First principle electronic structure theory for spintronics

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Intrinsic electronic structure

Intrinsic electronic structure

- Kohn-Sham equation

$$\mathcal{H}\,|\Psi_k\rangle = \left(\mathcal{T} + \mathcal{V}_{eff}\right)|\Psi_k\rangle = E_k\,|\Psi_k\rangle$$

- Green's function

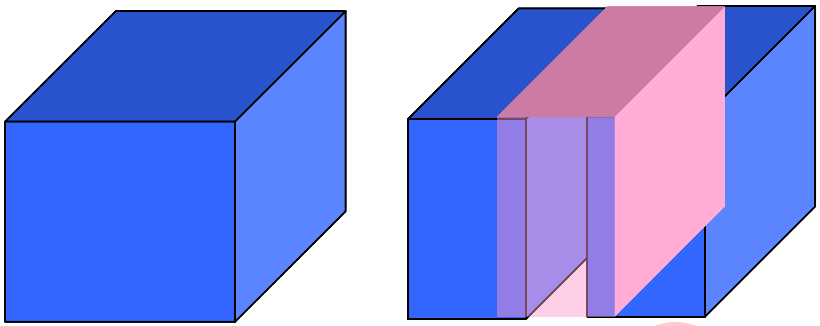
$$\left(E - \mathring{\mathcal{H}}\right)\mathring{\mathcal{G}} = \mathbf{1} \qquad\qquad (E - \mathcal{H})\,\mathcal{G} = \mathbf{1}$$

- Dyson equation

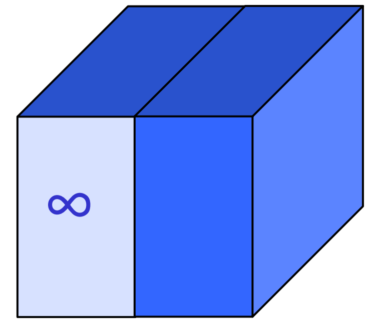
$$\begin{aligned} \mathcal{G} &= \mathring{\mathcal{G}} + \mathring{\mathcal{G}}\,\Delta\mathcal{V}_{eff}\,\mathcal{G} \\ \Delta\mathcal{V}_{eff} &= \mathcal{V}_{eff} - \mathring{\mathcal{V}}_{eff} \end{aligned}$$

Korringa-Kohn-Rostoker, Screened-KKR, LKKR

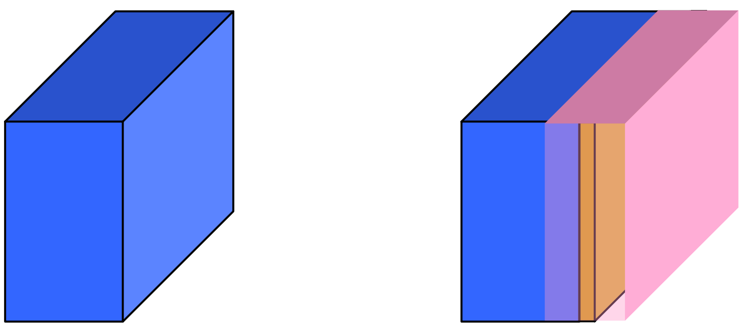
The power of Green functions



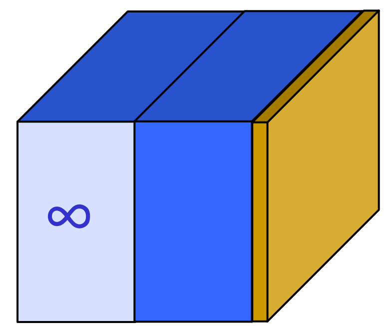
Surface



$$\mathcal{G}_{surf} = \mathcal{G}_{bulk} + \mathcal{G}_{bulk} \Delta V \mathcal{G}_{surf}$$



Adlayer



$$\mathcal{G}_{ad} = \mathcal{G}_{surf} + \mathcal{G}_{surf} \Delta V \mathcal{G}_{ad}$$

N scaling!

Output

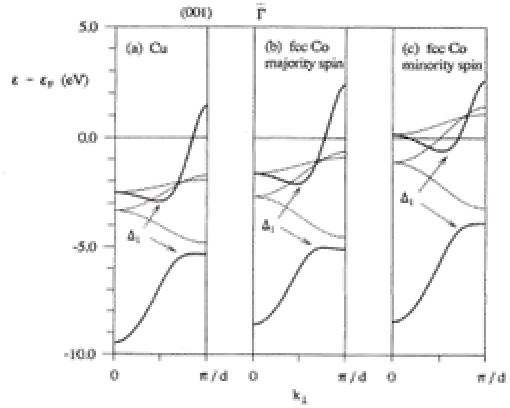
Dispersion relation: E_k^σ

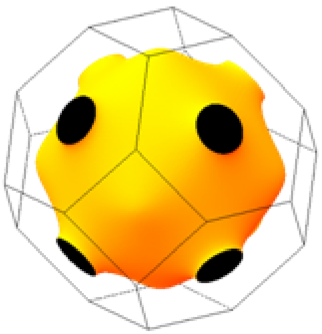
Fermi surface: $E_k^\sigma = E_F$

Group velocity: $\mathbf{v}_k^\sigma = \frac{1}{\hbar}\frac{\partial E_k^\sigma}{\partial k}$

Wave function: $\psi_k^\sigma(\mathbf{r})^o$

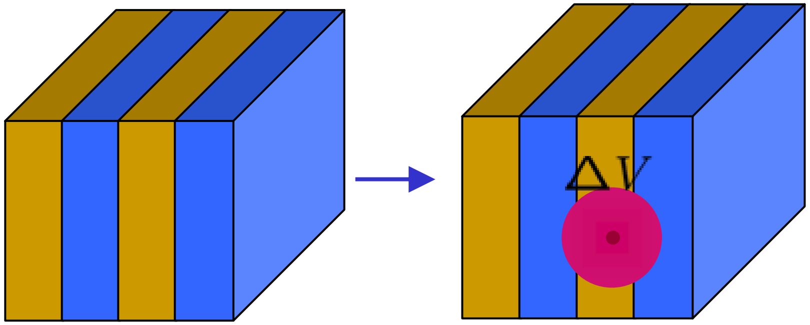
Green function: $G^{\sigma\,o}(\mathbf{r},\mathbf{r}',E)$





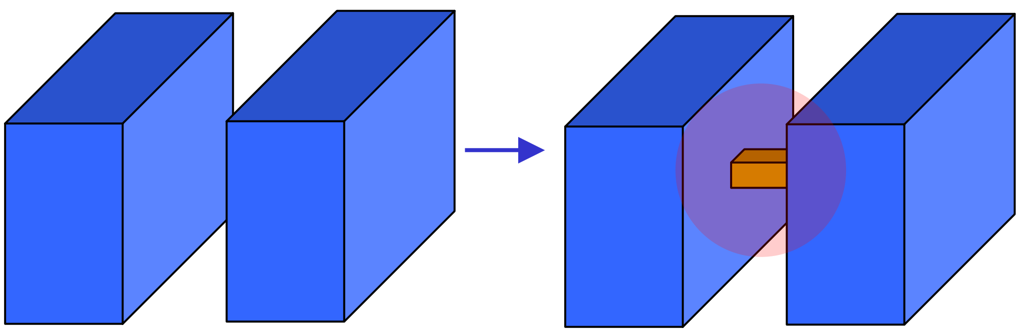
Extrinsic electronic properties

Bulk defects and nanocontacts



Defect in a
Bulk material

$$\mathcal{G}_{def} = \mathcal{G}_{bulk} + \mathcal{G}_{bulk} \Delta V \mathcal{G}_{def}$$



Nanocontact

$$\mathcal{G}_{def} = \mathcal{G}_{bulk} + \mathcal{G}_{bulk} \Delta V \mathcal{G}_{def}$$

Self-consistent potential for the region of interest!

Scattering properties

- T matrix

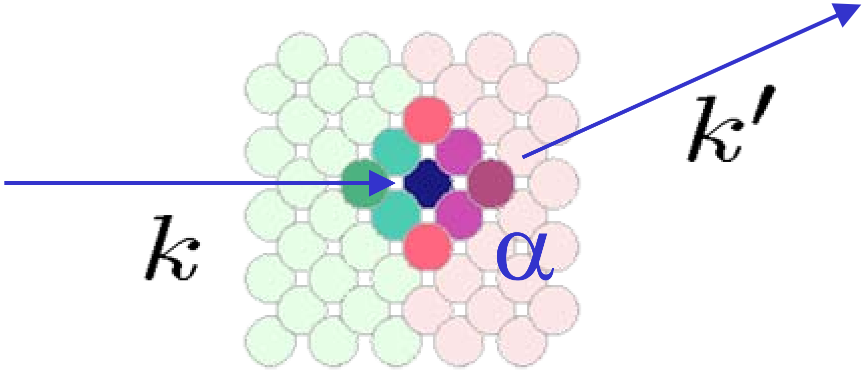
$$T_{kk'}^{\alpha} = \langle \tilde{\psi}_k | \Delta V^{\alpha} | \psi_{k'} \rangle = \langle \tilde{\psi}_k | \mathcal{T}^{\alpha} | \tilde{\psi}_{k'} \rangle$$

- Fermi's golden rule

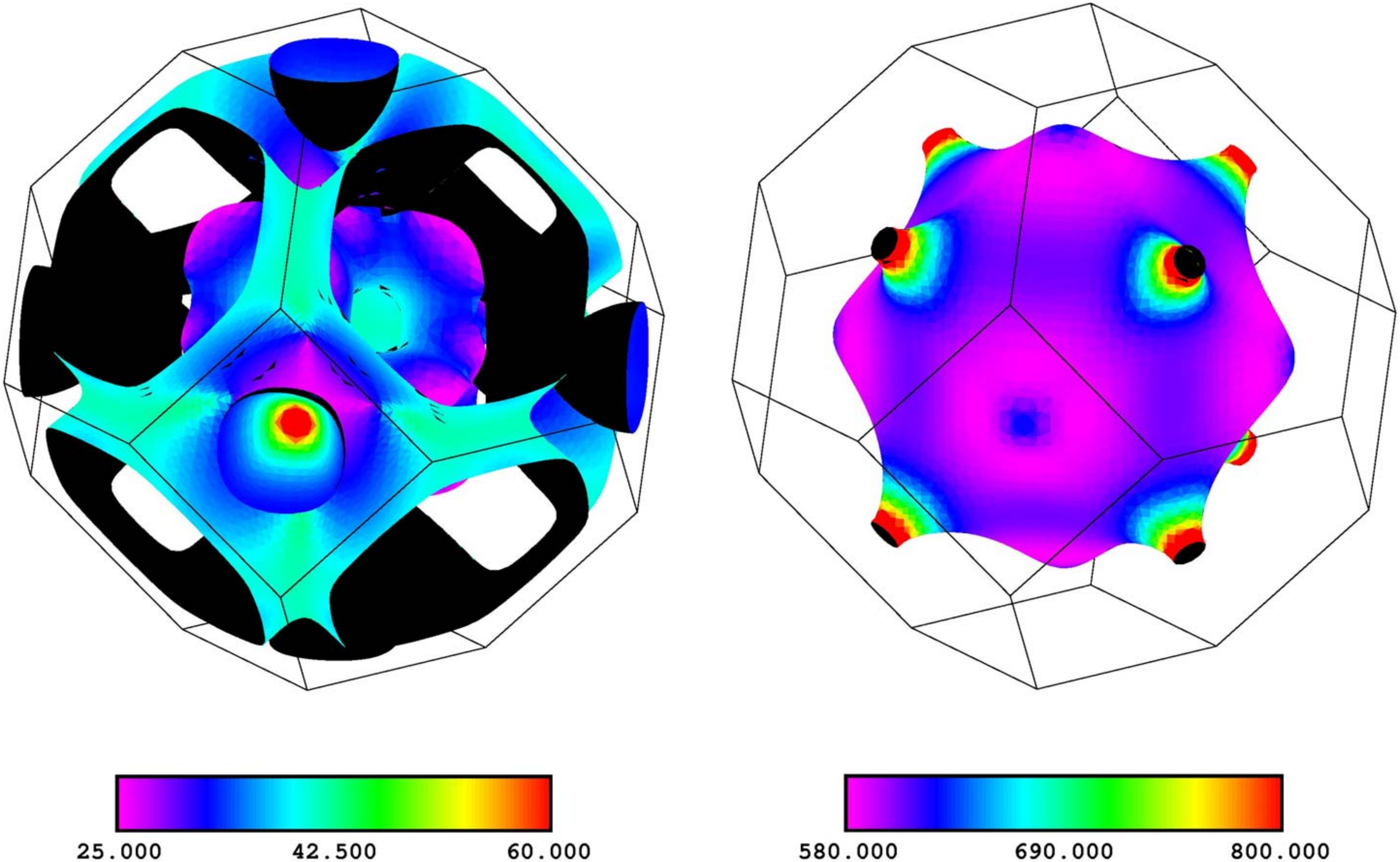
$$P_{kk'} = 2\pi \sum_{\alpha} c_{\alpha} N \left| T_{kk'}^{\alpha} \right|^2 \delta(E_k - E'_k)$$

- Relaxation time

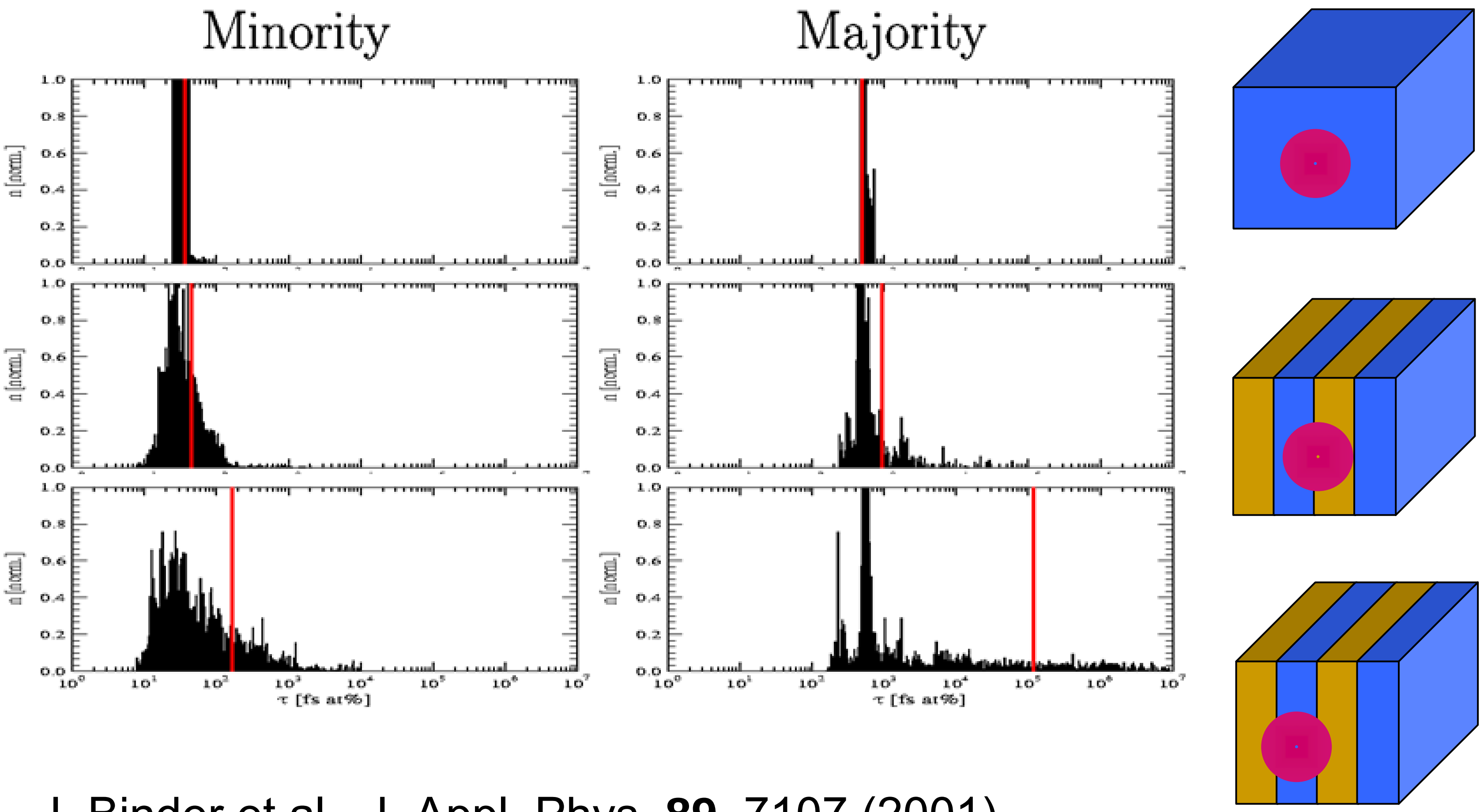
$$\tau_k = \left[\sum_{k'} P_{kk'} \right]^{-1}$$



Spin- and k-dependent relaxation time Co(Cu) [fs/at%]



Relaxation time of a Cu impurity in Co



J. Binder et al., J. Appl. Phys. **89**, 7107 (2001)

Transport properties in linear response

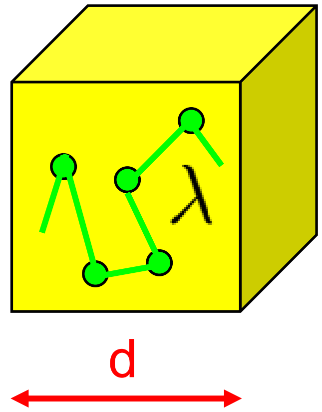
Transport properties

Diffusive limit

Resistance

$R = \rho \; L / A$

Resistivity: ρ



Conductance

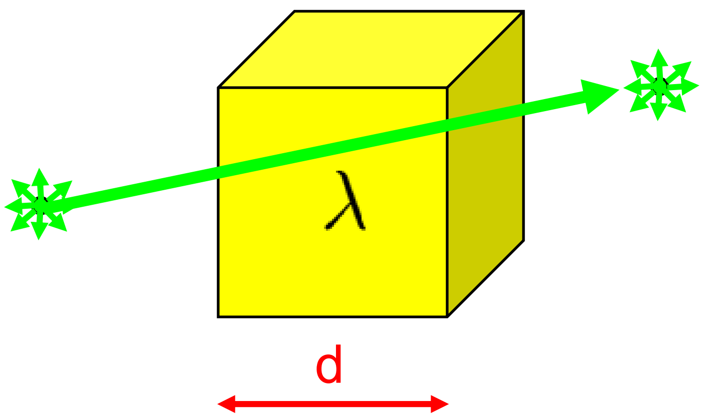
$G = \sigma \; A / L$

Conductivity: σ

Ballistic limit

$R \neq L / A$

$G \neq A / L$



Diffusive transport

- Boltzmann equation

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\frac{\partial f_k}{\partial \mathbf{r}} + \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t}\frac{\partial f_k}{\partial \mathbf{k}} - \left.\frac{\partial f_k}{\partial t}\right|_{scatt} = 0$$

- Scattering term

$$\left.\frac{\partial f_k}{\partial t}\right|_{scatt} = \sum_{k'} P_{kk'}\left(g_{k'} - g_k\right)$$

$$f_k = \mathring{f}_k + g_k$$

$$g_k = -e\frac{\partial \mathring{f}_k}{\partial E}\mathbf{\Lambda}_k\mathbf{E}$$

- Linearized Boltzmann equation

$$\mathbf{v}_k = \sum_{k'} P_{kk'}\mathbf{\Lambda}_k - P_{kk'}\mathbf{\Lambda}_{k'}$$

Diffusive transport

$$\mathbf{v}_k = \sum_{k'} P_{kk'} \mathbf{\Lambda}_k - P_{kk'} \mathbf{\Lambda}_{k'}$$

- Time-reversal symmetry

$$\mathbf{v}_{-k} = -\mathbf{v}_k$$

$$\mathbf{\Lambda}_{-k} = -\mathbf{\Lambda}_k$$

$$\mathbf{v}_k = \sum_{k'} P^S_{kk'} \mathbf{\Lambda}_k - P^A_{kk'} \mathbf{\Lambda}_{k'}$$

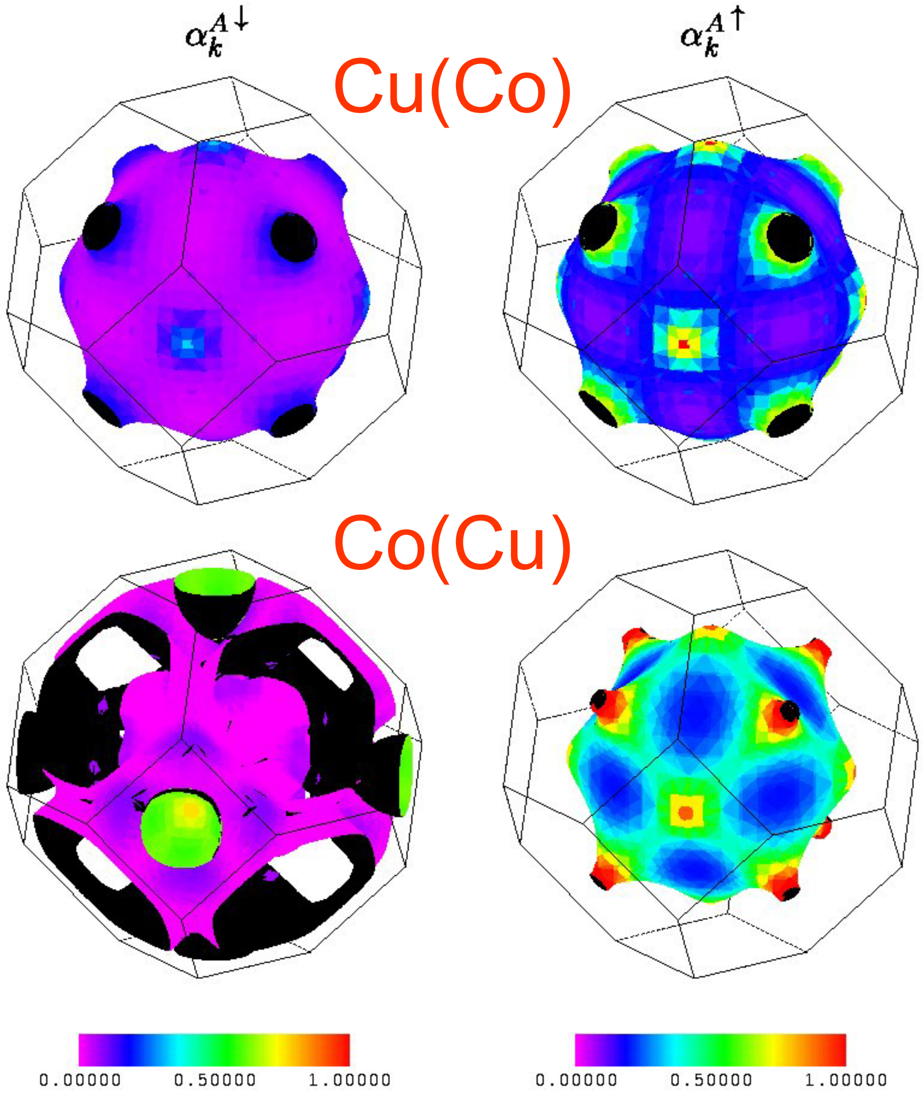
$$P^S_{kk'} = \frac{P_{kk'} + P_{k\,-k'}}{2} \qquad P^A_{kk'} = \frac{P_{kk'} - P_{k\,-k'}}{2}$$

Scattering anisotropy

$$P^S_{kk'} = \frac{P_{kk'} + P_{k\,-k'}}{2}$$

$$P^A_{kk'} = \frac{P_{kk'} - P_{k\,-k'}}{2}$$

$$\alpha^A_k = 2\frac{P^A_{kk}}{P_{kk}}$$

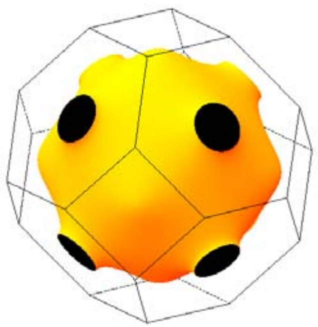


Two current model

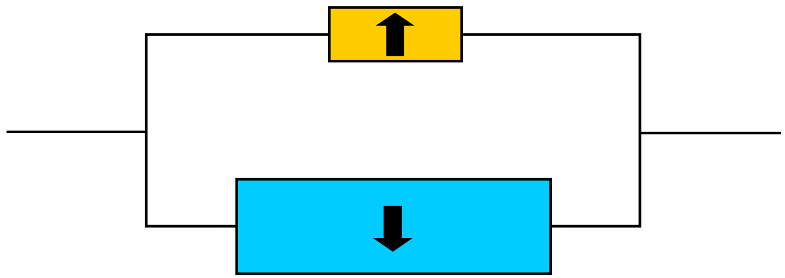
Conductivity tensor:

$$\hat{\sigma} = e^2 \sum_\sigma \sum_k \delta(E_k^\sigma - E_F)\mathbf{\Lambda}_\mathbf{k}^\sigma \cdot \mathbf{v}_\mathbf{k}^\sigma$$

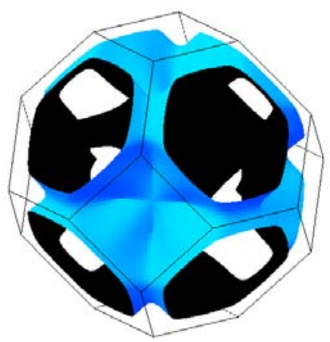
Co Majority Fermi Surface



Two current model:



Co Minority Fermi Surface



Coherent transport

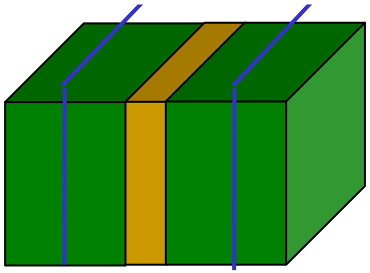
Landauer formula $$g = g_0 \sum_\sigma \int d\mathbf{k}_{\|} T^\sigma(\mathbf{k}_{\|}, E_F)$$

Green's function formulation (Baranger&Stone 1989)

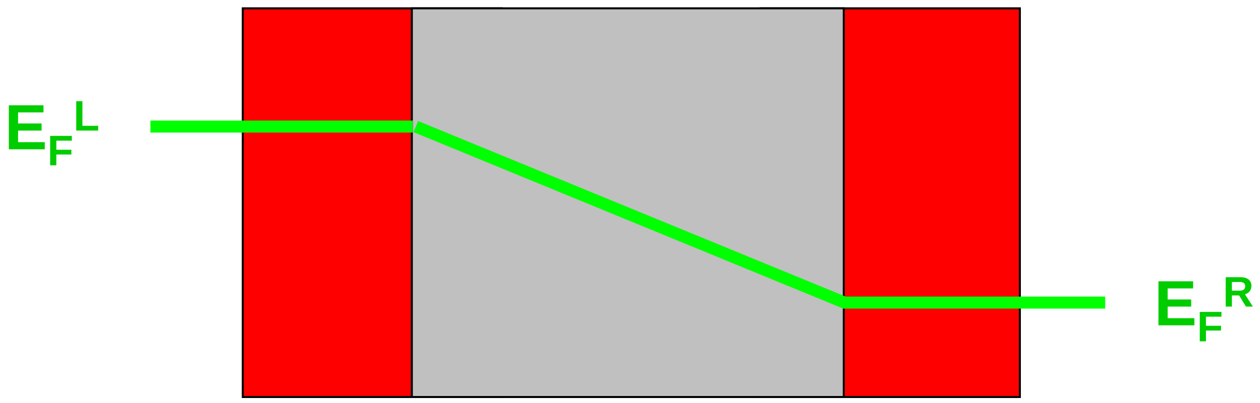
$$g \propto \sum_\sigma \left[\int d\mathbf{k}_{\|} \sum_{n_l n_r} \sum_{LL'L''L'''} J^{n_l}_{L'''L}\, G^{n_l n_r}_{LL'}\, J^{n_r}_{L'L''}\, G^{+\, n_r n_l}_{L''L'''} \right]^\sigma$$

Current matrix

$$J^{n\sigma}_{LL'} = \int_{V_n} d\mathbf{r} \left[R^n_L(\mathbf{r}) \partial_z R^{*\,n}_{L'}(\mathbf{r}) - R^{*\,n}_{L'}(\mathbf{r}) \partial_z R^n_L(\mathbf{r}) \right]^\sigma$$



Bias dependence



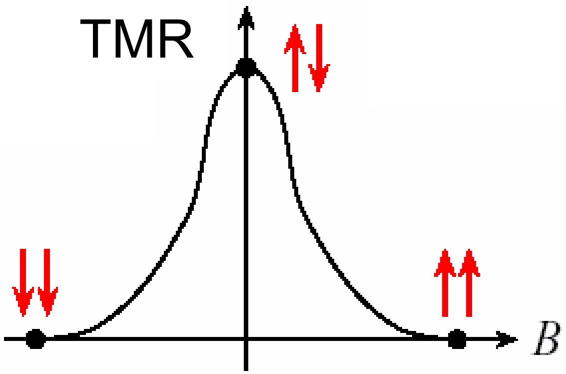
$E_F^L = E_F^R + eV_{Bias}$

$$\bar{T}^{\sigma}(k_{\|}) = \frac{1}{E_F^L - E_F^R} \int_{E_F^R}^{E_F^L} dE\, T^{\sigma}(E, k_{\|})$$

$$T = \sum_{\sigma} \bar{T}^{\sigma}(k_{\|})$$

Tunneling magnetoresistance

Tunneling magnetoresistance

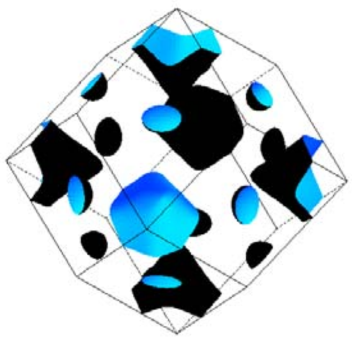


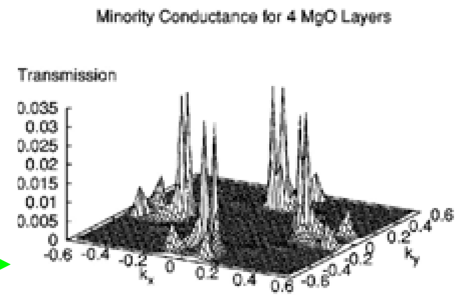
$$\mathrm{TMR} = (G^{P} - G^{AP}) / (G^{P} + G^{AP})$$

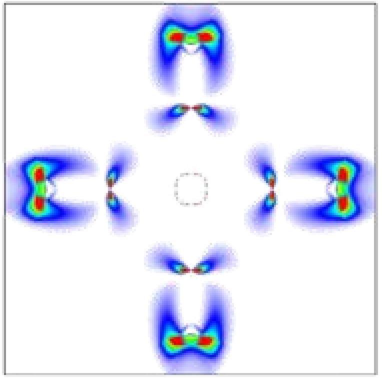
J. S. Moodera et al., Phys. Rev. Lett. **74**, 3273 (1995)

Fe/MgO/Fe

Fe Minority Fermi Surface

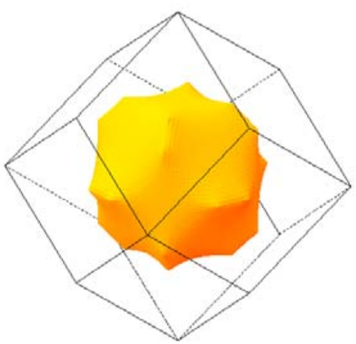


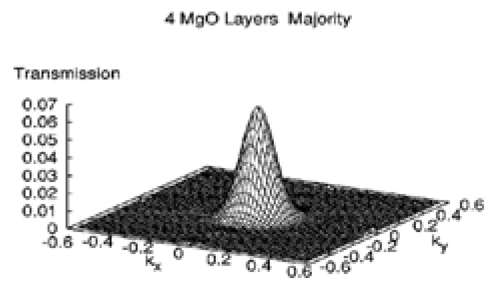


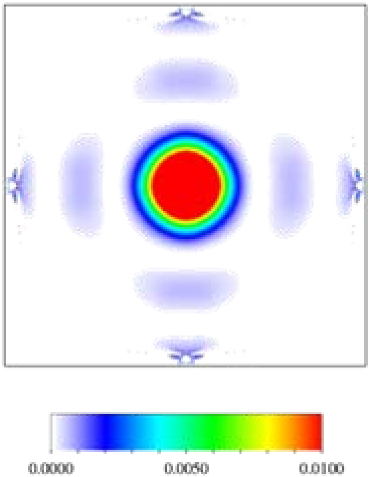


TMR = 1000 %

Fe Majority Fermi Surface



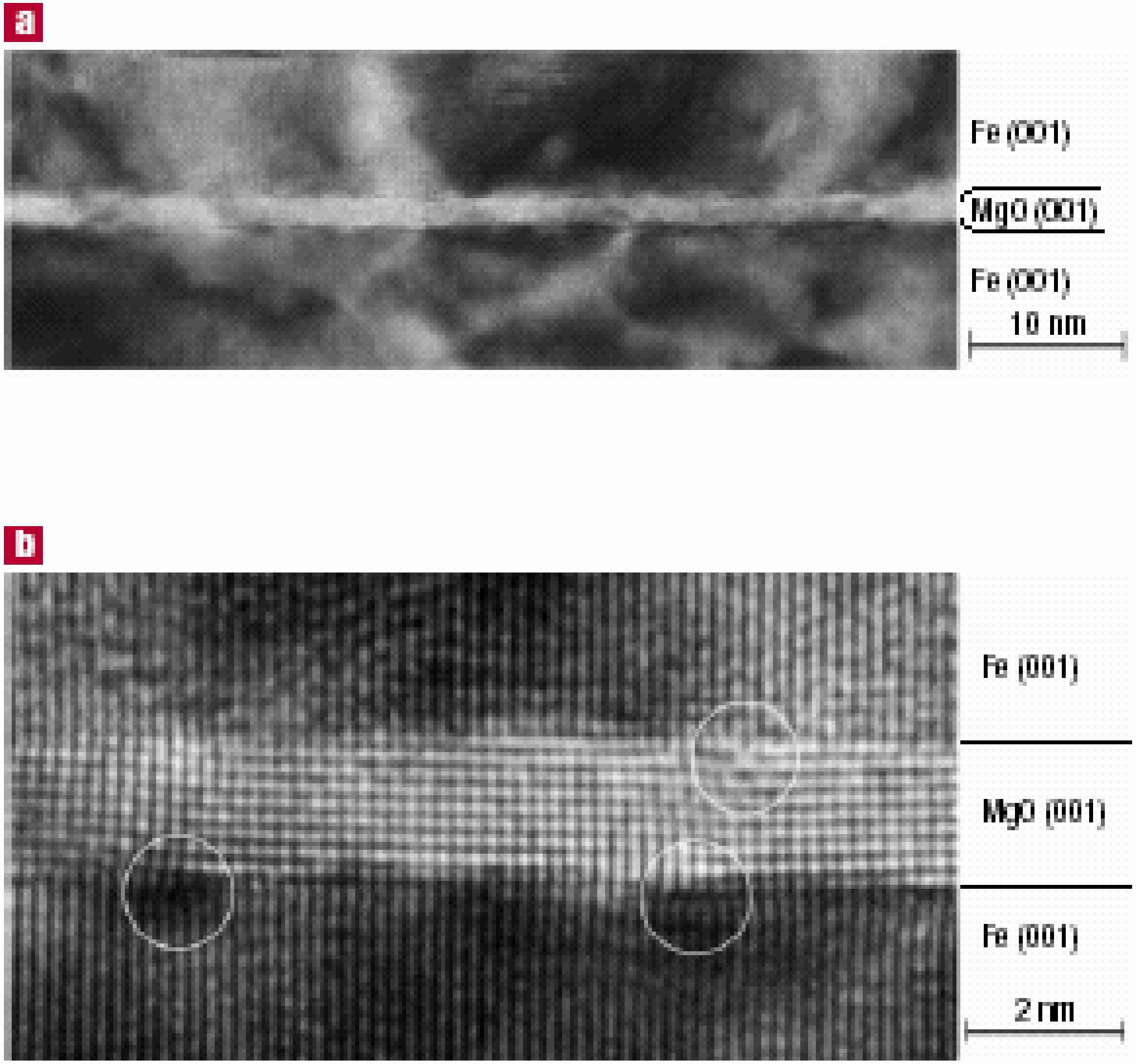




Butler et al. 2001

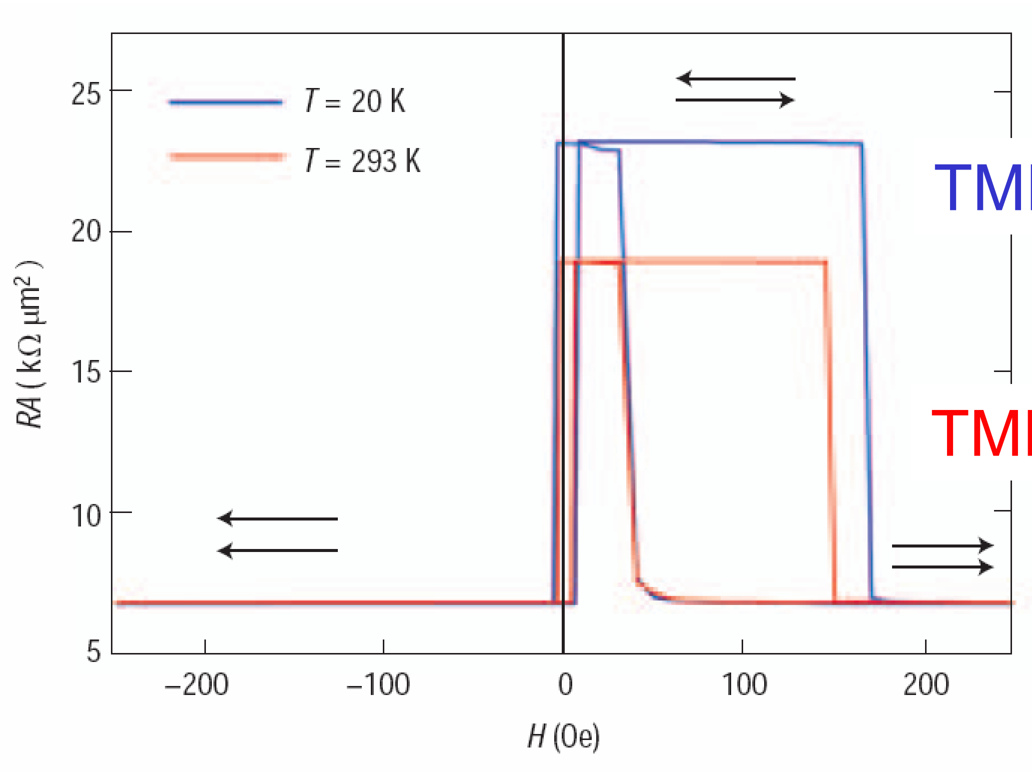
Zahn et al. 2004

Fe/MgO/Fe – sputtered TMR system



S. Yuasa et al. (2004)

Fe/MgO/Fe – experimental results



TMR=247 %

TMR=180 %

S. Yuasa et al. Nature Materials **3**, 868 (2004)

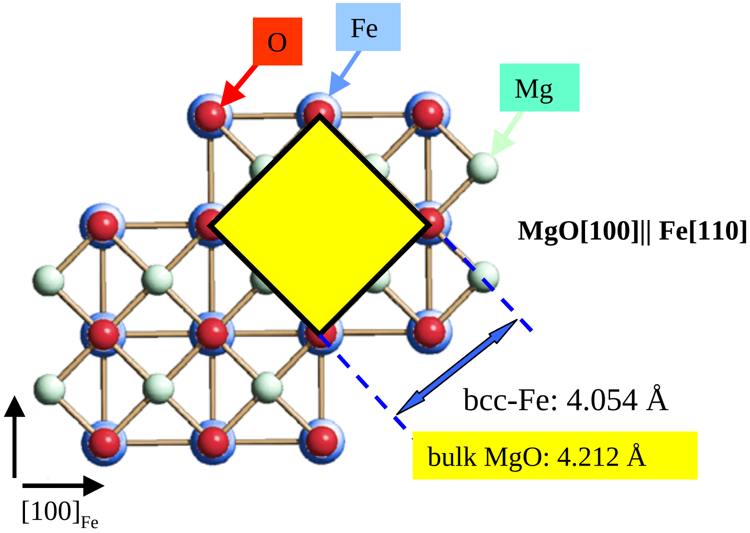
S. Parkin et al. Nature Materials **3**, 862 (2004)

P.G. Mather et al. cond-mat/0603734

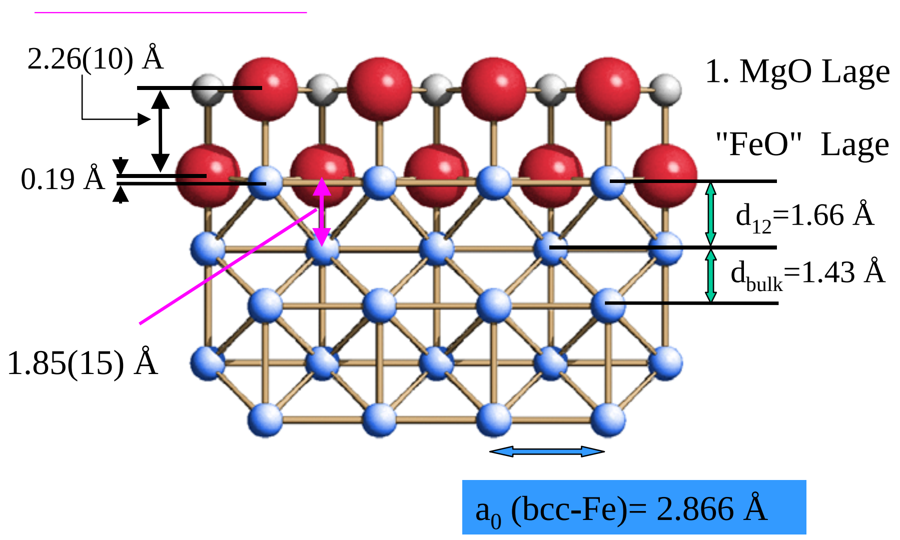
G. D. Fuchs et al. cond-mat/0510786

Fe/MgO – epitaxially grown TMR system

Top view



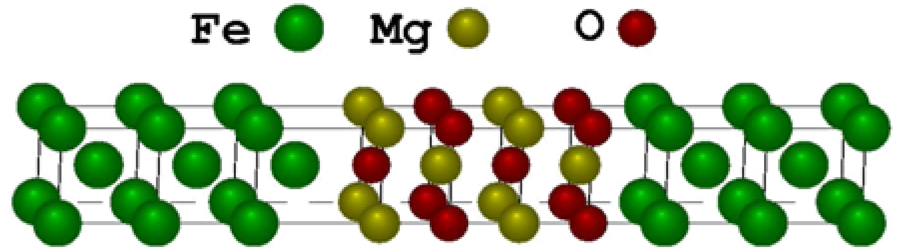
Side view



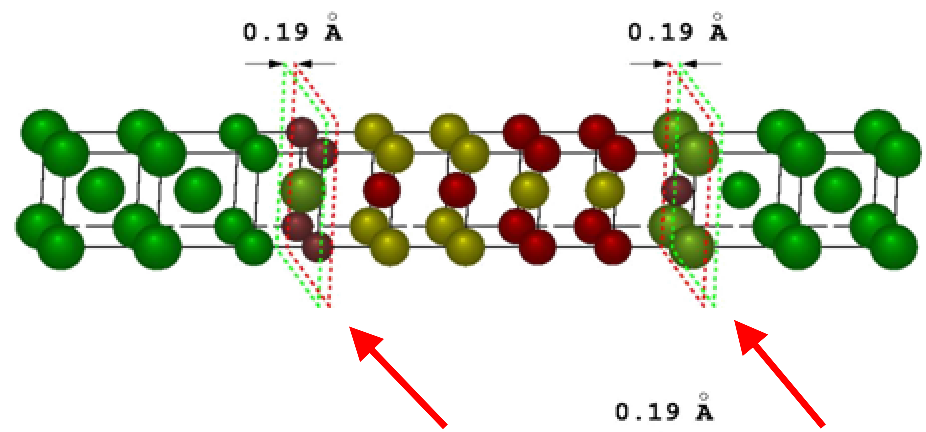
H.L. Meyerheim et al., Phys. Rev. Lett. **80**, 076102 (2001);
H.L. Meyerheim et al., Phys. Rev. B **65**, 144433 (2002)
C. Tusche et al., Phys. Rev. Lett. **95**, 176101 (2005)

Influence of interface structure

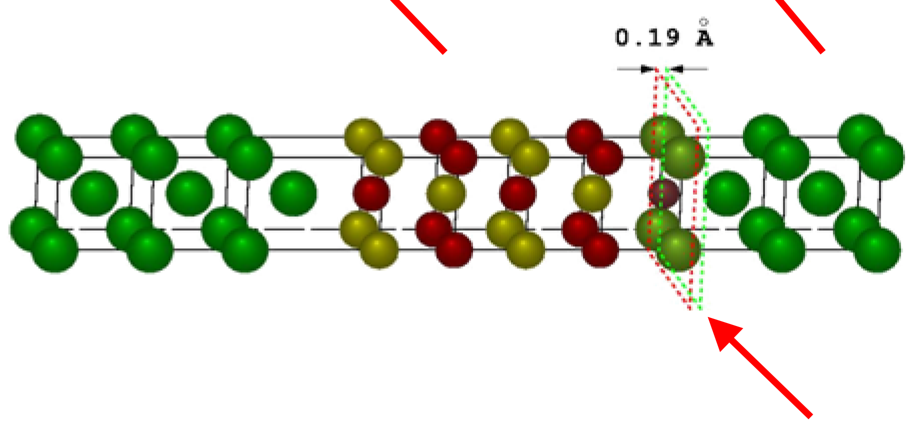
Ideal Interfaces:



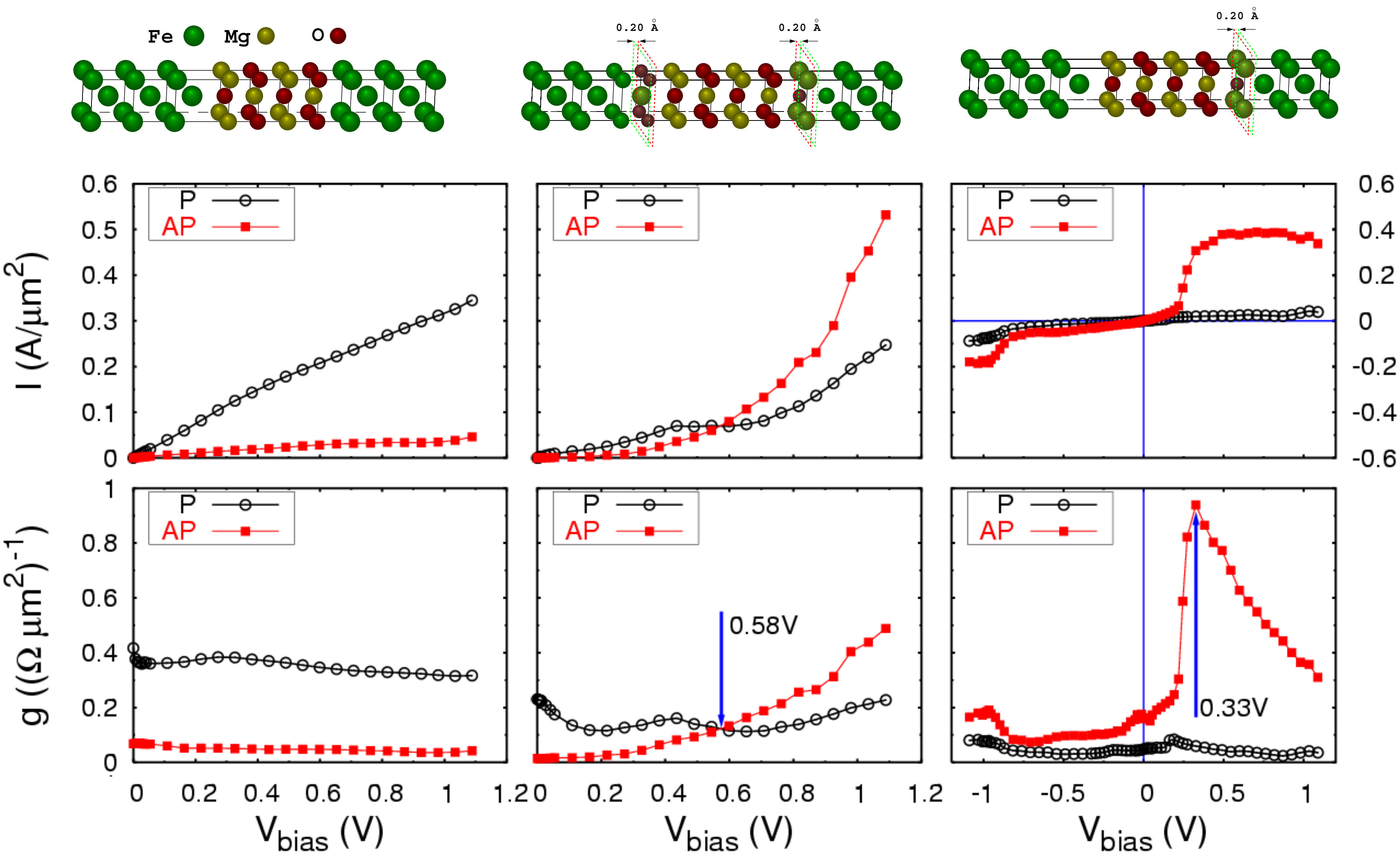
Two FeO interfaces:
symmetric



Single FeO interface:
asymmetric

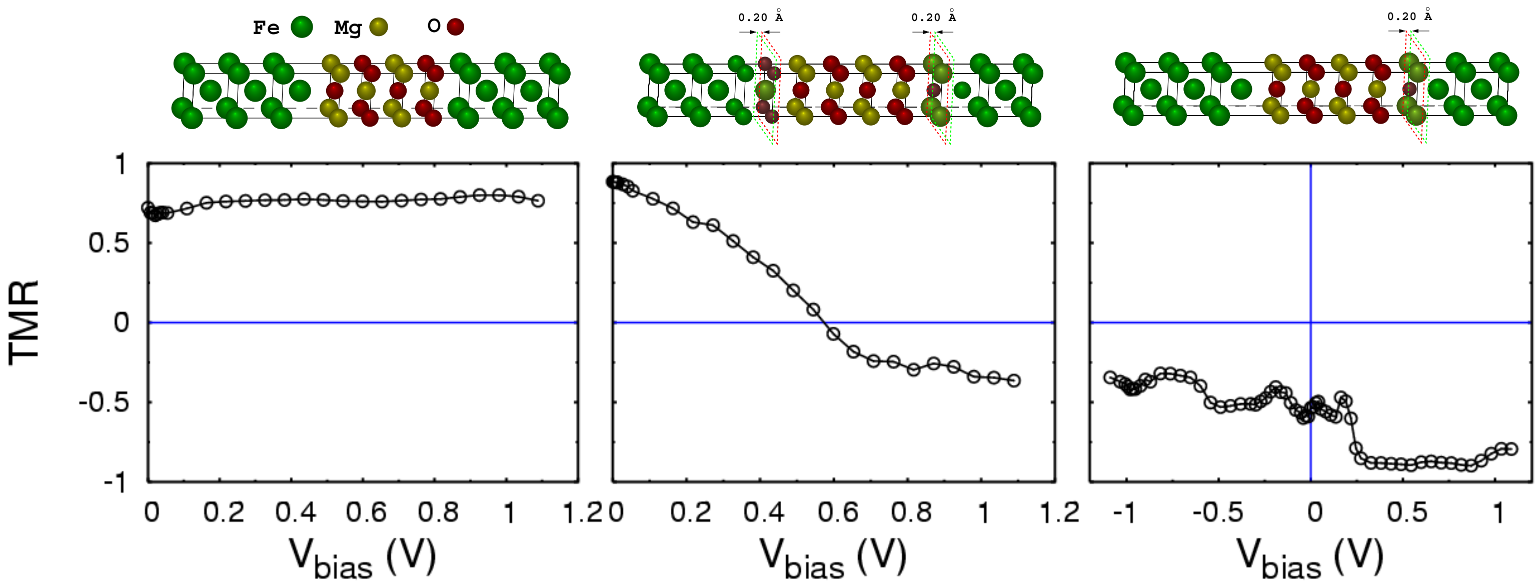


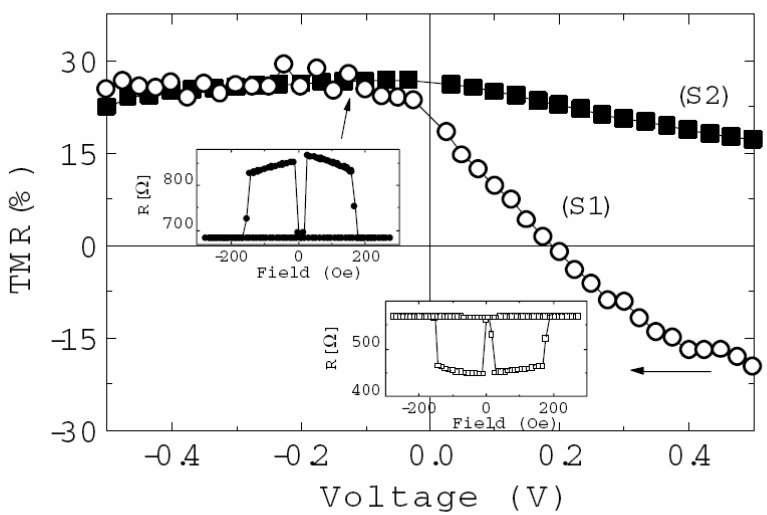
Bias dependence – theoretical results



C.Heiliger et al., PRB **72**, 180406 (2005)

Comparison with experiment



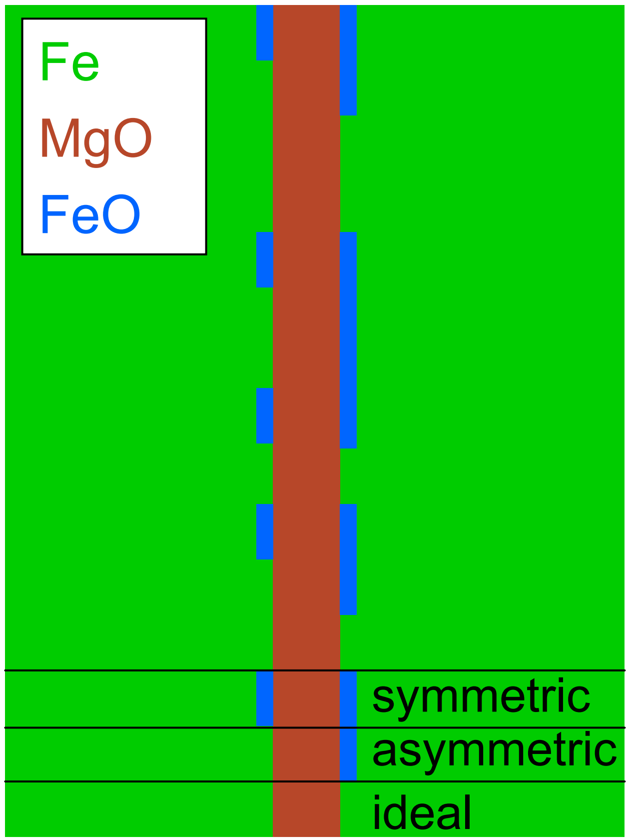


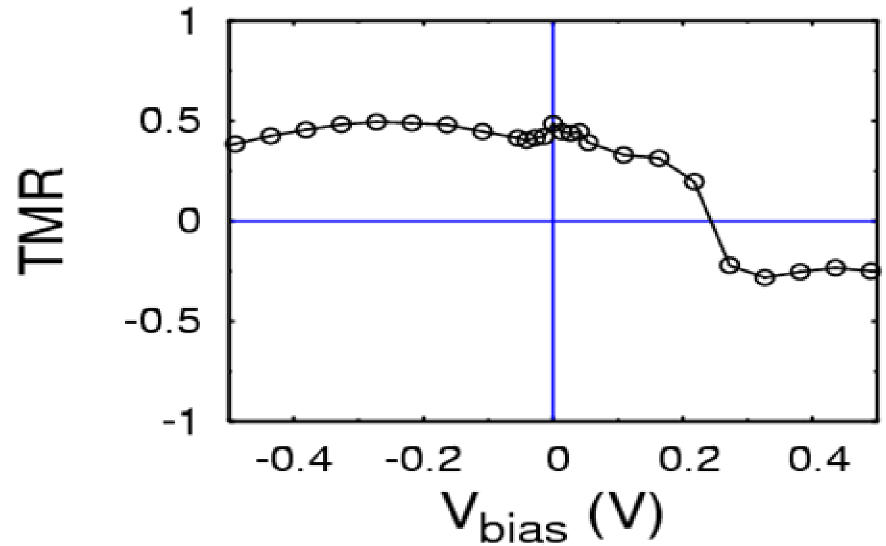
C.Heiliger et al., PRB **72**, 180406 (2005)

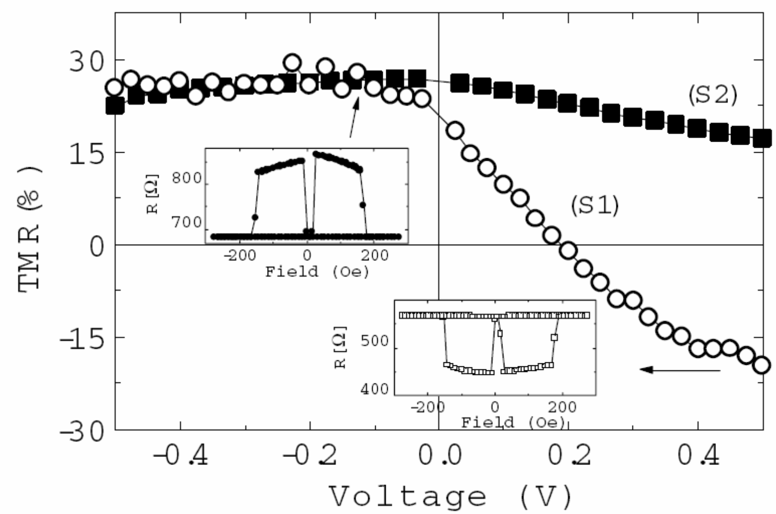
Tiusan et al. PRL 93, 106602 (2004)

Comparison with experiment

local variation
of interface structure







C.Heiliger et al., PRB **72**, 180406 (2005)

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