Journées
Nationales
en Nanosciences
et en Nanotechnologies

Ab initio Simulation of Transport in Nanospintronics

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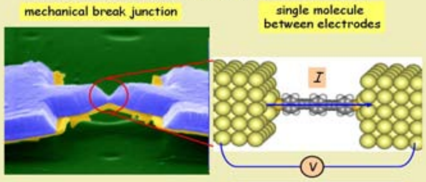
INTRODUCTION

Quantum transport: Molecular Electronics



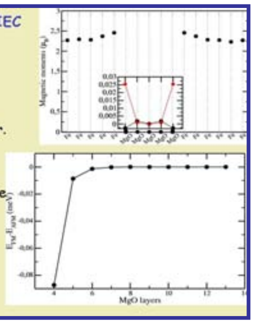
conductance: $\mathcal{G} = \frac{dI}{dV} = \frac{e^2}{\pi h} \times Transmission$

on the nanoscale electrons are (quantum) waves

Magnetic moments and IEC

The magnetic moments increase at the Interface and magnetic moments are Induced in the MgO spacer.

Exponential decrease of the IEC with the spacer size. The parallel alignment remains the ground-state magnetic configuration



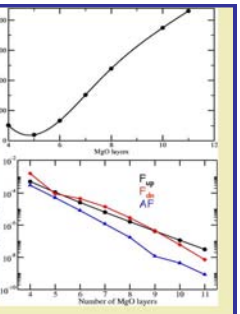
TMR

The TMR has a minimum at 5 layers (94%) and increases with increasing the spacer thickness to reach 2100% for 11 layers

$$TMR = \frac{G_{\uparrow\uparrow} - G_{\uparrow\downarrow}}{G_{\uparrow\downarrow}}$$

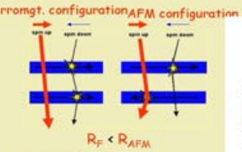
At small thickness, the conductance is dominated by spin down channel, at high thickness by the up channel

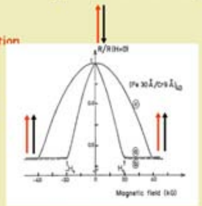
The conductance in the parallel configuration is larger than in the antiparallel one.



Geant Magneto-Resistance (GMR) mechanism (spin dependant currents)

Spin-up and spin-down currents





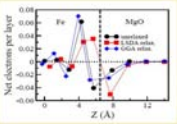
Gb hard drive

M. N. Balbich *et al.*, PRL ***61*** (1988).
G. Binasch *et al.*, PRB **39** (1989)

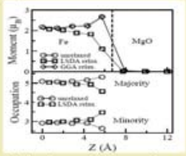
Relaxation effect on the magnetic and transport properties of Fe/MgO/Fe junctions

Case	DFT	d_{-4}	d_{-3}	d_{-2}	d_{-1}	d_0	d_1	d_2	d_3
I	unrelaxed	1.433	1.433	1.433	1.433	2.16	2.026	2.026	2.026
II	LSDA	1.297	1.313	1.343	1.120	2.002	2.130	2.119	2.119
III	GGA	1.380	1.414	1.427	1.350	2.219	2.199	2.177	2.185

Atomic relaxations along the junction direction in Å. The d_i are the inter plane distances (d_0 is the distance between Fe and MgO layers).



Charge transfer at the interface calculated using Bader analysis.



Calculated magnetic moments and occupations at the Fe/MgO interface.

Conclusions:

1. IEC favor parallel alignment of the magnetization at the interfaces of Fe/MgO/Fe
2. The calculated TMR values are higher than experiment -> Atomic relaxations have a strong effect on the TMR
3. Adding vanadium at the Fe interface acts as an extra barrier reducing the TMR, and its different magnetic states can change it considerably
4. The double barriers Fe/V/Fe/MgO/Fe offers many possibilities to change the TMR as a function of the different magnetic states.

Perspectives:

- ➡ Extend this study to molecular spacers
- ➡ Use half-metals (like SFMO) or DMS as leads
- ➡ Transport with finite bias (non-equilibrium Green's function formalism)

Spacer

The use of an amorphous spacer like Al_2O_3 gives a TMR ratio of at most 70%.

Calculated TMR for MgO spacers of the order of 1000% , much higher than the experimental values (240%)

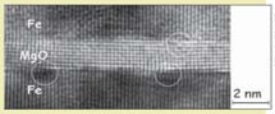
It seems that a better interface leads to a high TMR ratios.

For GaAs and MgO the small lattice misfit makes layer by layer growth possible.

Experimentally, a perfect interface is always complicated.

For Fe/GaAs/Fe, the so called dead magnetic layer of iron at the interface reduces the TMR ratio.

For Fe/MgO/ Fe, the presence of FeO layer at the interface destroys the TMR.



Yuasa et al, Nature Mat. 3, 868 (2004)

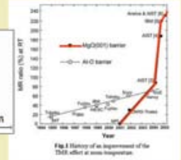
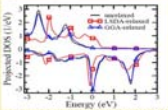
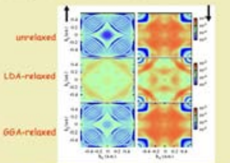


Fig.1 History of an improvement of the TMR effect at room temperature.

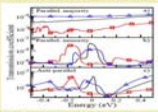
Effects of the atomic relaxation on the DOS, the transmission coefficient and TMR



Atomic relaxation effects on the DOS of the Fe atoms at the interface.



Relaxation effects on k-resolved DOS of interface Fe.



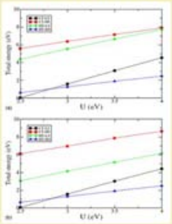
Atomic relaxation effects on the transmission coefficient. The colors are the same as for the DOS.

	G_P	G_{AP}	TMR
unrelaxed	1.21 × 10[illegible]	7.18 × 10[illegible]	173
LSDA relax.	7.32×10^{-6}	6.74×10^{-7}	9.86
GGA relax.	2.38×10^{-4}	3.23×10^{-6}	72.7
Expt.	-	-	2.47

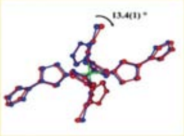
Atomic relaxation effects on the TMR of $Fe/(MgO)_5/Fe$

Molecular Magnetism

High-spin Low-spin transition in $FeX_2(NCS)_2$, X= btr, phen



LDA+U total energy of the HT and LT HS and LS versus U parameter for (a) $Fe(btr)_2(NCS)_2$ and (b) $Fe(btr)_2(NCS)_2$.



$FeX_2(NCS)_2$ HL atomic configurations

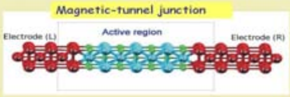
	btr	phen
Theory	16.5	13.6
Expt.		12.5

Calculated HL energy in KJ/mole for both $FeX_2(NCS)_2$, X=brt or phen as compared to experiment.

Materials-Specific Quantum Transport Codes in Development

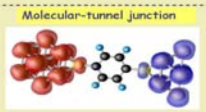
Fleur (Germany, France)

TB-LMTO (Czech Republic, France)

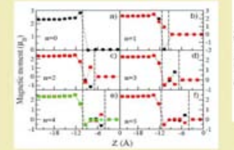


siesta (Spain)

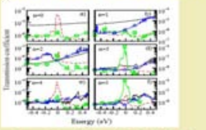
Smeagol Non-equilibrium Electronic Transport (Ireland, France)



Magnetic configuration of vanadium layers in Fe/V/MgO/Fe magnetic junction and its effect on the transport properties.



Stable (black) and instable magnetic configuration of $Fe/V_n/(MgO)_5/Fe$ magnetic junctions.



Transmission coefficient of $Fe/V_n/(MgO)_5/Fe$ magnetic junctions for different values of *n*

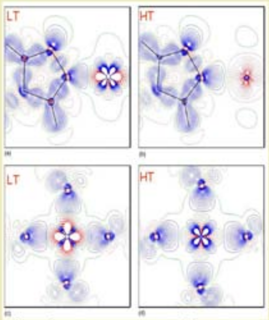
P: Black curve (LE majority) and blue triangles (LE minority).

AP: Green with squares curve (LE majority), and blue triangles (LE minority).

Calculated deformation densities of the LT and HT forms of btr complex

Plane of triazole ring including the Fe(II) ion.

Plane of the four triazole N ligands.

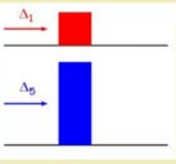


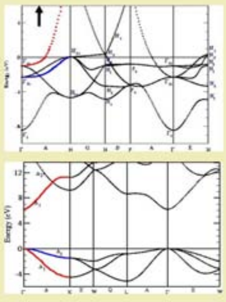
Positive contours are blue and negative contours are red. The contours are between ±1.05 e/Å³ and the charge density step is 0.05 e/Å³.

S. Lebègue, S. Pillet, J. G. Ángyán, Phys. Rev. B, 78, 024433 (2008).

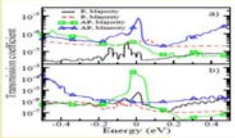
Band structure of Fe and MgO.

The Δ_1 band of Fe and the Δ_1 of MgO conductance bands have the smallest energy difference compared to Δ_5 and Δ_2.





Conductance and TMR of Fe/V/Fe/MgO/Fe magnetic junctions



Transmission of Fe/V/Fe/MgO/Fe magnetic junction for the Fe layer near MgO parallel and antiparallel to left iron electrode.

MTJ	Magnet.	Majority G	Minority G	Opt. TMR	Pess. TMR
n = 2,	↑↑↑	4.78 × 10[illegible]	3.19 × 10[illegible]	-0.93	-12
m = 4	↑↑↓	3.06 × 10[illegible]	4.65 × 10[illegible]		
	↑↓↑	4.50 × 10[illegible]	4.49 × 10[illegible]		
	↑↓↓	3.02 × 10[illegible]	8.41 × 10[illegible]	-0.98	-60
n = 2,	↑↑↑	4.62 × 10[illegible]	5.66 × 10[illegible]	115	0.99
m = 6	↑↑↓	9.89 × 10[illegible]	3.89 × 10[illegible]		
n = 4,	↑↑↑	1.60 × 10[illegible]	4.49 × 10[illegible]	49	0.98
m = 6	↑↑↓	5.85 × 10[illegible]	3.14 × 10[illegible]		

Conductance (in units of e2/h) and TMR of $Fe/V_n/Fe_m/MgO/Fe$. The arrows indicate the magnetizations of the left, middle and right iron layers.

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