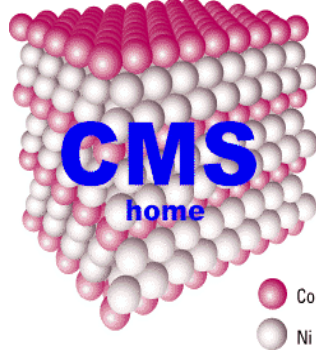
Materials-specific theory for Spin Electronics

P.J.Kelly

Computational Materials Science
Faculty of Science and Technology & MESA+
University of Twente

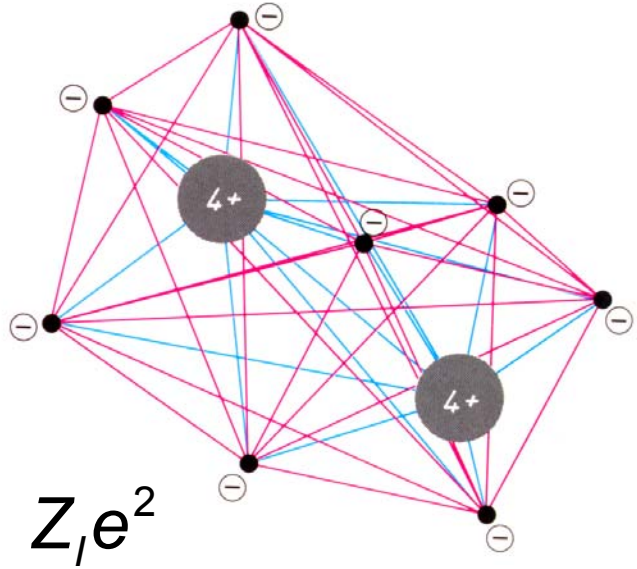


Computational Materials Science

Mission:

To understand the magnetic, optical, and electrical properties of condensed matter and the relationship between these physical properties and its chemical composition and atomic structure.

The problem ….



N particle Schrödinger equation

$$\hat{H}\Psi(r_1, r_2, \ldots, r_N) = E\Psi(r_1, r_2, \ldots, r_N)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j}^{N}\frac{e^2}{|r_i - r_j|} - \sum_{I}\sum_{i\neq j}^{N}\frac{Z_I e^2}{|r_i - R_I|}$$

If we know Ψ, then we know everything
… but the Schrödinger equation can only be solved exactly for VERY small systems:

- analytically for N=1 and quasi 1-D problems (free electron, H atom, harmonic oscillator)
- numerically for N small and high symmetry (light atoms, homogeneous electron gas)

Condensed Matter:

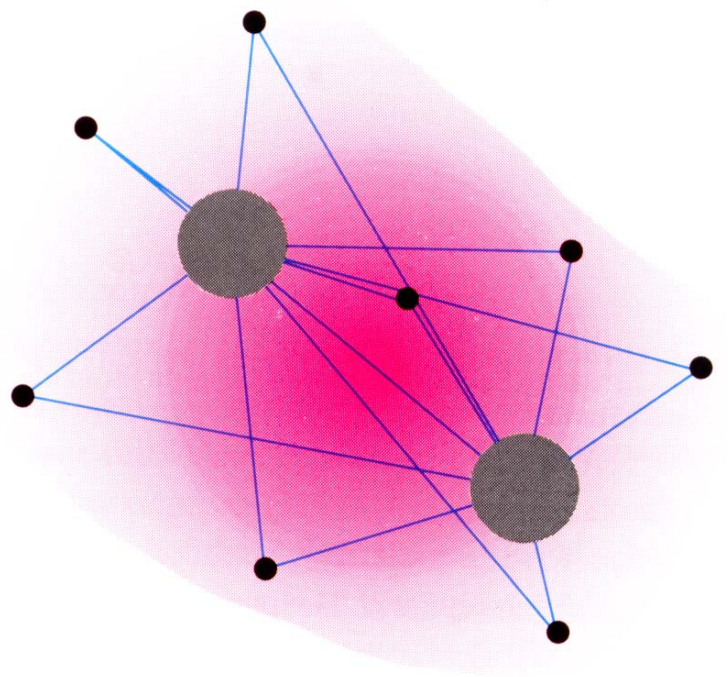
N ~ 10^{23} electrons/cm^3

The solution ….

"Density Functional Theory"

• valid for electronic ground state

Starting point for:
• structure of materials
• magnetism
• dynamics (phonons)
• transport theory
• excitations (optical properties)
etc.



Reduce linear differential equation for a function in 3N variables to N coupled non-linear integro-differential equations for N functions in 3 variables

DFT: For the electronic ground state, the total energy only depends on the electron density

$$E[n] = T[n] + \int \sum_I \frac{Z_I n(r)}{|r - R_I|}\, dr + \frac{1}{2}\sum \frac{n(r)n(r')}{|r - r'|} dr\, dr' + E_{xc}[n]$$

Use the variational principle for the ground state energy:

$$\left[-\frac{\nabla^2}{2} + \upsilon_{eff}(r)\right]\psi_i(r) = \varepsilon_i\, \psi_i(r)$$

Kohn-Sham equations of DFT

$$n(r) = \sum_i^N |\psi_i(r)|^2$$

electron density

$$\upsilon_{eff}(r) = \sum_I \frac{Z_I}{|r - R_I|} + \sum_{i \neq j}^N \frac{n(r')}{|r - r'|} dr' + \boxed{\frac{\delta E_{xc}(n)}{\delta n(r)}}$$

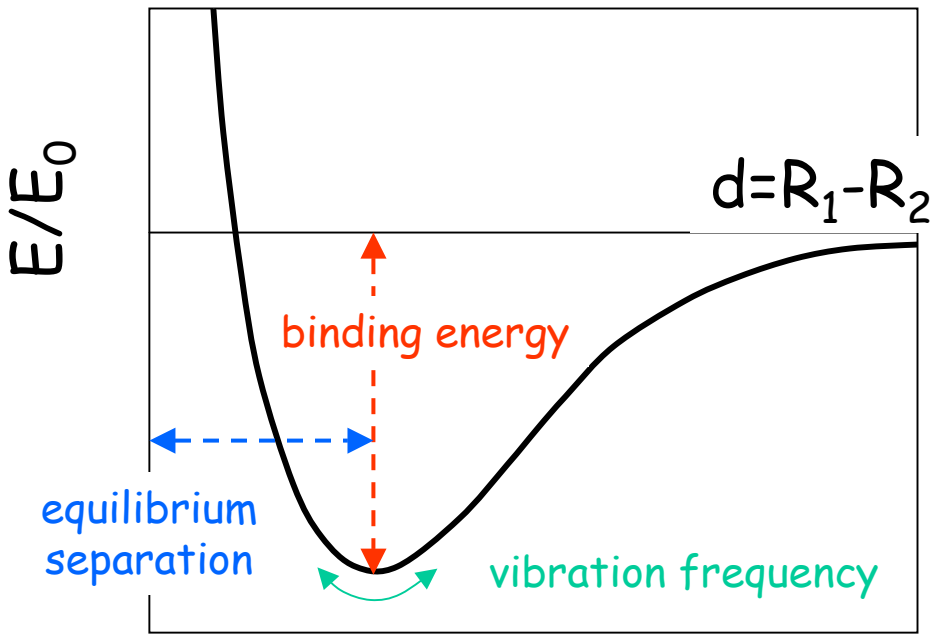
Effective potential:

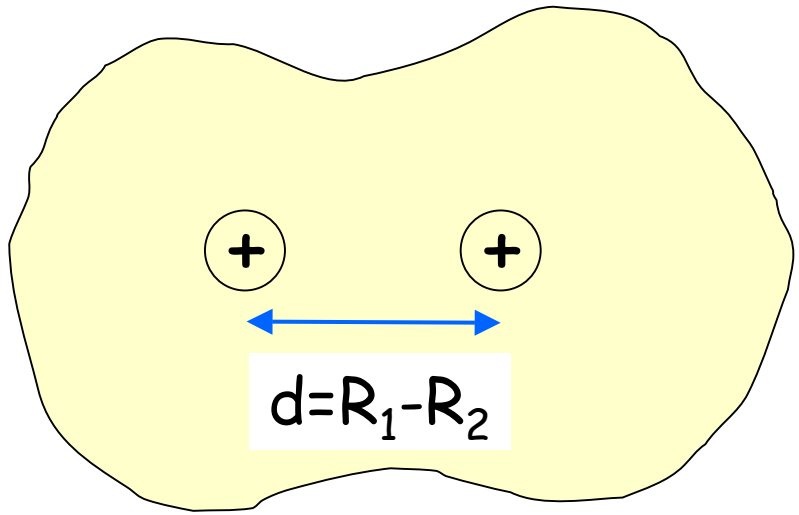
Local Density Approximation

… then calculate the total ground state energy

$$E[n] = T[n] + \int \sum_I \frac{Z_I n(r)}{|r - R_I|}\, dr + \frac{1}{2}\sum \frac{n(r)n(r')}{|r - r'|}\, dr\, dr' + E_{xc}[n]$$

e.g. the H_2 molecule





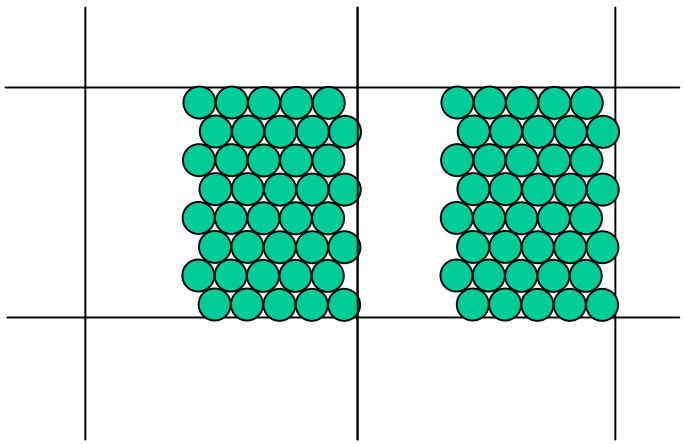
Theoretical Methods: ab-initio

Parameter-free: the only input to the calculations are the constants occuring in the Schrödinger Equation: e, h, m_e, c (Dirac eqn)

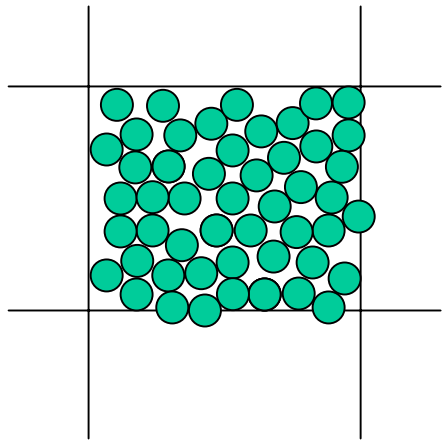
Translational symmetry

For a solid with N ~ 10^{23} per cm^3 we need to make use of translational symmetry to make solution of KSEs tractable.

Use repeated supercells to model:

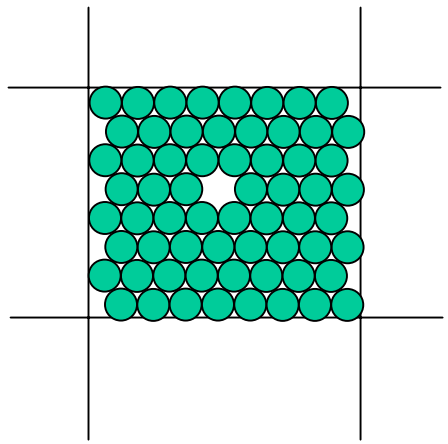


Amorphous or Liquid phases

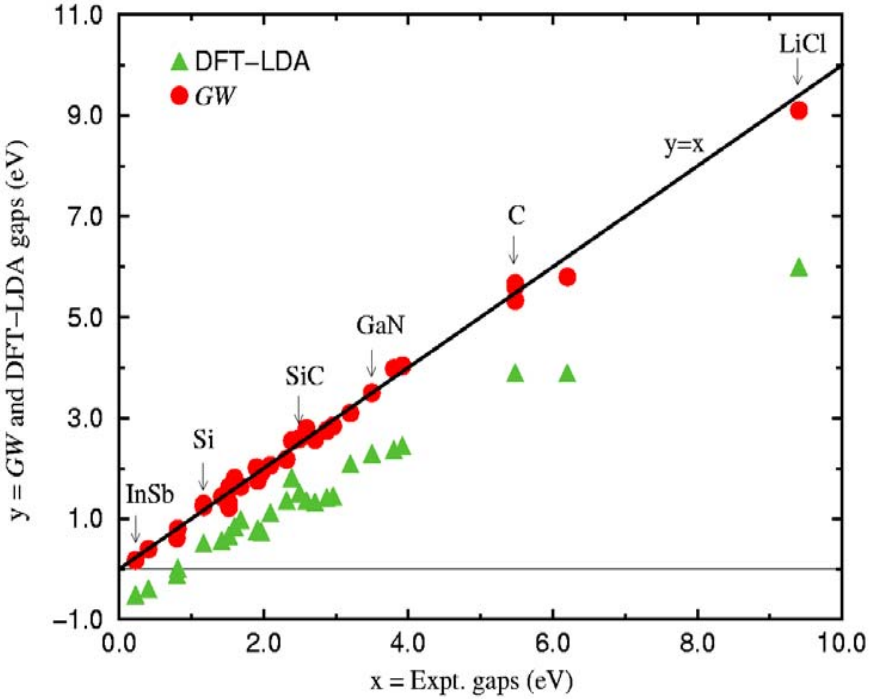


Surfaces

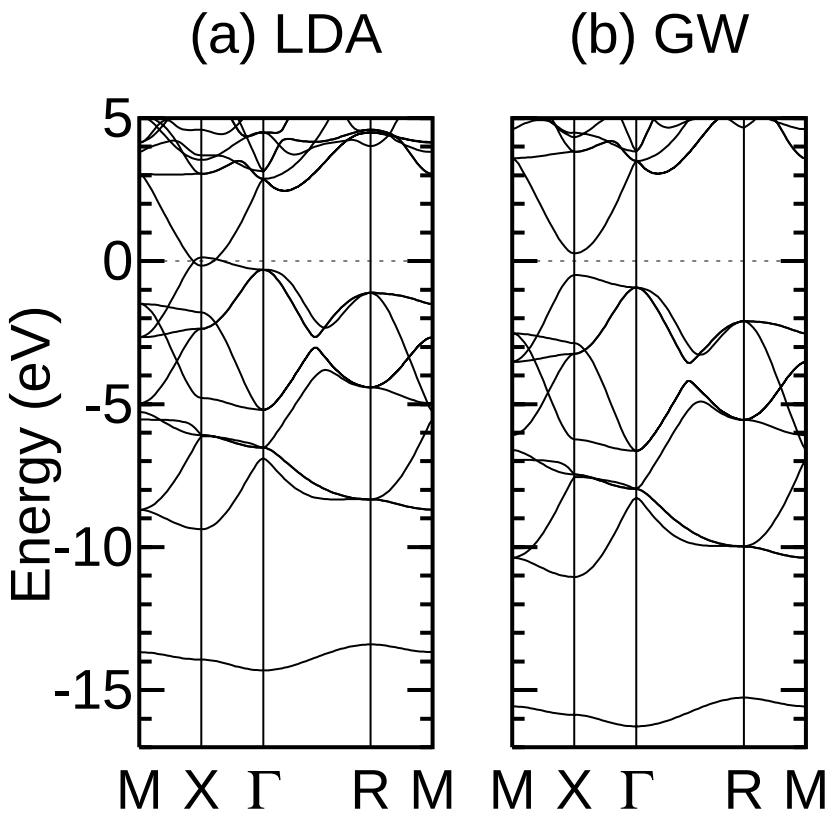
Point or extended defects etc.



DFT is a theory for ground state properties. The eigenvalue spectrum yields incorrect values of the gap



Doped divalent hexaborides CaB_6 are high temperature magnetic semiconductors

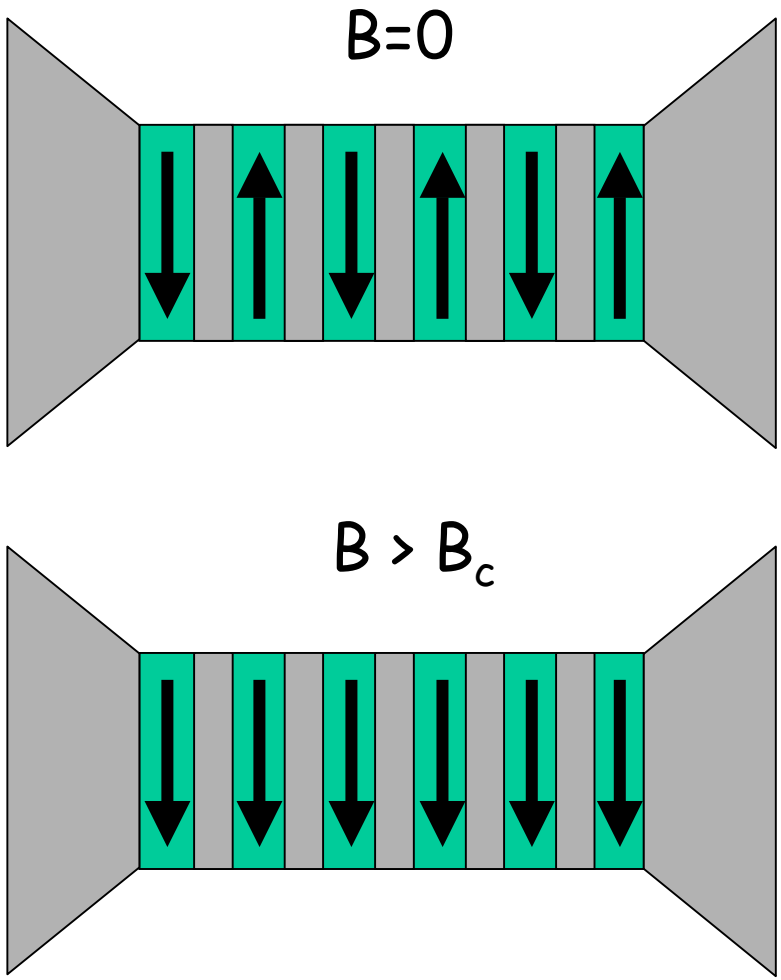


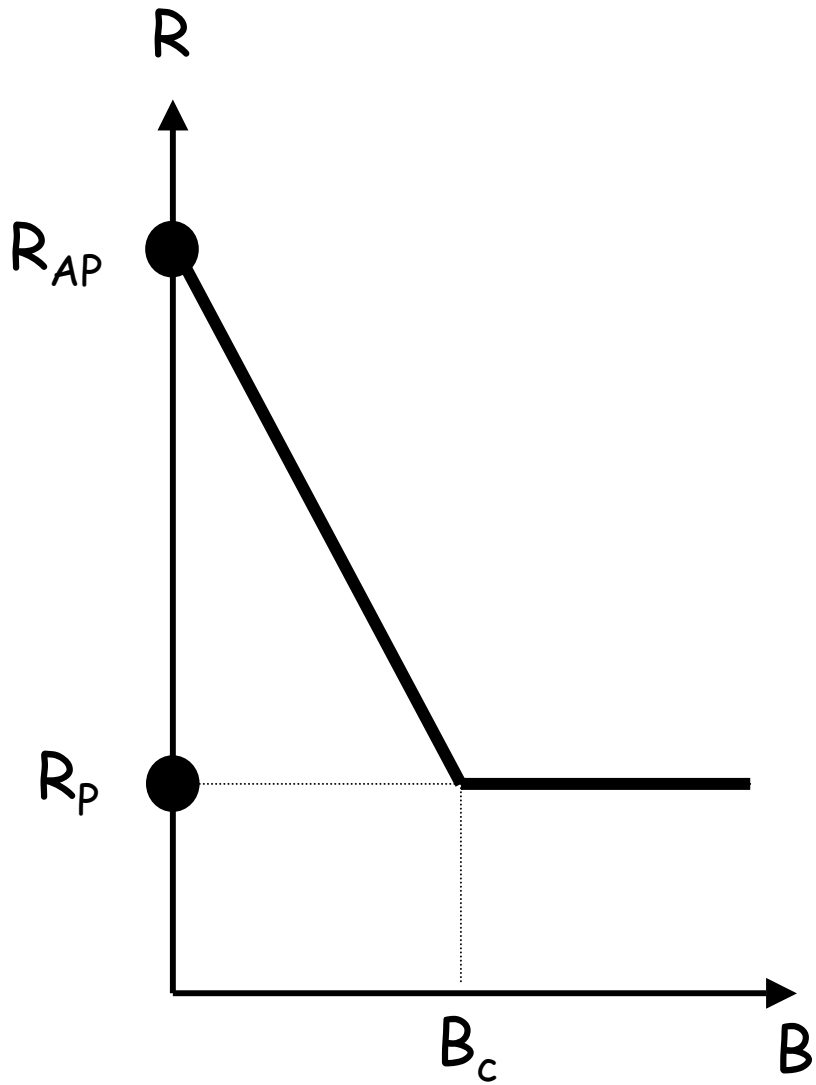
Solve a "quasiparticle" equation use the "GW" approximation

Tromp et al. PRL 87 (2001)

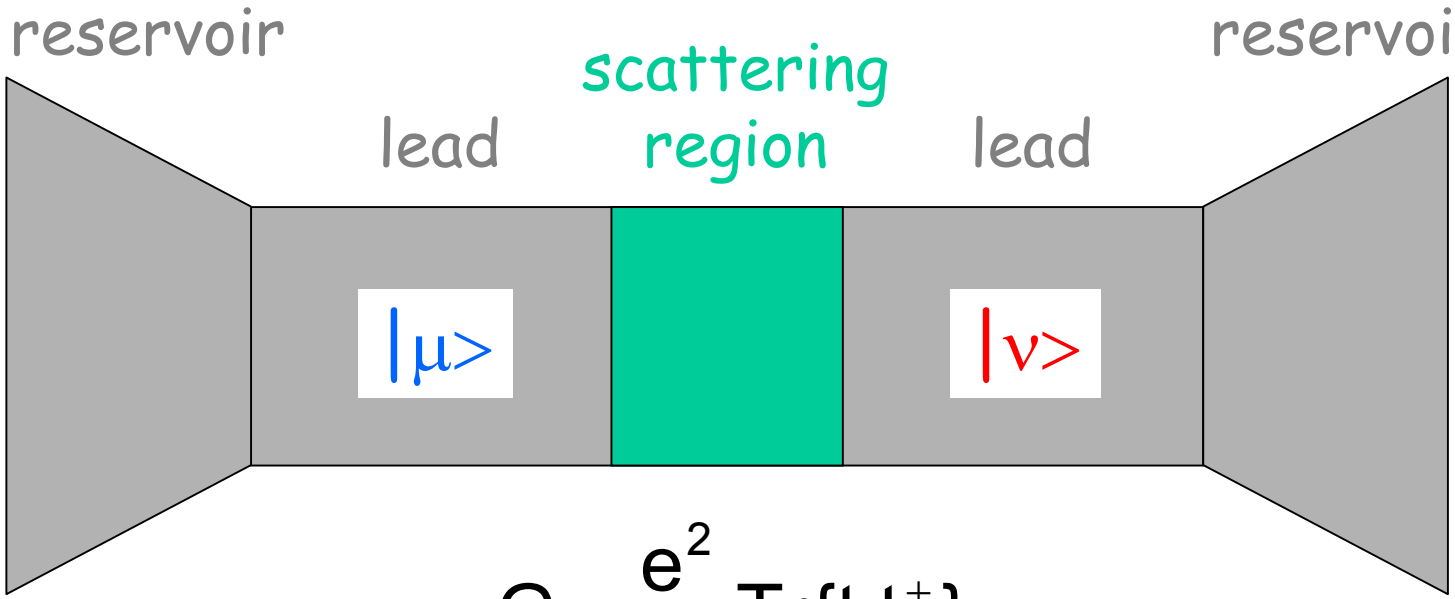
Spin Transport

Giant MagnetoResistance (GMR)





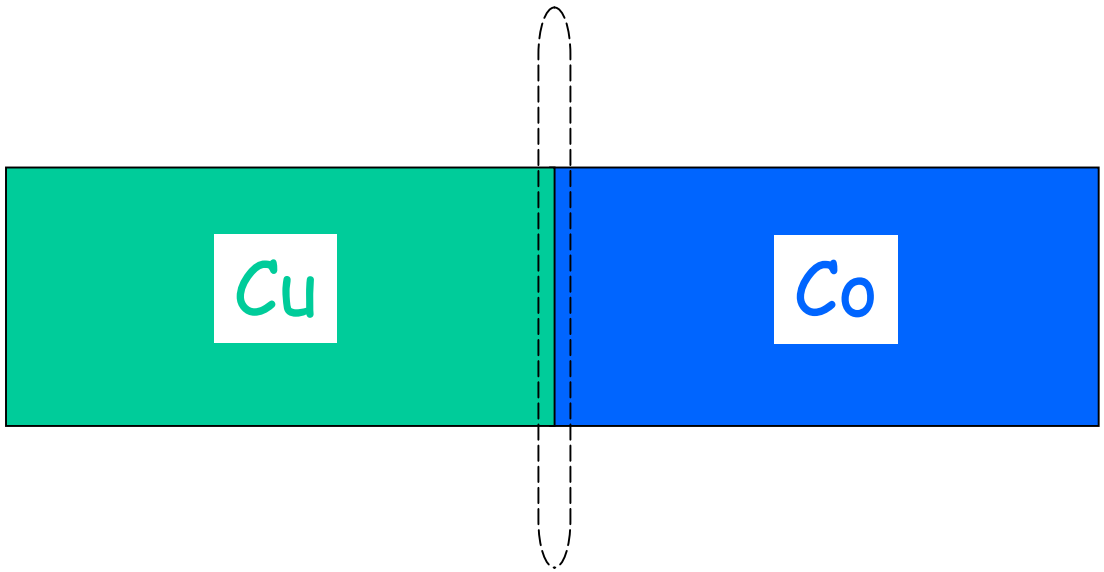
Transport theory: Landauer-Büttiker



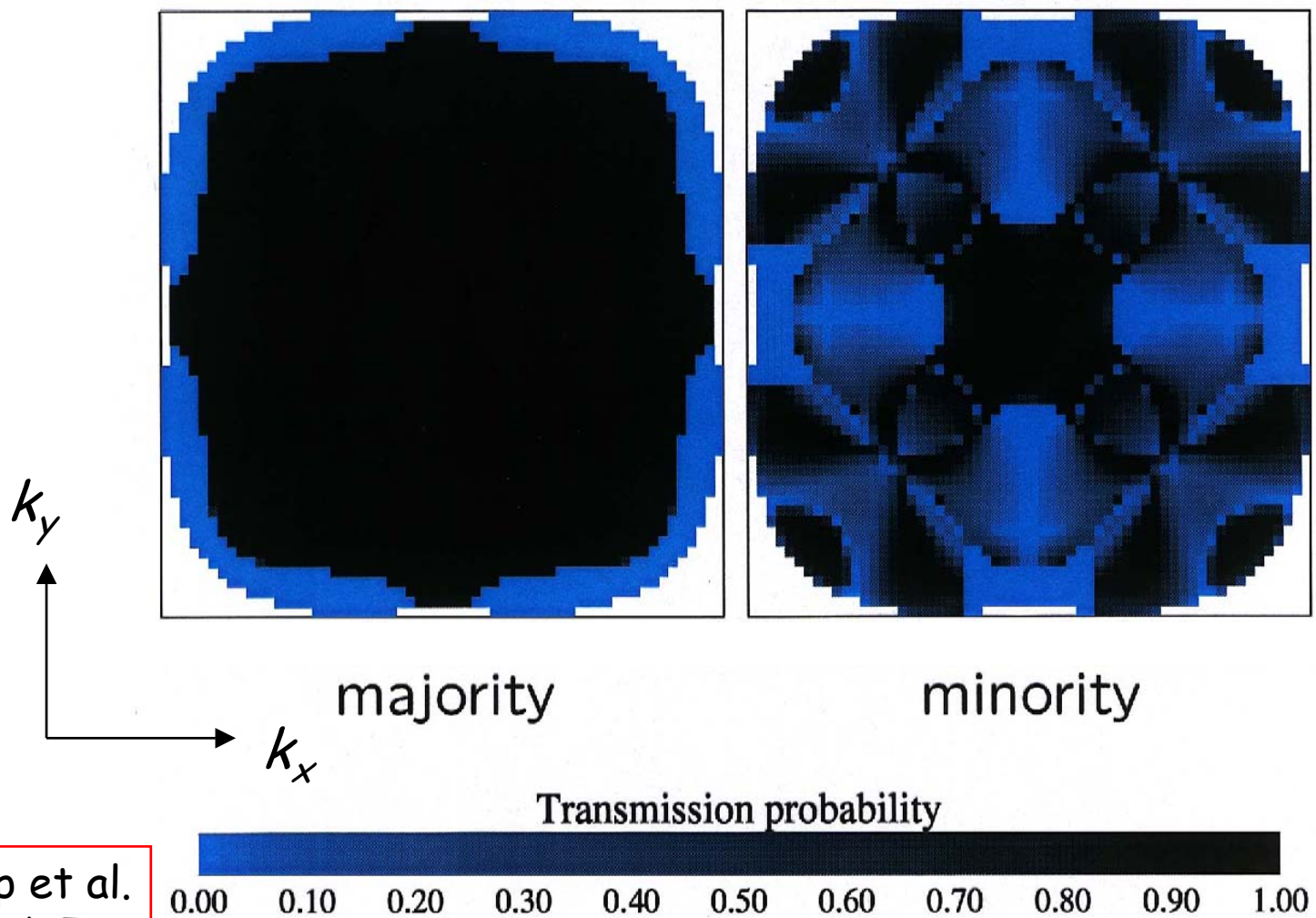
$$G = \frac{e^2}{h} Tr\{t\, t^{+}\}$$

The transmission matrix element $t_{\mu\nu}$ describes the probability amplitude that a state $|\mu\rangle$ in the left lead is transmitted through the scattering region into a state $|\nu\rangle$ in the right lead.

Single clean interface between (almost) perfectly lattice matched Cu and Co



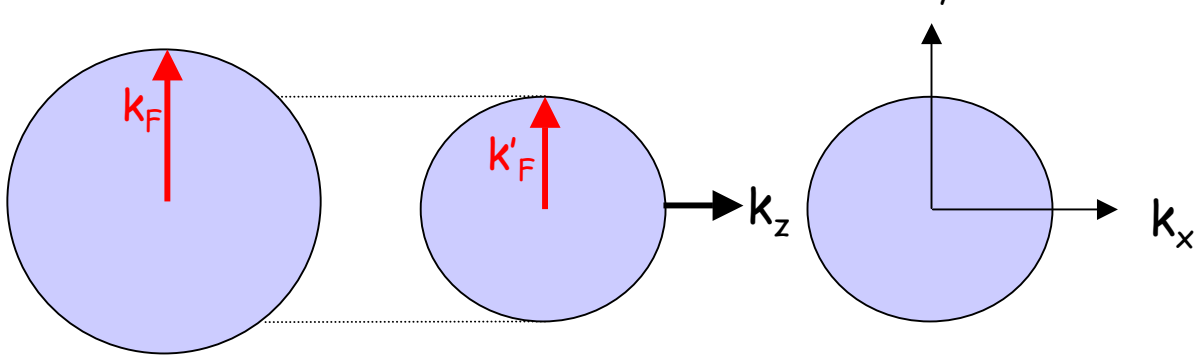
Ab initio transmission probabilities $T(k_x,k_y)$ for Cu → Co(100)



Schep et al.
PRB '97

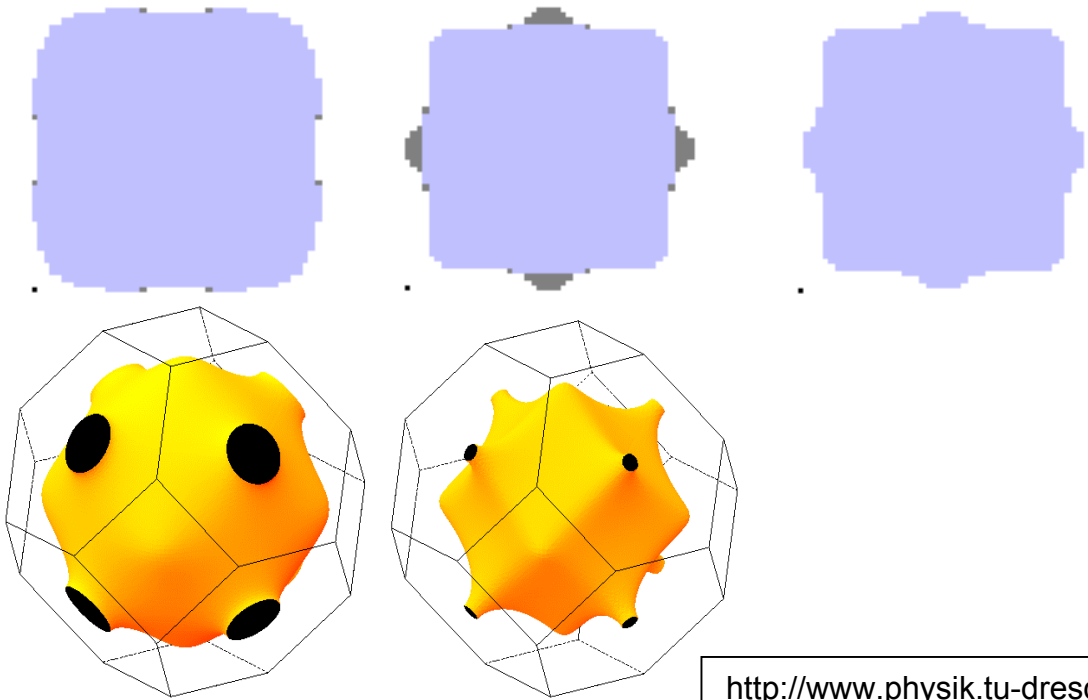
Fermi surface projections

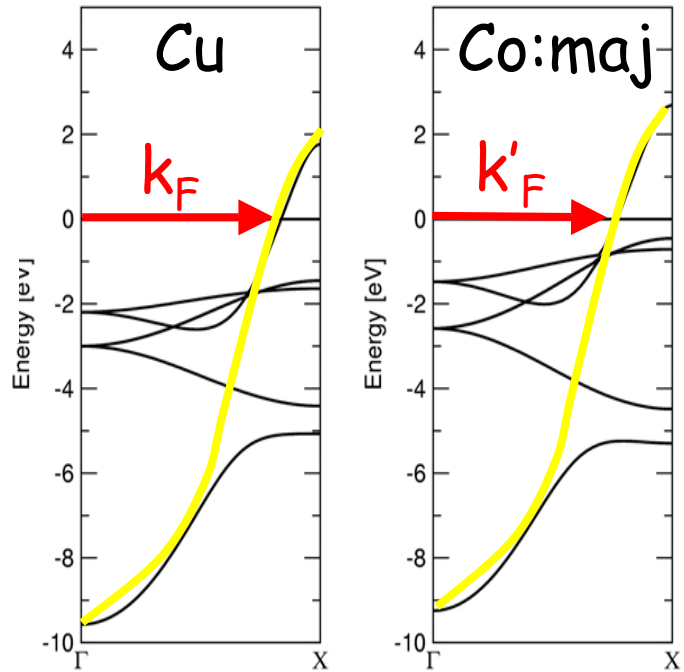
$T(k_x,k_y)$



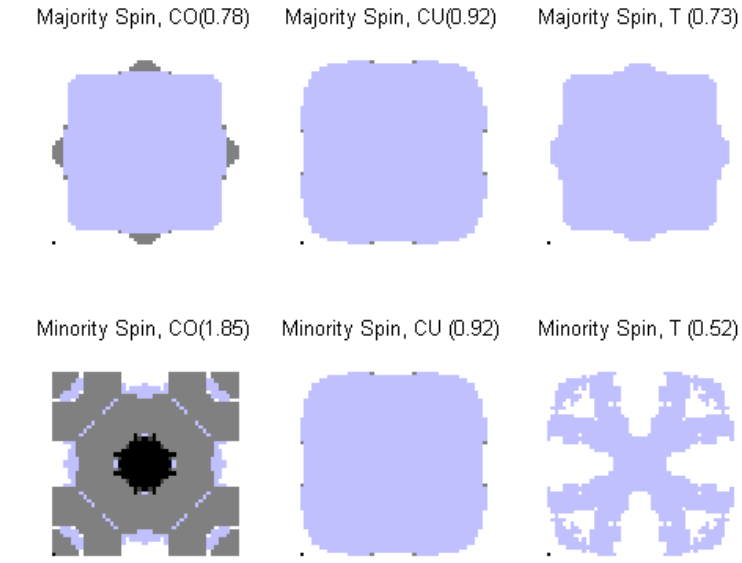
Majority spins

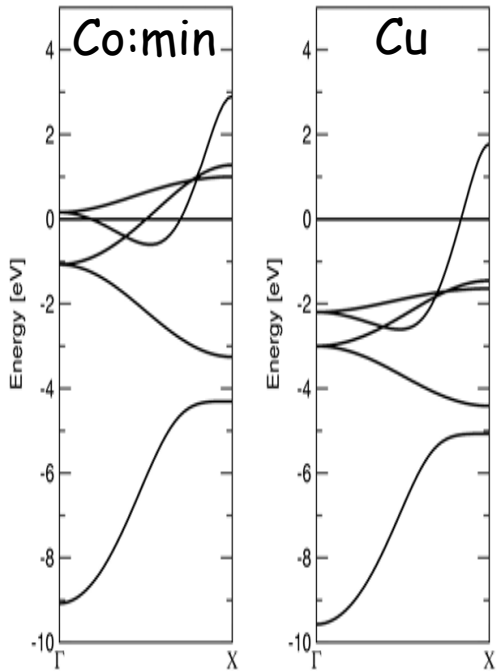
Majority Spin, CU(0.92) Majority Spin, CO(0.78) Majority Spin, T (0.73)



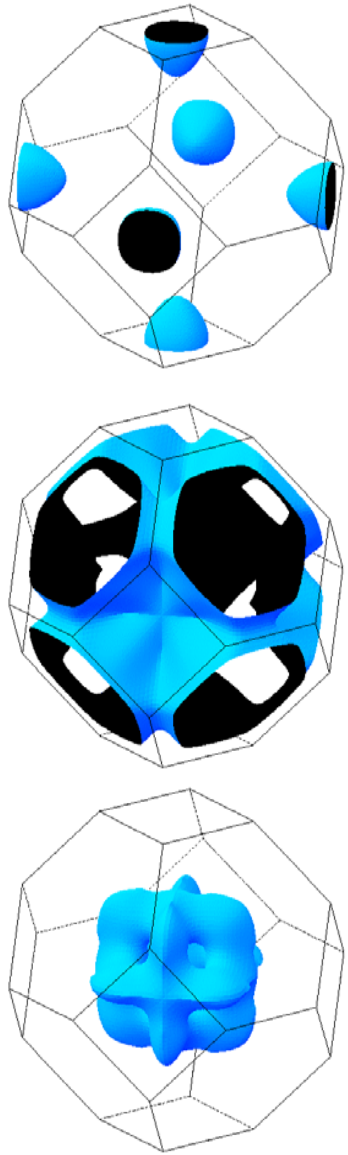


http://www.physik.tu-dresden.de/~fermisur/





Fermi surfaces of fcc-Co: minority-spin



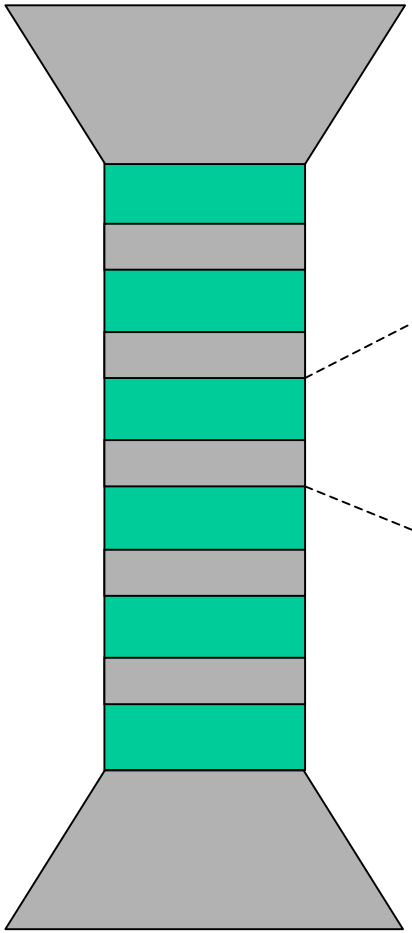
http://www.physik.tu-dresden.de/~fermisur/

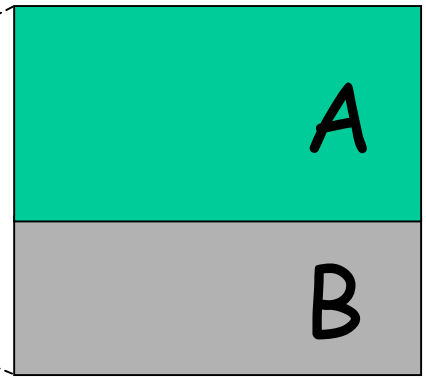
- Electrons can be strongly reflected at a perfect interface (no disorder) between two different metals because of bandstructure mismatch

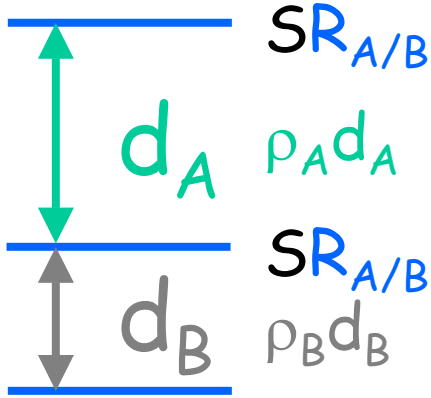
- Interface disorder can increase the interface transparency

- The transmission through an interface into a ferromagnetic material can be strongly spin-dependent

Resistor Model



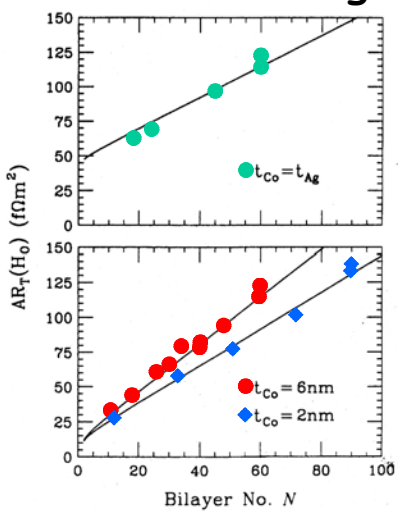


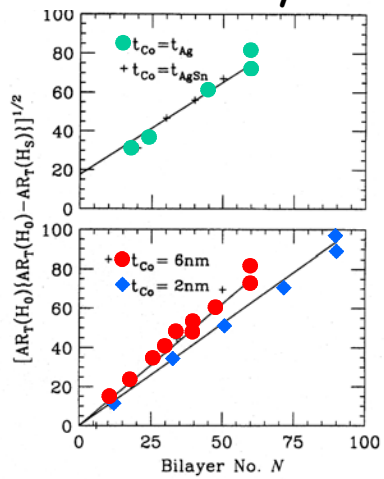


$$SR_T = N(SR_{A/B} + \rho_A d_A + SR_{A/B} + \rho_B d_B)$$

GMR is mainly determined by the spin-dependence of $R_{A/B}$

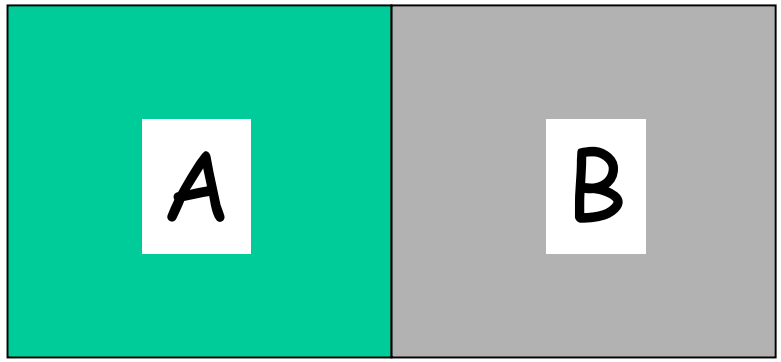
Michigan State University





Interface Resistances

- $$\frac{1}{R} = G = \frac{e^2}{h} Tr\{t\, t^+\}$$



But suppose A=B; then R≠0 ?

Correction for Sharvin resistance

$$SR_{A/B} = \frac{Sh}{e^2}\left[\frac{1}{tr\{t\, t^+\}} - \frac{1}{2}\left(\frac{1}{N_A} + \frac{1}{N_B}\right)\right]$$

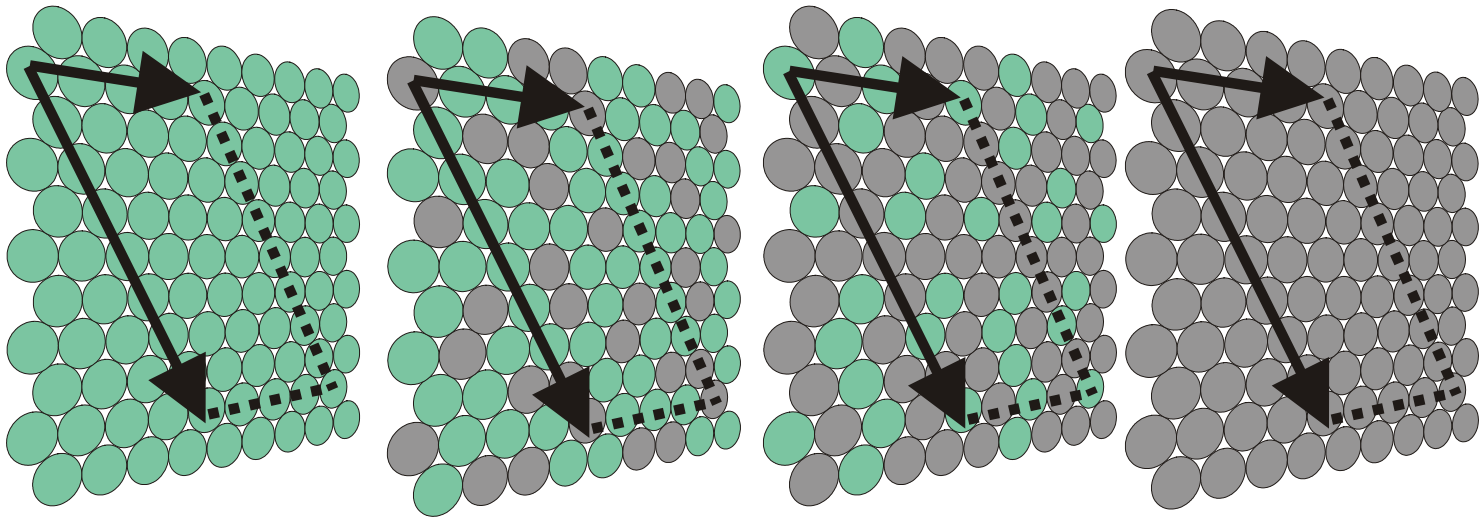
Co/Cu

fΩm²	Orientation	majority	minority
calculation	(100)	0.33	1.79
calculation	(111)	0.39	1.46
expt (MSU)	(111)	0.26±0.06	1.84±0.14

Schep et al. PRB '97

Model disorder in lateral supercells as two layers of alloy.

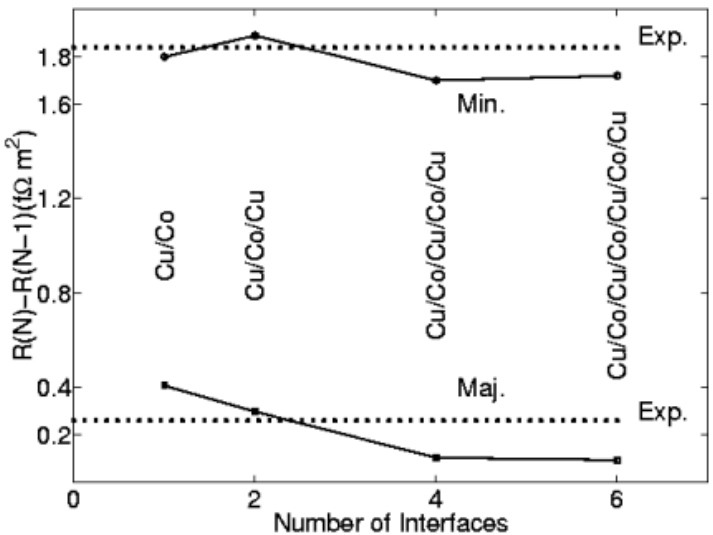
A



B

Cu/Co fcc(111)	R↑ fΩm²	R↓ fΩm²
Clean	0.39	1.46
2x50-50 alloy	0.41	1.82
Expt (MSU)	0.26±0.06	1.84±0.14

Xia et al. PRB '01



Applications

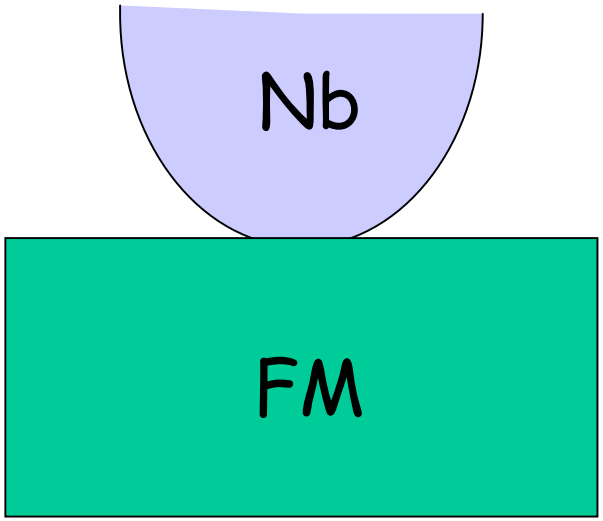
- GMR
  - CPP - Interface resistances
  - CIP
- Transport through domain walls
- JMR
- Current induced torque
- Spin injection in Fe/InAs
- Andreev reflection at F/S interfaces
- Enhancement of Gilbert damping
- ....

Applications

- GMR
  - CPP - Interface resistances
  - CIP
- Transport through domain walls
- JMR
- Current induced torque
- Spin injection in Fe/InAs
- Andreev reflection at F/S interfaces
- Enhancement of Gilbert damping

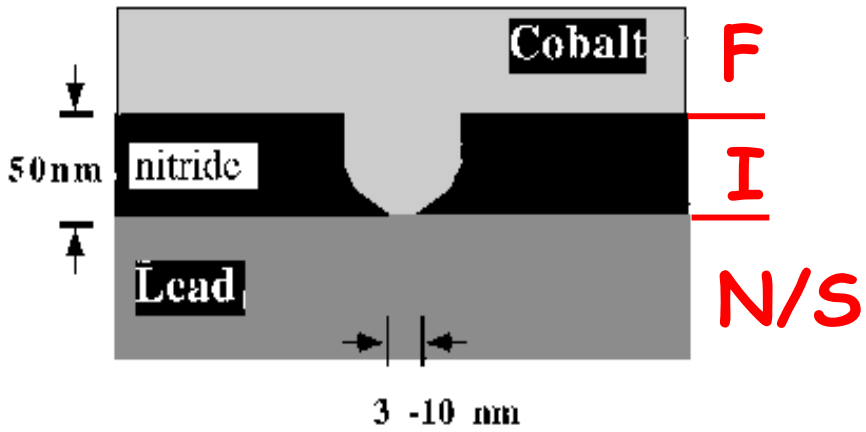
Measure spin-polarization with F/S point contacts

- Mechanical point contacts
  Soulen et al.
  Science **282** (1998)



- Simple
- Flexible
- Poorly characterized

- Thin-film point contacts
  Upadhyay et al.
  PRL **81** (1998)



- Well characterized
- Difficult
- Inflexible

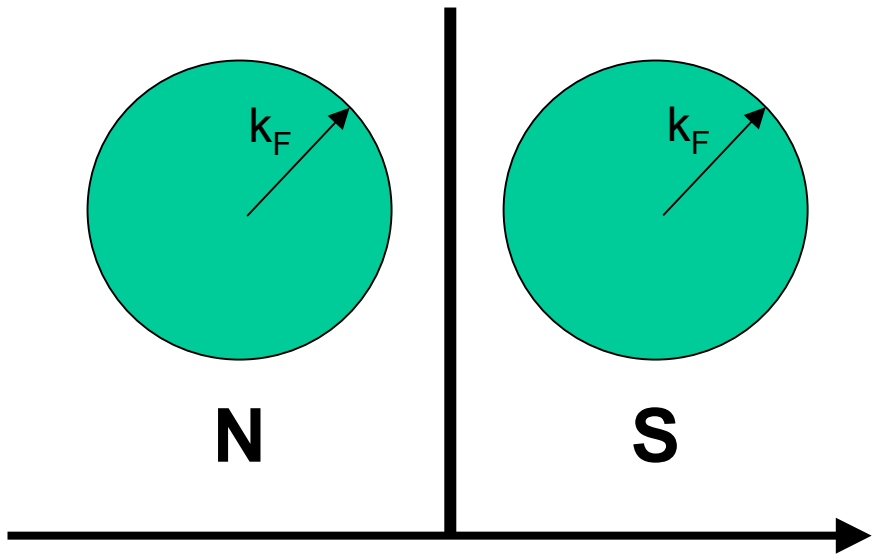
Near perfect fit to experiment using BTK theory without any spin dependent interface transparency !

BTK theory:

Model interfacial scattering (of free electrons) by $Z\upsilon_F\delta(x)$

Transmission $T = 1/(1+Z^2)$

Spin polarized situation
- two parameters: Z, P



Result of scattering theory for F/S interface:

$$G_{FS}(\varepsilon) = \frac{e^2}{h} \sum_{\sigma=\pm 1} Tr(1 - R_{ee}^{\sigma} R_{ee}^{\sigma\dagger} + R_{he}^{\sigma} R_{he}^{\sigma\dagger})$$

The conductance only depends on the normal state transmission and reflection matrices.

$$R_{ee}^{\sigma} = r_{FF}^{\sigma}(\varepsilon) + \alpha^2 t_{FN}^{\sigma}(\varepsilon) r_{NN}^{-\sigma *}(-\varepsilon) \frac{1}{1 - \alpha^2 r_{NN}^{\sigma}(\varepsilon) r_{NN}^{-\sigma *}(-\varepsilon)} t_{NF}^{\sigma}(\varepsilon)$$

and

$$R_{he}^{\sigma} = \alpha^* e^{-i\phi} t_{FN}^{-\sigma *}(-\varepsilon) \frac{1}{1 - \alpha^2 r_{NN}^{\sigma}(\varepsilon) r_{NN}^{-\sigma *}(-\varepsilon)} t_{NF}^{\sigma}(\varepsilon)$$

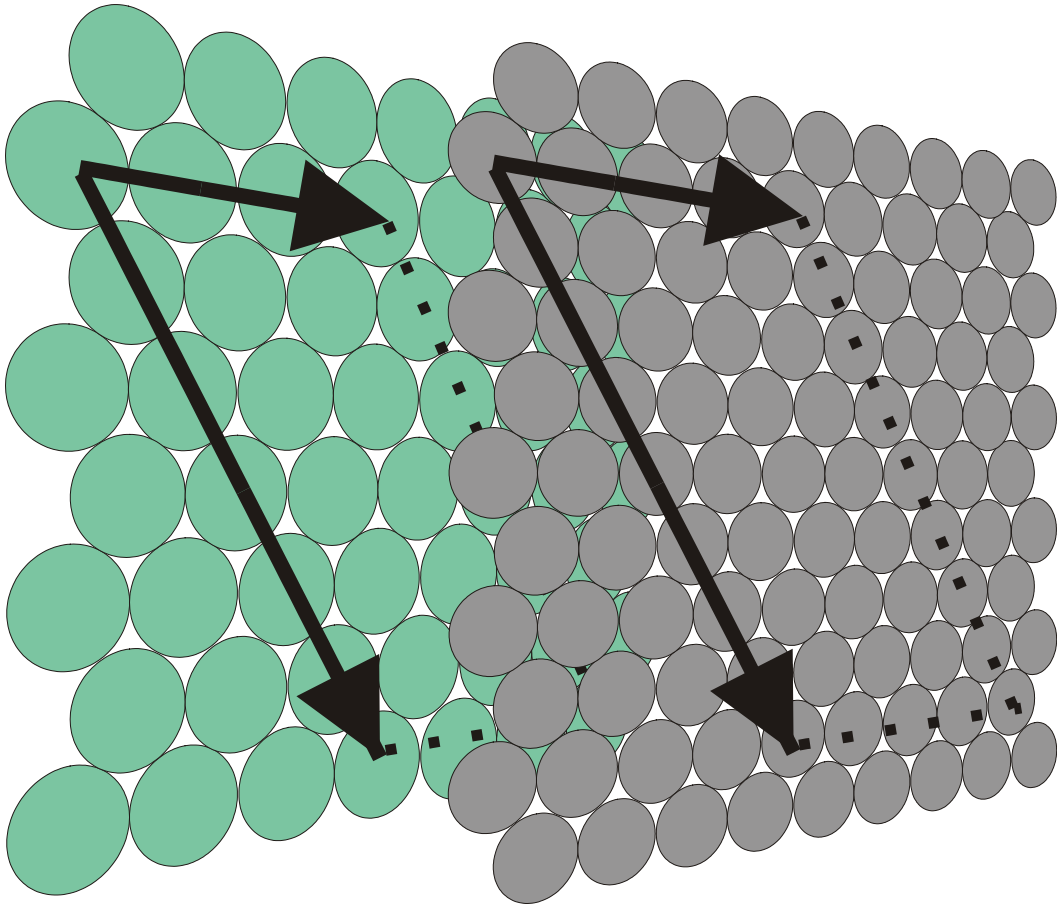
$$|\varepsilon| < \Delta_0 : \alpha = e^{-i \arccos(\varepsilon/\Delta_0)}$$

$$|\varepsilon| > \Delta_0 : \alpha = \left(\varepsilon - \mathrm{sgn}(\varepsilon)\sqrt{\varepsilon^2 - \Delta_0^2}\right)/\Delta_0, \; |\alpha| < 1$$

Rev. Mod. Phys. **69** (1997);
J. Phys. Cond. Matt. **10** (1998)

$$eI(V) = \int d\varepsilon \left[f(\varepsilon) - f(\varepsilon + eV) \right] G_{FS}(\varepsilon)$$

Large lattice mismatch

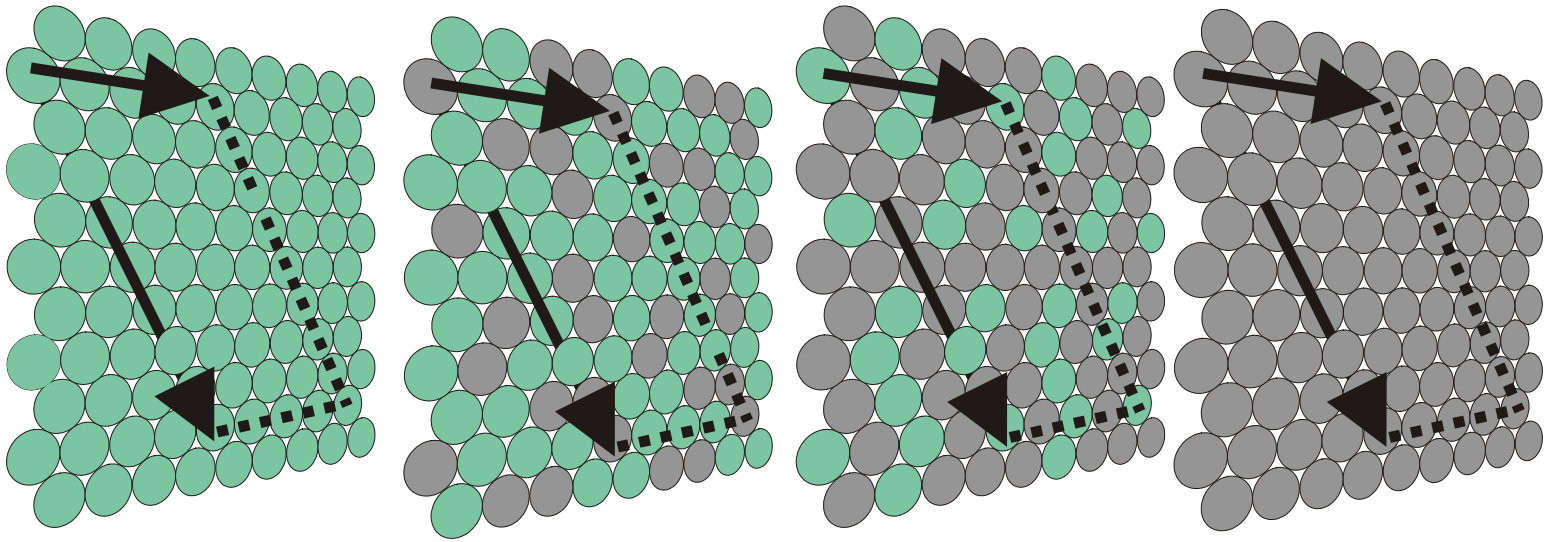


Pb: 4x4 Cu: 5x5

Because of the large lattice mismatch we use a lateral supercell with
3x3 Pb atoms to match
to
4x4 Cu (Ni, Co) atoms
or
4x4 Pb atoms to match
to
5x5 Cu (Ni, Co) atoms.

Model disorder in lateral supercells as two layers of alloy.

A

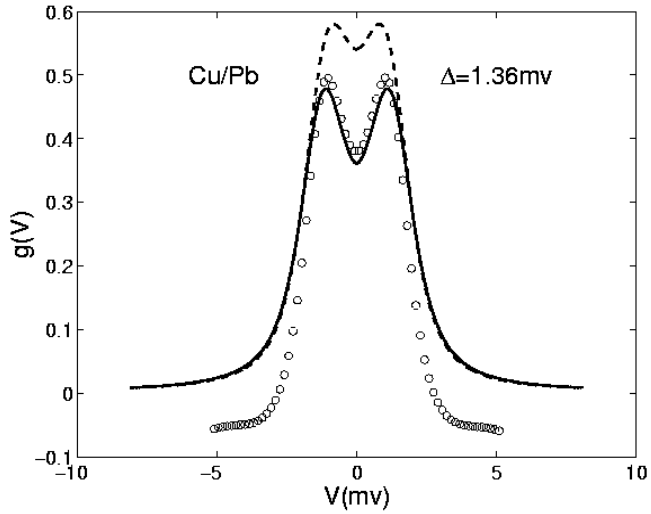


B

Andreev Reflection

Results: V=0

$G_{FS}(0)/G_{FN}(0)$	Cu/Pb	Ni/Pb	Co/Pb
Clean	1.54	1.29	1.08
Rough	1.36	1.16	1.00
Expt.	1.38	1.18	1.13



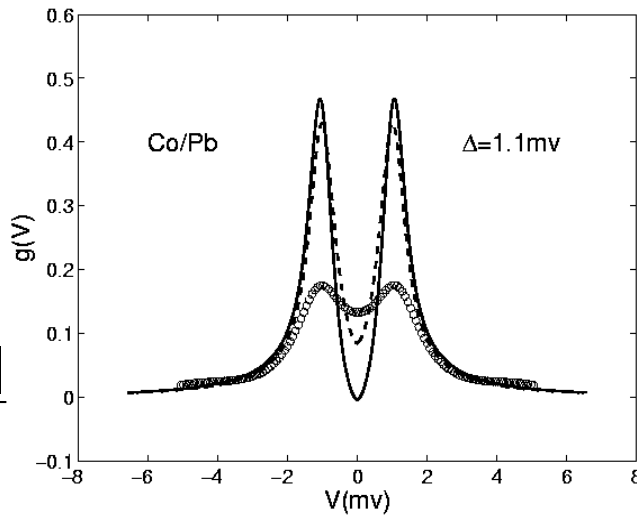
Interface

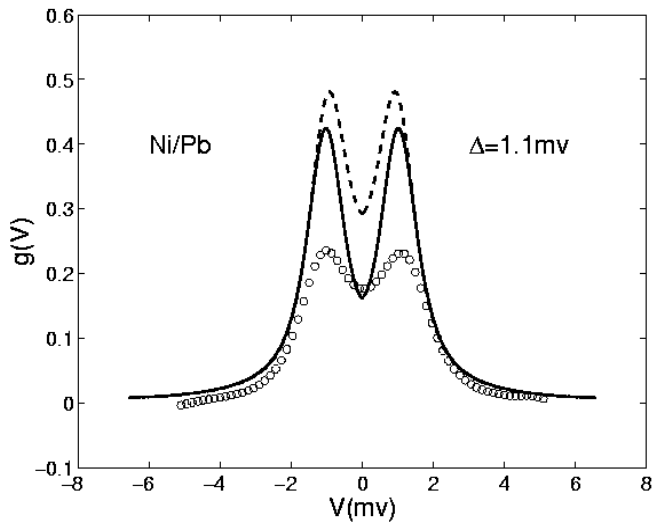
Clean

Disordered

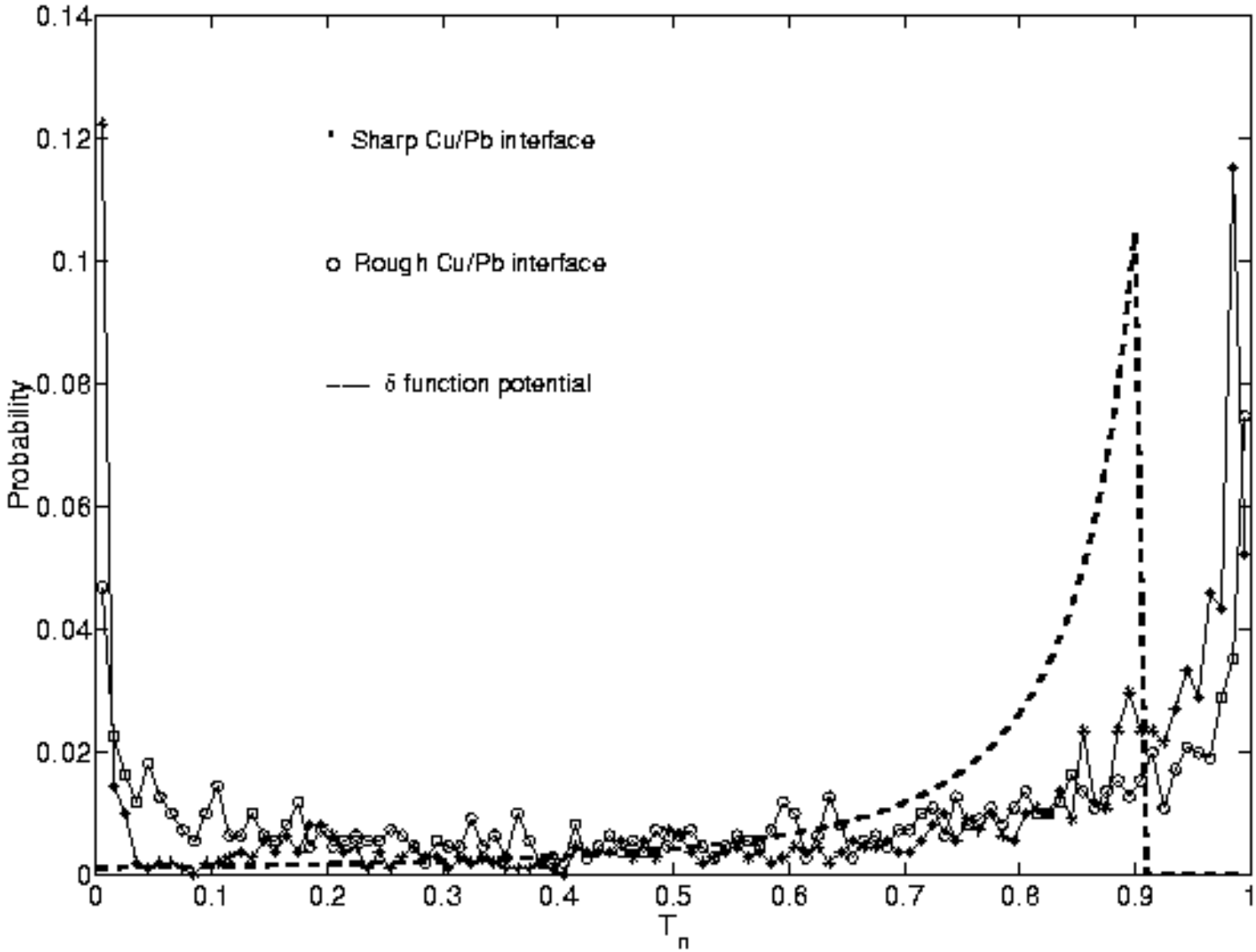
Expt.

$$g(V) = \frac{|G_{FS}(V) - G_{FN}(0)|}{G_{FN}(0)}$$





Distribution function of tranmission matrix eigenvalues



Xia et al. PRL **89** (2002)

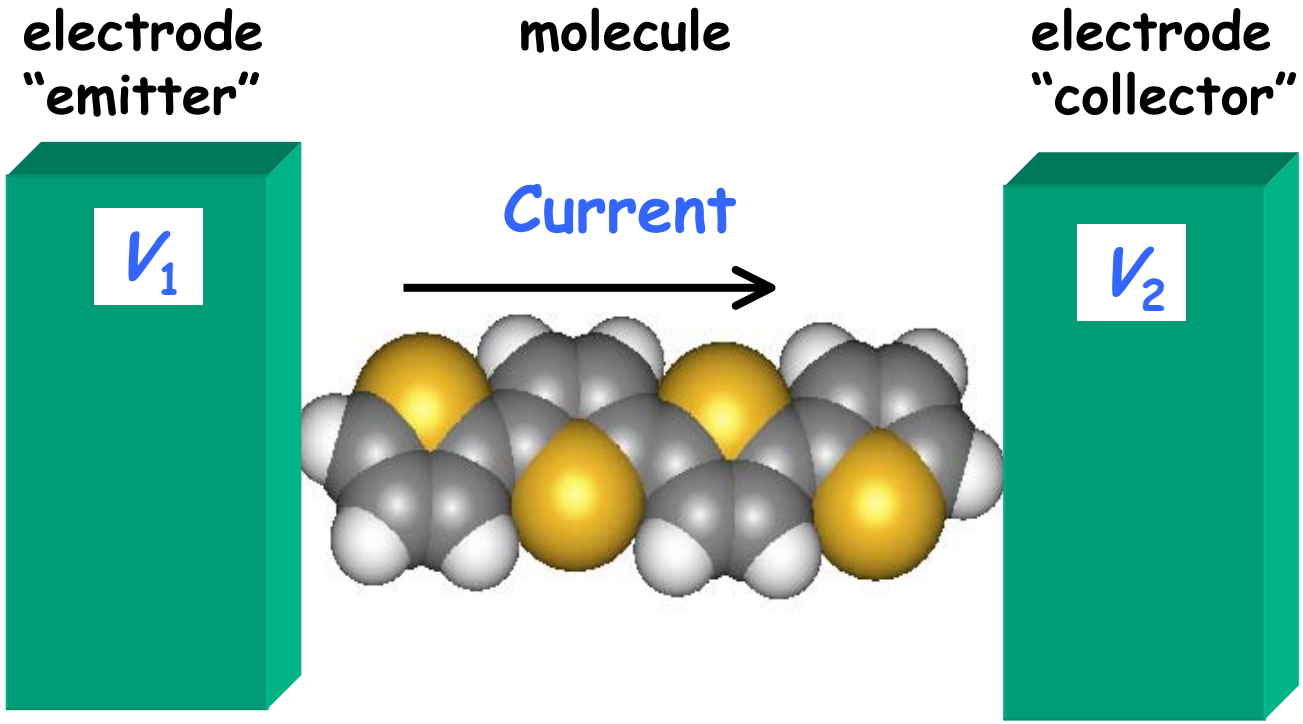
Conclusions

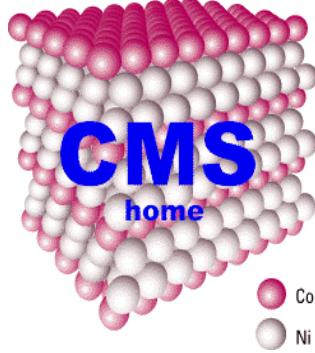
The good agreement obtained fitting theory with a simple generalization of BTK theory to ferromagnets is misleading (also Lancaster group).

The spin-dependent transmission through an A/B interface $T_{A/B}$ is a property of the interface and cannot be factored into an A part and a B part characteristic of the bulk materials.

BTK theory doesn't describe transport at a F/S interface and needs to be extended – include Zeeman splitting in fringing fields ?

Molecular Electronics





Work done in collaboration with:

Twente

K. Xia (Beijing)
M. Zwierzycki
S. Gerritsen
M. Talanana

I. Turek (Brno)

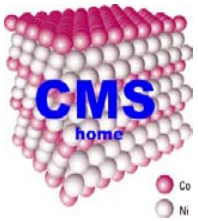
Delft

G.E.W. Bauer
A. Brataas (Harvard, Trondheim)

Philips

K. Schep
J. van Hoof

MESA+
NEDO New Energy and Industrial Technology Development Organization
NAME
FOM
CW
University of Twente
The Netherlands



The End