Nanoelectronics with ALACANT: An application to Ni nanocontacts

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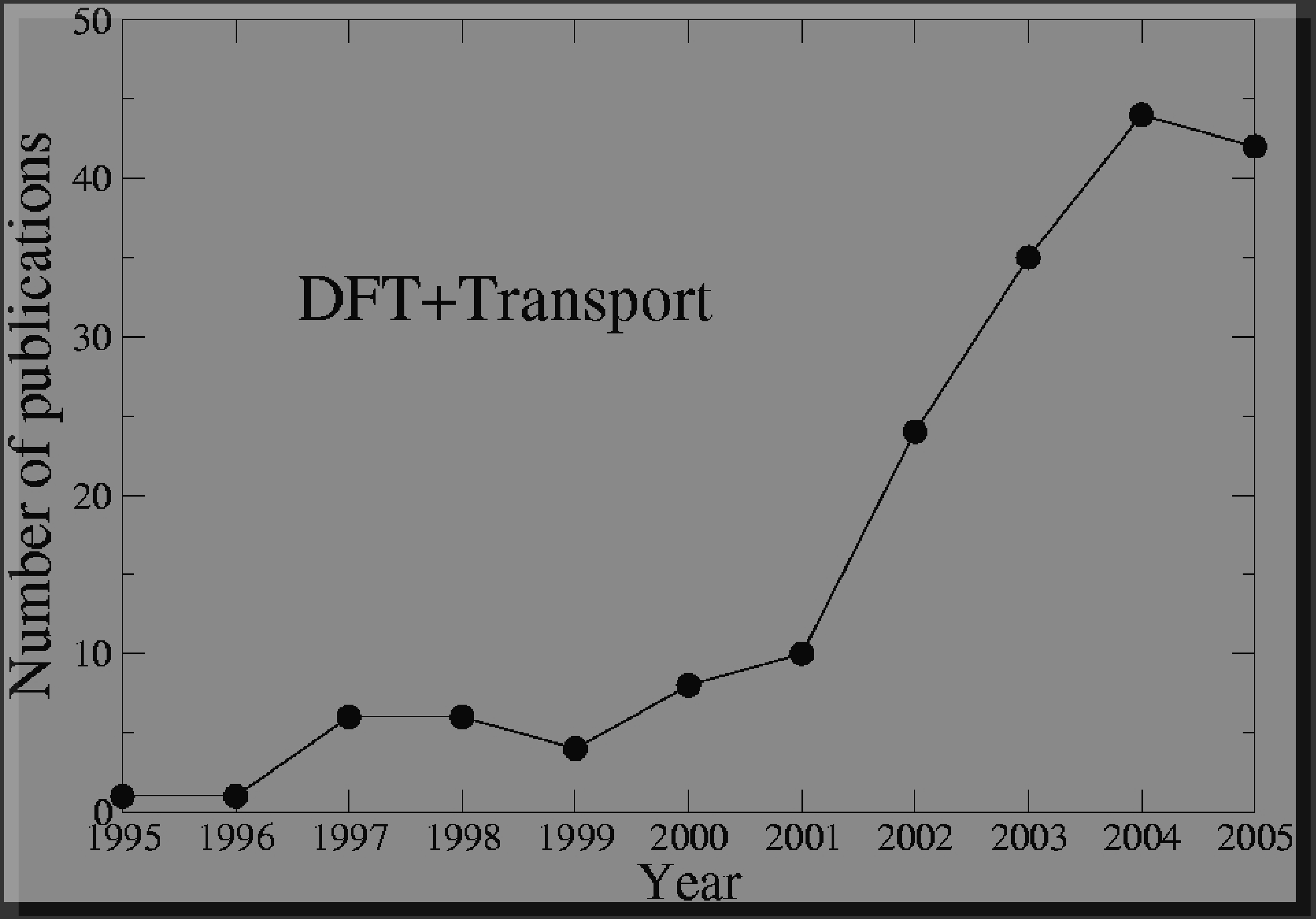
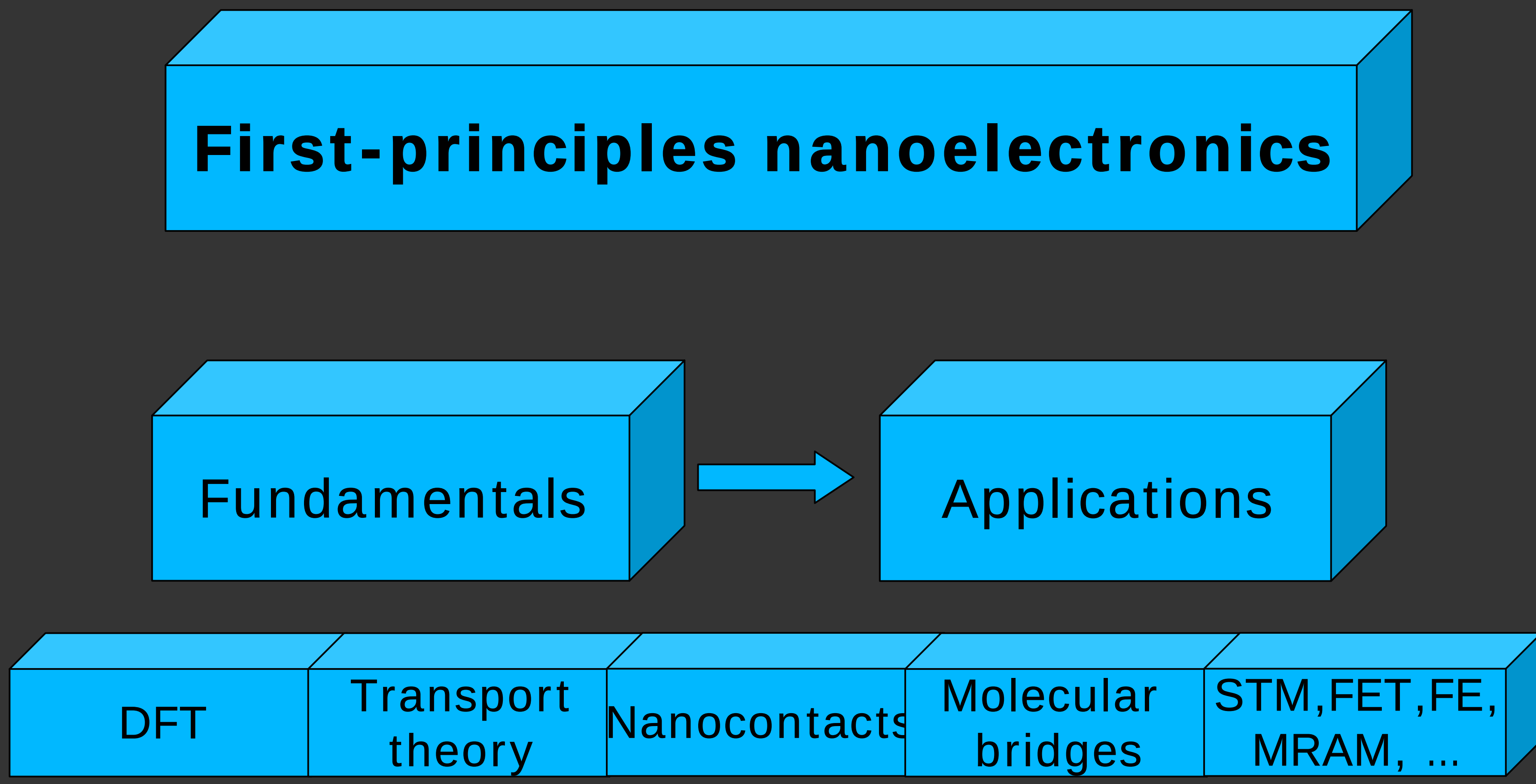
Universitat d'Alacant
Universidad de Alicante

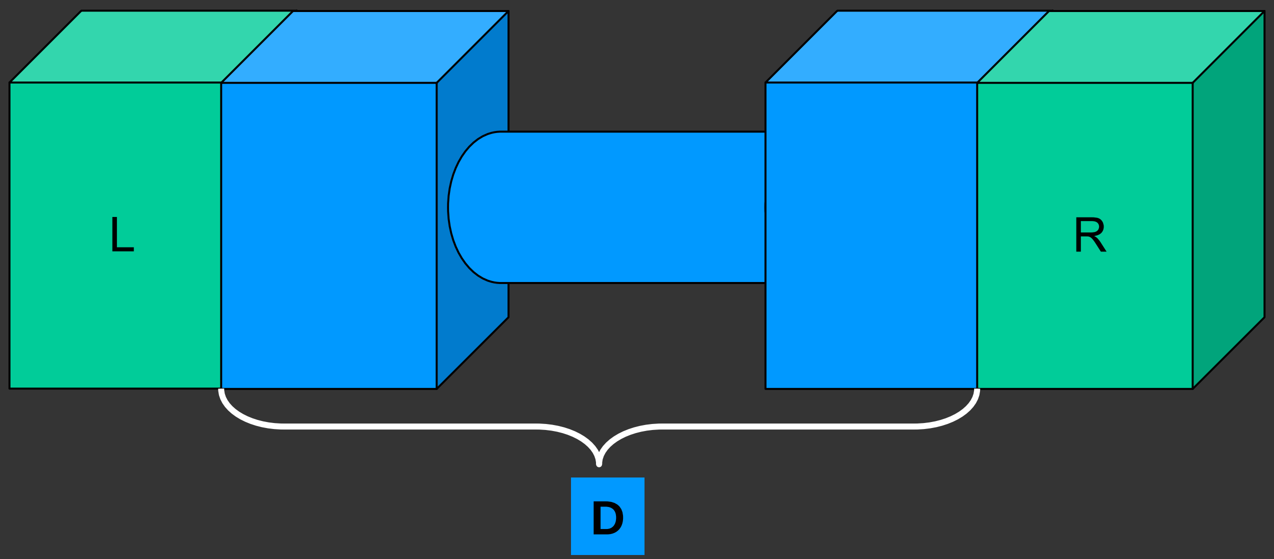
M4nano
Symposium
Madrid (Spain)

First-principles quantum transport: A tool to stay




First-principles nanoelectronics
Fundamentals
Applications
DFT
Transport theory
Nanocontacts
Molecular bridges
STM,FET,FE, MRAM, ...

Green’s function formalism



$$\hat{G}_D(E) = \left[E\hat{S}_D - \hat{H}_D - \hat{\Sigma}_L(E) - \hat{\Sigma}_R(E)\right]^{-1} \rightarrow T = Tr\left[\hat{\Gamma}_L \hat{G}_D^r \hat{\Gamma}_R \hat{G}_D^a\right]$$

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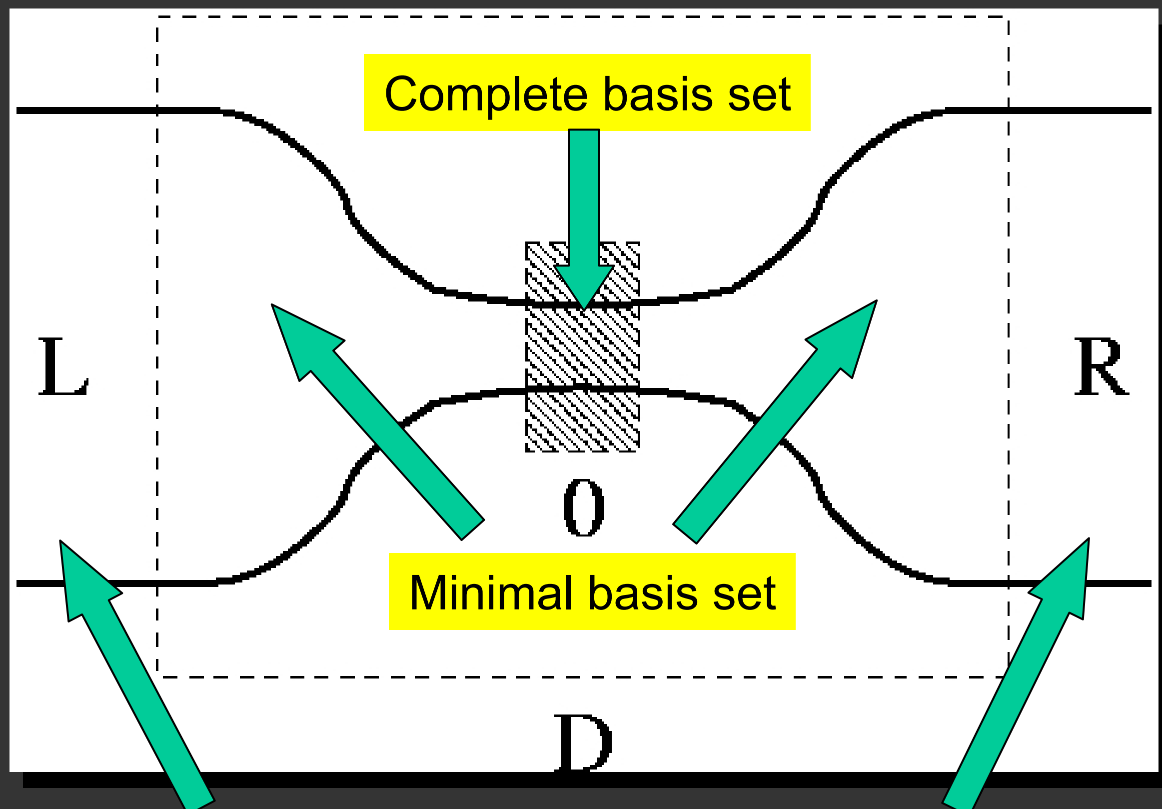
ALicante Ab initio Computation Applied to NanoTransport



Parametrized tight-binding model

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ALicante Ab initio Computation Applied to NanoTransport

Available at http://www.guirisystems.com/alacant

- Interface to Gaussian03
- NEGF/Landauer formalism
- Spin-resolved transport

$$\hat{\rho}$$

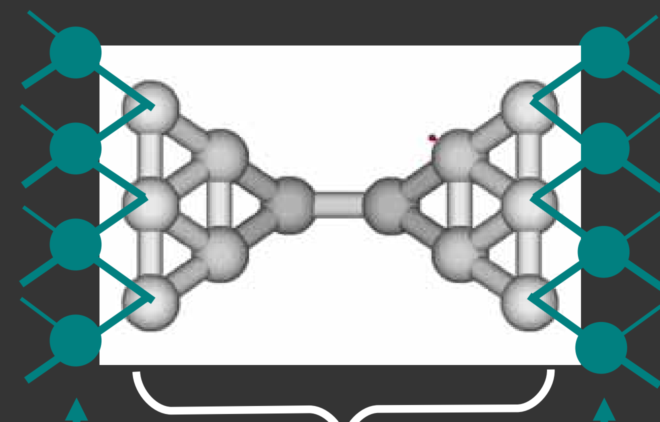
$$\hat{H}_D = \hat{H}_{KS}\left[\hat{\rho}\right]$$

$$\hat{\rho} = -\frac{\pi}{2}\int_{-\infty}^{E_F} dE\,\Im[\hat{G}_D(E)]$$

$$N_e = Tr[\hat{\rho}]$$

$$G = \frac{e^2}{h} Tr\left[\hat{\Gamma}_L \hat{G}_D^a \hat{\Gamma}_R \hat{G}_D^r\right]$$

$$\hat{G}_D = [E\hat{S} - \hat{H}_D - \hat{\Sigma}_R - \hat{\Sigma}_L]^{-1}$$



Device: *Ab initio*

Electrodes: Tight-binding Bethe lattice

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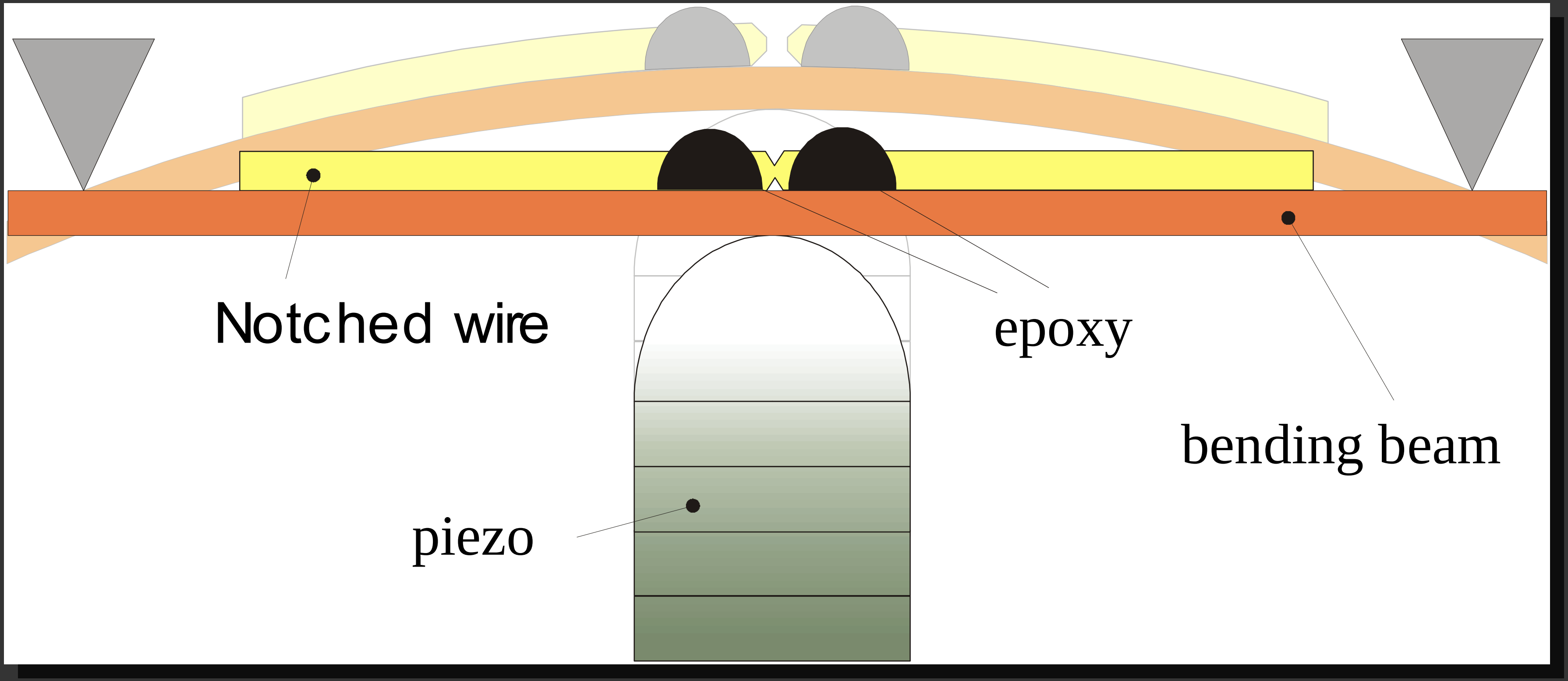
First-principles nanoelectronics

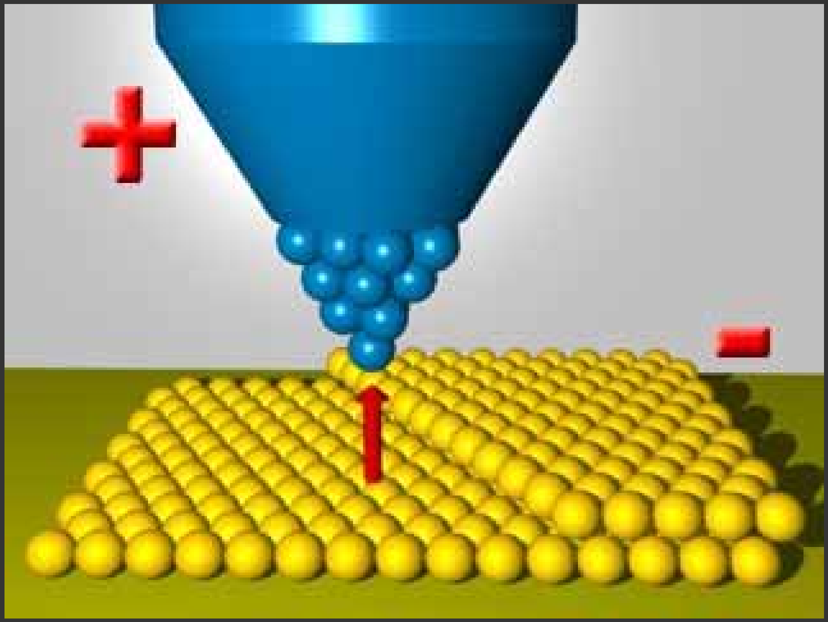
Fundamentals → Applications

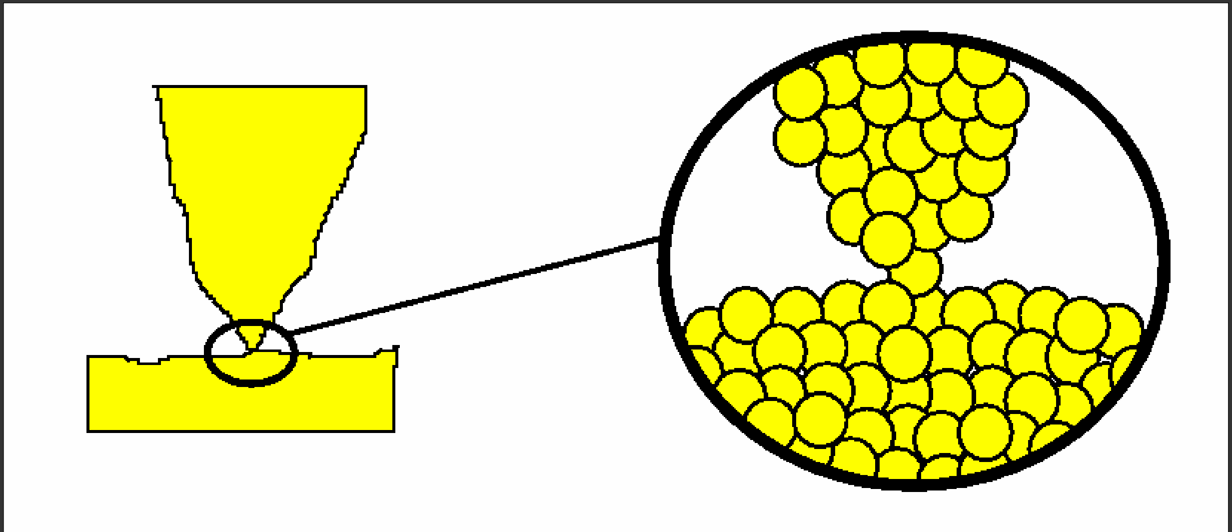
DFT	Transport theory	Nanocontacts	Molecular bridges	STM,FET,FE, MRAM, ...

MCBJ nanocontacts

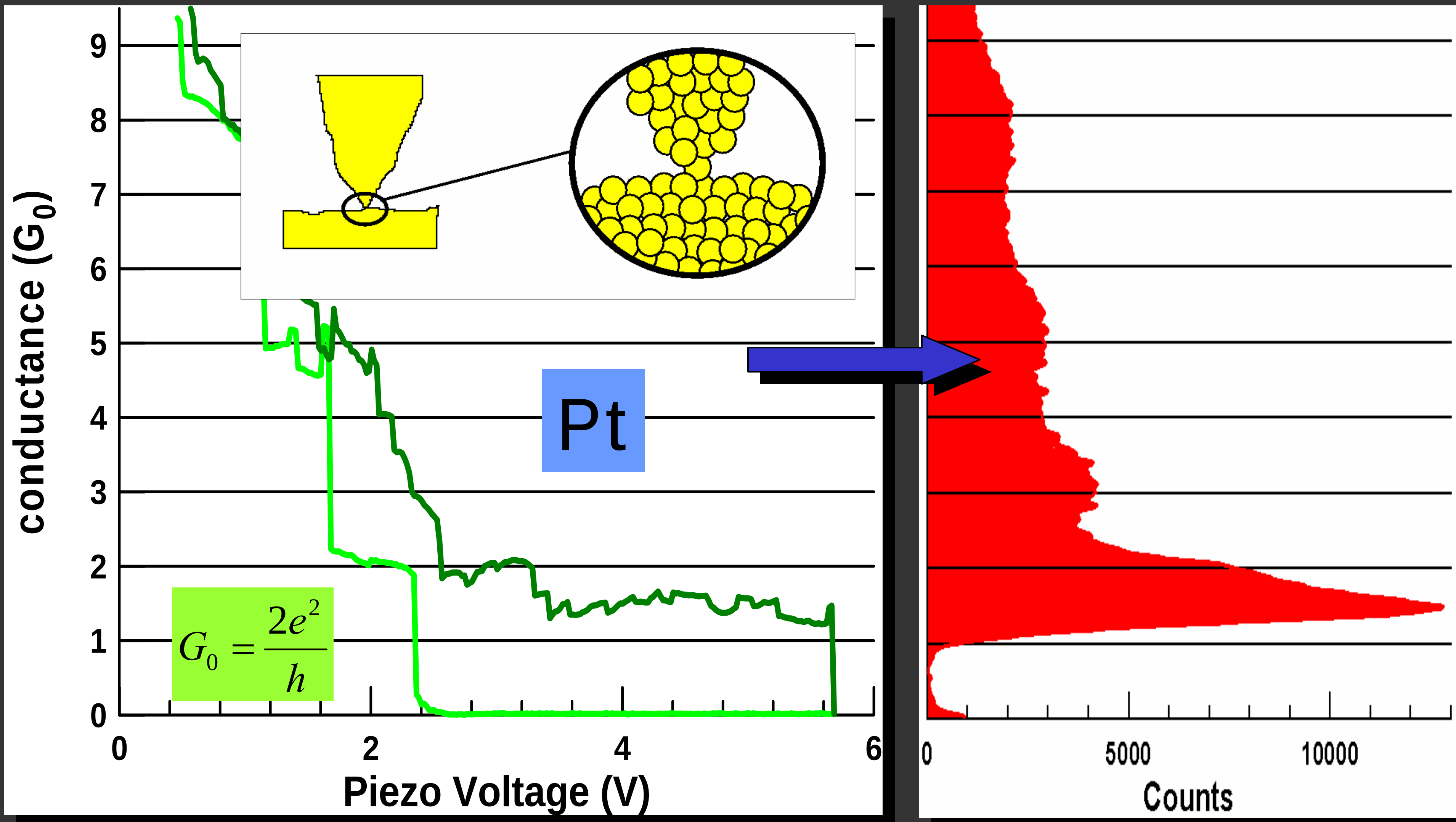


STM nanocontacts



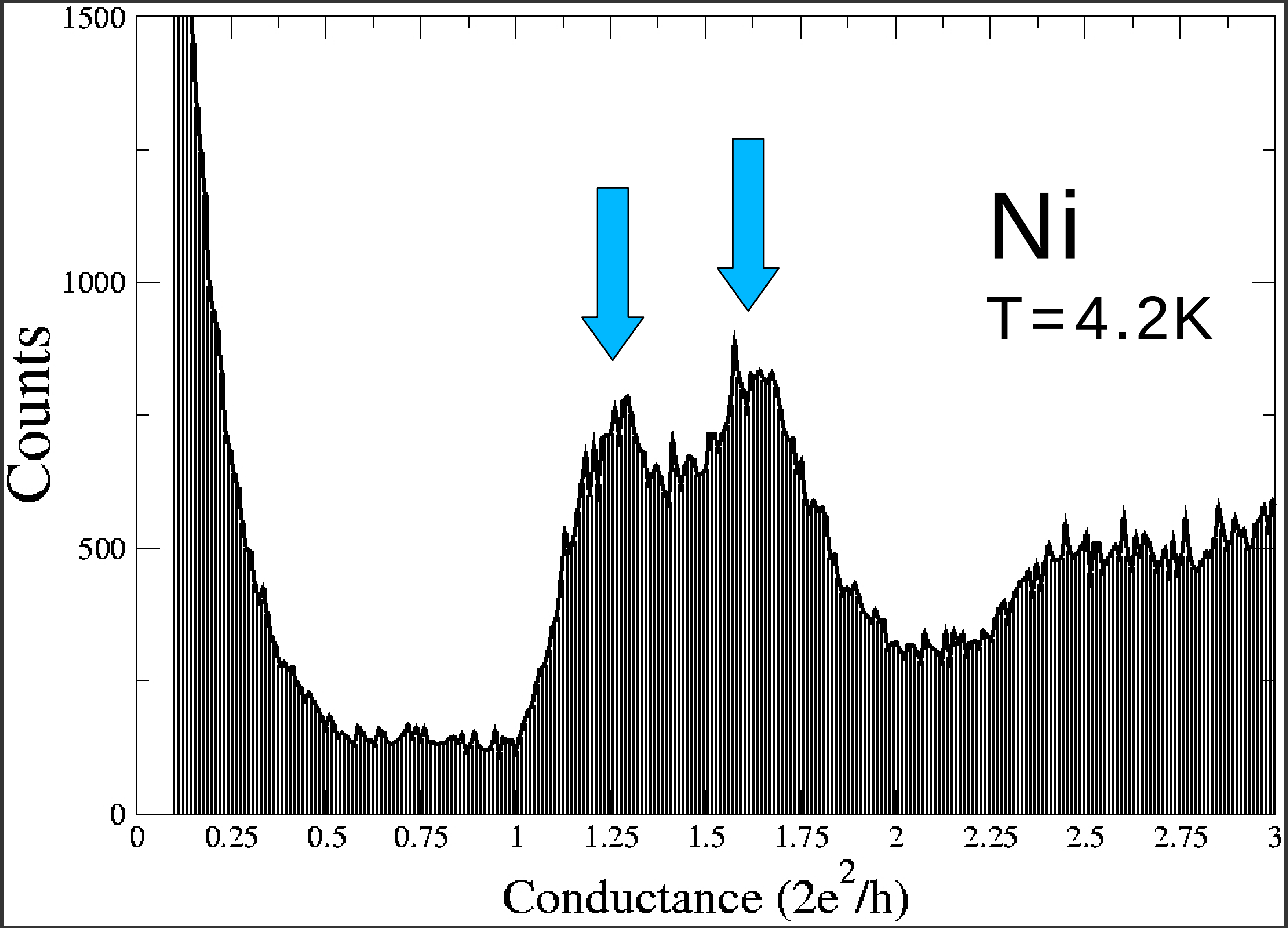


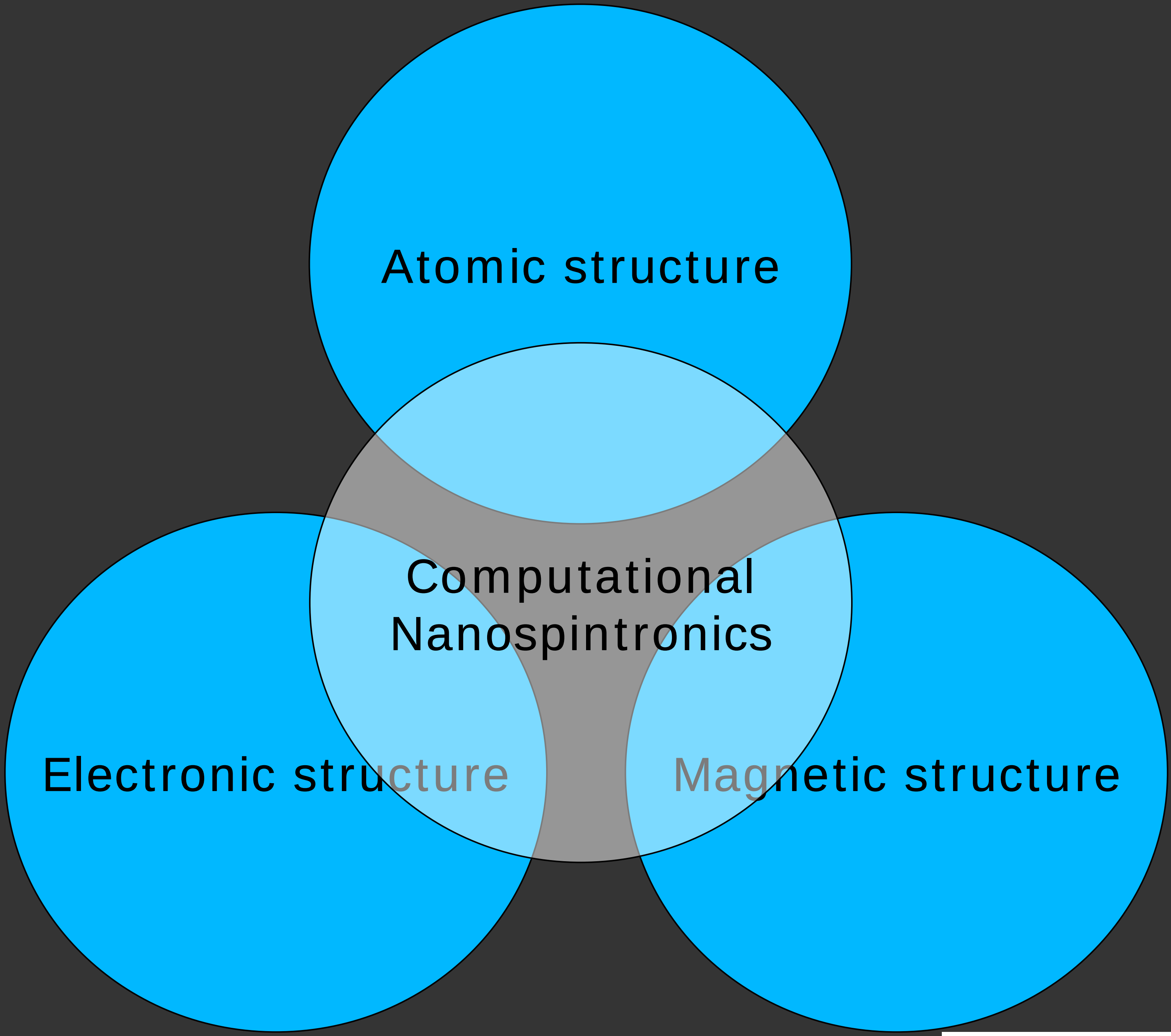
Histograms



conductance (G_0)
9
8
7
6
5
4
3
2
1
0
0
2
4
6
Piezo Voltage (V)
Pt
$G_0 = \frac{2e^2}{h}$
0
5000
10000
Counts

Ni histograms

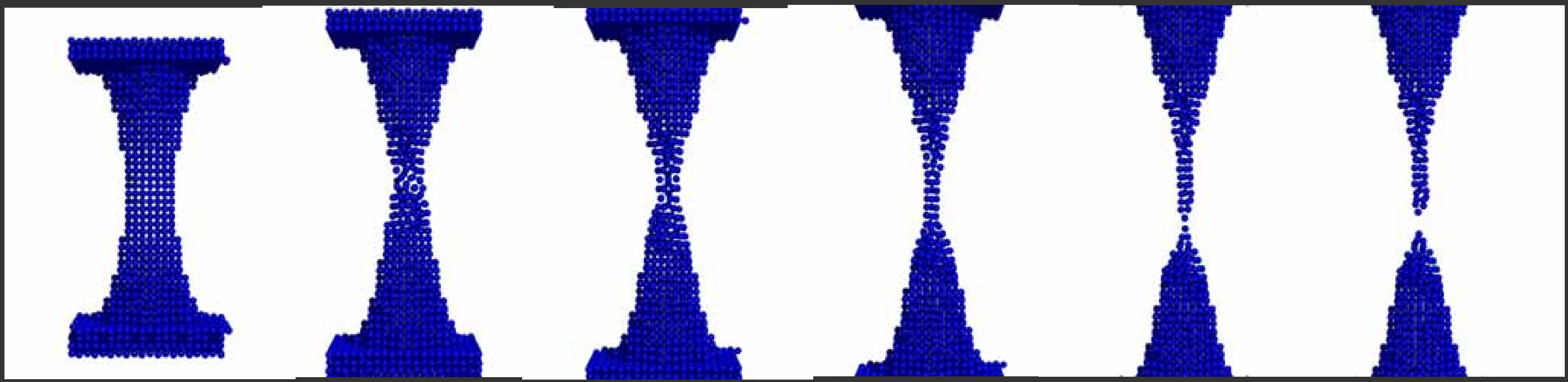



Atomic structure
Computational Nanospintronics
Electronic structure
Magnetic structure

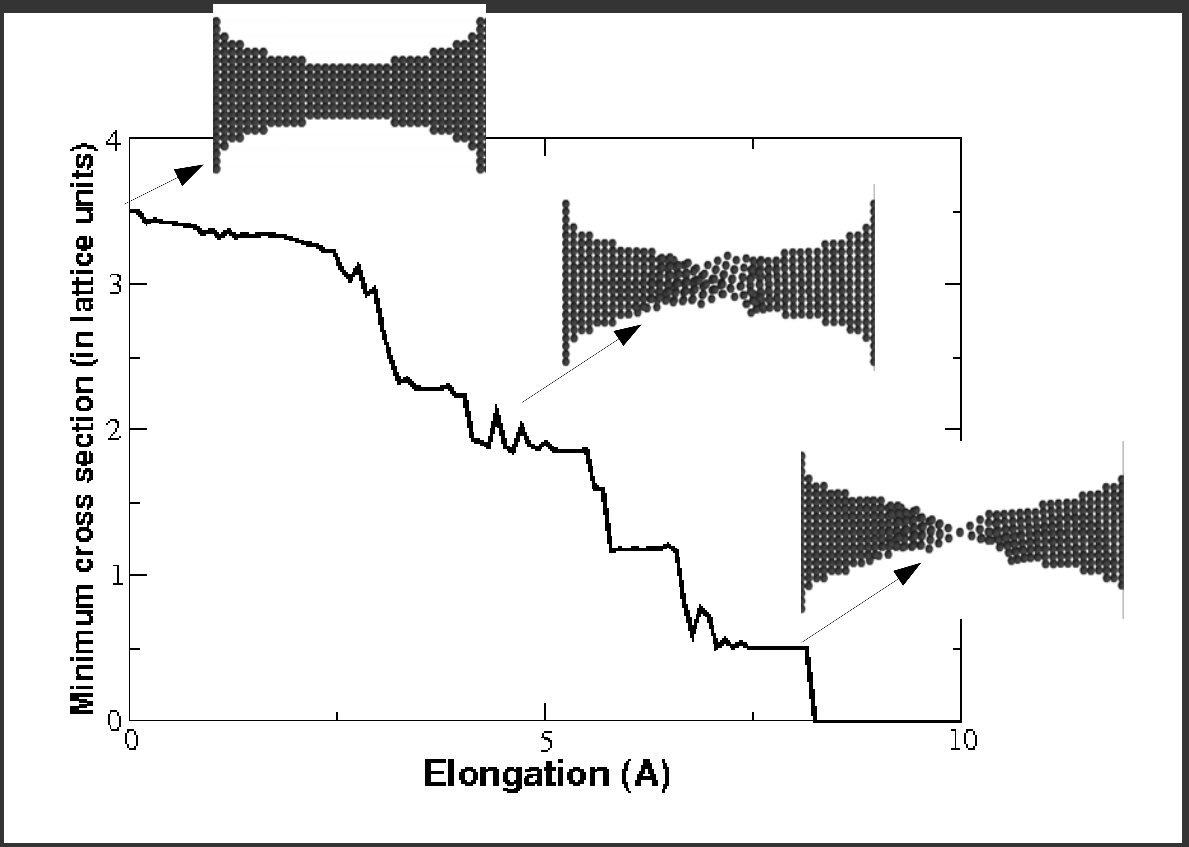
Molecular dynamics simulations of deformation of Ni nanowires

- Simulation characteristics:
  - Interatomic potential for Ni: Mishin et al., Phys. Rev. B59 (1999), 3393
  - System sizes: 77, 102, 463, 631 and 2645 atoms
  - Initial cross sections: 1.5 - 3.5a_0
  - Tension applied perpendicular to the [100] surface

- Studies:
  - Histograms of minimum cross section during elongation
  - Preferential configuration before breaking



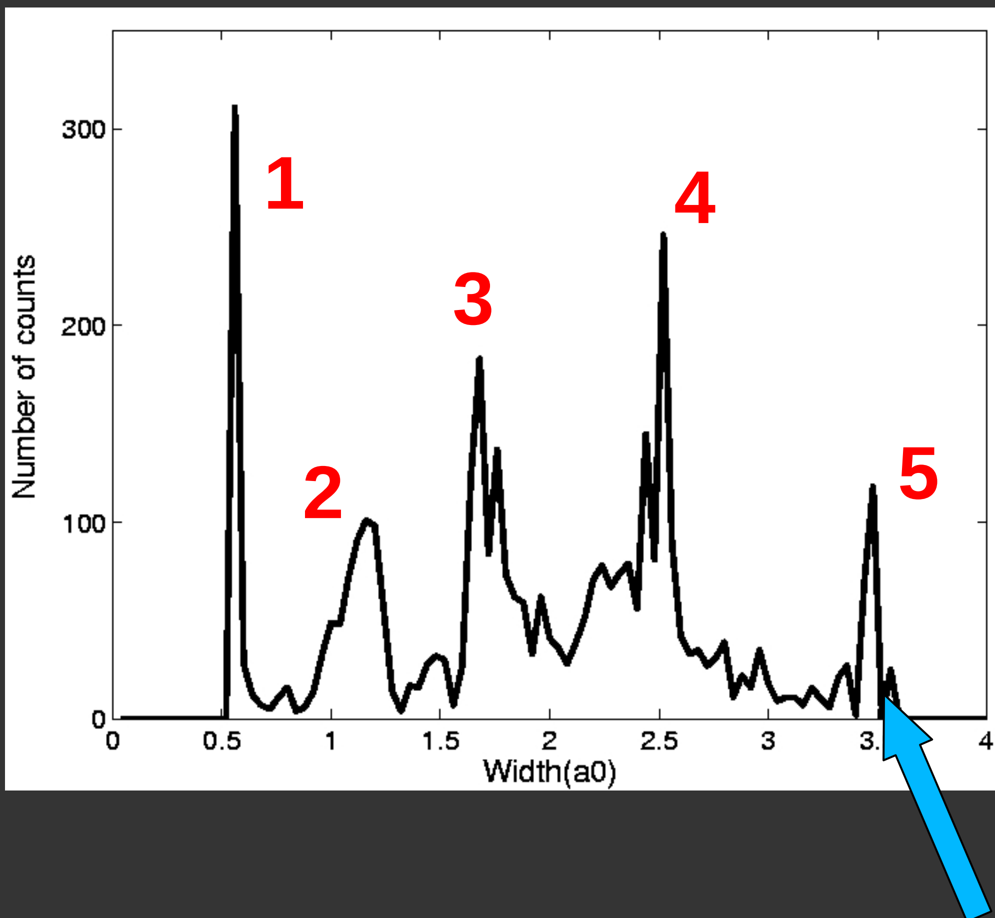
Minimum cross section during elongation



The smallest cross section is computed during elongation for 25 different cases
Preferential cross sections are clearly observed

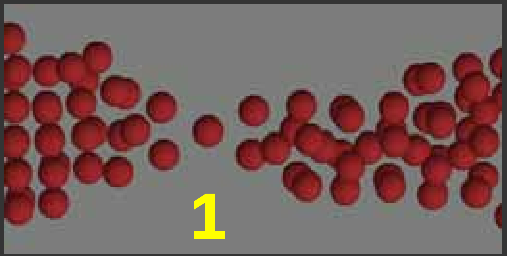
Minimum cross section histogram
Preferential configurations

Cross section histogram
T = 4.2 K

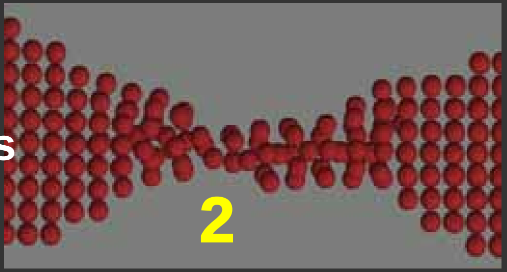


initial configuration

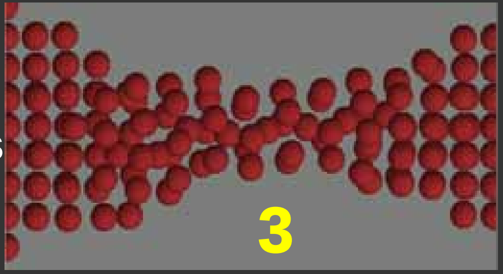
monoatomic
cross section



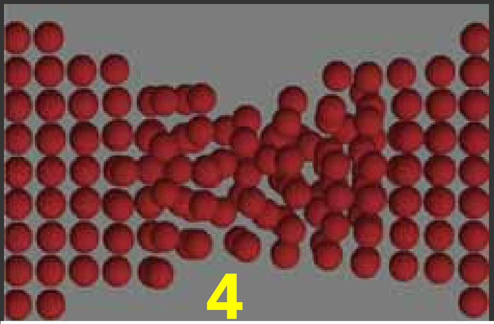
two atoms across



three atoms across

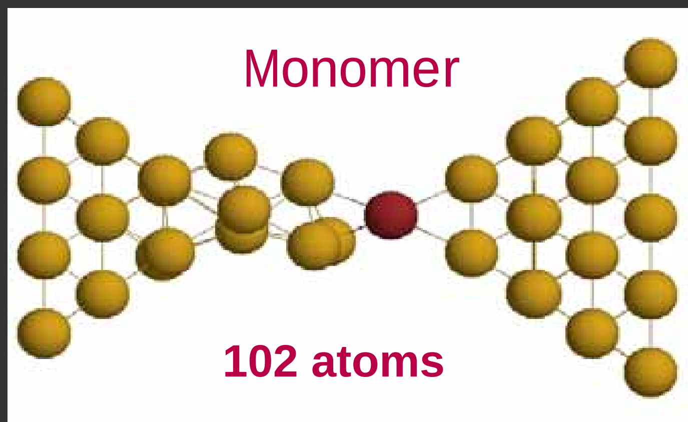


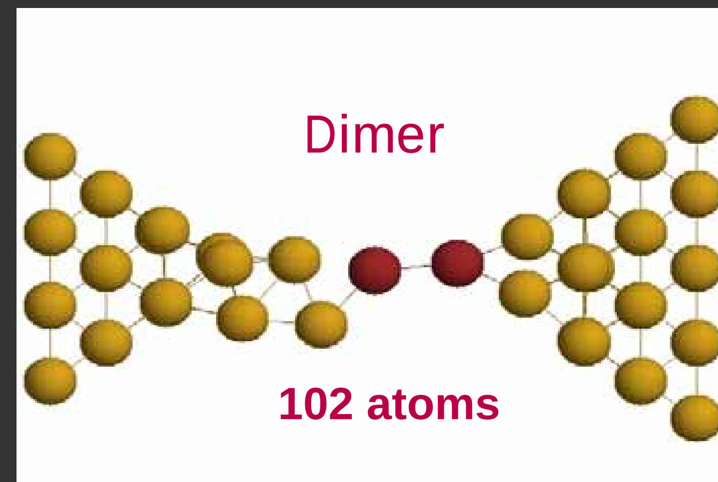
four – five
atoms across

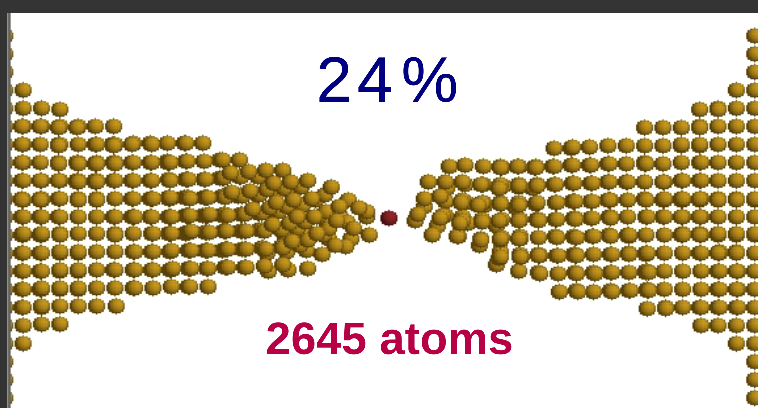


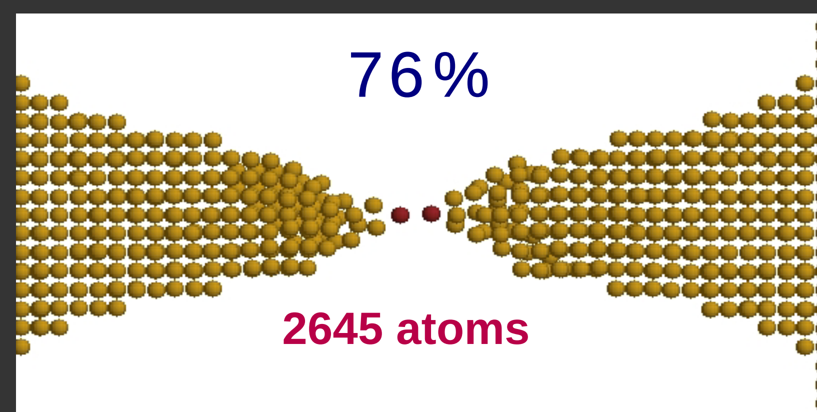
Preferential configurations before breaking

Two preferential structures identified before breaking for 125 cases studied including all sizes

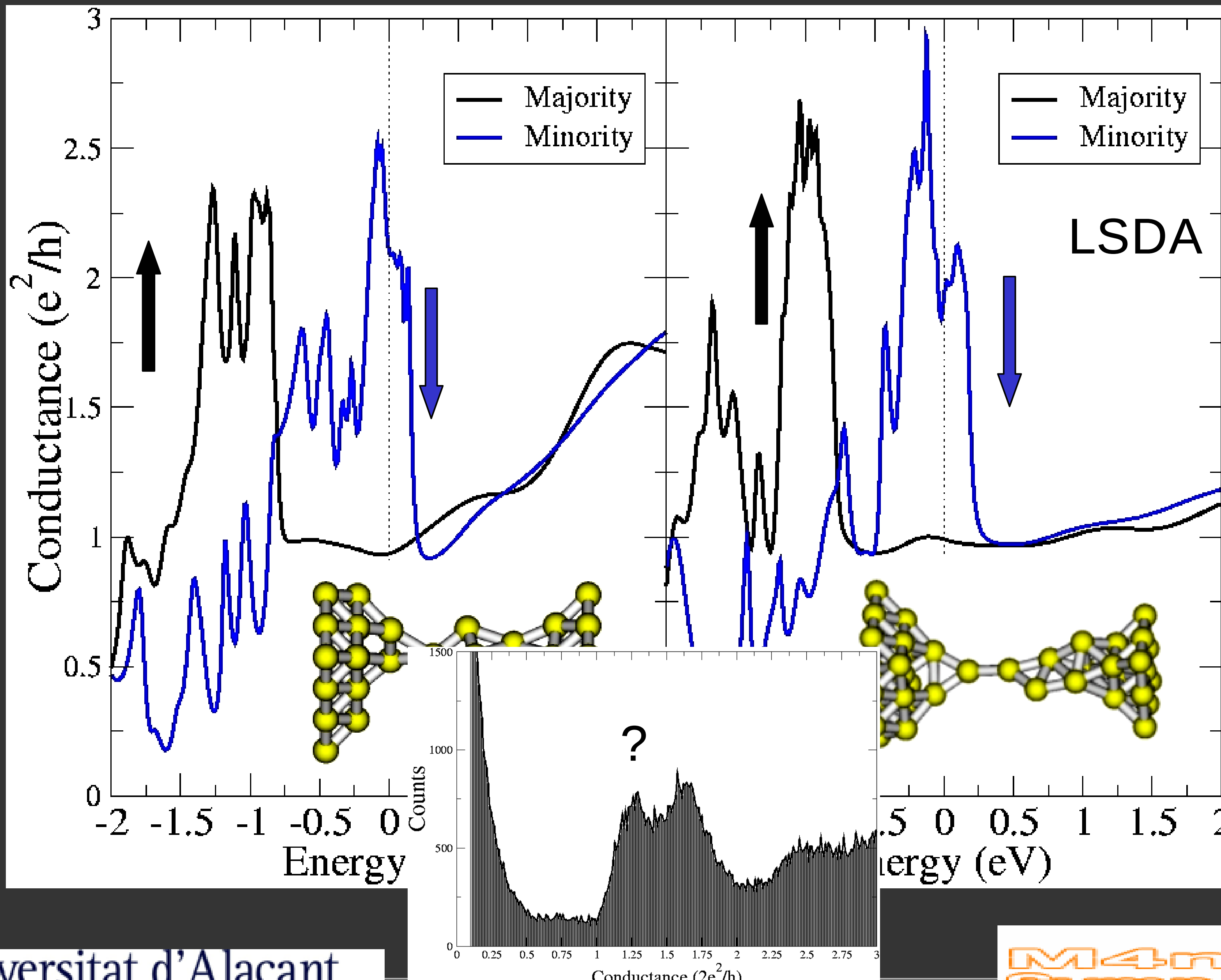






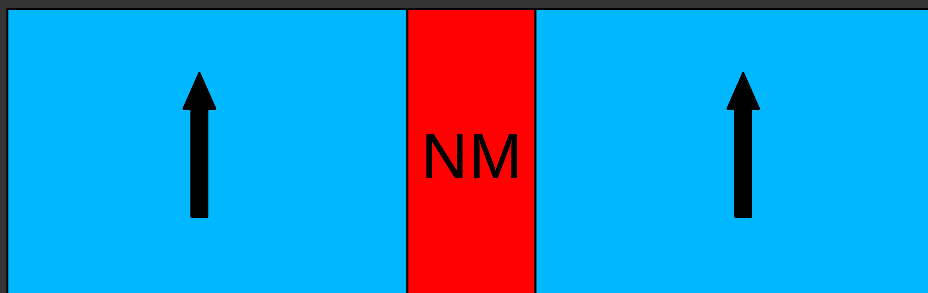


Spin-resolved conductance



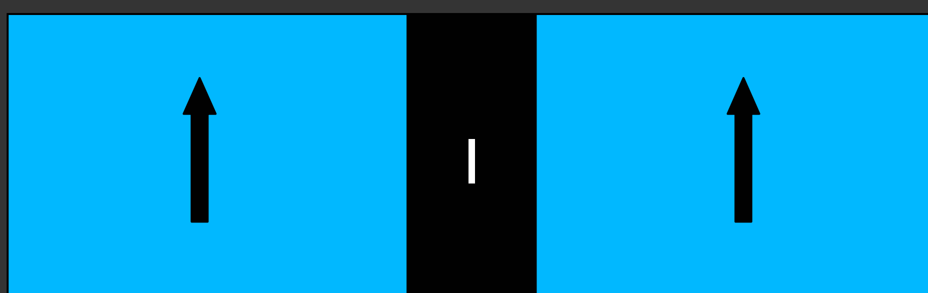
Magnetoresistance

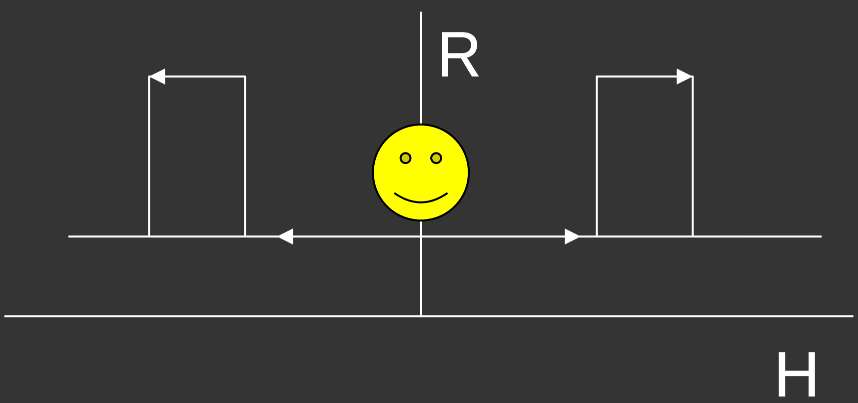
GMR



$$MR = 100 \times \left(\frac{G_P}{G_{AP}} - 1 \right) \leq \infty$$

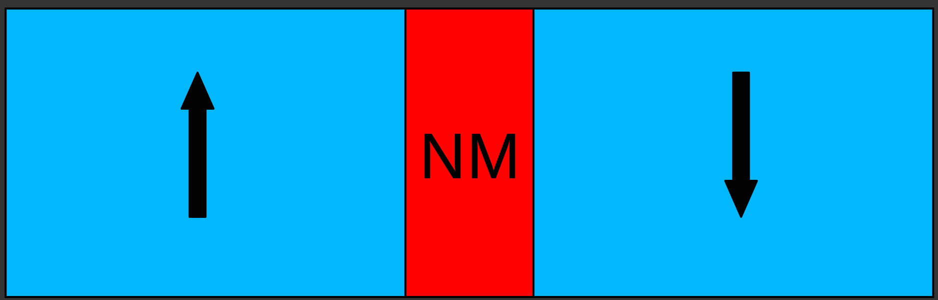
TMR





Magnetoresistance

GMR



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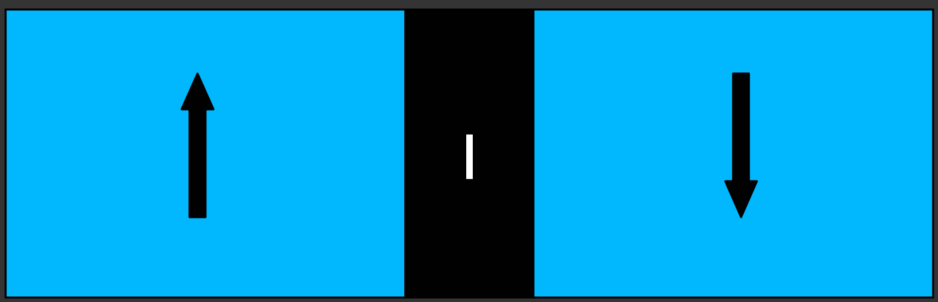
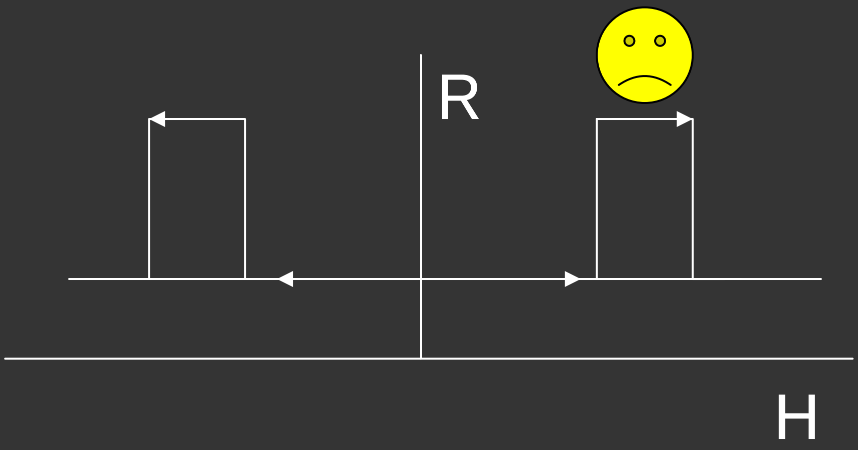
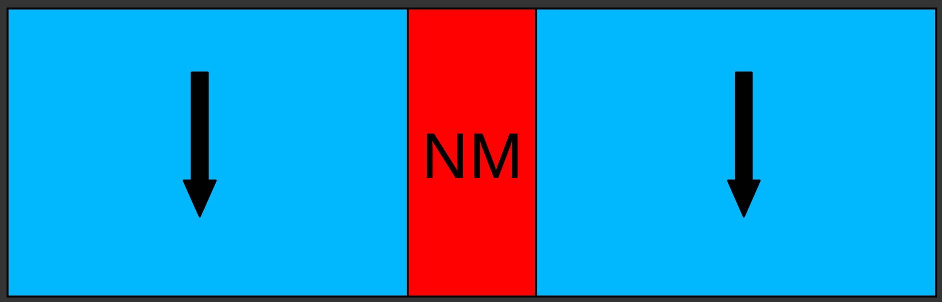
TMR





Magnetoresistance

GMR



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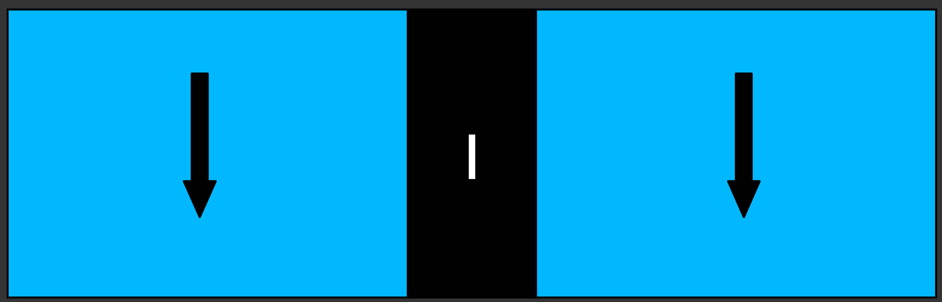
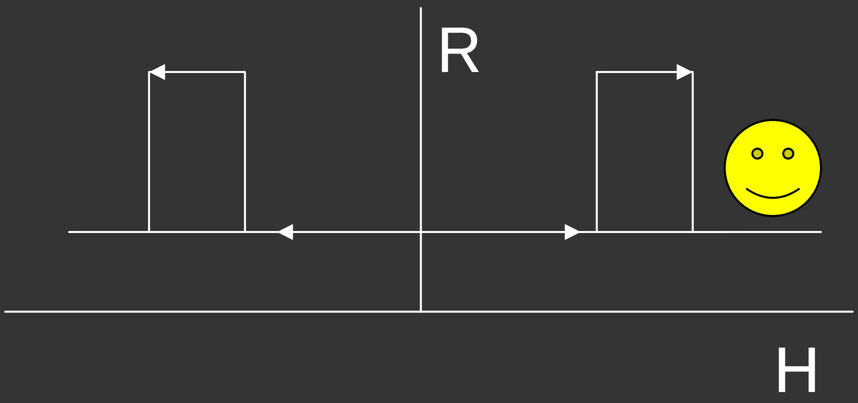
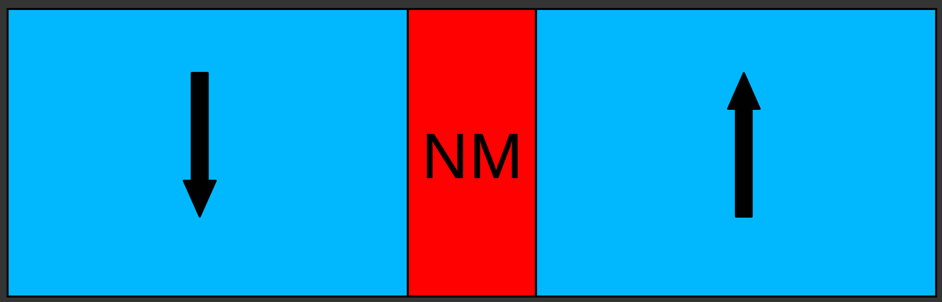
TMR





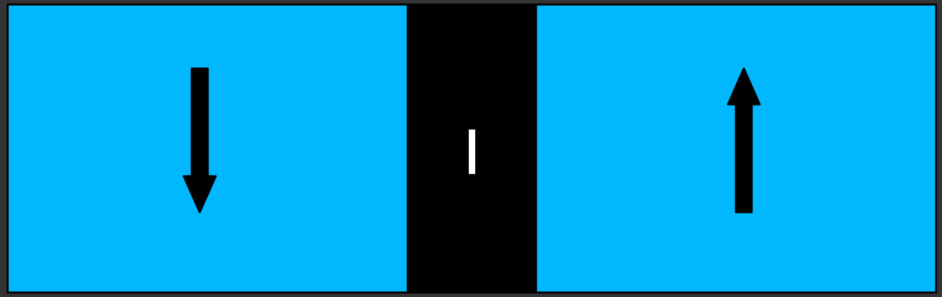
Magnetoresistance

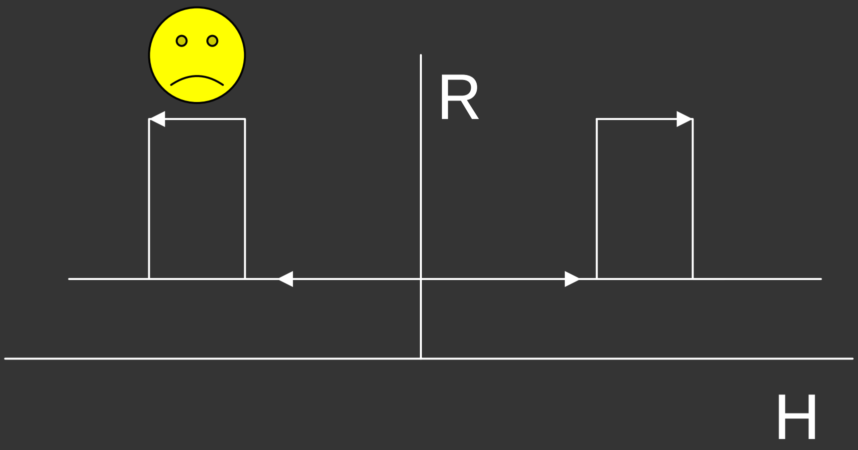
GMR



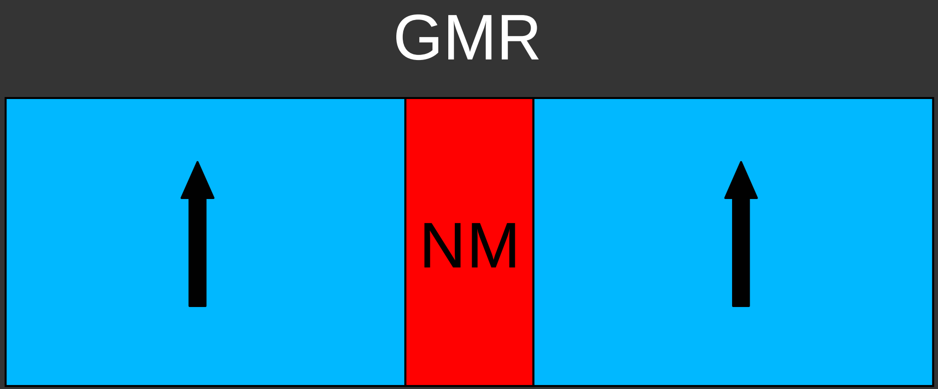
$$MR = 100 \times \left(\frac{G_P}{G_{AP}} - 1 \right) \leq \infty$$

TMR





Magnetoresistance



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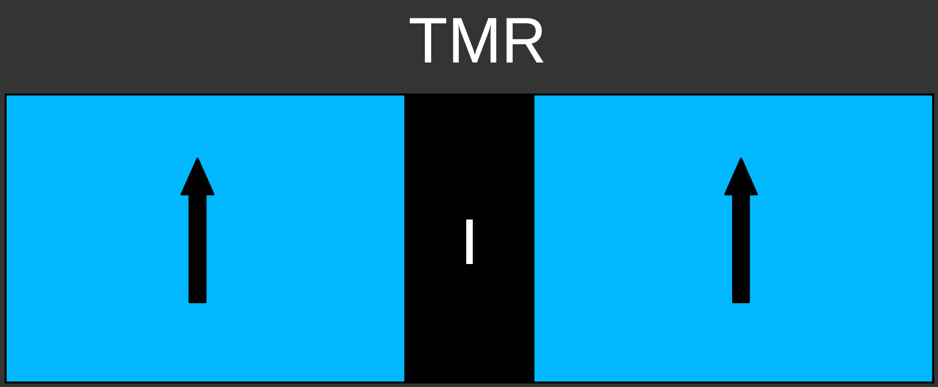
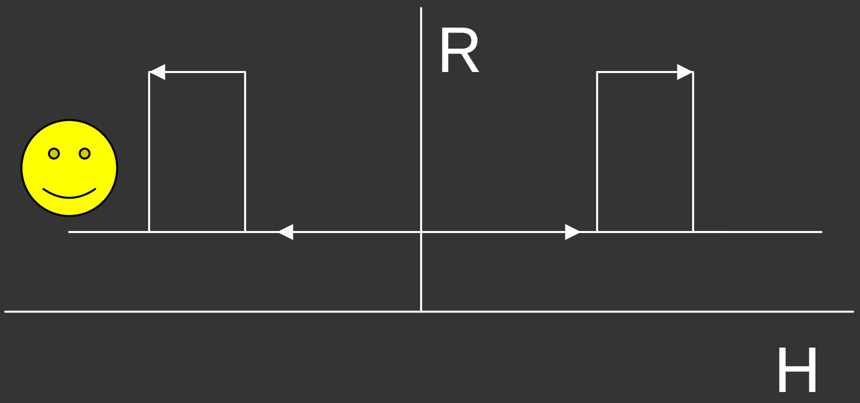
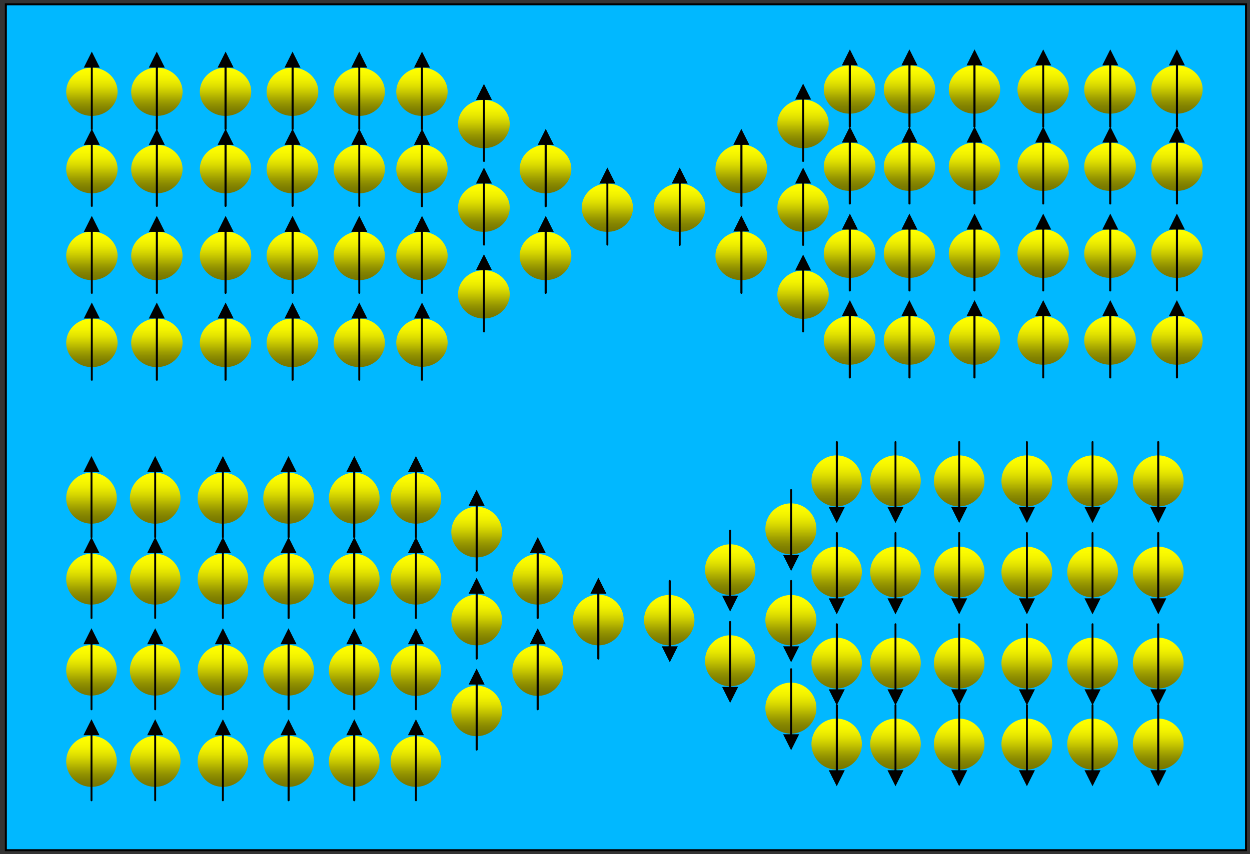


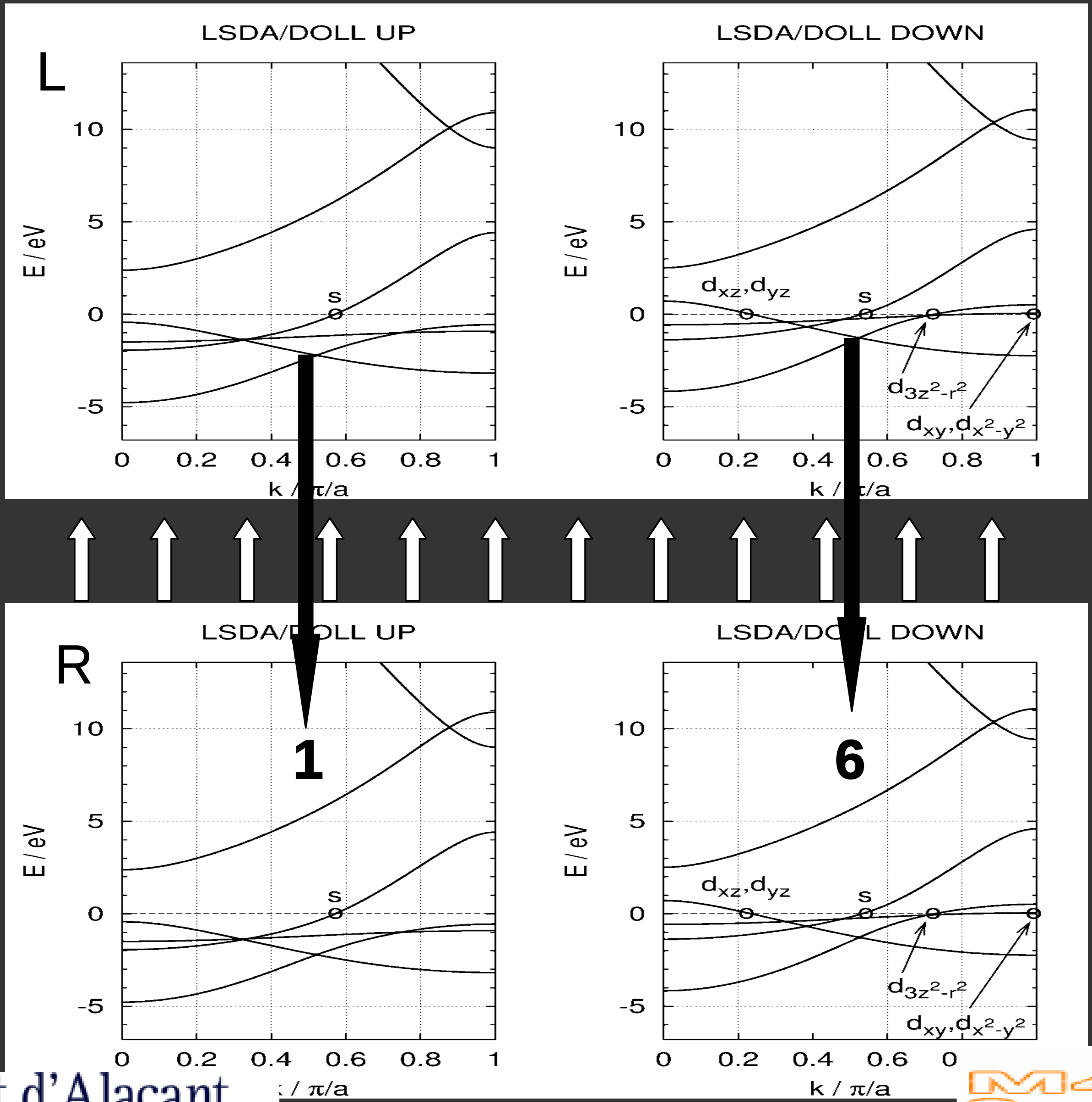


Domain-wall scattering



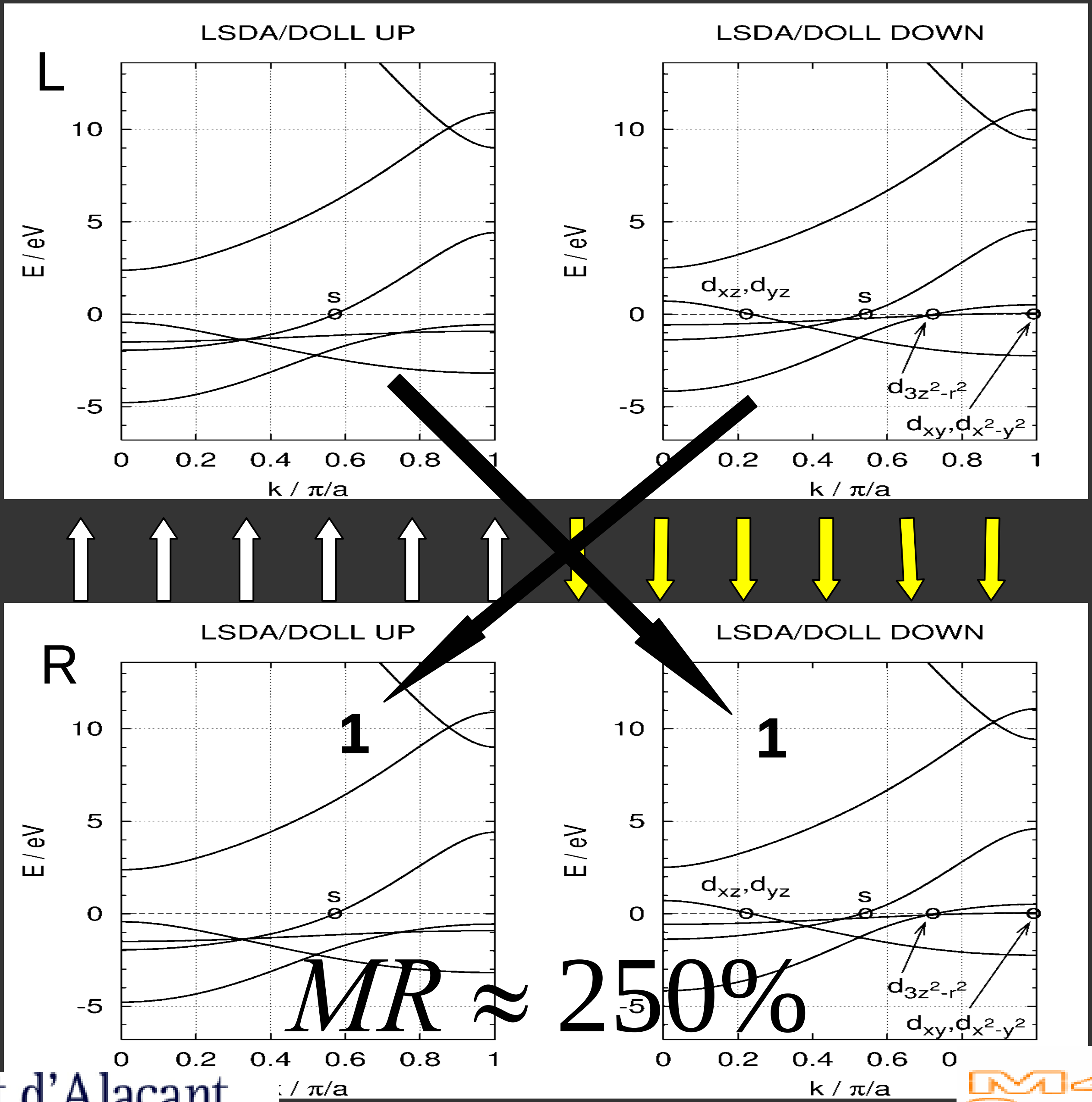
Tatara et al., PRL (1997)
Levy et al., PRL (1997)
Tatara et al., PRL (1999)
van Hoof et al., PRB (1999)
García, APL (2000)
Imamura et al. PRL (2000)
García et al., APL (2001)
Tagirov et al., PRB (2002)
Zhuravlev et al., APL (2003)
Dugaev et al., PRB (2003)
...

1-dimensional Ni chains



D. Jacob et al.
PRB (2005)

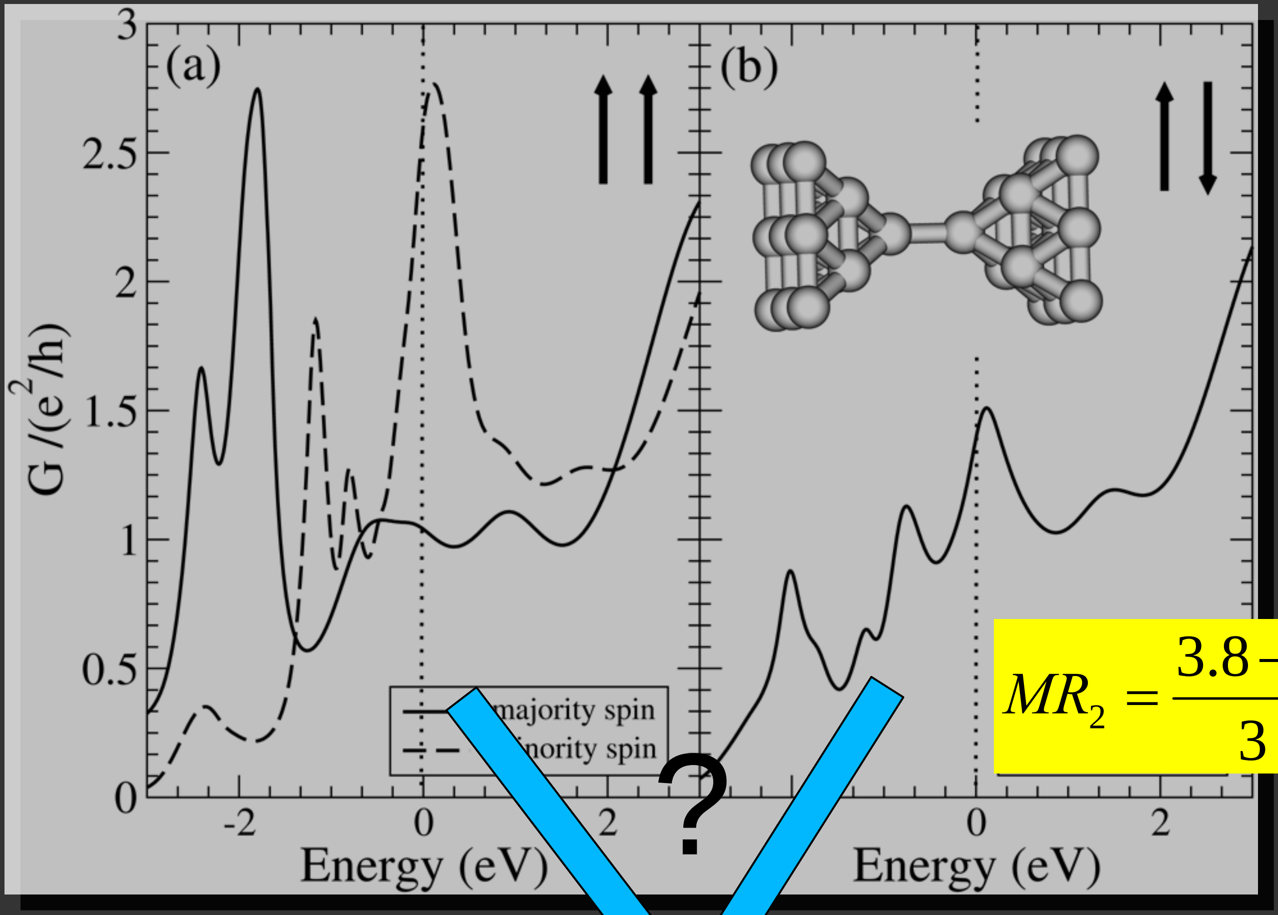
1-dimensional Ni chains



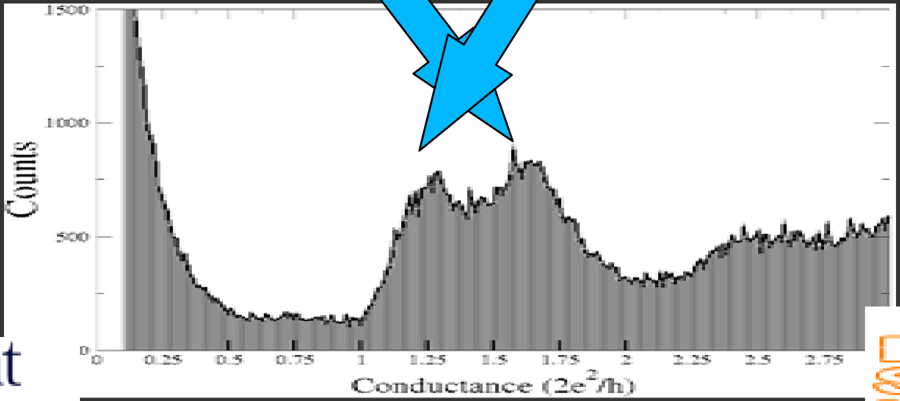
$MR \approx 250\%$

D. Jacob et al.
PRB (2005)

Domain wall in nanocontacts



$$MR_2 = \frac{3.8-3}{3} x100 \approx 26\%$$



Acknowledgements

Transport theory

J. Fernández- Rossier

D. Jacob

Experimental

C. Untiedt

R. Calvo

Molecular dynamics

M. J. Caturla

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