From quantum mechanics to spintronics

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Outline

- Ab initio calculations
- Tunneling magnetoresistance on the sub-nanometer scale
- Multiferroic interfaces and magnetoelectric coupling
- Magnetic molecules
- Summary

Ab initio calculations

Green function method

- 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

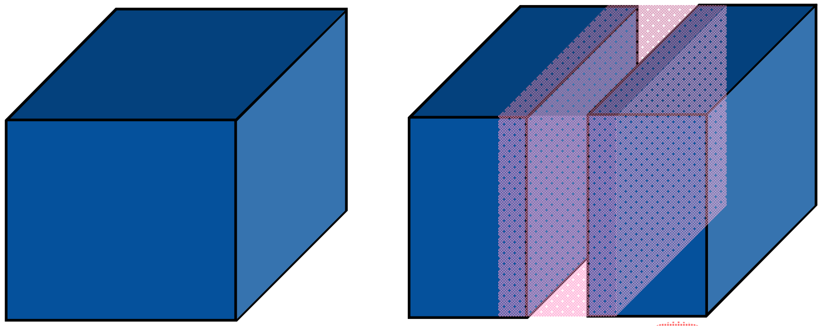
$$\left(E - \bar{\mathcal{H}}\right)\bar{\mathcal{G}} = 1 \qquad\qquad (E - \mathcal{H})\,\mathcal{G} = 1$$

- Dyson equation

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

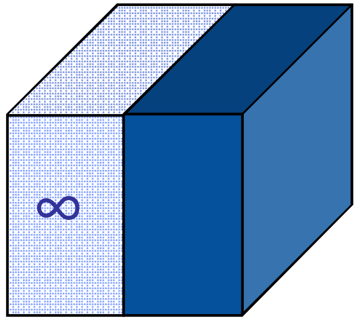
N scaling!

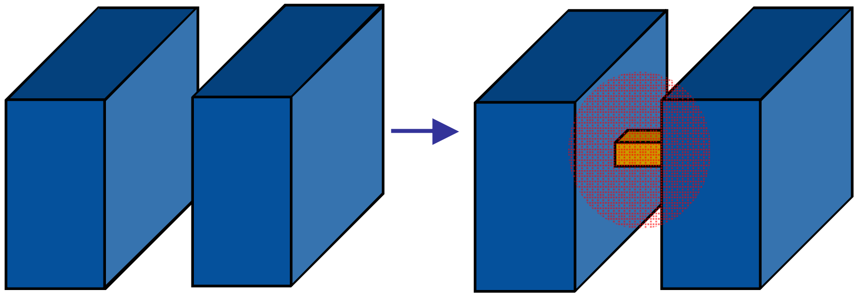
The power of Green functions



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

Surface





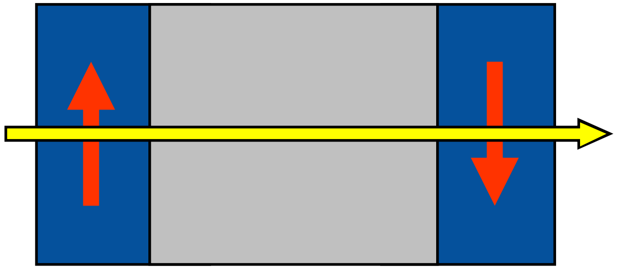
Nanocontact

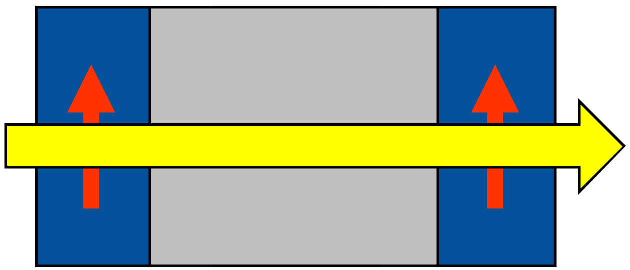
$$\mathcal{G}_{imp} = \mathcal{G}_{surf} + \mathcal{G}_{surf} \Delta V \mathcal{G}_{imp}$$

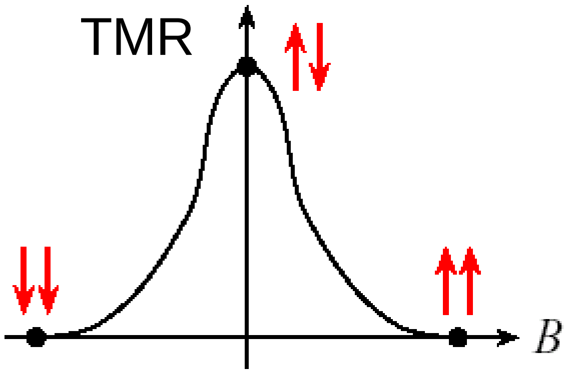
Tunneling magnetoresistance


Martin Gradhand
Peter Zahn
Christian Heiliger

Tunneling magnetoresistance



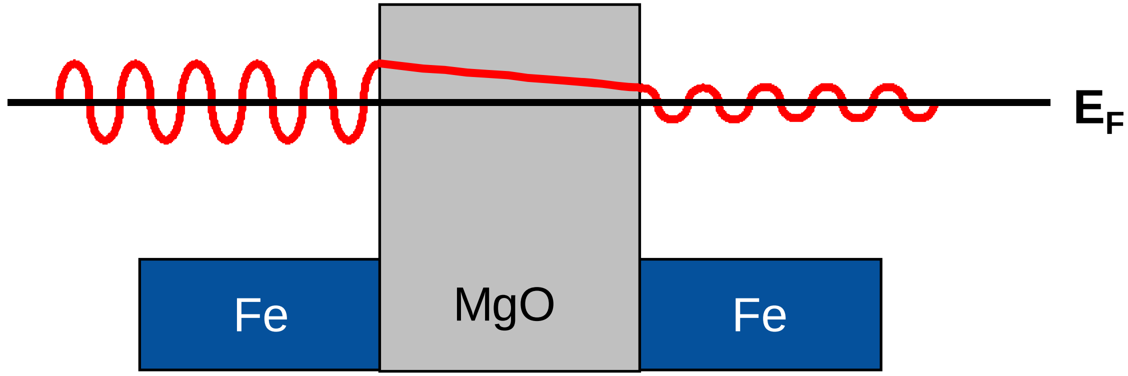




$$TMR = (g^{P} - g^{AP}) / (g^{P} + g^{AP})$$

M. Julliere, Phys. Lett. **54A**, 225 (1975)
J. S. Moodera et al., Phys. Rev. Lett. **74**, 3273 (1995)

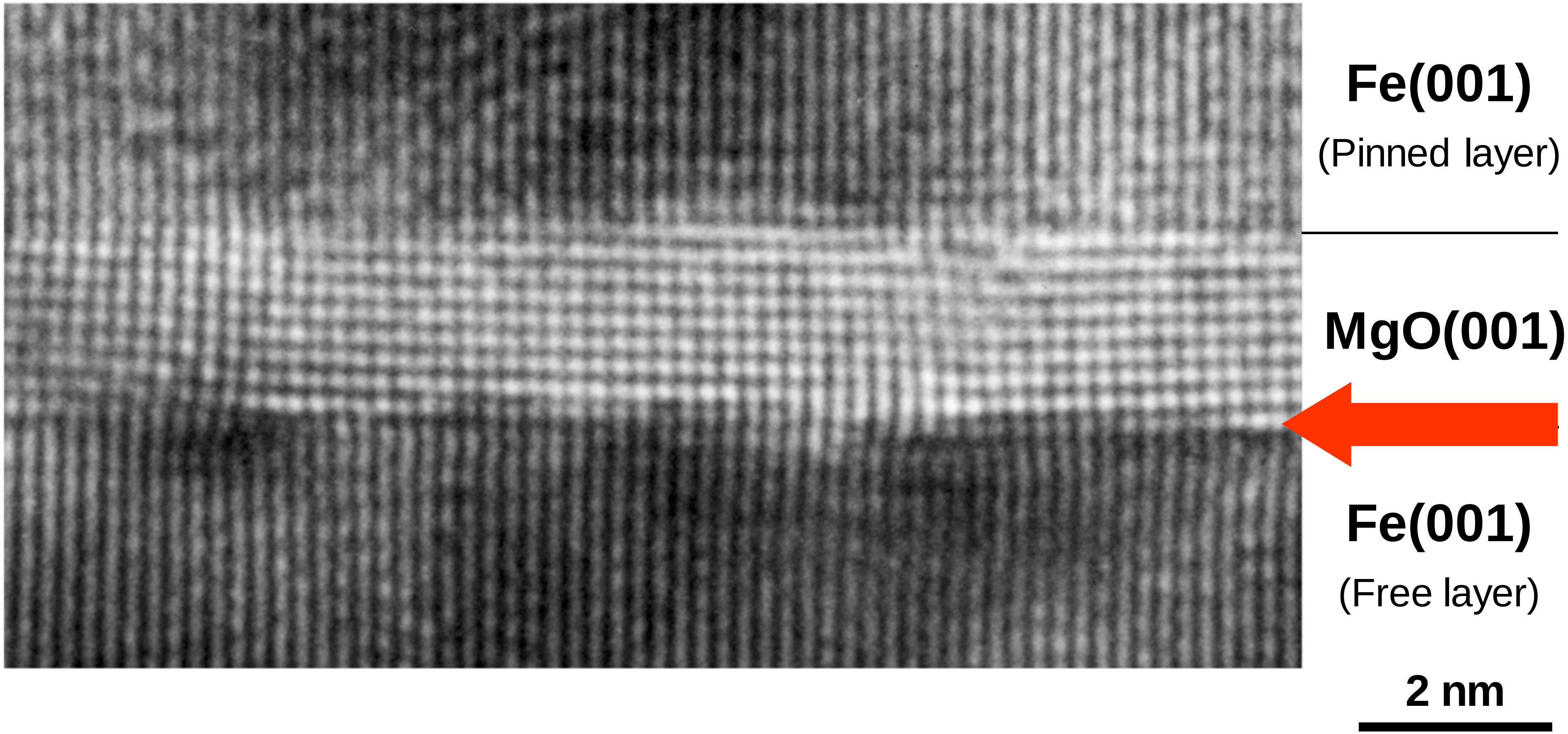
Ab initio calculation – coherent limit



TMR > 1000 %

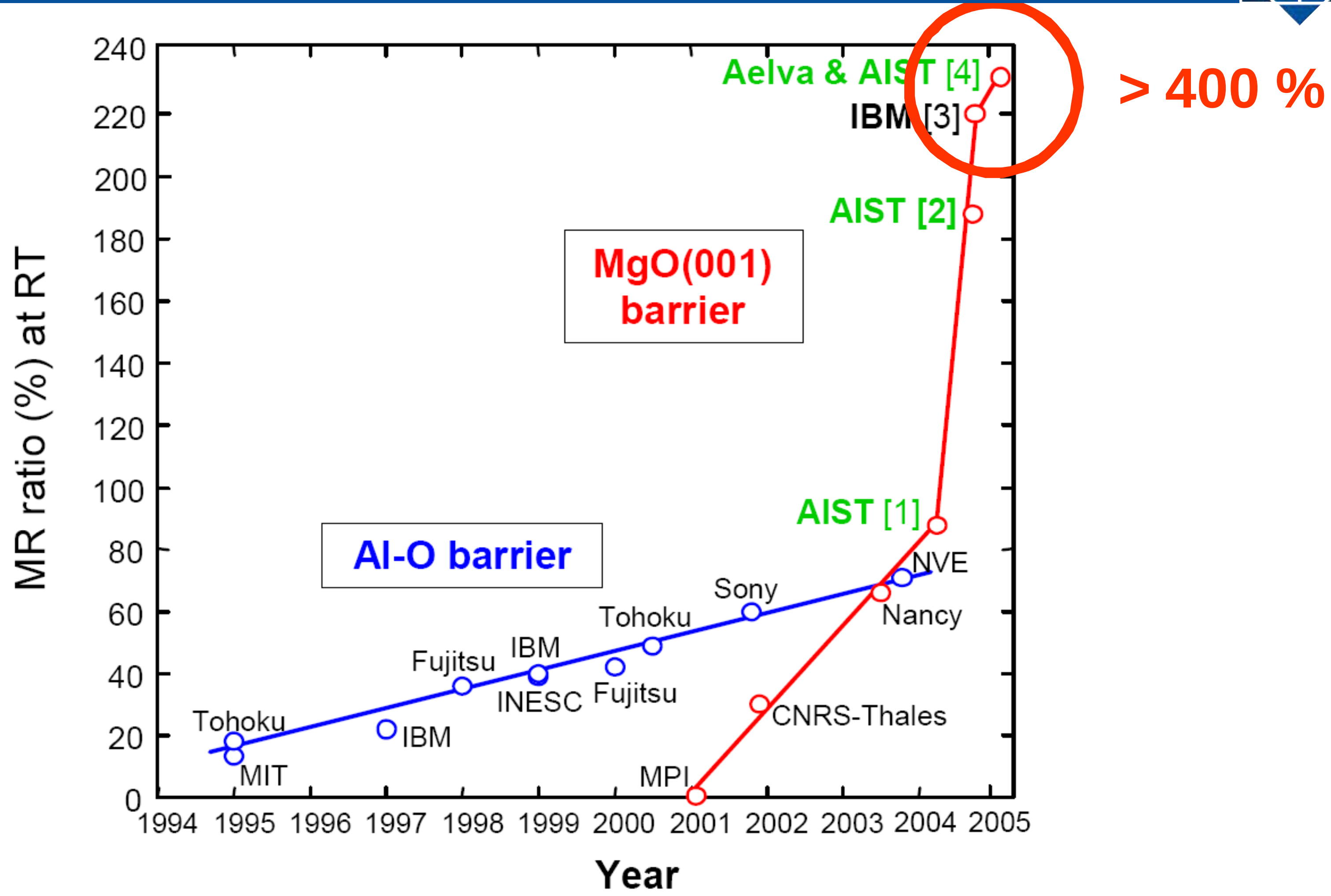
W. H. Butler et al., Phys. Rev. B **63**, 054416 (2001)
G. Mathon et al., Phys. Rev. B **63**, 220403(R) (2001)
C. Heiliger et al., Phys. Rev. B **72**, 180406(R) (2005)

High quality MgO barriers



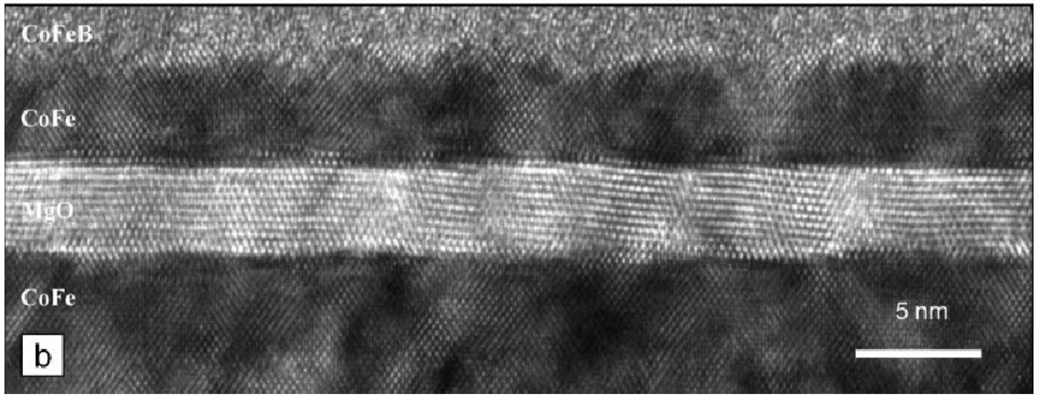
S. Yuasa et al., Nature Materials **3**, 868 (2004)

Development of the TMR effect



[1] Yuasa: *Jpn. J. Appl. Phys*. **43**, L558 (2004).
[2] Yuasa: *Nature Materials* **3**, 868 (2004).
[3] Parkin: *Nature Materials* **3**, 862 (2004).
[4] Djayaprawira: *Appl. Phys. Lett*. **86**, 092502 (2005).

Role of the electrodes



S. Parkin, MRS Bulletin **31,** 389 (2006)

amorphous CoFeB

MgO

TMR ratio

as depoited: 60%

after annealing: 350%

Fe_{bcc}

. . .

. . .

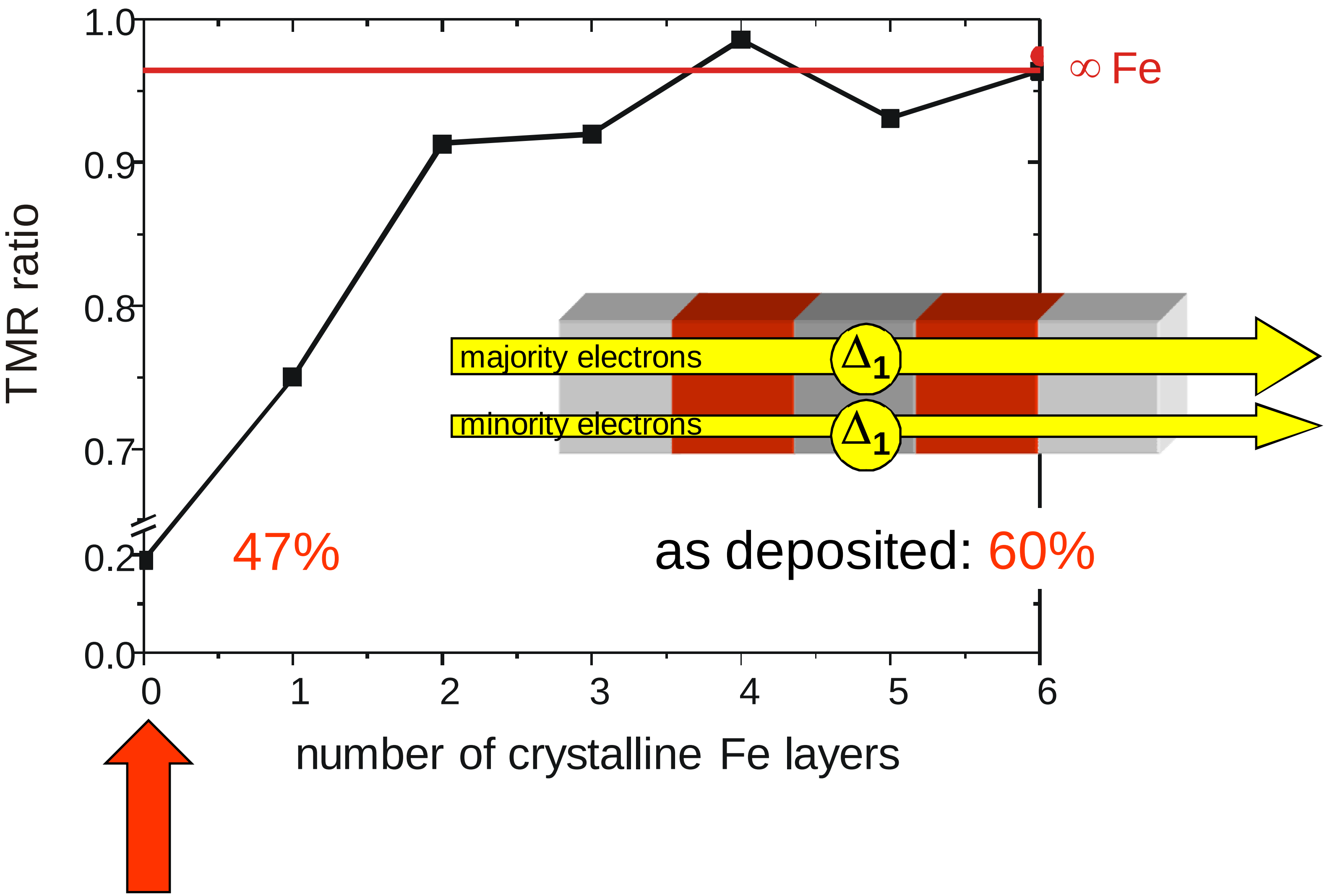
free electron-like
reservoir
Cu-bcc

MgO

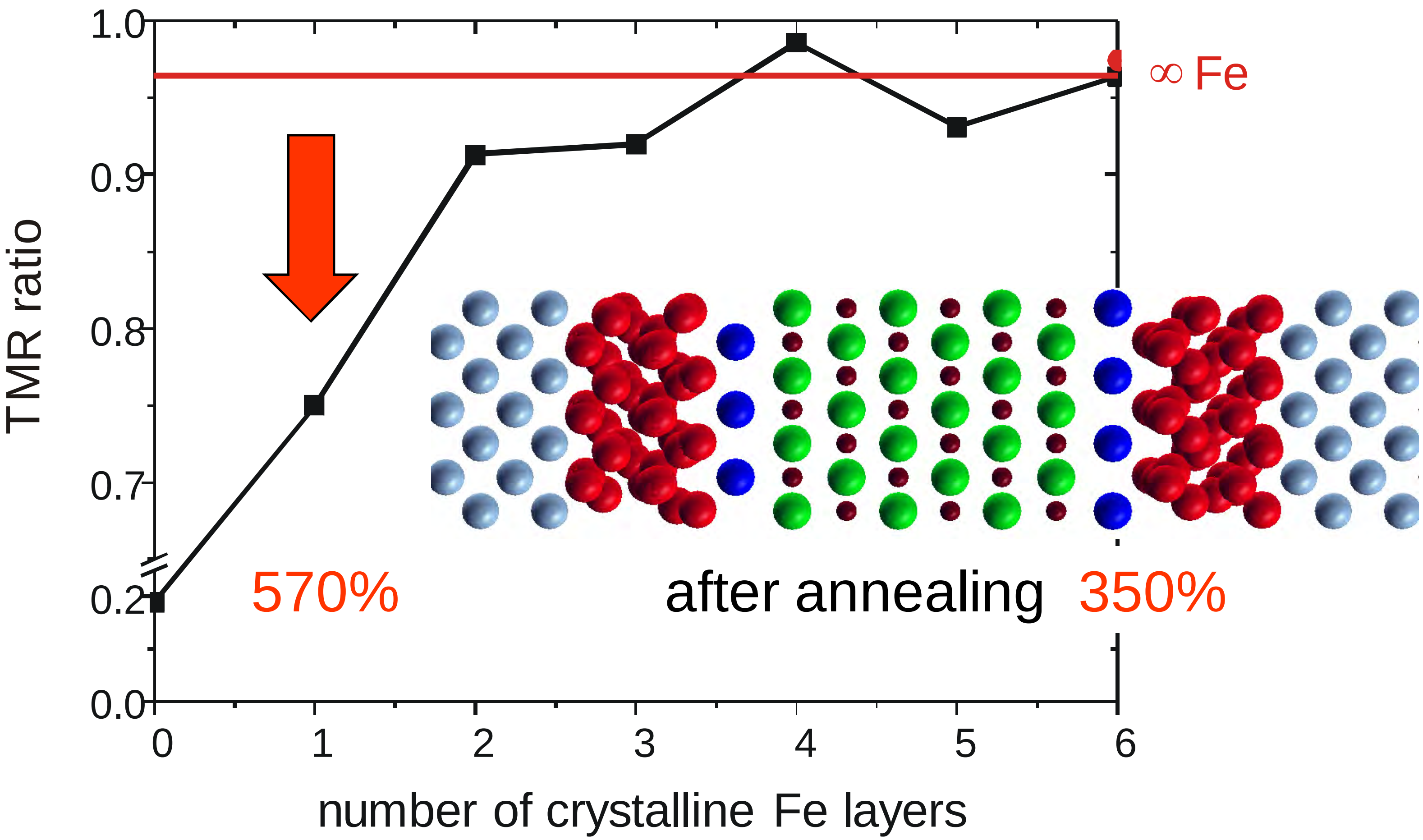
amorphous Fe electrodes

free electron like
reservoir
Cu-bcc

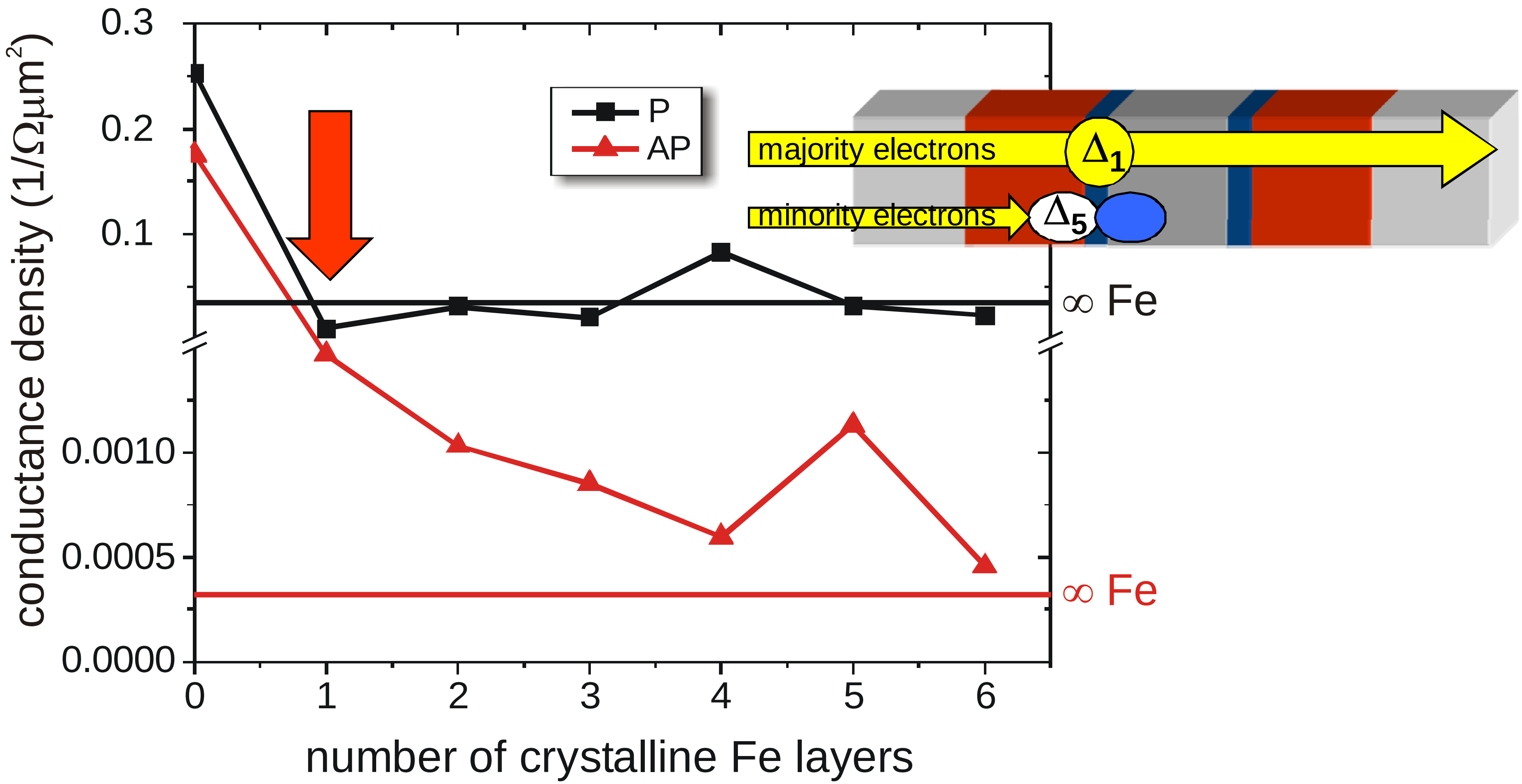
TMR for amorphous Fe electrodes



TMR – 1ML of Fe and amorphous Fe electrodes

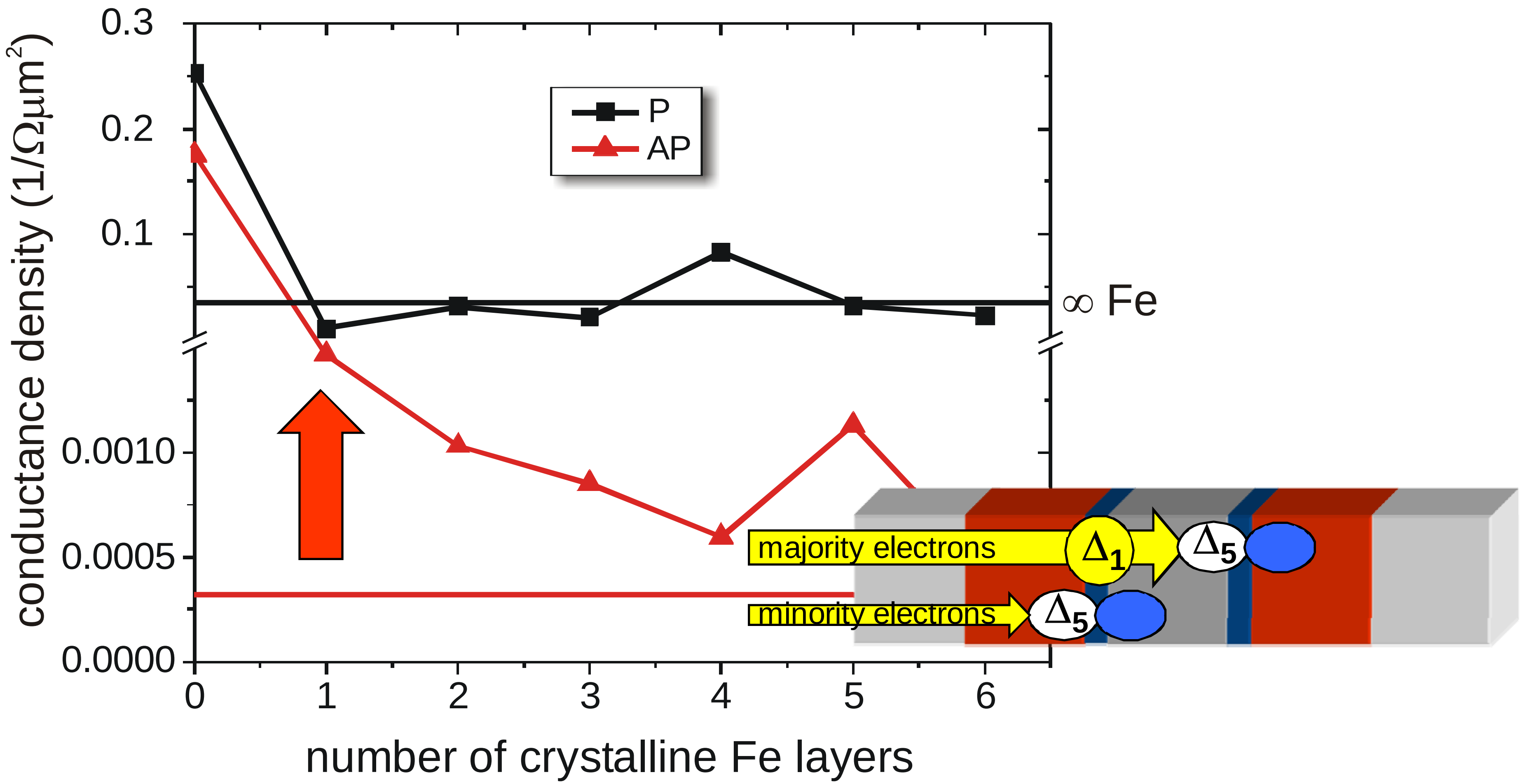


Conductance for P and AP configuration



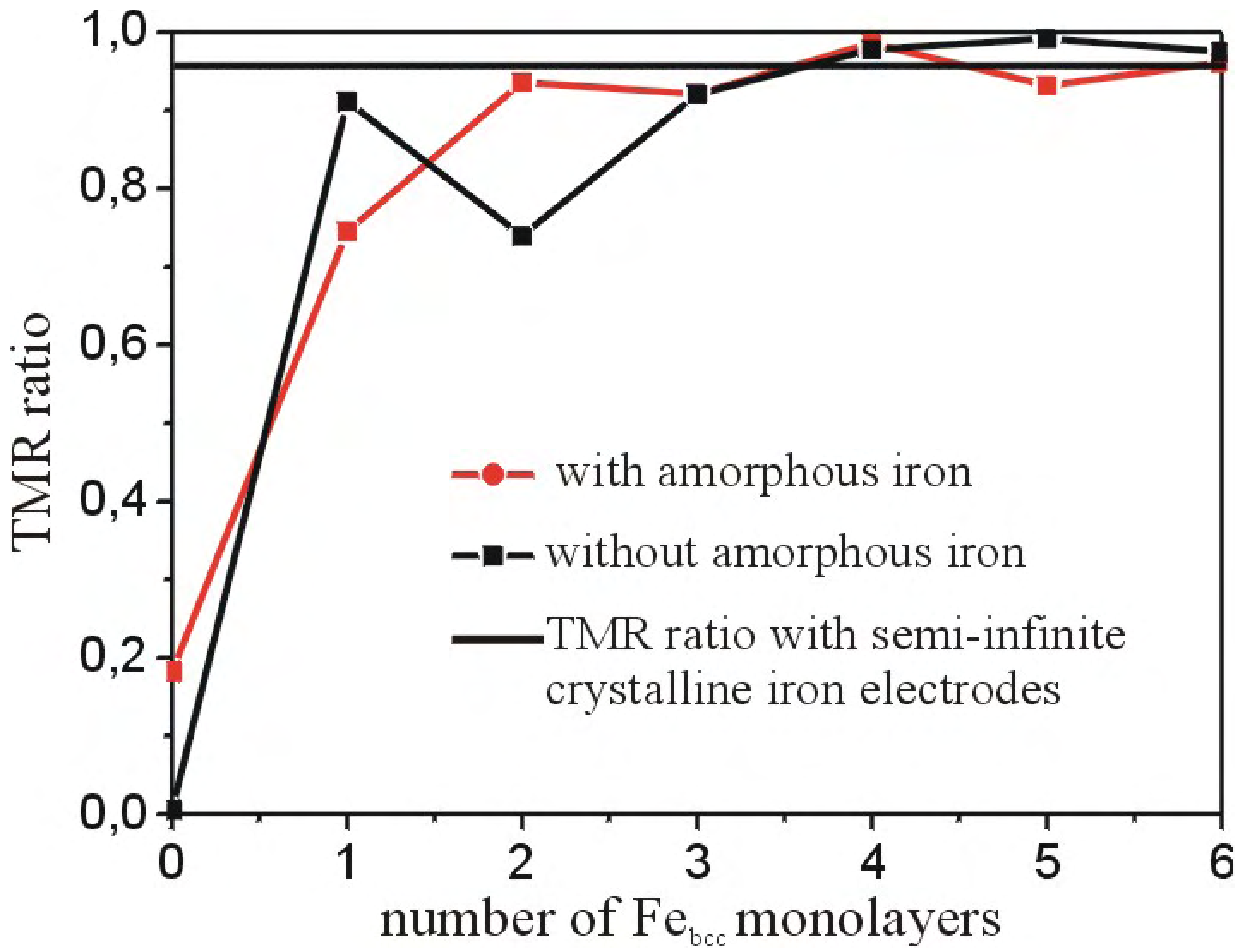
C. Heiliger et al., Phys. Rev. Lett. **99,** 066804 (2007)
M. Gradhand et al., Phys. Rev. B **77**, 134403 (2008)

Conductance for P and AP configuration



C. Heiliger et al., Phys. Rev. Lett. **99,** 066804 (2007)
M. Gradhand et al., Phys. Rev. B **77**, 134403 (2008)

Amorphous versus free electron like electrodes

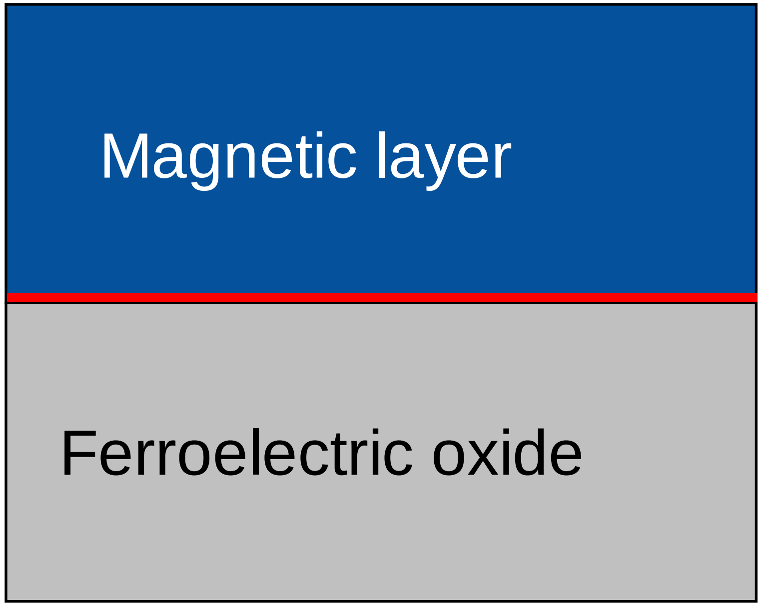


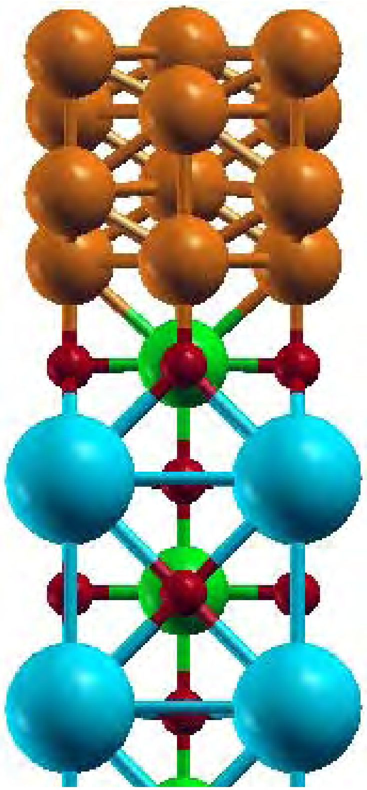
C. Heiliger et al., Phys. Rev. Lett. **99,** 066804 (2007)
M. Gradhand et al., Phys. Rev. B **77**, 134403 (2008)

Multiferroic interfaces


Igor Maznichenko
Sergey Ostanin
Michael Fechner
Arthur Ernst

Multiferroic interfaces





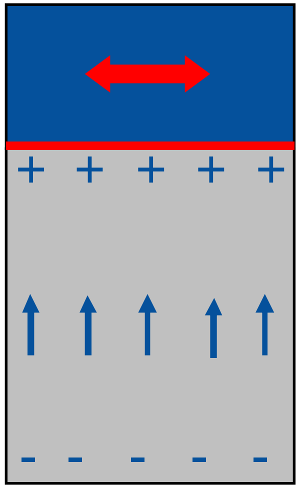
$BaTiO_3$

Magnetoelectric coupling

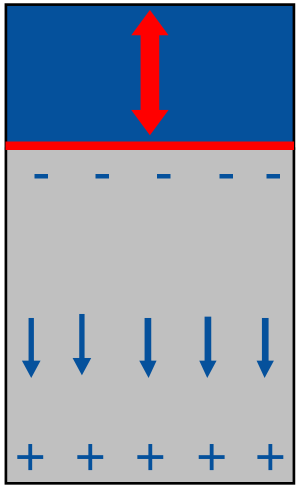
Magnetisation

External magnetic field

M



B



M

P

E

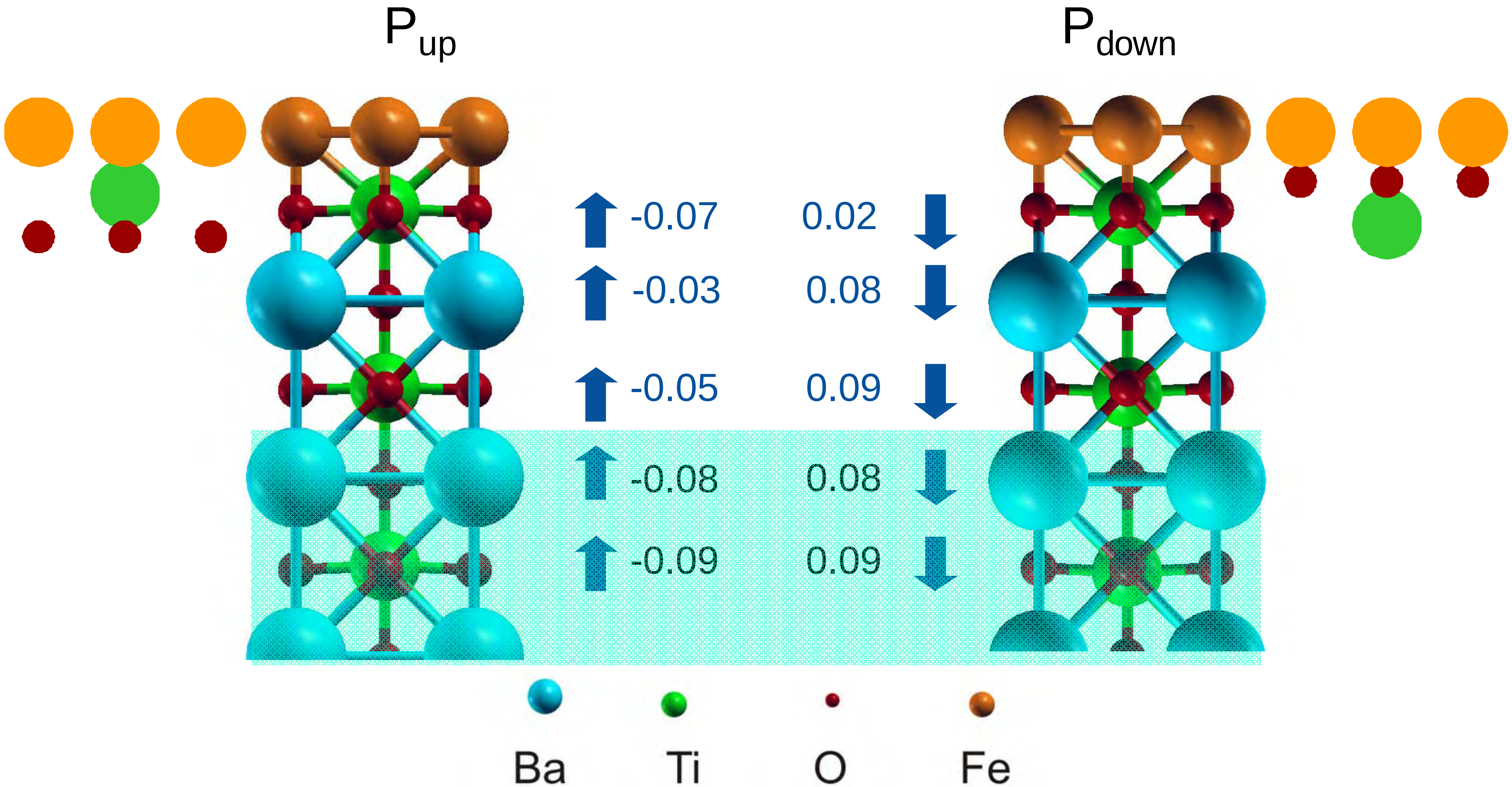
P

Electrical polarisation

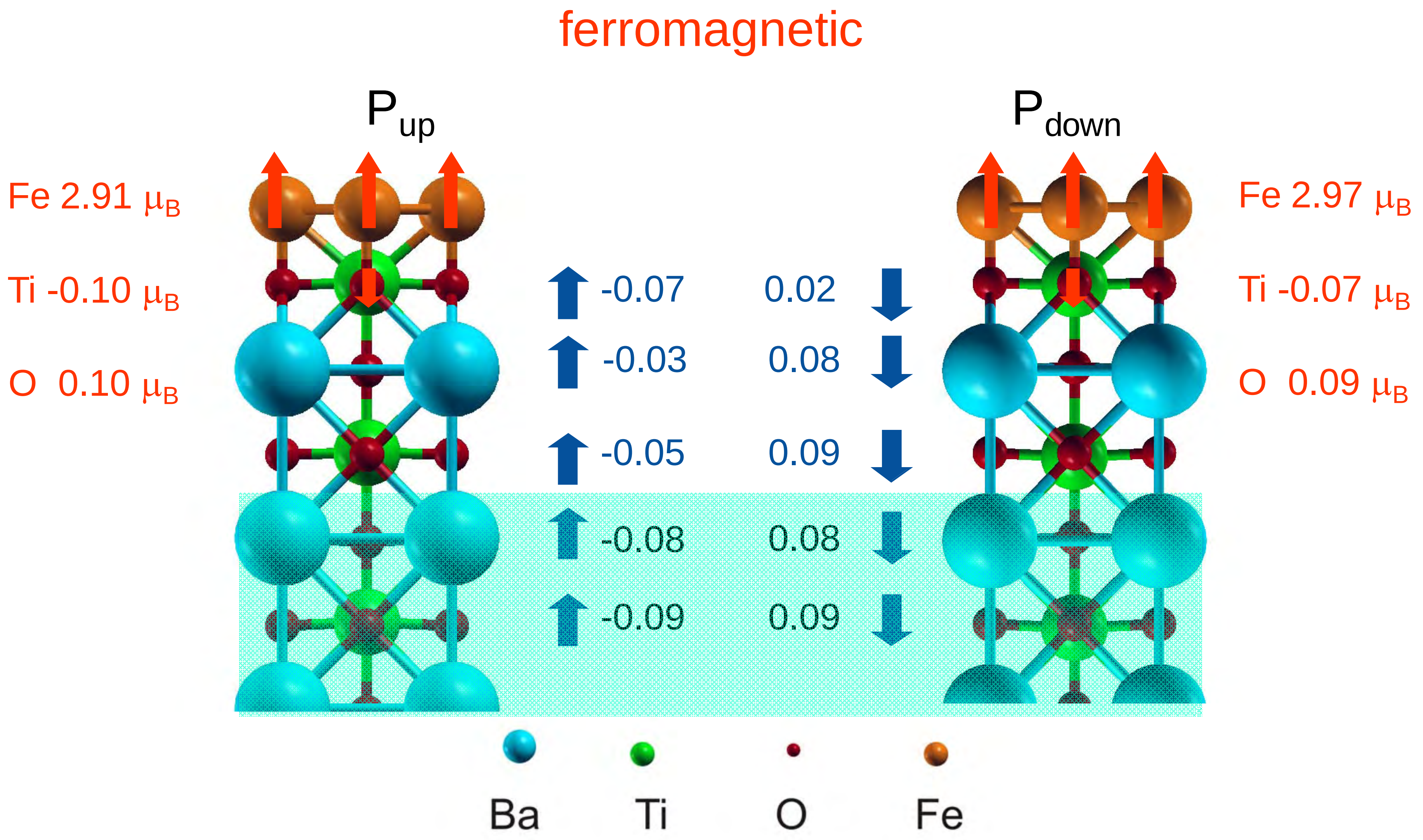
External electric field

One monolayer of Fe on $BaTiO_3$

$$\delta = z(O) - z(Kation)$$

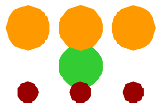


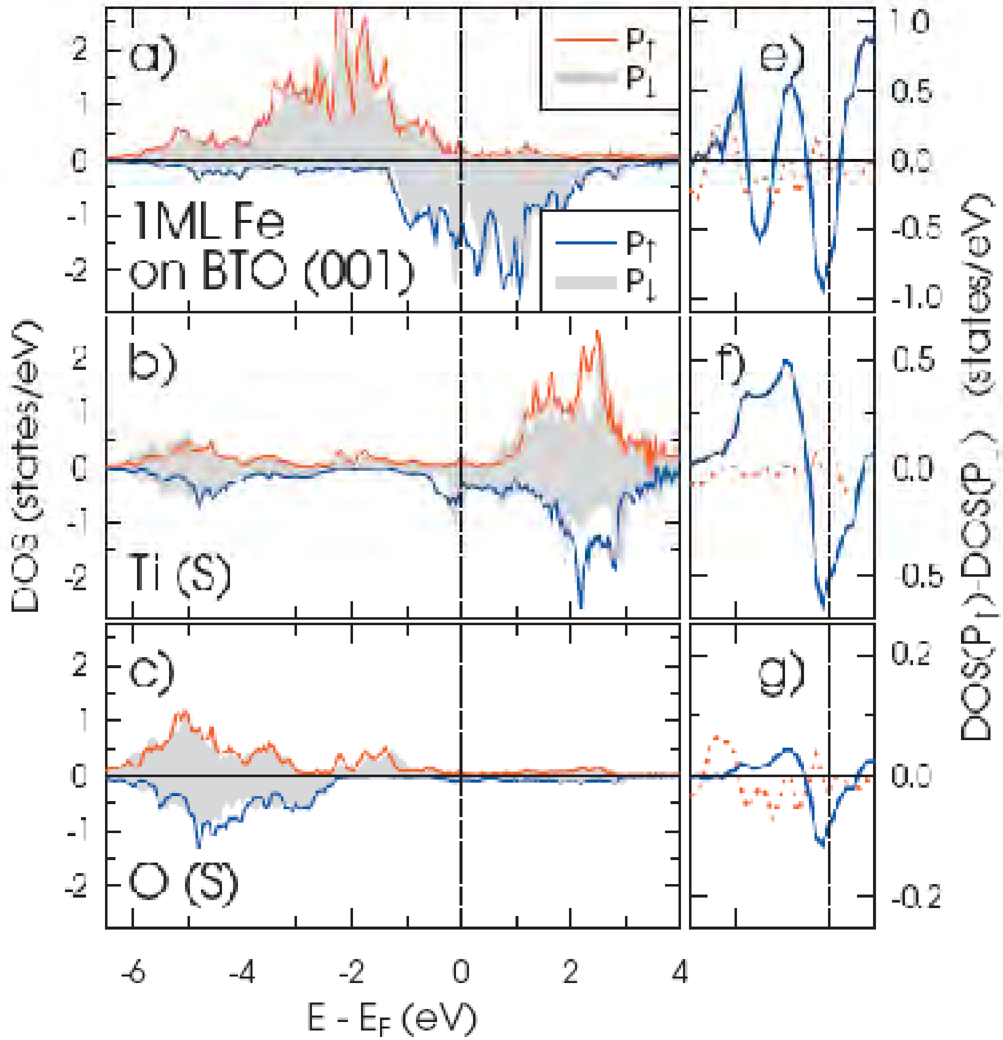
Magnetic order of Fe on $BaTiO_3$



Charge transfer from Fe to Ti under switching

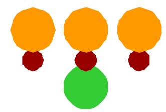
P_{up}





M. Fechner et al., PRB **78,** 212406 (2008)

P_{down}

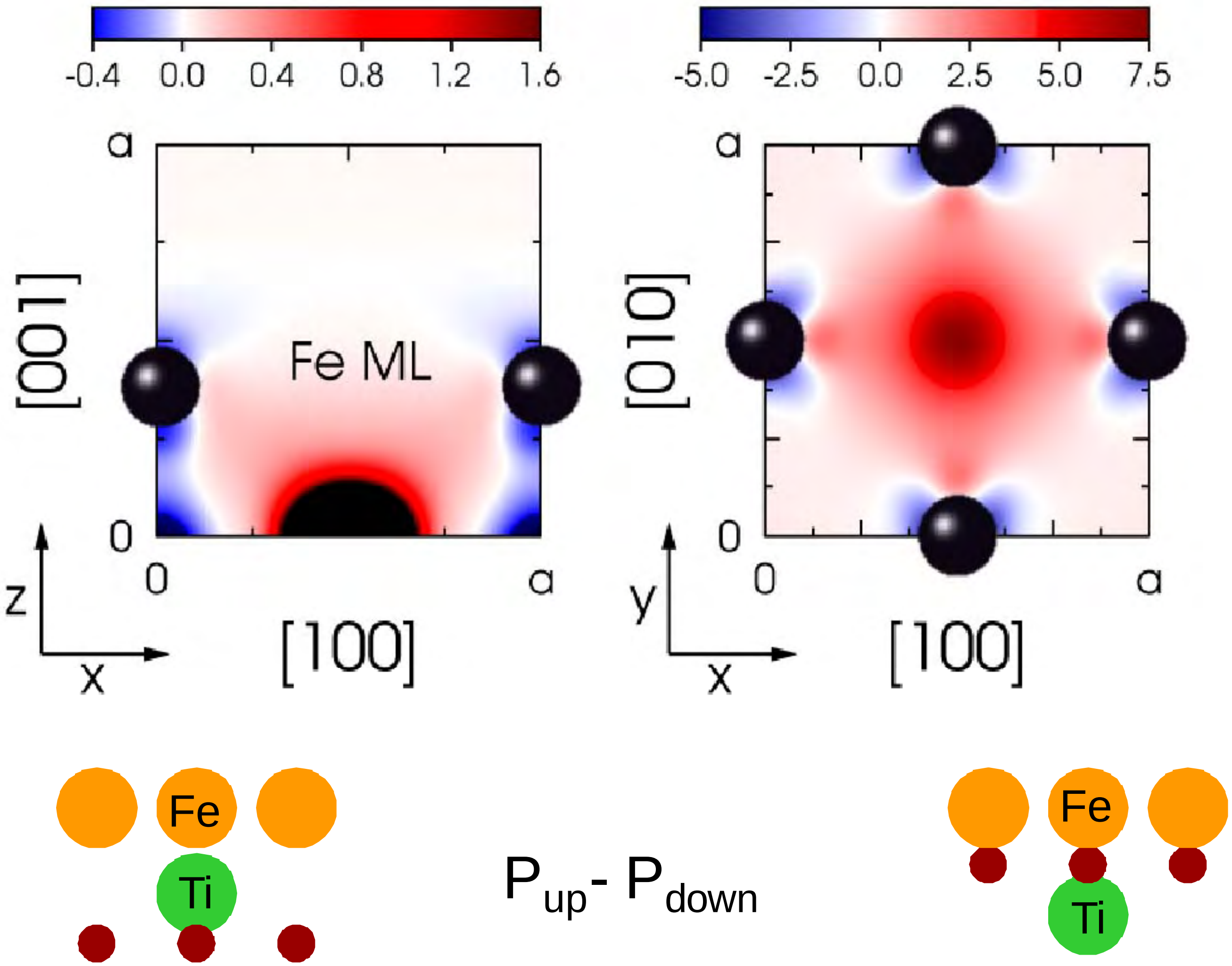


Change of charge on the Fe layer:

$\Delta q = 0.56$ e

$\Delta M = 0.13\ \mu_B$

Charge transfer from Ti to Fe



P_{up}- P_{down}

Magnetic order in the Fe layer on $BaTiO_3$

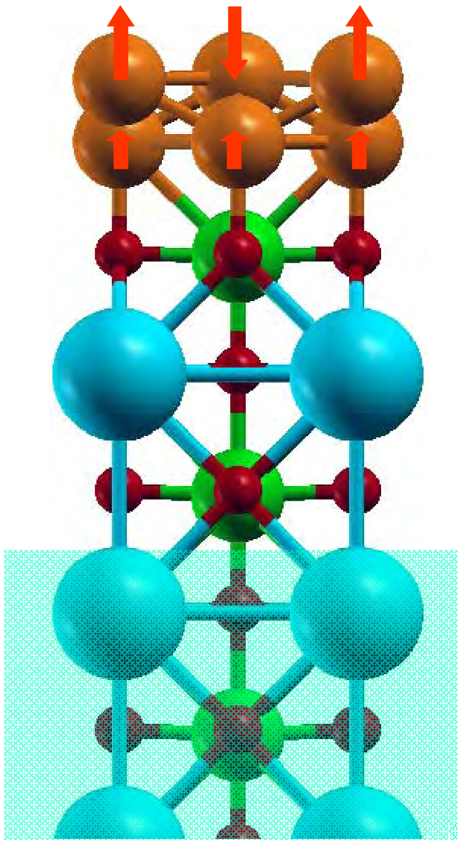
antiferrimagnetic

P_{up}

Fe^{2ML}_{Ti} -2.71 μ_B

Fe^{2ML}_{Ba} 2.38 μ_B

Fe^{1ML} 0.37 μ_B



P_{down}

Fe^{2ML}_{Ti} -2.36 μ_B

Fe^{2ML}_{Ba} 2.18 μ_B

Fe^{1ML} 0.33 μ_B

Structure:

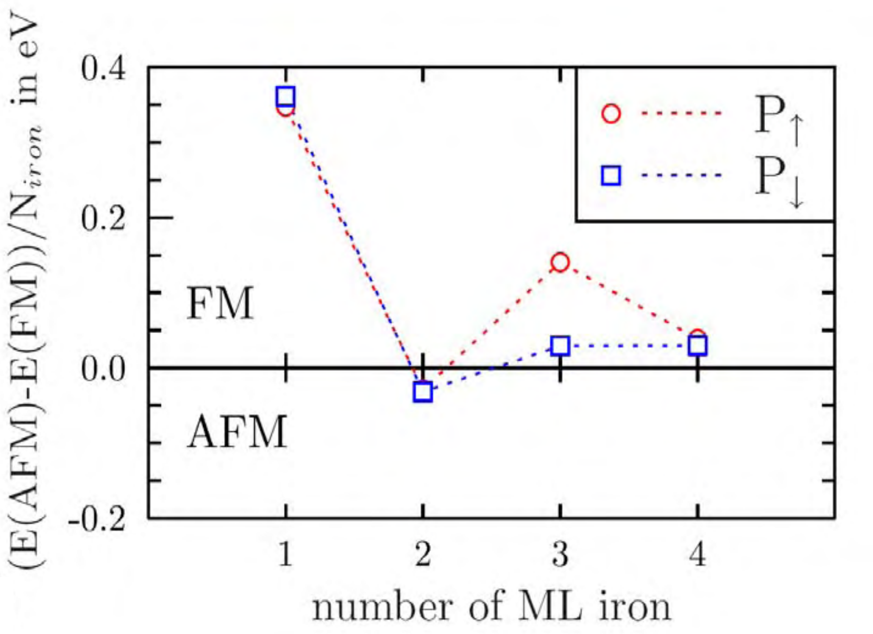
$Fe_{\text{in plane}}$ 2.79

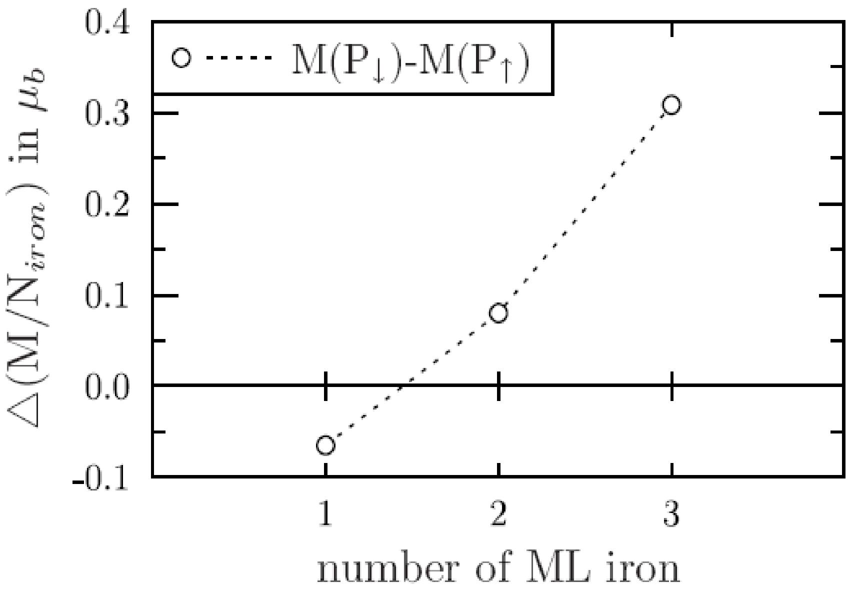
$Fe_{\text{between planes}}$ 1.1

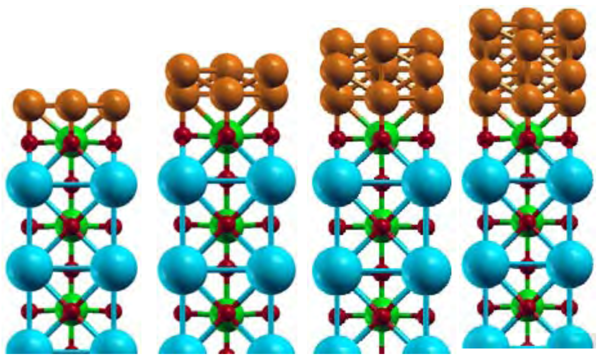
T_c = 205 K

M. Fechner et al., PRB **78,** 212406 (2008)

Magnetic order in the Fe layer on $BaTiO_3$







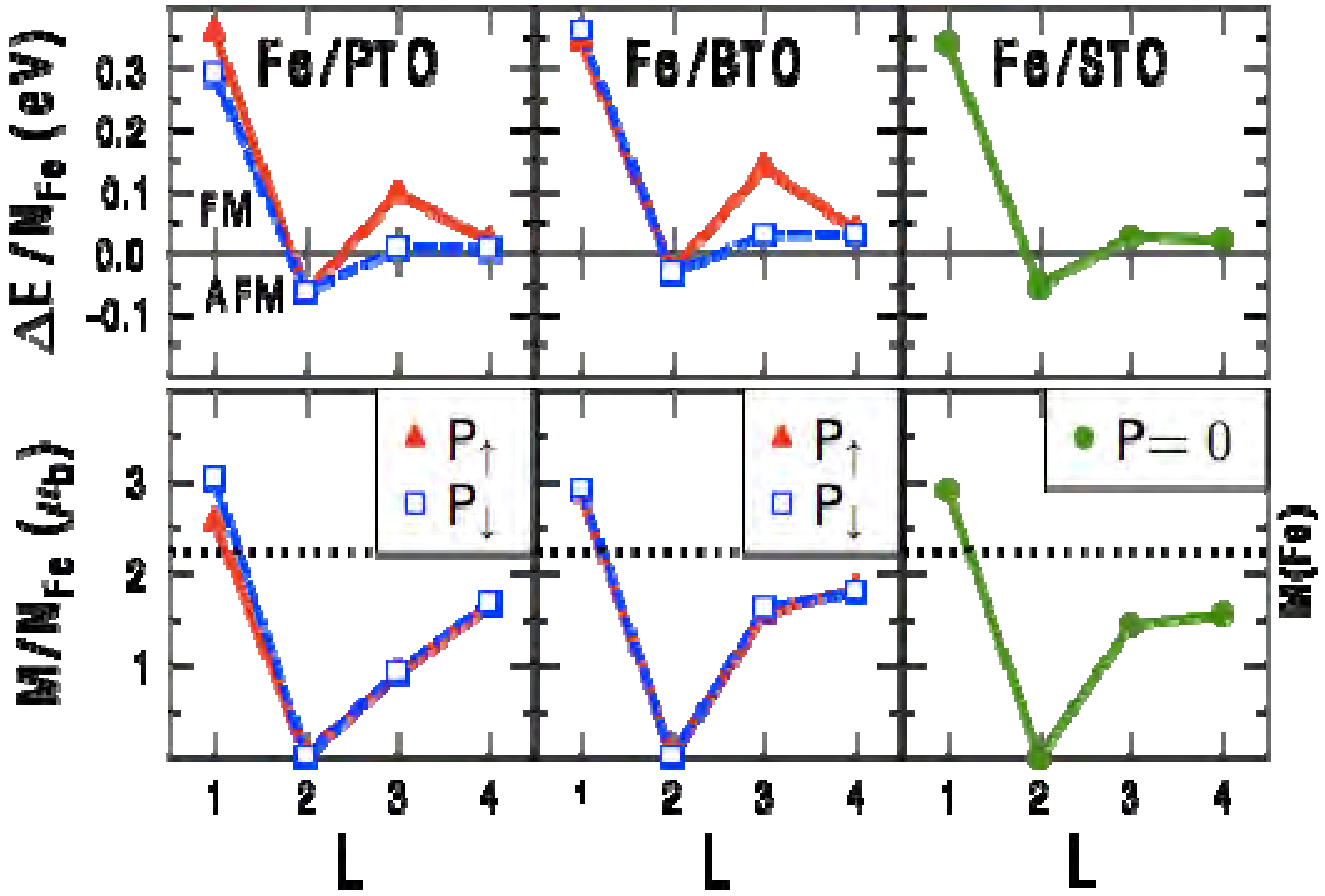
Magnetoelectric coefficient:

$$\alpha = \mu_0 \Delta M / E_c \approx 0.01 Gcm/V$$

$$\mu_0 \Delta M \approx 100G$$

$$E_c \approx 10kV/cm$$

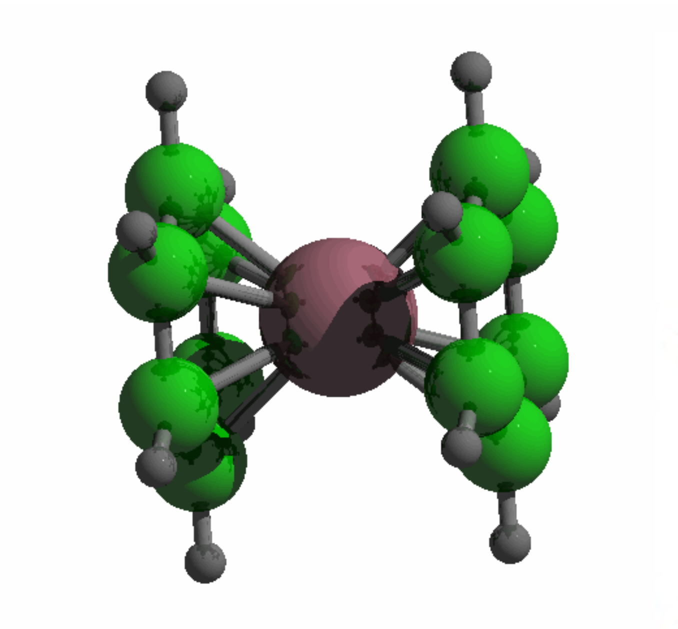
Magnetic order in the Fe layer on $BaTiO_3$

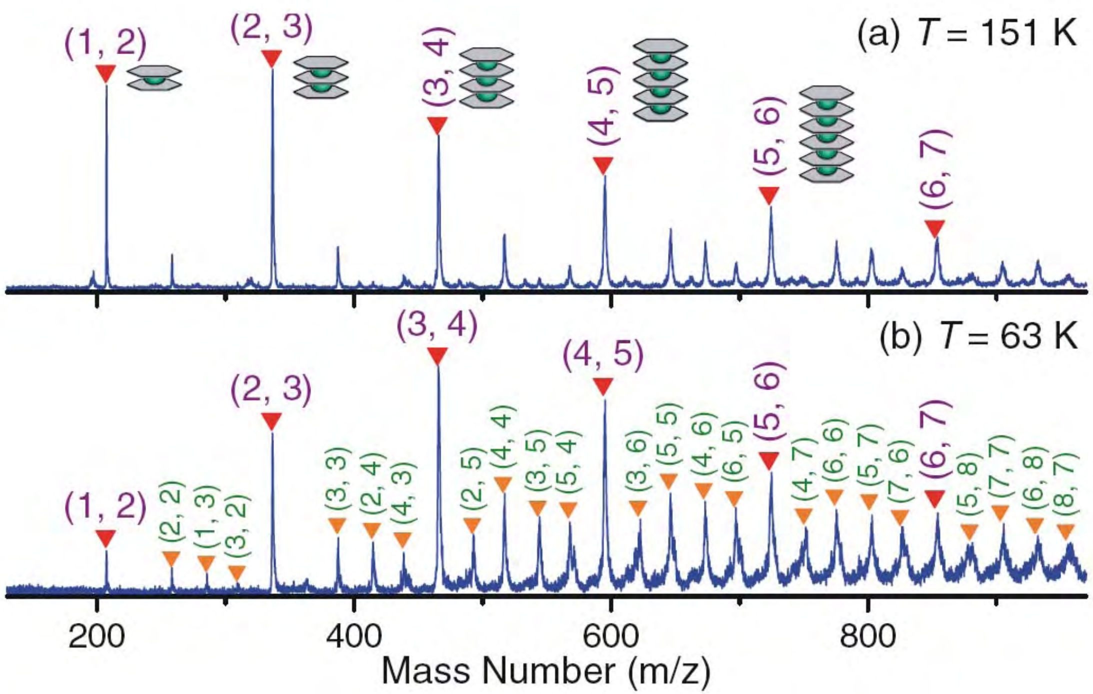


Magnetic molecules


Vova Maslyuk

Organometallic benzene-vanadium wires



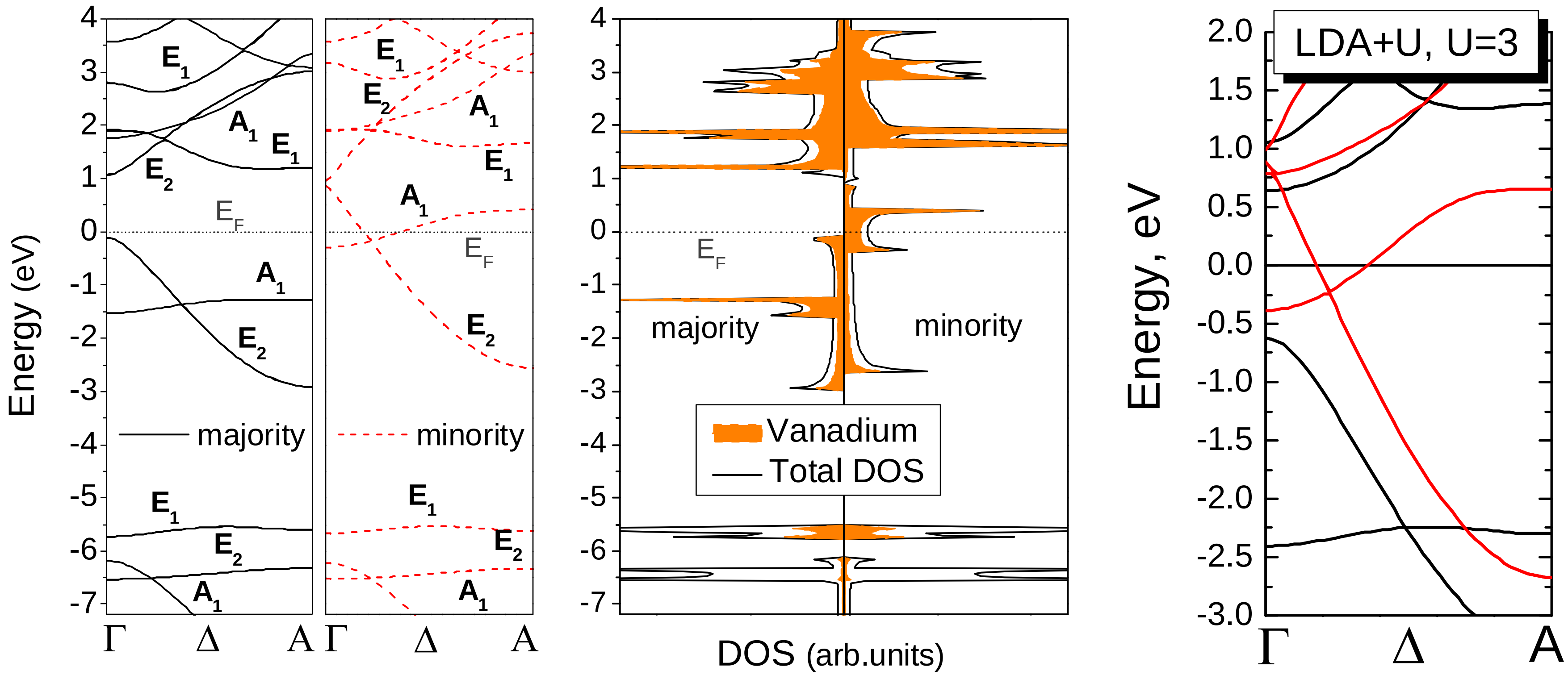


K. Miyajima, *et al.* Eur. Phys. J. D **34** 177 (2005)

Organometallic benzene-vanadium wires

ferromagnetic

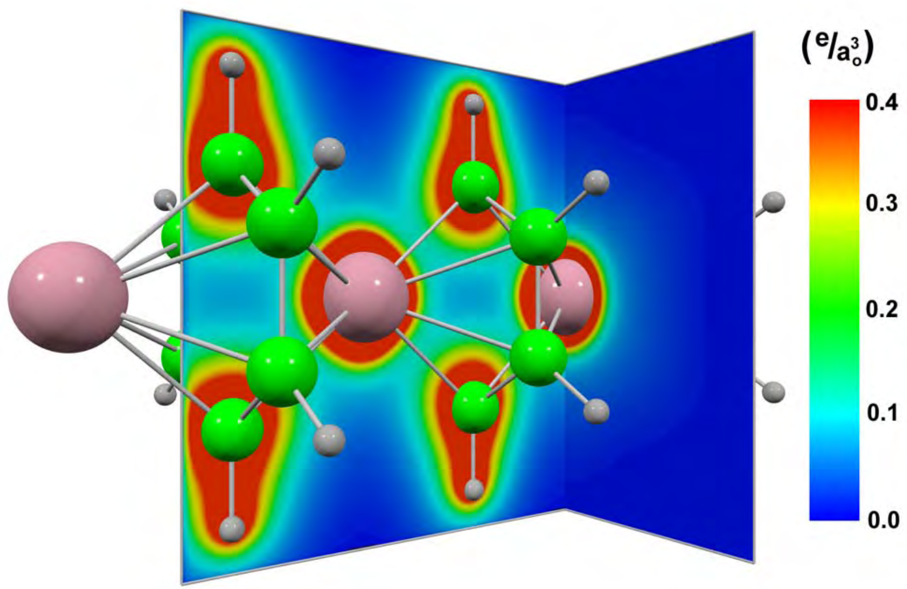
half-metallic



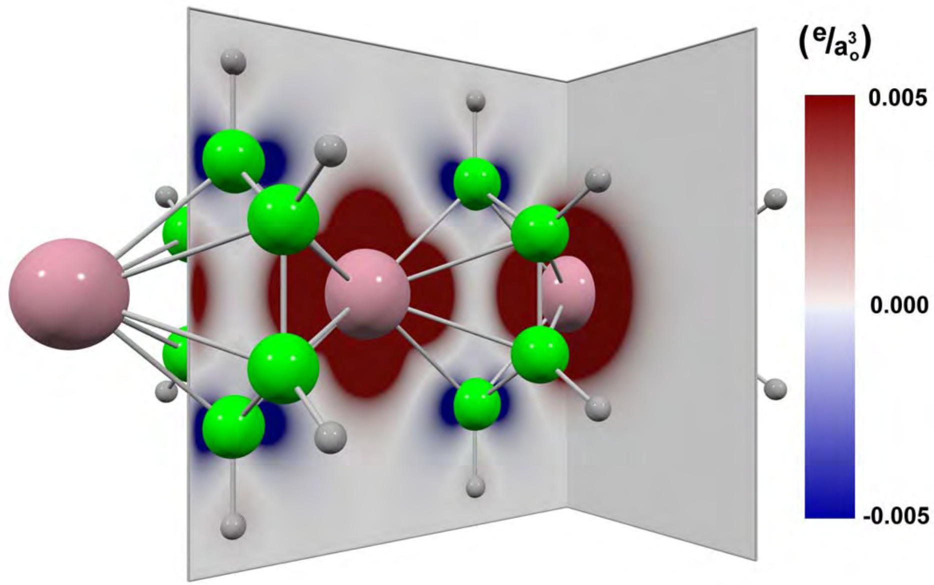
W. Maslyuk et al. PRL **97**, 097201(2006)

Organometallic benzene-vanadium wires

Charge density

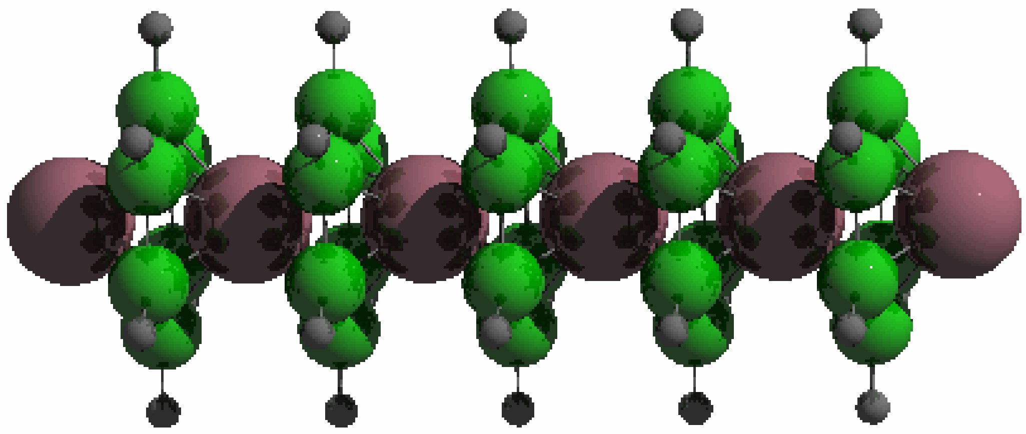


Spin density

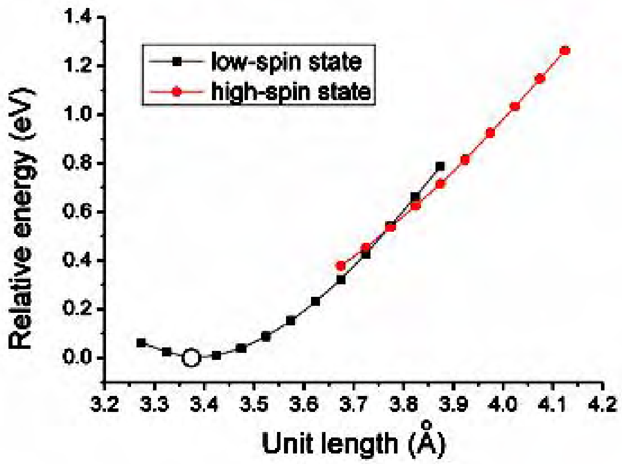


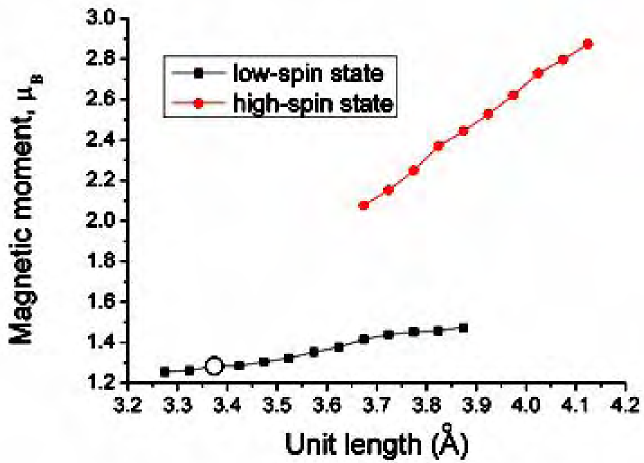
W. Maslyuk et al. PRL **97**, 097201(2006)

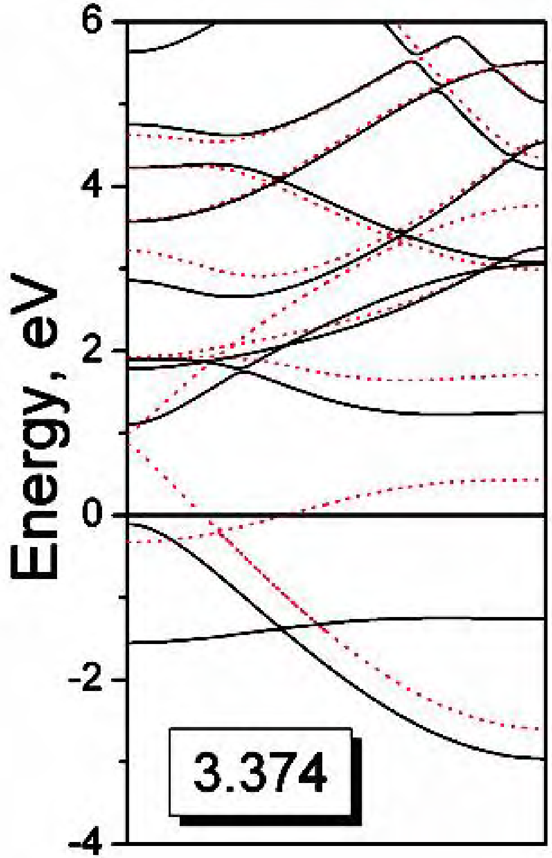
Stretching



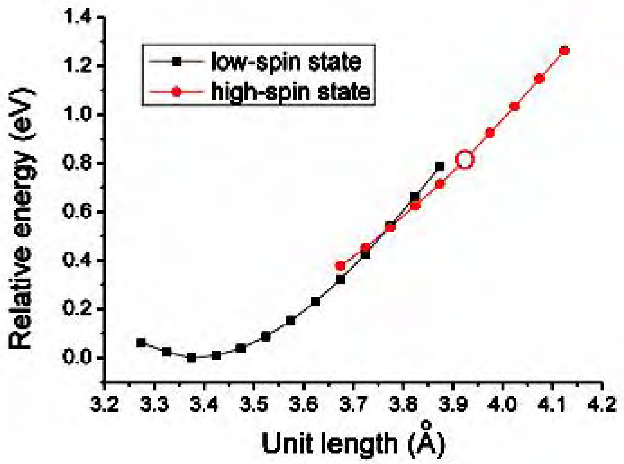
Low spin - high spin transition

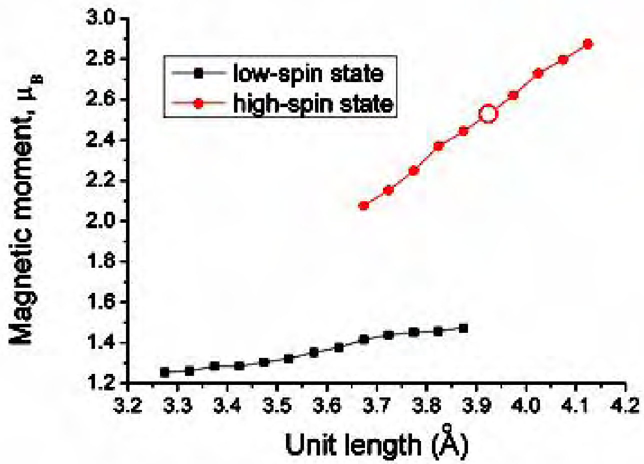


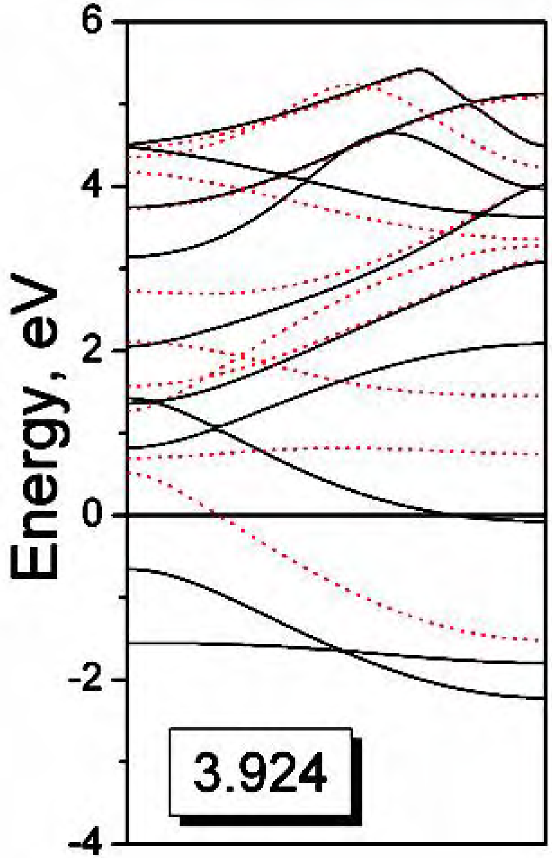




Low spin - high spin transition

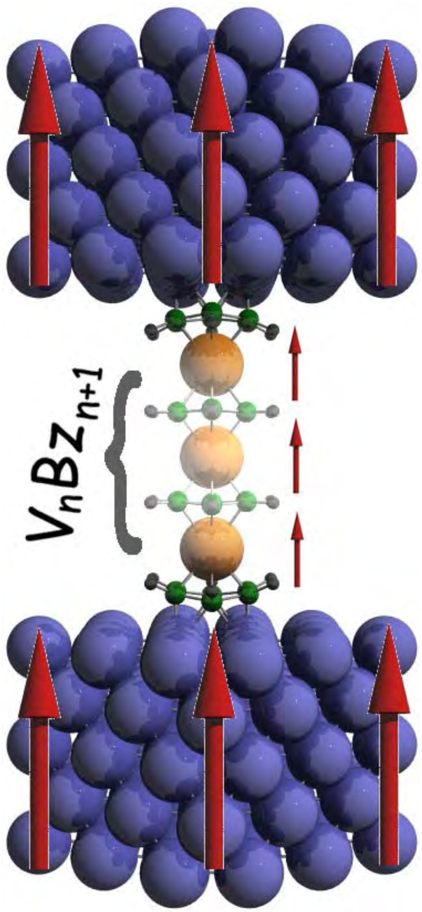


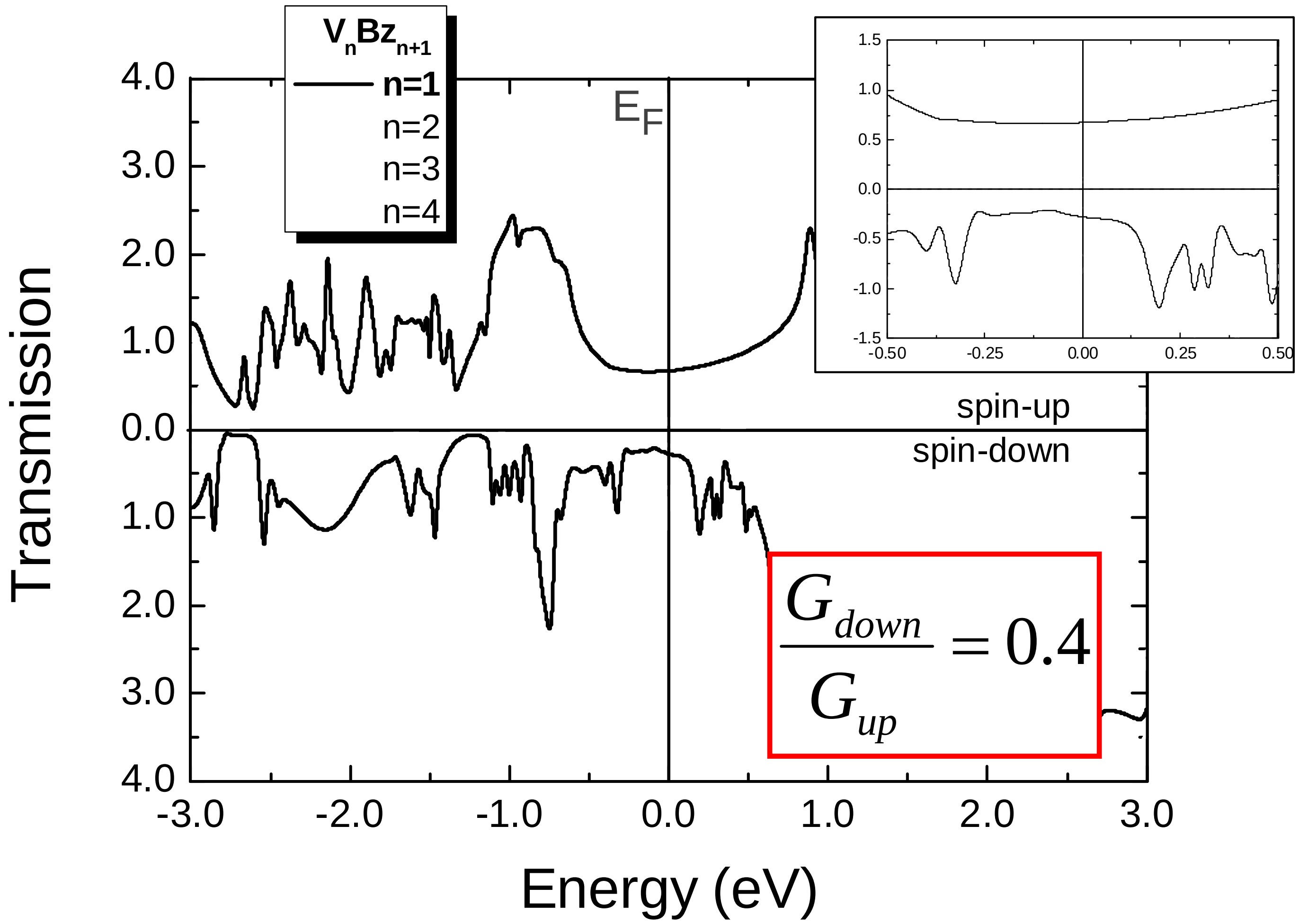




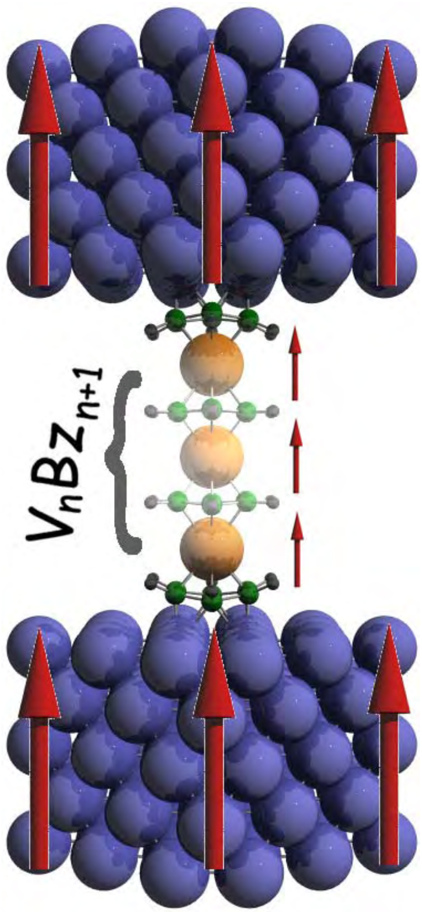
Transport through the molecule

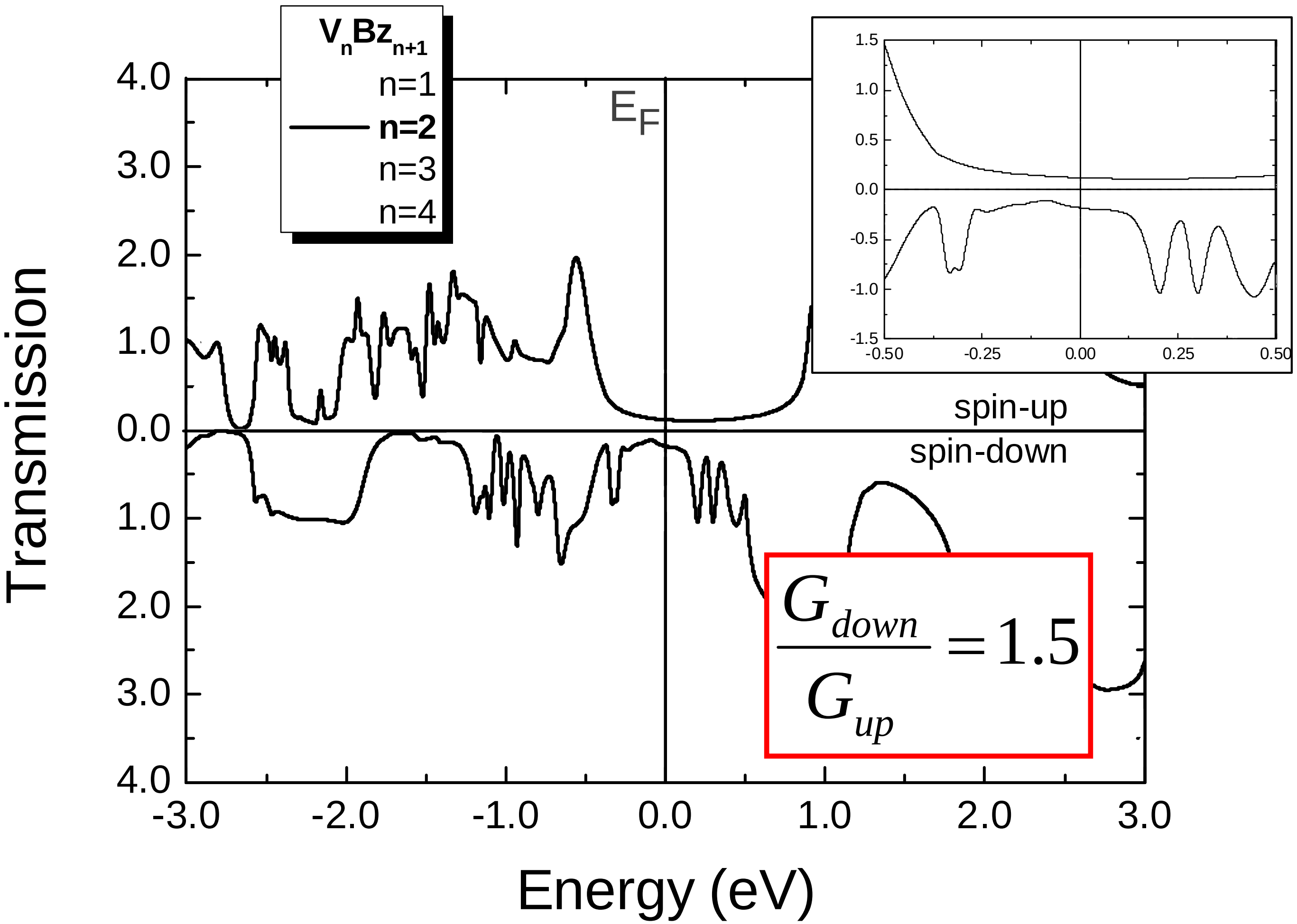
Transport through V_nBz_n+1 between Co(100) electrodes



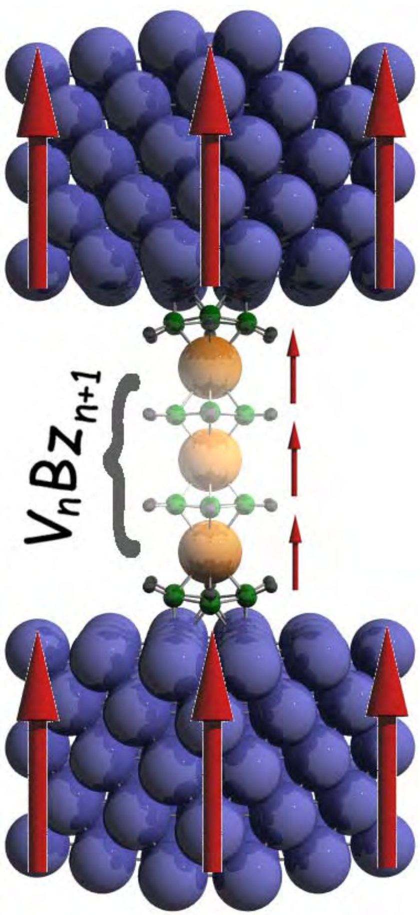


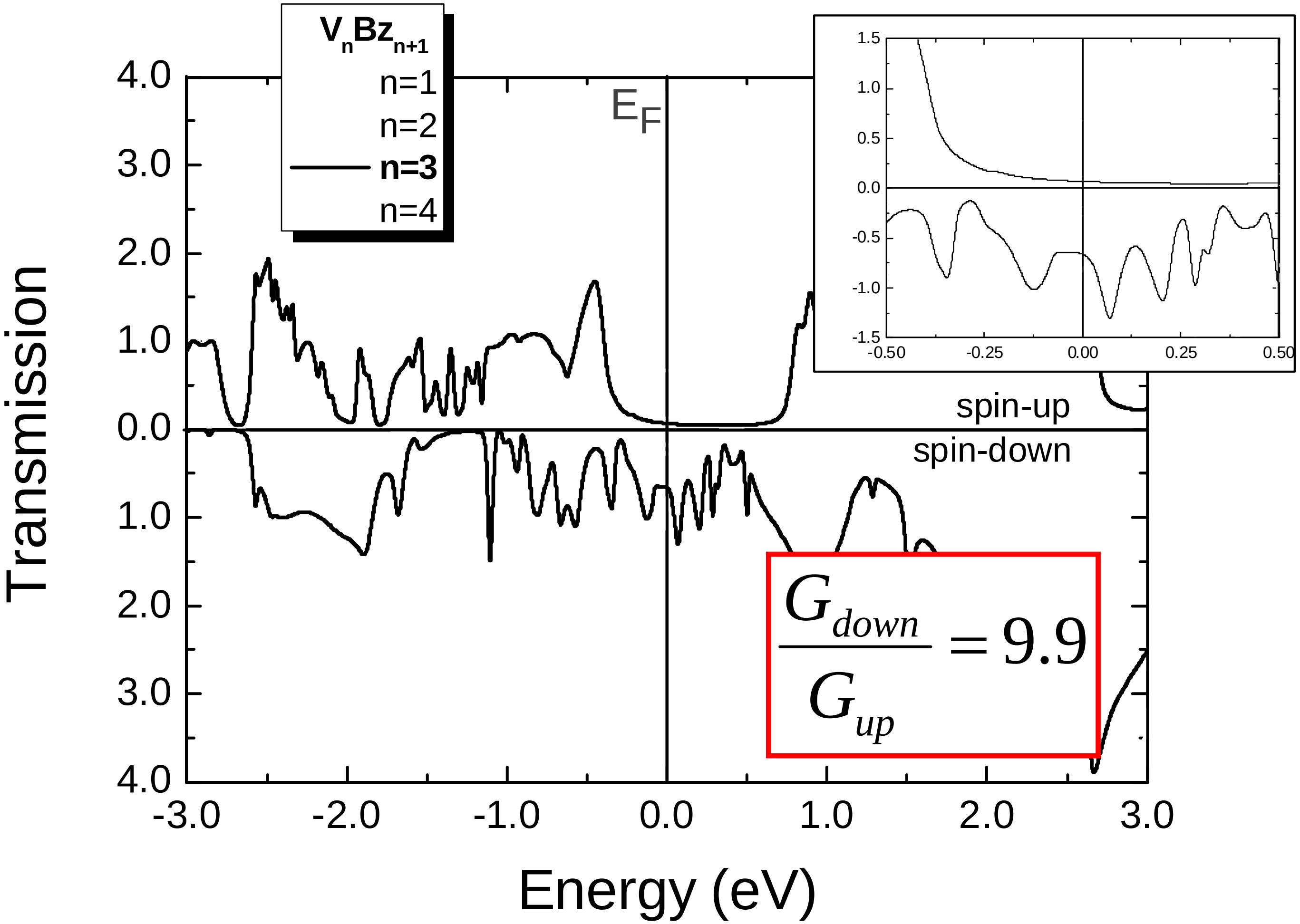
Transport through V_nBz_n+1 between Co(100) electrodes





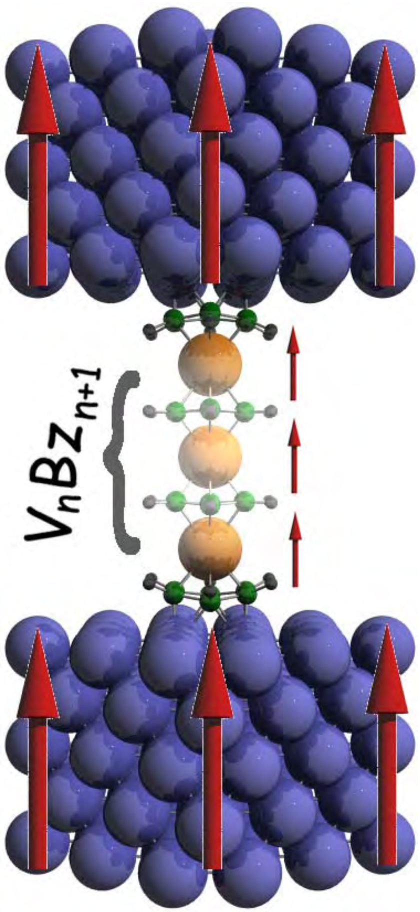
Transport through V_nBz_n+1 between Co(100) electrodes

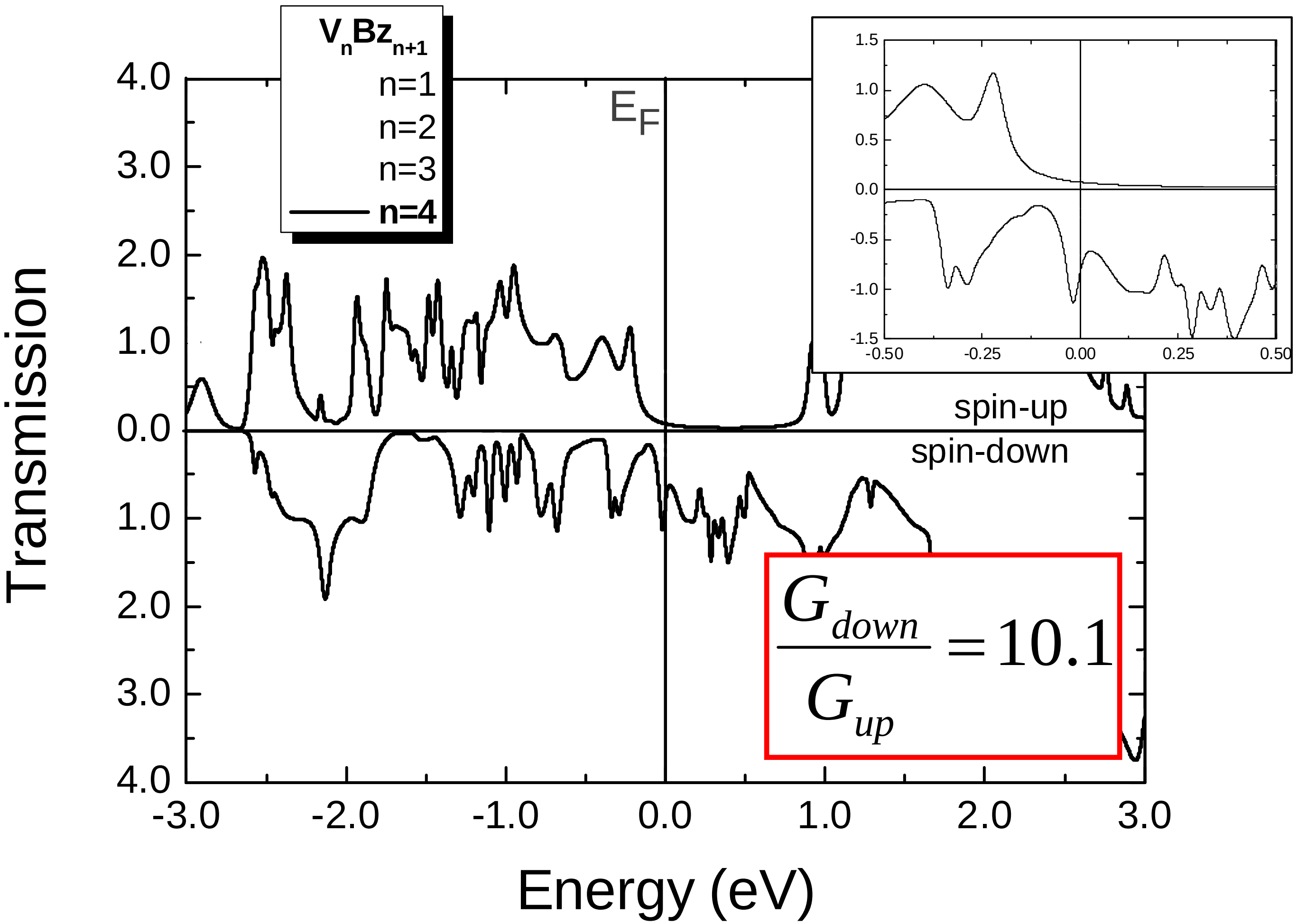




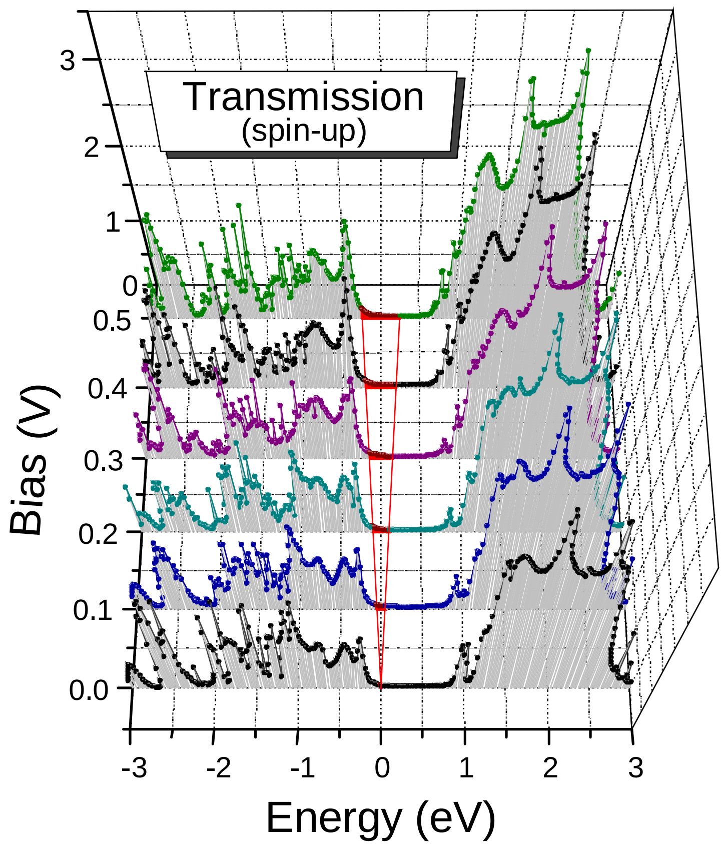
$$\frac{G_{down}}{G_{up}} = 9.9$$

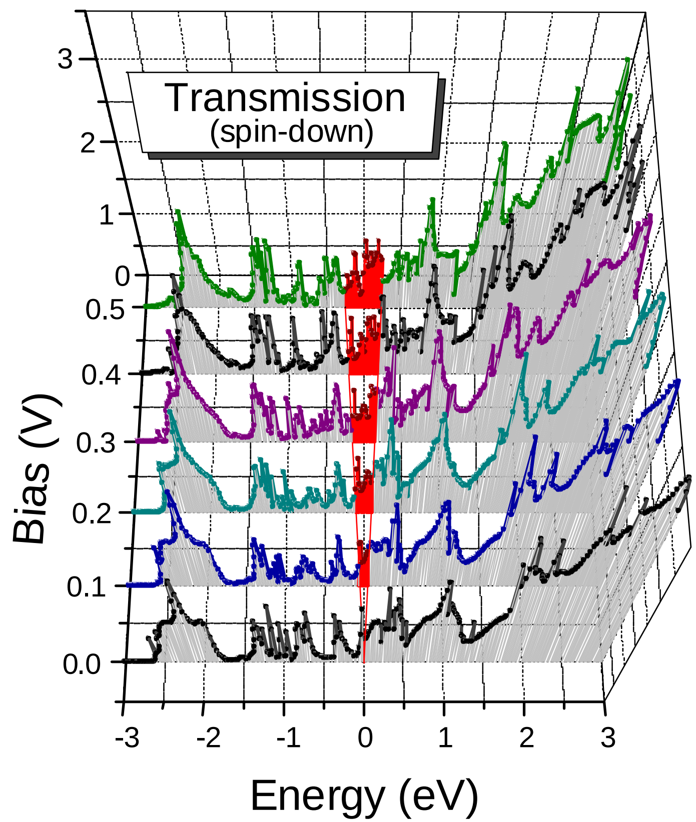
Transport through V_nBz_n+1 between Co(100) electrodes





Bias dependence





Co(100)-V_4Bz_5-Co(100)

Summary

- Tunneling current and TMR effect are tailored by the interface between oxide barrier and first layer of the electrodes!
- Ferroelectricity changes at the surface!
- We predict magnetoelectric coupling via the interface caused by charge transfer!
- Organometallic contacts show pronounced spin-dependent transport

Collaborations and funding

A. Ernst, J. Henk, L. Sandratski,

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MAX-PLANCK-GESELLSCHAFT