



# Spin-Dependent Tunneling in Magnetic Tunnel Junctions

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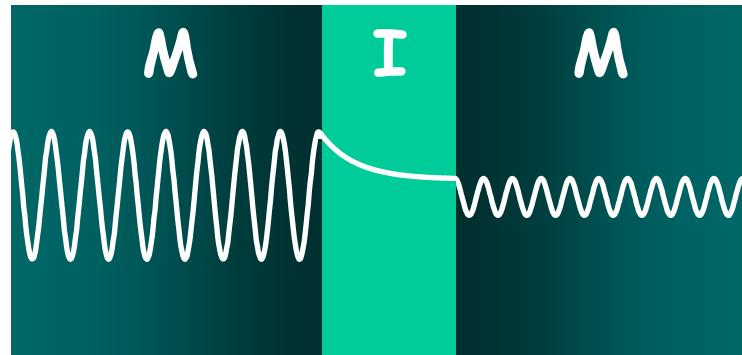
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# Electron Tunneling

## Tunnel junction



- quantum-mechanical effect
- observed in tunnel junctions

## Some applications:

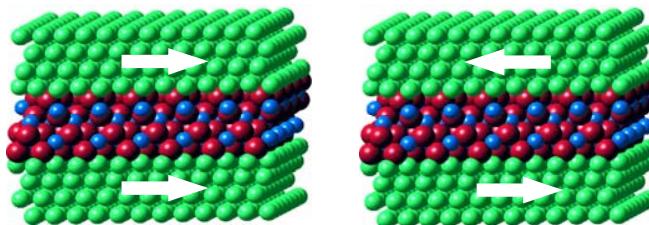
- Scanning tunneling microscopy (STM)
- Josephson junctions: superconducting quantum interference devices (SQUIDs)
- Field emission (Fowler-Nordheim tunneling): electron source in flash memories, electron microscopy and field emission displays
- Magnetic tunnel junctions: magnetic field sensors, magnetic random access memories (MRAM)



# Tunneling magnetoresistance (TMR)

## Magnetic tunnel junction (MTJ)

$$TMR = \frac{G_{AP} - G_P}{G_{AP}}$$



Ferromagnet  
Insulator  
Ferromagnet

Jullière, Phys. Lett. A 54, 225 (1975) - realization of a MTJ

Maekawa and Gafvert, IEEE Trans. Magn. 18, 707 (1982) -

TMR-magnetization switching correlation

Miyazaki and Tezuka, JMMM 139, L231 (1995) - large TMR

Moodera et al., PRL 74, 3273 (1995) - large reproducible TMR

Parkin et al., Nat. Mat. 3, 862 (2004) - giant TMR, MgO-based MTJ

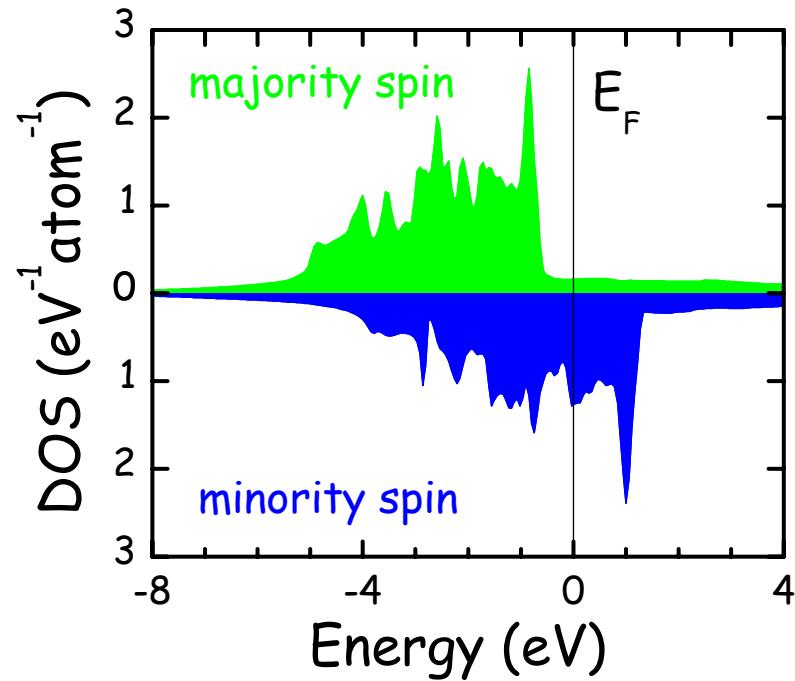
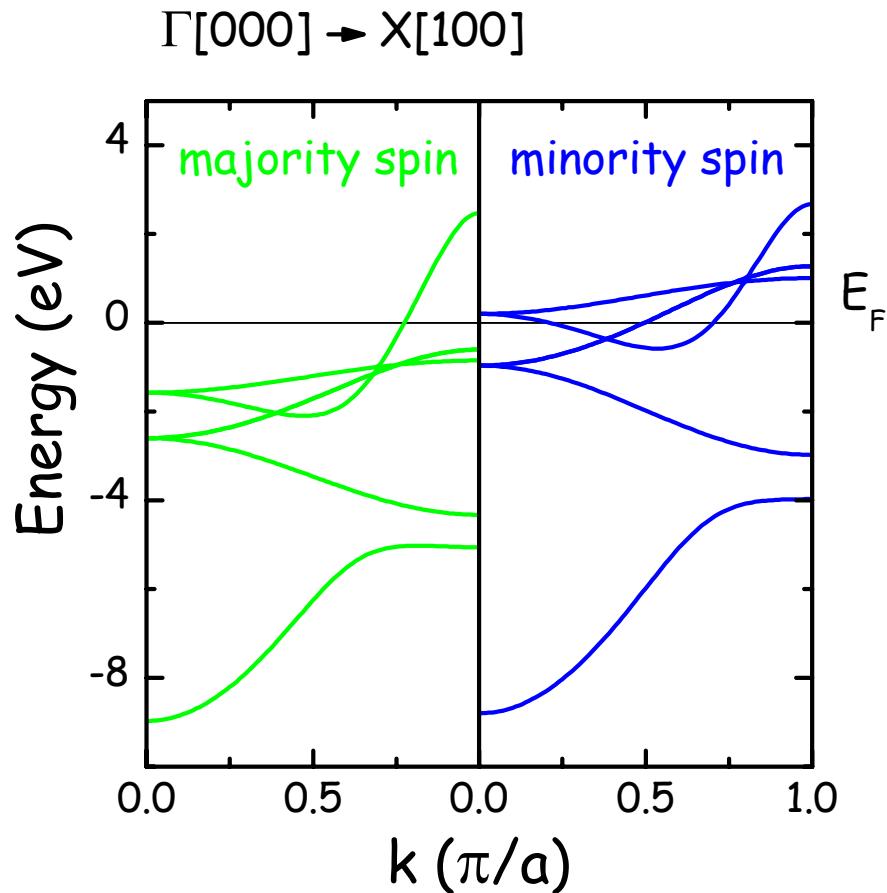
Yuasa et al., Nat. Mat. 3, 868 (2004) - giant TMR, MgO-based MTJ

FM|Al<sub>2</sub>O<sub>3</sub>|FM MTJs: TMR~70%

FeCo|MgO|FeCo MTJs: TMR>300%



# Band structure of Co

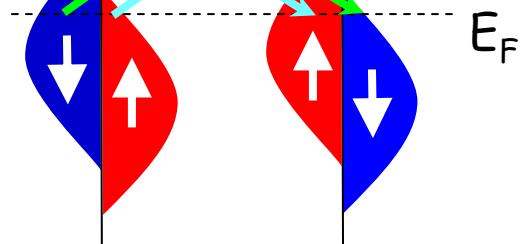
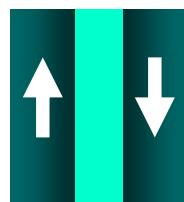
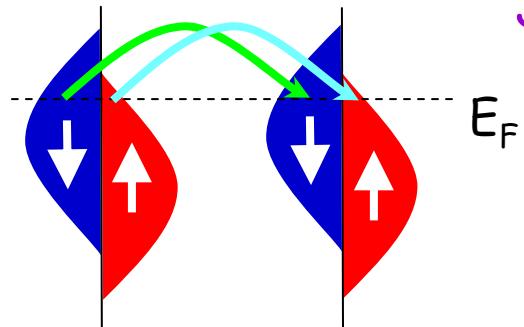
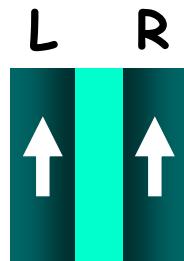


$$3d^7 4s^2 \quad n = 9 \quad n_{\uparrow} = 5.3 \quad n_{\downarrow} = 3.7$$
$$m = (n_{\uparrow} - n_{\downarrow})m_s = 1.6\mu_B$$

- Majority- and minority-spin electrons
- Exchange-split bands



# Origin of TMR



Jullière, Phys. Lett. A 54, 225 (1975)

$$G_{\uparrow\uparrow} \propto n_L^{\uparrow} n_R^{\uparrow} + n_L^{\downarrow} n_R^{\downarrow}$$

$$G_{\uparrow\downarrow} \propto n_L^{\uparrow} n_R^{\downarrow} + n_L^{\downarrow} n_R^{\uparrow}$$

Jullière's formula:

Tunneling spin polarization  
of ferromagnets:

$$\text{TMR} \equiv \frac{G_{\uparrow\downarrow} - G_{\uparrow\uparrow}}{G_{\uparrow\downarrow}} = \frac{2P_L P_R}{1 - P_L P_R}$$

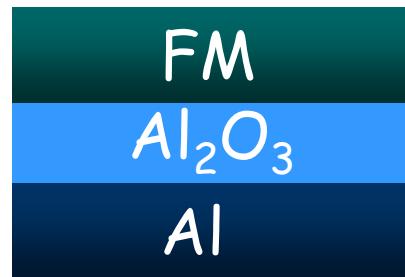
$$P_L = \frac{n_L^{\uparrow} - n_L^{\downarrow}}{n_L^{\uparrow} + n_L^{\downarrow}}$$

$$P_R = \frac{n_R^{\uparrow} - n_R^{\downarrow}}{n_R^{\uparrow} + n_R^{\downarrow}}$$



# Spin-polarized tunneling

Tedrow and Meservey PRL 26, 192 (1971)

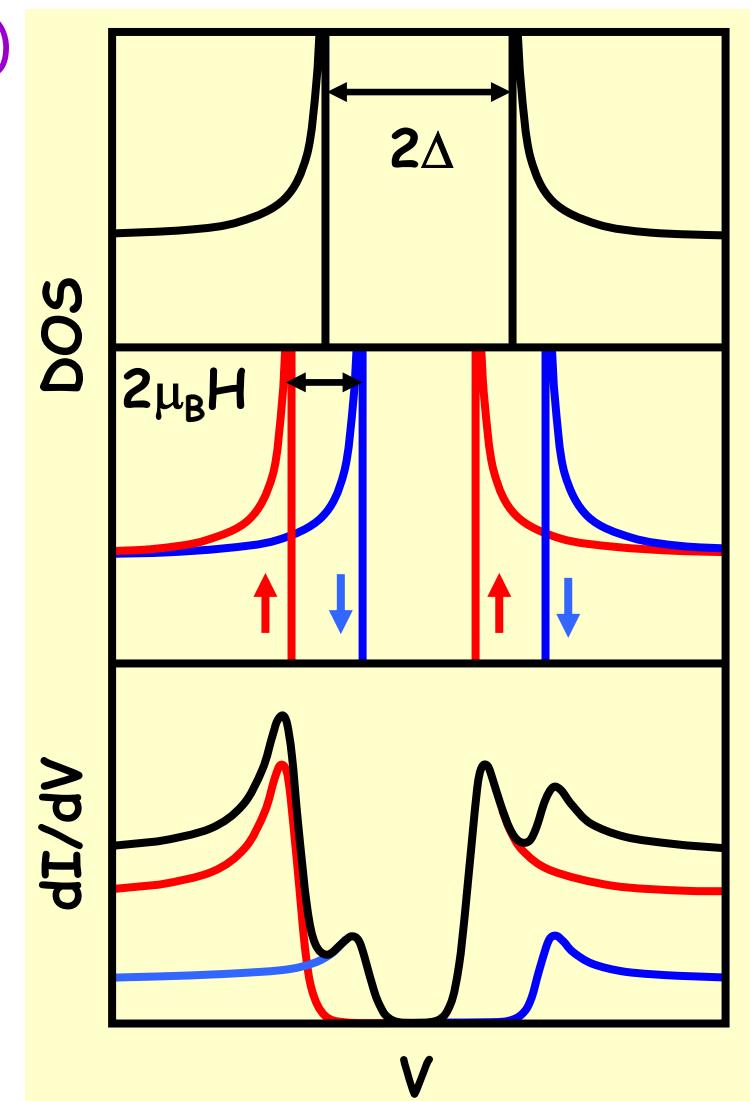


Ferromagnet  
Insulator  
Superconductor

- Quantum tunneling
- Spin-split bands of ferromagnets
- DOS of superconductors

Tunneling spin polarization:

$$P_{\text{exp}} = \frac{G^{\uparrow} - G^{\downarrow}}{G^{\uparrow} + G^{\downarrow}}$$





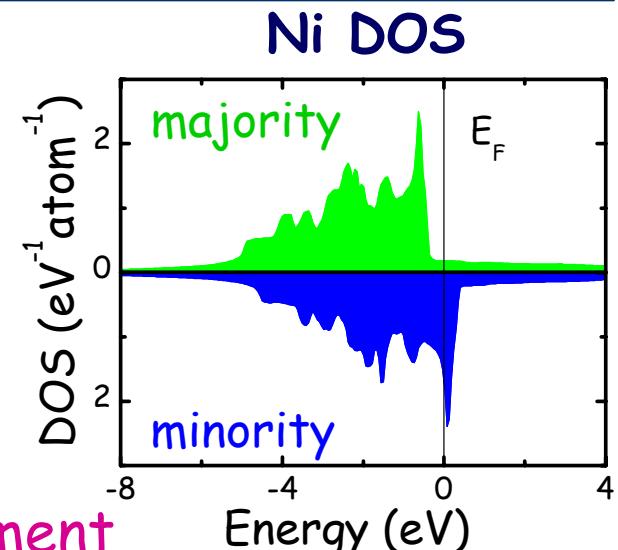
# Spin polarization and TMR

## Spin polarization

$$\text{FM} \quad P_{\text{exp}} = \frac{G^{\uparrow} - G^{\downarrow}}{G^{\uparrow} + G^{\downarrow}} \quad P_{\text{calc}} = \frac{n^{\uparrow} - n^{\downarrow}}{n^{\uparrow} + n^{\downarrow}}$$

Fe	+45%	+61%
Co	+42%	-77%
Ni	+32%	-81%

- Contradiction between theory and experiment



## Tunneling Magnetoresistance

### MTJ

Ni/Al<sub>2</sub>O<sub>3</sub>/Ni  
Co/Al<sub>2</sub>O<sub>3</sub>/Co  
Co<sub>75</sub>Fe<sub>25</sub>/Al<sub>2</sub>O<sub>3</sub>/Co<sub>75</sub>Fe<sub>25</sub>  
Co<sub>70</sub>Fe<sub>30</sub>/MgO/Co<sub>70</sub>Fe<sub>30</sub>

### Julliere      Experiment

25%	23%
42%	37%
70%	69%
520%	~600%

- Consistency between measured SP and TMR values

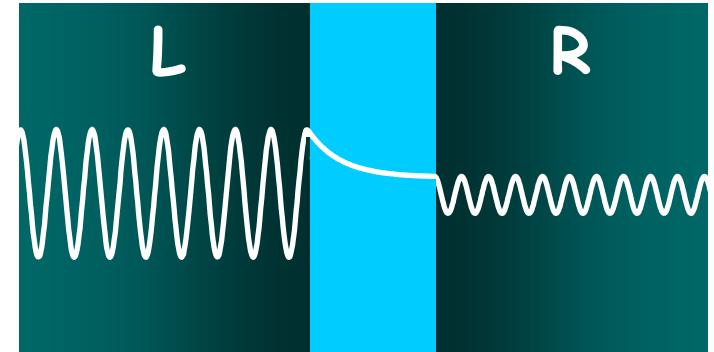


# Interface Transmission Function

Belashchenko et al., PRB 69, 174408 (2004)

$$G^\sigma = \frac{e^2}{h} \sum_{k_\parallel} T^\sigma(k_\parallel) \quad - \text{conductance}$$

$$T^\sigma(k_\parallel) = T_L^\sigma(k_\parallel) e^{-2\kappa(k_\parallel)d} T_R^\sigma(k_\parallel)$$



$T_L^\sigma(k_\parallel), T_R^\sigma(k_\parallel)$  - interface transmission functions (ITF)

$$T_{L,R}^\sigma(k_\parallel) = \frac{4\kappa k_{L,R}^\sigma}{\kappa^2 + k_{L,R}^{\sigma 2}} \quad - \text{for free electrons}$$

- Tunneling spin polarization is largely controlled by ITF

for thick crystalline barrier

$$P_{L,R} = \frac{T_{L,R}^\uparrow(0) - T_{L,R}^\downarrow(0)}{T_{L,R}^\uparrow(0) + T_{L,R}^\downarrow(0)}$$

for amorphous barrier

$$P_{L,R} = \frac{\langle T_{L,R}^\uparrow \rangle - \langle T_{L,R}^\downarrow \rangle}{\langle T_{L,R}^\uparrow \rangle + \langle T_{L,R}^\downarrow \rangle}$$



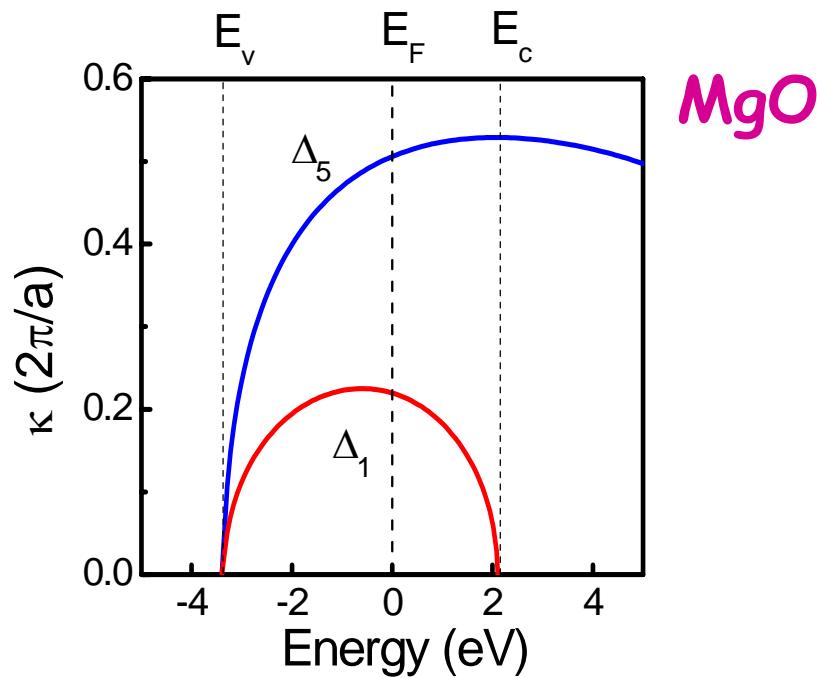
# Symmetry of bands

Mavropoulos et al., PRL 85, 1091 (2000)

## Insulator

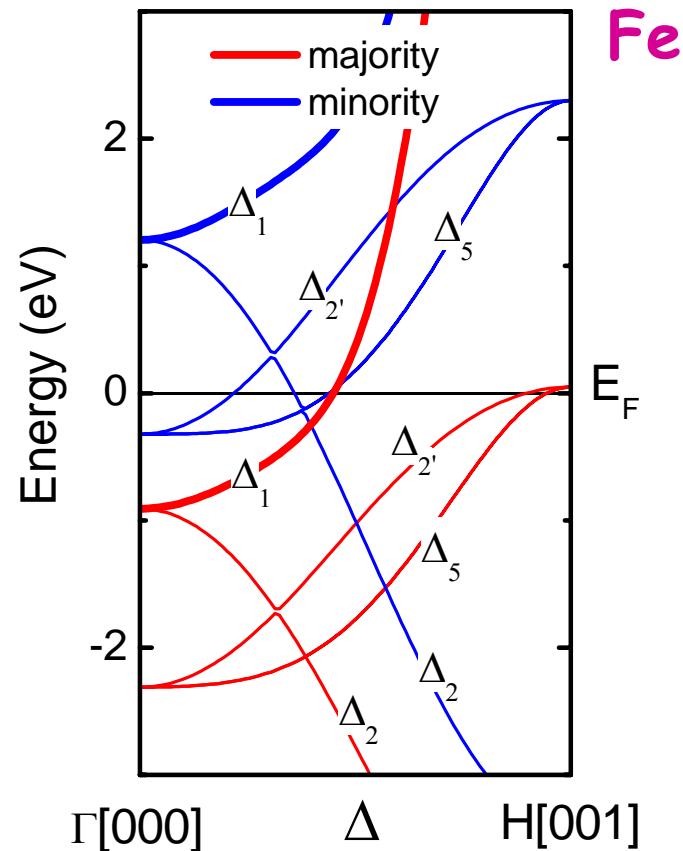
Complex band structure:

$$E = E(k_{||}, k_z), \text{ where } k_z = q + i\kappa, \psi \propto e^{-\kappa z}$$



MgO

## Ferromagnet



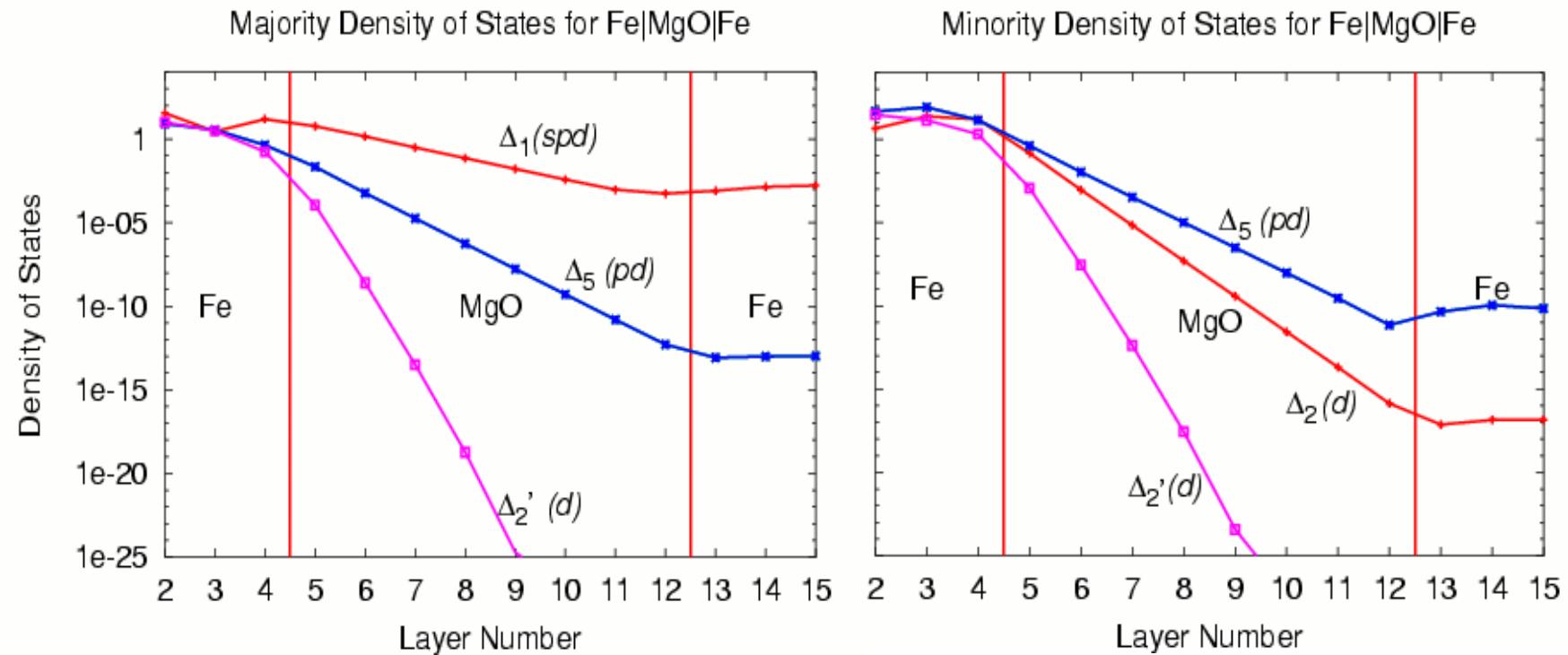
Fe

- Fe(001) behaves as a half metal if coupled with MgO



# Fe/MgO/Fe junctions

Butler et al., PRB 63, 054416 (2001)

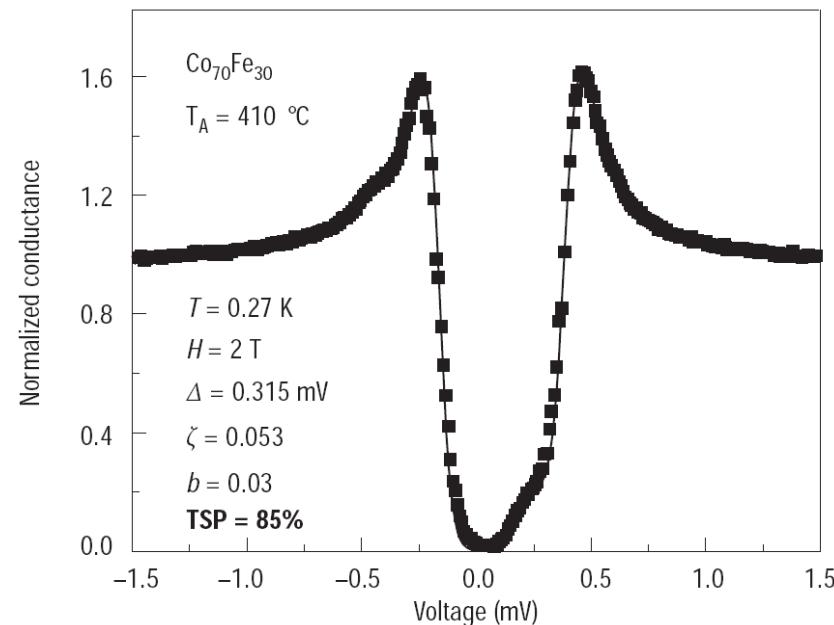


- Giant TMR for Fe/MgO/Fe (001)



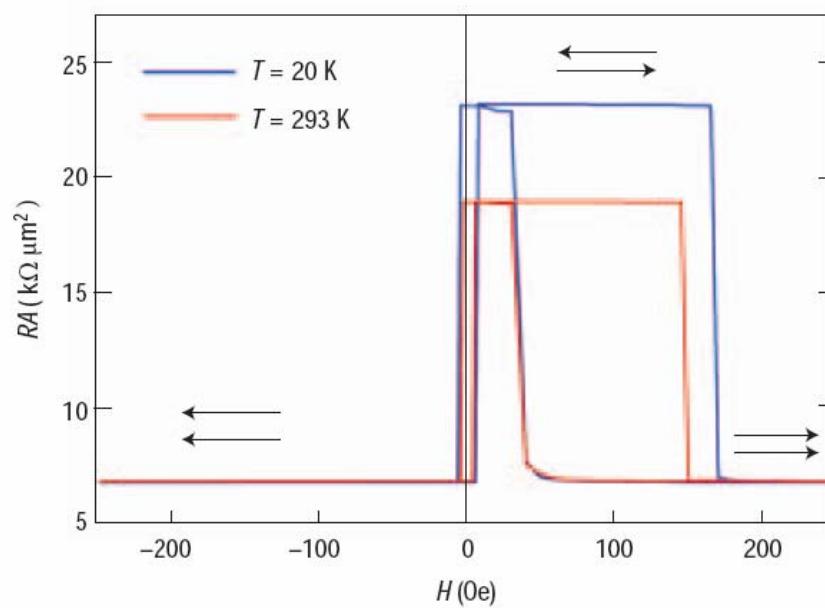
# Experimental results on Fe(Co)/MgO/Fe(Co)

Parkin et al., Nat.Mat. 3, 862 (2004)



**SP = 85%**

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



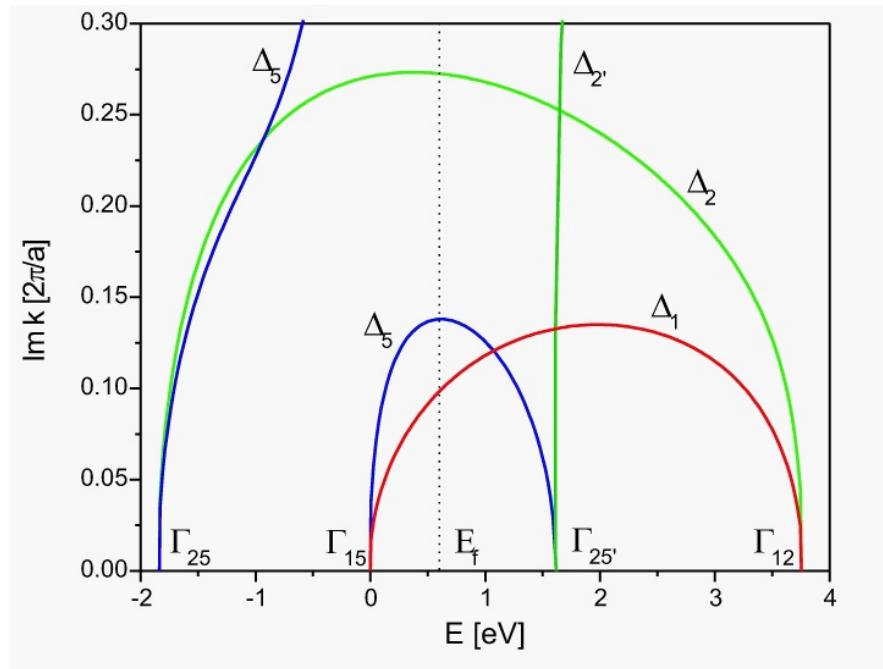
**TMR = 250%**



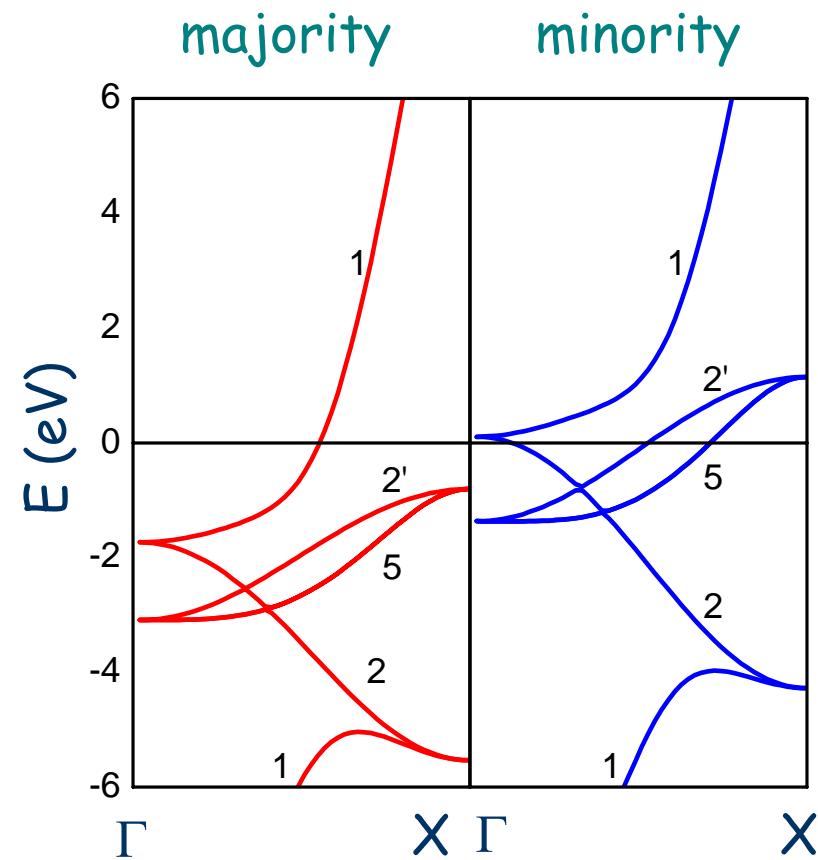
# Co/SrTiO<sub>3</sub>/Co junctions

Velev et al., PRL 95, 216601 (2005)

SrTiO<sub>3</sub>



bcc Co



- Significant contribution to conductance from Co d bands

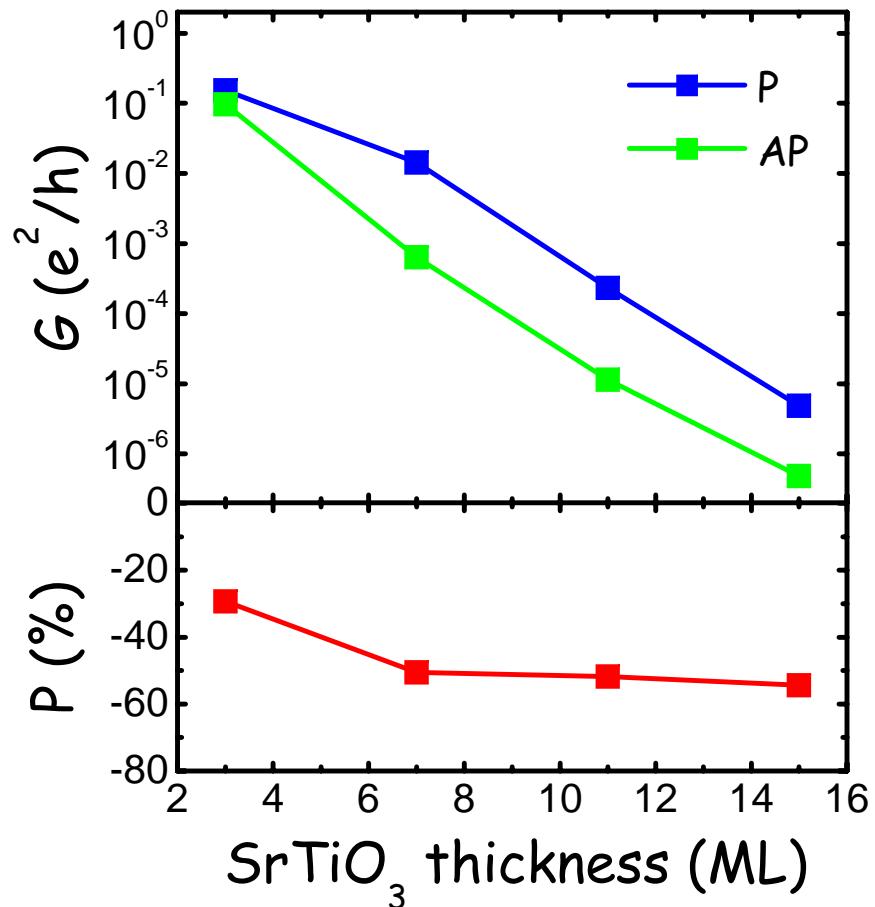
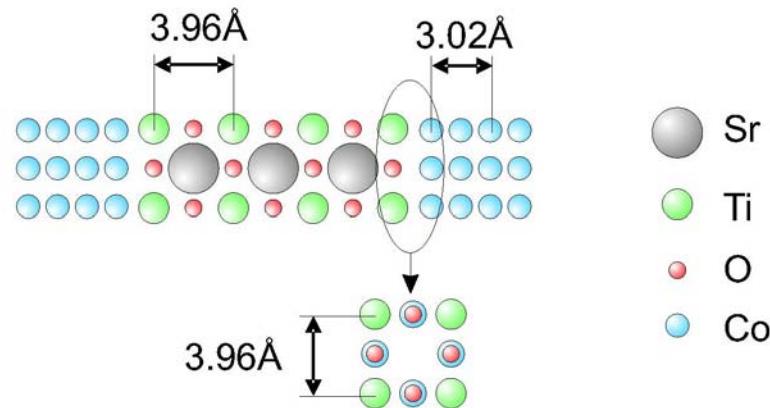


# Conductance and spin polarization

Velev et al., PRL 95, 216601 (2005)

$\text{SrTiO}_3$  - perovskite,  
 $\text{TiO}_2$  terminated

$\text{Co}$  - bcc coordination

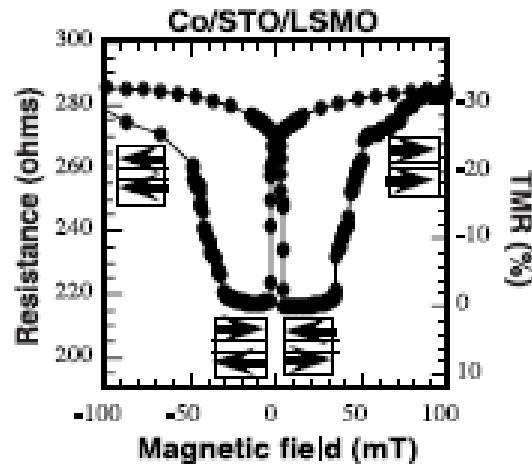


- Negative spin polarization and a very large TMR

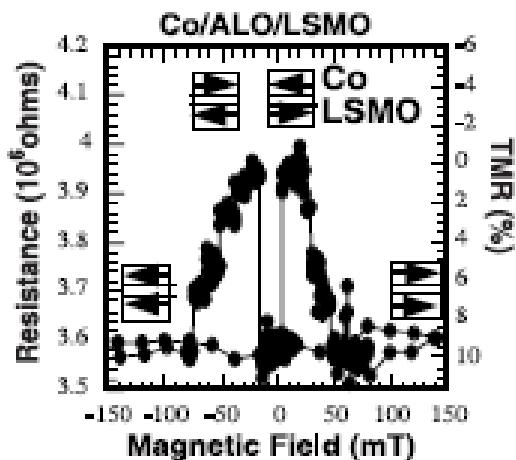


# Transport spin polarization of Co/SrTiO<sub>3</sub> interface

De Teresa et al., Science 286, 507 (1999)



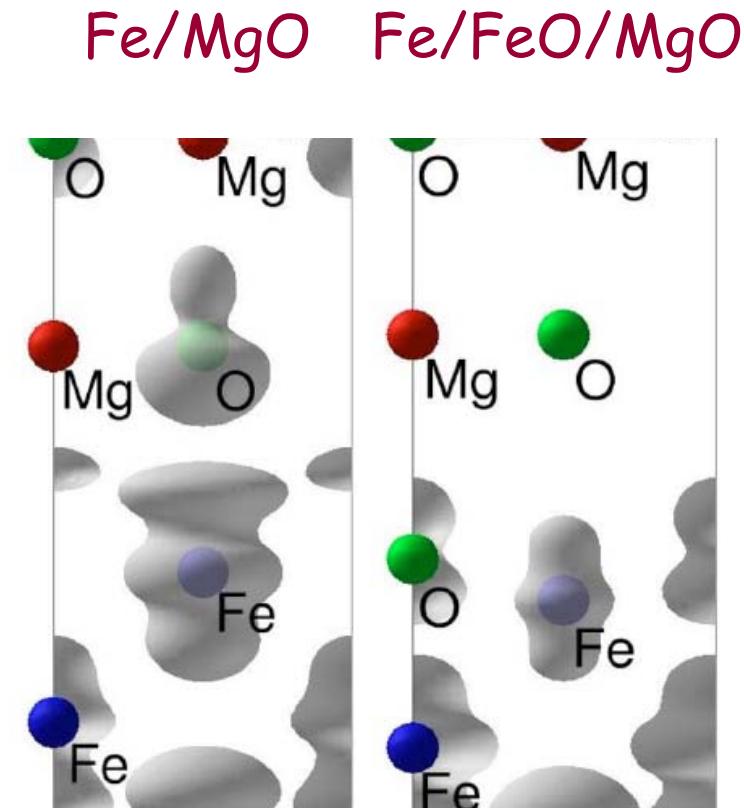
- LSMO as spin analyzer (100% positive SP)
- large inverse TMR (-50%) for Co/SrTiO<sub>3</sub>/LSMO
- negative spin polarization for Co/SrTiO<sub>3</sub>



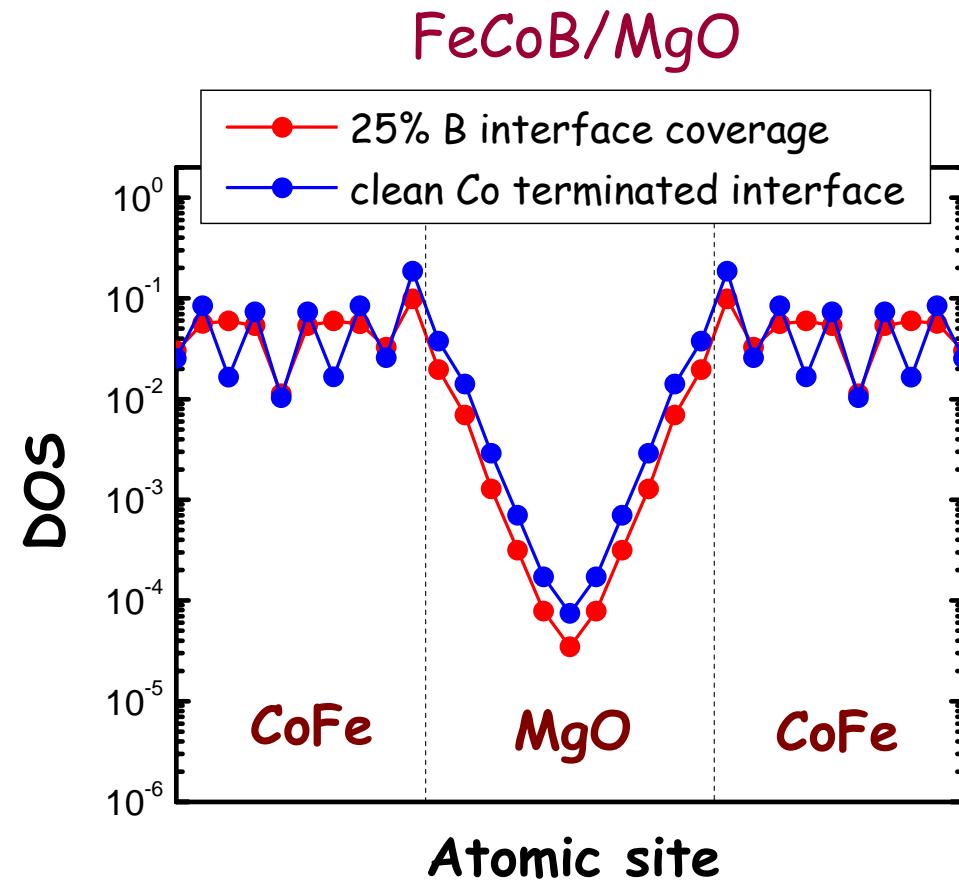


# Detrimental effect of O and B at the interface

Zhang et al., PRB 68, 092402 (2003)



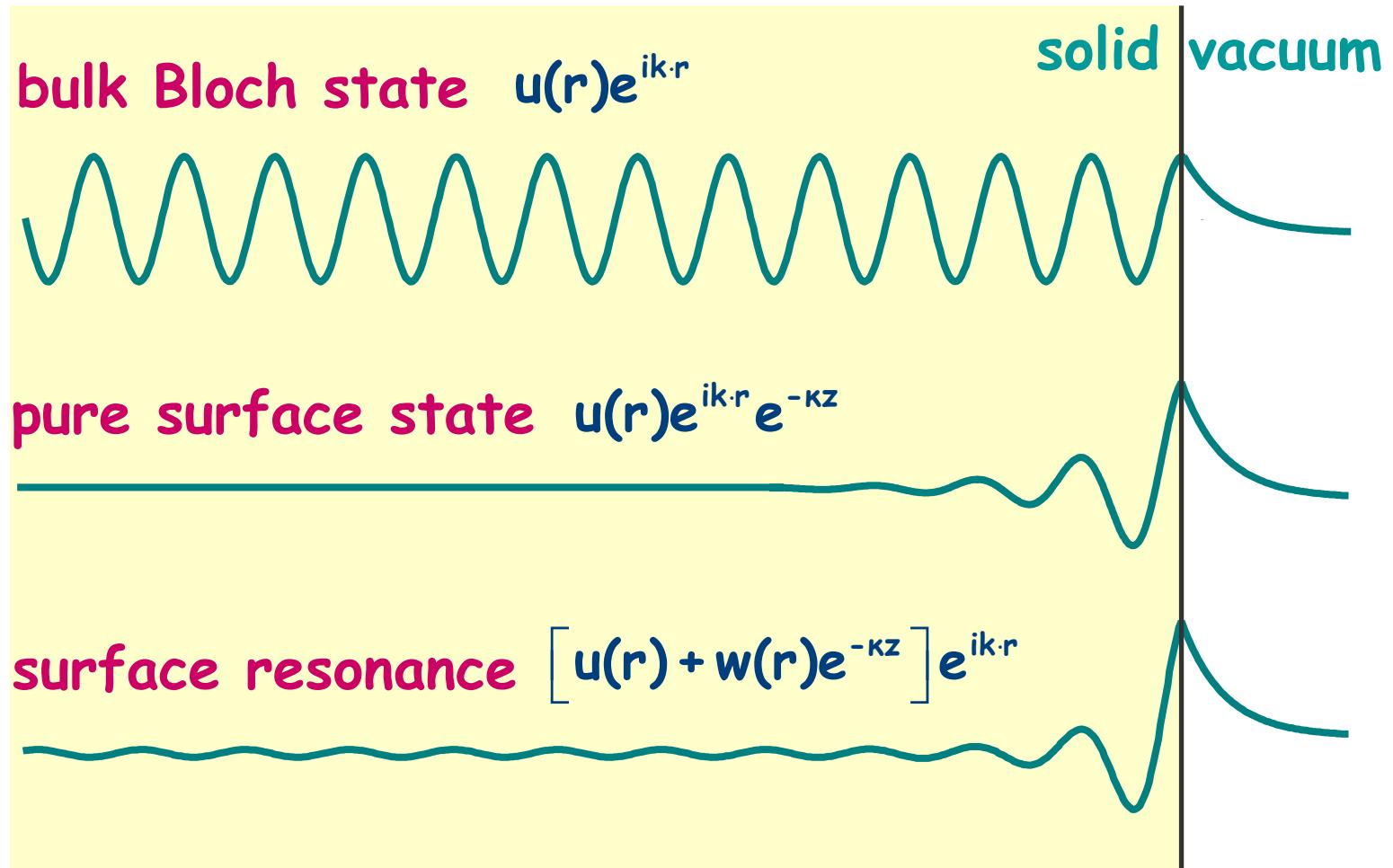
Burton et al., APL (2006)



- Bonding at the interface controls the spin polarization

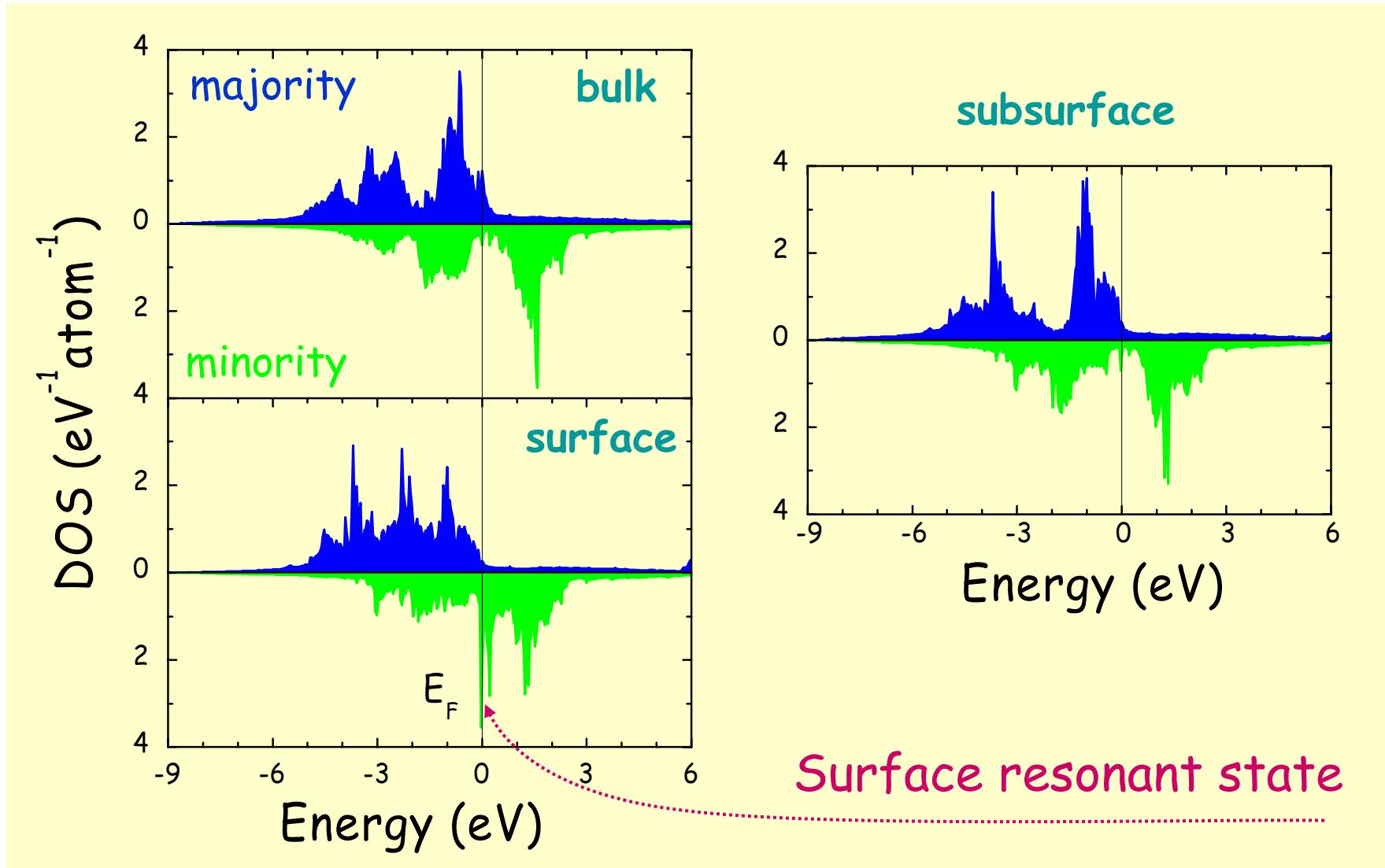


# Surface states





# Surface states in Fe(100)





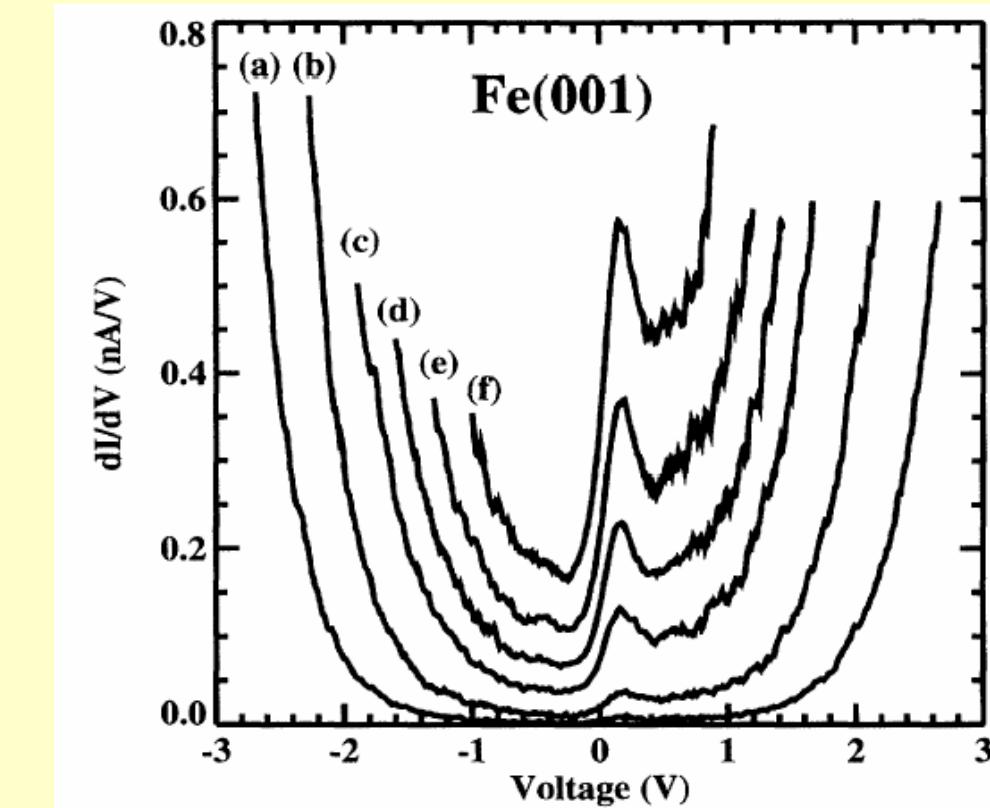
## Tunneling Spectroscopy of bcc (001) Surface States

Joseph A. Stroscio, D. T. Pierce, A. Davies, and R. J. Celotta

*Electron Physics Group, National Institute of Standards and Technology, Gaithersburg, Maryland 20899*

M. Weinert

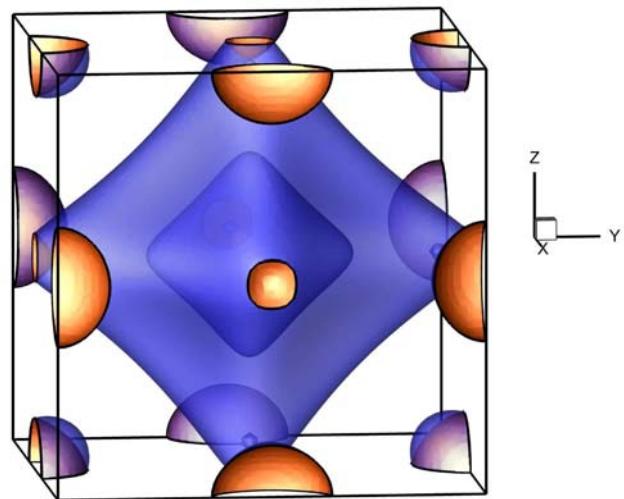
*Physics Department, Brookhaven National Laboratory, Upton, New York 11973*



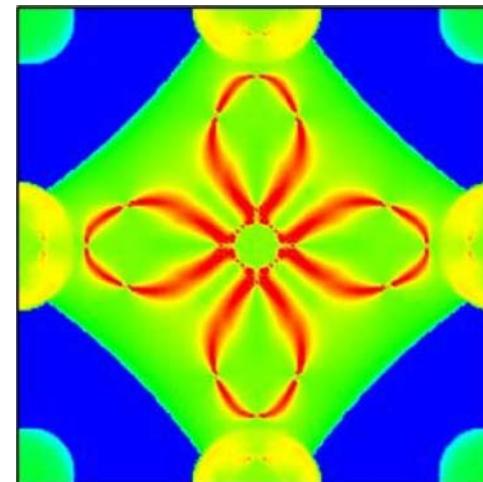


# Minority-spin states in Fe(100)

Fermi surface



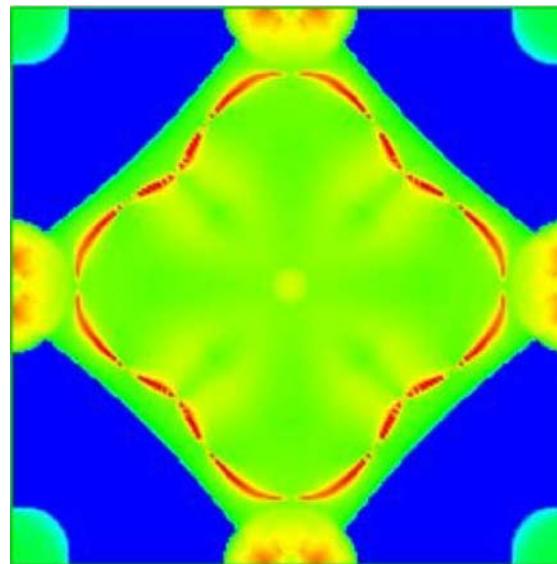
$K_{||}$ -resolved  
surface DOS at  $E_F$





# Energy dependence

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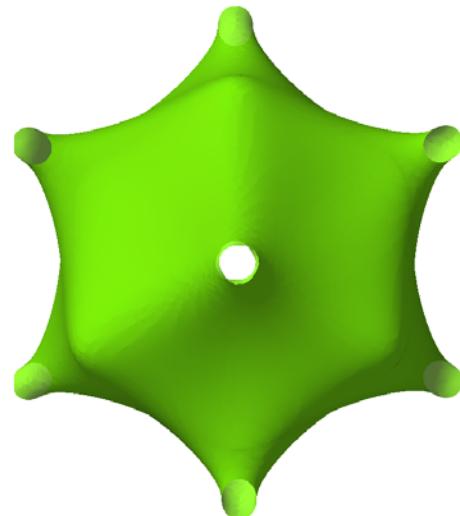
$$E = E_F + 0.125\text{eV}$$



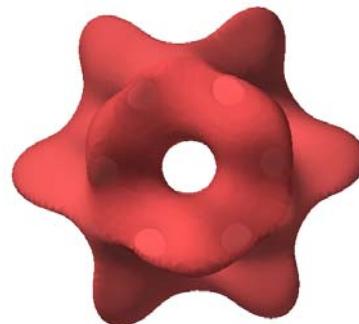
# Spin-dependent tunneling from clean and oxidized Co surface

## Fermi surface

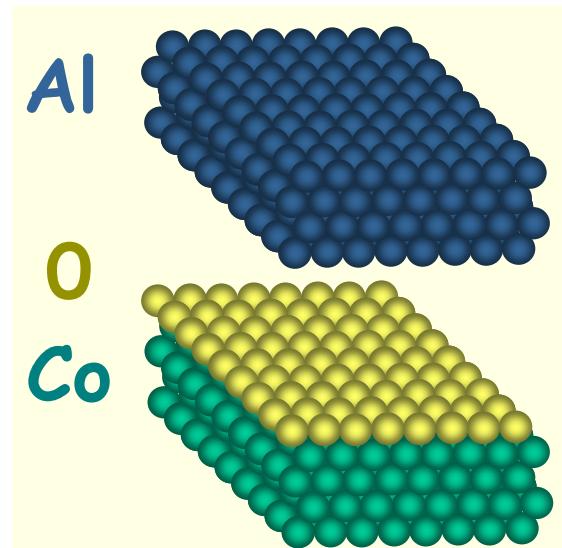
Majority spin



Minority spin



Belashchenko et al.,  
PRB 69, 174408 (2004)



$$\kappa(k_{\parallel}) = \sqrt{\frac{2m}{\hbar^2}U + k_{\parallel}^2}$$

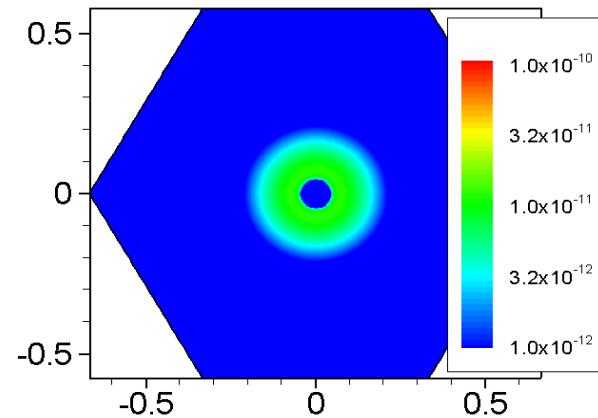
- decay constant in vacuum

- Majority-spin conductance is expected to dominate in the asymptotic regime of a thick barrier

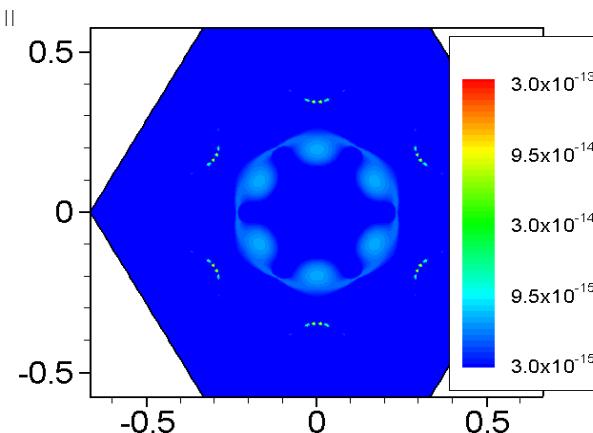
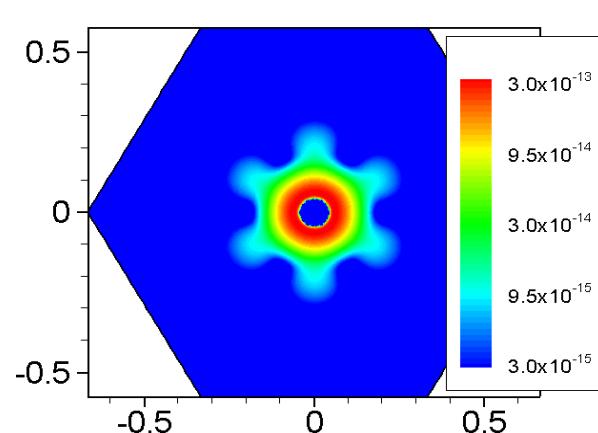
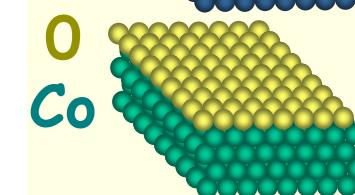
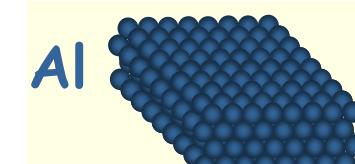
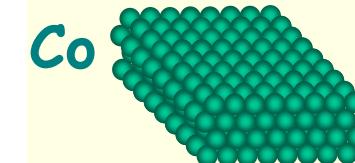
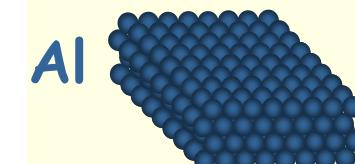
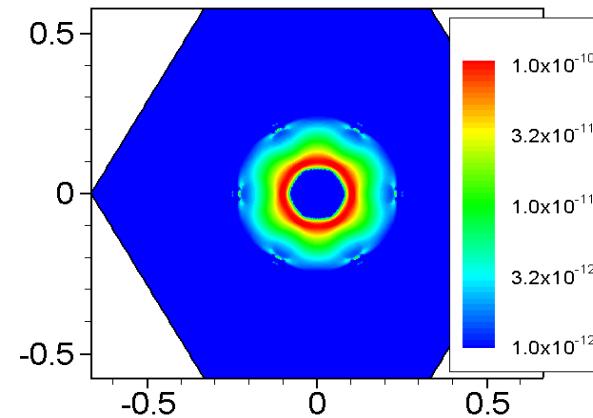


# $k_{||}$ -resolved transmission

Majority spin



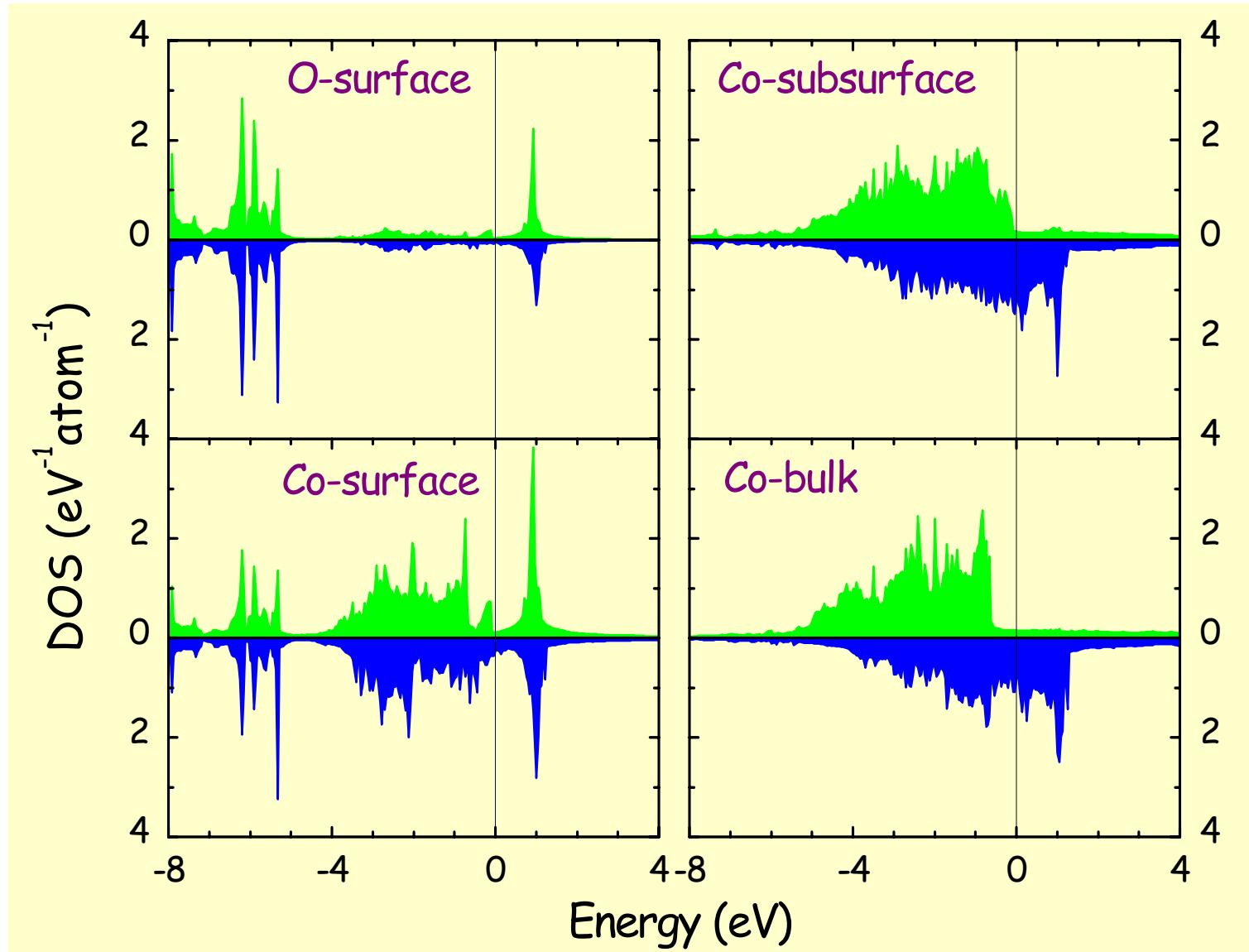
Minority spin



- Minority-spin conductance is filtered out by O layer
- Reversal of spin polarization



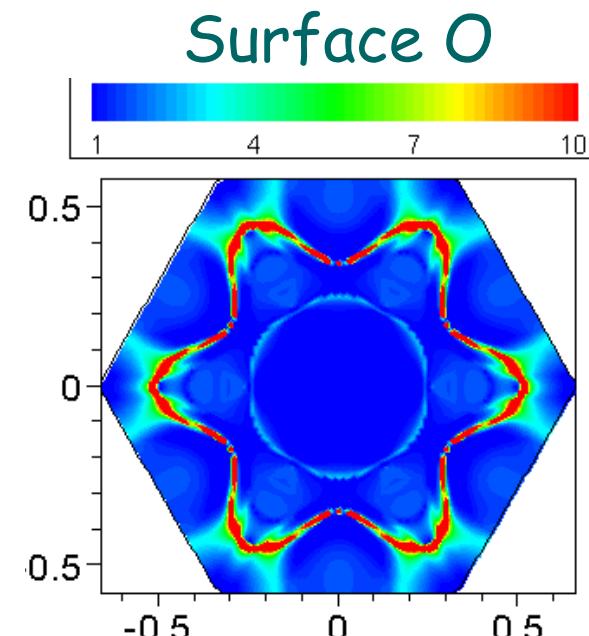
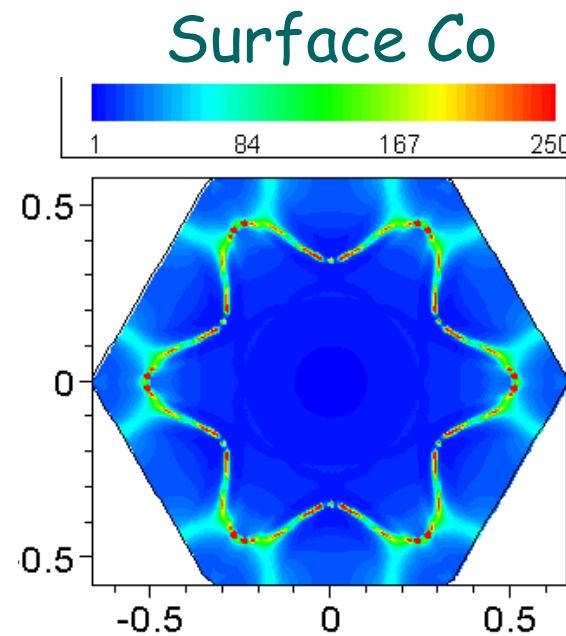
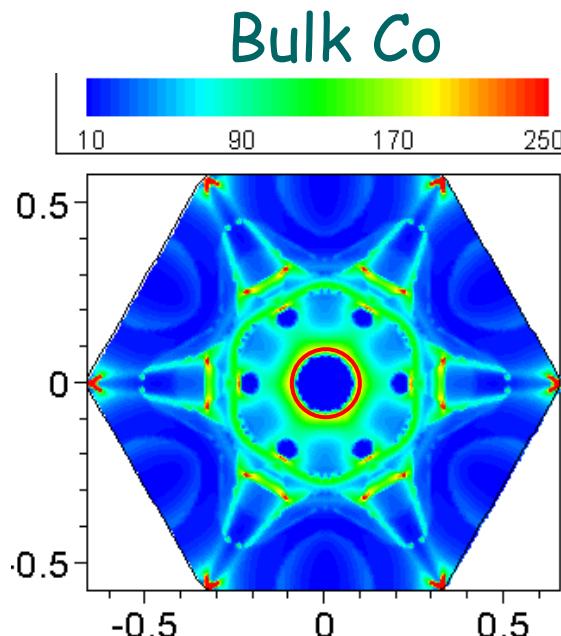
# Density of states for oxidized Co surface





# $k_{||}$ -resolved DOS for oxidized Co surface

Minority spin

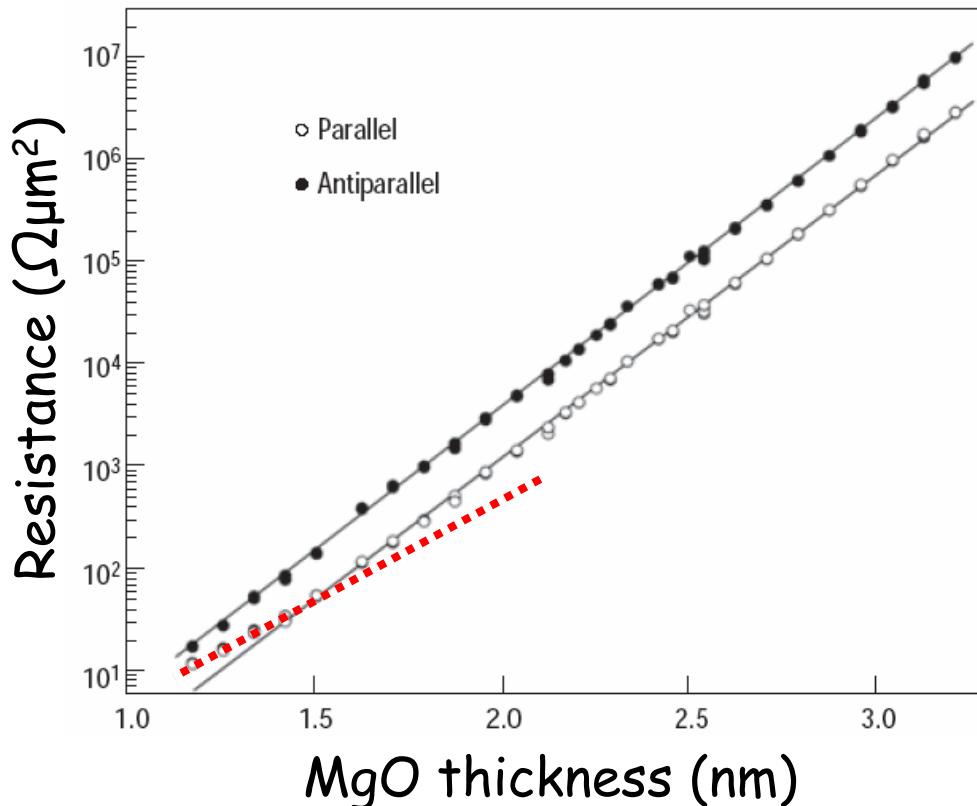


- Surface Co-O antibonding state creates an additional tunneling barrier in minority-spin channel

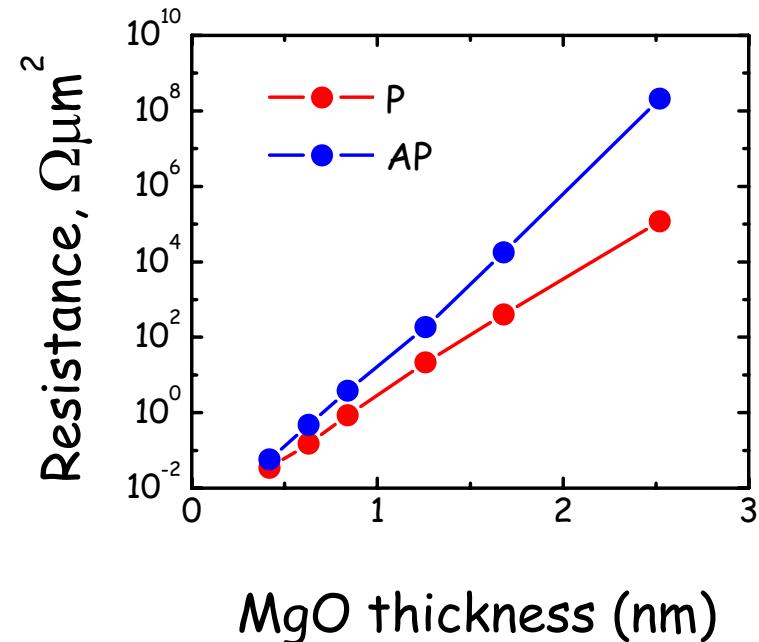


# Ballistic or diffusive ?

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



Belashchenko et al.,  
PRB 72, R140404 (2005)

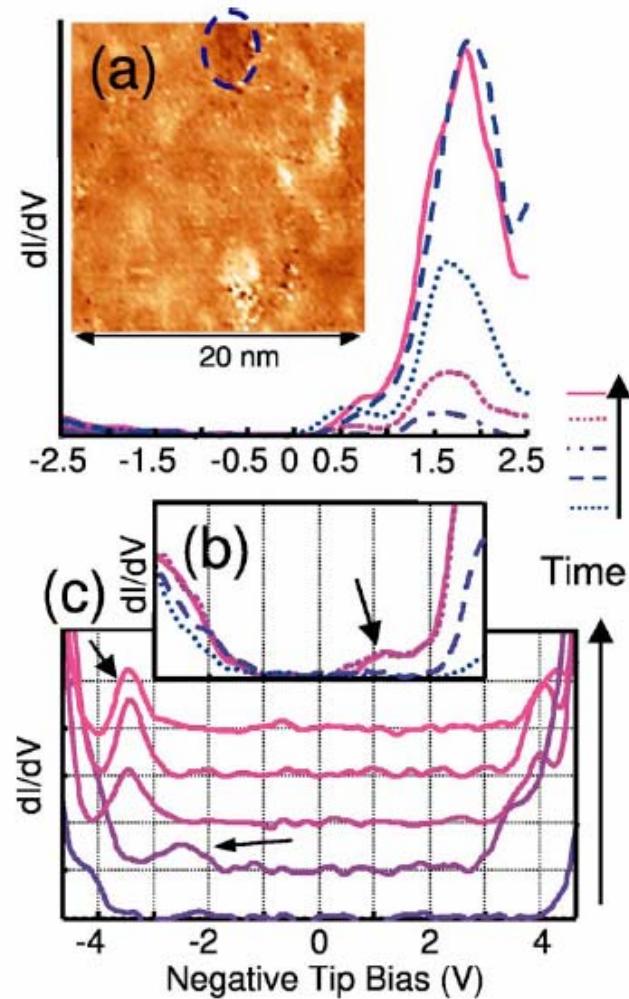


- Ballistic conductance only for thin barriers
- Diffusive transport for MgO thickness above 1.5 nm

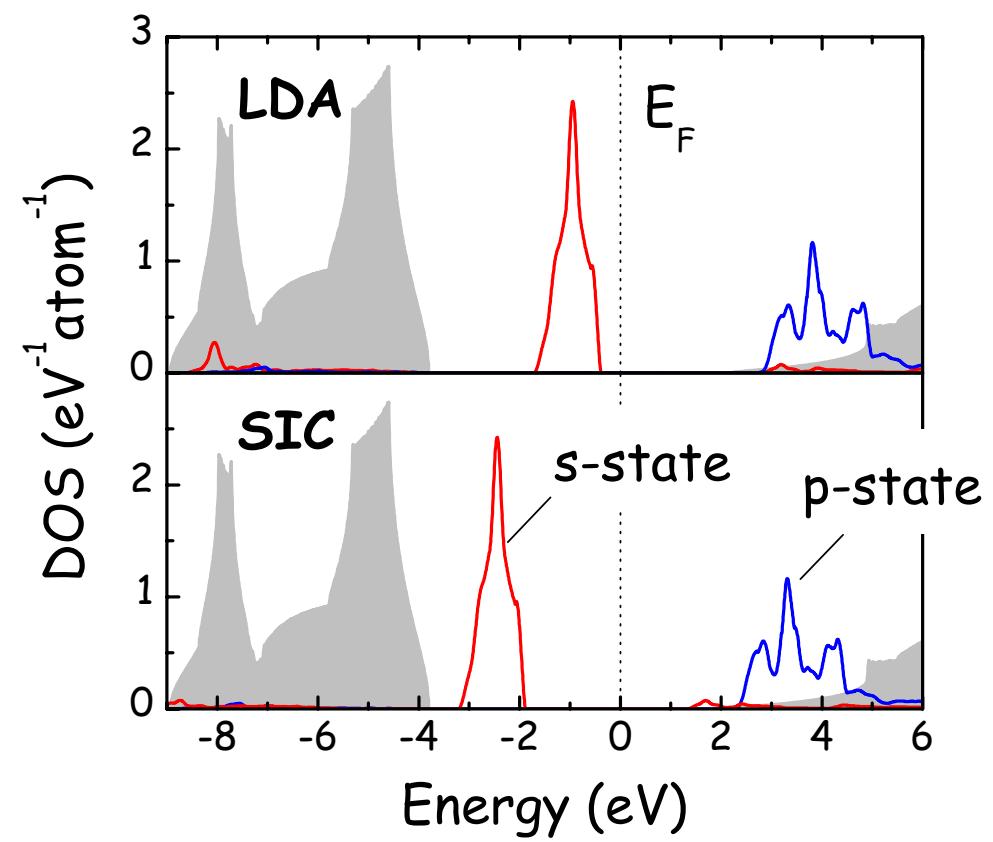


# O vacancies in MgO

Mather et al., PRB 73, 205412 (2006)



Velev et al., APL (2007)

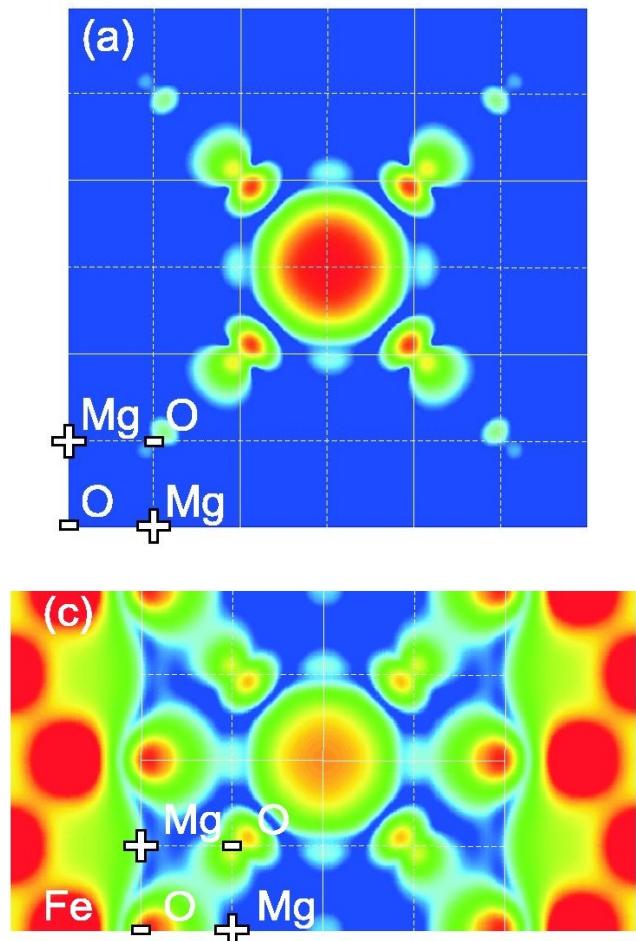


- Agreement between theory and experiment

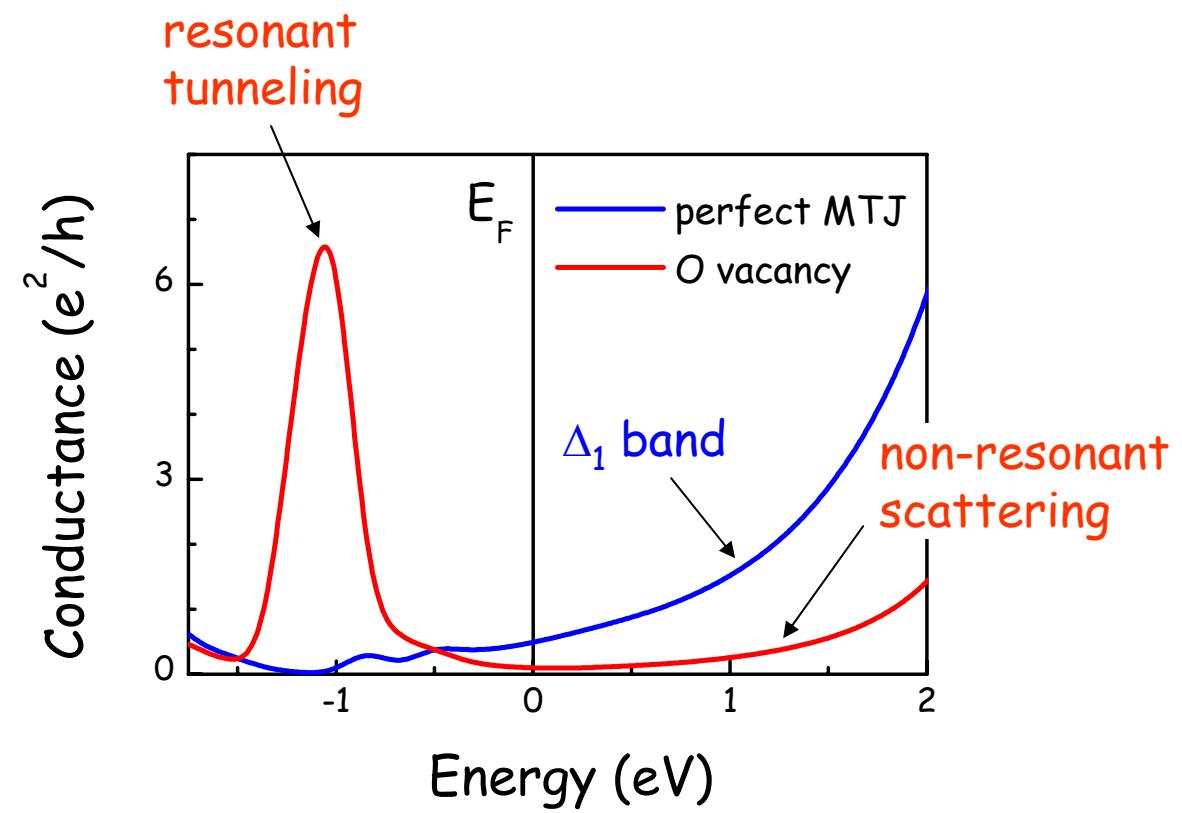


# Effect of O vacancies on transport

Charge density



Velev et al., APL (2007)



- Reduction of TMR due to O vacancies



# Conclusions

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- Tunneling spin polarization in magnetic tunnel junctions is determined by the interface transmission function which depends on electronic properties of ferromagnets, insulator and interfaces
- Symmetry arguments, though important, are not sufficient to make overall conclusions regarding the spin polarization in magnetic tunnel junctions
- Critical role of electronic band structure of interfaces: interface bonding and interface states are important
- Diffusive mechanism of tunneling conduction has to be considered to interpret experimental data quantitatively