Copenhagen University
June 23rd 2008

Ph.D. Defence

Morten Stilling
Ph.D. student
Nano-Science Center/Atomistix

Goals of the industrial Ph.D. project

- **Market development**

- Visits at IBM, Fujitsu, Hitachi, Grandis, Toshiba, Crocus, Thales Samsung, Seagate, KIST, KAIST, Spintec, TSMC, IMEC, Panasonic...
- Participation in MMM, MRS, Nanotech, NTNE, Nanofair, NNIN...
- Set up of the Magnetoresistive Storage and Memory Consortium

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Magnetoresistance in MgO-based magnetic tunnel junctions with Fe, Co, and FeCo electrodes

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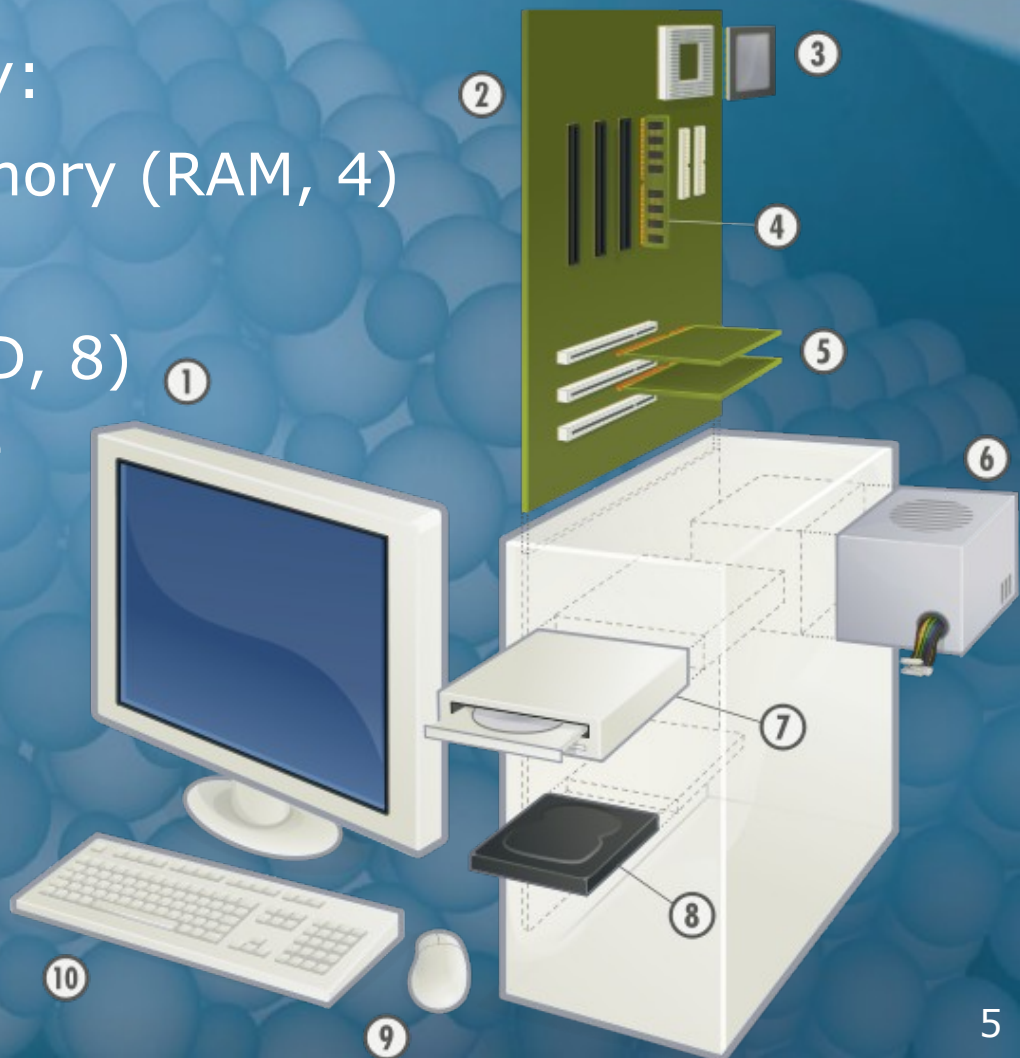
Here's what I want to tell you

- Hard disk drives with read heads incorporating MgO-based magnetic tunnel junctions are emerging in the data storage market
- We have modeled the spin-transport properties of MgO-based magnetic tunnel junctions using first-principles DFT/NEGF methods
- The tunneling magnetoresistance in MgO-based magnetic tunnel junctions is high but decreases with increasing bias voltage

The personal computer (PC)

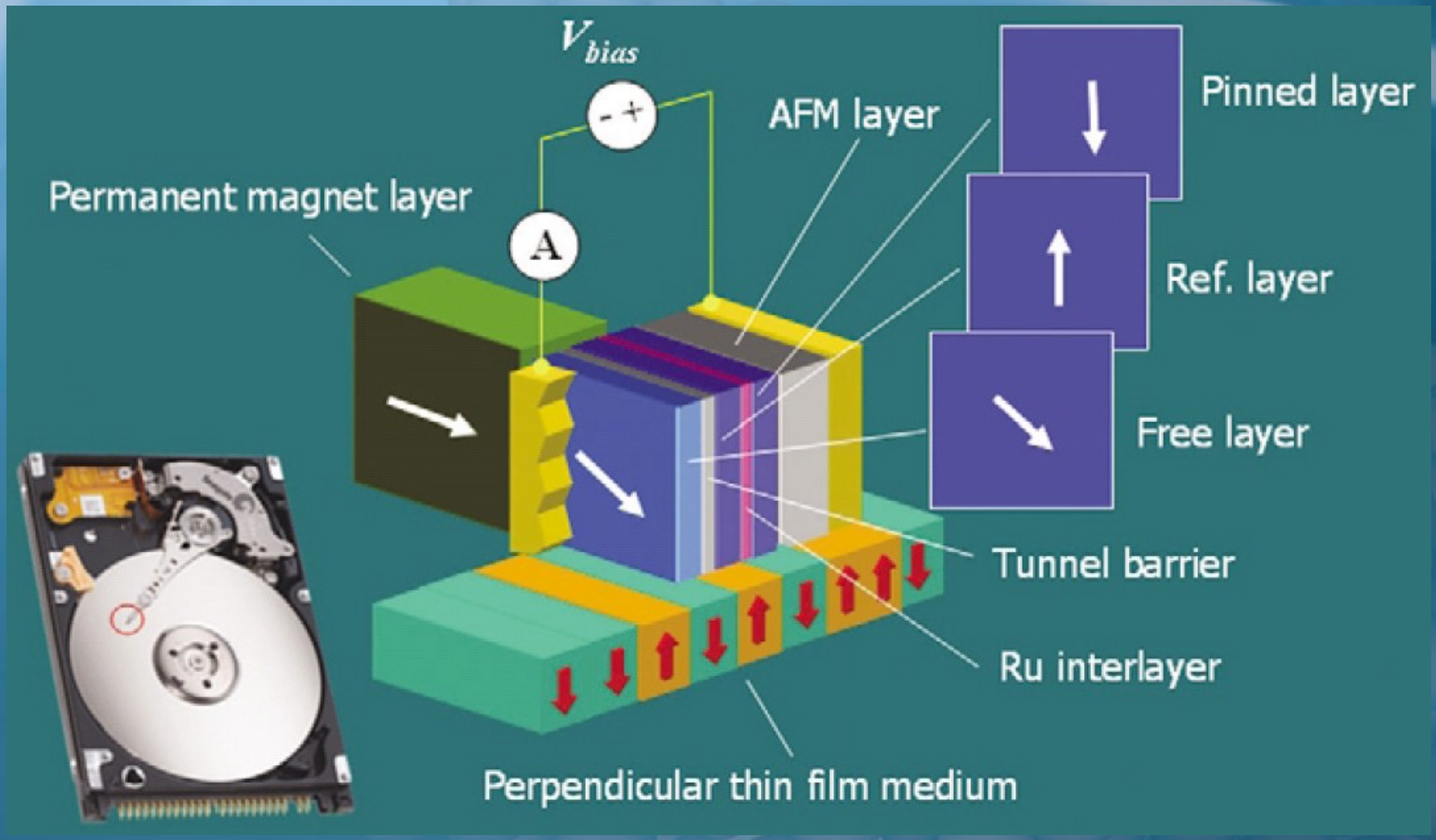
- Two types of memory:
  - Random access memory (RAM, 4)
    - RAM is volatile
  - Hard disk drive (HDD, 8)
    - HDD is non-volatile



The world's first hard disk drive

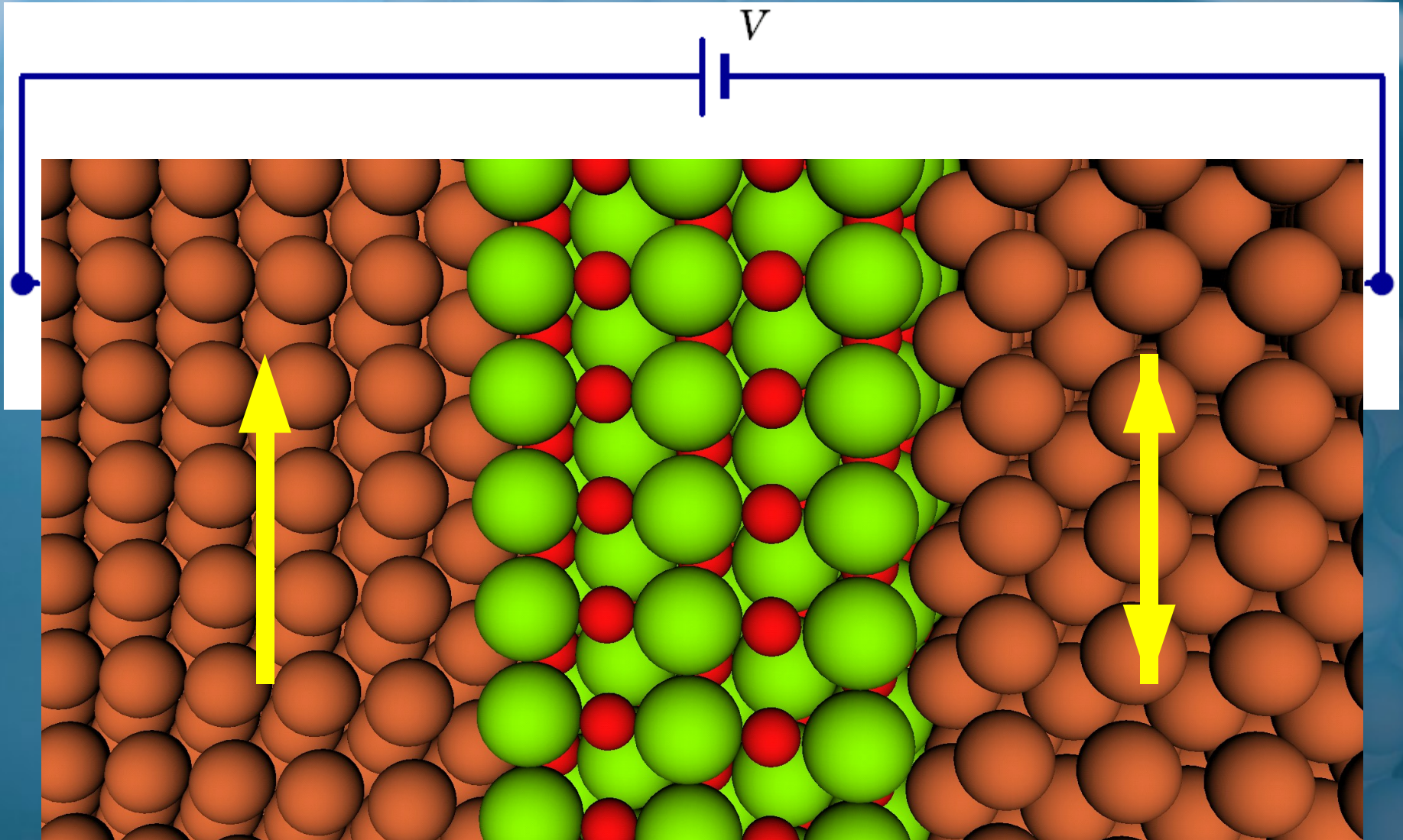


The read head in the hard disk drive



Zhu and Park, Materials Today **9**, 36-45 (2006)

The magnetic tunnel junction in the read head in the hard disk drive



Tunneling magnetoresistance in MgO-based magnetic tunnel junctions

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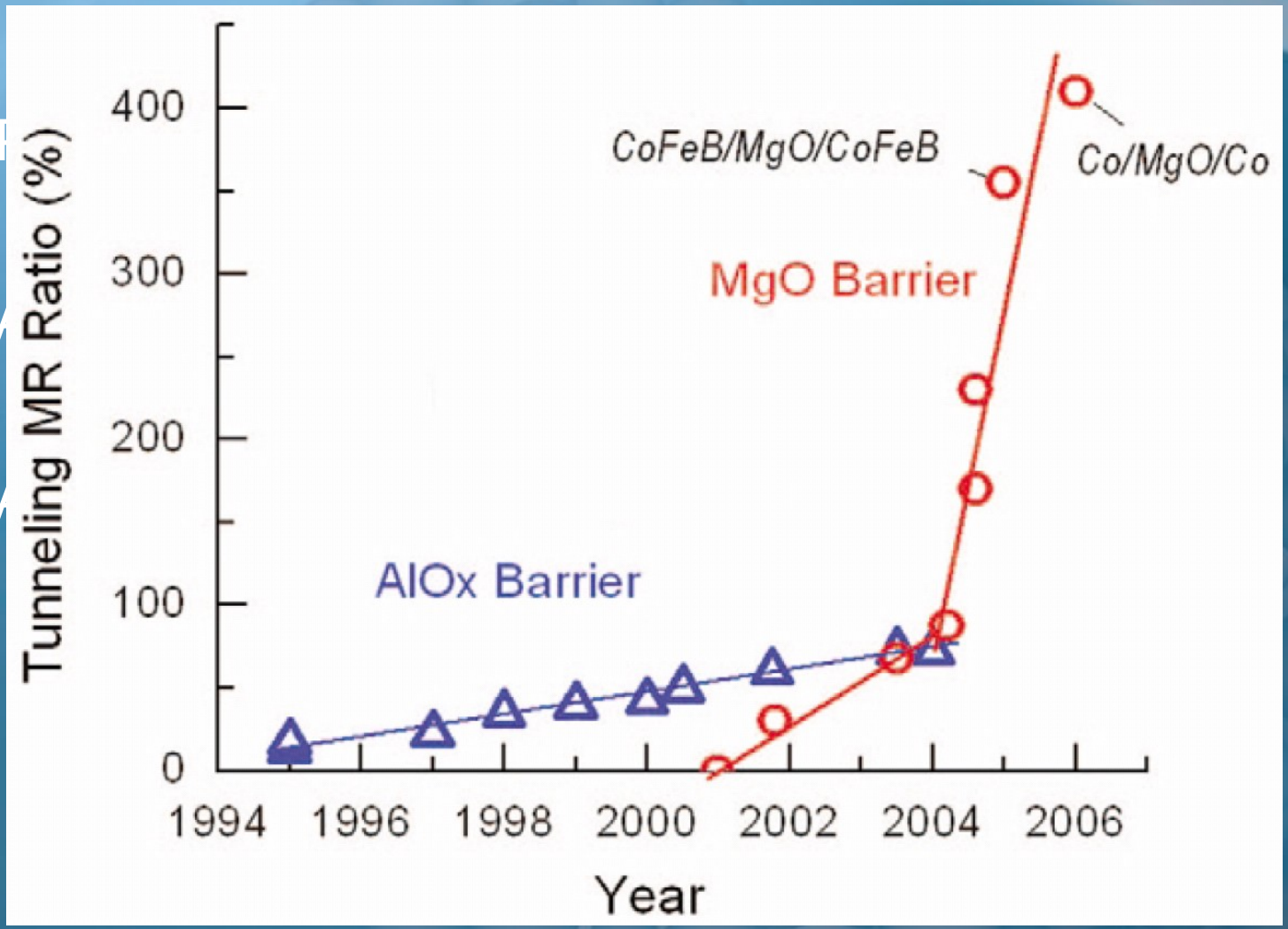
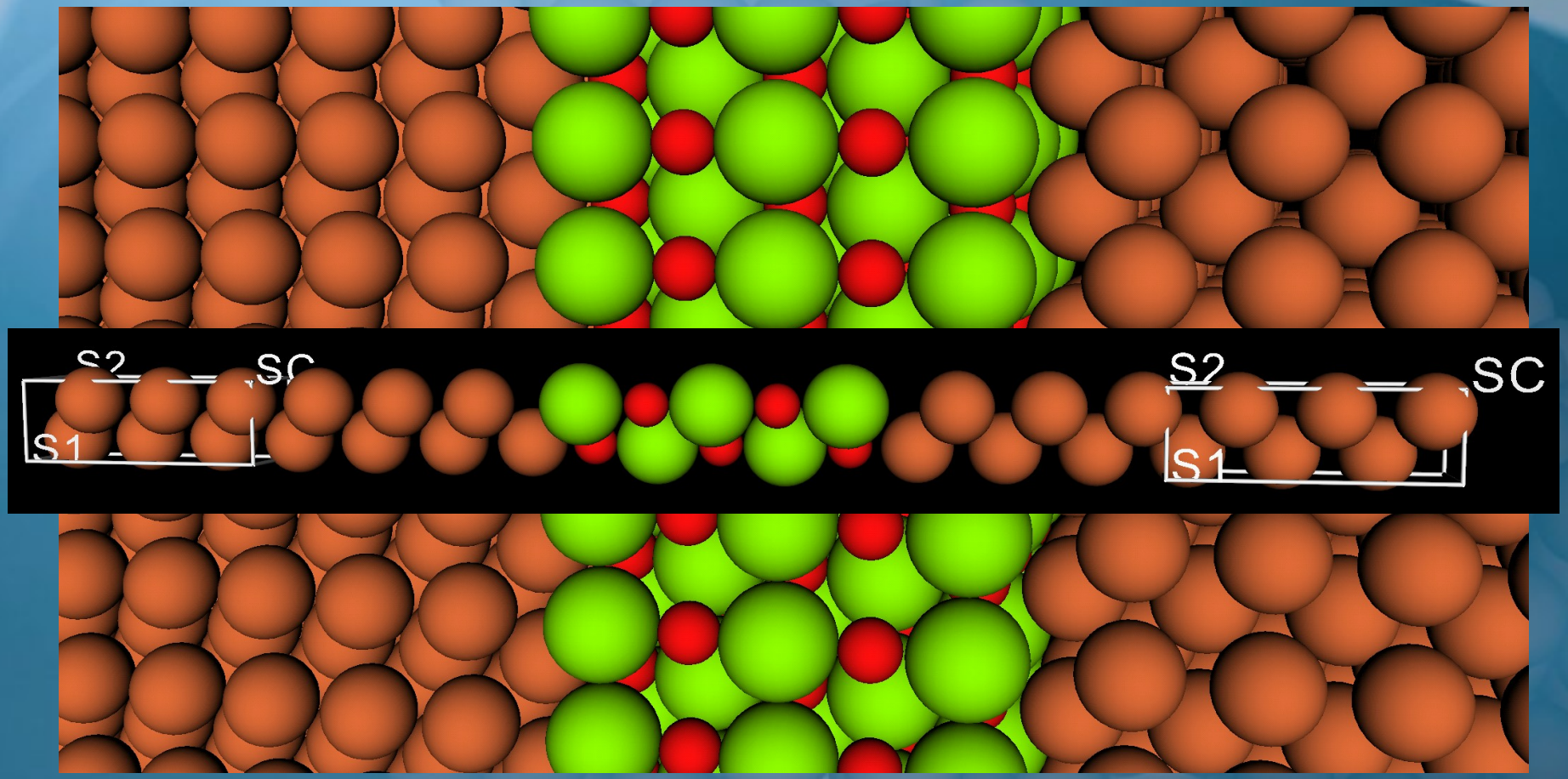
- A



Zhu and Park, Materials Today **9**, 36-45 (2006)

We assume ideal crystalline structure



We calculate the electronic structure using density functional theory (DFT)

- Th
  - d
- Th
  - d

$$\left\{ -\frac{\hbar^2}{2m_e}\nabla^2 + v_{eff}(\mathbf{r}) \right\} \psi_i(\mathbf{r}) = E_i \psi_i(\mathbf{r})$$

$$v_{eff}(\mathbf{r}) = v(\mathbf{r}) + v_H(\mathbf{r}) + v_{xc}(\mathbf{r})$$

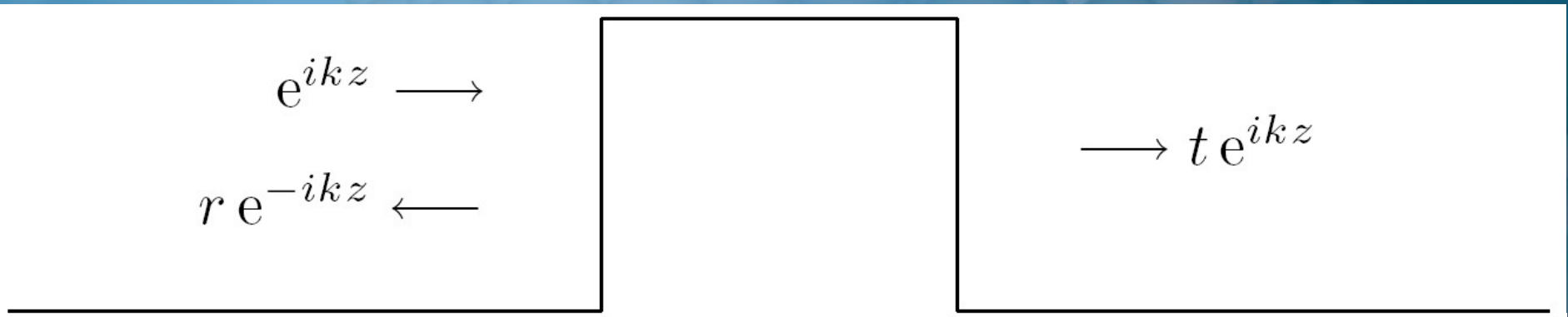
Effective potential — External potential — Hartree potential — Exchange-correlation potential

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2$$

Hohenberg and Kohn, Phys. Rev. **136**, B864 (1964)
Kohn and Sham, Phys. Rev. **140**, A1133 (1965)

We calculate the current using the Landauer approach

- The conductance and current are related to the transmission probability of incident electrons



$$I_\sigma(V) = \frac{e}{h}\int_{-\infty}^{\infty} T_\sigma(V,E)\,[f_R(E;\mu_R+eV/2) - f_L(E;\mu_L-eV/2)]\,\mathrm{d}E$$

$$G_\sigma = \frac{e^2}{h}\,T_\sigma(0,E_F)$$

We calculate the transmission coefficient using non-equilibrium Green's functions

$$T_\sigma^k(V, E, \mathbf{k}_\parallel) = \mathrm{Tr}\left\{\bar{\Gamma}^L_{CC}\,\bar{G}^r_{CC}\,\bar{\Gamma}^R_{CC}\,\bar{G}^a_{CC}\right\}$$

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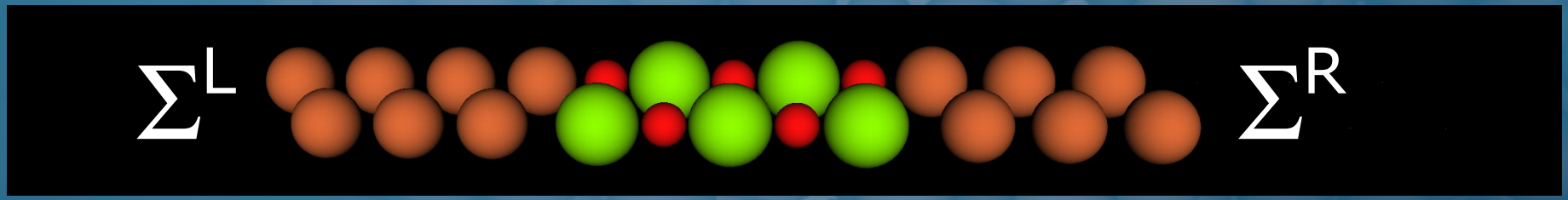
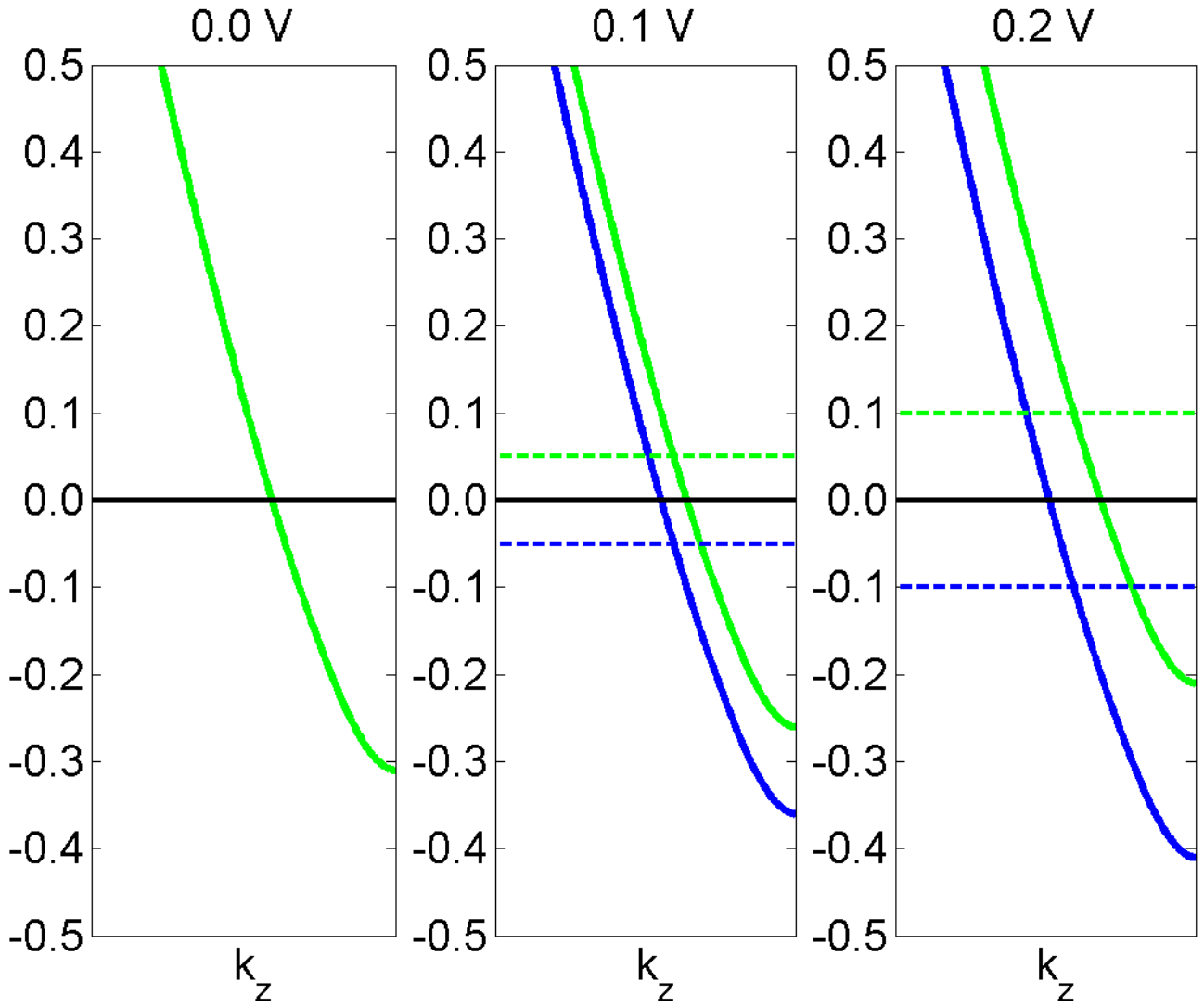
en the

$$\begin{aligned}
\bar{G}^r_{CC} &= \left[\bar{\mathcal{H}}_{CC} - \bar{\Sigma}^L_{CC} - \bar{\Sigma}^R_{CC}\right]^{-1} \\
\bar{G}^a_{CC} &= \left(\bar{G}^r_{CC}\right)^\dagger \\
\bar{\Gamma}^L_{CC} &= -2\mathrm{Im}\left\{\bar{\Sigma}^L_{CC}\right\} \\
\bar{\Gamma}^R_{CC} &= -2\mathrm{Im}\left\{\bar{\Sigma}^R_{CC}\right\}
\end{aligned}$$



Taylor *et al.*, Phys. Rev. B. 63, 245407 (2001)
Brandbyge *et al.*, Phys. Rev. B. 65, 165401 (2002)

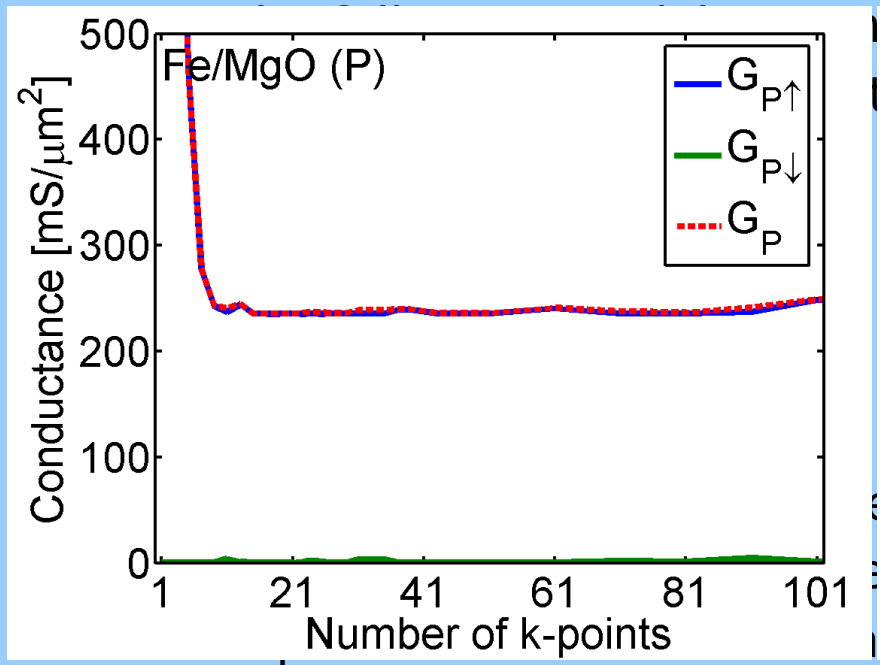
We use a “ramp approximation”

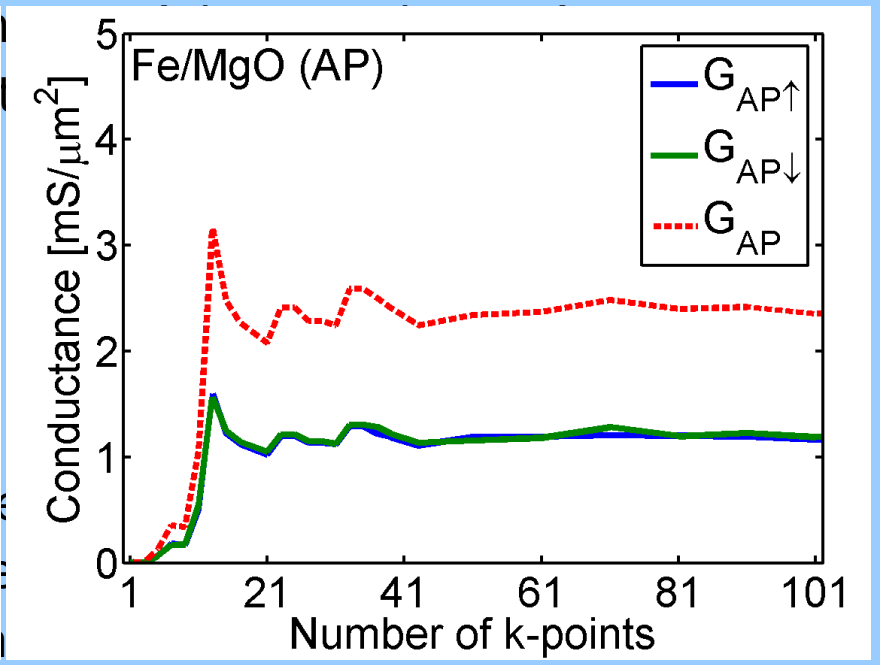


Majority-spin band structure of FeCo electrode (blue: left electrode – green: right electrode)

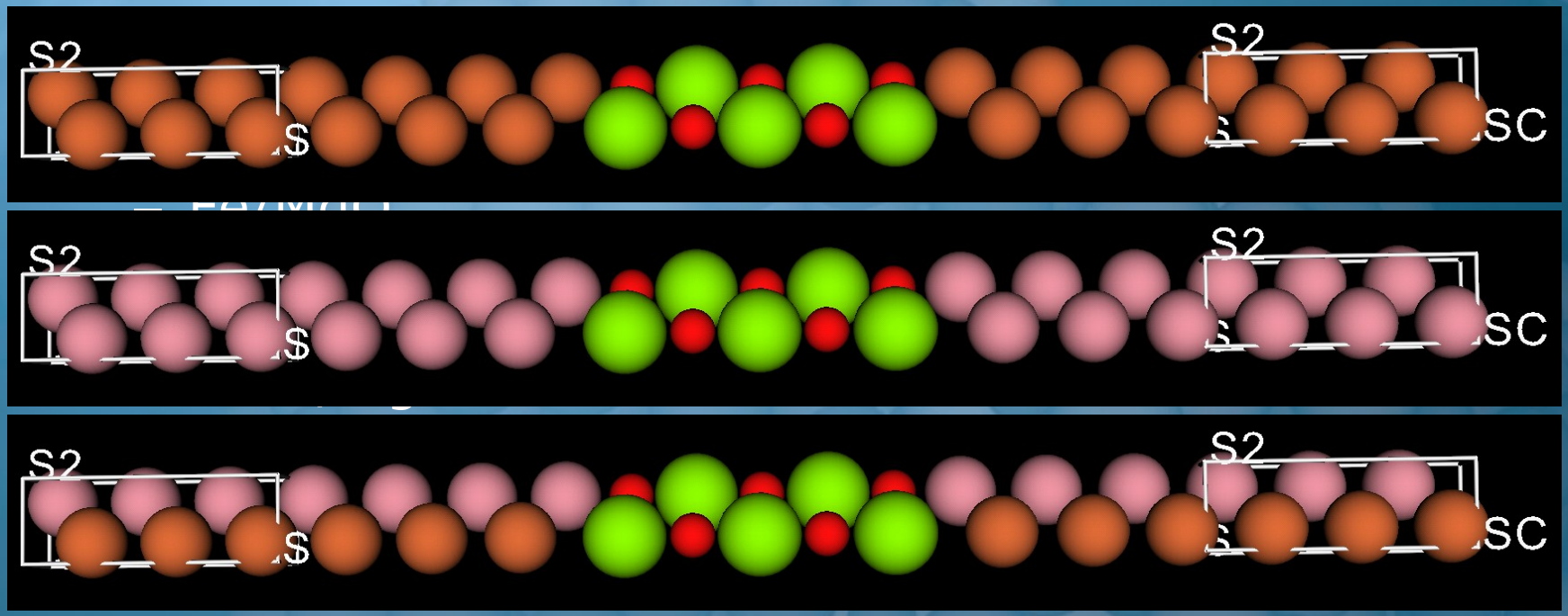
Reliability/accuracy of our results

- **Numerical accuracy**
-





We have calculated the TMR of three magnetic tunnel junctions



Calculation results – zero-bias

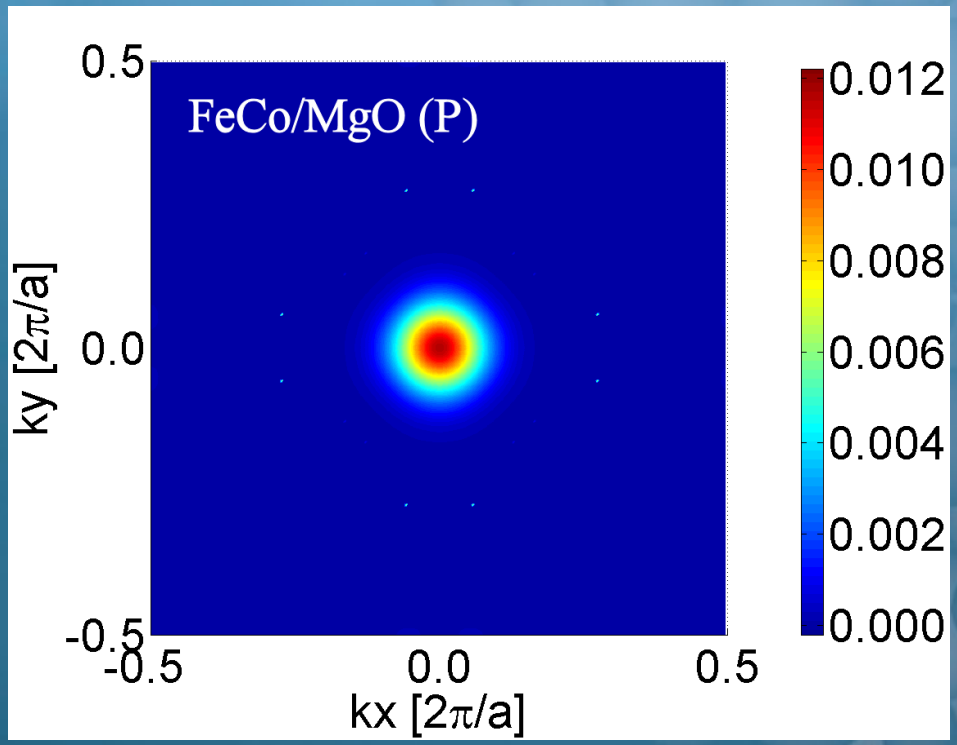
	G_P	G_{AP}	TMR (num.)	TMR (exp.)
Fe/MgO	239	3.23	$\approx 7300\%$	247%
Co/MgO	179	4.88	$\approx 3600\%$	507%
FeCo/MgO	106	1.54	$\approx 6800\%$	300%

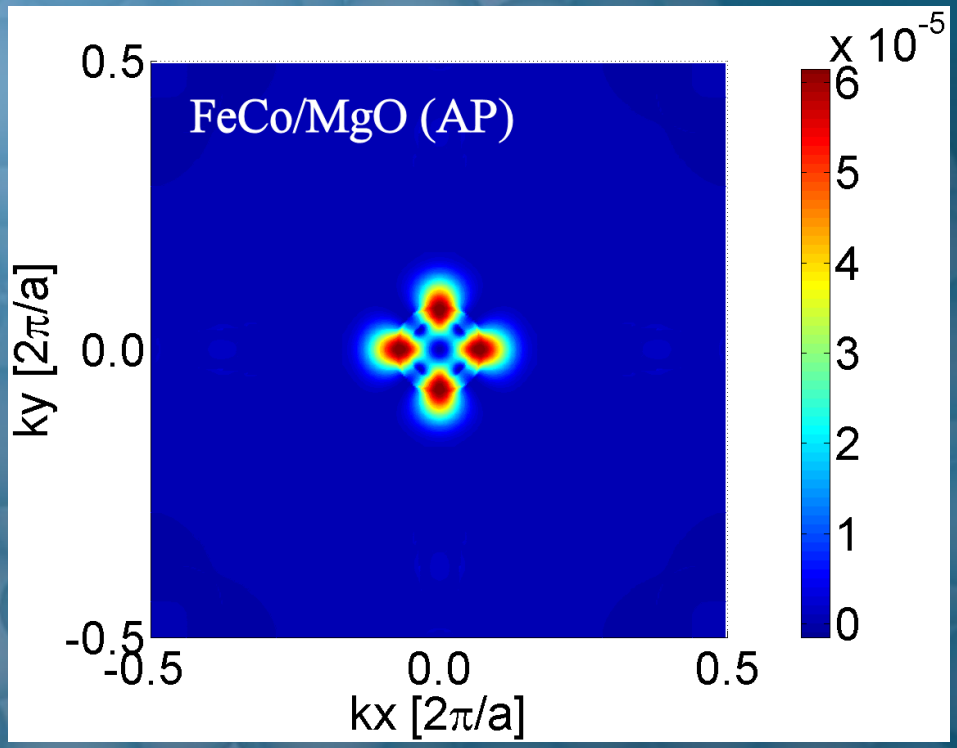
- The TMR values are large
- The TMR values are of similar size (an order of magnitude larger than experimental values)

Yuasa *et al.*, Nat. Mater. **3**, 868 (2004)
Yuasa *et al.*, Appl. Phys. Lett. **89**, 042505 (2006)
Parkin *et al.*, Nat. Mater. **3**, 862 (2004)

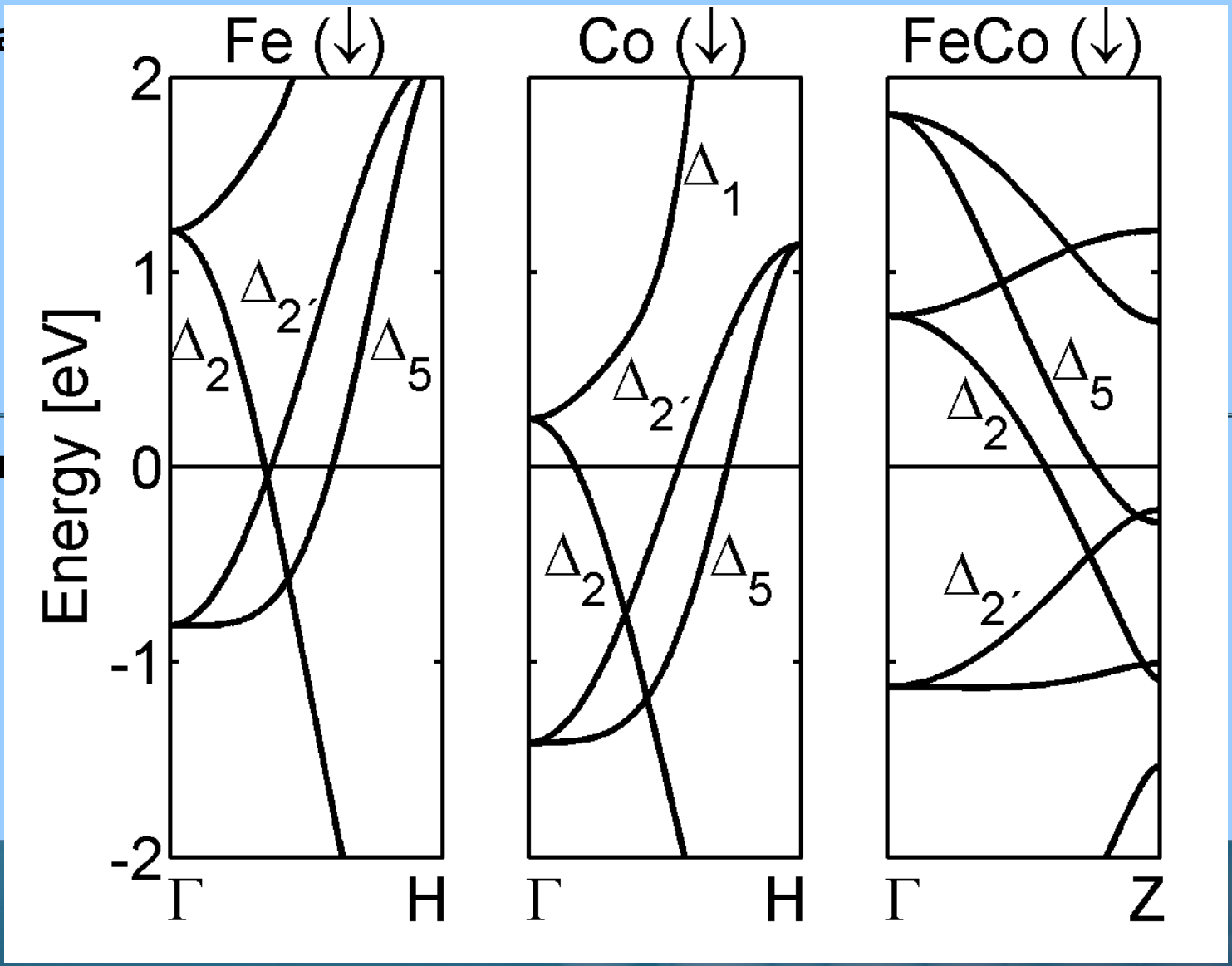
Tunneling mechanisms (transmission spectra)

- Transmission as function of k-vector for the parallel- and anti-parallel configurations

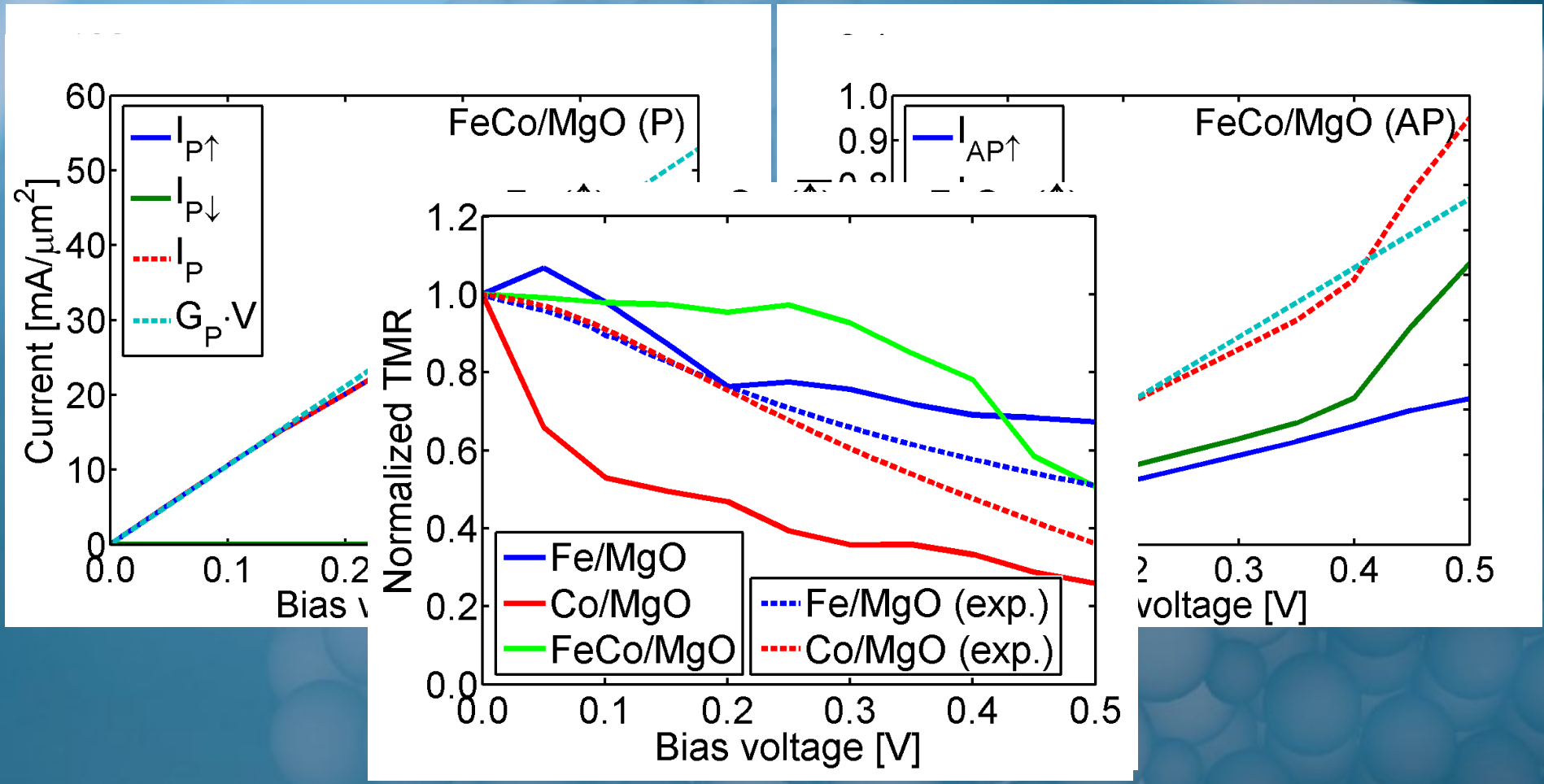




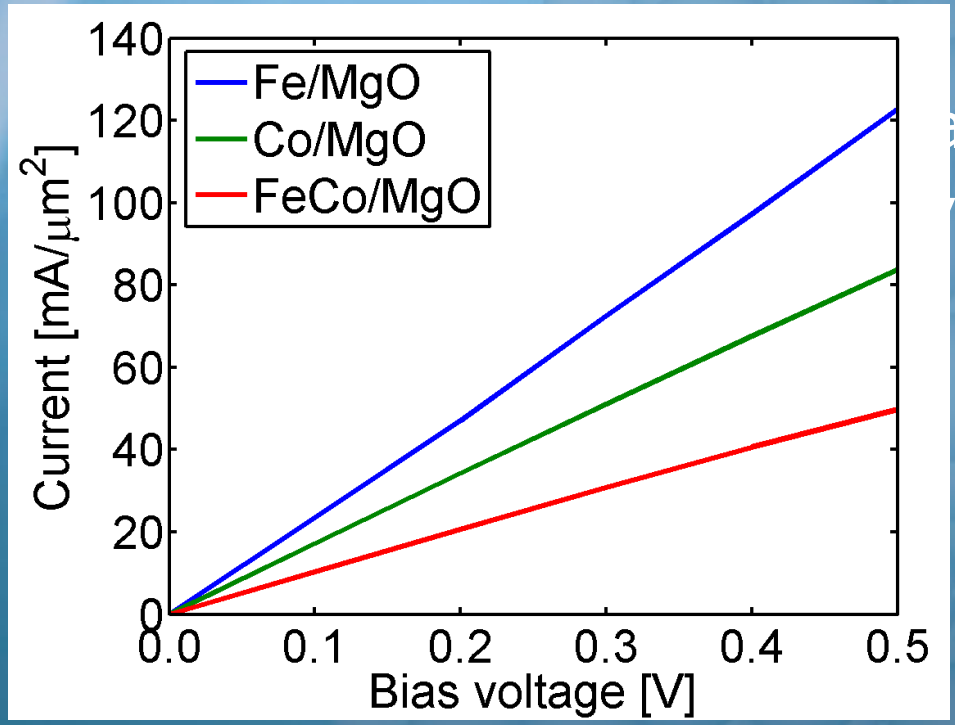
Tunneling mechanisms (transmission eigenstates)

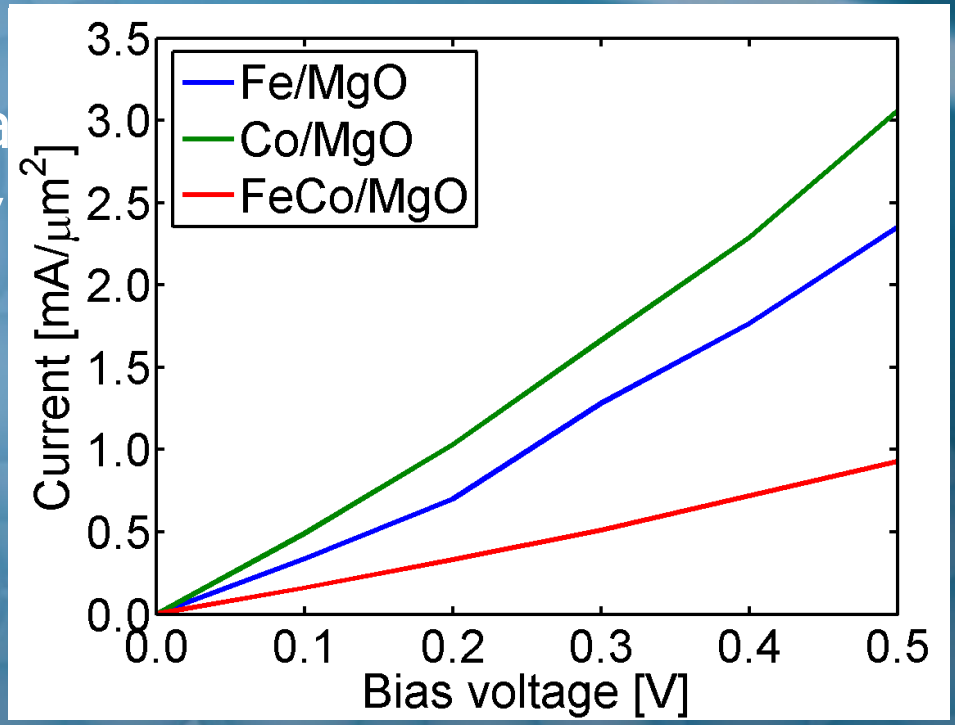


Effects of an applied bias voltage



Voltage dependence of the tunneling mechanisms





- The t… stly on the e…
- The effect of an increasing bias voltage is to "sample" an increasingly larger energy window

$$I_\sigma(V) = \frac{e}{h}\int_{-eV/2}^{eV/2} T_\sigma(0,E)\,\mathrm{d}E$$

Here's what I wanted to tell you

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Thank you for your attention...

... and thank you for your contribution





atomistix