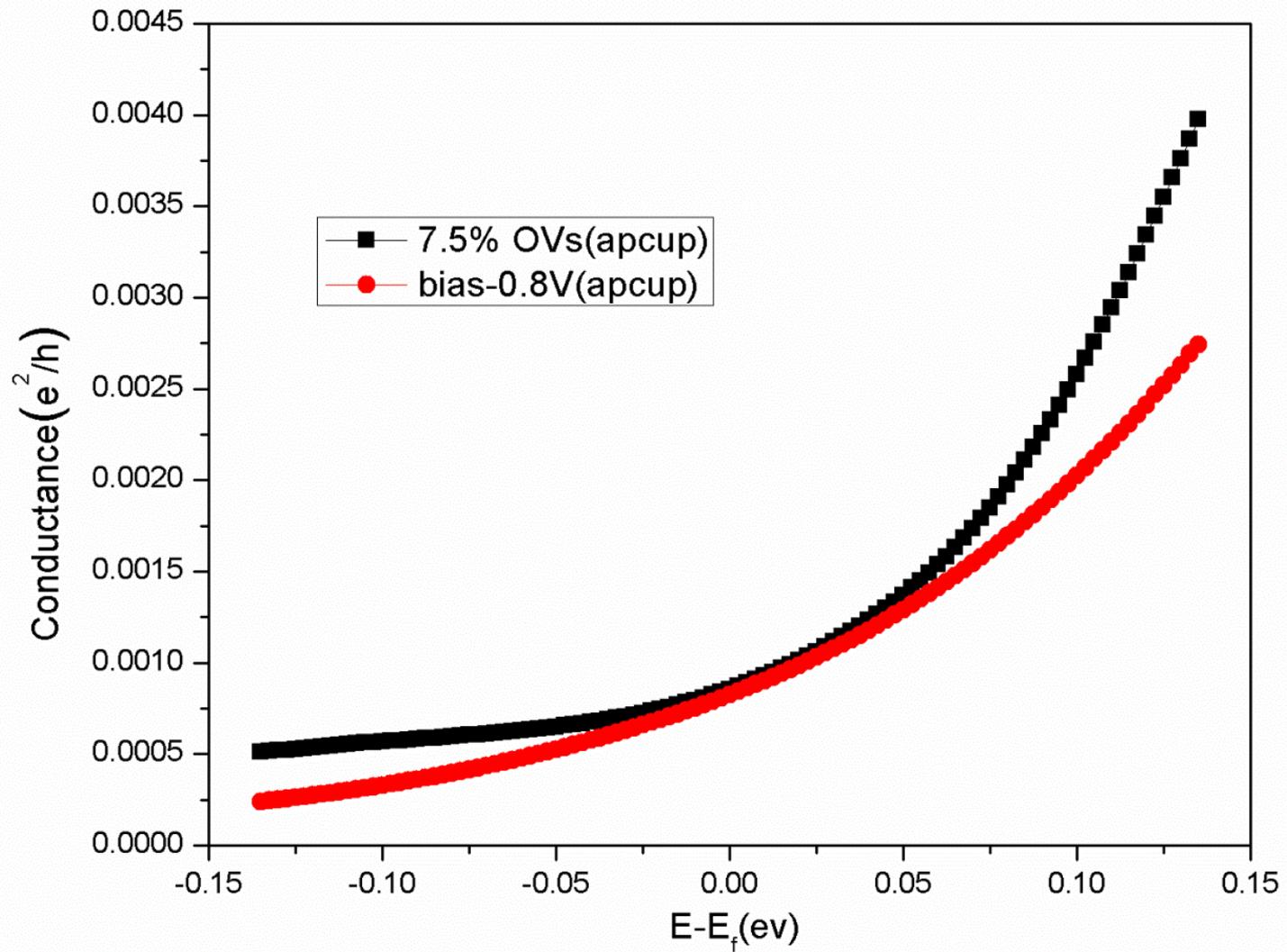
	TMR(%)	Thermal torkance (nJK <sup>-1</sup> m <sup>-2</sup> )
5%OVs	90	-0.052
7%OVs	22.8	1.02
10%OVs	15	11.24
<b>15%OVs</b>	<b>65.6</b>	<b>27.37</b>
20%OVs	34	6.52
L10%R5%	-2.64	2.88
L5%R10%	2.38	-0.26
10%N	1240	-0.0095
15%N	1018	-0.0037

Fe-MgO(3ML)-Fe

~ -112.3 nJK<sup>-1</sup>m<sup>-2</sup>

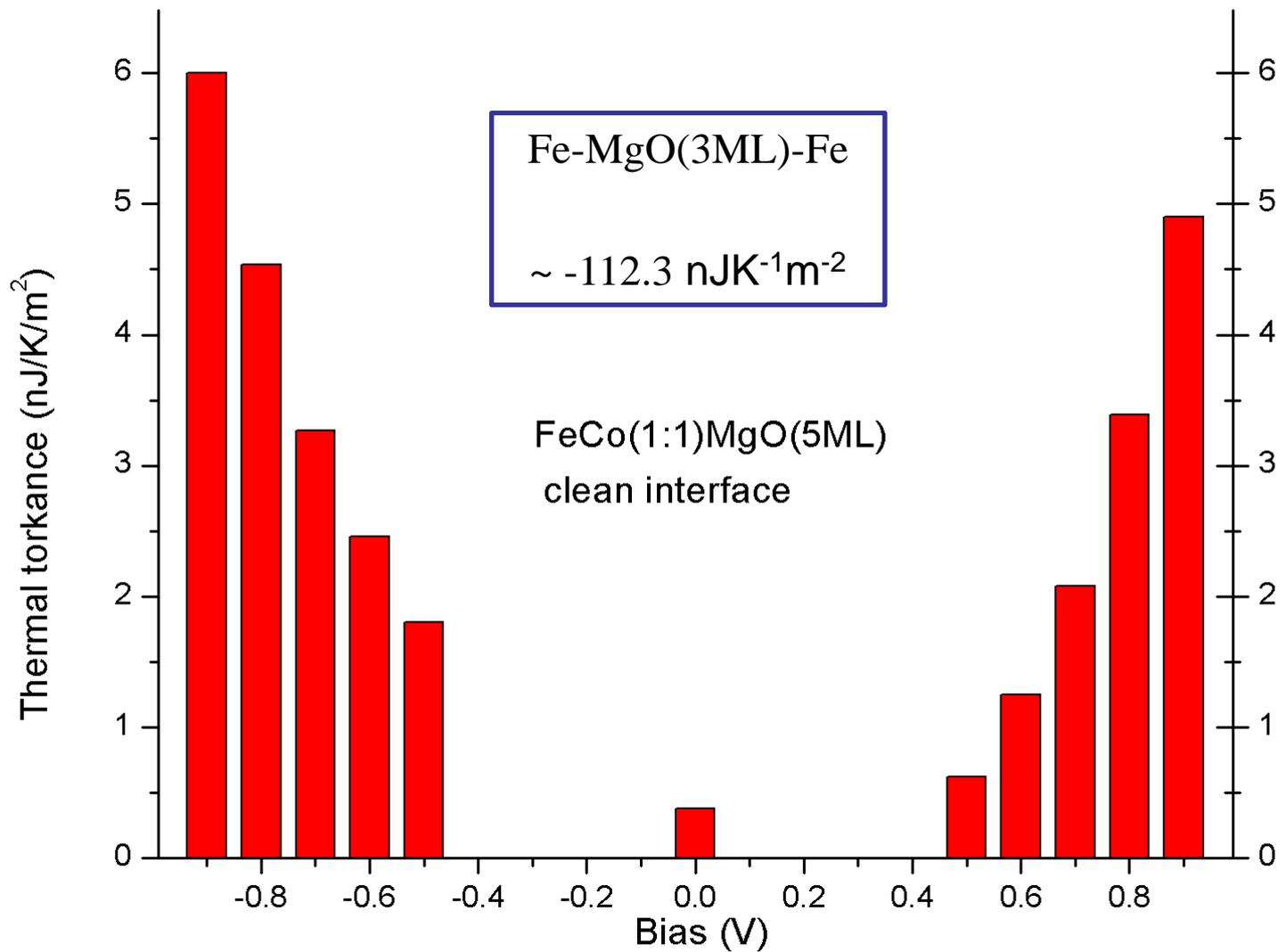
Direct calculated :

~ -195 nJK<sup>-1</sup>m<sup>-2</sup>



Similarity of bias and interfacial defects

# Thermal torkance ( $\text{nJK}^{-1}\text{m}^{-2}$ )



# Spin Mixing Conductance



$$\hat{I} = (\hat{I}I_0 + \hat{\sigma} \cdot \vec{I}_s) / 2$$

$I_0$  is the scalar particle current

$\vec{I}_s$  is the vector spin current which directly contributes to the spin-torque

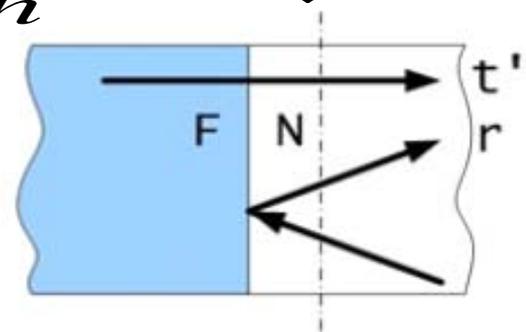
$\vec{I}_s$  is a function of the normal conductance

$$G_{\uparrow} = \frac{e^2}{h} \text{Tr}(t_{\uparrow}^{\dagger} t_{\uparrow}) \quad G_{\downarrow} = \frac{e^2}{h} \text{Tr}(t_{\downarrow}^{\dagger} t_{\downarrow})$$

and mixing conductance

$$G_{\uparrow\downarrow} = \frac{e^2}{h} \text{Tr}(I - r_{\uparrow}^{\dagger} r_{\downarrow})$$

(Brataas et al. PRL 2000)

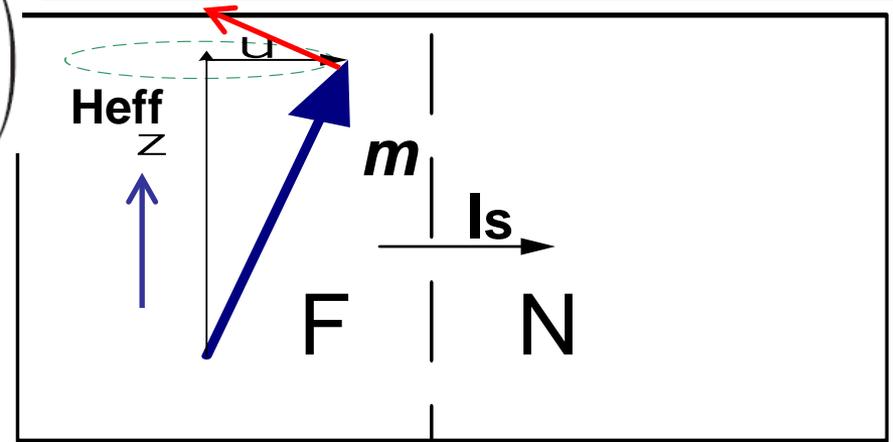


# Spin Pumping & magnon-electron coupling @interfaces

$$\mathbf{I}_s = \frac{\hbar}{4\pi} \left( \text{Re } \mathcal{A}_{\text{eff}}^{\uparrow\downarrow} \mathbf{m} \times \frac{d\mathbf{m}}{dt} + \text{Im } \mathcal{A}_{\text{eff}}^{\uparrow\downarrow} \frac{d\mathbf{m}}{dt} \right)$$

$\mathcal{A}_{\text{eff}}^{\uparrow\downarrow}$  Mixing Conductance of F/N interface

Ferromagnet/Normal Metal

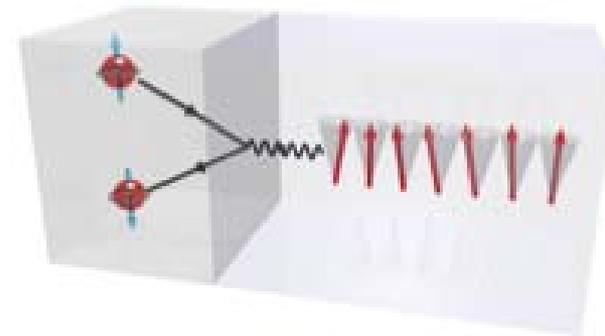


Theory: Tserkovnyak, Y. *et al Phys. Rev. B* **66**, 224403 (2002)

Experiment: Urban, R *et al Phys. Rev. Lett.* **87**, 217204(2001)

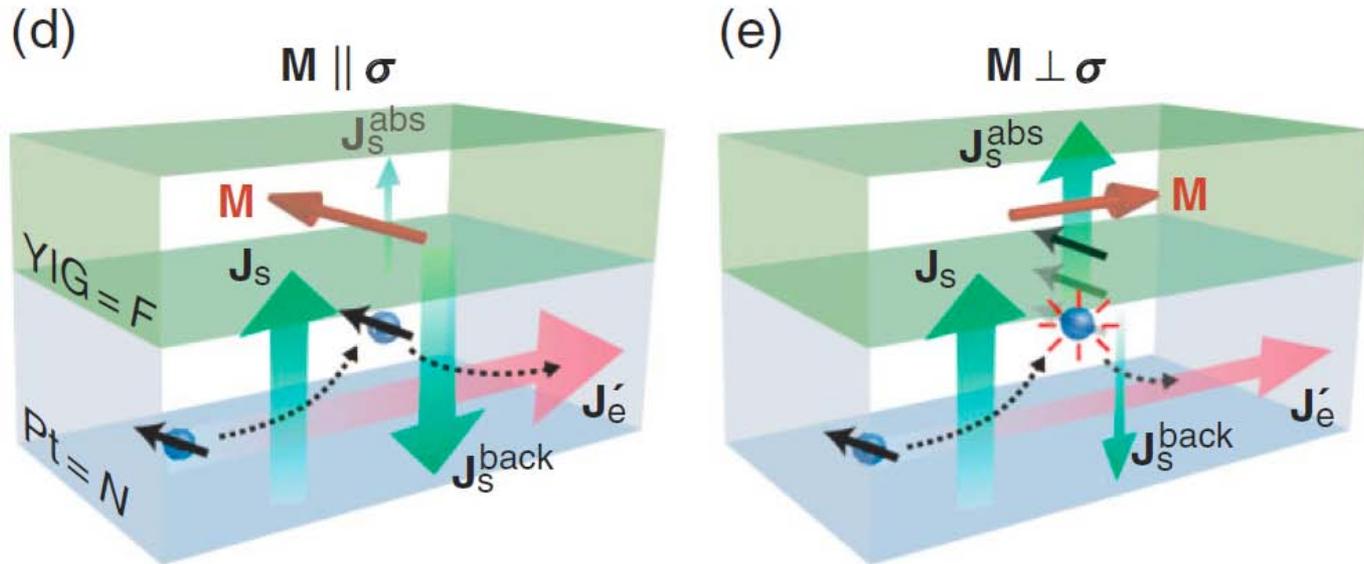
Heinrich, B. *et al, J. Appl. Phys.* **93**, 7545(2003)

magnon-electron coupling



S. Bender *et.al.*, PRL **108**, 246601 (2012)

# Spin Hall Magnetoresistance (SHMR)



$$\frac{\Delta\rho_1}{\rho} = \theta_{SH}^2 \frac{\lambda_{NM}}{d_{NM}} \operatorname{Re} \frac{2\lambda_{NM} G_{mix} \tanh^2 \frac{d_{NM}}{2\lambda_{NM}}}{\sigma + 2\lambda_{NM} G_{mix} \coth \frac{d_{NM}}{\lambda_{NM}}}$$

$$\frac{\Delta\rho_2}{\rho} = -\theta_{SH}^2 \frac{\lambda_{NM}}{d_{NM}} \operatorname{Im} \frac{2\lambda_{NM} G_{mix} \tanh^2 \frac{d_{NM}}{2\lambda_{NM}}}{\sigma + 2\lambda_{NM} G_{mix} \coth \frac{d_{NM}}{\lambda_{NM}}}$$

Yan-Ting Chen *et al.* Phys. Rev. B **87**, 144411 (2013).

H. Nakayama *et al.* Phys. Rev. L **110**, 206601 (2013).

$$G^{\uparrow\downarrow} = \frac{e^2}{h} (M - \sum_{nm} |r_{\uparrow}^{nm}| |r_{\downarrow}^{nm}| \exp[i(\phi_{\uparrow}^{nm} - \phi_{\downarrow}^{nm})])$$

$$G_{\uparrow\downarrow} = \frac{e^2}{h} M (r_{\uparrow} = 0)$$

$$G_{\uparrow\downarrow} = \frac{e^2}{h} (M - \sum e^{i\delta\phi_{mn}})$$

$$G_{\uparrow\downarrow} = \frac{e^2}{h} M$$

For CoFe|Ta interface:

$$G_{\uparrow\downarrow} \approx \frac{e^2}{2h} M$$

Ta Co <sub>50</sub> Fe <sub>50</sub>	G_Up	G_Dn	Sharvin	G_Re	G_Im
Alloy 20 layers	<b>1.58</b>	<b>0.97</b>	<b>9.35</b>	<b>4.84</b>	<b>-0.92</b>

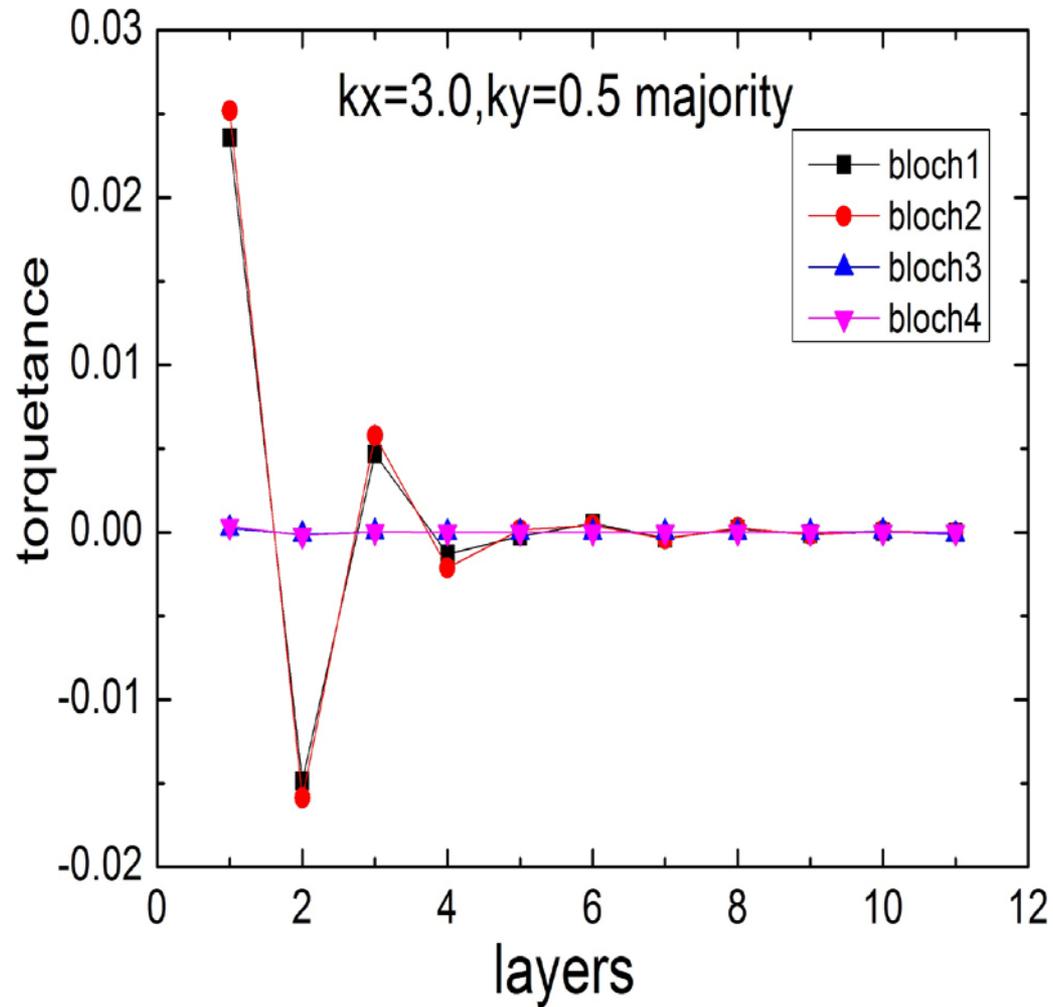
$10^{14} \Omega^{-1} \text{m}^{-2}$

$$\tau = \theta_{SH} J_e f(G_{\uparrow\downarrow}, G_{\uparrow}, G_{\downarrow})$$

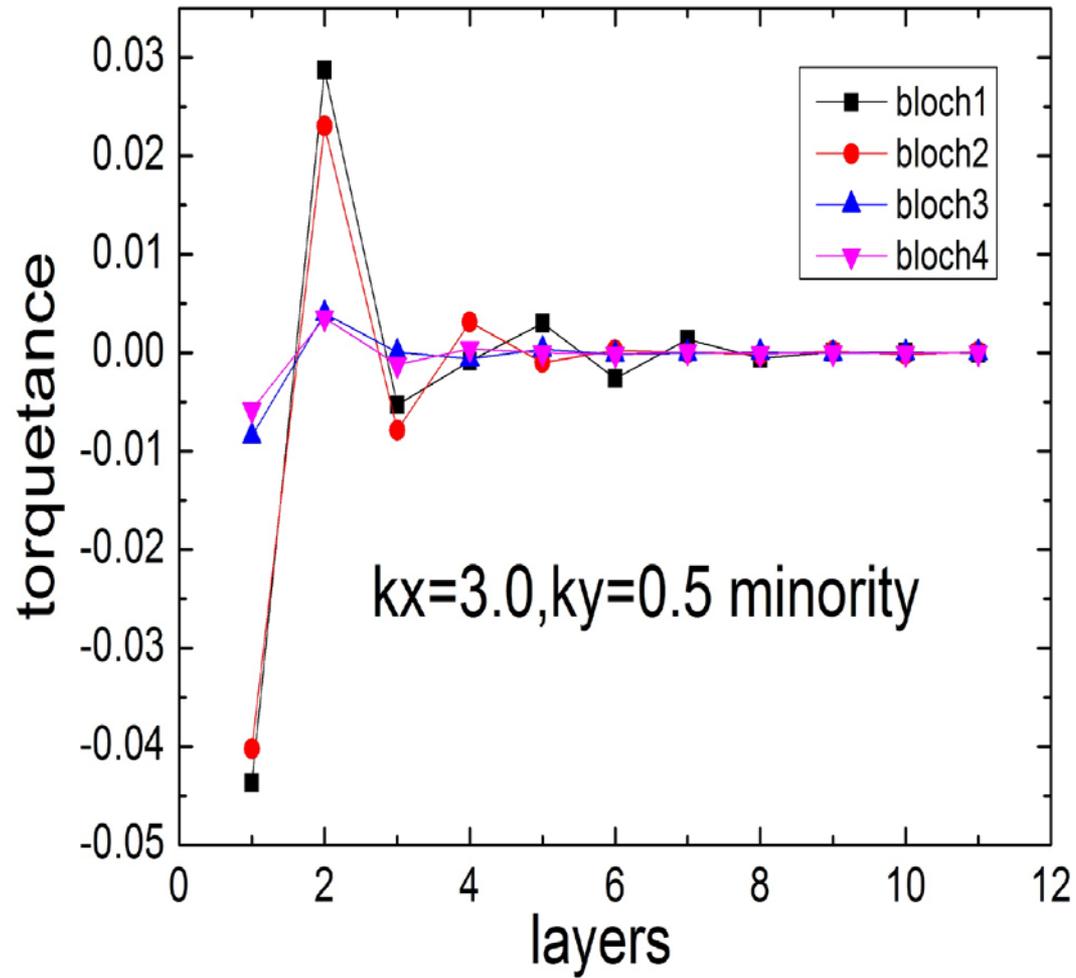
# G\_mix for multi shell metals ( $10^{14}\Omega^{-1}\text{m}^{-2}$ )

	<b>G_up</b>	<b>G_dn</b>	<b>G_sh</b>	<b>G_r</b>	<b>G_i</b>
Ta Fe	2.78	2.00	9.35	4.89	-1.70
Pt Fe	0.36	1.37	7.00	4.37	-0.45
Pd Fe	3.43	0.68	5.92	5.72	-1.03
<b>Au Fe</b>	<b>4.01</b>	<b>0.90</b>	<b>4.62</b>	<b>4.59</b>	<b>0.05</b>

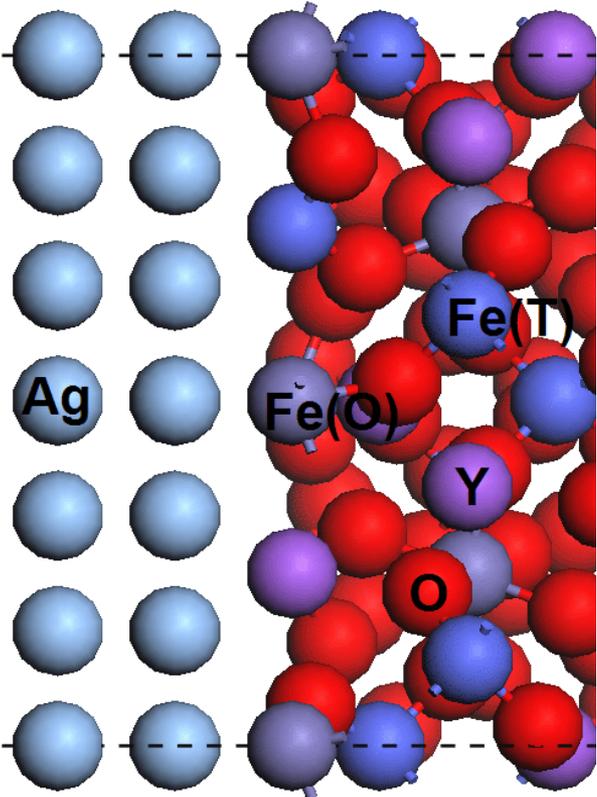
# Pt|Fe interface each bloch state of majority spin



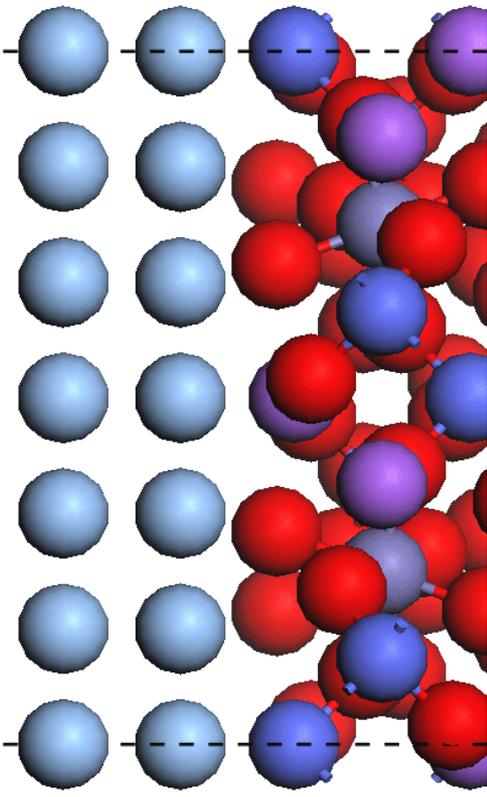
# Pt|Fe interface each bloch state of minority spin



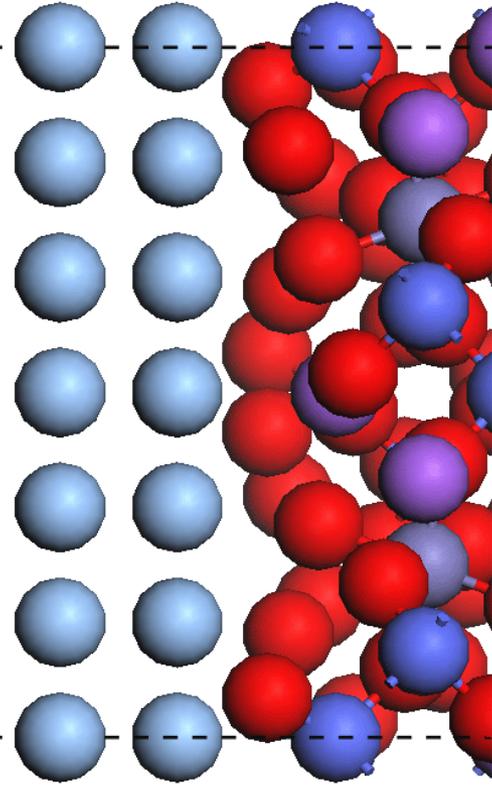
# Ag|YIG interface



YFe(001)



Fe(001)



O(001)

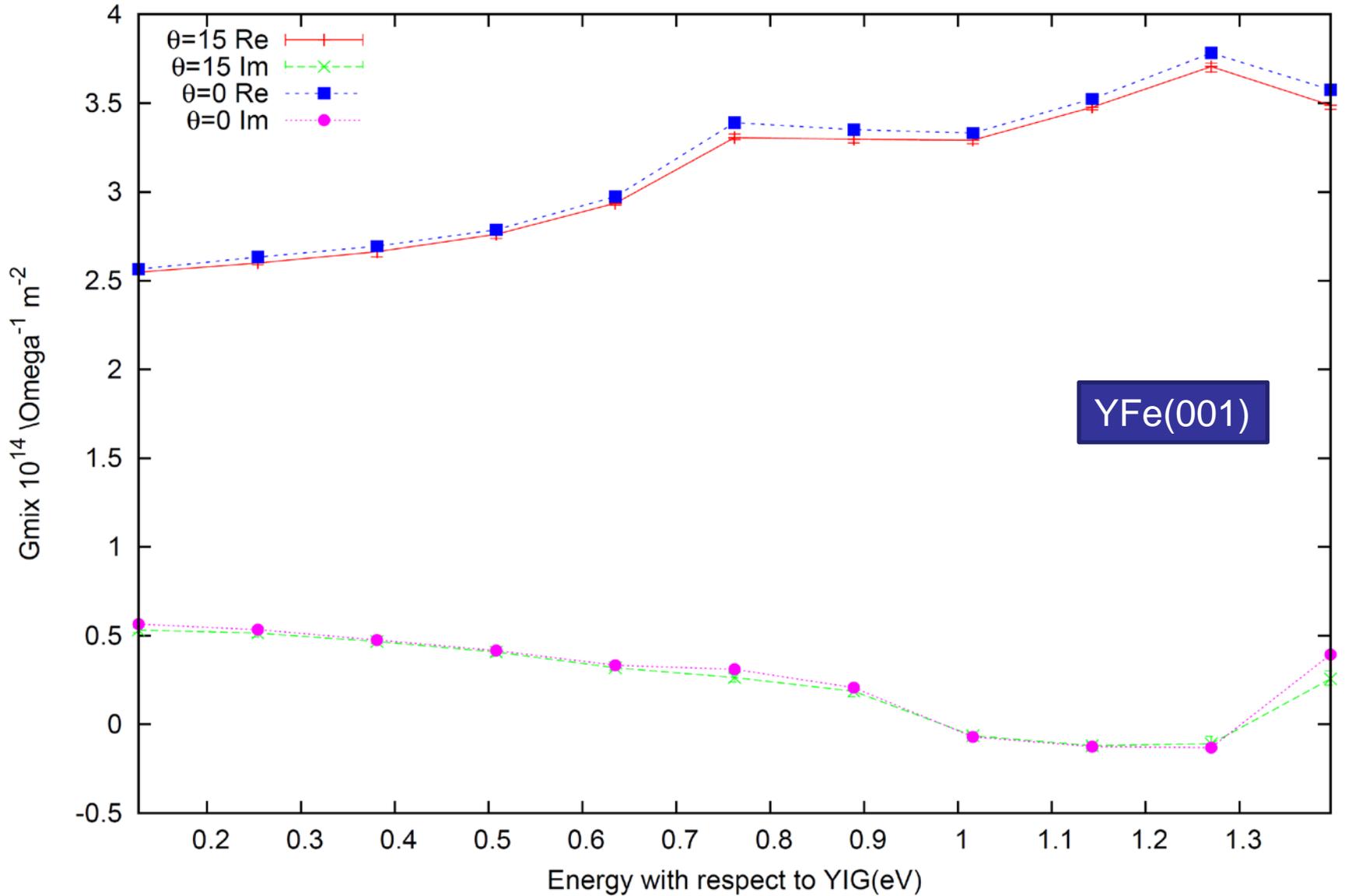
# $G^{\uparrow\downarrow}$ is as large as metallic contact

- Band Gap?
- Band dispersion and band alignment?
- Distance effect and ASA overlap?
- Ferromagnetic proximity effect?

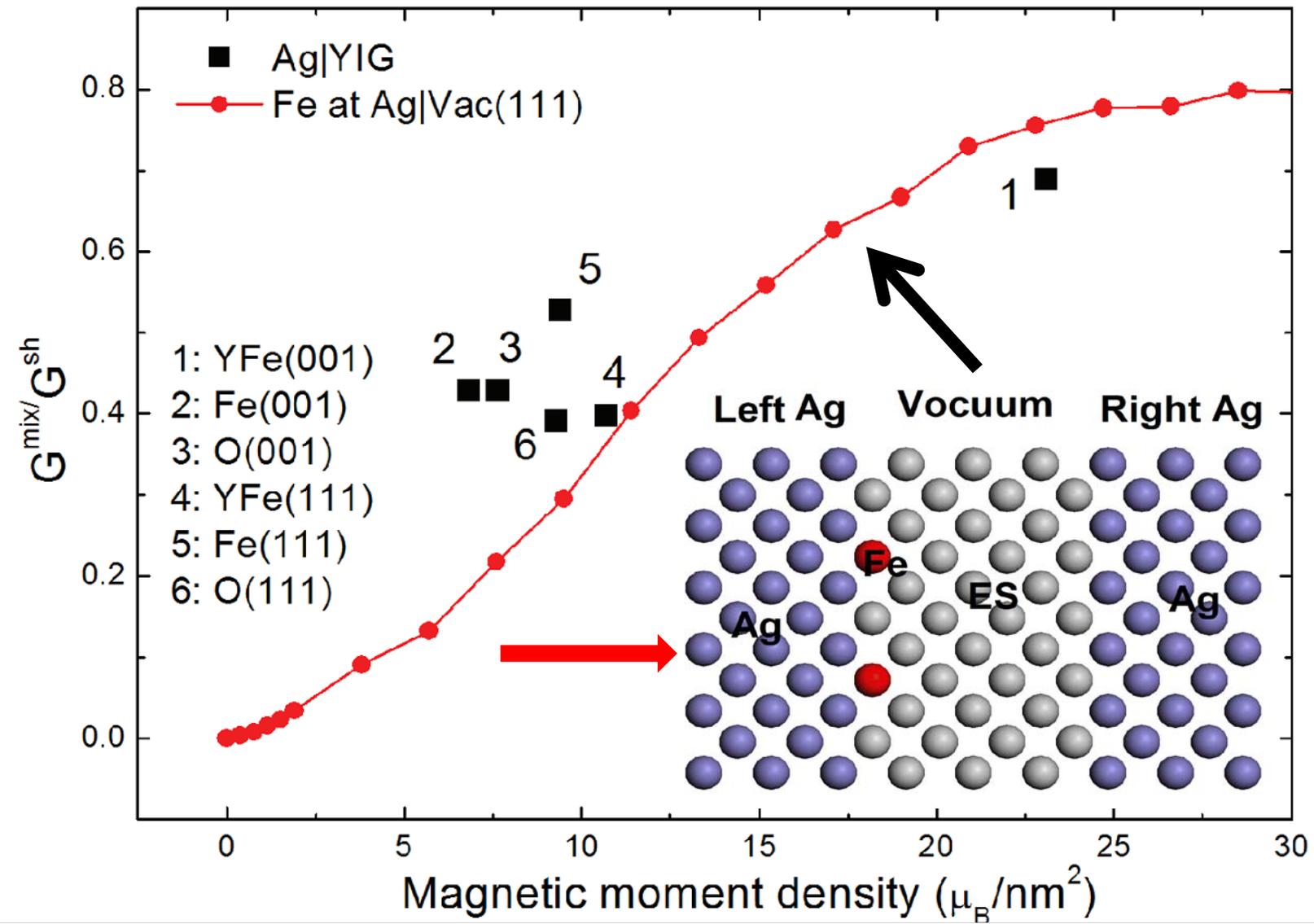
## Band gap

Effect of band gap, considering  $E=0.5(E_V+E_C)$

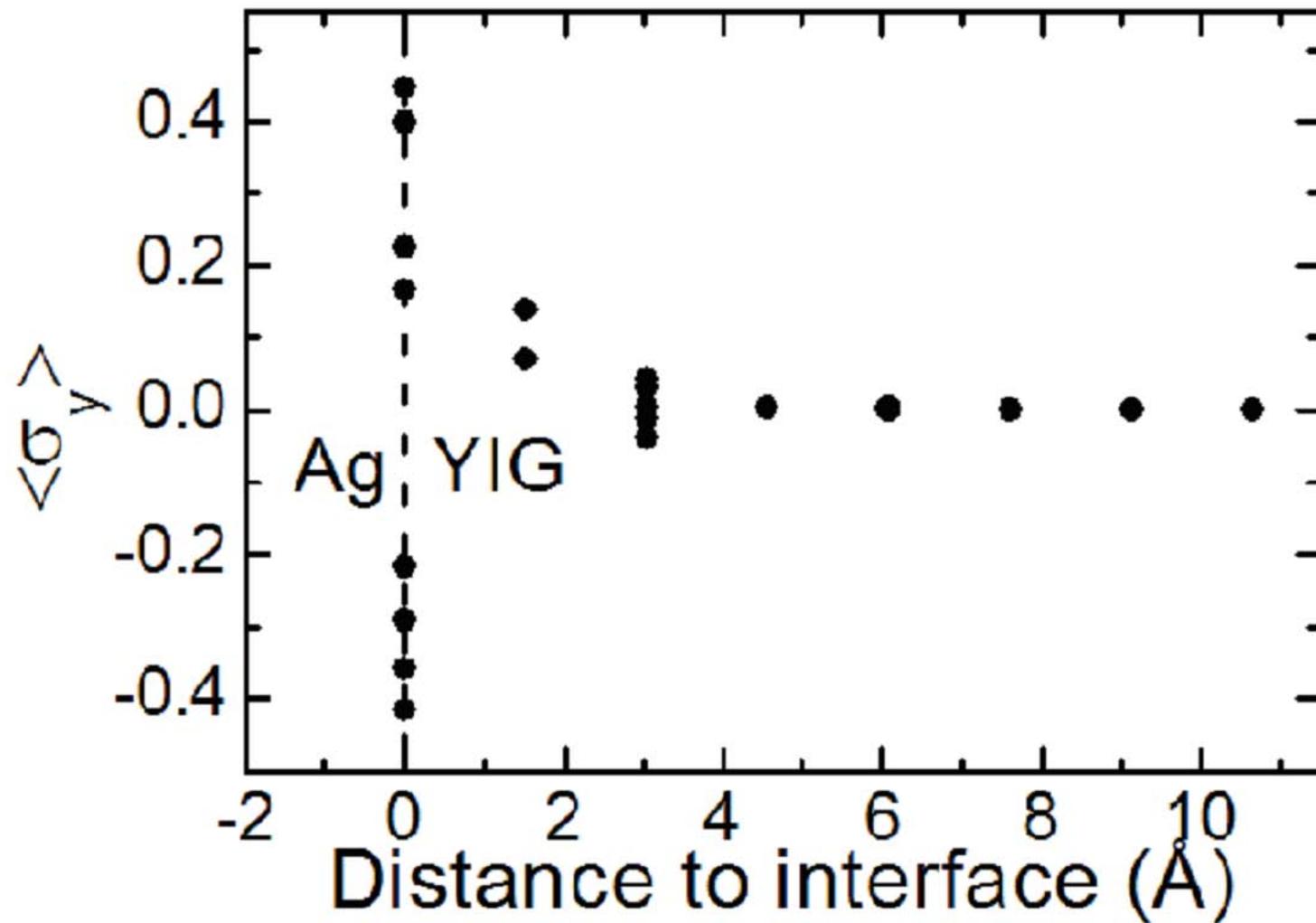
C (eV)	0	2	4	7.2
$E_g$ (eV)	0.35	0.65	0.95	1.4
$G_r^{\uparrow\downarrow}$ ( $10^{14}\Omega^{-1}\text{m}^{-2}$ )	3.46	3.89	3.43	3.01



# Local Moments Picture



# Penetration length of spin injection



# Enhanced spin pumping in YIG/Au structures

C.Burrowes,<sup>1</sup> B.Heinrich,<sup>1, a)</sup> B.Kardasz,<sup>1</sup> E.A. Montoya,<sup>1</sup> E. Girt,<sup>1</sup> Yiyan Sun,<sup>2</sup> Young-Yeal Song,<sup>2</sup> and Mingzhong Wu<sup>2</sup>

<sup>1)</sup>Physics Department, Simon Fraser University, 8888 University Dr., Burnaby, BC, V5A 1S6, Canada

<sup>2)</sup>Physics Department, Colorado State University Fort Collins CO 80523 USA

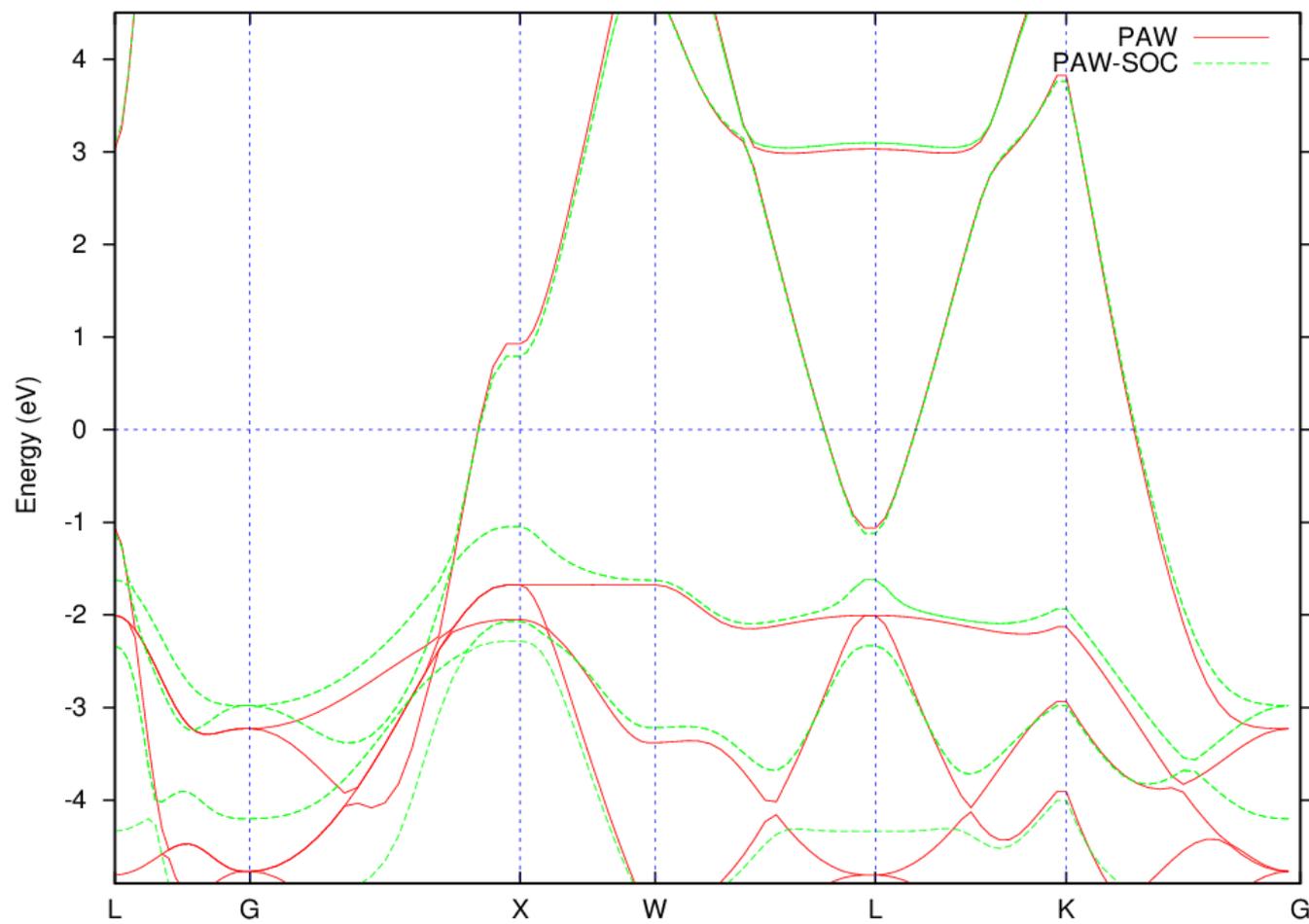
(Dated: 21 November 2011)

Spin injection across the ferrimagnetic resonance (FMR). The parameter  $\alpha$  in single magnetic l

Exp.:  $5.2 \times 10^{14} \text{cm}^{-2}$

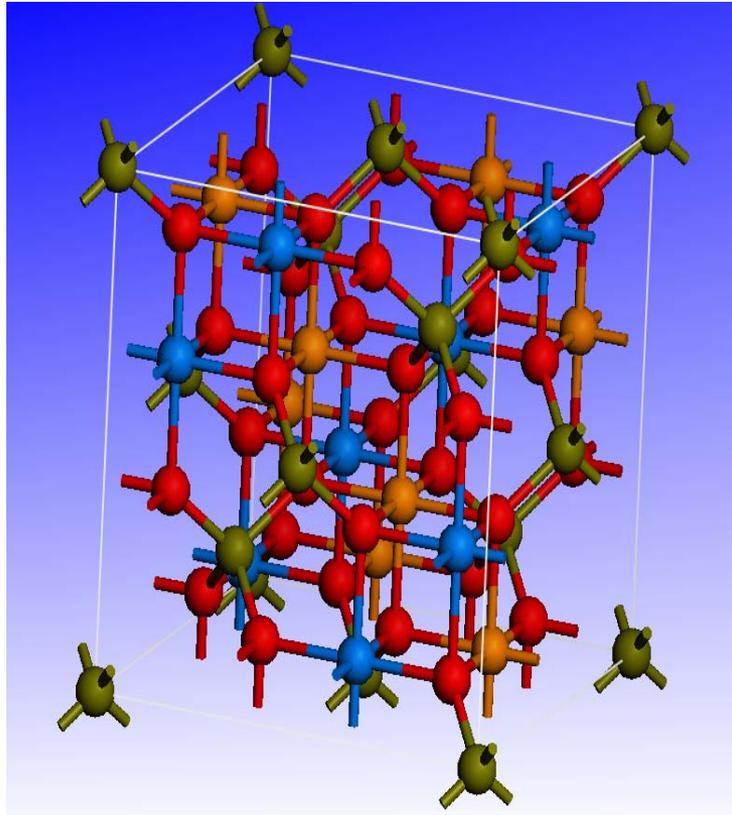
Theory:  $7 \times 10^{14} \text{cm}^{-2}$

ferromagnetic structure

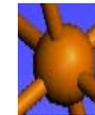
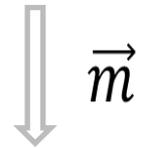


the damping parameter  $\alpha$  was to correlate the spin *in situ* etching and deposition to increase the spin mixing represents factor of 5 increase  $\gamma$  the recent first principle related with changes in the

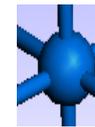
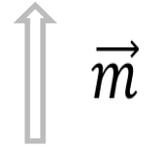
# Structure



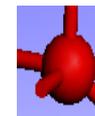
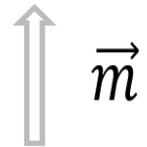
Fe



Fe  
1



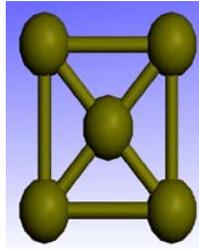
Co



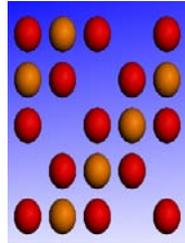
O

Sketch of the  $\text{CoFe}_2\text{O}_4$  of  $\beta$ -type which we concern.

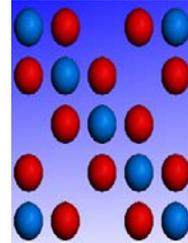
# Terminal on the interface



Fe

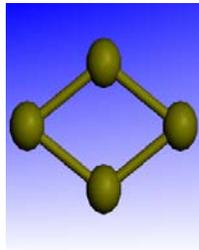


Fe1O

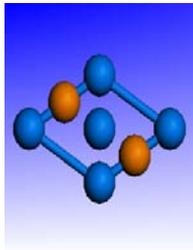


CoO

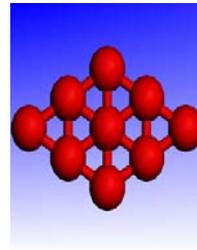
001



Fe



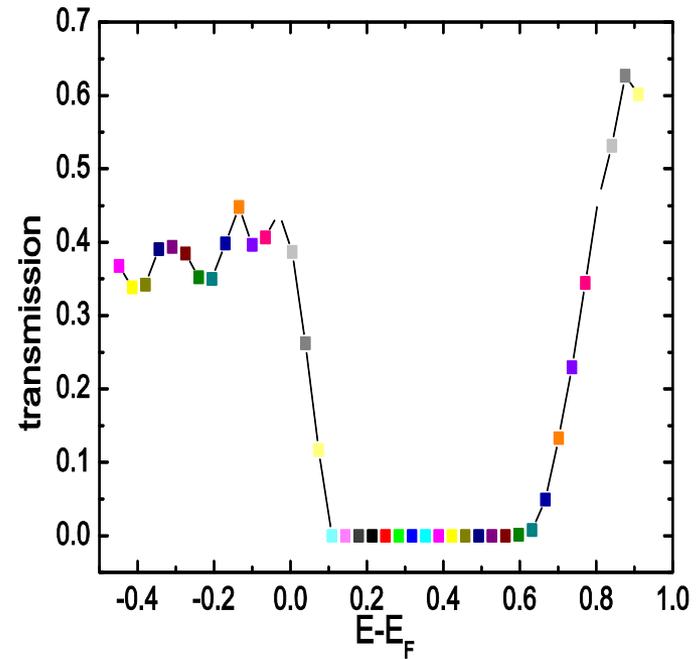
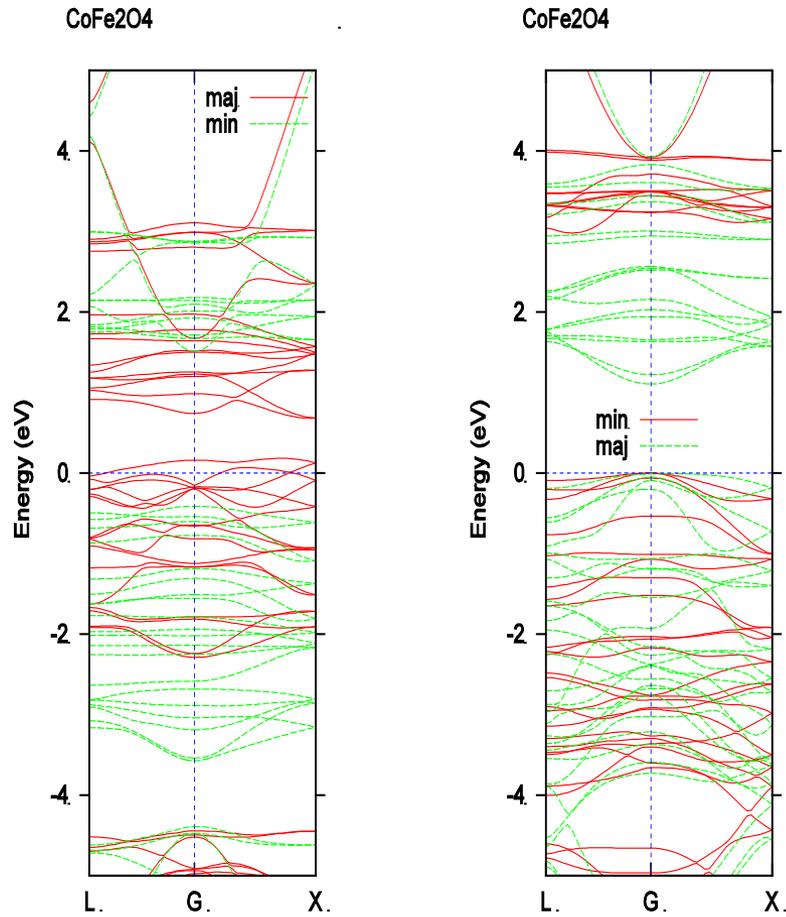
Fe1Co



O

111

# Band structure and magnetic moment



Transmission through CoFeO

GGA+C(left) & GGA+U(right)

# Results

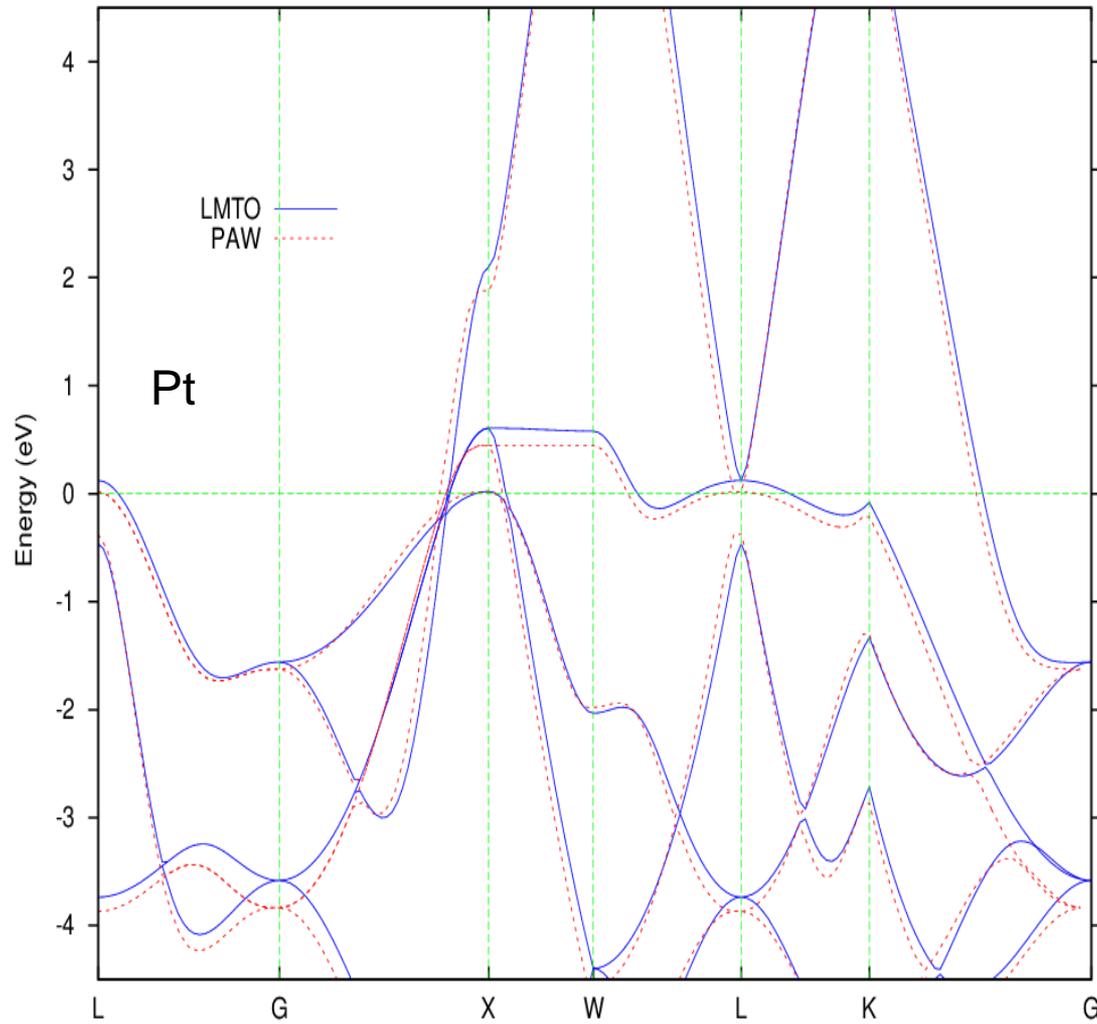
	001			111		
Terminal	Fe	Fe1O	CoO	Fe	Fe1Co	O
$G_{\uparrow\downarrow} (10^{14}\Omega^{-1}\text{m}^{-2})$	2.82	1.28	3.26	1.15	9.00	0.63
Exp ( $10^{14}\Omega^{-1}\text{m}^{-2}$ )		6.5~15			0.14~0.36	
MMD( $\mu_B/\text{nm}^2$ )	10.50	21.51	15.64	12.12	30.48	<0.1
MMD2( $\mu_B/\text{nm}^2$ )	15.64	<0.1	10.50	<0.1	<0.1	<0.1

Exp. Miren Isasa et. al. arXiv: 1307.1267

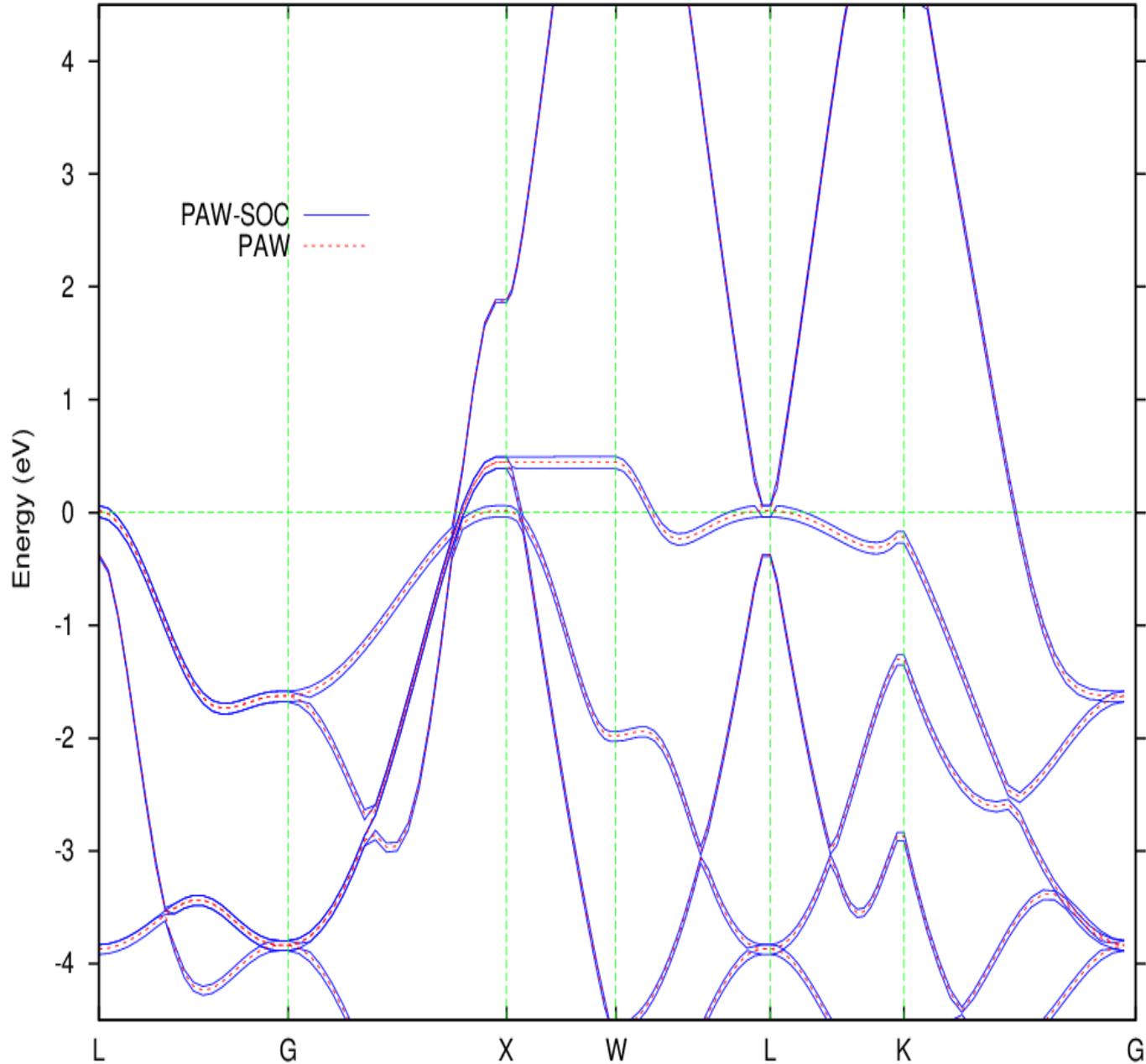
Mixing conductance & surface magnetic moment density(MMD)

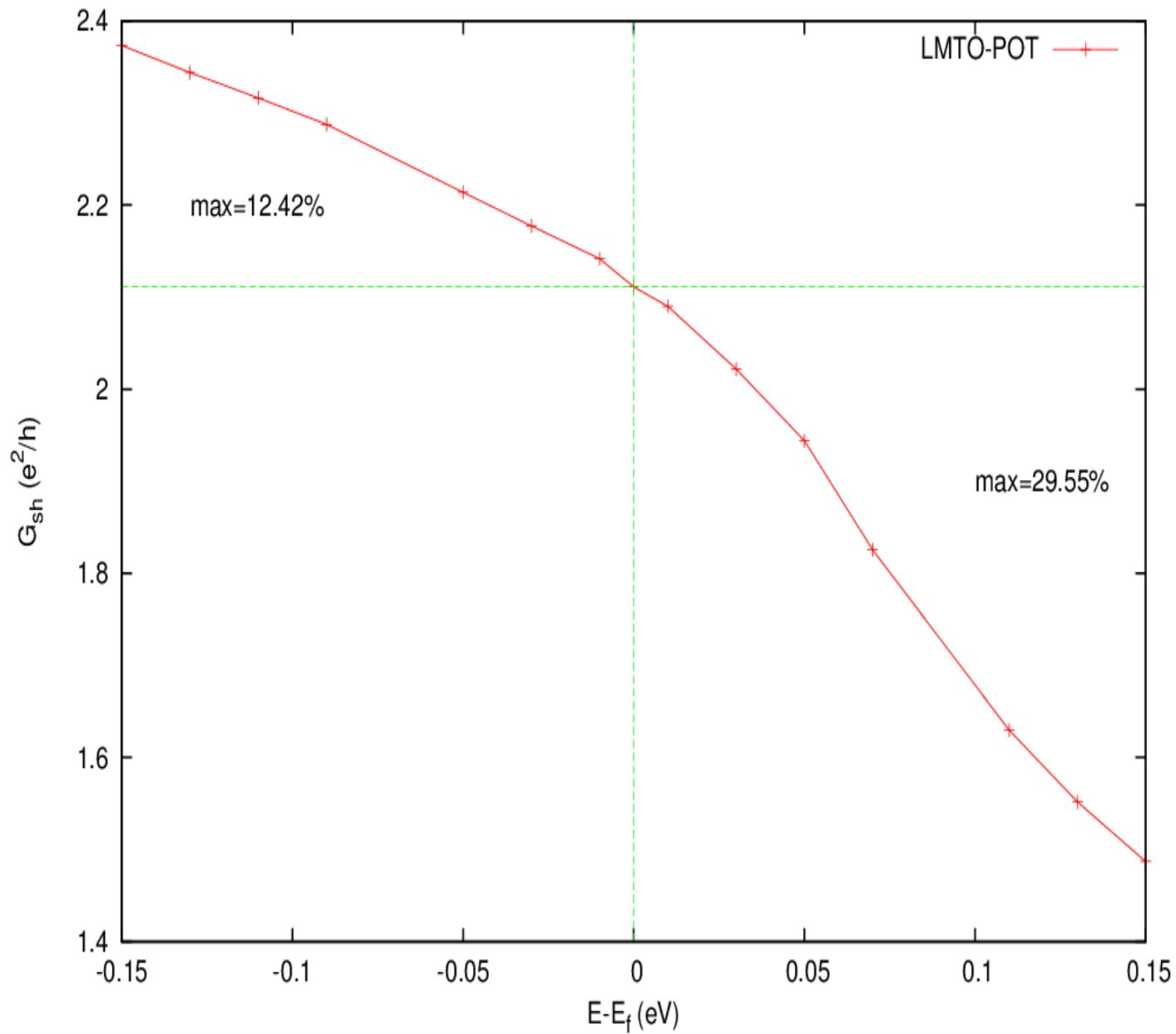
$$\frac{1}{\widetilde{G}_{\uparrow\downarrow}} = \frac{1}{G_{\uparrow\downarrow}} - \frac{1}{2G_{Au}^{sh}}$$

# LMTO Vs VASP(PAW) error bar $\sim 0.12$ eV



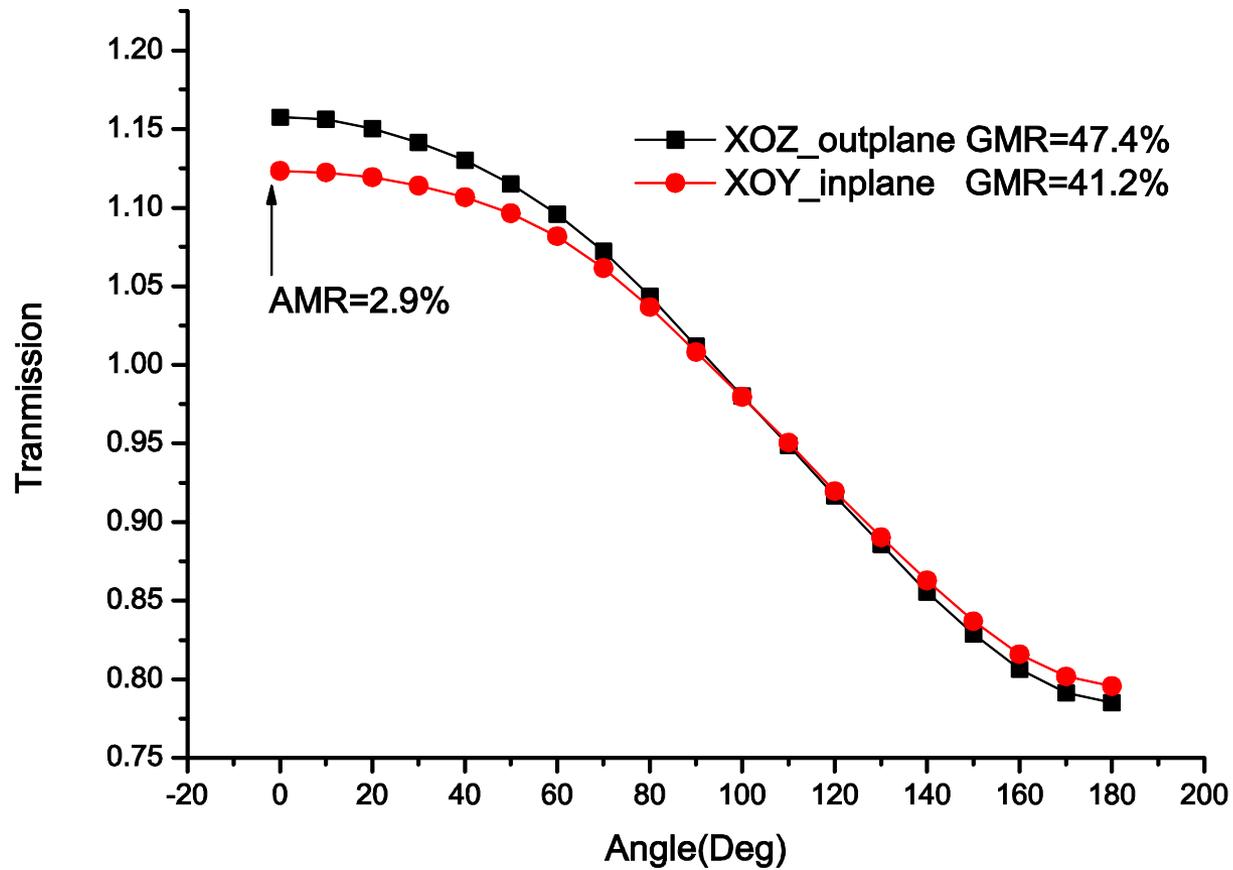
# With and without SO





# Fe|Pt(8ML)|Fe with Pt lattice constants

30MLPt GMR still 40%



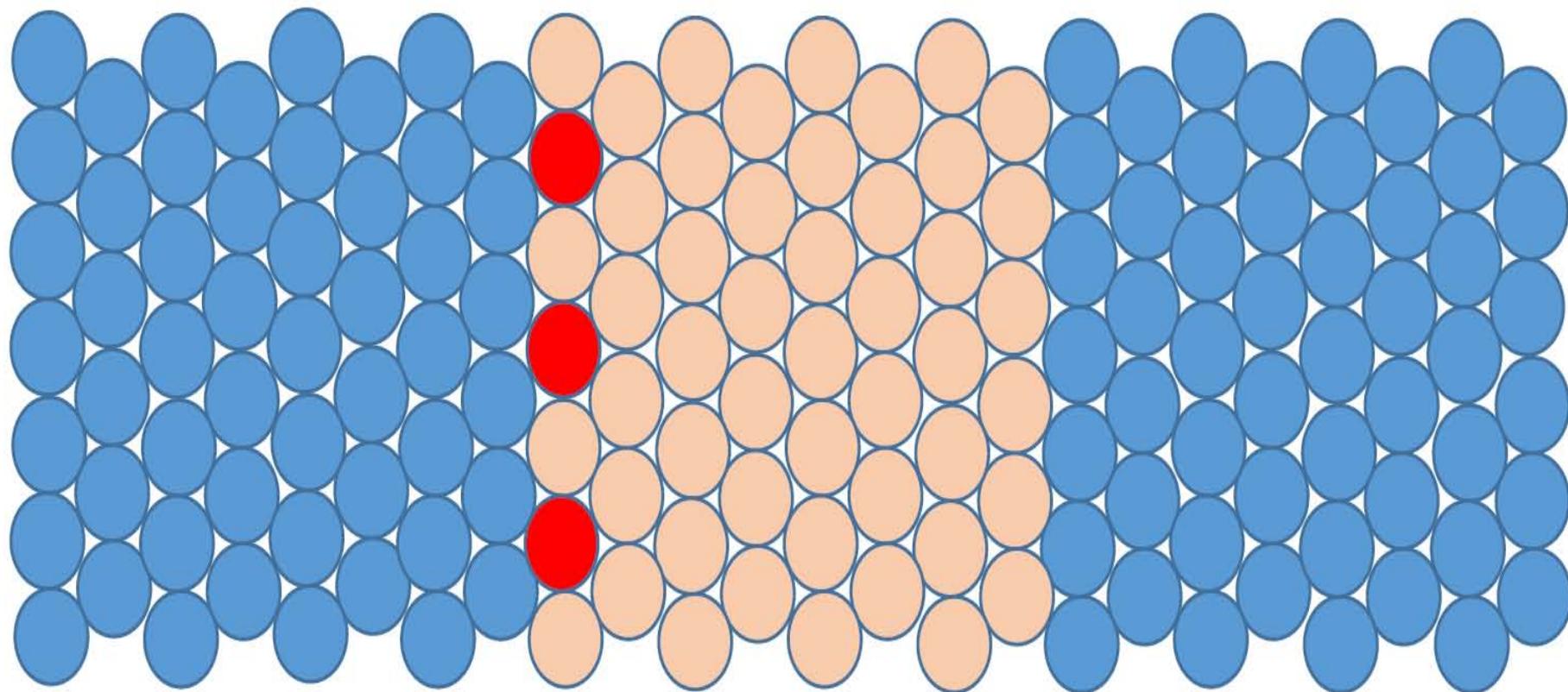
model of Au-vac-Au

with  $M_{\text{Fe}} = 2.8\mu$

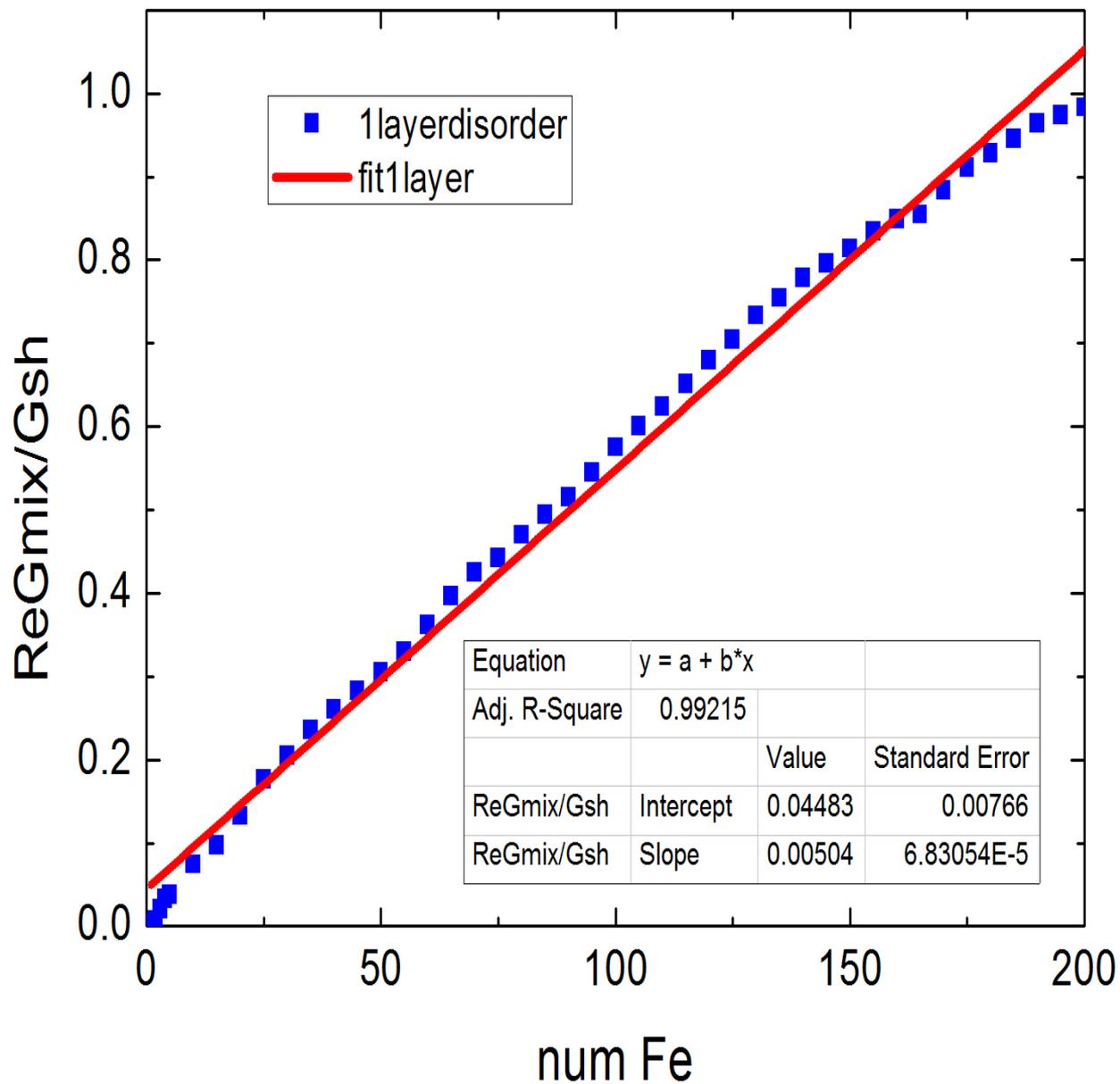
● Pt/Au

● Es

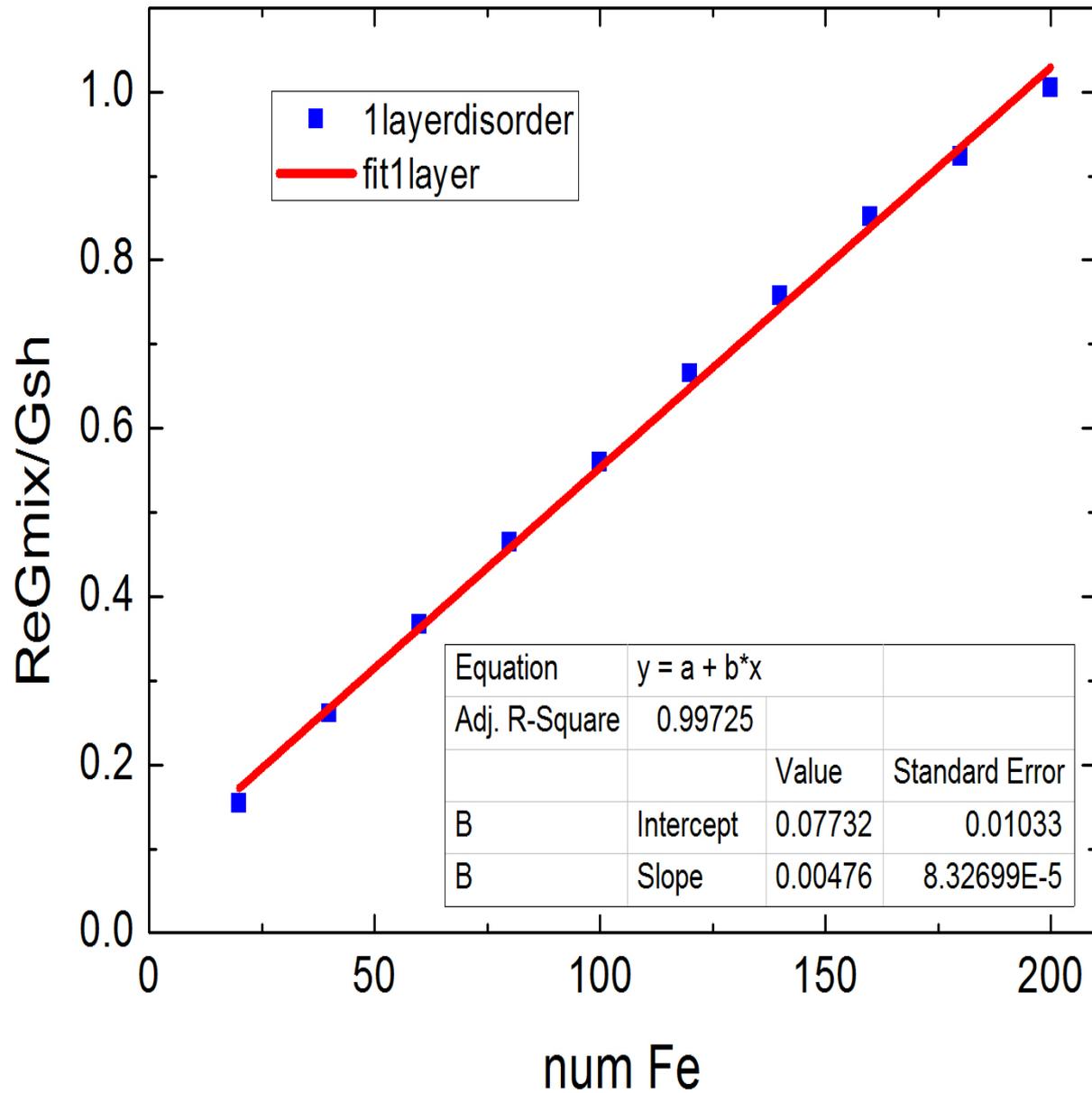
● Fe



# Au|Vac|Au



# Pt|vac|Pt

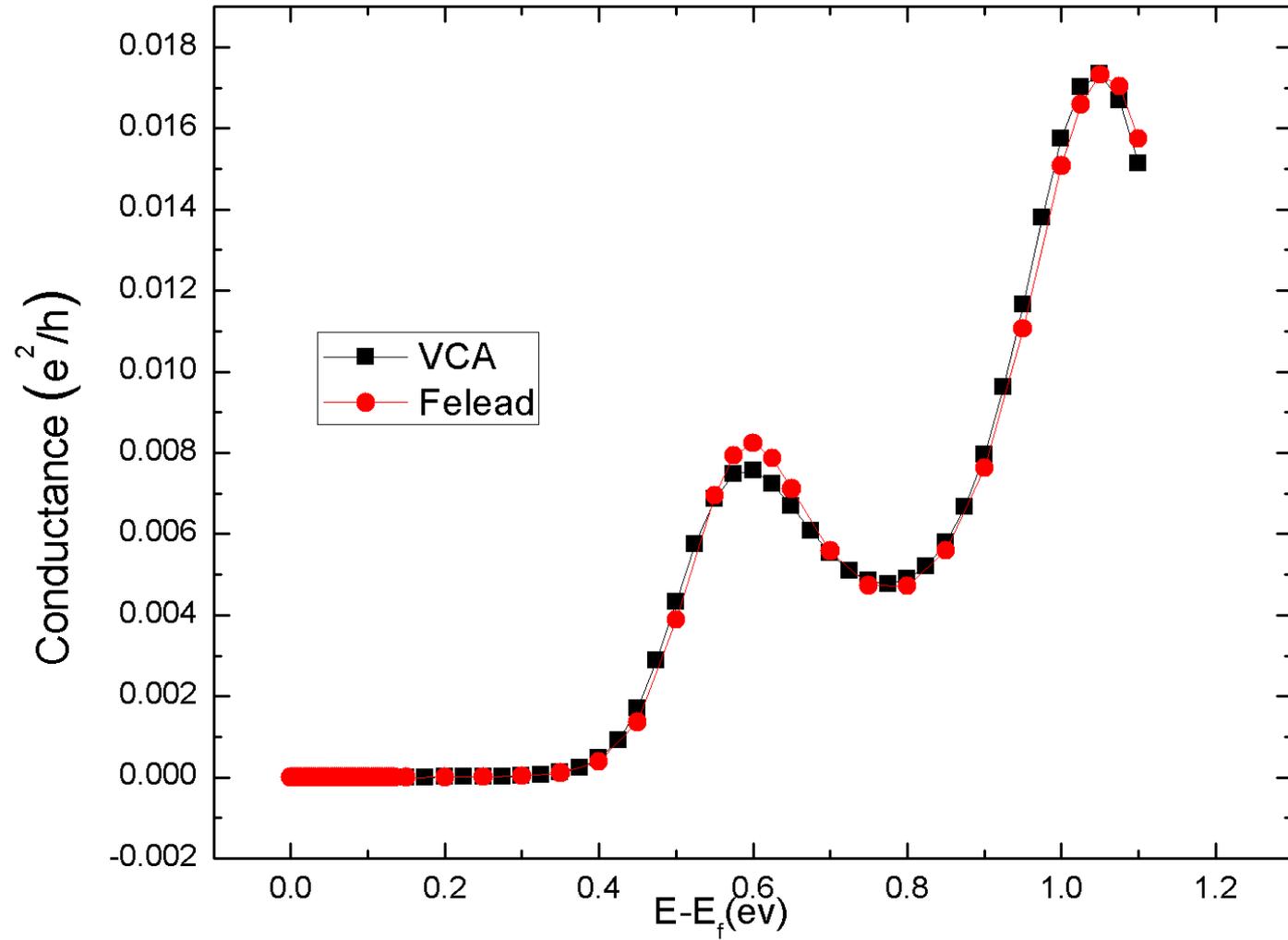


# Summary

- Bias enhanced Thermo-STT
- Efficient spin coupling at metal-magnetic insulator

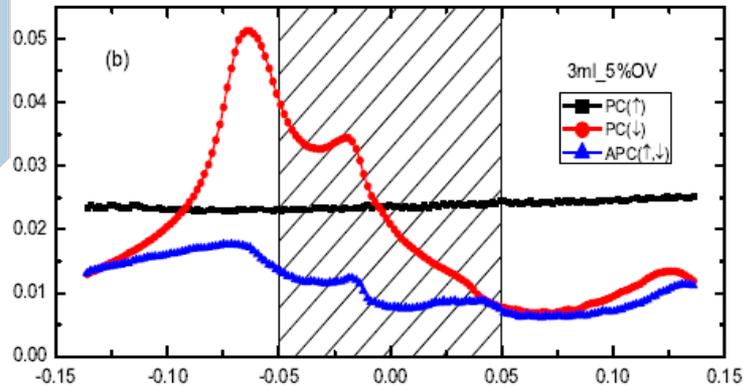
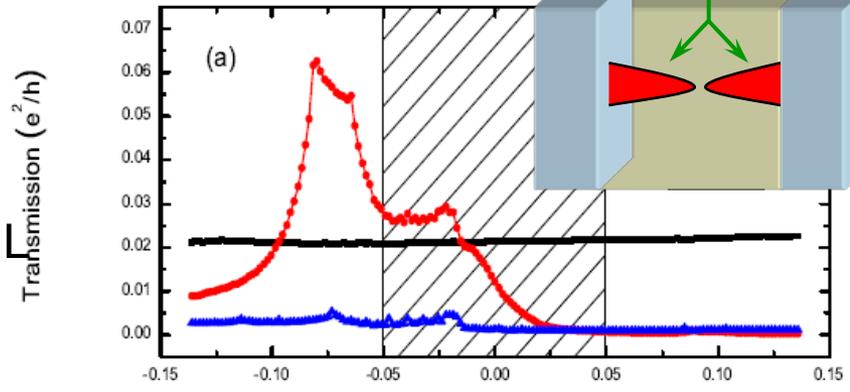
Thank you

# Comparison Energy dependent of transmission for clean interface of PC\_min 7MgO\_FeCo between VCA and Fe\_lead

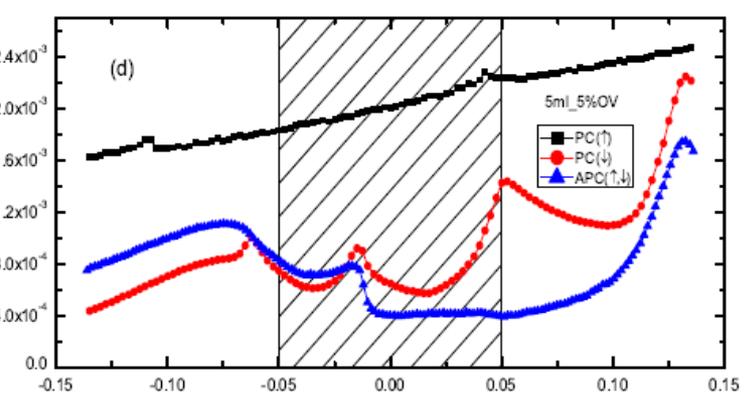
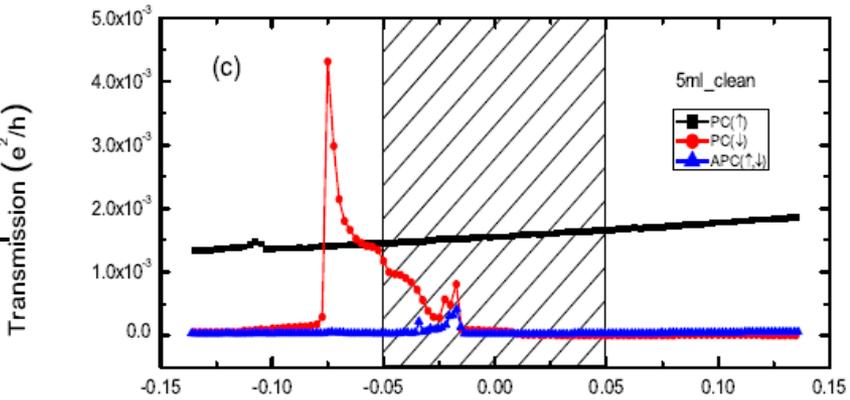


# surface states

3ML



5ML



7ML

