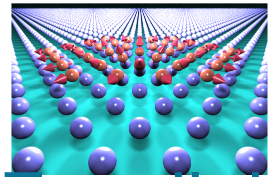


Funsilab

JÜLICH
FORSCHUNGSZENTRUM

Mitglied der Helmholtz-Gemeinschaft

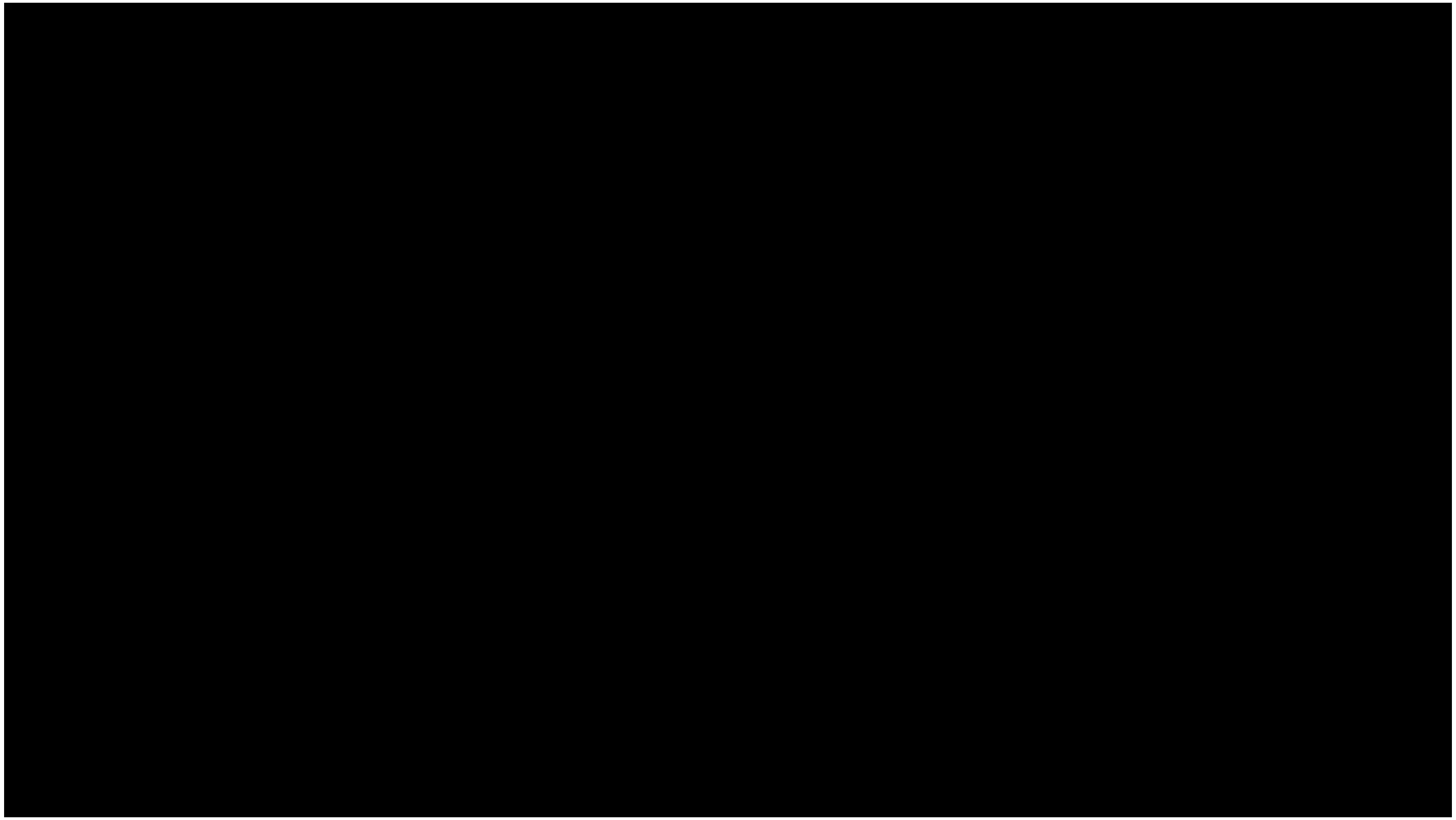
Novel applications II: Magnetic nanostructures

Samir Lounis

July 10, 2013

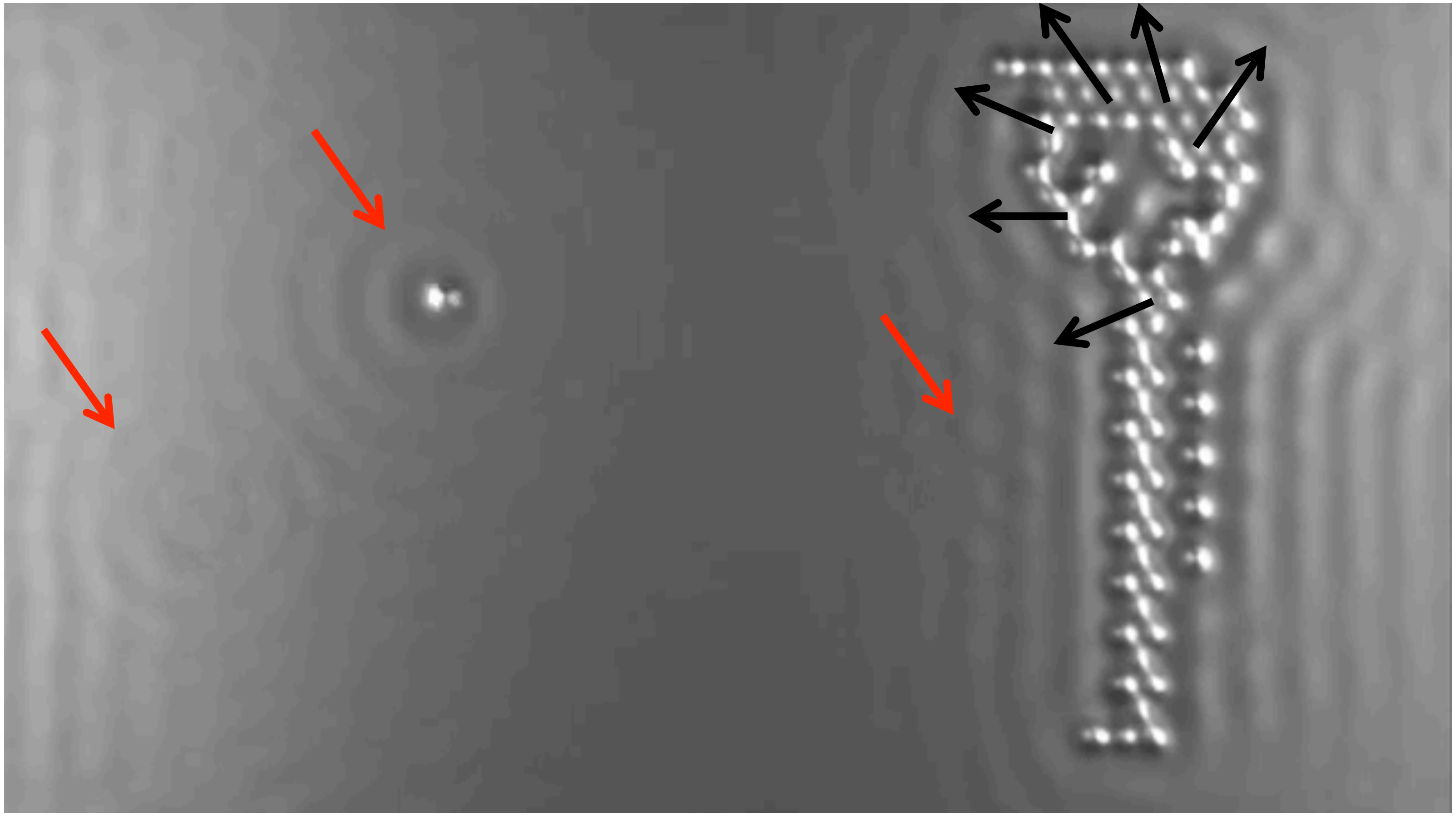
Peter Grünberg Institut & Institute for Avdanced Simulation

World’s smallest movie



- Heinrich et al. IBM Almaden

World's smallest movie

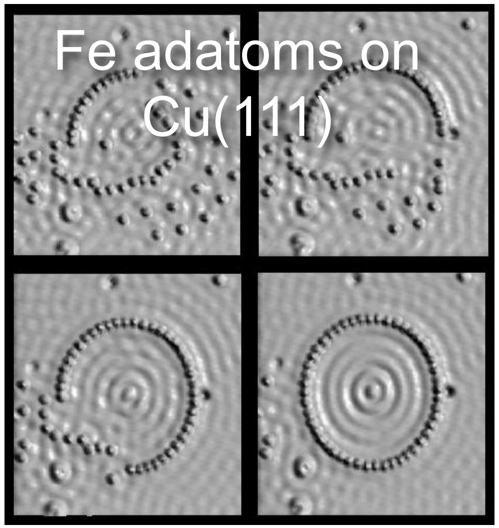


- Heinrich et al. IBM Almaden

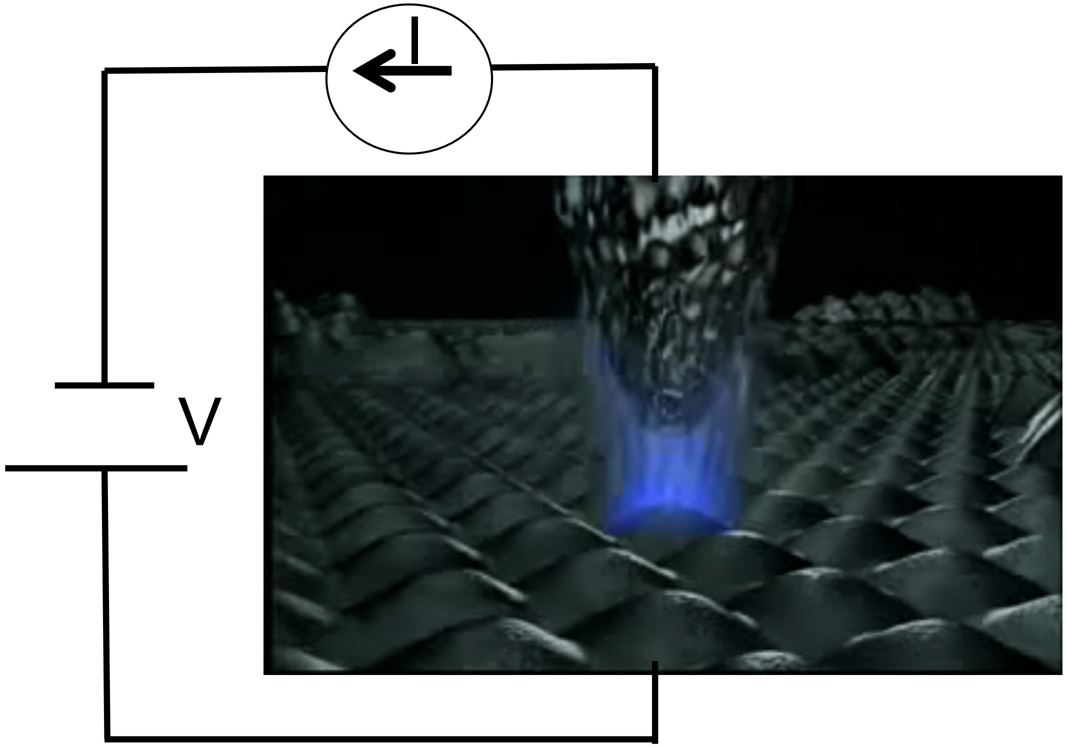
$$H = -\frac{1}{2}\sum_{i\neq j} J_{ij}\vec{e}_i\cdot\vec{e}_j - \frac{1}{2}\sum_{i\neq j} D_{ij}\vec{e}_i\times\vec{e}_j - \sum_i K_i(\vec{e}_i\cdot\vec{e}_j^{\,z})^2 - \ldots$$

Manipulation of surface states

- Silly, Pivetta, Ternes, Patthey, Pelz, Schneider, PRL (2004)

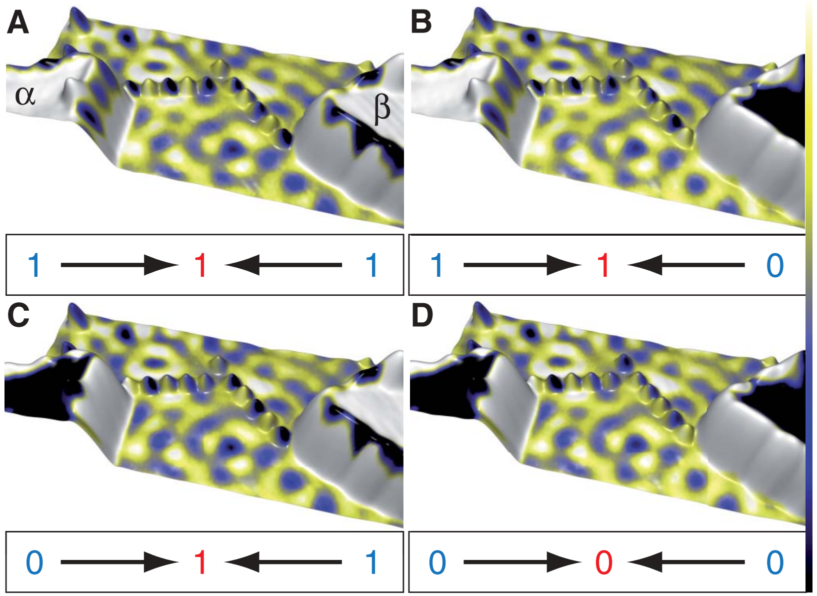


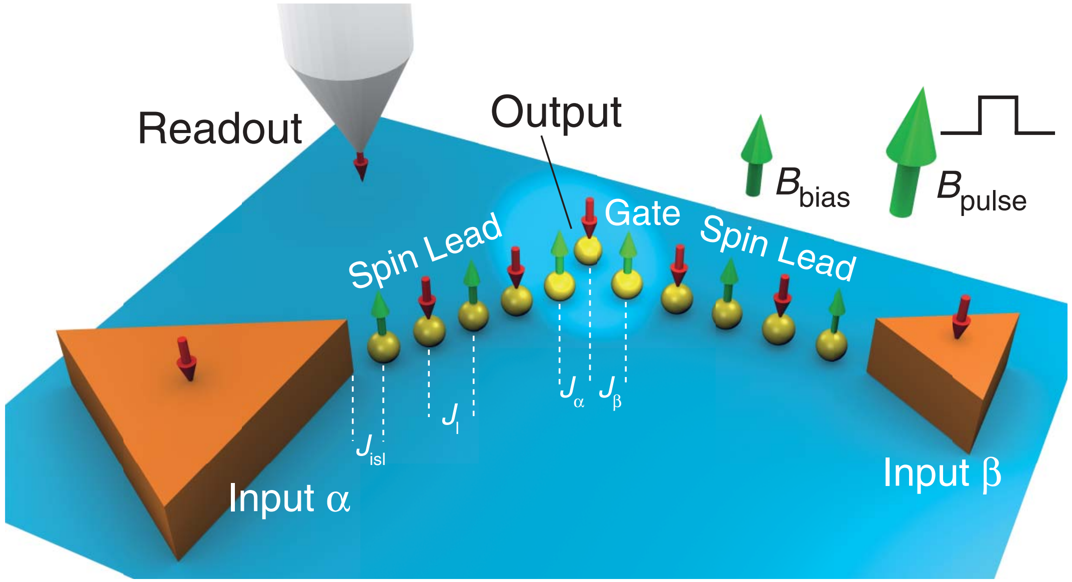
- Crommie, Lutz, Eigler, Science (1993)



From youtube.com: look at STM!

Magnetic logic gates



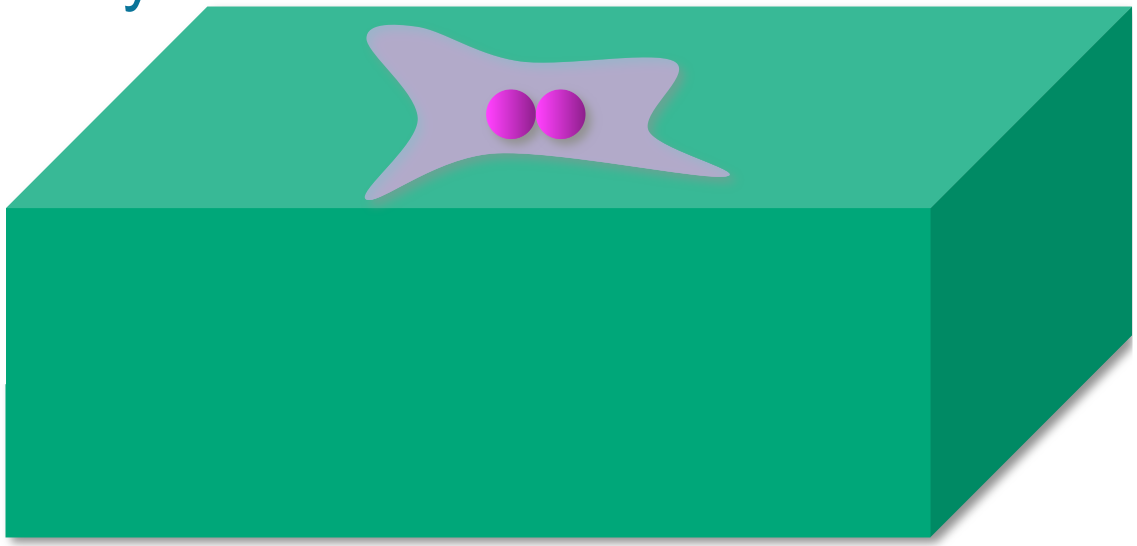


Khajetoorians, Wiebe, Chilian, Wiesendanger, Science (2011)

KKR Green-function method

within density-functional theory

juDFT
www.judft.de



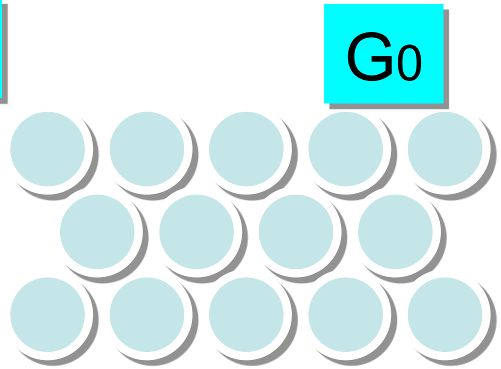
Embedding the clusters
is a non-trivial task

Dyson eq.: Reference system → New system

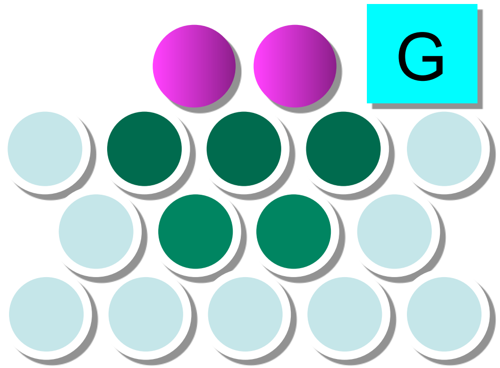
$$G(E) = G_0(E) + G_0(E) V G(E)$$

No periodic supercell needed
Takes into account the infinite system

$$n(E) = -1/\pi \, \mathrm{Im}\, G(E)$$



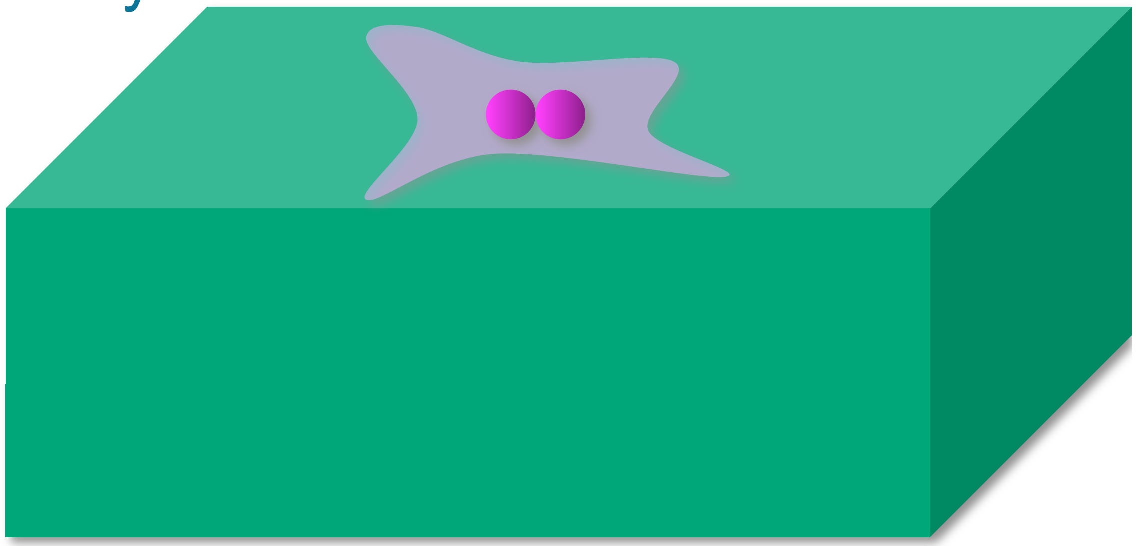
Crystal surface



Cluster on surface

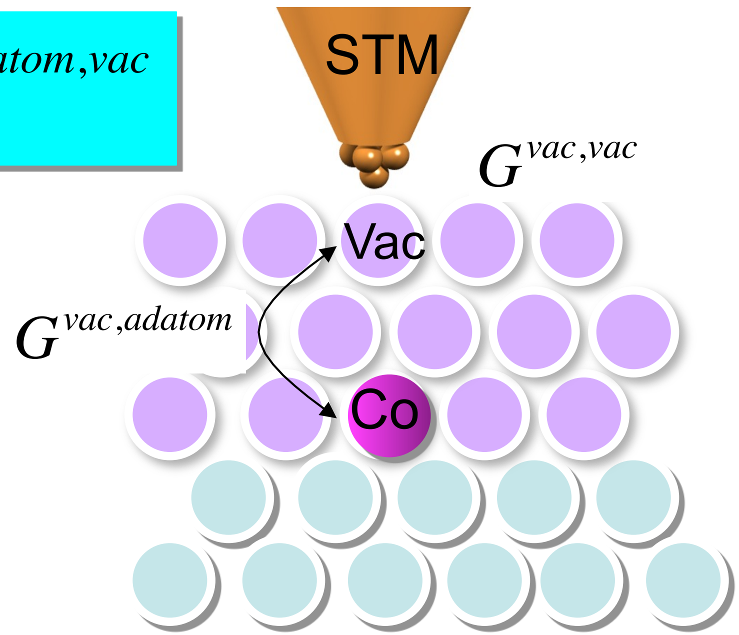
KKR Green-function method
within density-functional theory

juDFT
www.judft.de



Embedding the clusters
is a non-trivial task

$$G^{vac,vac} = G_0^{vac,vac} + G_0^{vac,adatom} V^{adatom} G^{adatom,vac}$$



Tersoff-Hammann approximation:

$$\frac{dI}{dV} \propto -\frac{1}{\pi} \mathrm{Im}\, G^{vac,vac}$$

Magnetism of single adatoms

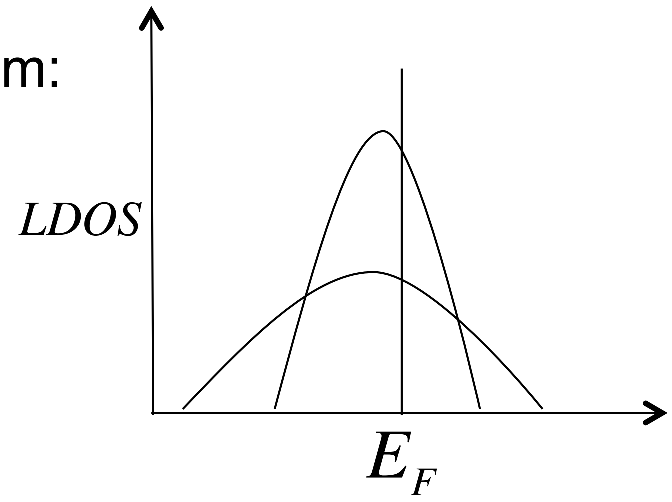
Appetizer: Adatoms and small clusters
Transition from atomic to monolayer & bulk behaviour

Stoner model & Stoner criterion for ferromagnetism:

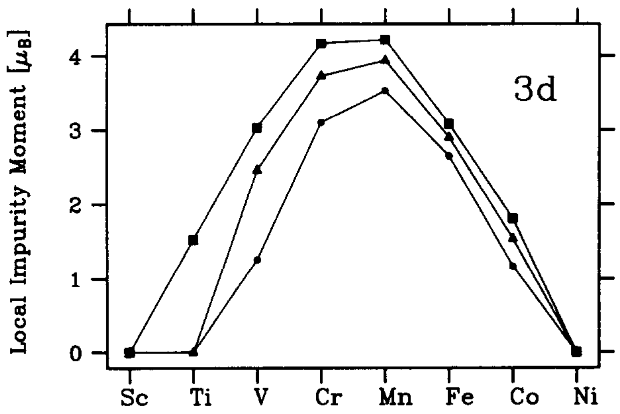
$$\delta M = \chi \delta B$$

$$\chi = \frac{1}{1 - I n^0(E_F)} n^0(E_F)$$

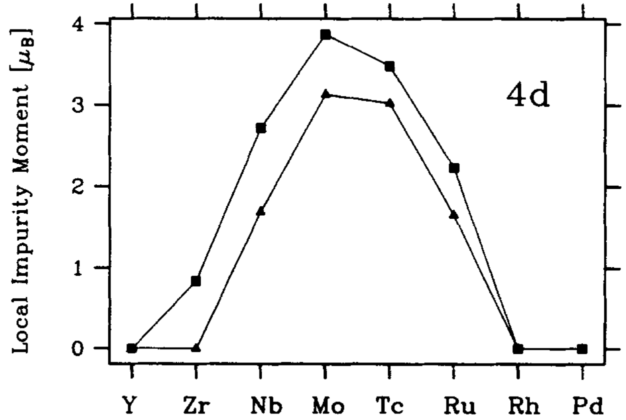
$$I n^0(E_F) > 1$$



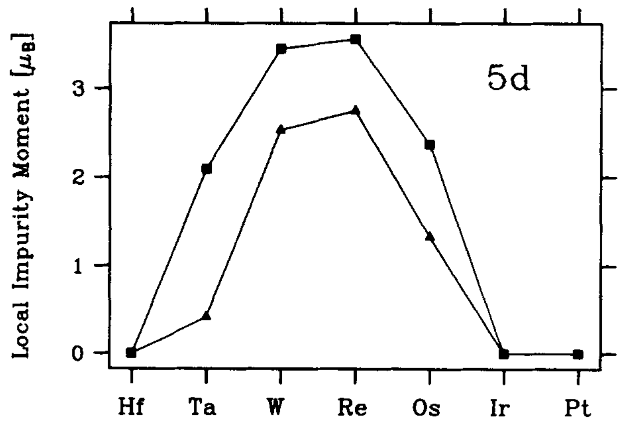
3d atoms/Cu(001)



4d atoms/Ag(001)



5d atoms/Ag(001)

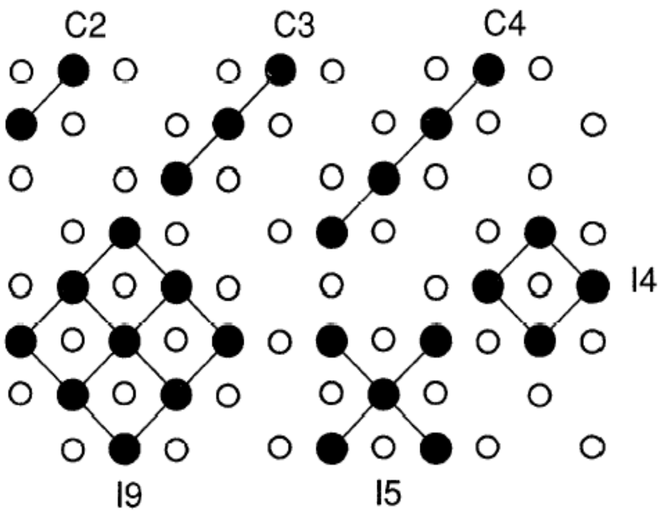


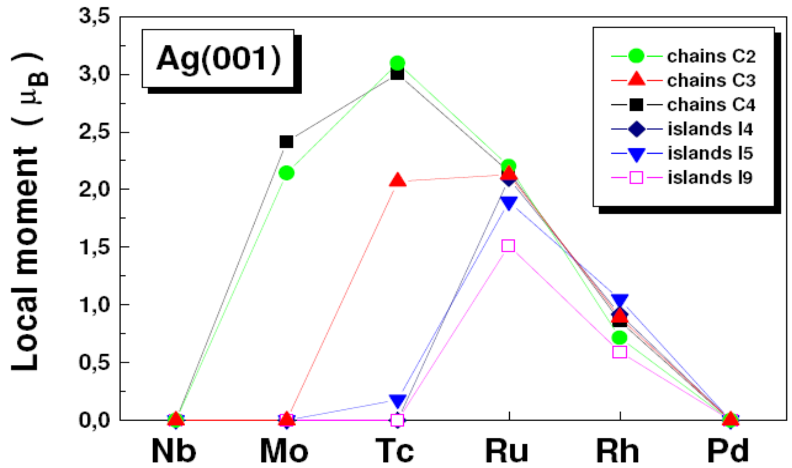
- Lang, Stepanyuk, Wildberger, Zeller, Dederichs, Solid state Comm. (1994)

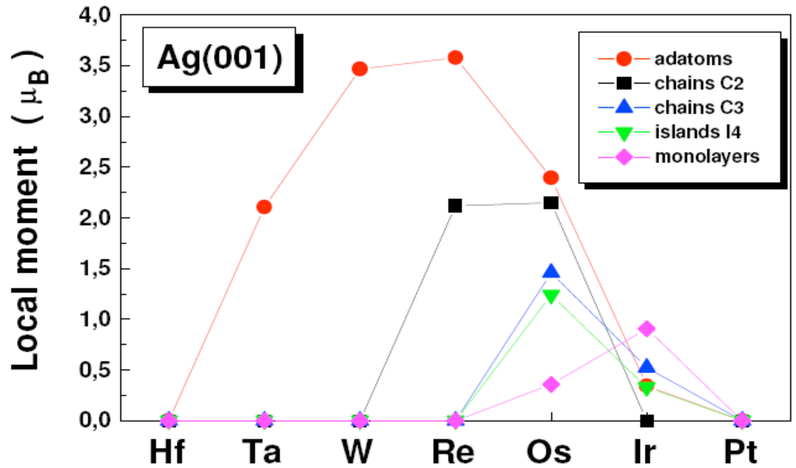
Transition from atomic to monolayer & bulk behaviour

Spin moments: 4d & 5d on Ag(001), shape & size dependence

Dependence on:
- Size
- Shape
- Interactions:
  - Intra-cluster
  - Cluster-substrate







Wildberger, Stepanyuk, Lang, Zeller, Dederichs, PRL (1995)

Nanowires
&
magnetic frustration

Non-collinear magnetism

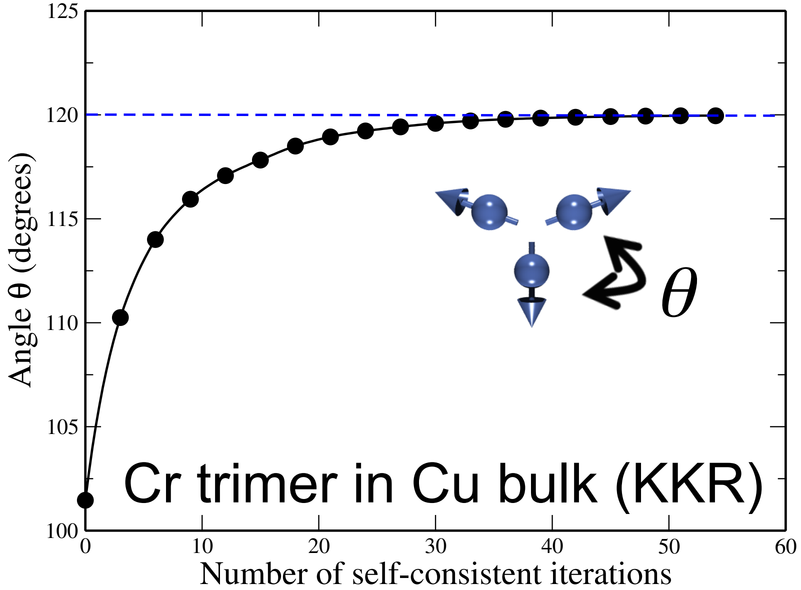
Classical Heisenberg Hamiltonian:

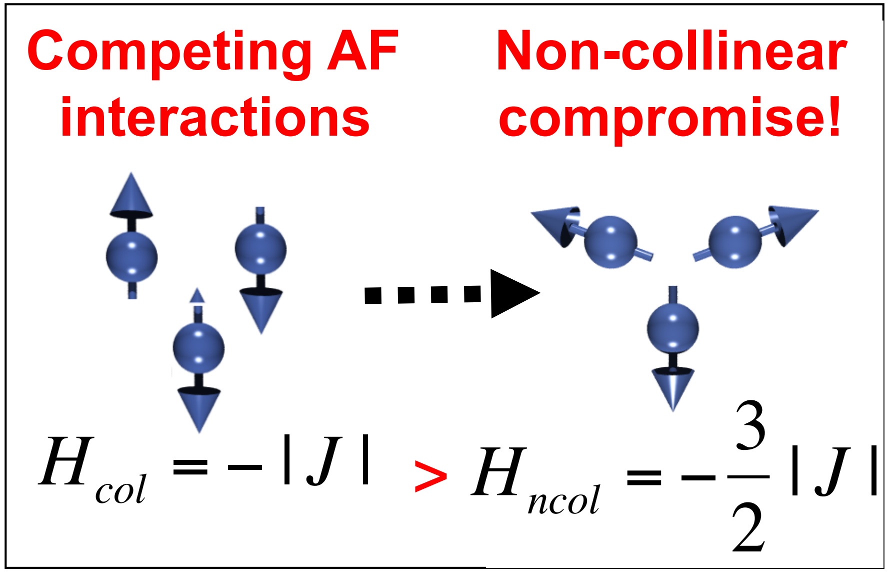
$$H = -\frac{1}{2}\sum_{i\neq j} J_{ij}\vec{e}_i \cdot \vec{e}_j$$

Driving mechanism:

Competing interactions:

Ferromagnetism or antiferromagnetism



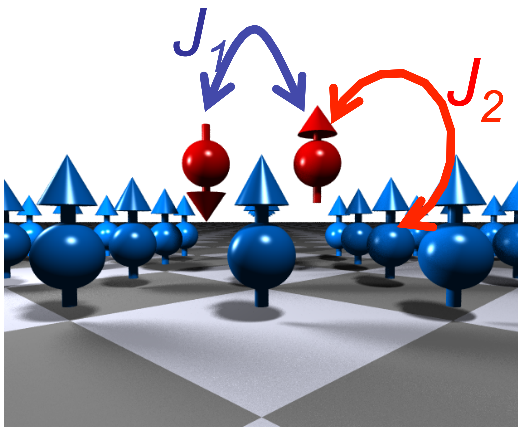


Mn or Cr atoms couple AF

Non-collinear magnetism:

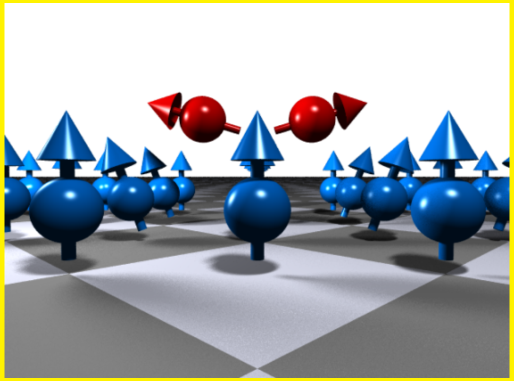
Mn on Ni(001)

collinear result:
frustrated



$H(ferri) = J_1$

Total E minimum (–13meV)

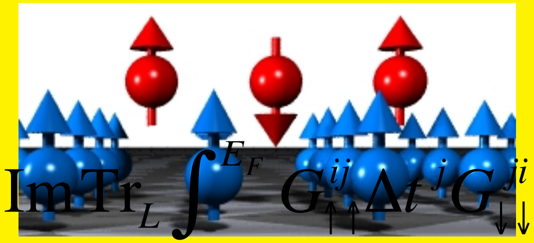


θ=72.5°

$H(ncol) = -J_1 \cos(2\theta) - J_2 \cos(\theta)$

Total E minimum (–9meV)

col

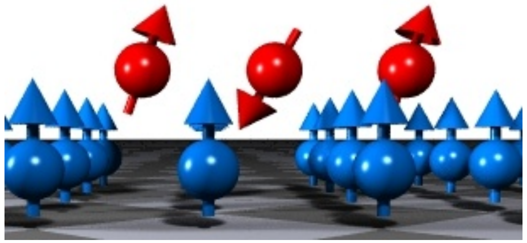


$$J_{ij} = \frac{1}{4\pi} \mathrm{Im\,Tr}_L \int^{E_F} G^{ij}_{\uparrow\uparrow} \Delta t^j G^{ji}_{\downarrow\downarrow} \Delta t^i$$

$J_1 = J(Mn\text{-}Mn) = -138$ meV

$H(ferri) = 2J_1 - J_2$

$J_2 = J(Mn\text{-}Ni) = 4 \times 13$ meV



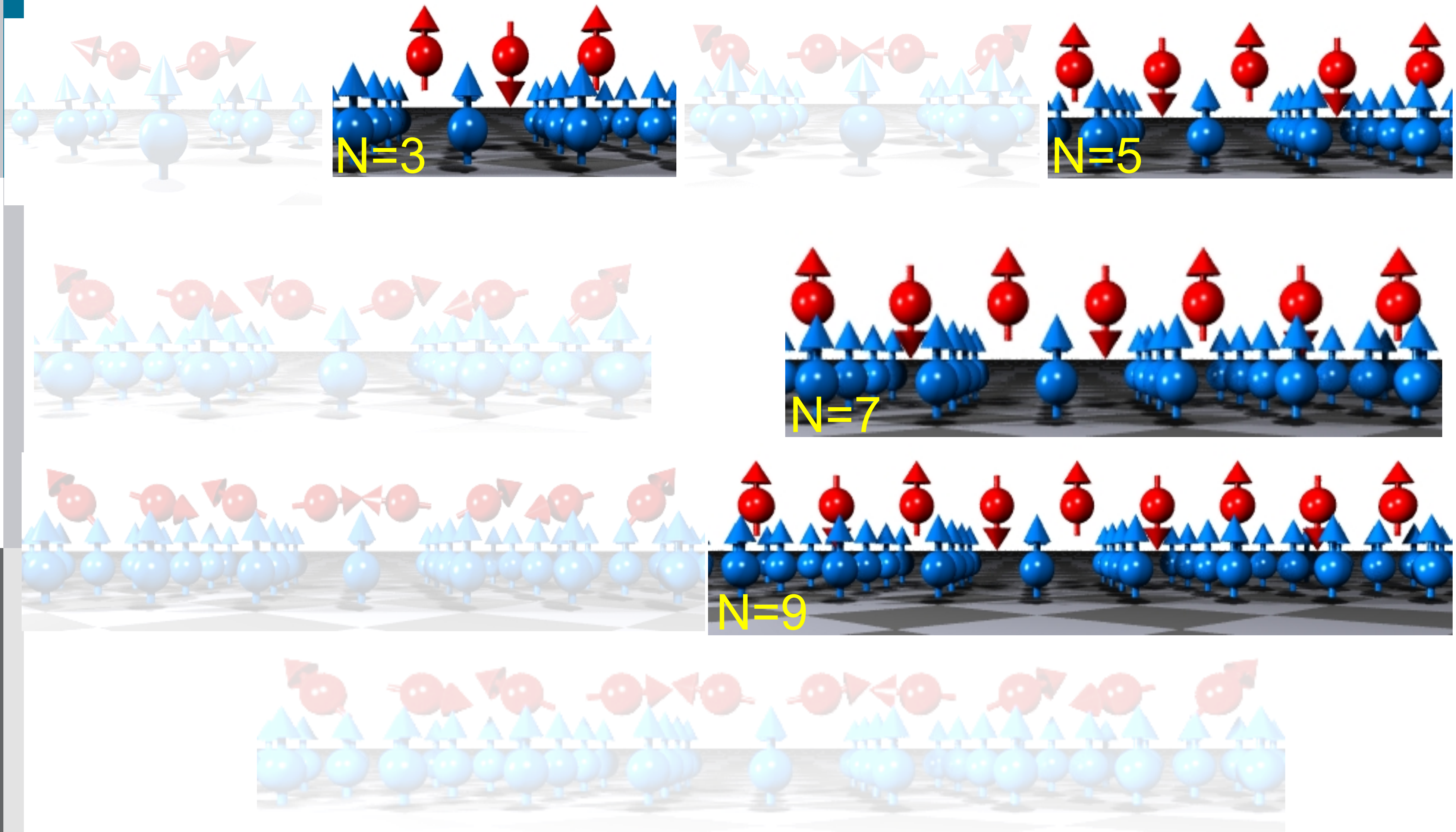
ncol

$H(ncol) = -2J_1 \cos(\alpha) - J_2 \cos(\theta)$

- Lichtenstein, Katsnelson, Antropov, Gubanov, JMMM, (1987)

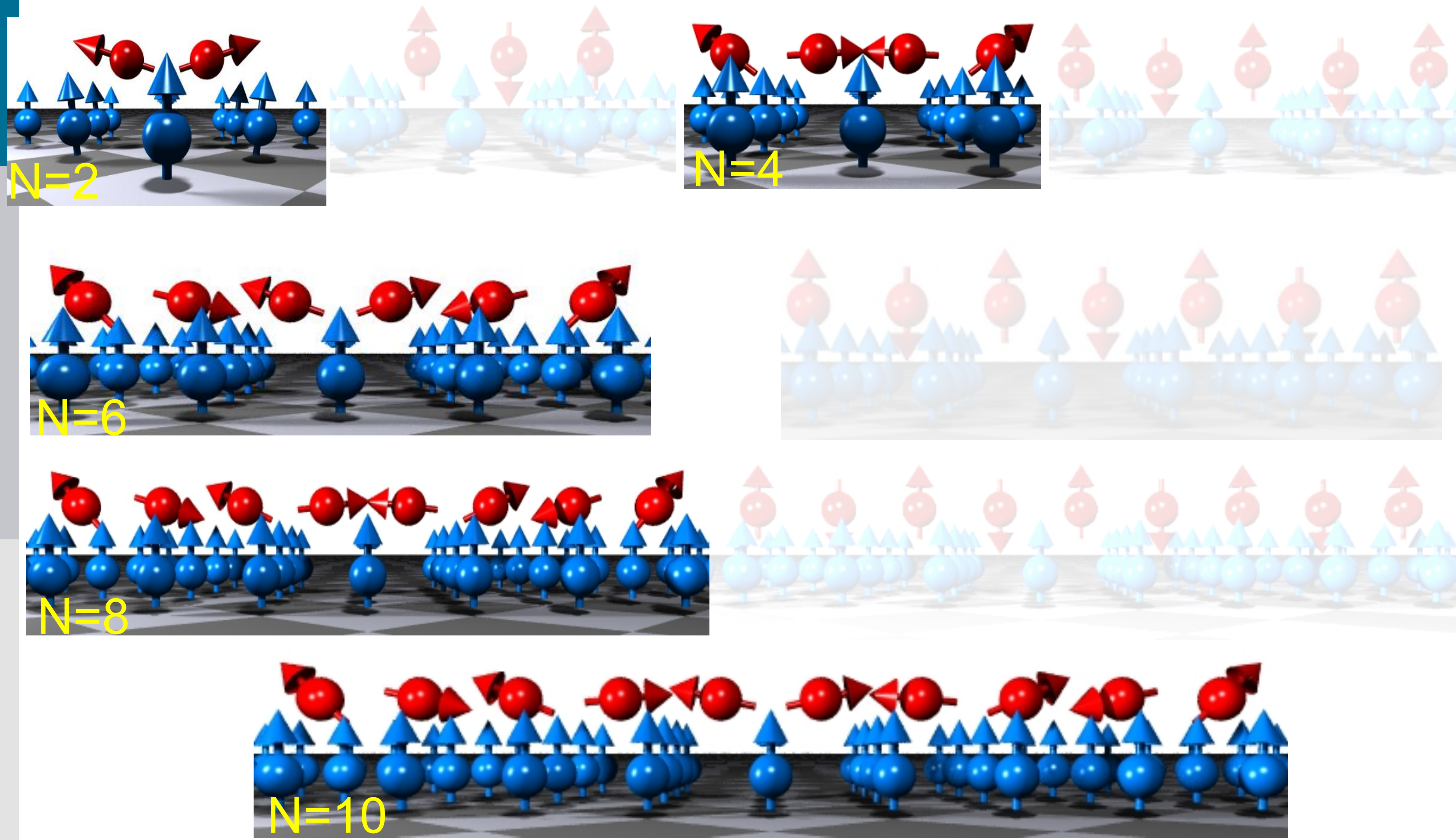
Odd numbered wires

odd = anti-parallel

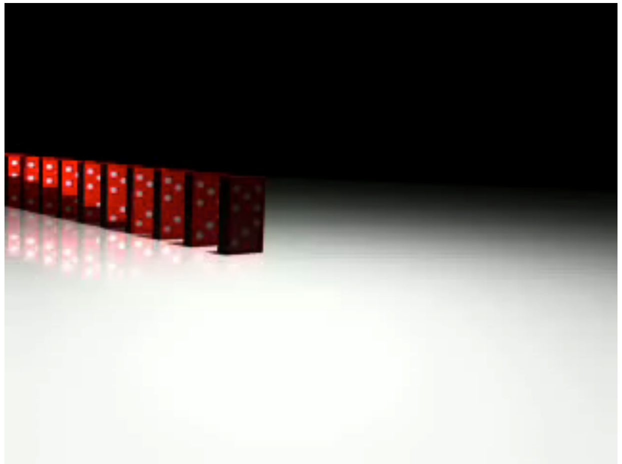


Even-numbered wires: Frustration

even = non-collinear



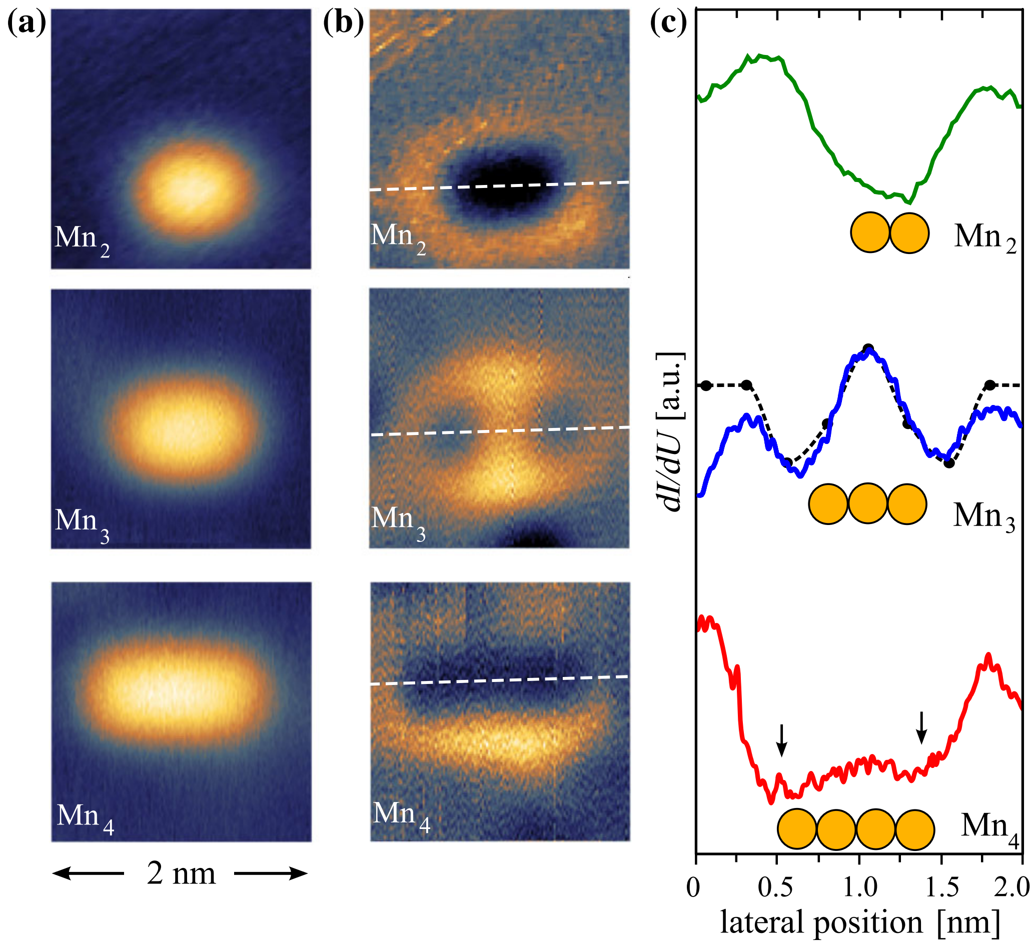
Domino effect in nanowires



From youtube.com: look at Domino

- Lounis, Dederichs, Blügel, Phys. Rev. Lett. **101**, 107204 (2008)

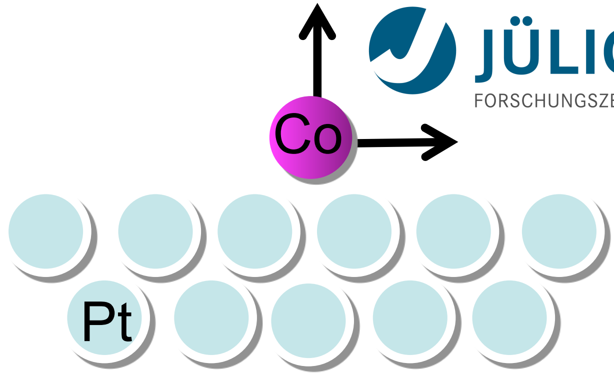
Experiment: Mn wires/Ni(110)



Holzberger, Schuh, Blügel, Lounis, Wulfhekel, PRL (2013)

Magnetic crystalline anisotropy energy (MAE)

XMCD measurements on MAE of Co adatoms/Pt(111)



$$H = -\frac{1}{2}\sum_{i \neq j} J_{ij}\vec{e}_i \cdot \vec{e}_j - \sum_i K_i \left(\vec{e}_i \cdot \vec{e}_j^{\,z}\right)^2$$

$$\sum_i K_i = H_x - H_z$$

A

n	**S**	**L**	$\Delta\mathbf{L}_{x\text{-}z}$	$K_{x\text{-}z}$
1	2.14	0.60 (1.50)	- 0.25	+ 18.45
2	2.11	0.38 (0.74)	- 0.11	+ 4.11
3 chain	2.08	0.34 (0.67)	- 0.06	+ 3.69
3 triangle	2.10	0.25 (0.43)	- 0.05	+ 2.22
4	2.08	0.22 (0.33)	- 0.01	+ 0.75
5	2.08	0.27 (0.45)	- 0.09	+ 1.81

B

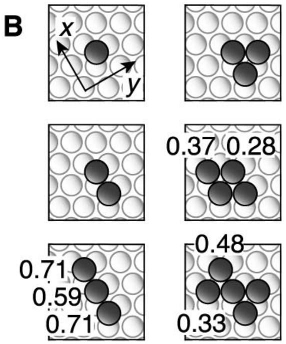
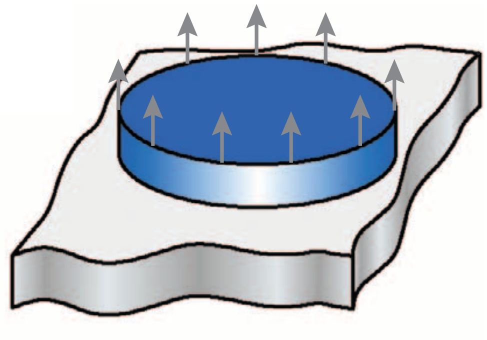
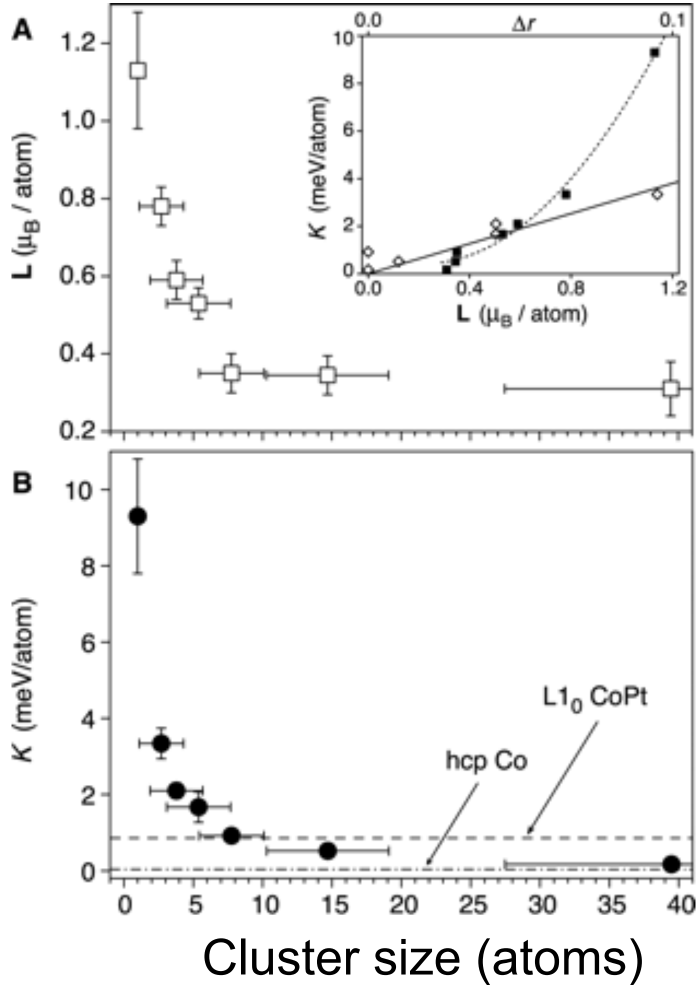


Fig. 4. (**A**) Values of **S**, **L**, $\Delta\mathbf{L}$ (μ_B), and K (meV) per Co atom calculated by the SPR-KKR method for Co particles on Pt(111) as shown in (B). The values of **L** in parentheses have been computed within the OP scheme with a 50% reduced Racah parameter. (**B**) Hard-sphere representation of the Co particles considered in the theoretical calculations. The labels indicate the OP values of **L** for nonequivalent Co sites. **S**, **L**, $\Delta\mathbf{L}$, and K in (A) are averaged over all Co sites.





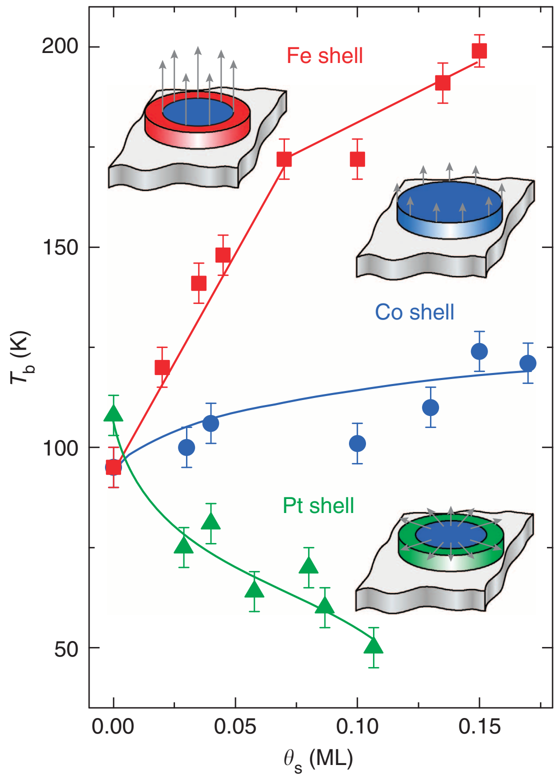
P. Gambardella et al., Science (2003)

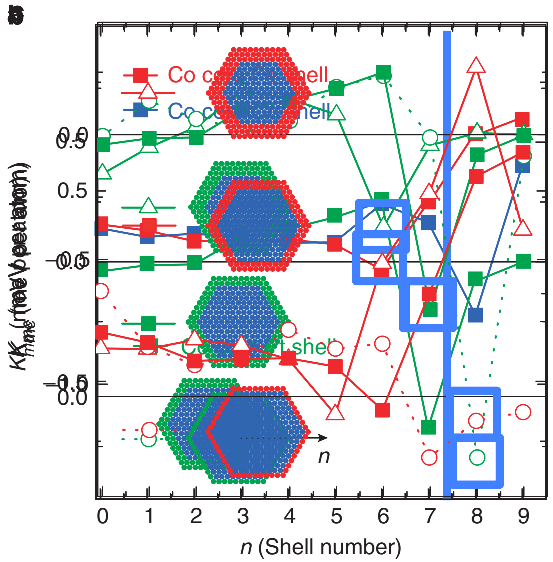
Engineering of MAE of nanostructures

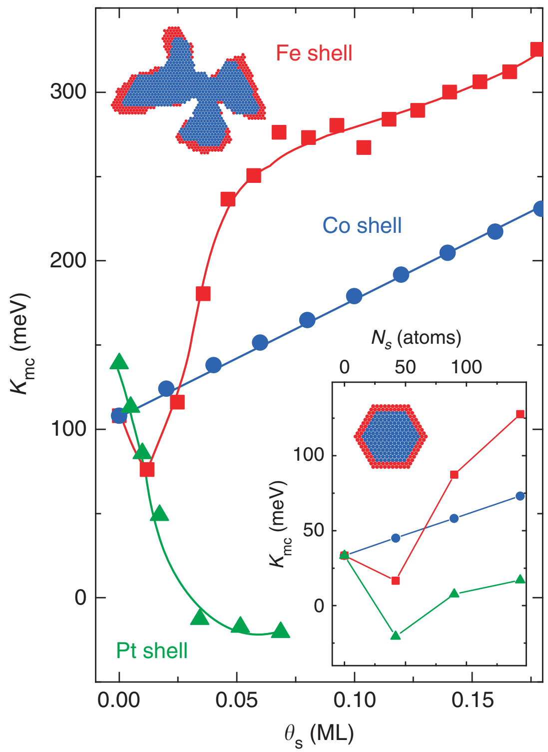
JÜLICH
FORSCHUNGSZENTRUM

Blocking temperature is related to MAE

Calculated MAE for experimental island sizes and shapes.





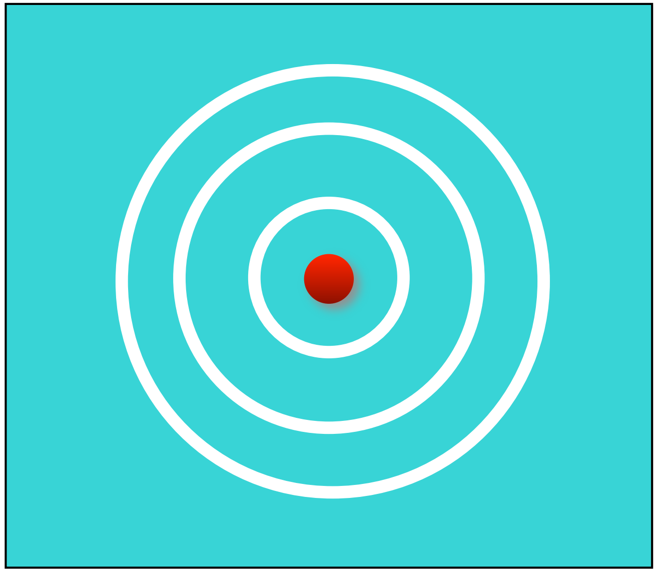


- Ouazi, Vlaic, Rusponi, Moulas, Bulushek, Halleux, Bornemann, Mankovsky, Minar, Staunton, Ebert, Brune, Nature Communications,(2012)

Friedel oscillations & confinement

Friedel oscillations and confinement

Stone in water



3D jellium $\Delta n(r) \propto \frac{\cos(2k_F r)}{r^3}$

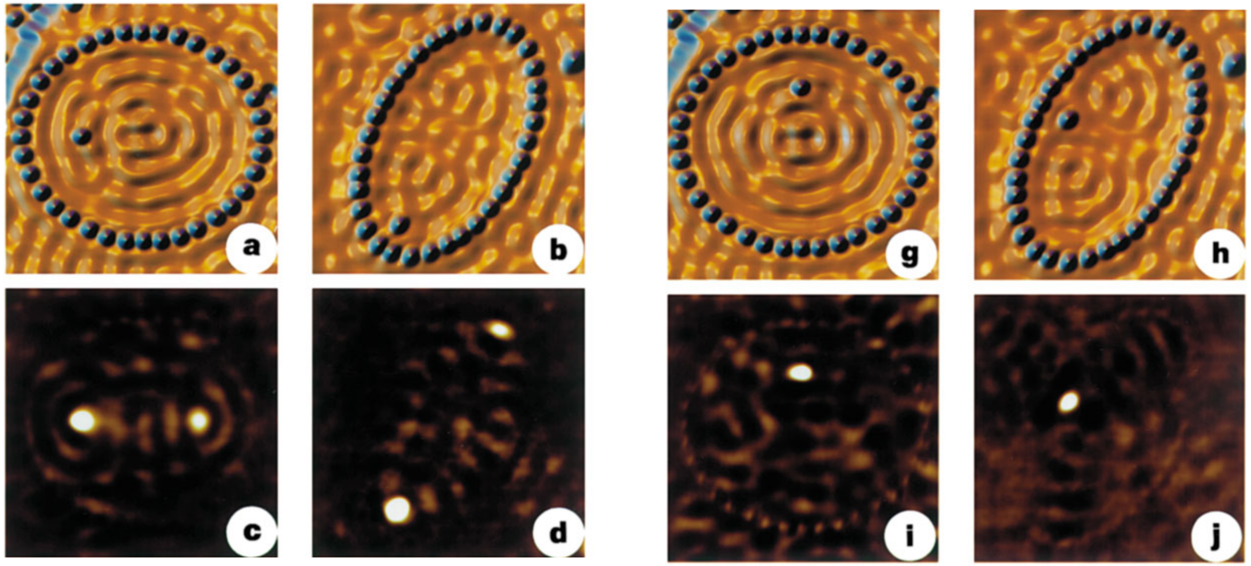
2D jellium $\Delta n(r) \propto \frac{\cos(2k_F r)}{r^2}$

Quantum Corals & Quantum Mirage

Atom at focal point; mirage at second focal point!

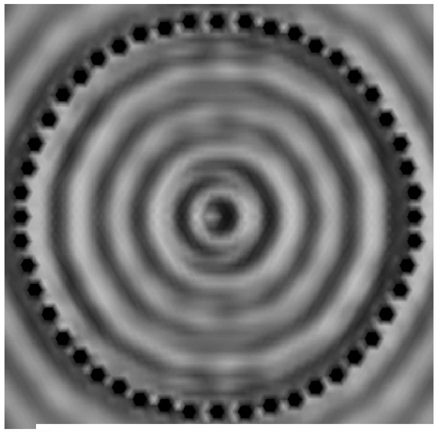
STM image:
Co corral
on Cu(111)

Significant
role of
surface state



- Manoharan, Lutz, and Eigler, Nature (2000)

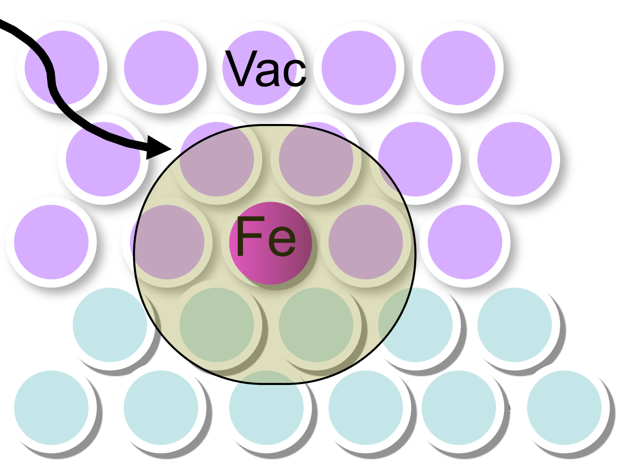
Related *ab-initio* calculations:



- Lazarovits, Ujfalussy, Szunyogh, Gyorffy, Weinberger, J.Phys. Cond. Matt. (2005)

1-Self-consistent calculations

Side view

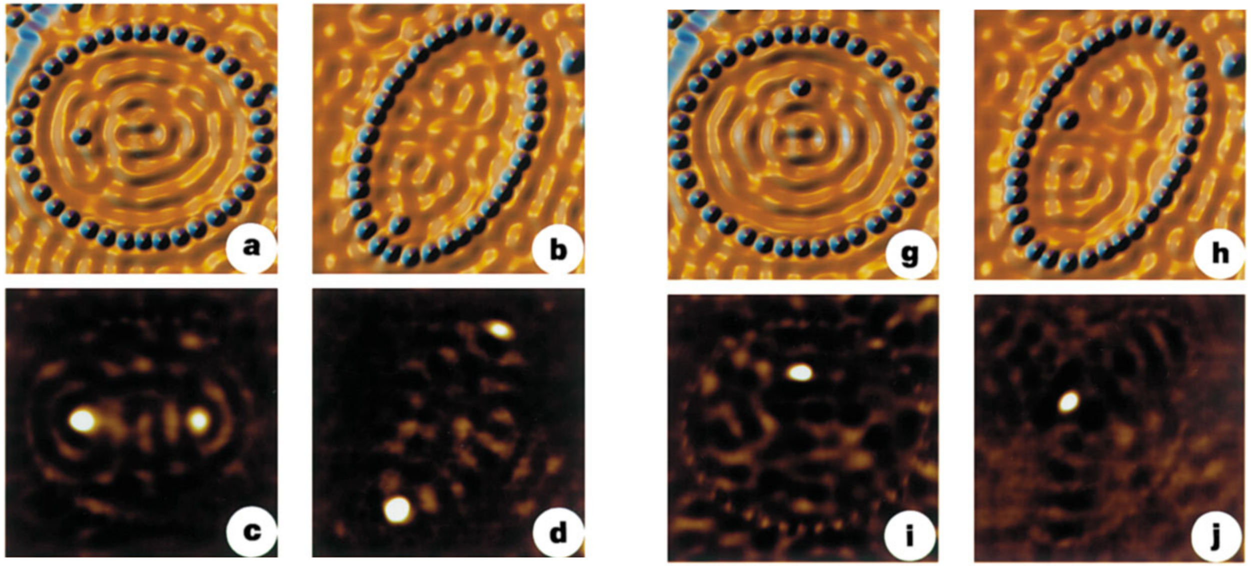


Quantum Corals & Quantum Mirage

Atom at focal point; mirage at second focal point!

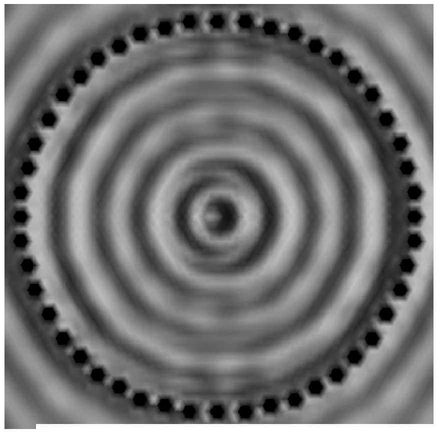
STM image:
Co corral
on Cu(111)

Significant
role of
surface state



Manoharan, Lutz, and Eigler, Nature (2000)

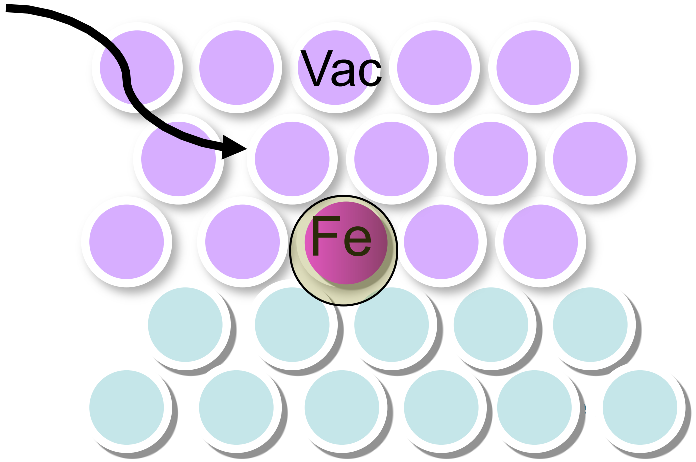
Related *ab-initio* calculations:



Lazarovits, Ujfalussy, Szunyogh,
Gyorffy, Weinberger, J.Phys. Cond. Matt. (2005)

2-Use of potential of
single Fe atoms

Side view



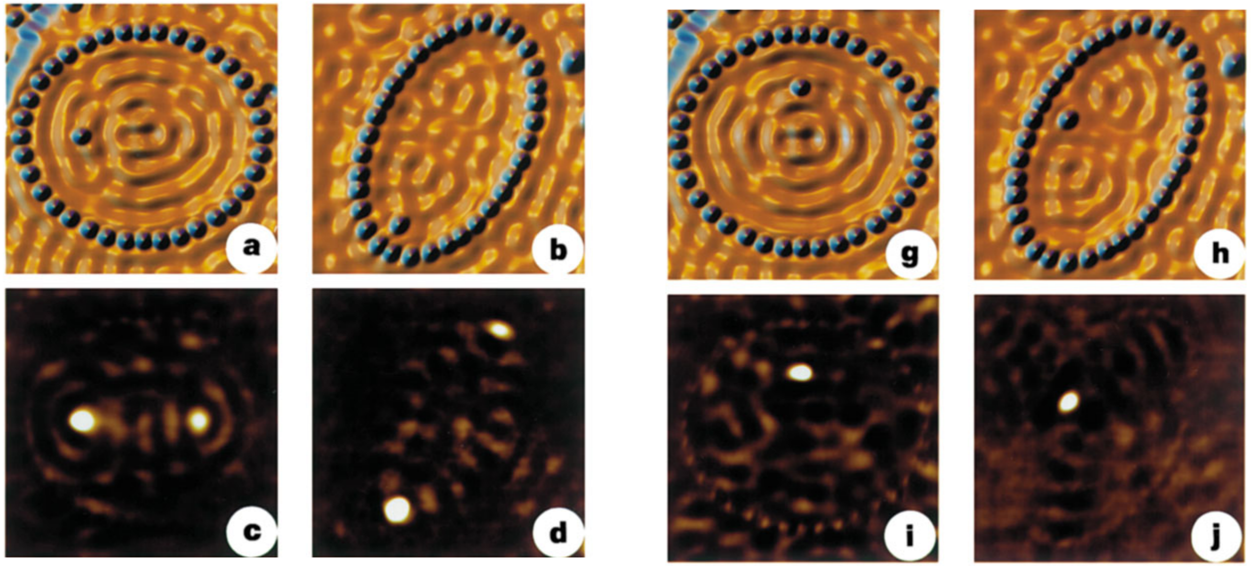
Quantum Corals & Quantum Mirage

JÜLICH FORSCHUNGSZENTRUM

Atom at focal point; mirage at second focal point!

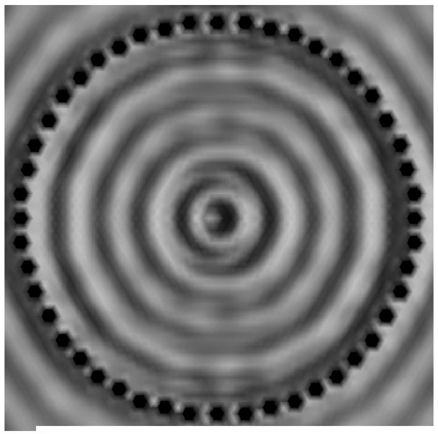
STM image:
Co corral
on Cu(111)

Significant
role of
surface state



Manoharan, Lutz, and Eigler, Nature (2000)

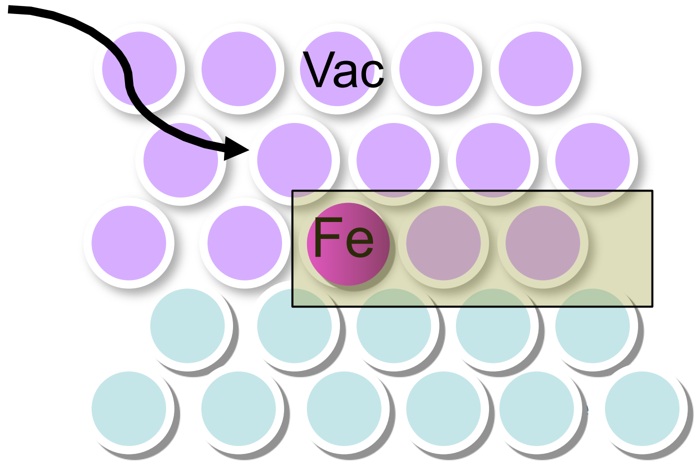
Related *ab-initio* calculations:



Lazarovits, Ujfalussy, Szunyogh,
Gyorffy, Weinberger, J.Phys. Cond. Matt. (2005)

3-Solve the Dyson eq.
for corral + vacuum sites

Side view

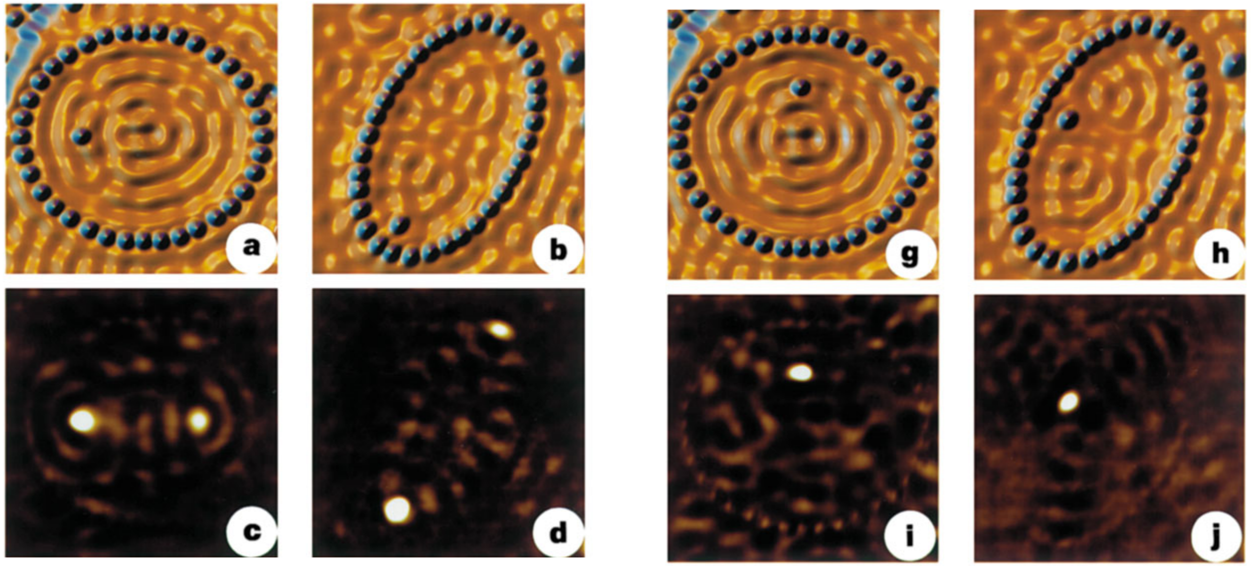


Quantum Corals & Quantum Mirage

Atom at focal point; mirage at second focal point!

STM image:
Co corral
on Cu(111)

Significant
role of
surface state

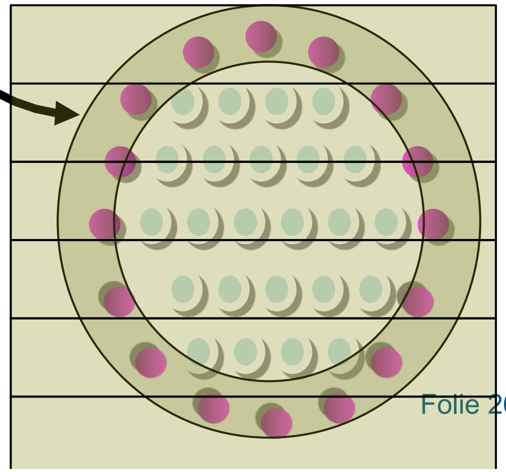


Manoharan, Lutz, and Eigler, Nature (2000)

Related *ab-initio* calculations:

3-Solve the Dyson eq.
for corral + vacuum sites

top view



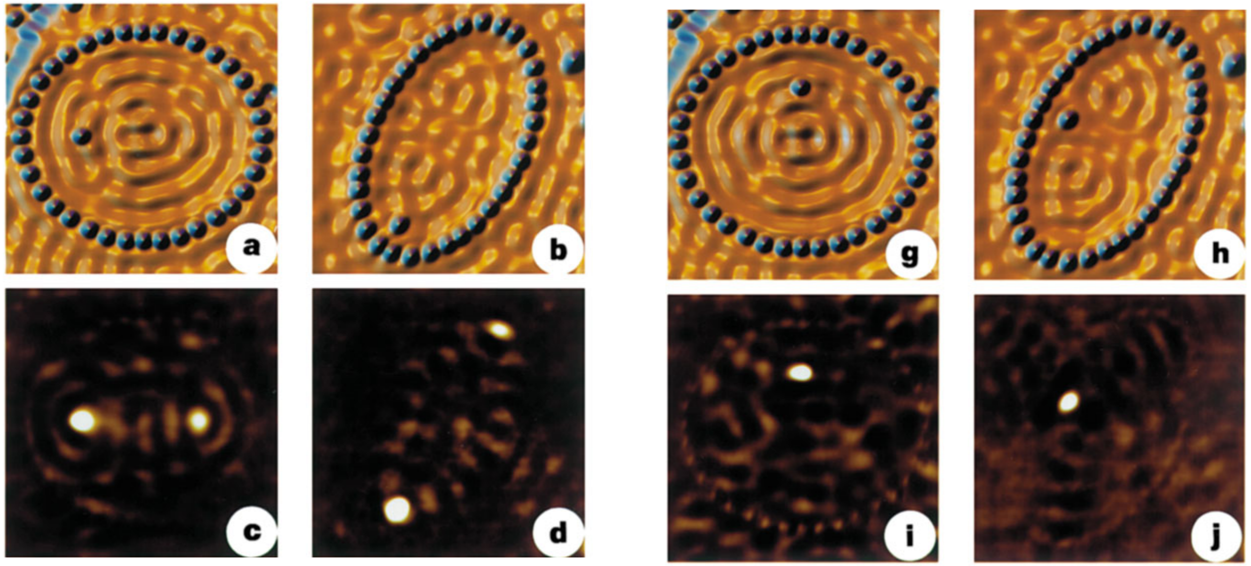
Lazarovits, Ujfalussy, Szunyogh,
Gyorffy, Weinberger, J.Phys. Cond. Matt. (2005)

Quantum Corals & Quantum Mirage

Atom at focal point; mirage at second focal point!

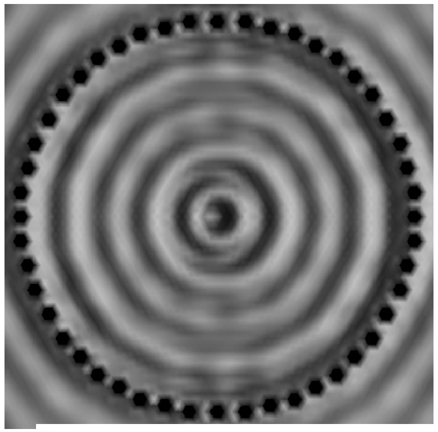
STM image:
Co corral
on Cu(111)

Significant
role of
surface state



- Manoharan, Lutz, and Eigler, Nature (2000)

Related *ab-initio* calculations:

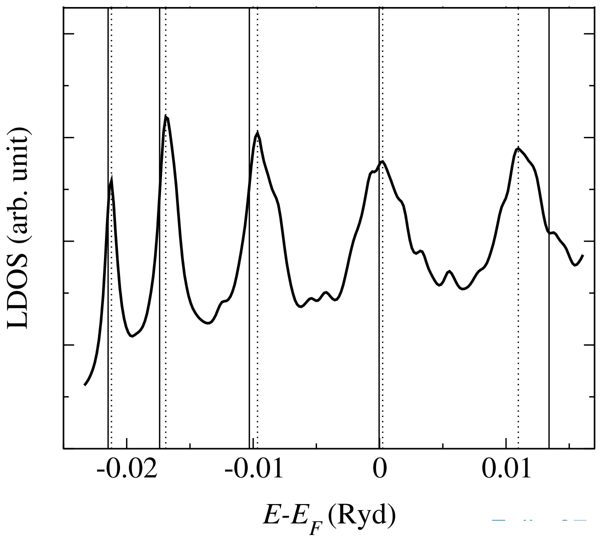


- Lazarovits, Ujfalussy, Szunyogh, Gyorffy, Weinberger, J.Phys. Cond. Matt. (2005)

Circular quantum well model

$$V(\vec{r}) = \begin{cases} 0 & \text{if } r < R \\ +\infty & \text{if } r \geq R \end{cases}$$

Solutions are bessel functions of the first kind



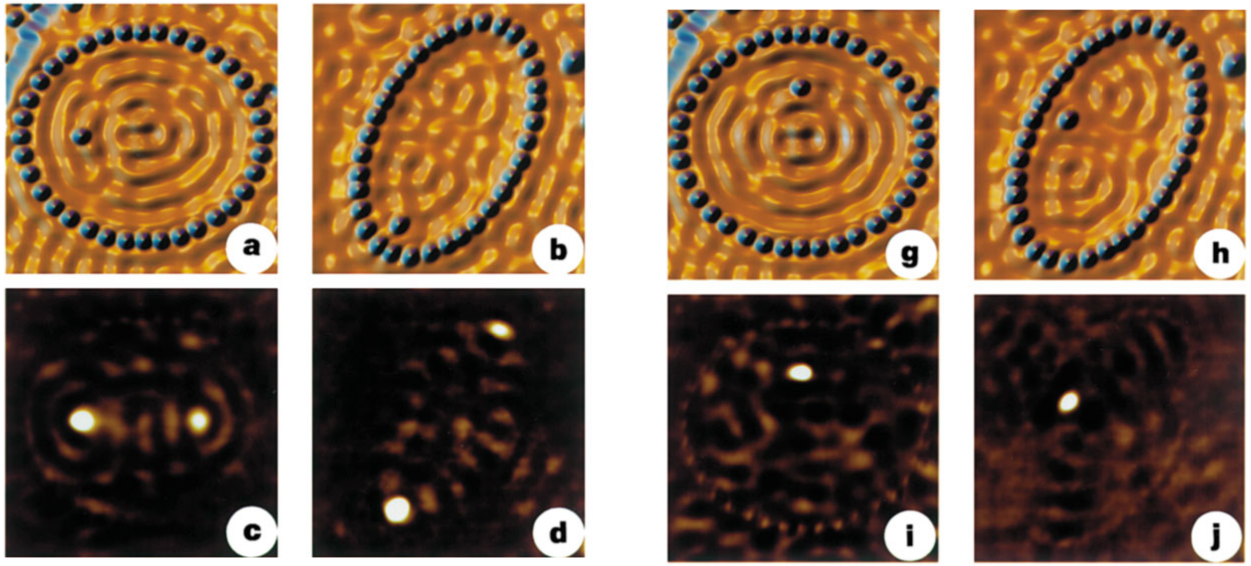
Center of quantum corrals

Quantum Corals & Quantum Mirage

Atom at focal point; mirage at second focal point!

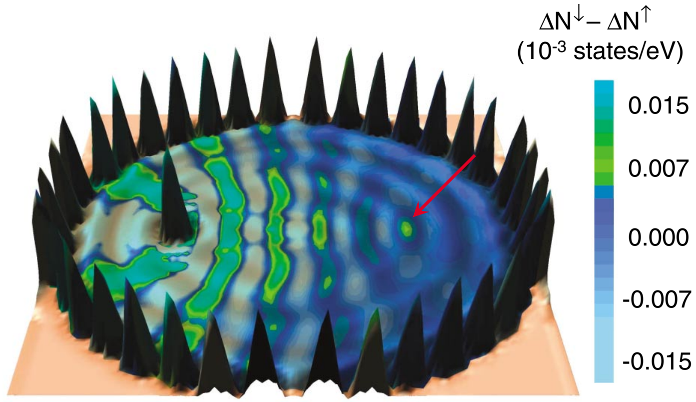
STM image:
Co corral
on Cu(111)

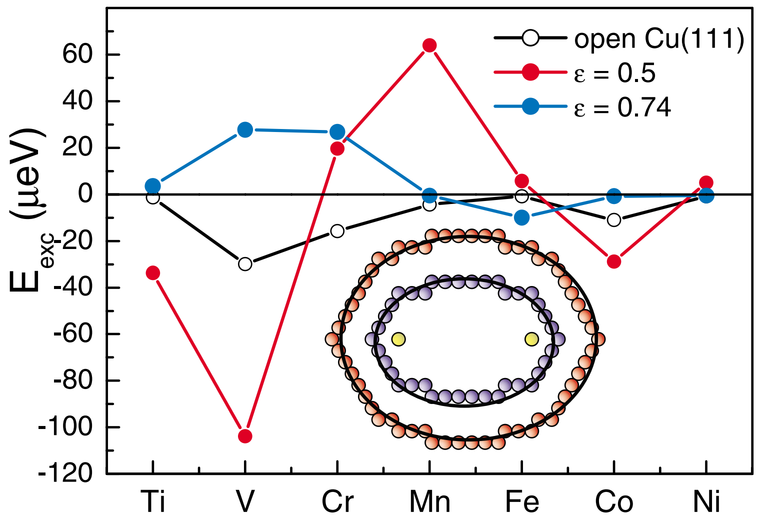
Significant
role of
surface state



- Manoharan, Lutz, and Eigler, Nature (2000)

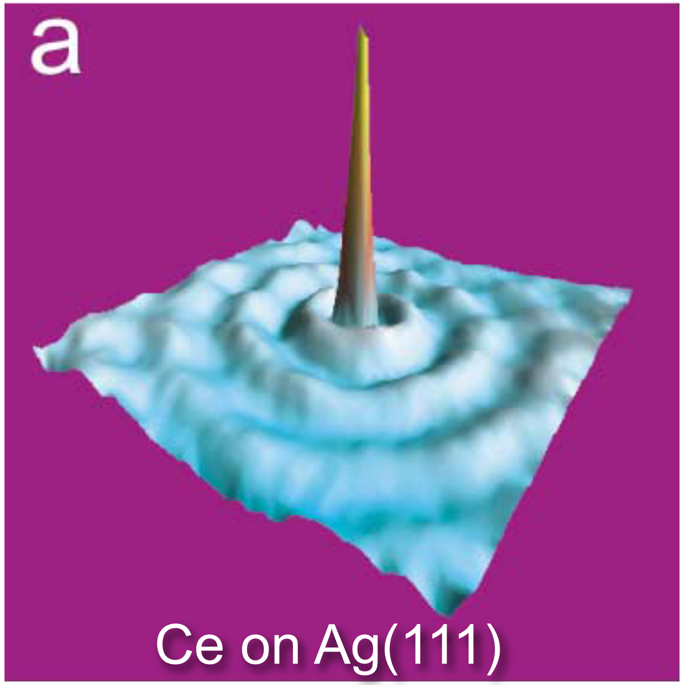
Related *ab-initio* calculations:



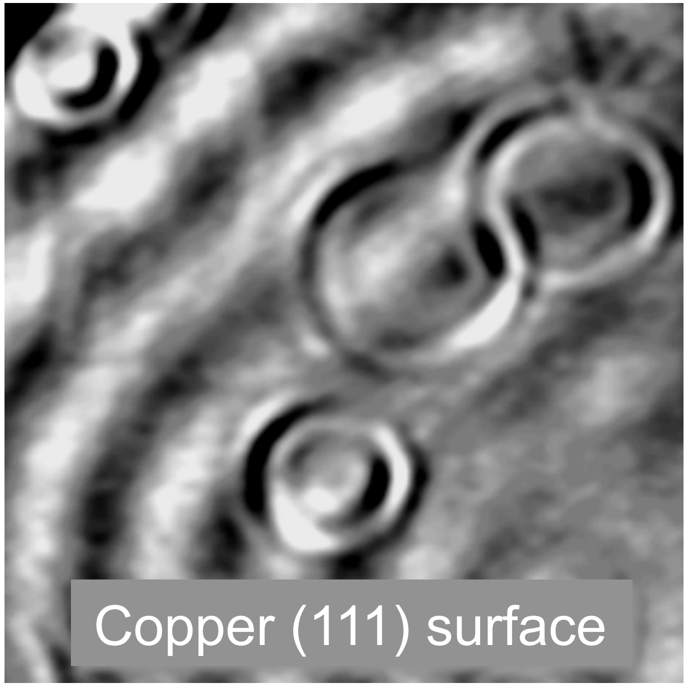


- Stepanyuk, Niebergall, Hergert, Bruno, PRL (2005)

Electron distribution induced by adatoms or buried atoms



Silly et al., PRL 92, 16101 (2004)



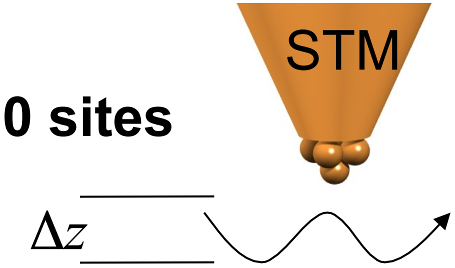
STM picture by
A. Weismann, M. Wenderoth, R.G. Ulbrich
University of Göttingen

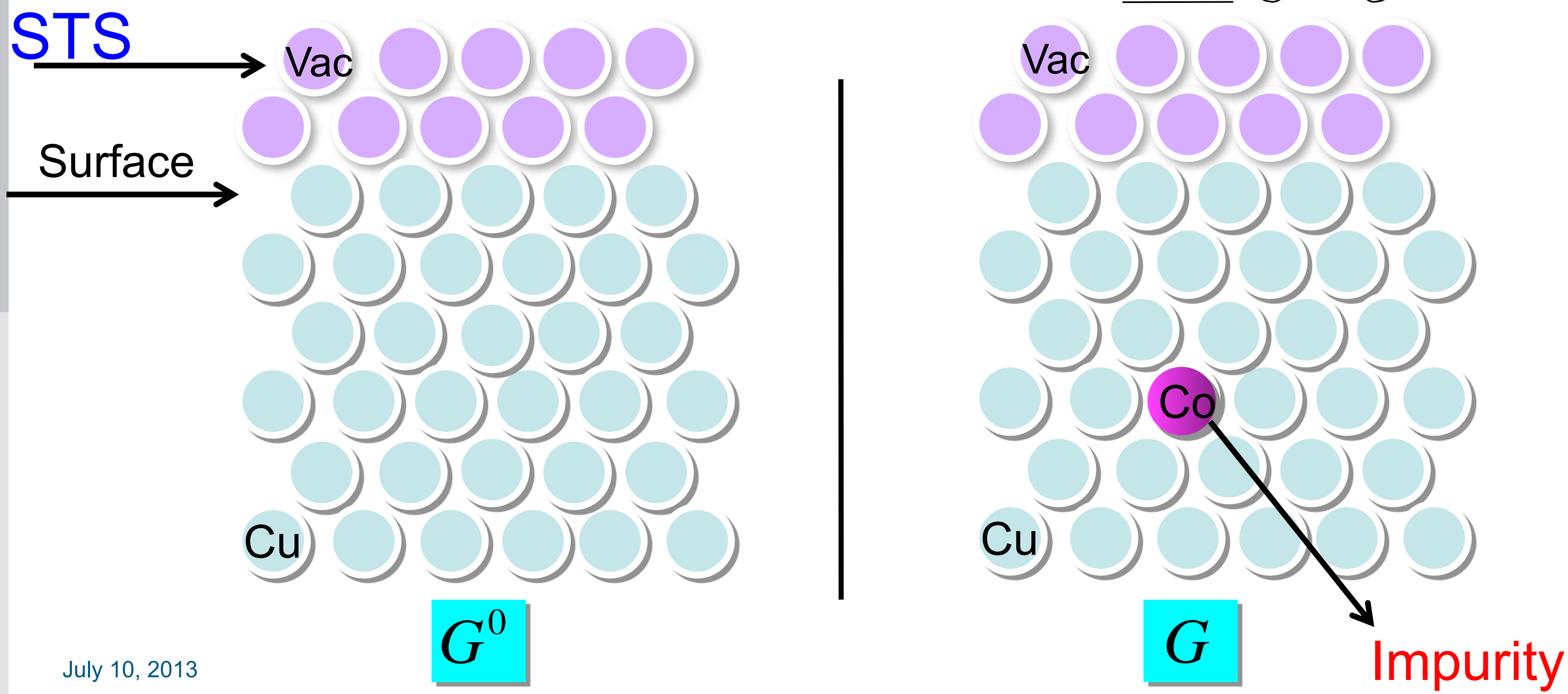
Method

Tersoff-Hamann Model:
$$I(\vec{r}_{\|}, z, V) \propto n_T \int_{E_F}^{E_F+eV} n(\vec{r}_{\|}, z, \epsilon)\, d\epsilon$$

$$G(E) = G^0(E) + G^0(E)V\,G(E)$$

~ few 1000 sites



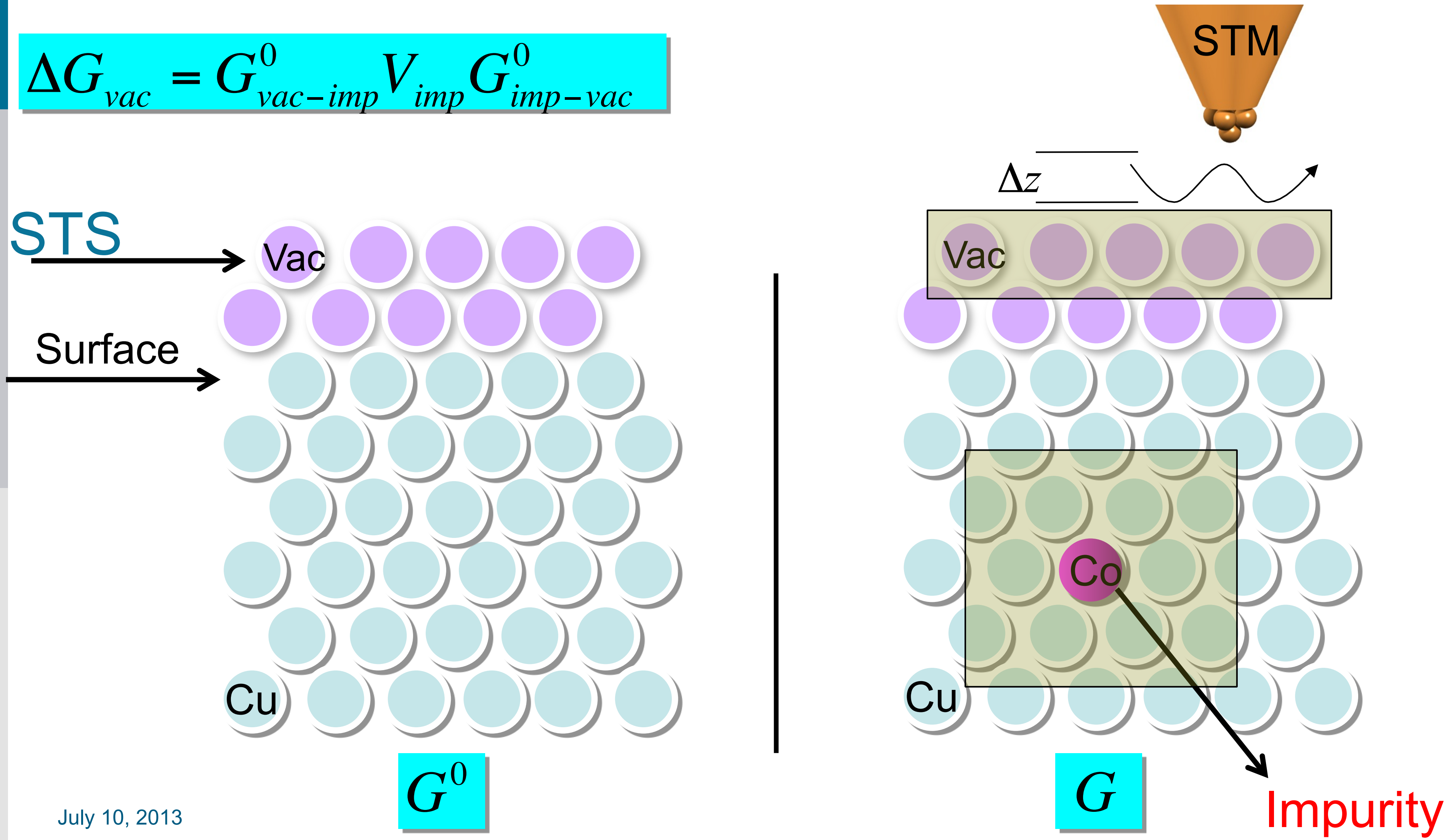


Method

Tersoff-Hamann Model:

$$I(\vec{r}_\parallel, z, V) \propto n_T \int_{E_F}^{E_F+eV} n(\vec{r}_\parallel, z, \epsilon)\, d\epsilon$$

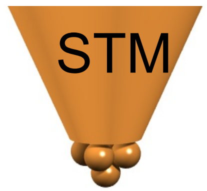
$$\Delta G_{vac} = G^0_{vac-imp} V_{imp} G^0_{imp-vac}$$



Method

Tersoff-Hamann Model:

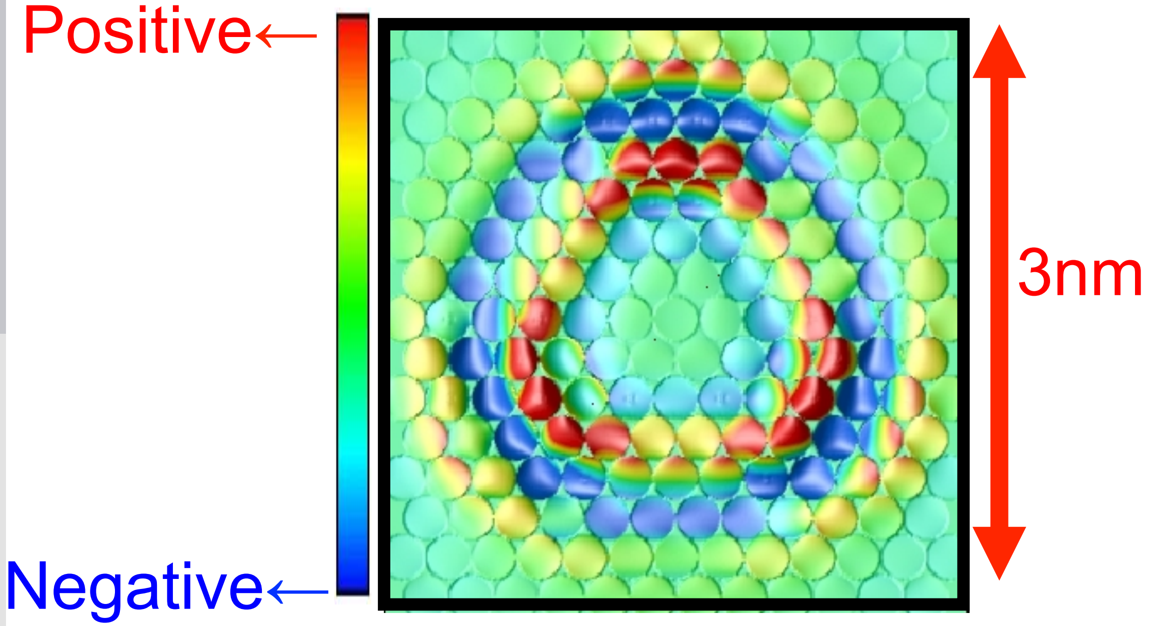
$$I(\vec{r}_{\parallel}, z, V) \propto n_T \int_{E_F}^{E_F+eV} n(\vec{r}_{\parallel}, z, \epsilon)\, d\epsilon$$

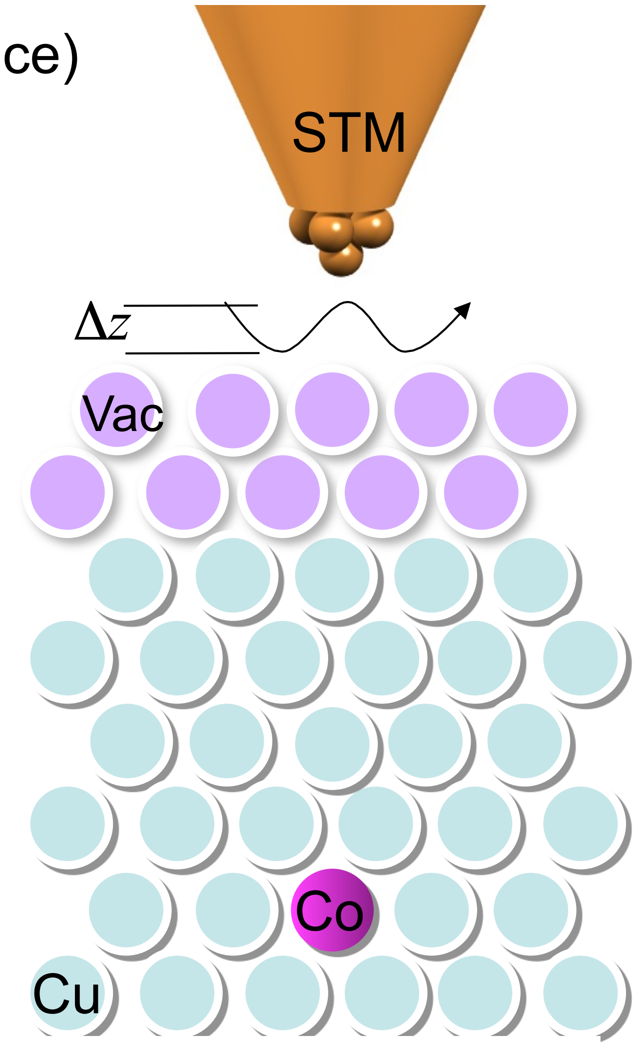


$$\Delta G_{vac} = G^0_{vac-imp} V_{imp} G^0_{imp-vac}$$

Result: Constant Current STM-image
Co buried below Cu(111) surface

- Charge density in vacuum (~6.1Å above the surface)
- Bias Voltage V: 100 meV below E_F
- Co at 6th layer below the surface (~12.1Å)

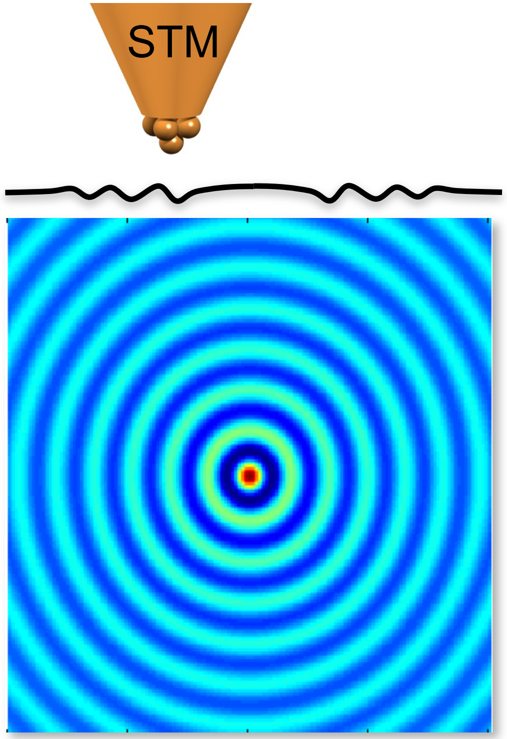


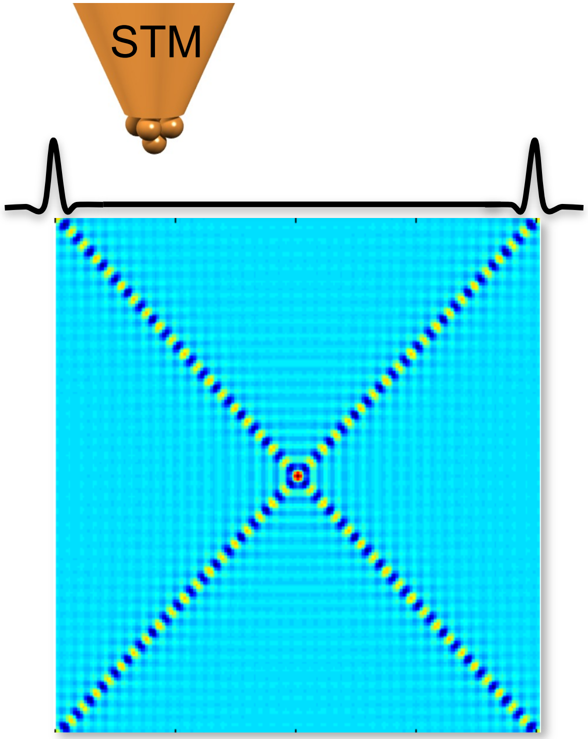


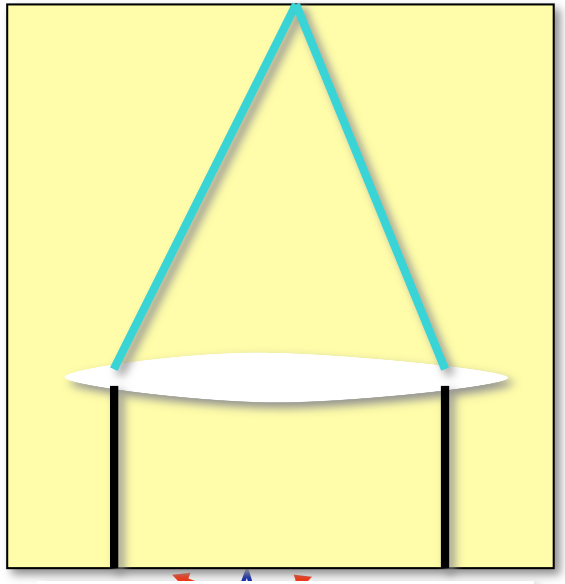
- Weismann,Wenderoth, Lounis, Zahn, Quaas, Ulbrich, Dederichs, Blügel, *Science* (2009)
- Lounis, Zahn, Weismann,Wenderoth, Ulbrich, Mertig, Dederichs, Blügel, *PRB* (2011)

Origin of effect

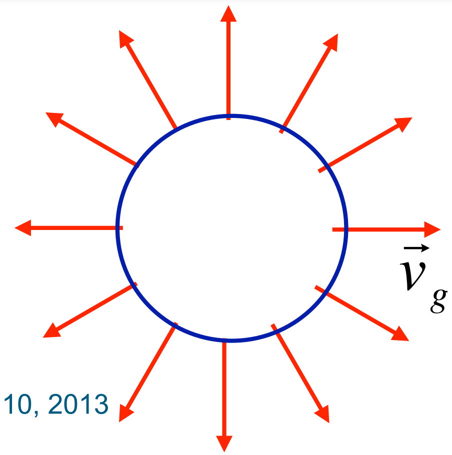
Dyson eq.: $G(E) = G_0(E) + G_0(E)V\,G(E)$



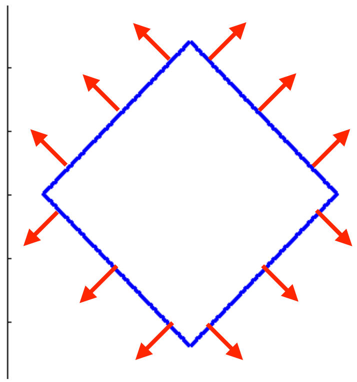


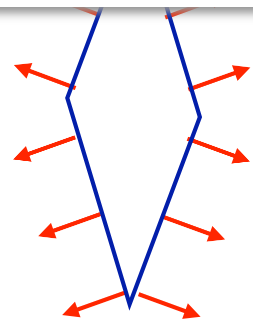


Lens focusing light



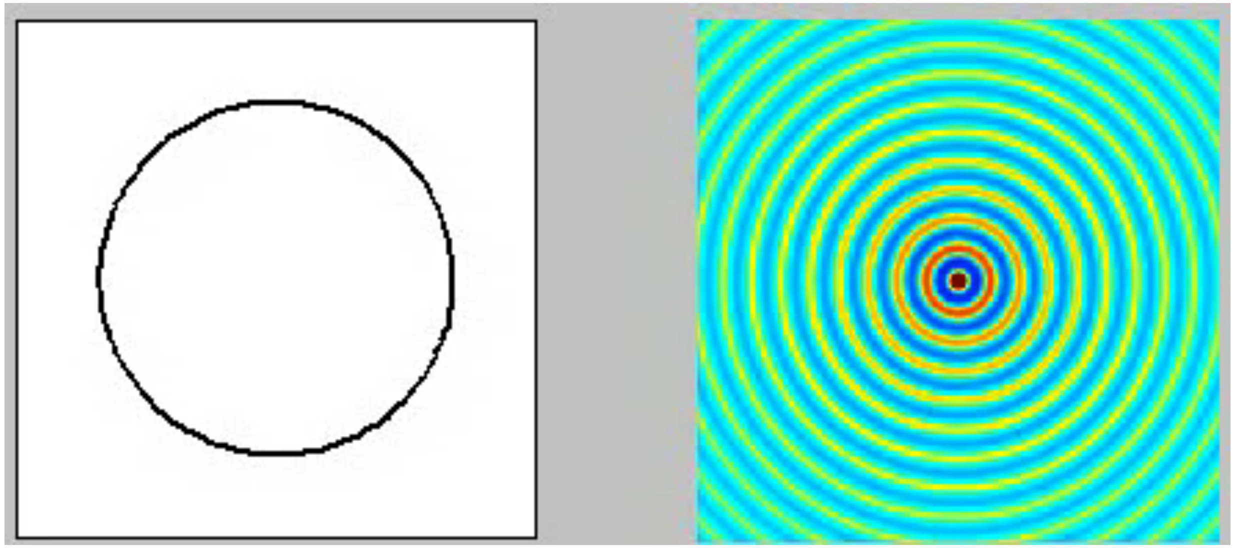
$$\vec{v}_g = \frac{\partial E}{\partial \vec{k}}$$





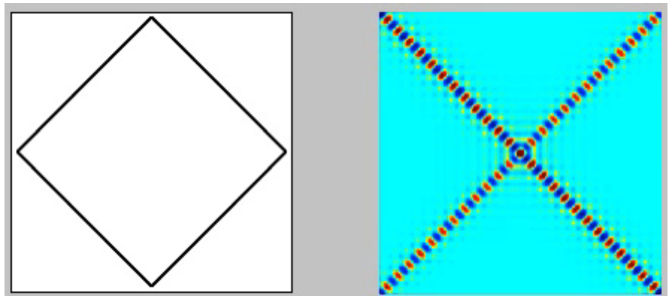
Origin of effect

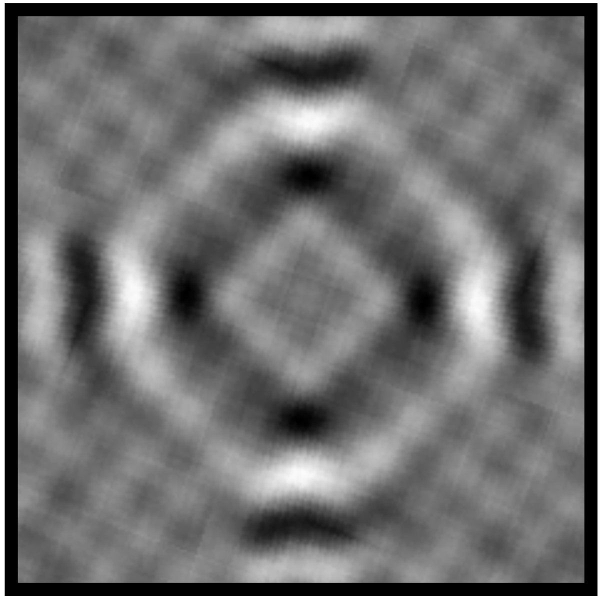
Dyson eq.: $$G(E) = G_0(E) + G_0(E) V G(E)$$



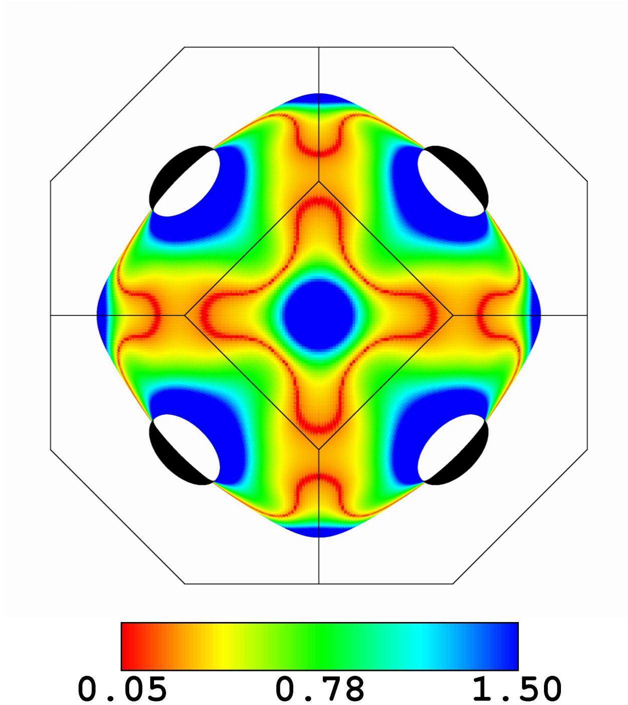
- Weismann,Wenderoth, Lounis, Zahn, Quaas, Ulbrich, Dederichs, Blügel, *Science* (2009)
- Lounis, Zahn, Weismann,Wenderoth, Ulbrich, Mertig, Dederichs, Blügel, *PRB* (2011)

Origin of effect





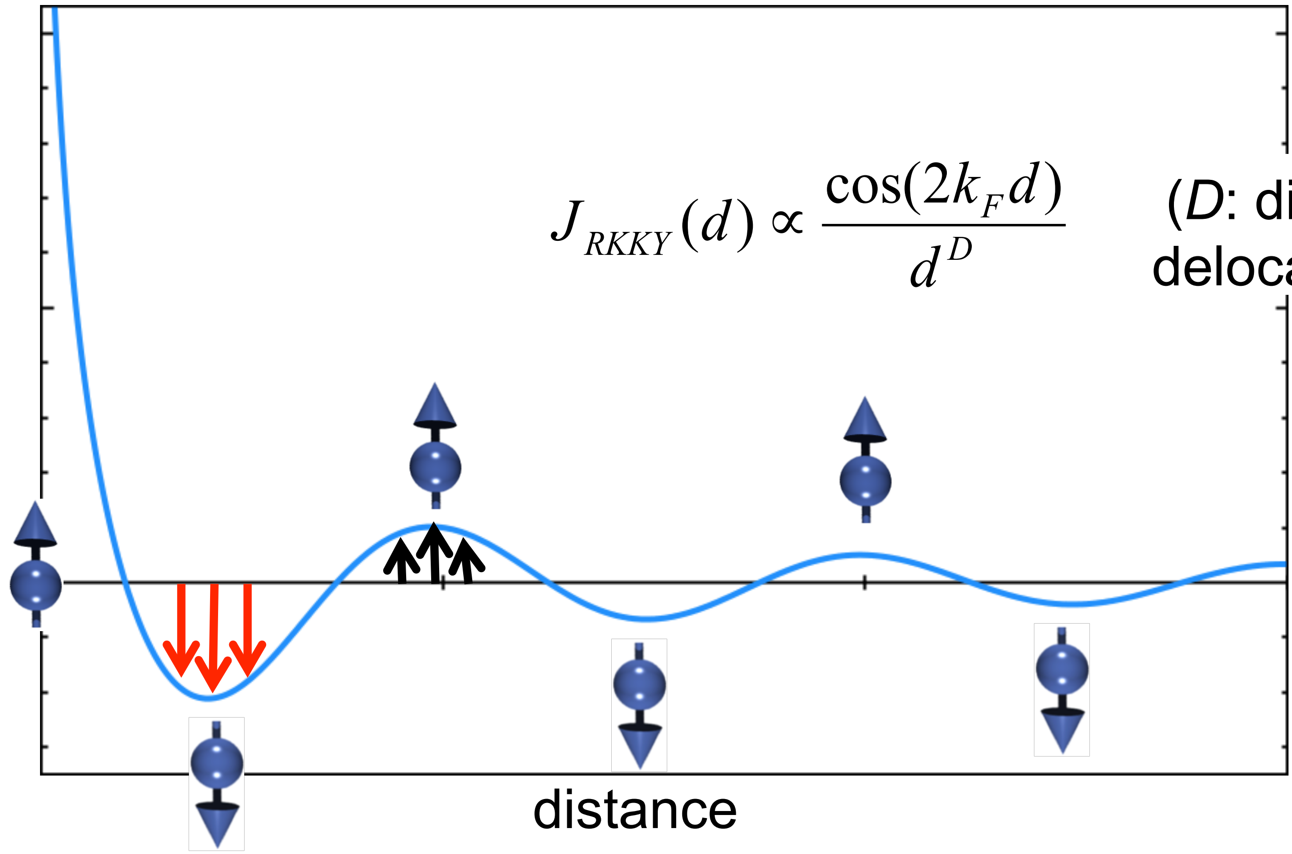
Co at 8th layer below Cu(001)surface



Measure of curvature

Real space visualisation of Fermi surfaces with STM!

Magnetic Friedel oscillations & RKKY interac.

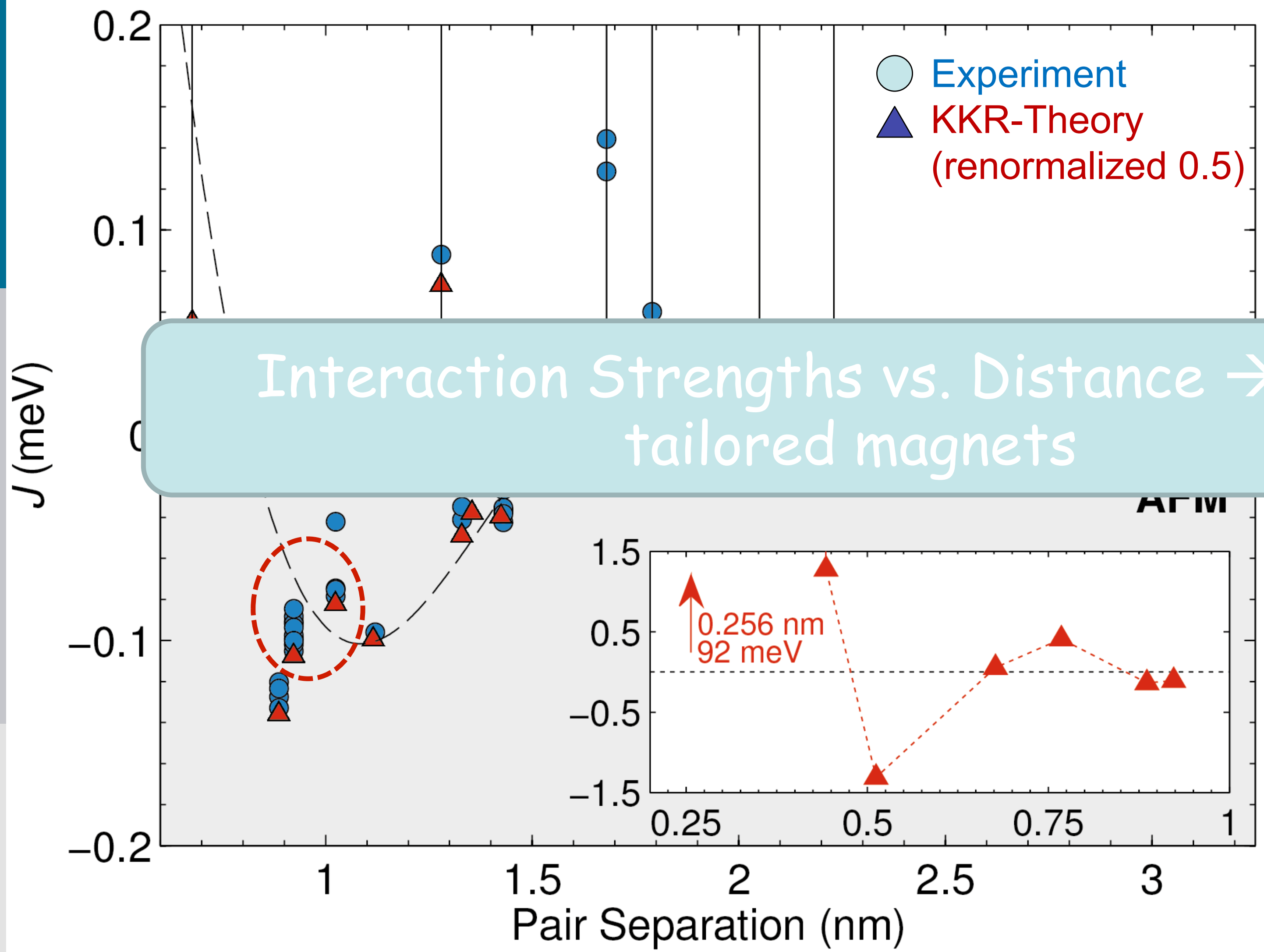


$$J_{RKKY}(d) \propto \frac{\cos(2k_F d)}{d^D}$$

(*D*: dimensionality of delocalized electrons)

- M. A. Ruderman, C. Kittel, *Phys. Rev.* (1954);
  T. Kasuya, *Prog. Theor. Phys.* (1956);
  K. Yosida, *Phys. Rev.* (1957)

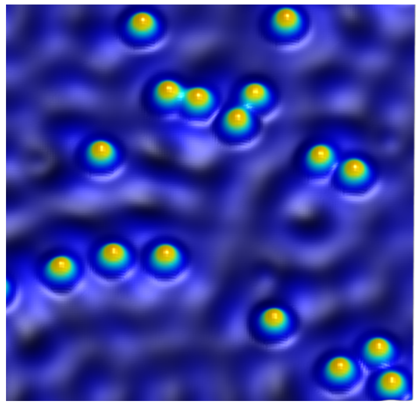
RKKY Interaction in Fe Pairs on Cu(111)



Interaction Strengths vs. Distance → build tailored magnets

Ab initio calculations:

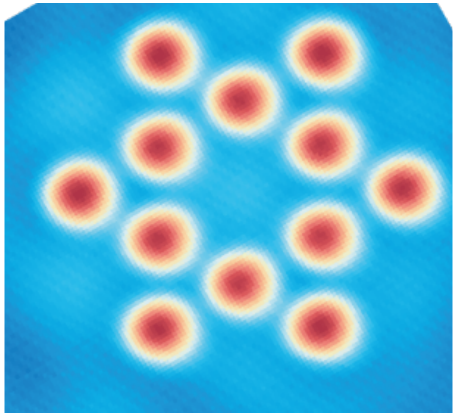
- fully-relativistic KKR Green function method
- LDA
- relaxed



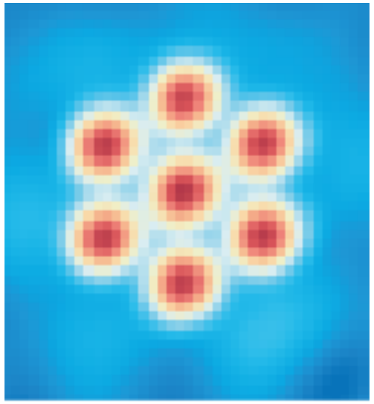
Khajetoorians, Wiebe, Chilian, Lounis, Blügel, and Wiesendanger, Nature Physics (2012)

Manufacturing and investigating antiferromagnetic nano-objects

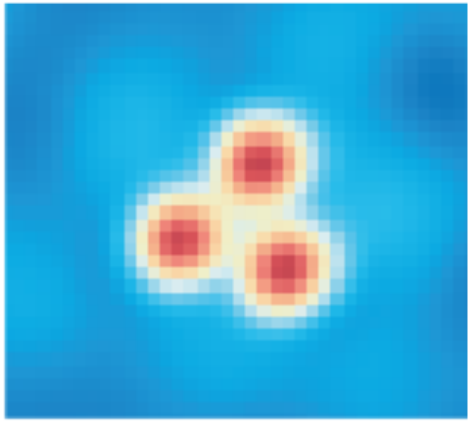
JÜLICH FORSCHUNGSZENTRUM



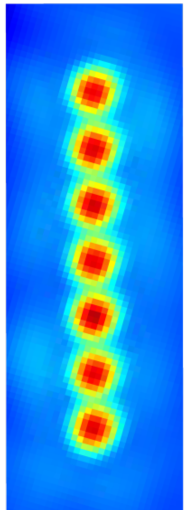
"Kagome"



Flower



Trimer



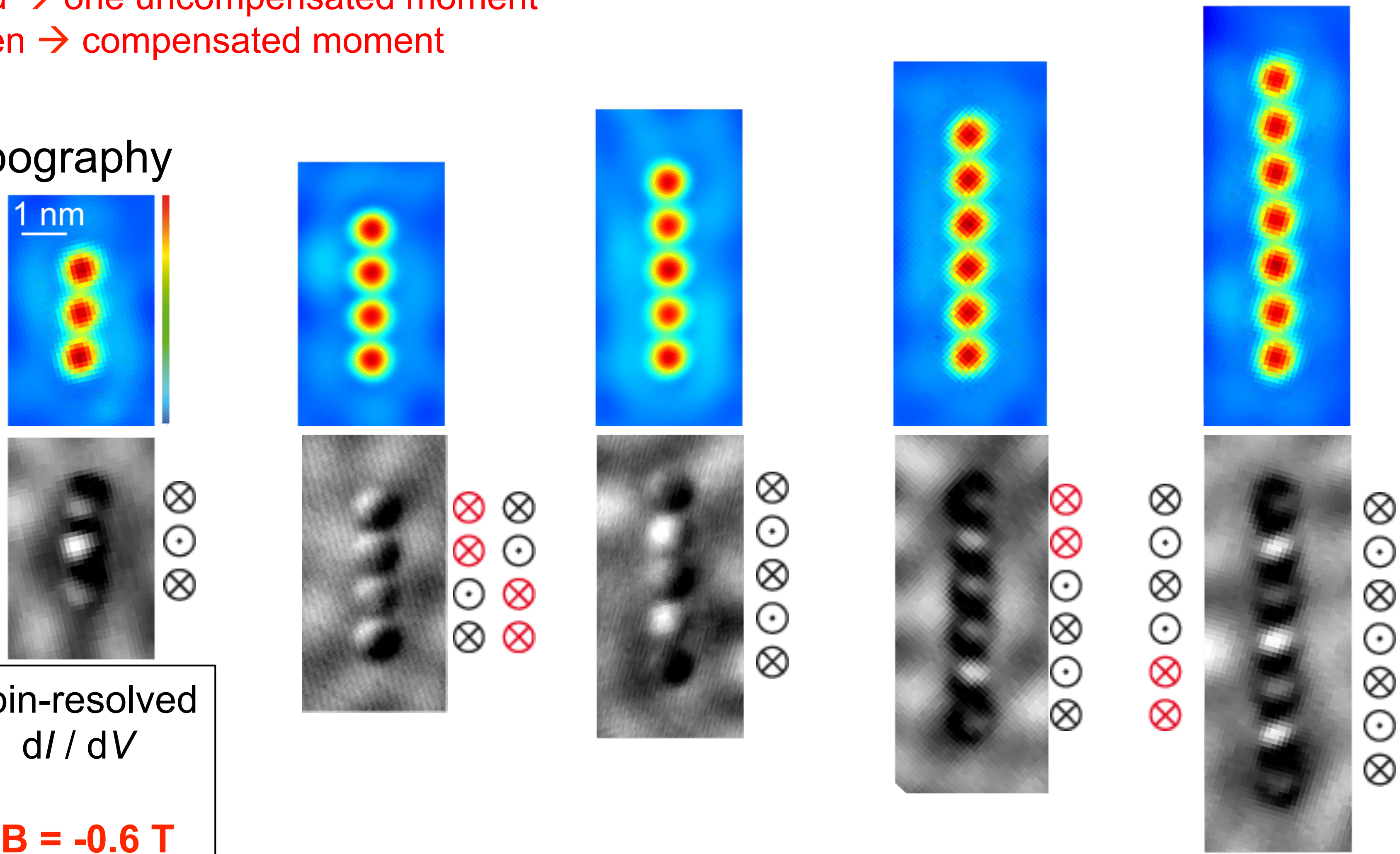
Wires

- Khajetoorians, Wiebe, Chilian, Lounis, Blügel, and Wiesendanger, Nature Physics (2012)

Odd and Even Antiferromagnetic Chains

odd → one uncompensated moment
even → compensated moment

topography



spin-resolved
d*I* / d*V*

B = -0.6 T

Here: J_2 = B and MAE K >> J_1 and B → Ising-like system

- Khajetoorians, Wiebe, Chilian, Lounis, Blügel, and Wiesendanger, Nature Physics (2012)

Summary

- Overview of recent novel applications of the KKR method
- One atom more or less matters!
- Impact on magnetism, frustration, electronic confinement, interactions
- KKR = elegant tool to investigate nanostructures

s.lounis@fz-juelich.de