The Abdus Salam
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Spring College on Computational Nanoscience

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Magnetism at the Nanoscale

S. BLUEGEL

Quantum Theory of Materials, IFF
Juelich
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Magnetism at the nanoscale (Part I)

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www.fz-juelich.de/iff//Bluegel_S

Lecture notes:

www.fz-juelich.de/iff/e_th1

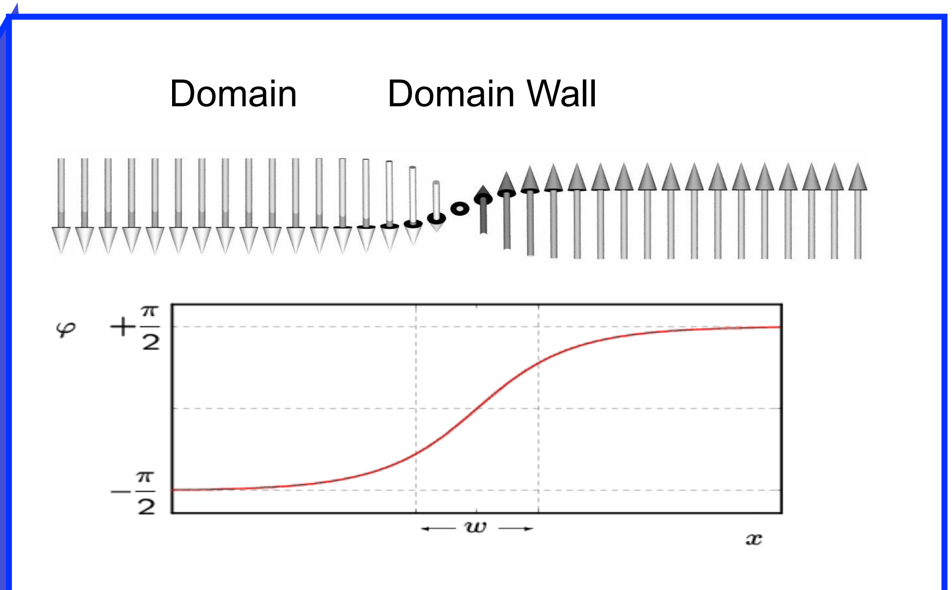
- S. Blügel and G. Bihlmayer,
  Magnetism of Low-dimensional Systems: Theory,
  in: Handbook of Magnetism and Advanced Magnetic Materials,
  H. Kronmüller and S.S.P. Parkin (eds), pp 598-640
  (John Wiley & Sons Ltd, Chichester, UK, 2006).

- http://www.fz-juelich.de/iff/datapool/pdfs/C1_Blugel.pdf

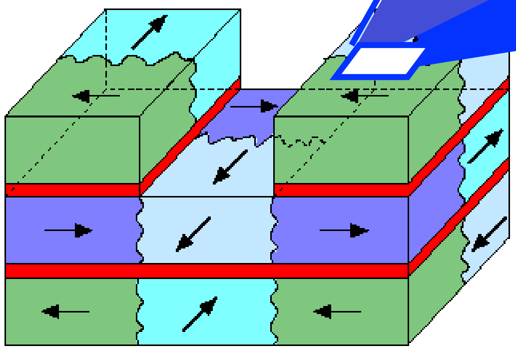
Magnetism from Large to Small:

www.fz-juelich.de/iff/e_th1

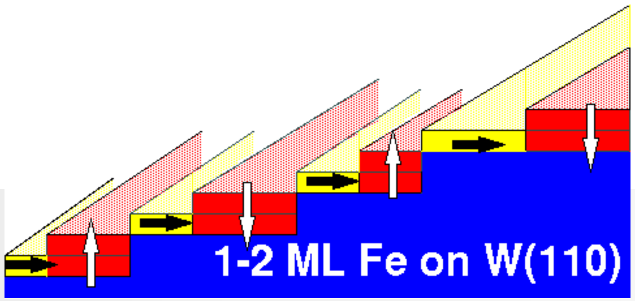
macroscopic



micrometer scale



nano-scale



quantum tunneling,
quantization
quantum interference

"Single Molecule"
Magnets

Magnetism from Large to Small

www.fz-juelich.de/iff/e_th1

macroscopic nanoscopic

permanent magnets | micron particles | nanoparticles | clusters | molecular magnets

S=10^{20} 10^{10} 10^{8} 10^{6} 10^{5} 10^{4} 10^{3} 10^{2} 10 1

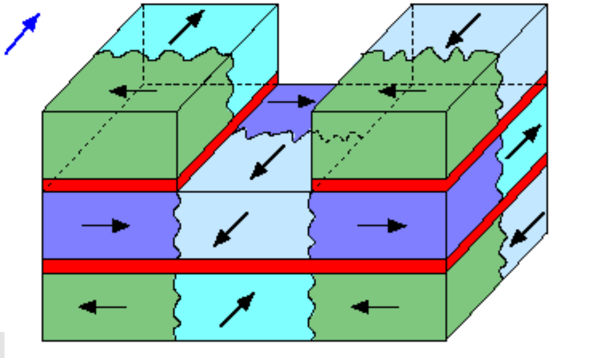
complex systems

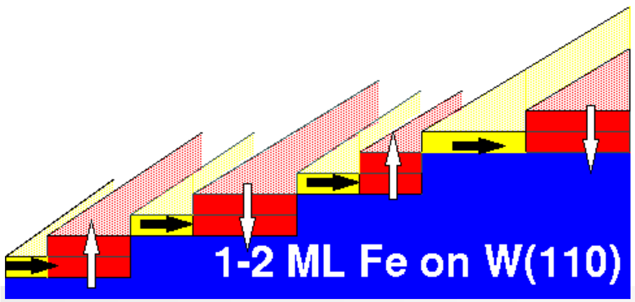
giant spin

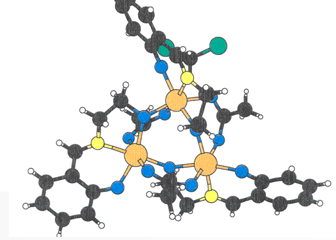
micrometer scale

nano-scale

quantum tunneling, quantization quantum interference







Outline of the lectures

- Some fundamental facts about magnetism
- Itinerant magnetism in metals
- Reduction of dimensionality on magnetic moments
- Reduction of dimensionality on magnetic order
- Critical Temperature
- Kondo effect
- Spin-Orbit related Phenomena: Magnetic Anisotropy
- Spin-Orbit related Phenomena: Dzyaloshinskii-Moriya Int
- Spin-polarized Density Functional Theory

1. Some Fundamentals of Magnetism

Magnetism

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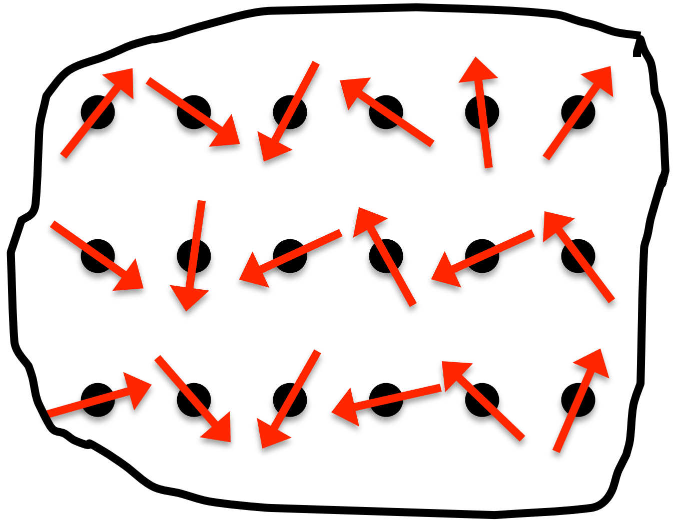
Magnetism is response of a solid to an external magnetic field

Magnetization:

$$\vec{M}(B_{\text{ext}},T) = \frac{1}{V} < \sum_i \vec{m}_i(B_{\text{ext}}) >$$

Linear Response: $\vec{M} = \vec{\vec{\chi}} * \vec{B}_{\text{ext}}$



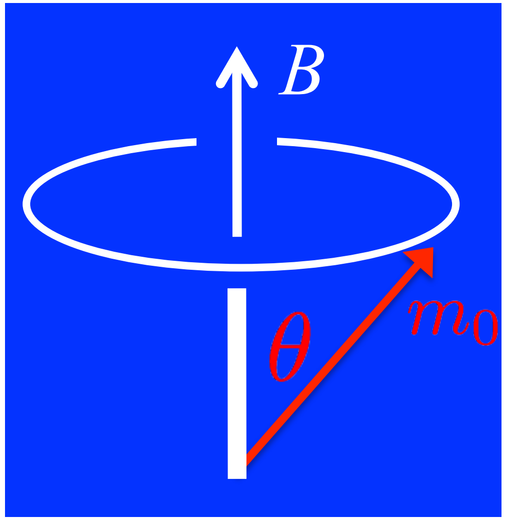
Solid

Susceptibility: $\vec{\vec{\chi}}$

Longitudinal Susceptibility: $\vec{\vec{\chi}}_{||}$ $\qquad \delta m \parallel \vec{m}$

Transversal Susceptibility: $\vec{\vec{\chi}}_{\perp} = \vec{\vec{\chi}}^{+-}$ $\qquad \delta\vec{m} \perp \vec{m}$

Magnetism of noninteracting moments



Assumption: Atomic magnetic moment=m_0

$$E(\theta) = -\vec{m}_0 \cdot \vec{B} = -m_0 B \cos\theta$$

$$\vec{M}(B_{\text{ext}}, T) = \frac{N}{V} < \vec{m}(B_{\text{ext}}) >$$

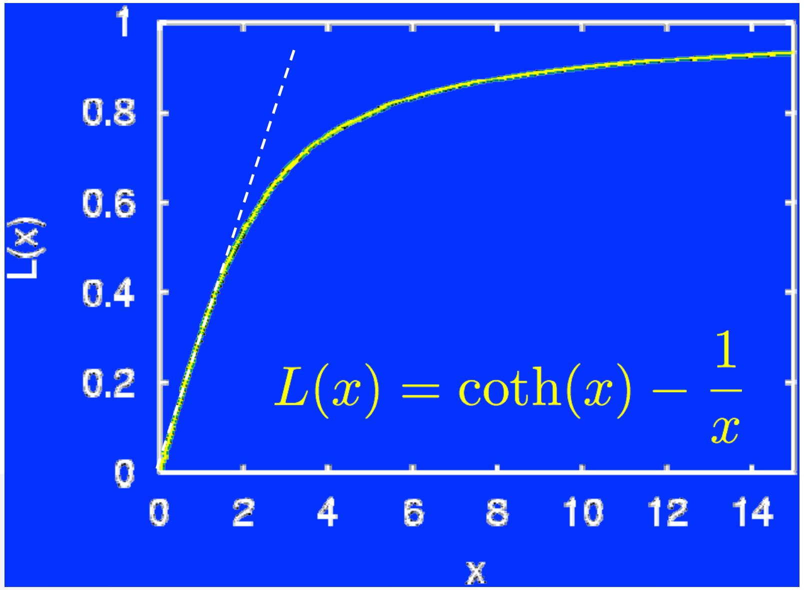
Free energy: $F = -k_{\text{B}} T \ln Z$

Partition function: $Z = \int_0^\pi 2\pi \exp\left(\frac{-E(\theta)}{k_{\text{B}}T}\right) \sin\theta \, d\theta$

Average magnetic moment:

$$m(T) := \langle m_z \rangle = -\frac{\partial F}{\partial B} = k_{\text{B}} T \frac{1}{Z} \frac{dZ}{dB}$$

$$= \cdots = m_0 L\left(\frac{m_0 B}{k_{\text{B}} T}\right)$$



For large T: $m(T) \approx \frac{m_0^2}{3k_B T} B := \chi(T) \frac{B}{\mu_o}$
(Curie law)

Magnetism of interacting moments

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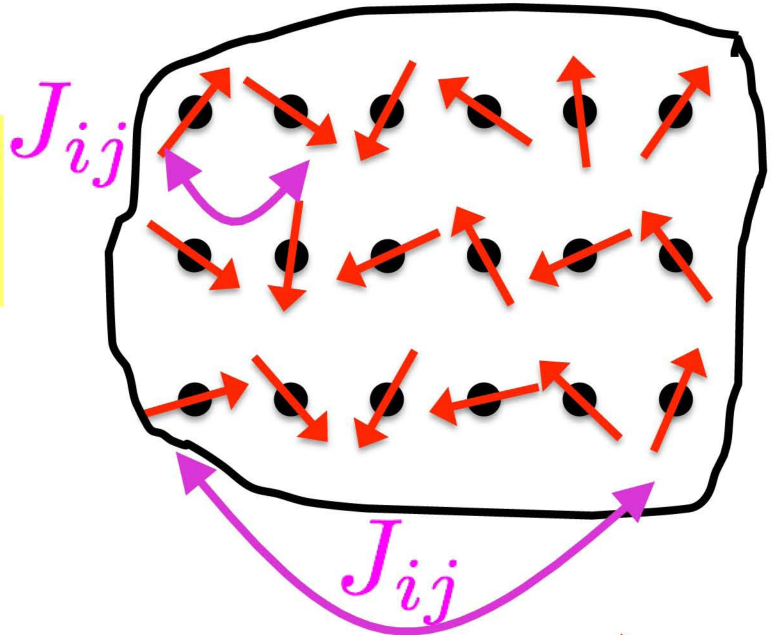
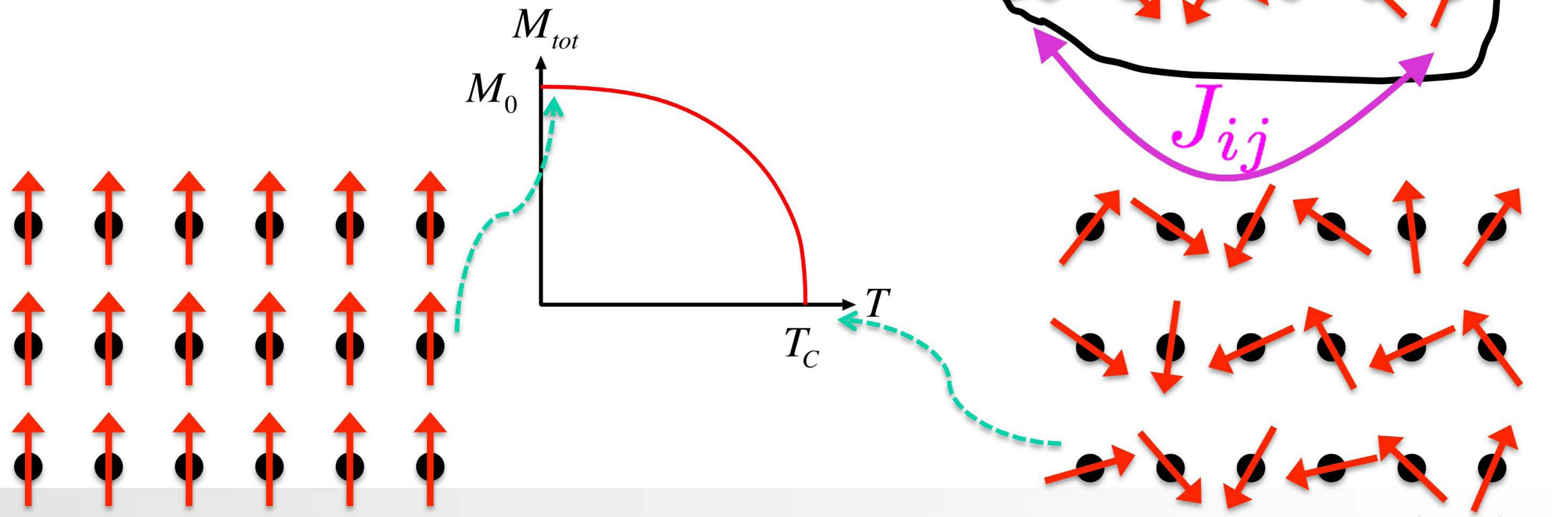
Susceptibility diverges:

$$\chi \rightarrow \infty$$

Two Questions:
1) How does M_o change in low Dim?
2) How does T_C change in low Dim?

Spontaneous magnatization:



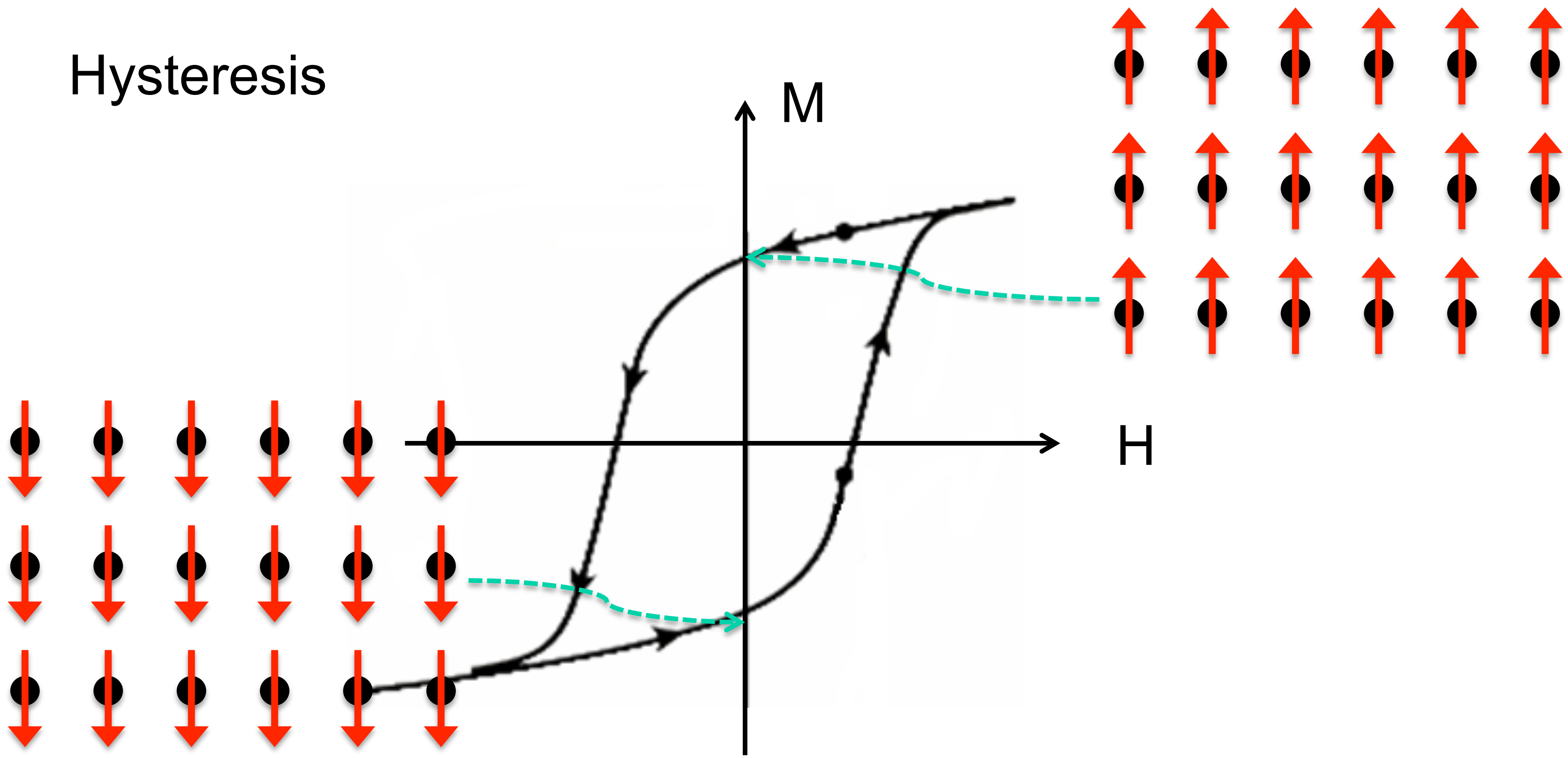


$T = 0$ Ordered spins

$T > T_C$ Long-range disorder Short-range order

Permanent Magnetization

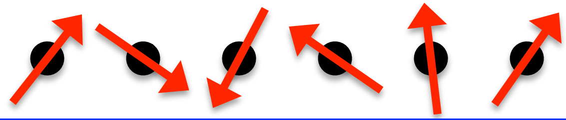
Hysteresis

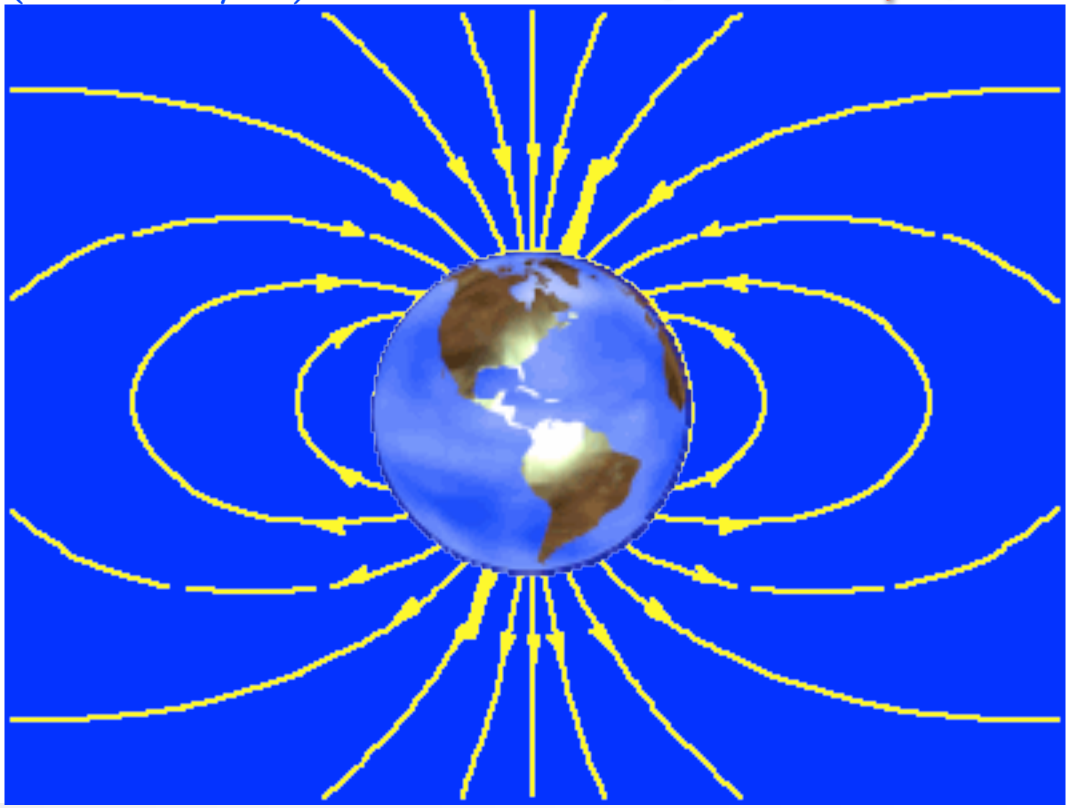


Magnetostatics: magnetic dipoles

Magnetic dipole $\vec{m}$ at site creates $\vec{r}\,' = 0$ magnetic field at point $\vec{r}$

$$\vec{B} = \frac{\mu_o}{4\pi} \frac{3(\vec{m}\cdot\hat{r})\hat{r} - \vec{m}}{r^3} \qquad (\hat{r} := \vec{r}/r)$$





Energy of a dipole $\vec{m}$ in an induction $\vec{B}$:

$$E = -\vec{m}\cdot\vec{B}$$

Order of magnitude of dipolar interactions

$$E_{\mathrm{dip}} \approx \frac{\mu_o}{4\pi}\frac{\mu_B^2}{a^3}$$

$$E_{\mathrm{dip}} \approx 5\times 10^{-5}\,\mathrm{eV} \approx k_{\mathrm{B}}\times 0.5\,\mathrm{K} \ll k_{\mathrm{B}}T_{\mathrm{C}}\ (T_{\mathrm{C}} \approx 100 \text{ to } 1000\,\mathrm{K})$$

Exchange Interactions

Magnetostatics never the origin of magnetism

Origin of
magnetism, magnetic interaction and magnetic order
is due to exchange interactions
Combined effect of

1. Pauli principle
2. Coulomb and/or exchange kinetic energy

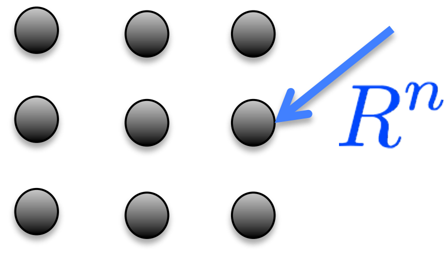
Microscopic Exchange mechanism depends on materials

e.g.:
1) Direct exchange
2) Kinetic exchange
3) Double exchange
4) Superexchange
5) RKKY interaction
6) Biquadratic exchange
7) ……

Origin of Exchange Interaction

- Hamiltonian

$$H = \sum_i \left\{ \frac{p_i^2}{2m} - \sum_n \frac{Z^n}{|r_i - R^n|} + \frac{1}{2} \sum_{j \neq i} \frac{1}{|r_i - r_j|} \right\}$$

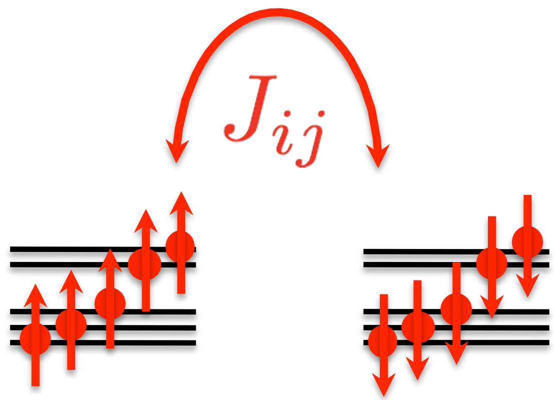


- Surprise ! Hamiltonian not explicit spin dependent:

$$[H, S^2] = 0 \quad \wedge \quad [H, S_z] = 0$$

- Effective Spin-Hamiltonian

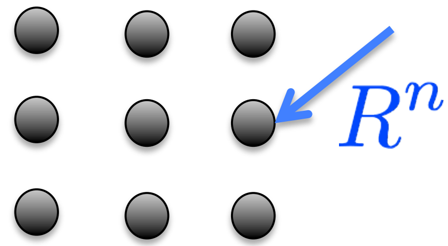
$$H_{2\text{-spin}} = \sum_{i,j} J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j$$



Origin of Exchange Interaction

- Hamiltonian

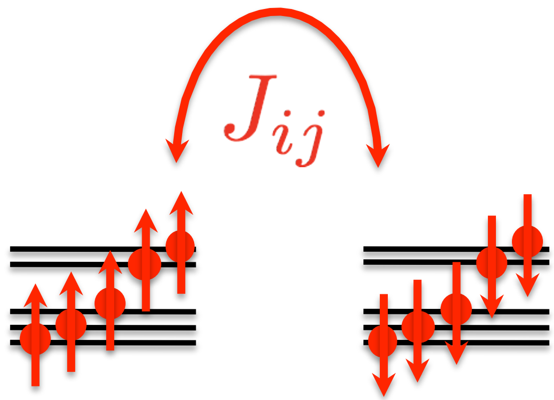
$$H = \sum_i \left\{ \frac{p_i^2}{2m} - \sum_n \frac{Z^n}{|r_i - R^n|} + \frac{1}{2} \sum_{j \neq i} \frac{1}{|r_i - r_j|} \right\}$$



- Hamiltonian not explicit spin dependent:

$$[H, S^2] = 0 \quad \wedge \quad [H, S_z] = 0$$

- Effective Spin-Hamiltonian



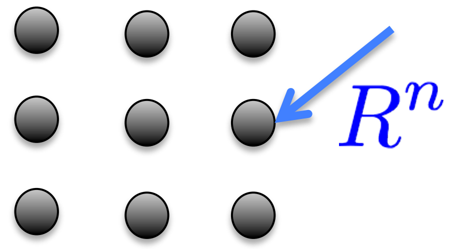
$$H_{2\text{-spin}} = \sum_{i,j} J_{ij} \, \mathbf{S}_i \cdot \mathbf{S}_j$$

$$H_{4\text{-spin}} = \sum_{ijkl} K_{ijkl} \left[(\mathbf{S}_i\mathbf{S}_j)(\mathbf{S}_k\mathbf{S}_l) + (\mathbf{S}_j\mathbf{S}_k)(\mathbf{S}_l\mathbf{S}_i) - (\mathbf{S}_i\mathbf{S}_k)(\mathbf{S}_j\mathbf{S}_l) \right]$$

Origin of Exchange Interaction

- Hamiltonian

$$H = \sum_i \left\{ \frac{p_i^2}{2m} - \sum_n \frac{Z^n}{|r_i - R^n|} + \frac{1}{2} \sum_{j \neq i} \frac{1}{|r_i - r_j|} \right\}$$



- It is the wavefunction

$$H \neq H(s_1, s_2, \cdots)$$

$$H(\cdot \vec{r}_i \cdots \vec{r}_j \cdot) = H(\cdot \vec{r}_j \cdots \vec{r}_i \cdot)$$

$$\Psi(x_1, x_2, \ldots) = \underbrace{\psi(\vec{r}_1, \vec{r}_2, \cdots)}_{\text{realspace}} * \underbrace{\chi(s_1, s_2, \cdots)}_{\text{spinor}}$$

- Minimization leads to spin dependent interaction

$$-\overbrace{\Psi(x_2, x_1, \ldots)}^{\text{fermion}} \qquad H\psi = E\psi \qquad \psi \in \begin{cases} \text{symmetric} \\ \text{antisymmetric} \end{cases}$$

$$\min_{\Psi} \left\langle \Psi \left| \sum_i \left\{ \frac{p_i^2}{2m} - \sum_n \frac{Z^n}{|r_i - R^n|} + \frac{1}{2} \sum_{j \neq i} \frac{1}{|r_i - r_j|} \right\} \right| \Psi \right\rangle$$

Origin of Exchange Interaction

- Minimization leads to spin dependent interaction

$$\min_{\Psi} \left\langle \Psi \middle| \sum_i \left\{ \underbrace{\frac{p_i^2}{2m}} - \sum_n \frac{Z^n}{|r_i - R^n|} + \underbrace{\frac{1}{2} \sum_{j \neq i} \frac{1}{|r_i - r_j|}} \right\} \middle| \Psi \right\rangle$$

Indirect exchange

- kinetic exchange
  - superexchange
- double exchange

Direct exchange

- intra-atomic exchange
- inter-atomic exchange

Historic Remark: Magnetite Fe_3O_4

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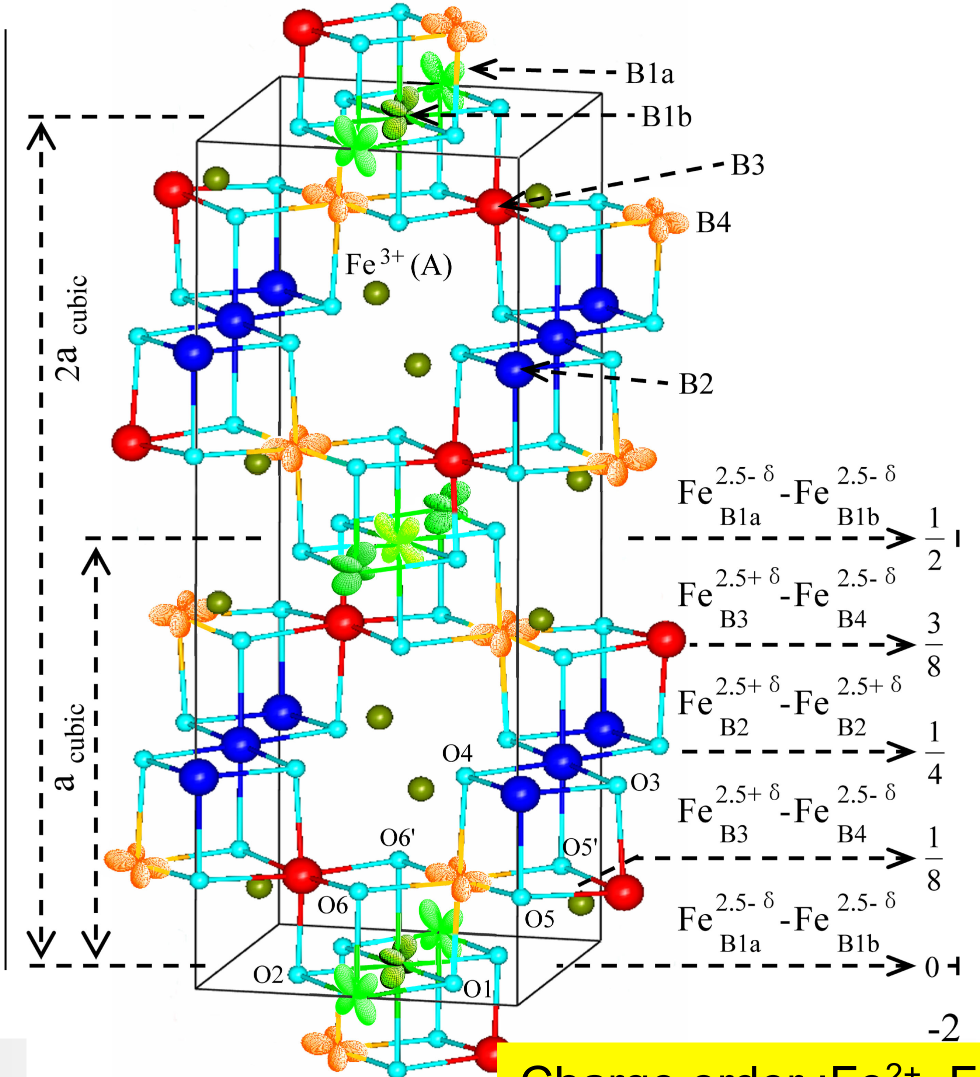
First magnetic material known to mankind

"Loadstone"

"Chinese South-Pointer"

(220 BC)

- Ferrimagnet with T_N ~ 860 K
- Candidate for *Spintronics* with 100% spin-polarization at E_F



Charge order :Fe^{2+}, Fe^{3+}
Orbital order

2. Itinerant Magnetism of Metals

Reminder : Bulk Magnetism

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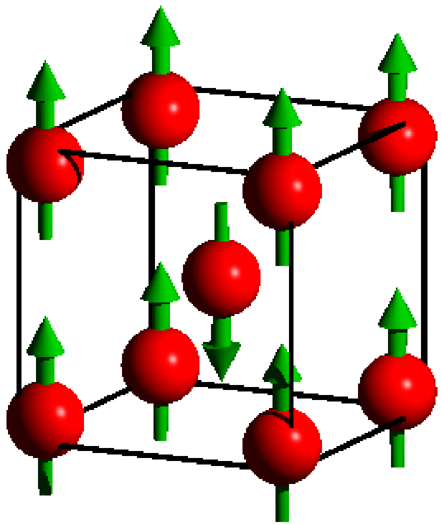
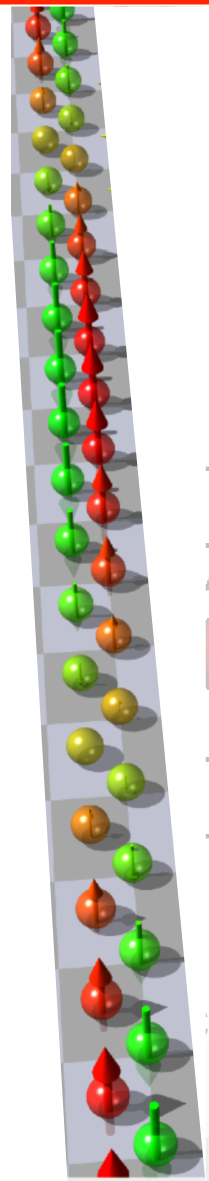
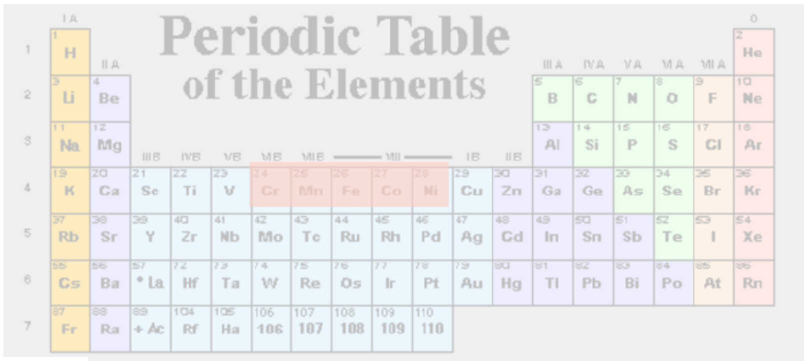
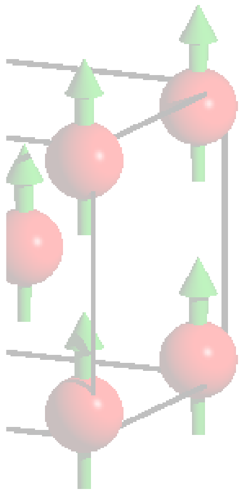
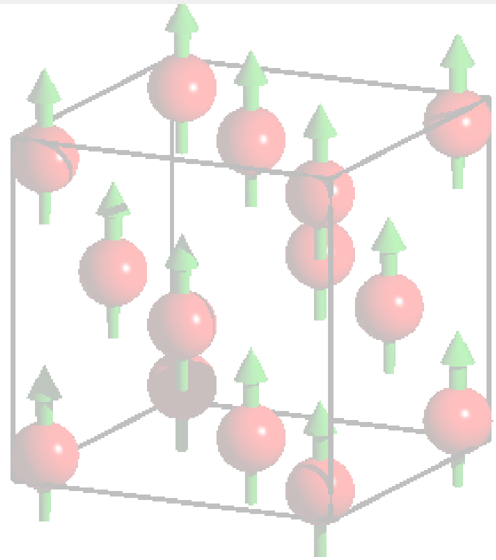










bcc-Cr:

M= 0.59 μ_B

c-Fe:

2.12 μ_B

fcc-Ni:

M= 0.55 μ_B

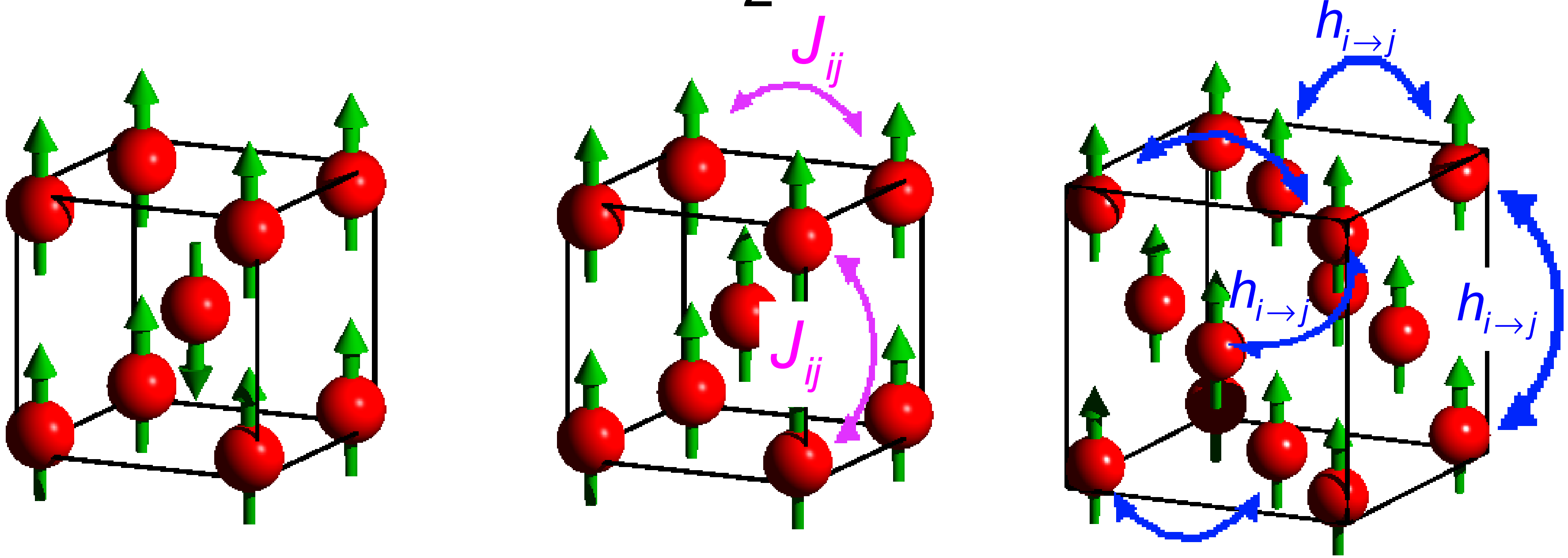
Reminder : Bulk Magnetism

www.fz-juelich.de/iff/e_th1

Itinerant magnets

$$H = -\frac{1}{2}\sum J_{ij}\vec{S}_i\vec{S}_j$$

$$J_{ij} \propto \frac{\cos(2k_F|\mathbf{R}_i - \mathbf{R}_j|)}{|\mathbf{R}_i - \mathbf{R}_j|^3}$$



bcc-Cr:

M= 0.59 $\mu_B \times \cos(1-\delta)\frac{\pi}{a}na$

bcc-Fe:

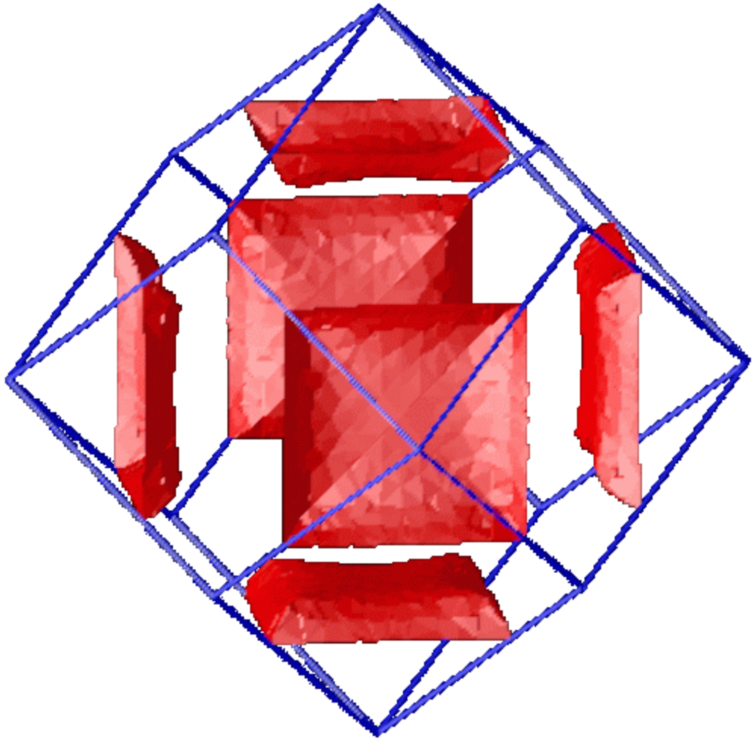
M= 2.12 μ_B

fcc-Ni:

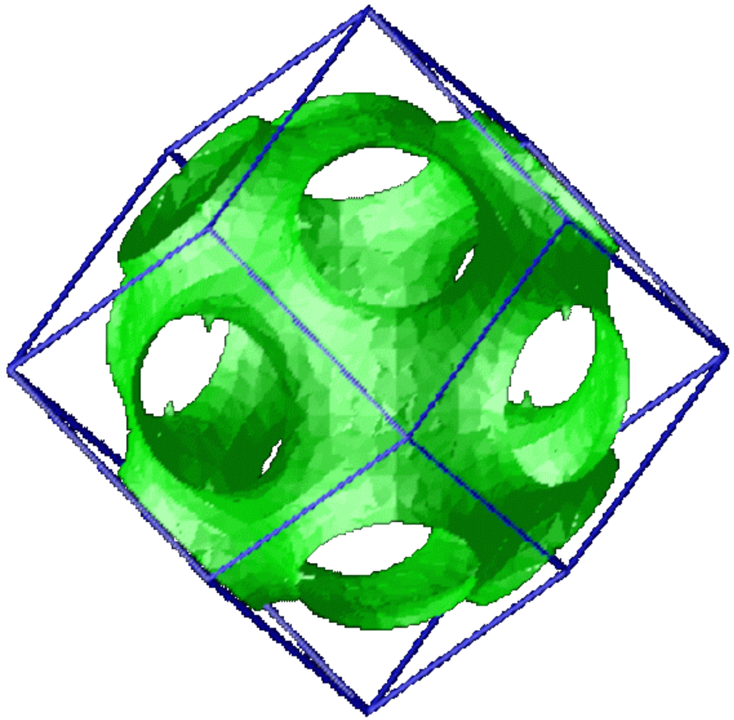
M= 0.55 μ_B

Fermi Surface of bulk Eu

Fermi Surface
Majority Electrons
(spin-up)



Fermi Surface
Minority Electrons
(spin-down)



G. Bihlmayer and Stefan Blügel, unpublished

Fermi surface of Pt(111)

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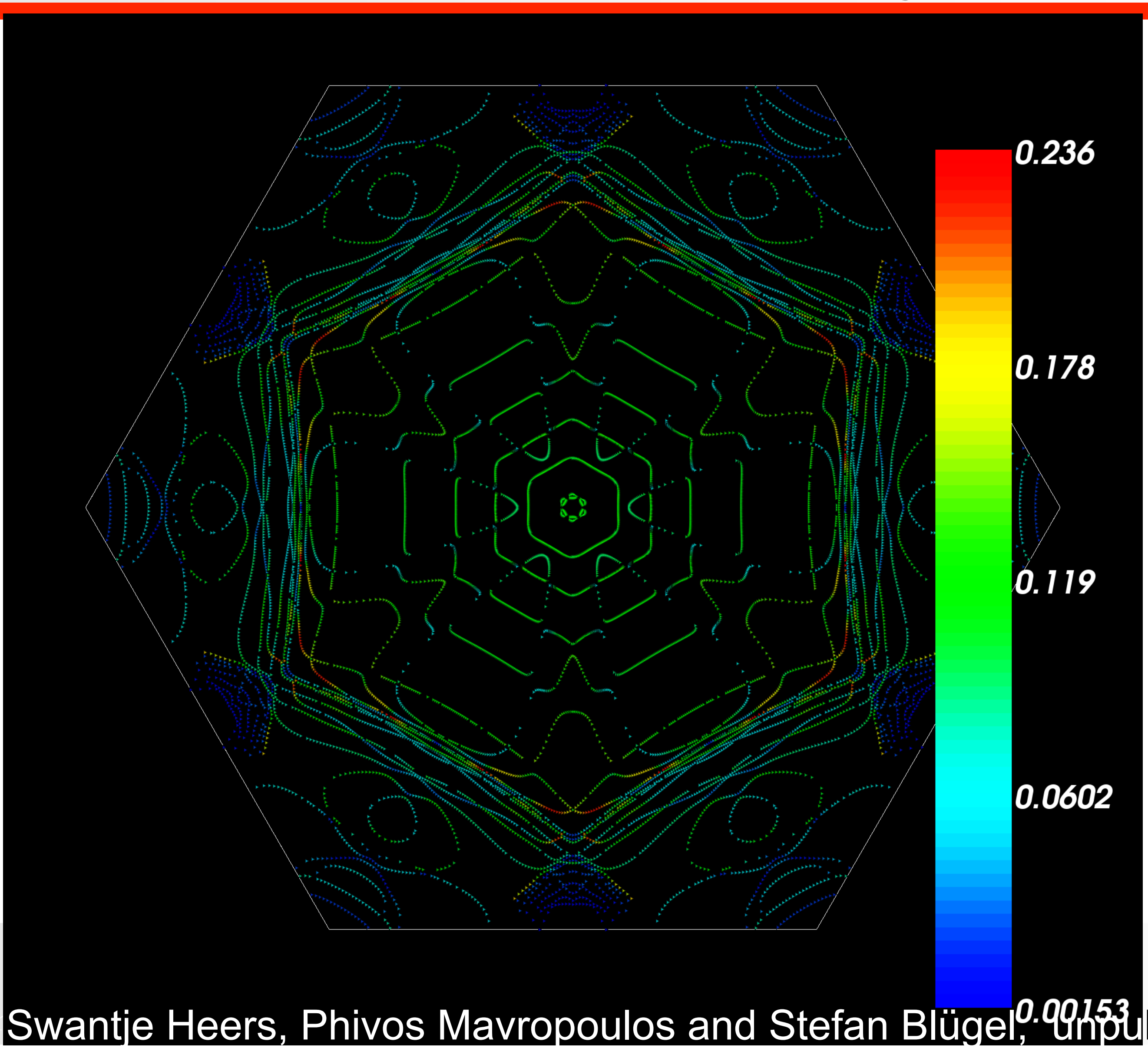
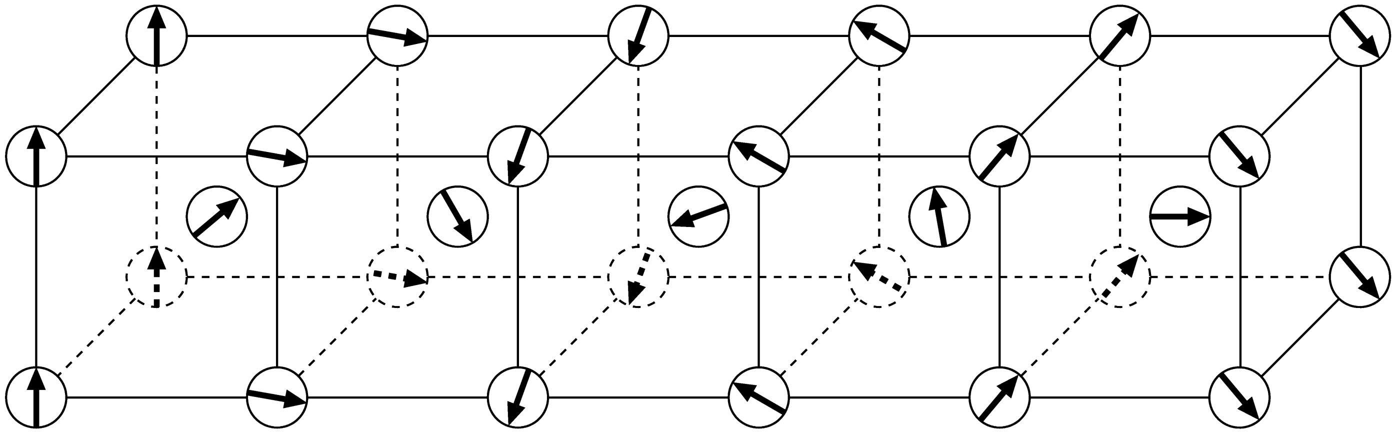
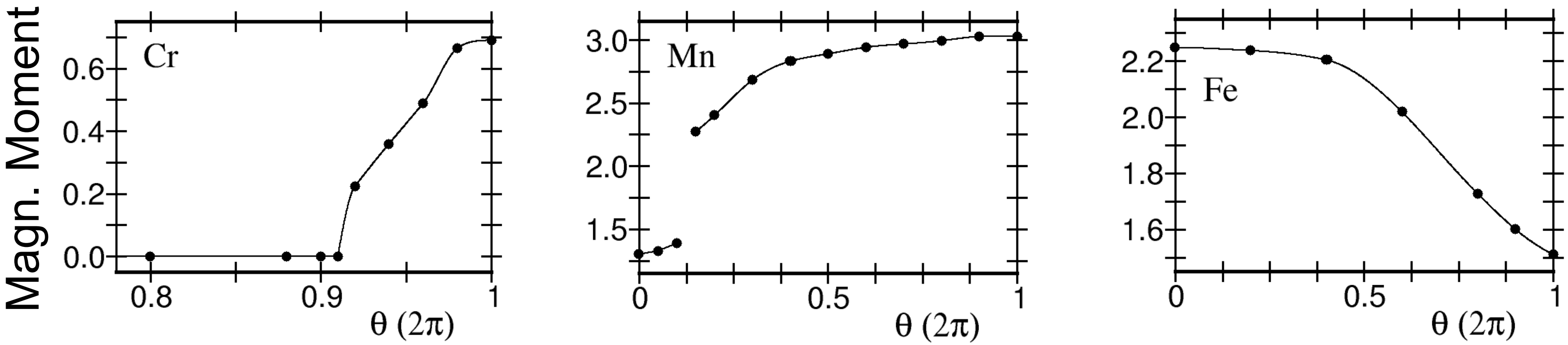


Swantje Heers, Phivos Mavropoulos and Stefan Blügel, unpublished

Reminder: Bulk Magnetism





S. Blügel, G. Bihlmayer in: Handbook of Magnetism and Advanced Magnetic Materials (2007)

Density of states for bulk Fe & Co

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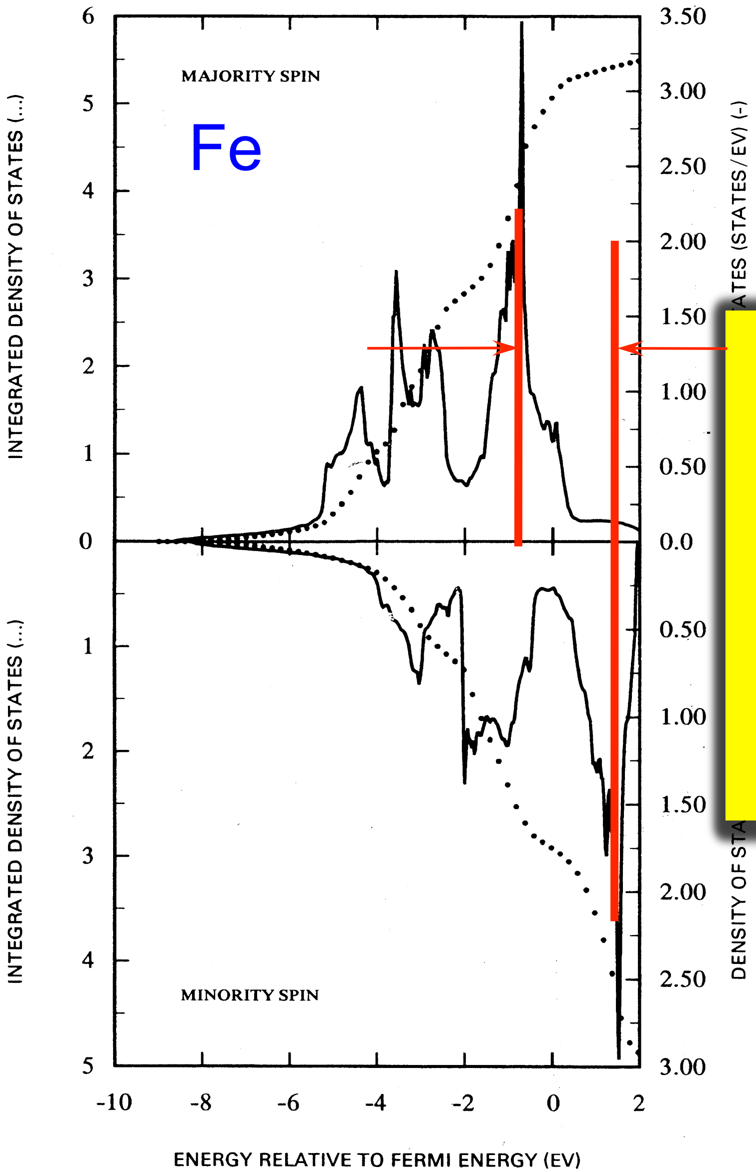
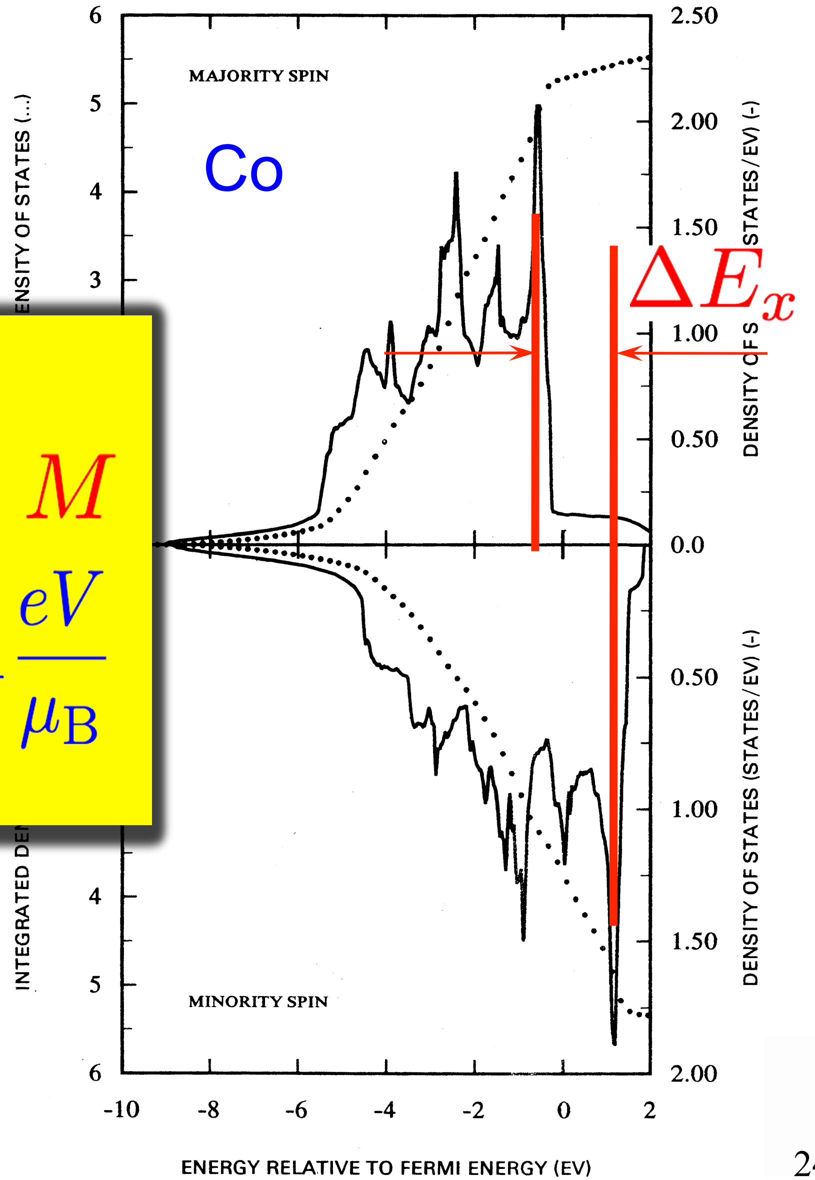


$$\Delta E_x = I \cdot M$$

$$I = 1\frac{eV}{\mu_B}$$



What happens in reduced Dimensions?

Magnetism at reduced dimensions

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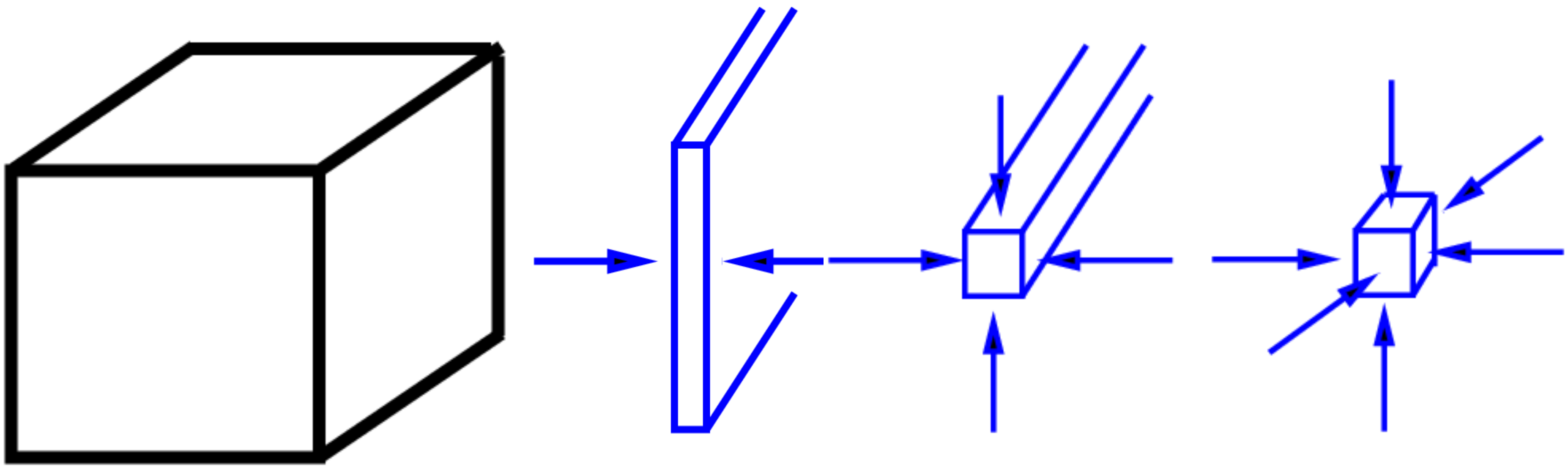
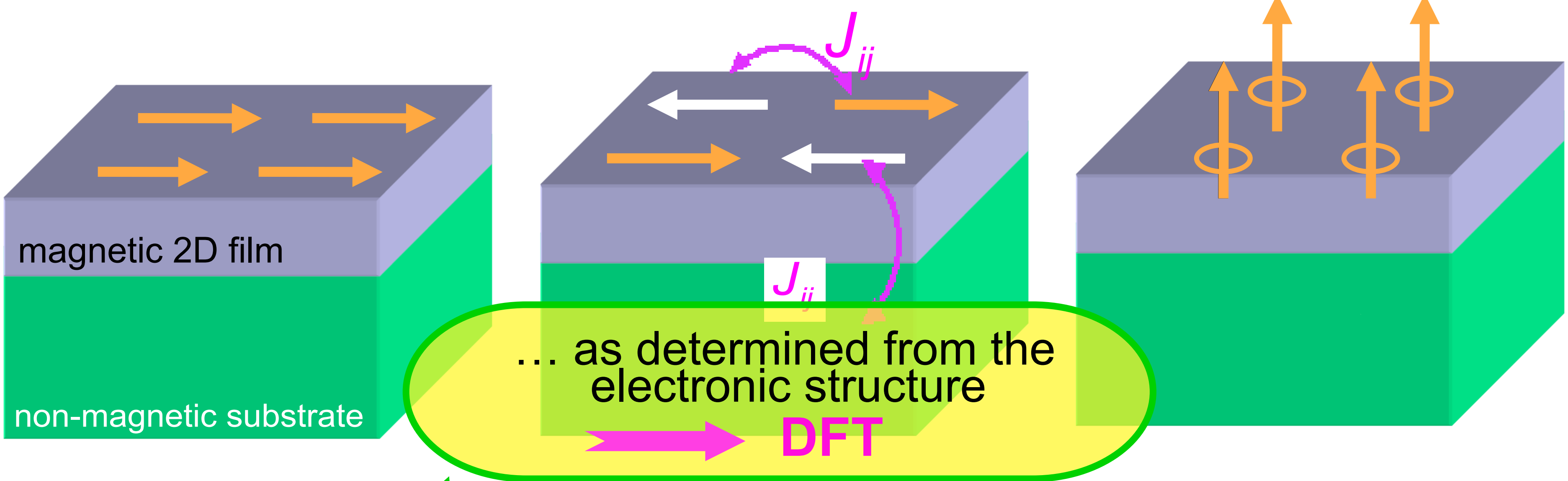
Bulk → Film Wire Cluster



Outline of lecture

www.fz-juelich.de/iff/e_th1

Typical Energies: ≈1 eV ≈0.2 eV ≈0.0005 eV

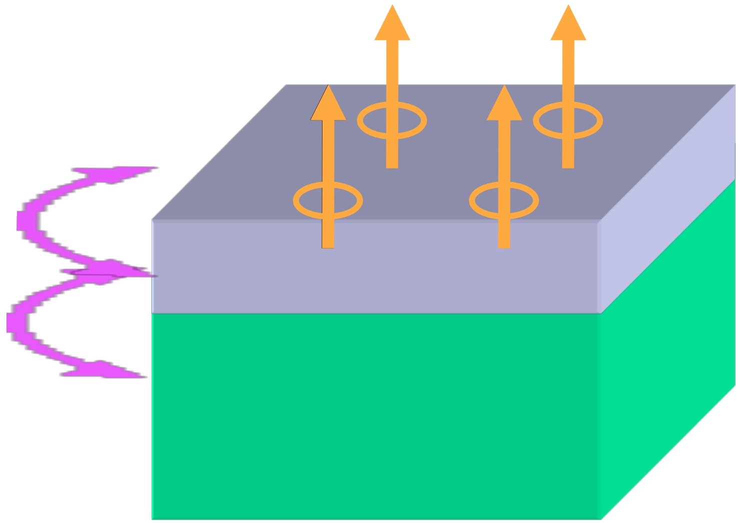


Magnetic Moments	Magnetic Order	Magnetic Orientation
Magnetism: Yes or No?	Ferro ⟺ Antiferro	In-plane ⟺ Out-of-plane
Intra-atomic Exchange	**Inter-atomic Exchange**	**Spin-Orbit + Dipole-Dip**
$H = -\frac{1}{2}\sum_i I_i m_i^2$	$H = -\frac{1}{2}\sum_{i,j} J_{i,j}\vec{m}_i\vec{m}_j$	$H = \sum_i K_i(\vec{m}_i\,\vec{e}_i)^2 + \sum_{i,j}\frac{1}{r^3_{i,j}}[\cdots]$

Outline of the lecture

Break of inversion symmetry

$P(z) \neq P(-z)$



Magnetic Orientation

In-plane ⟺ Out-of-plane

- o Rashba Effect
- o Chiral magnetic interaction (Dzyaloshinskii-Moriya)

Typical Ground State Energies

	E(eV/atom)
• Cohesive energy	5.5
• Local moment formation	1.0
• Alloy formation	0.5
• Magnetic order	0.2
• Structural relaxation	0.05
• Magnetic anisotropy	0.0005

[Of course: Thermal excitation, dynamics,….]

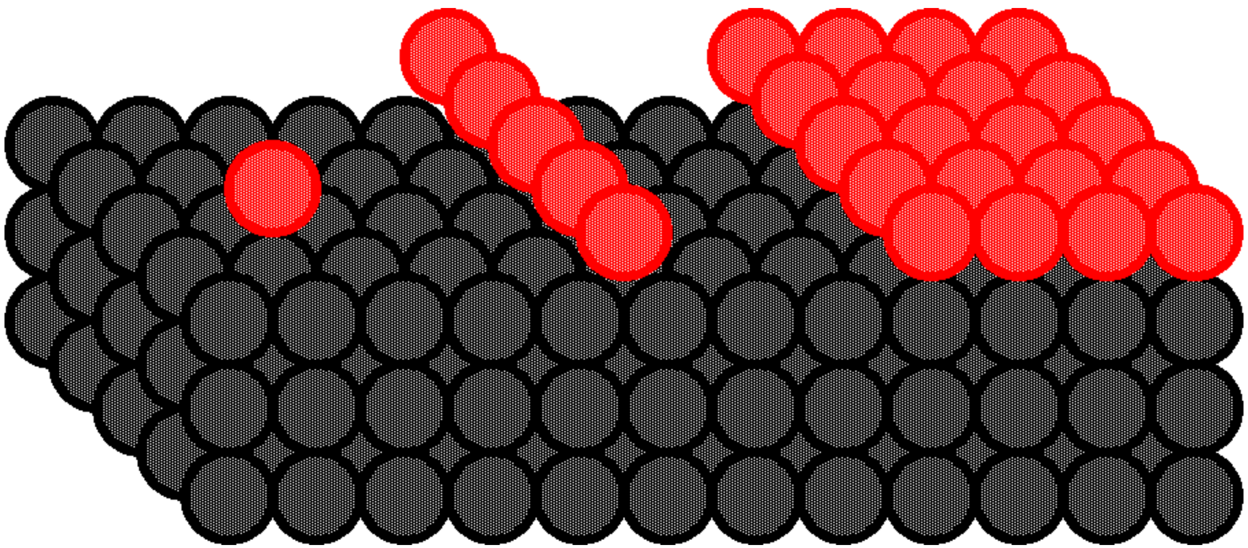
Systems in reduced dimensions

Reduced Dim.: Restrict hopping $h_{i \to j}$

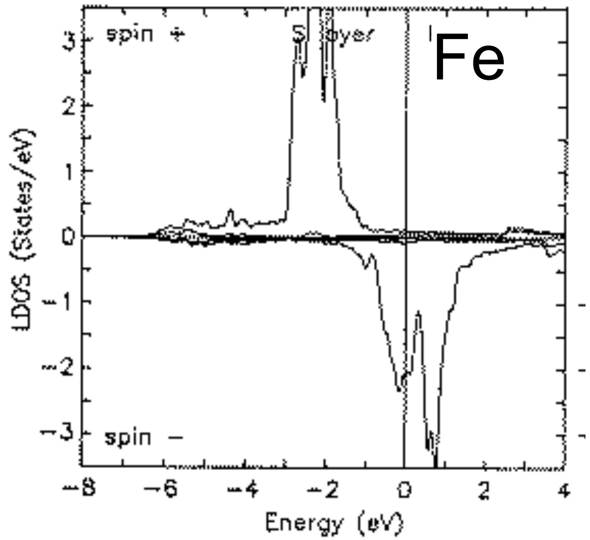
Restrict exchange interaction $J_{i \to j}$

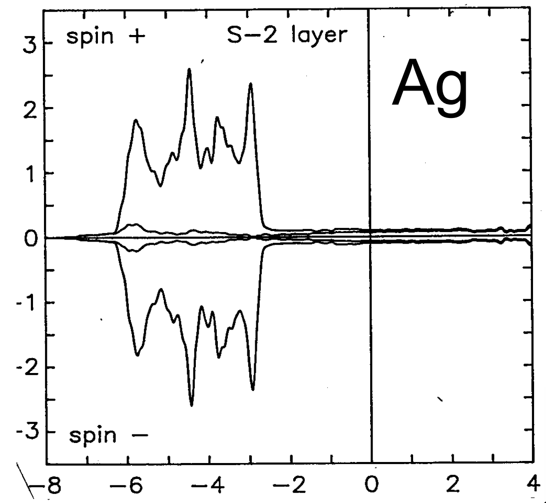
- two-dimensional films
- one-dimensional chains
- zero-dimensional cluster, molecules and atoms

$$\boxed{J_{\parallel} \gg J_{\perp}}$$



Example: Fe on Ag(100)





Competing Interactions: Mn cluster on Ni(100)

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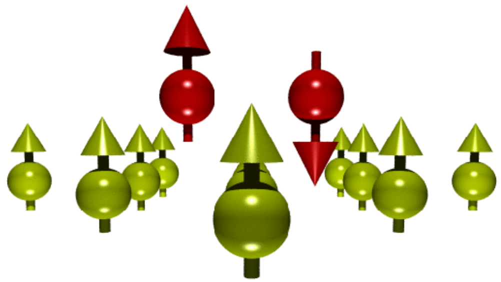
Mn-Dimer

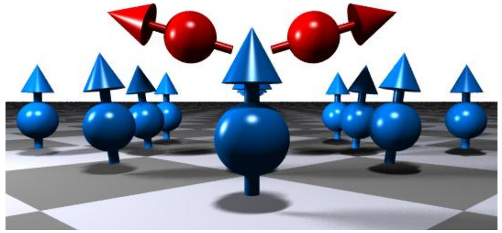


$$J_{\parallel} = J_{Mn-Mn} < 0$$

$$J_{\perp} = J_{Mn-Ni} > 0$$

$$J_S = J_{Ni-Ni} > 0$$

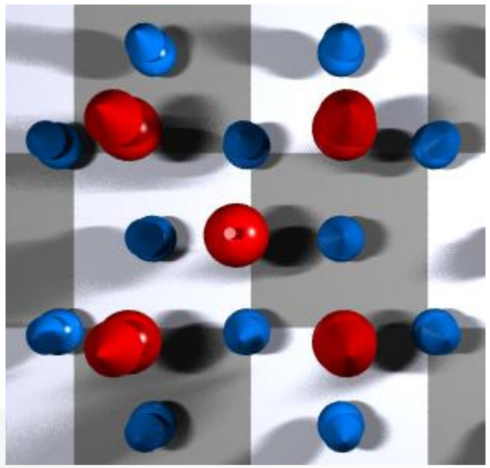
$$|J_{\perp}| \approx |J_{\parallel}|$$



Non-collinear result

θ=72.5º

Pentamer



S. Lounis, Ph.Mavropoulos, Ru.Zeller, P.H.Dederichs, S.Blügel, PRB **78**, 174436 (2007).

Rich field

- Surface/interface orientation: (100), (110), (111) ….
- Substrate: Non-, Ferro-, Antiferromagnetic
  Metal, Semiconductor, Oxide, ….
- Chemical Order/Disorder: Alloys, Compounds
- Structural Order/Disorder: Roughness, Islands, Steps
- Adsorbate: Adatoms, Clusters, Magnetic Molecules,
  Chains, Films
- Films $\Longleftrightarrow$ Multilayers, Laterally Patterned Structures

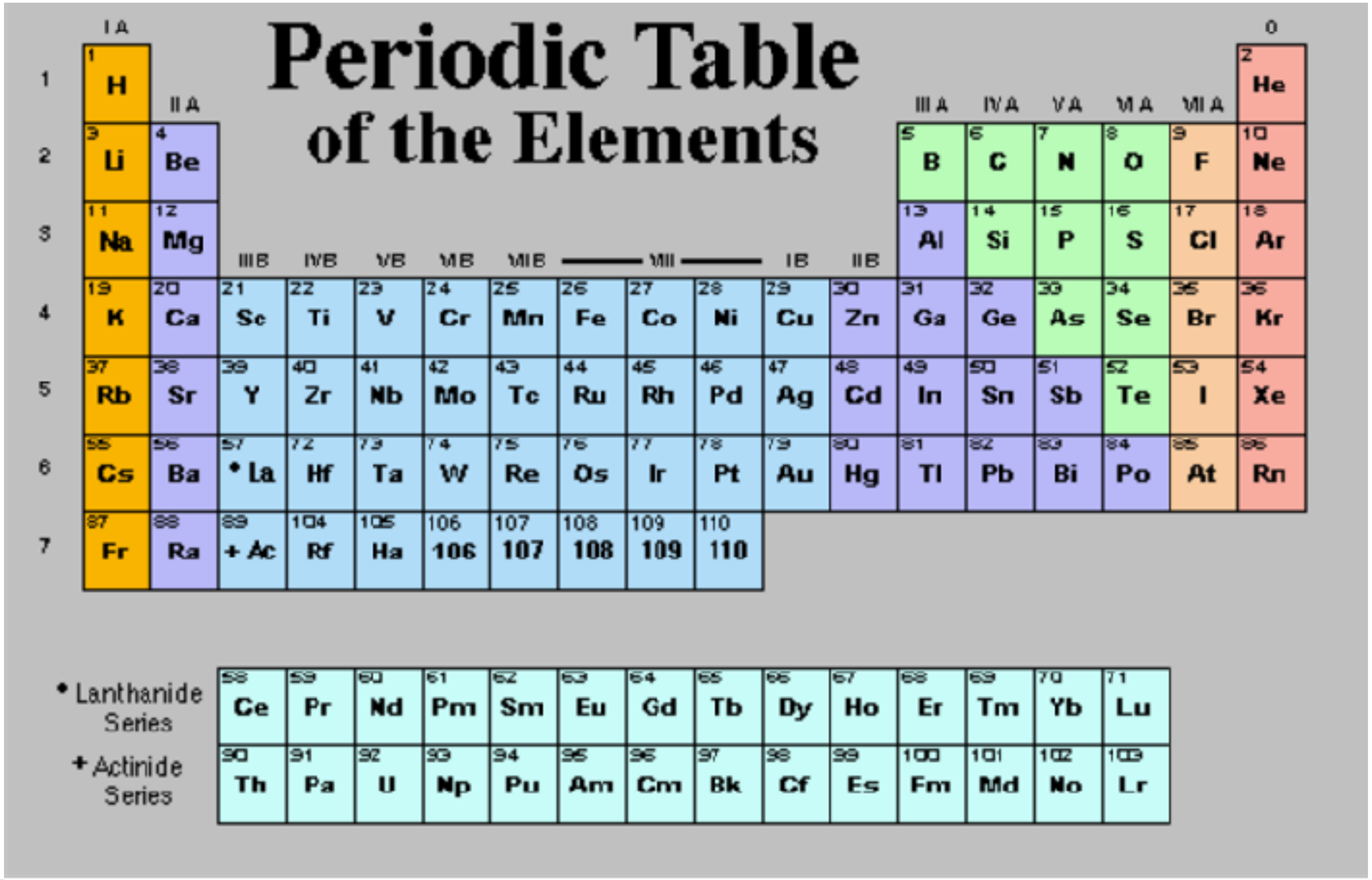
Some topics selected

3. General Aspects

Magnetism of Atoms (#=0)

www.fz-juelich.de/iff/e_th1

"almost all" atoms are magnetic



Magnetism of Atoms (#=0)

www.fz-juelich.de/iff/e_th1

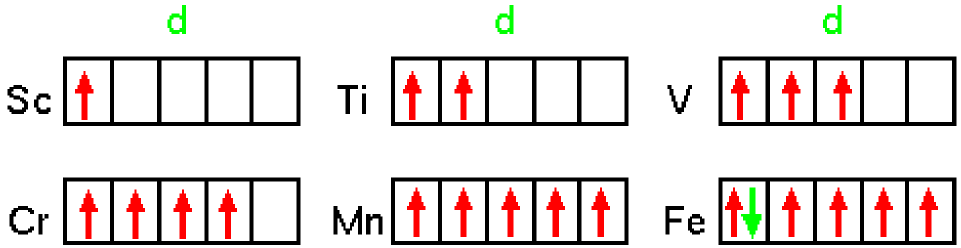
“almost all” atoms are magnetic

1.Hund’s Rule

(Exchange Interaction)

Example: 3d Transition Metal Series

	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu
$4s^2$	$3d^1$	$3d^2$	$3d^3$	$3d^4$	$3d^5$	$3d^6$	$3d^7$	$3d^8$	$3d^{10}$



Exchange Interaction

$$\Psi(\mathbf{r}_1\sigma_1,\cdots\mathbf{r}_i\sigma_i,\cdots,\mathbf{r}_j\sigma_j,\cdots\mathbf{r}_5\sigma_5) =$$

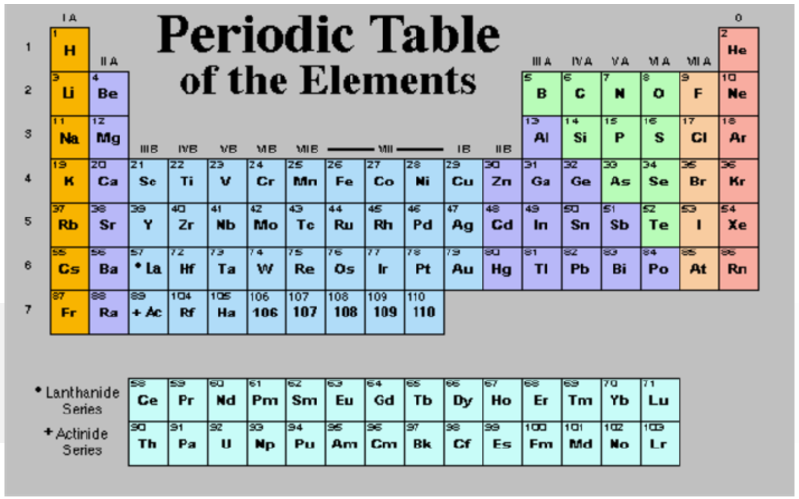
$$= -\Psi(\mathbf{r}_1\sigma_1,\cdots\mathbf{r}_j\sigma_j,\cdots,\mathbf{r}_i\sigma_i,\cdots\mathbf{r}_5\sigma_5)$$

$$= \underbrace{\Psi^{\mathrm{Mn}}(\mathbf{r}_1,\cdots,\mathbf{r}_5)}_{\text{antisymmetric}} \cdot \underbrace{\chi_{\uparrow\uparrow\uparrow\uparrow\uparrow}}_{\text{symmetric}}$$

$$\lim_{\mathbf{r}_i \to \mathbf{r}_j} \Psi^{\mathrm{Mn}}(\mathbf{r}_1,\cdots,\mathbf{r}_5) \longrightarrow 0$$

$$U(\mathbf{r}_i,\mathbf{r}_j) = \frac{1}{2}\int d\mathbf{r}_1\cdots\mathbf{r}_5 \frac{|\Psi^{\mathrm{Mn}}(\mathbf{r}_1,\cdots,\mathbf{r}_5)|^2}{|\mathbf{r}_i-\mathbf{r}_j|}$$

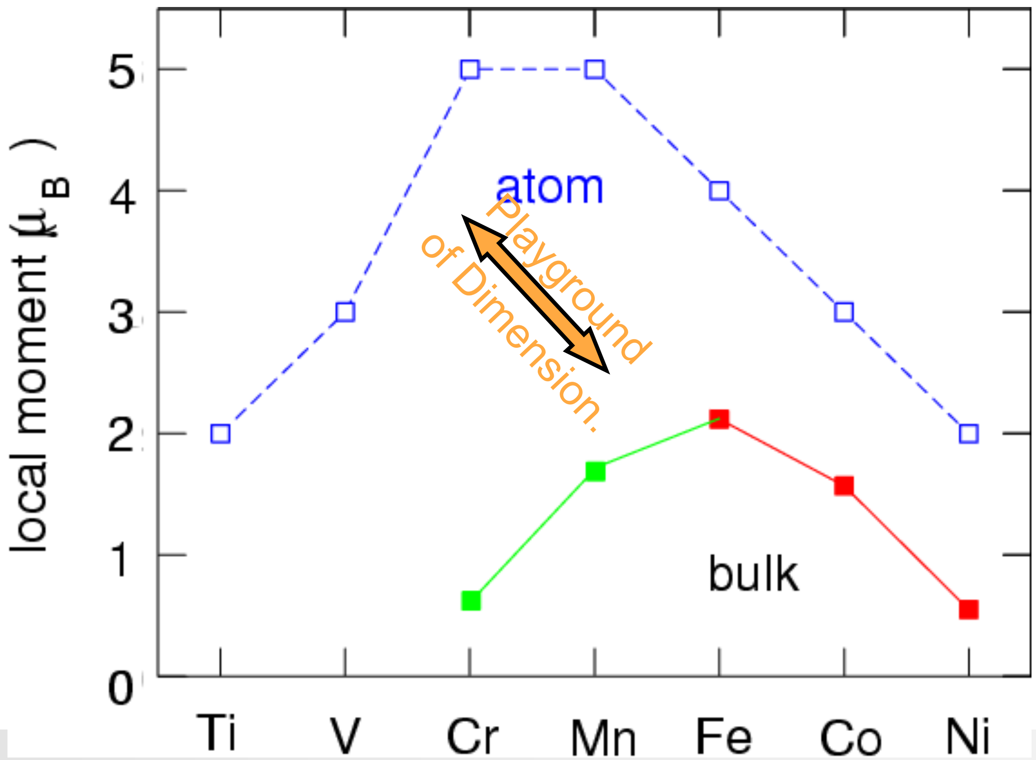
$$= \text{small}$$

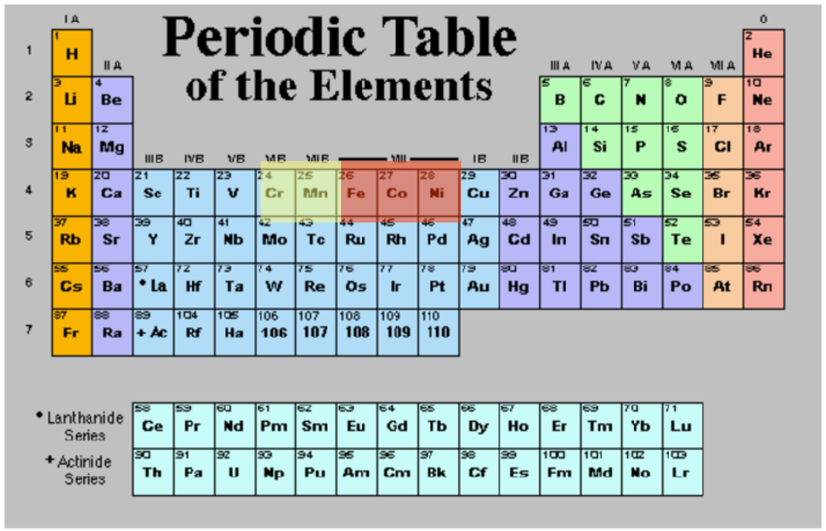


Magnetism in Reduced Dimension

www.fz-juelich.de/iff/e_th1

“New Magnets” in reduced dimensions





Stoner Model for Ferromagnetism

www.fz-juelich.de/iff/e_th1

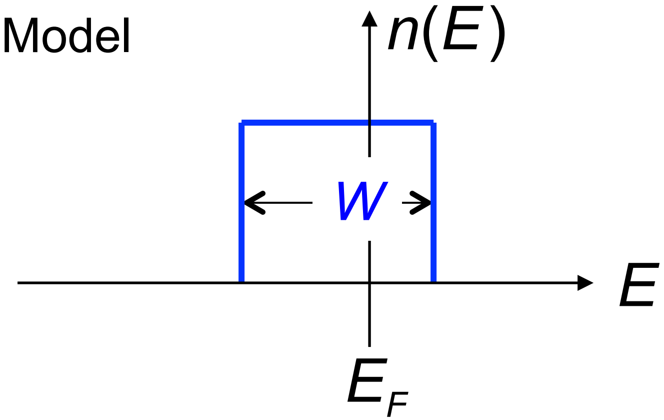
$$\vec{M} = \vec{\vec{\chi}} * \vec{B}_{\text{ext}}$$

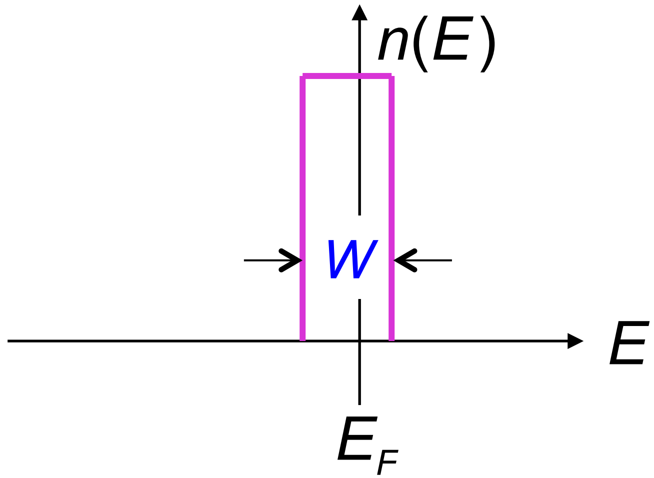
$$\chi \propto \frac{1}{1 - I \cdot n(E_{\text{F}})}$$

- Stoner criterion: $I \cdot n(E_F) > 1$
  (for d-electrons)

- Density of states: $n(E_F) \sim \dfrac{1}{W}$ $[\; n \cdot W = 5 \;]$

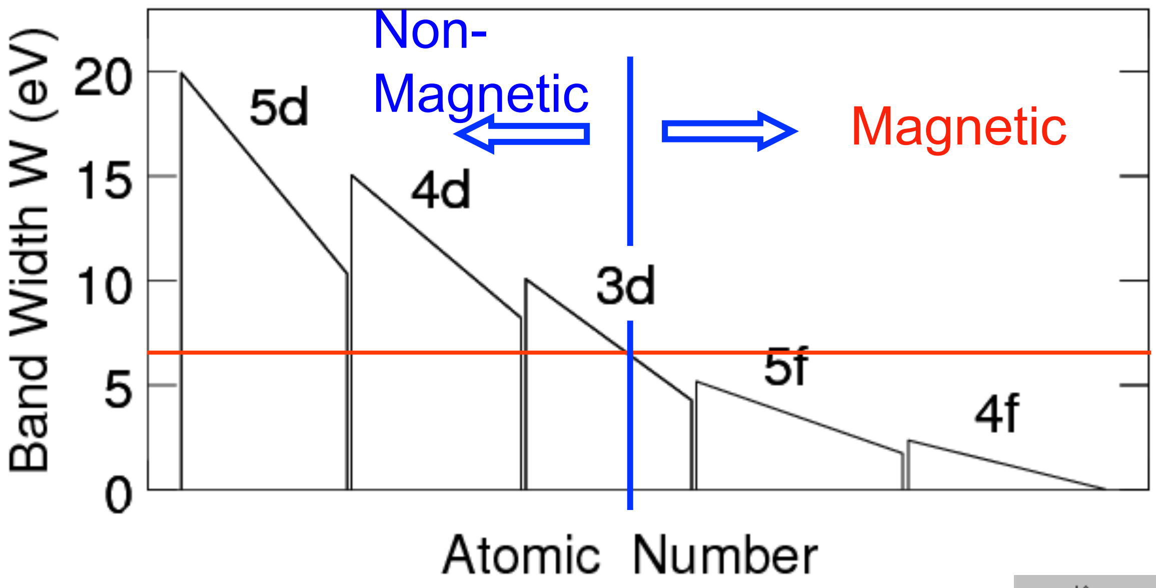
Model

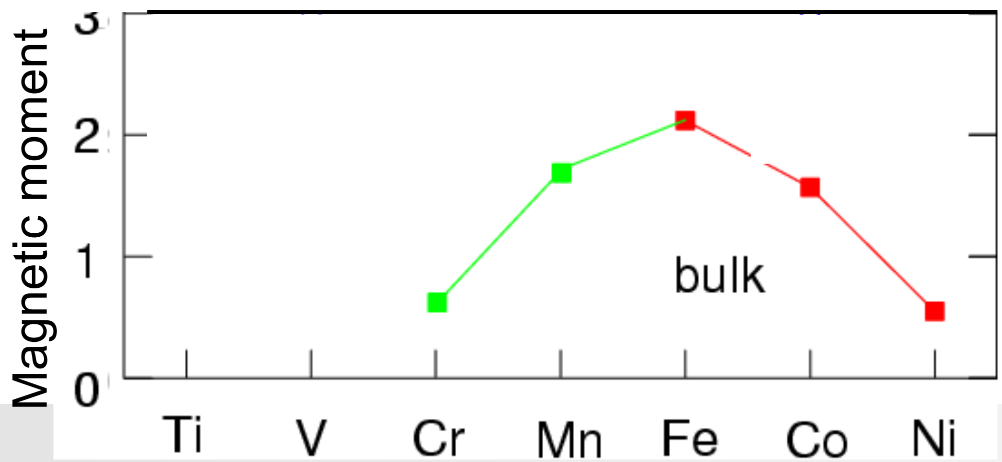


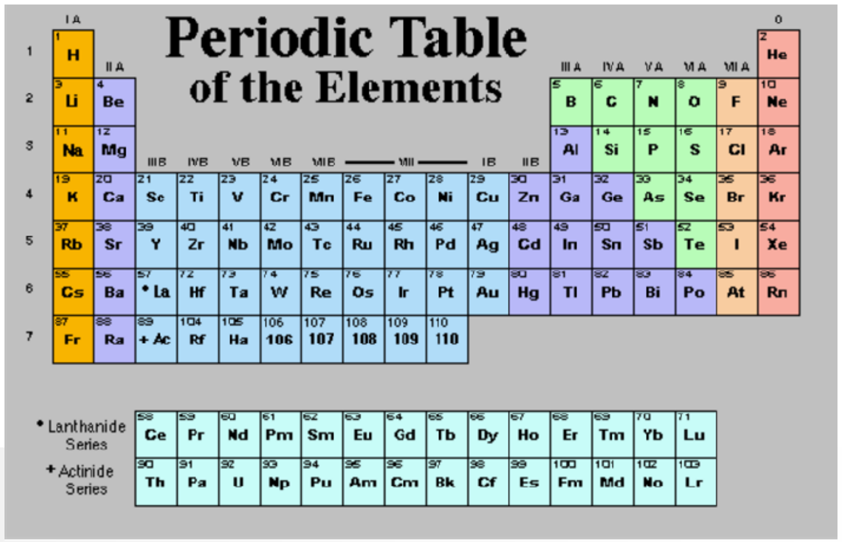


Bandwidths of bulk metals

www.fz-juelich.de/iff/e_th1







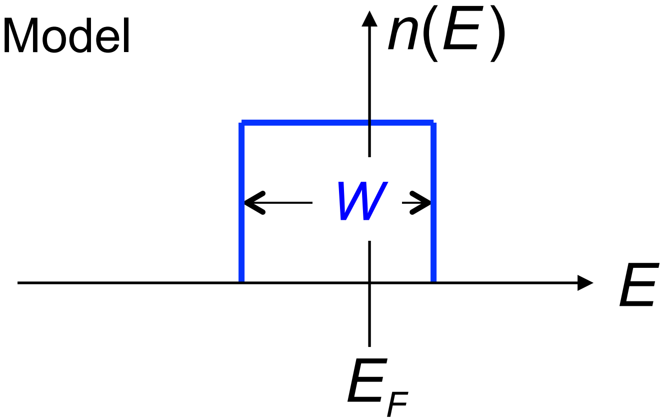
Stoner Model for Ferromagnetism

www.fz-juelich.de/iff/e_th1

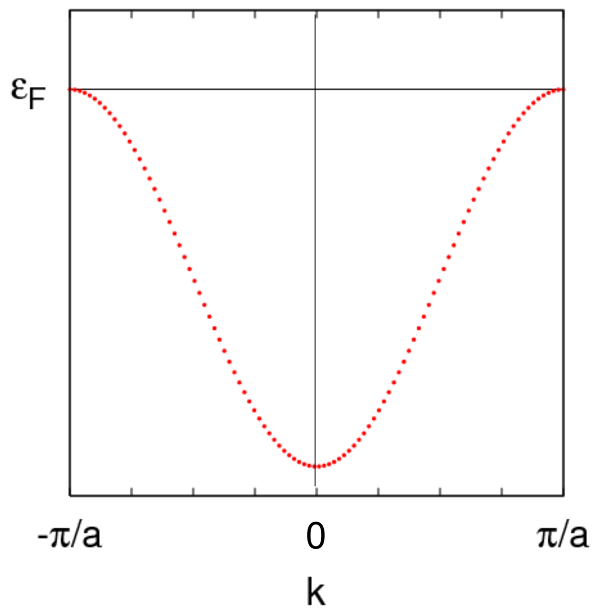
- Stoner criterion: $I \bullet n(E_F)$
  (for d-electrons)

- Density of states: $n(E_F)$

Model

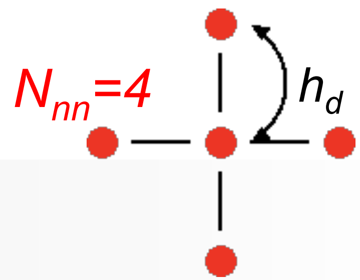


1D: $\varepsilon(k) = \varepsilon_0 + 2\sqrt{N_{\mathrm{nn}}}h_d \cos(ka)$



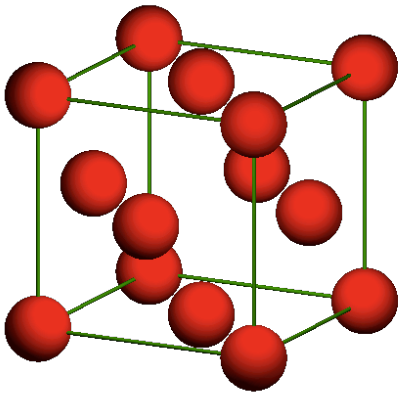
E_F

- Coordination N°: $\bar{W} = 2\sqrt{N_{nn}}h_d(R_{nn})$



Role of coordination number

$$n(E_F) \propto \frac{1}{\sqrt{N_{nn}}}$$

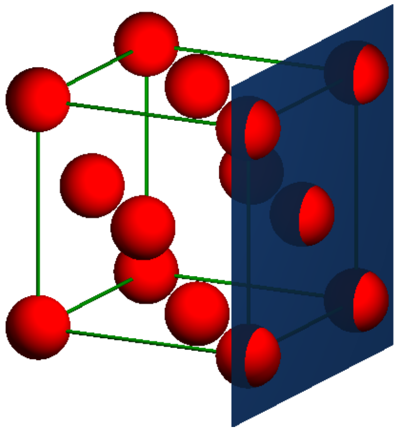


fcc-bulk:

$N_{fcc}=12$

$W_{fcc}:=1$

$n_{fcc}:=1$

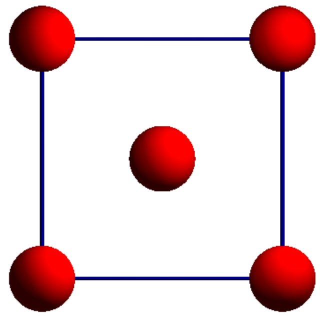


(100)-surface:

$N_{(100)}=8$

$W_{(100)}=0.82$

$n_{(100)}=1.22$



(100)-monolayer:

$N_{ML}=4$

$W_{ML}=0.58$

$n_{ML}=1.73$

1. Surfaces

$J_{||} \sim J_{\perp}$

V(100), Cr(100), Fe(100), Co(100), Ni(100)

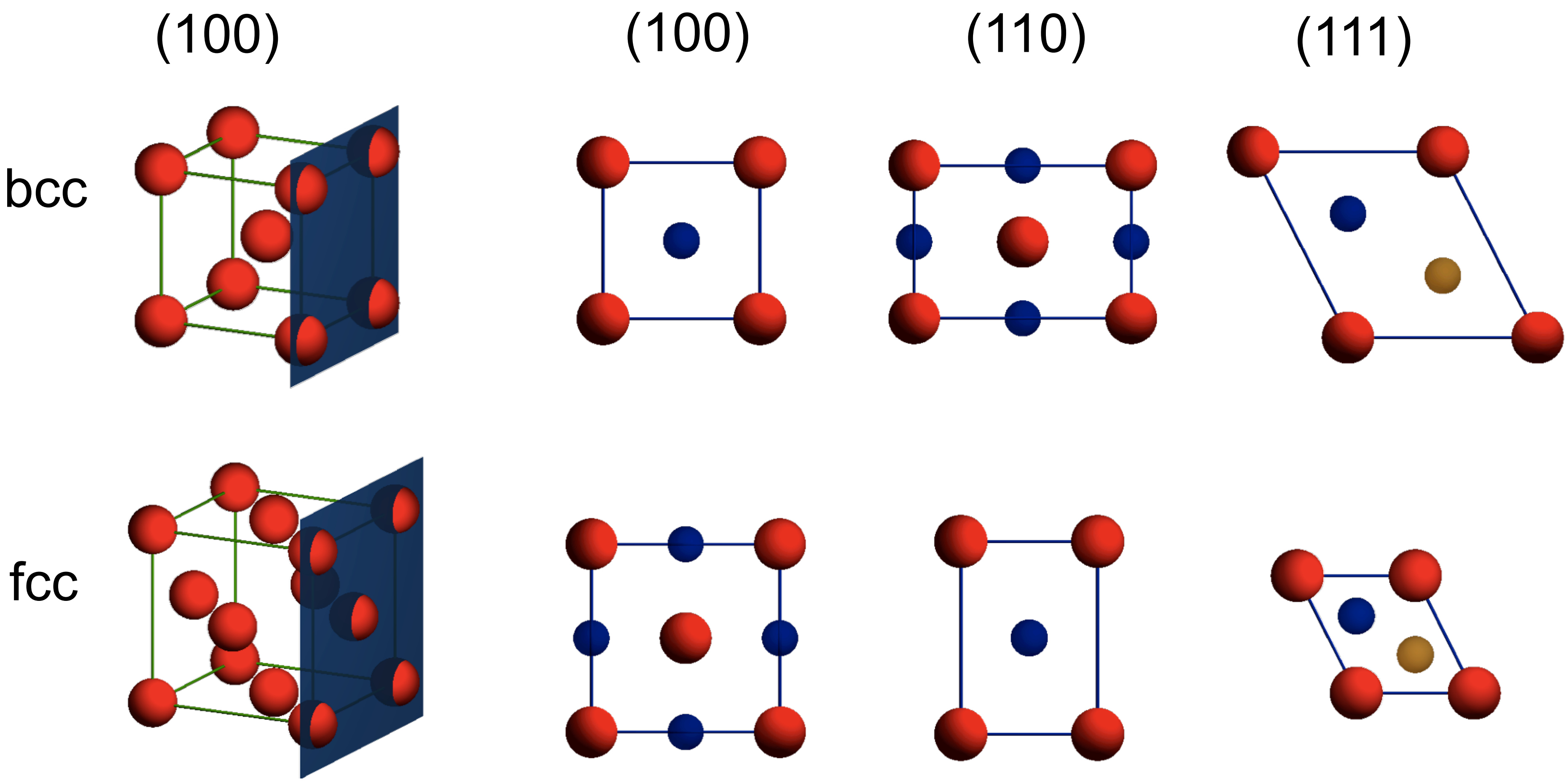
Surfaces: Magnetic Moments

www.fz-juelich.de/iff/e_th1

M [μ_B]	Cr (bcc)	Fe (bcc)	Co (hcp)	Ni (fcc)
(100)	2.55	2.88	1.85	0.68
Bulk	±0.60	2.13	1.62	0.61

$M^{(100)} / M^{Bulk} =$ 4.25 1.35 1.14 1.12

Surface Unit Cells



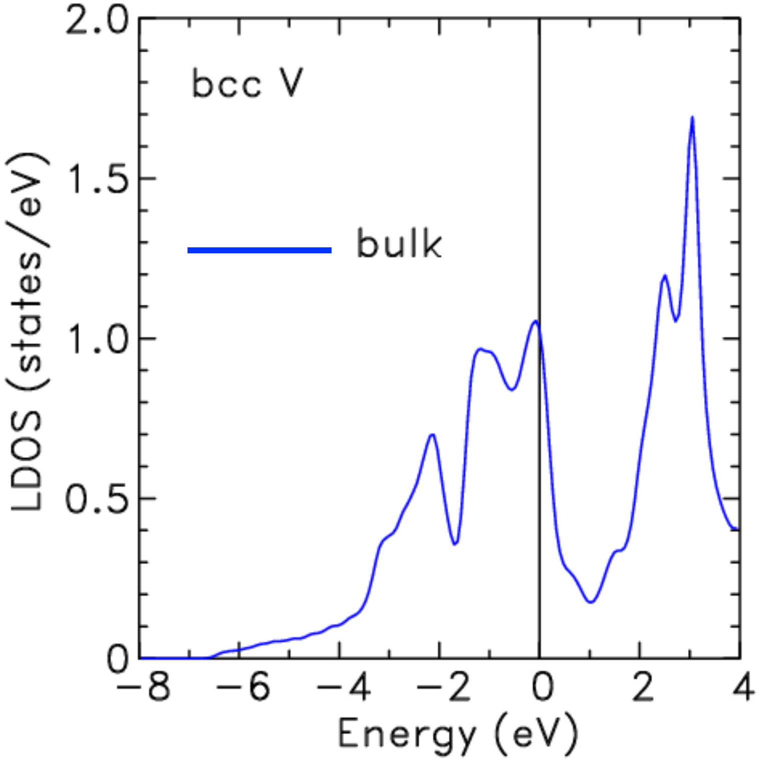
Figures: Manfred Niesert

Surfaces: Magnetic Moments

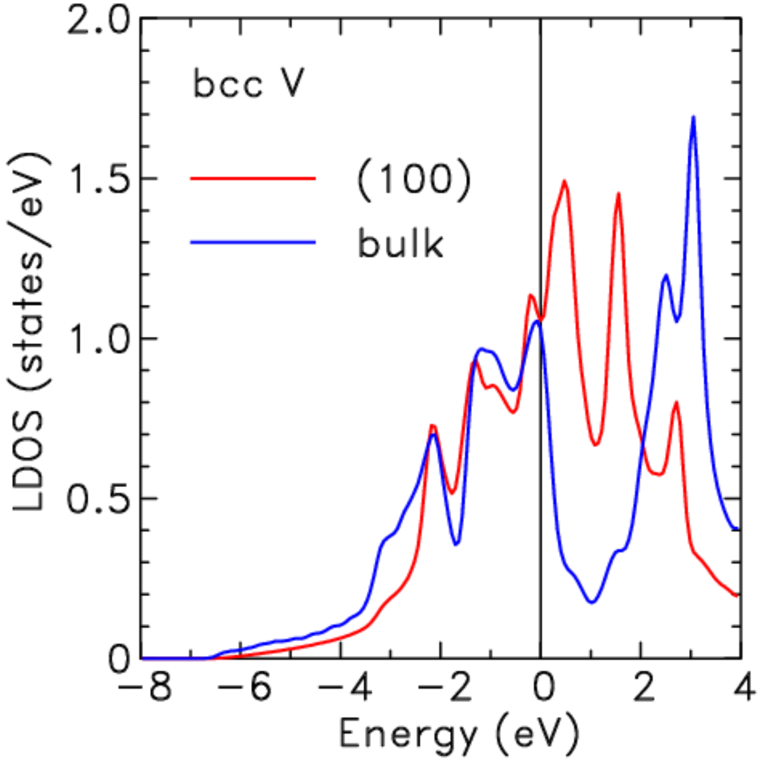
M [μ_B]	Cr (bcc)	Fe (bcc)	Co (hcp)	Ni (fcc)
(100)	2.55	2.88	1.85	0.68
(110)	—	2.43	—	0.74
(111) (0001)	—	2.48	1.70	0.63
Bulk	±0.60	2.13	1.62	0.61

V(100): LDOS

Local Density of States
bulk V



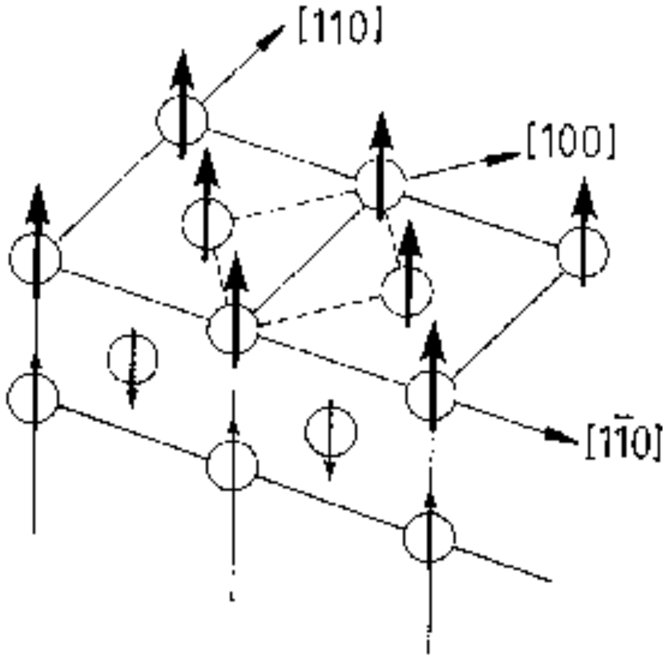
Local Density of States
bulk V
surface V(100)

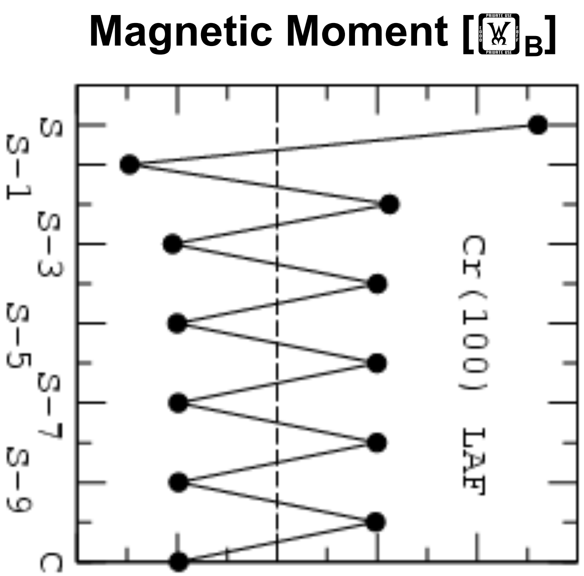


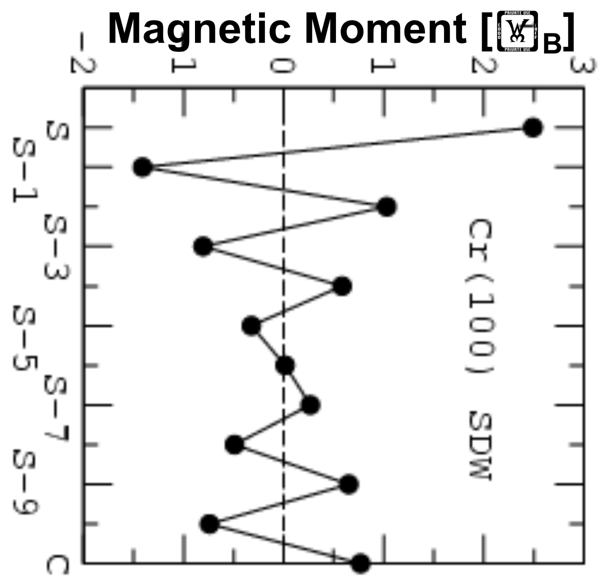
V bulk and surface (100) : nonmagnetic

Cr(100): Layered AntiFerromagnetism

www.fz-juelich.de/iff/e_th1





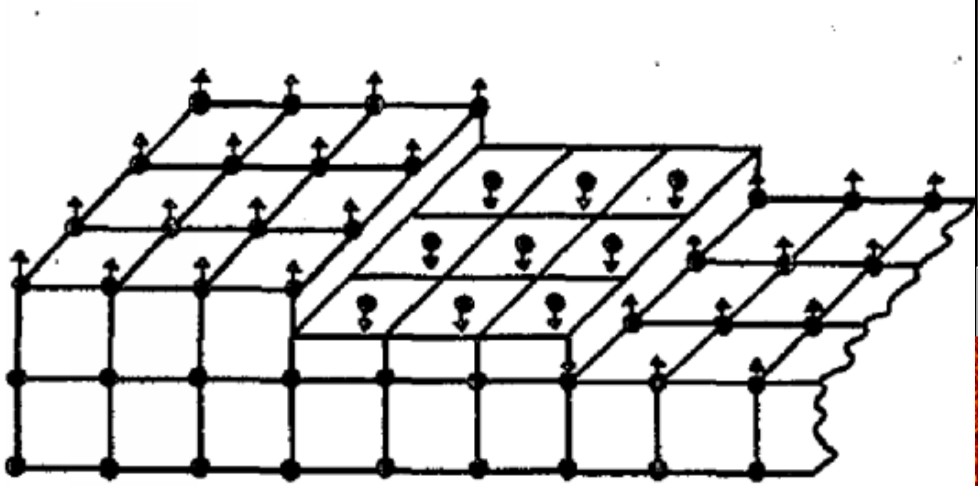


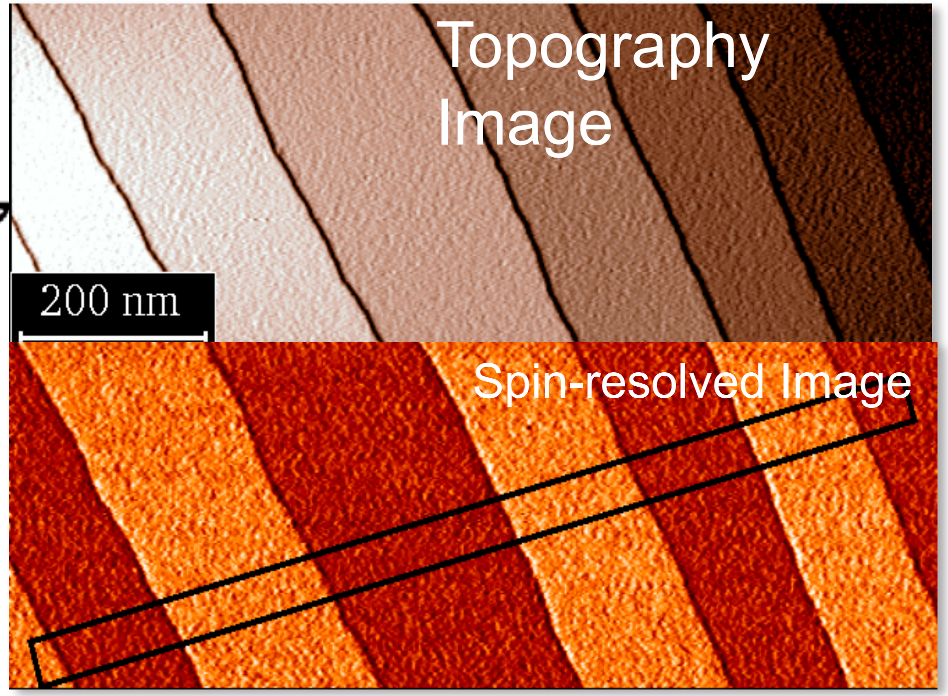
G. Bihlmayer, T. Asada, S. Blügel, PRB **62**, R11937 (2000)

Topological Antiferromagnetism of stepped Cr(001)

www.fz-juelich.de/iff/e_th1

Experiment (Wiesendanger)
Scanning Tunneling Microscopy (STM)

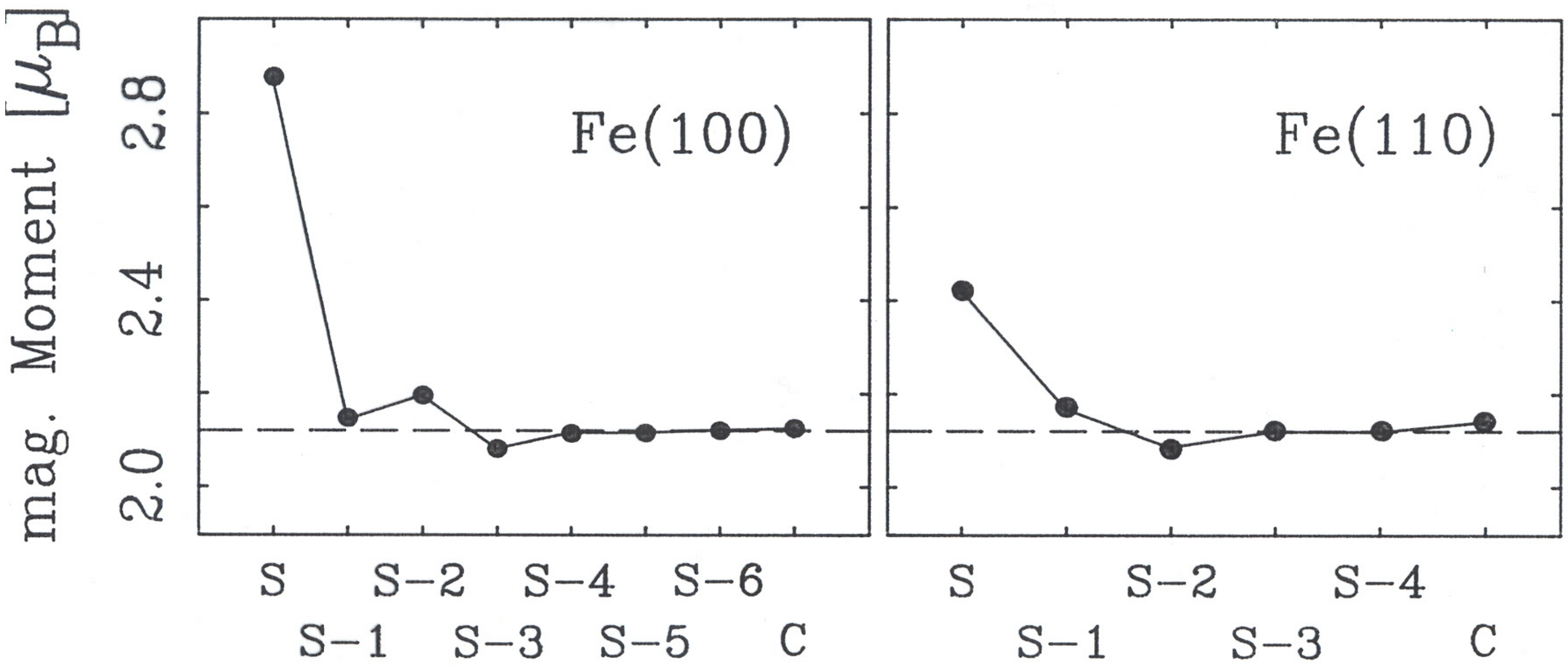




S. Blügel *et al.*, Phys. Rev. B **39**, 1392 (1989)

Kleiber *et al.*, Phys. Rev. Lett. **85**, 4606 (2000)

Fe(100) and Fe(110)

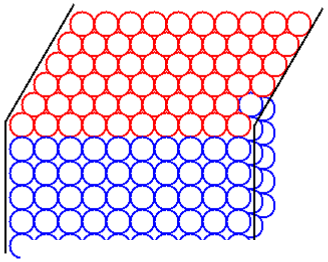


Susanne Handschuh, PhD thesis, Uni Köln

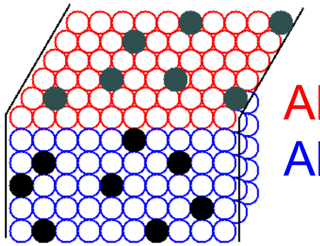
(100) Surfaces of VRu, VRh, VPd Alloys

www.fz-juelich.de/iff/e_th1

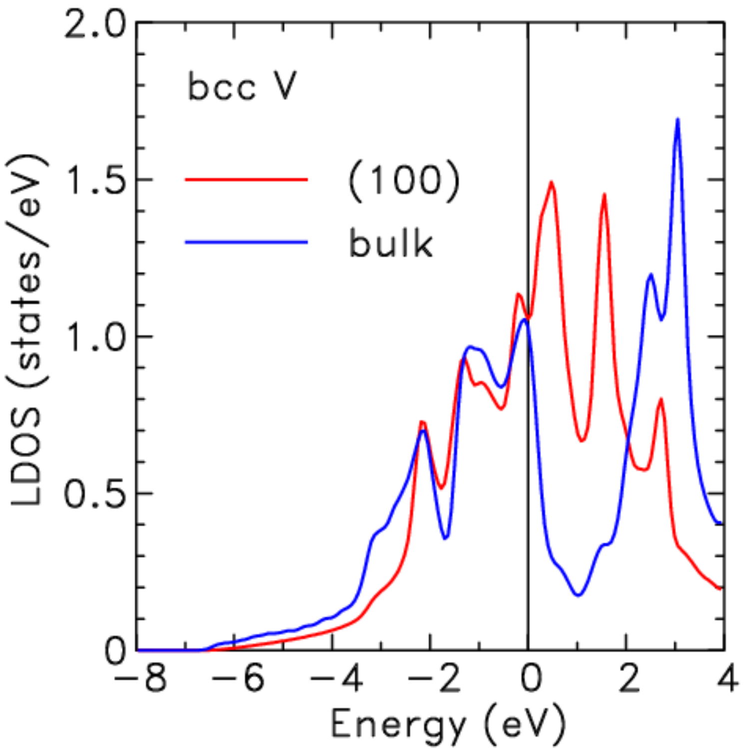
Local Density of States

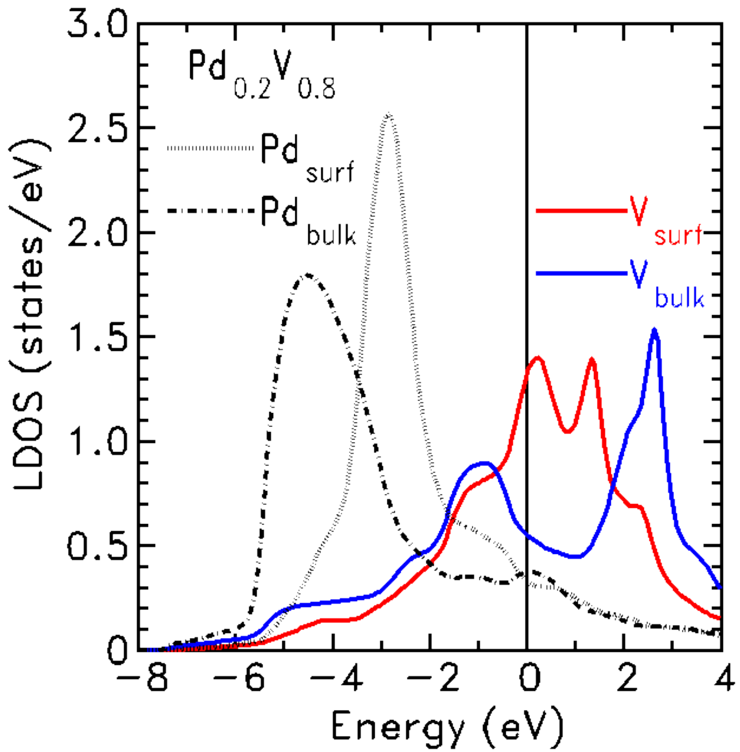


Clean surface V(100)
bulk V



Alloyed surface VPd(100)
Alloyed bulk VPd



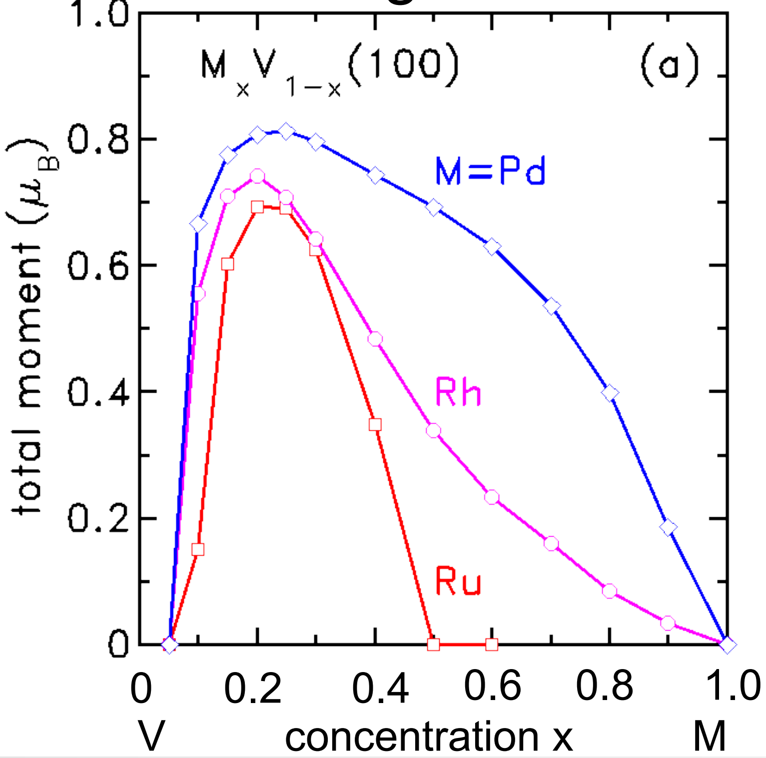


I. Turek, S. Blügel, and J. Kudrnovsk'y, PRB **57**, R11065 (1998)

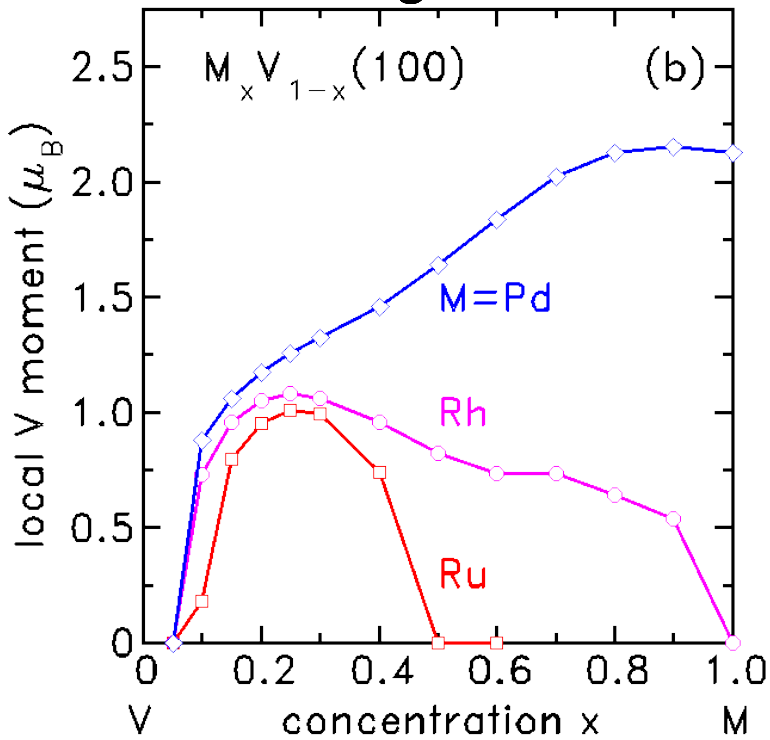
(100) Surfaces of VRu, VRh, VPd Alloys

Magnetic Moment

Total magnetic moment



Local magnetic moment V



I. Turek, S. Blügel, and J. Kudrnovsk'y,PRB **57**, R11065 (1998).

Magnetism at the nanoscale (Part II)

Stefan Blügel

Institut für Festkörperforschung
& Institute for Advanced Simulation

Forschungszentrum Jülich

www.fz-juelich.de/iff//Bluegel_S

Effects of “nano” on magnetism

- Reduction of neigboring atoms: $N_n \searrow$
- Reduction of local symmetry: $S \searrow$
- Finiteness of nano-object: $L \searrow$

Effects of “nano” on magnetism

- Reduction of neigboring atoms: N_n

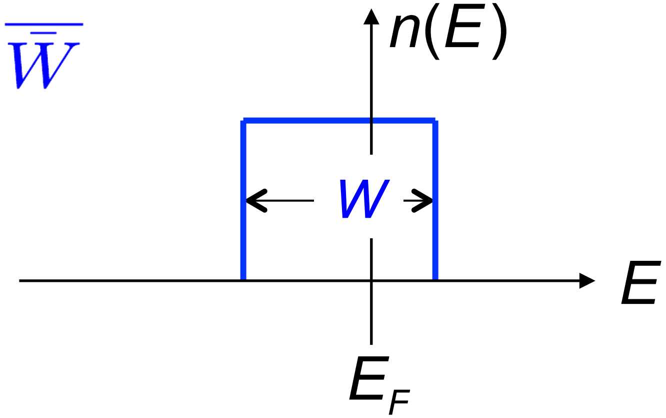
N_n

Kinetic energy

Coulomb energy

$$\bar{W} = 2\sqrt{N_{nn}}\, h_d(R_{nn})$$

$$n \sim \frac{1}{\bar{W}}$$



- Stoner criterion:

(for d-electrons)

$$I \bullet n(E_F) > 1$$

Effects of “nano” on magnetism

- Reduction of neigboring atoms: $N_n \searrow$

$N_n \searrow$

Kinetic energy $\searrow$

Coulomb energy $\nearrow$

- Many more nanomagnets than bulk magnets
- With large magnetic moments
- Immediate consequence for :
  - Nanostructure formation
  - Alloying
  - Relaxation

2. Thin Films

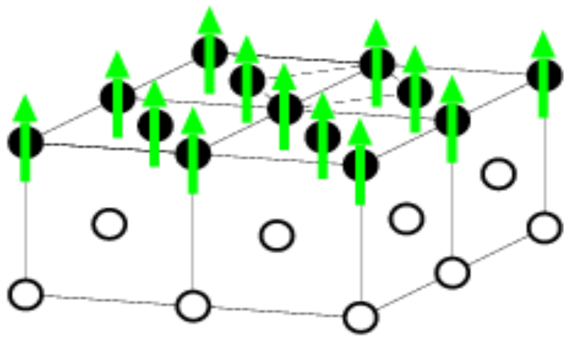
$J_{||} >> J_{\perp}$: e.g. 3d on Ag(100)

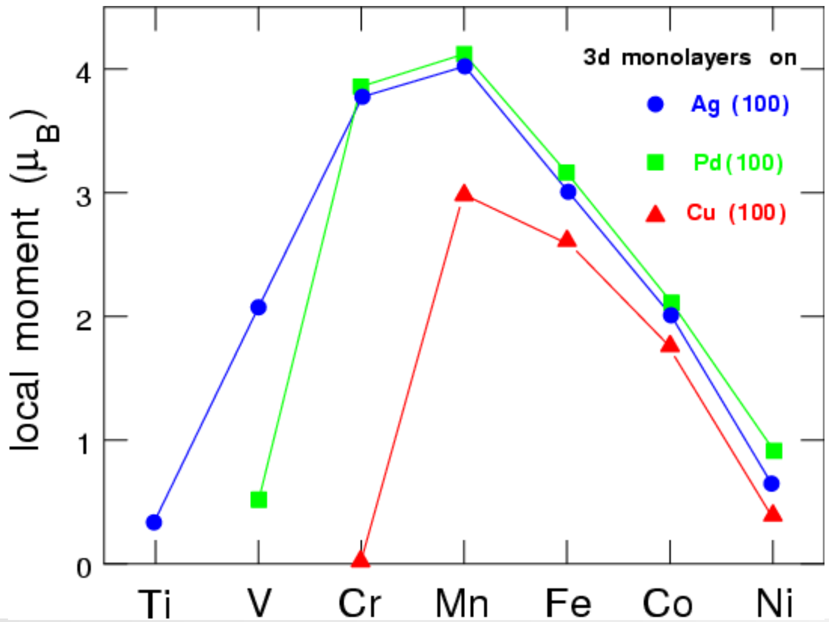
$J_{||} << J_{\perp}$: e.g. 3d on W(100)

$J_{||} \sim J_{\perp}, J_{s} > 0$: e.g. 3d on Fe(100)

$J_{||} \sim J_{\perp}, J_{s} < 0$: e.g. 3d on Cr(100)

2D-Ferromagnetism of 3d-Monolayers on NM(100)

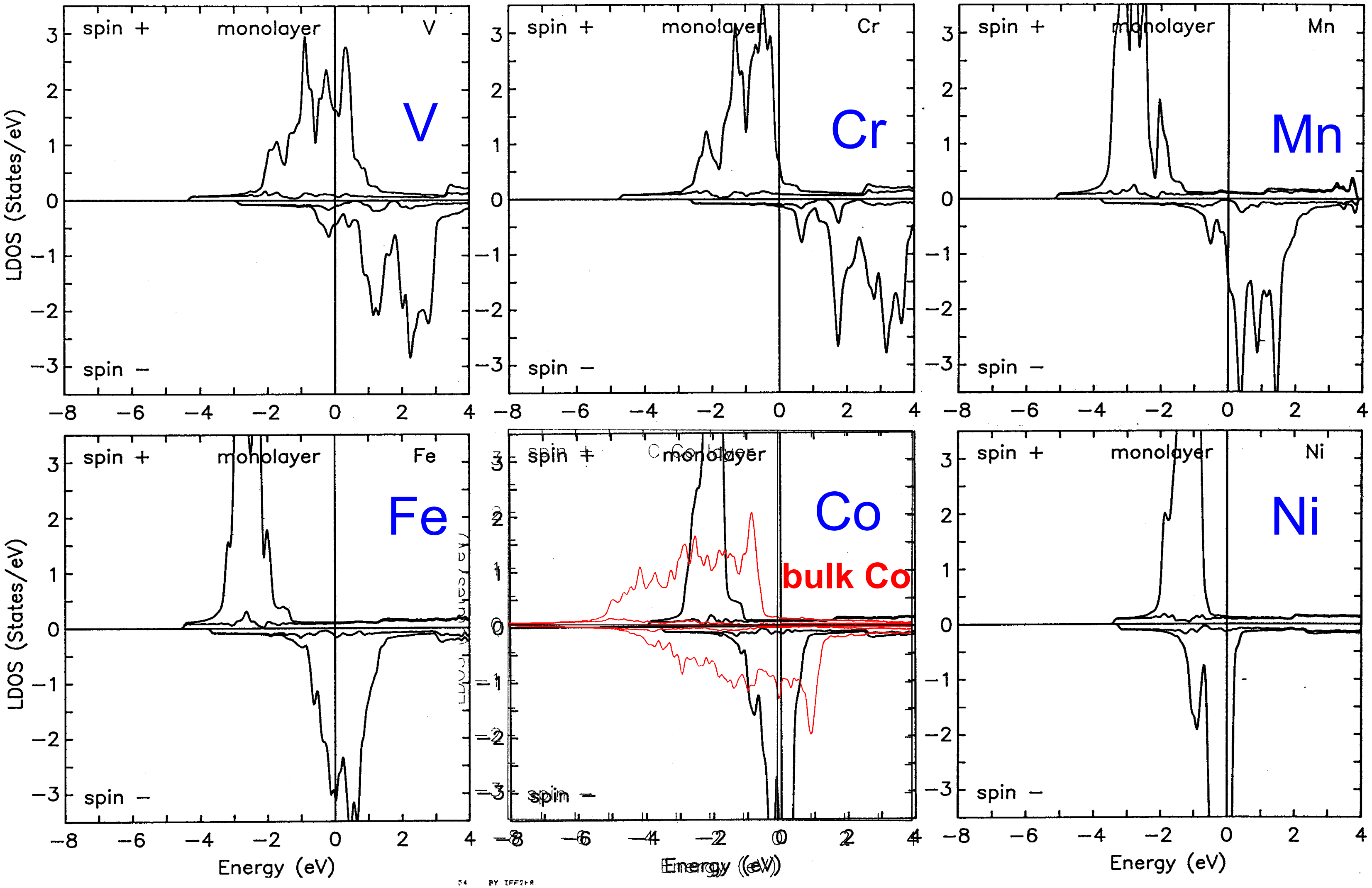




S. Blügel, D. Drittler, R. Zeller, and P.H. Dederichs, Appl. Phys. A **49**, 547 (1989)

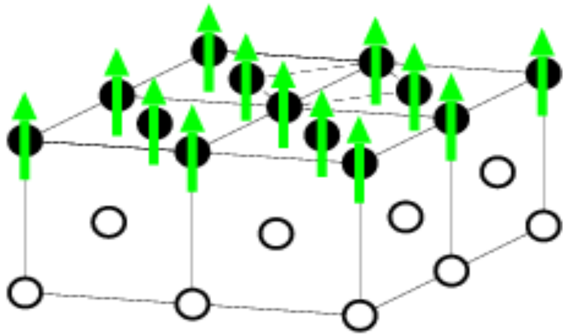
Ferromagnetic LDOS 3d/Ag(100)

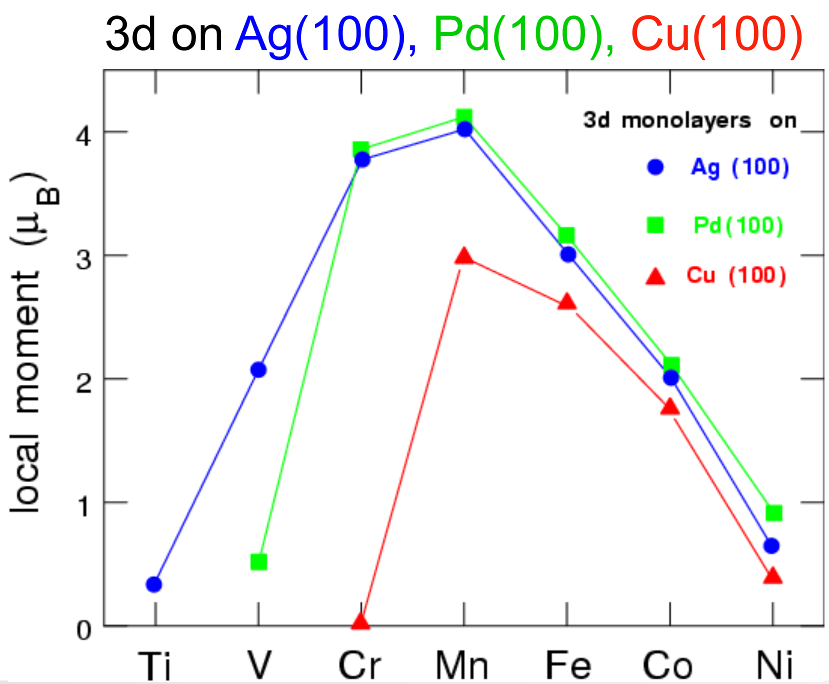
www.fz-juelich.de/iff/e_th1

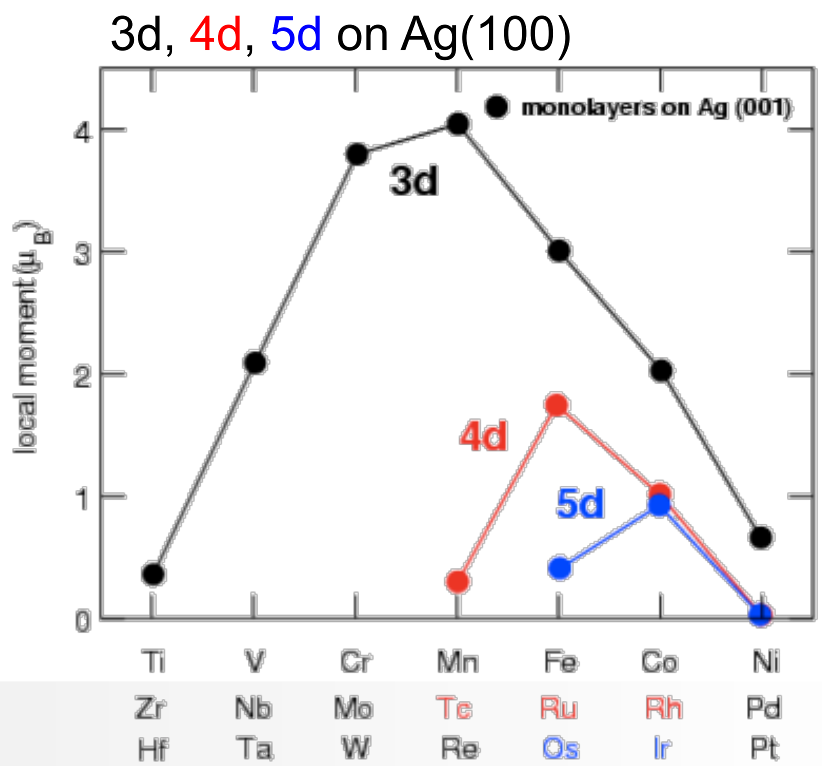


S. Blügel, D. Drittler, R. Zeller, and P.H. Dederichs, Appl. Phys. A **49**, 547 (1989)

2D-Ferromagnetism of 3d, 4d, 5d Monolayers on NM(100)



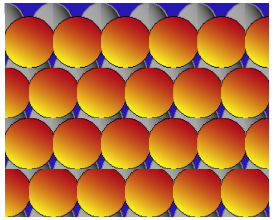


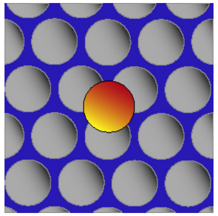


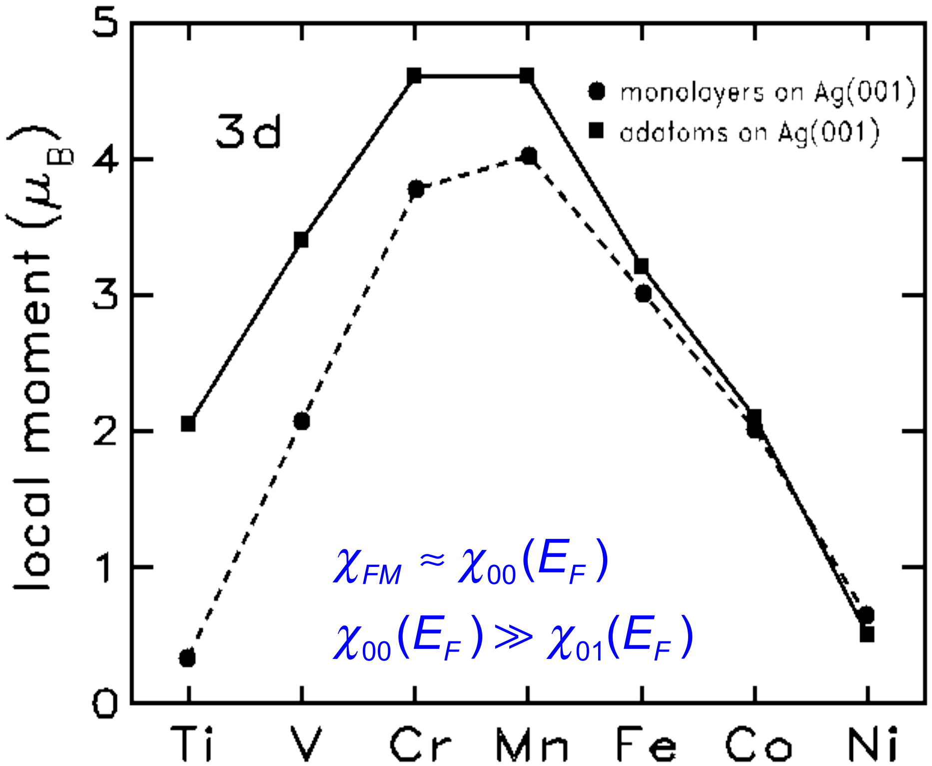
S. Blügel, PRL **68**, 851 (1992)

Monolayer vs Adatom: 3d, 4d, 5d/Ag(100)

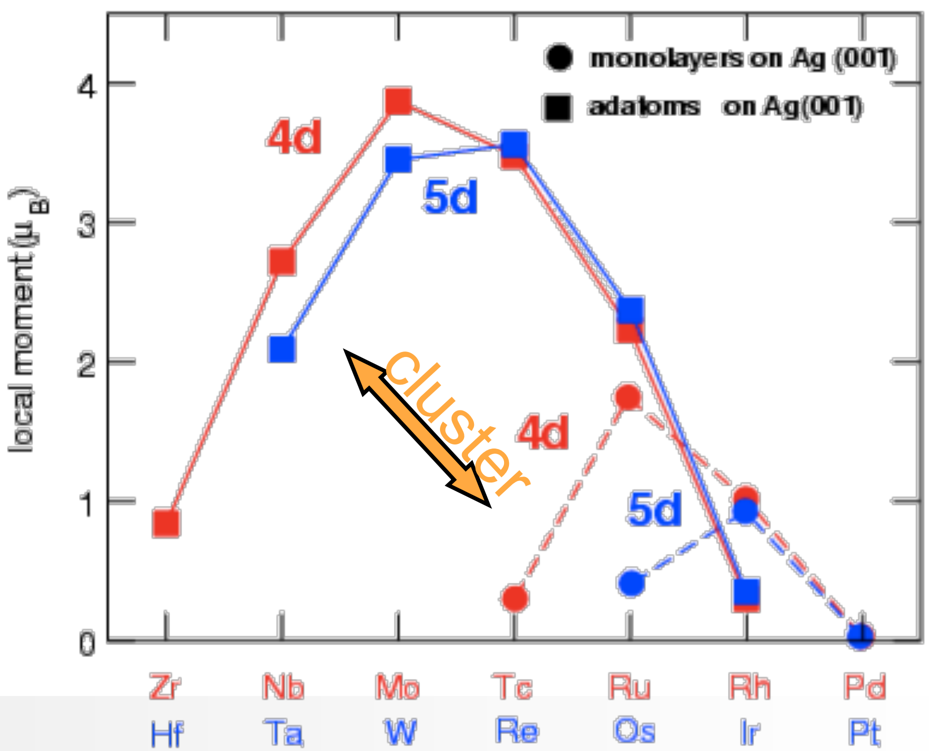
www.fz-juelich.de/iff/e_th1







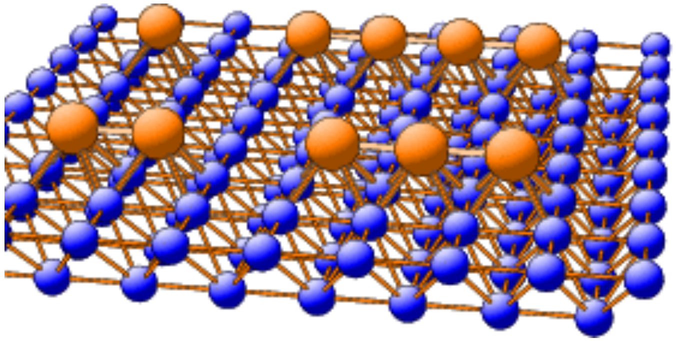
$$\chi_{FM} \approx \chi_{00}(E_F) + \chi_{01}(E_F) + \cdots + \chi_{0j}(E_F)$$

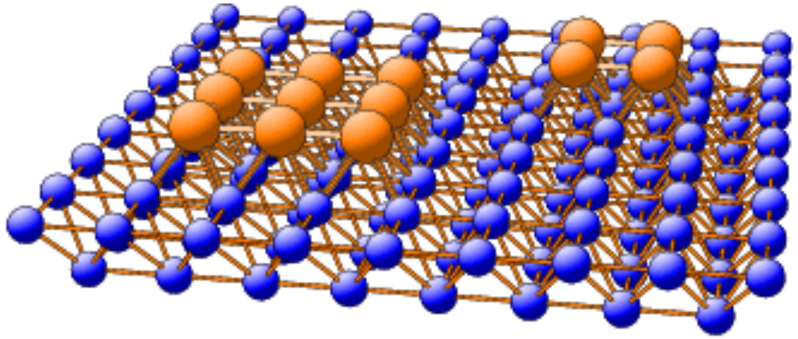


P. Lang, V. S. Stepanyuk*, K. Wildberger, R. Zeller, P. H. Dederichs, SSC **92**, 755 (1994)

3. Deposited Clusters

4d and 5d metal clusters on Ag(100)

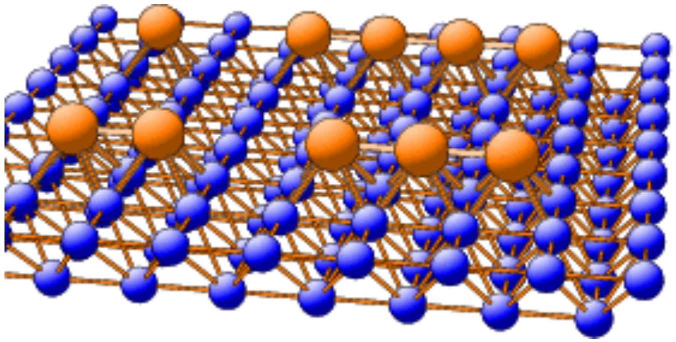


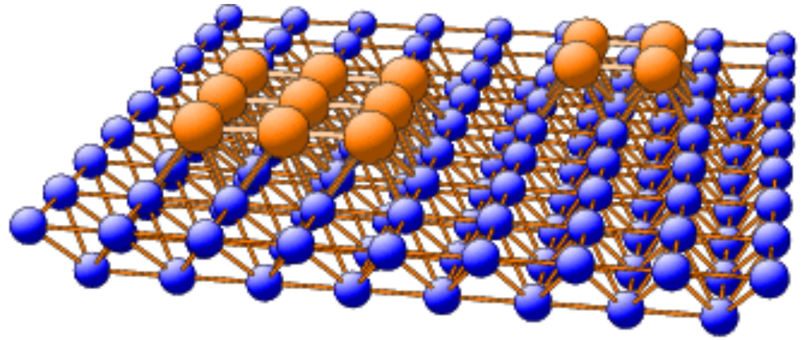


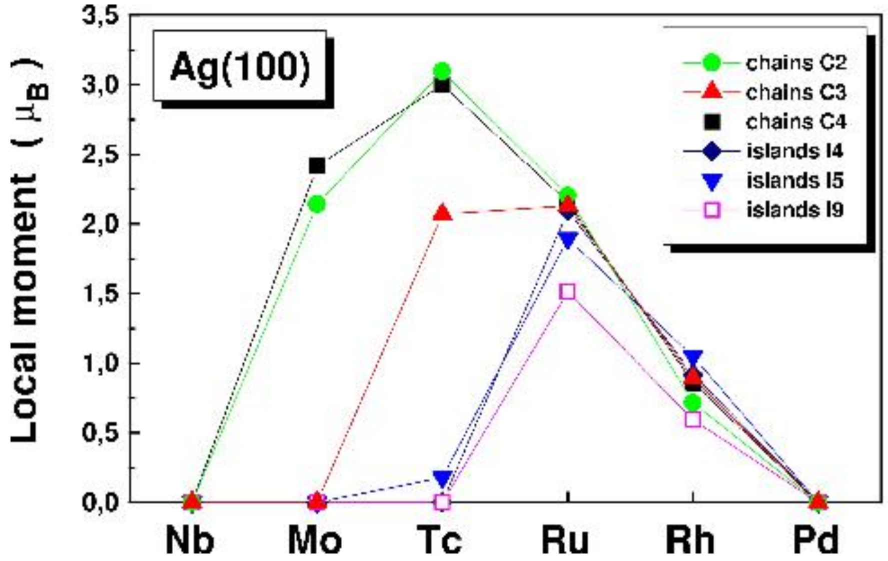
Properties depend on

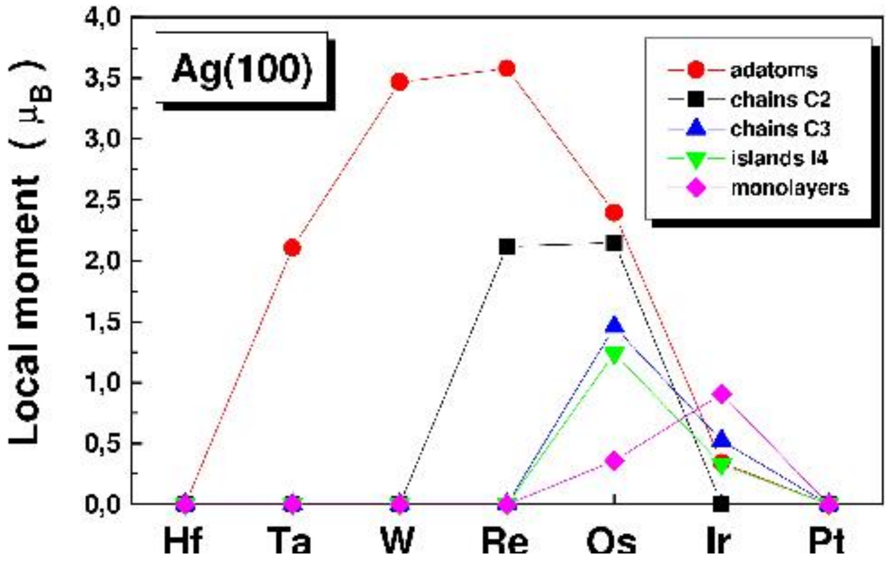
- cluster shape
- cluster size
- substrate

Magnetic Clusters







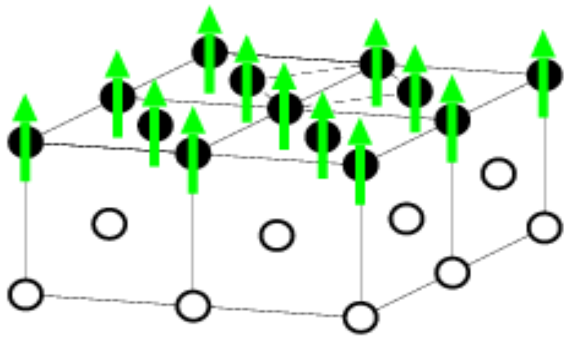


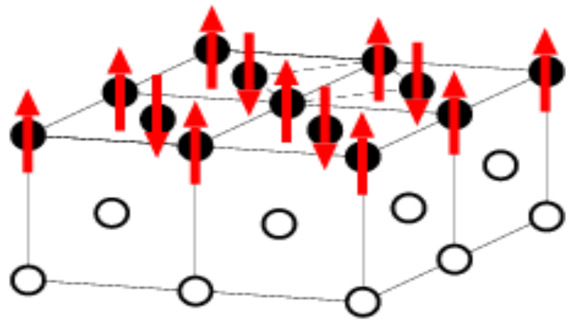
S. Blügel, PRL 68, 851 (1992)

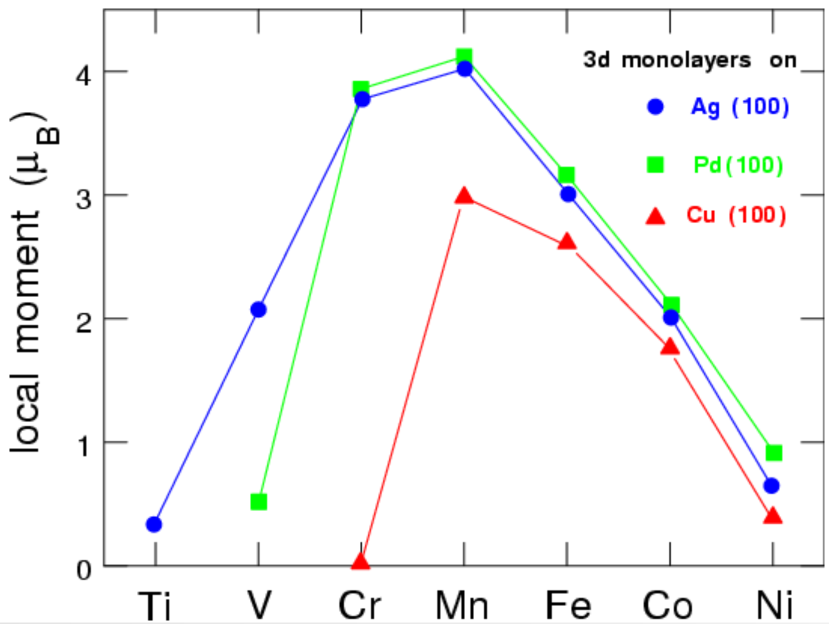
K. Wildberger, V.S. Stepanyuk, P. Lang, R. Zeller, P.H. Dederichs, PRL **75**, 509 (1995)

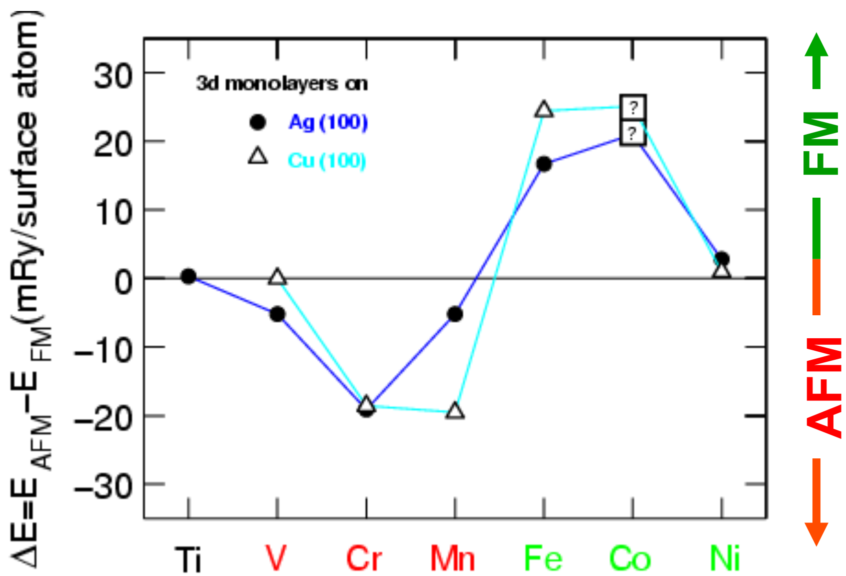
4. Magnetic Phases

2D-Antiferromagnetism of Monolayers on NM(100)







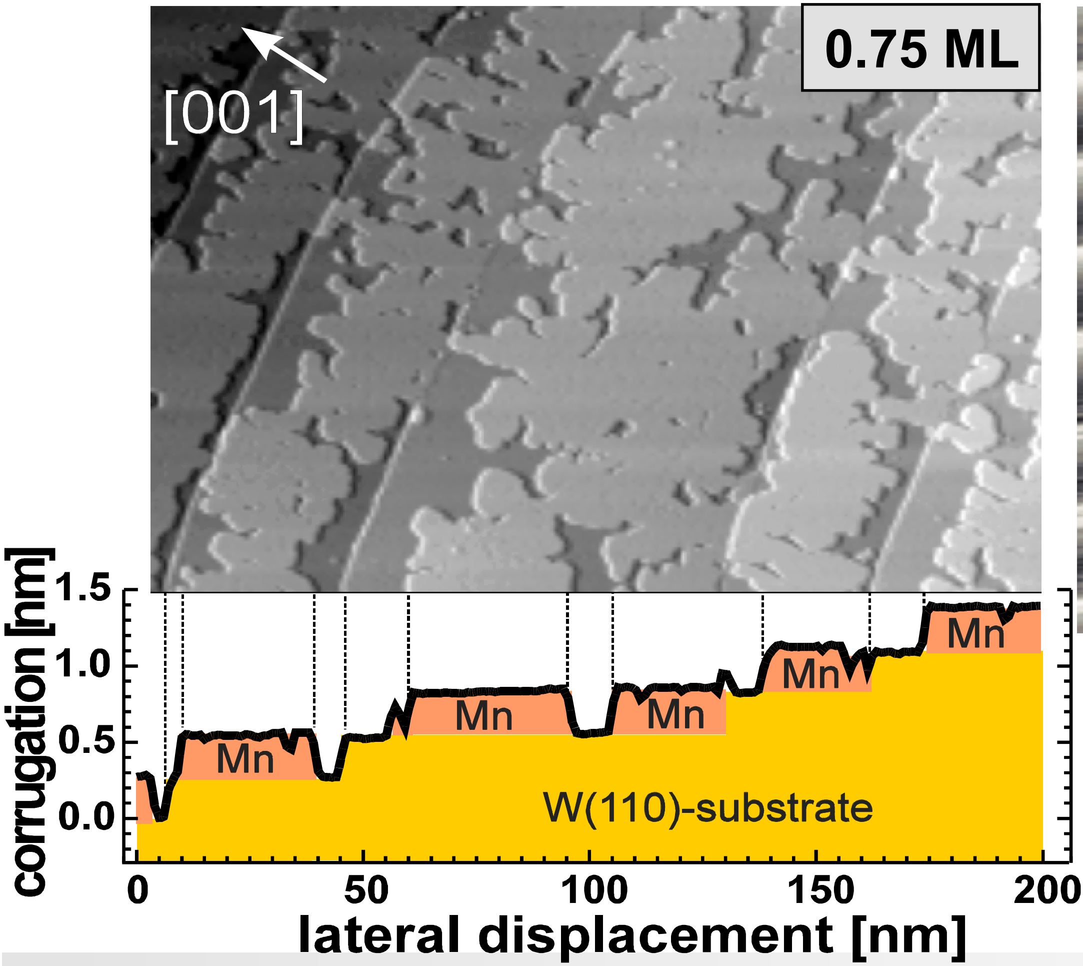


Blügel, Weinert, Dederichs, PRL **60** (1988)

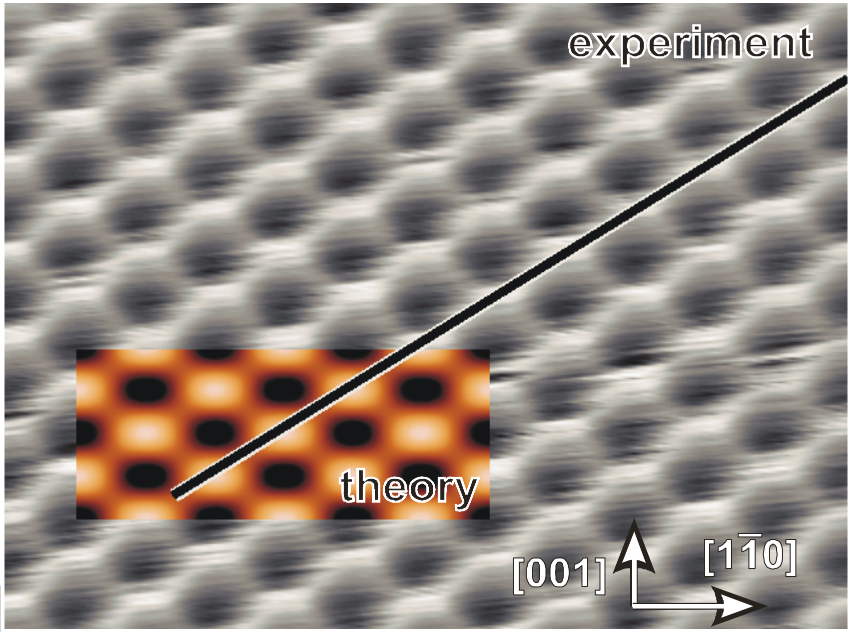
Experiment: Monolayer Mn/W(110)

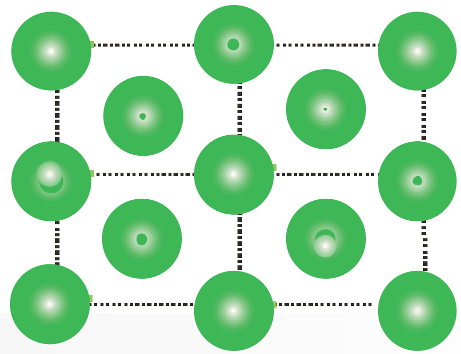
www.fz-juelich.de/iff/e_th1

Pseudomorphic Growth:



STM topography image



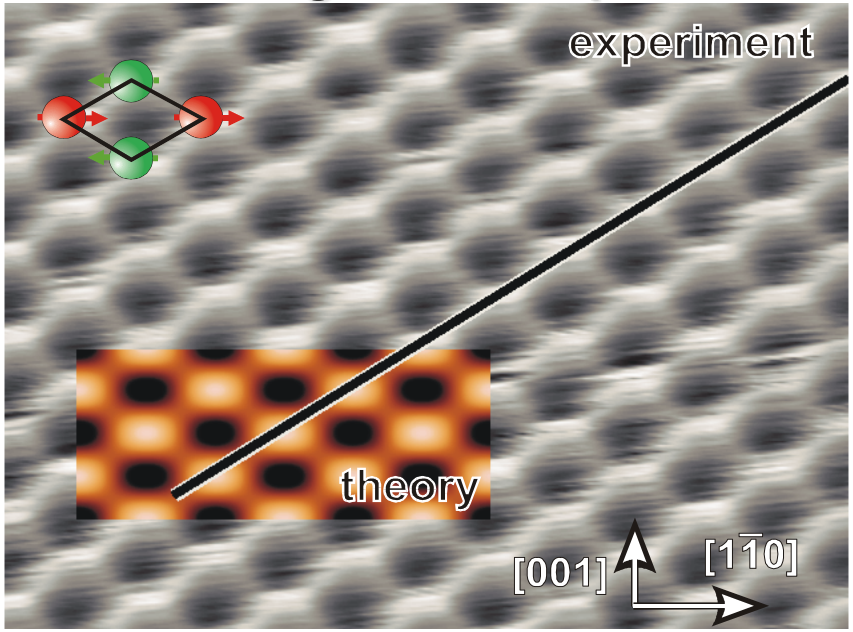


M. Bode et al., Surf.Sci 432, 8 (1999)

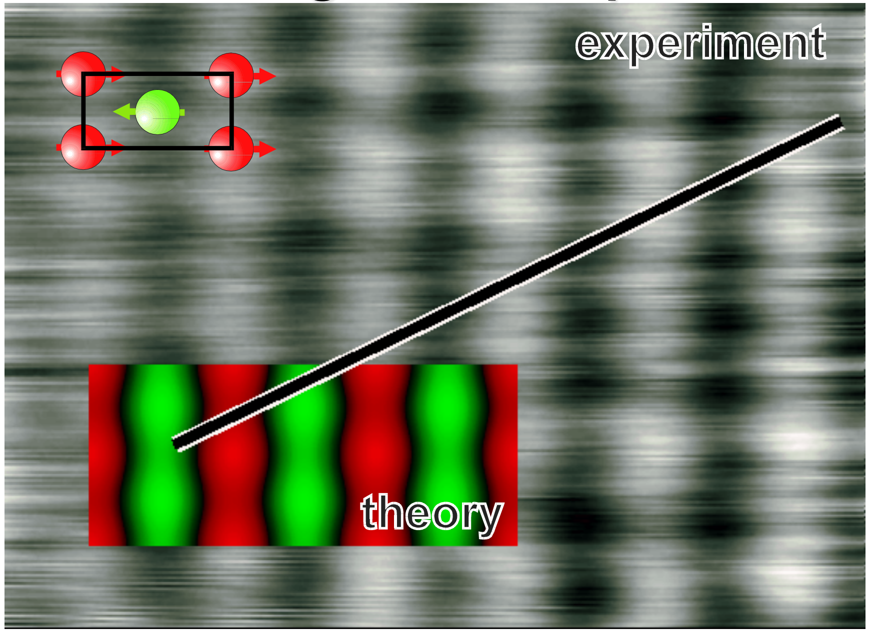
Imaging the Magnetic Ground State of 1ML-Mn/W(110)

www.fz-juelich.de/iff/e_th1

Non-magnetic W-Tip

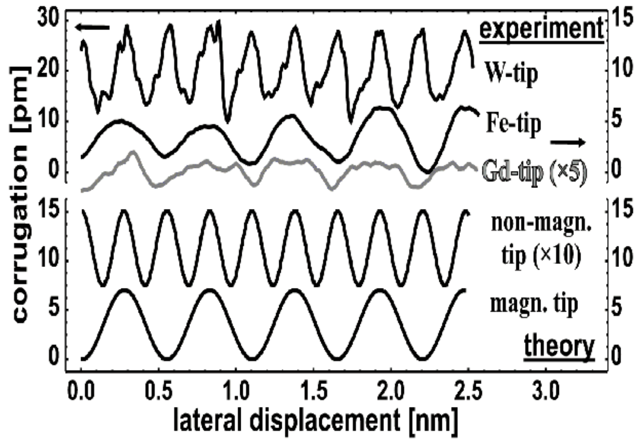


Magnetic Fe-Tip



➪ **First experimental Proof of the 2D-AFM!**

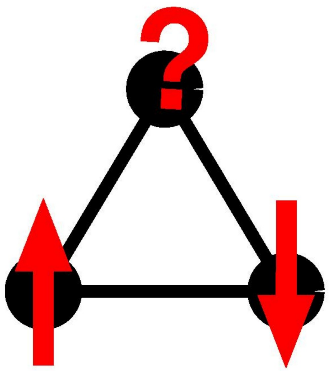
S.Heinze et al., Science **288** (2000)



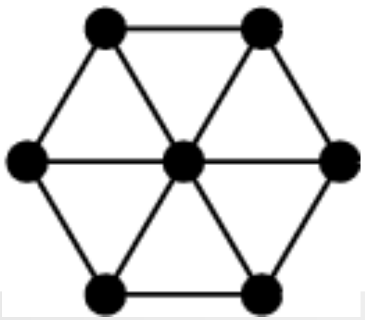
4. Magnetic Frustration

Frustrated itinerant Magnetism

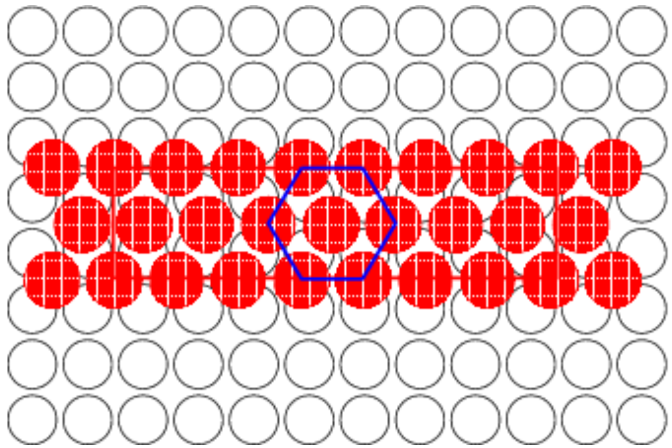
Geometric Frustration



Cr/Mn on
fcc(111) or hcp(0001)



Pseudo-hexagonal Mn:
c(8x2)Mn ML on Cu(100)



T. Flores et.al, Surf. Sci. 279 (1992)

Localized Antiferromagnets
With TAF-Lattice: VBr_2, $LiCrO_2$

Spin configurations

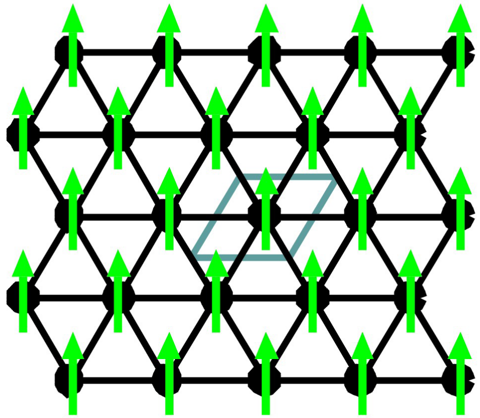
$$H_{2-spin} = -\sum_{ij} J_{ij} S_i S_j$$

www.fz-juelich.de/iff/e_th1

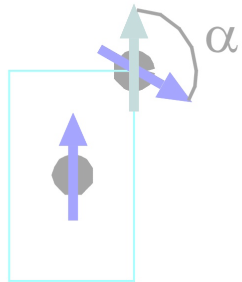
Itinerant Antiferromagn.

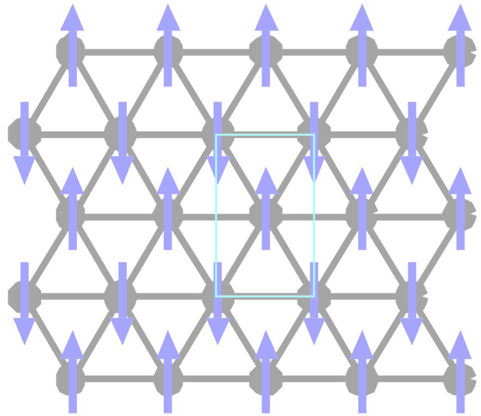
Only n.n. interaction:

Beyond n.n. interaction:

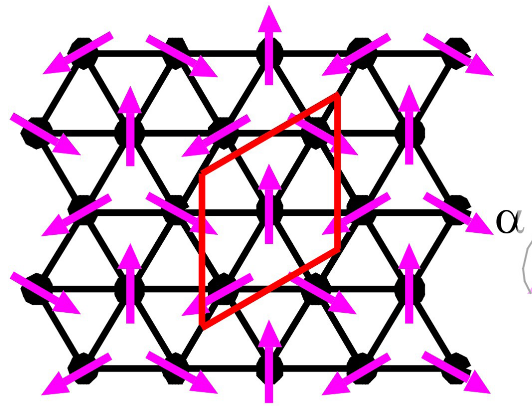


$J_1>0$: FM

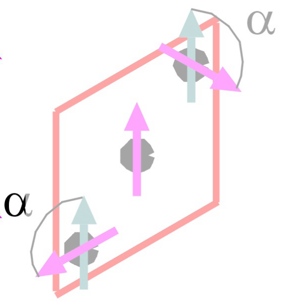




c(2x2)AFM



$J_1<0$: Neel State



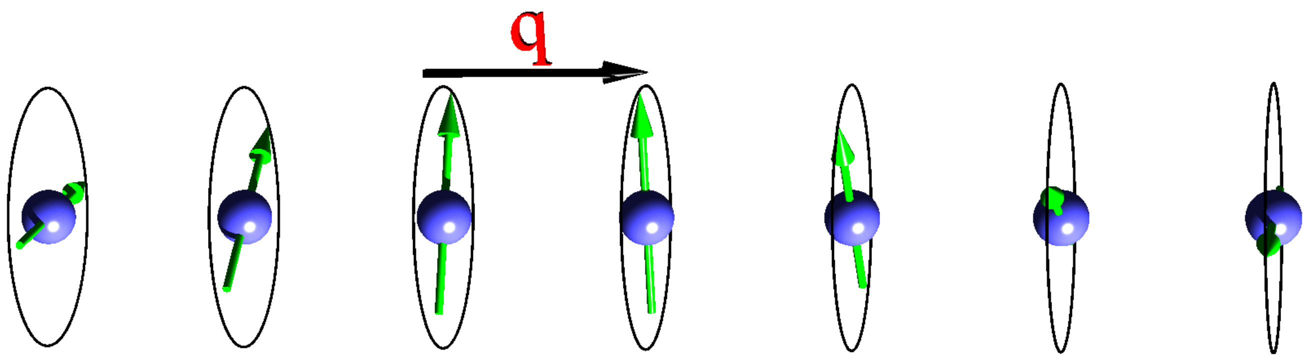
$(\sqrt{3} \times \sqrt{3})\ 180^\circ$

Incommensurate Spin Spirals (SSDW)

www.fz-juelich.de/iff/e_th1

Spiral magnetic structure

$$M^n = M\begin{pmatrix}\cos\varphi\sin\vartheta\\ \sin\varphi\cos\vartheta\\ \cos\vartheta\end{pmatrix},\ \varphi = \vec{q}\vec{R}^n$$



Generalized Bloch Theorem:

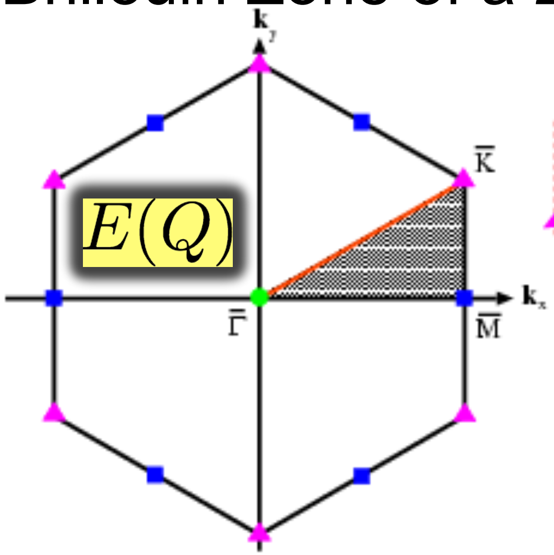
$$H(\vec{r}+\vec{R}^n) = U(\vec{r}+\vec{R}^n)H(\vec{r})U^*(\vec{r}+\vec{R}^n)$$

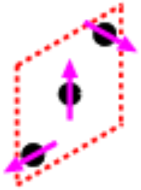
$$H_{2-spin} = -\sum_{ij} J_{ij} S_i S_j \longrightarrow \boxed{E(q)}$$

Ph. Kurz, F. Förster, L. Nordström, G. Bihlmayer, and S. Blügel, PRB **69**, 024415 (2004).

Huge number of possible Magnetic Structures

Brillouin Zone of a 2D Hexagonal Lattice:



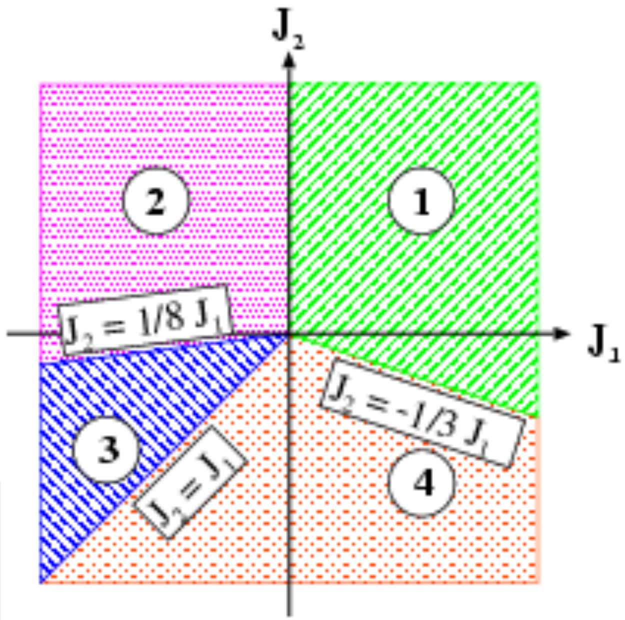


Néel State

Row-wise AFM (1Q-state)

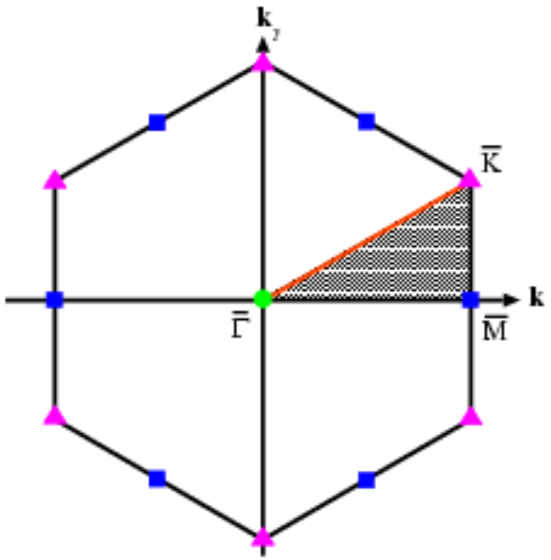
$$H_{2-spin} = -\sum_{ij} J_{ij} S_i S_j$$

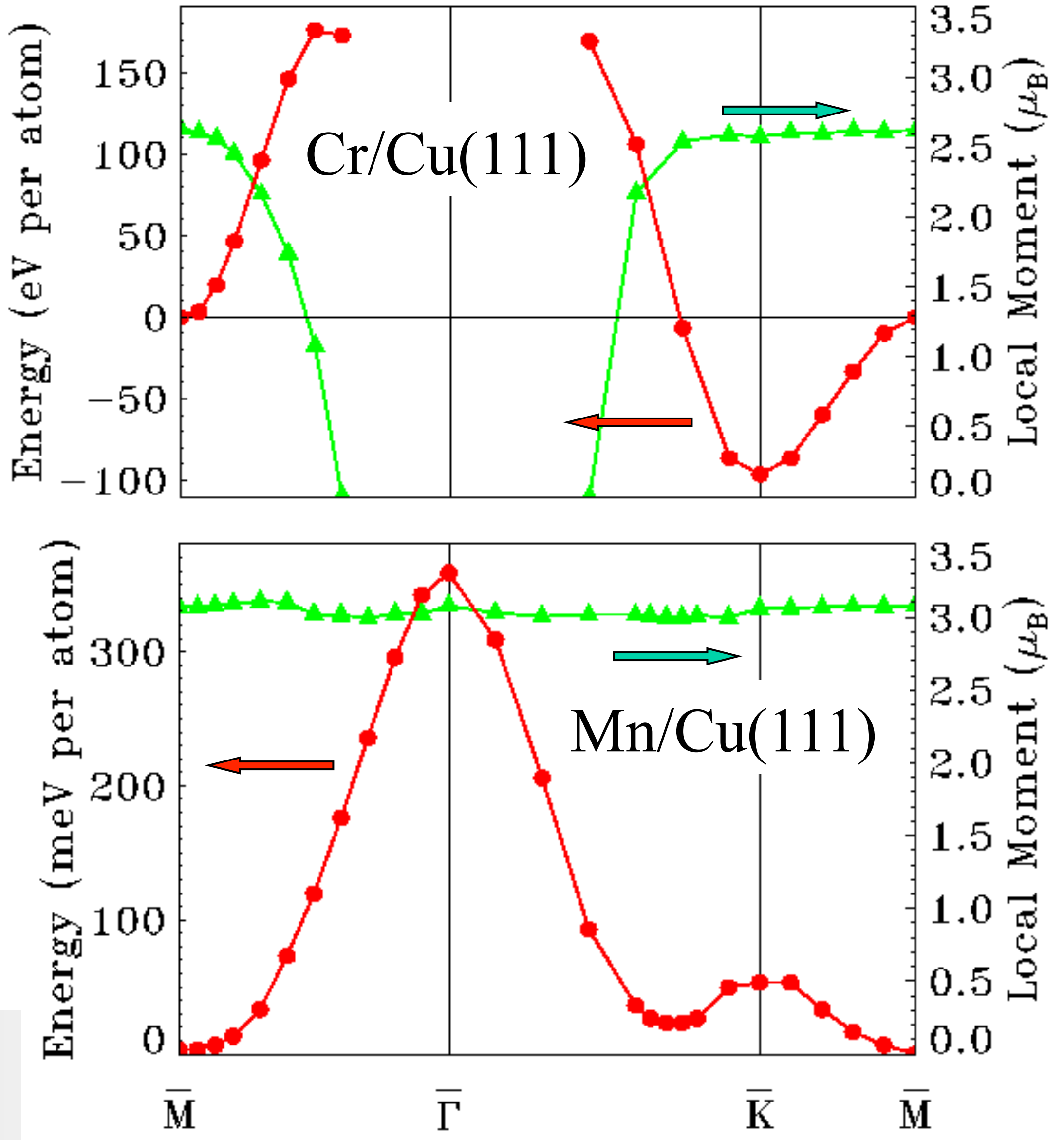
T=0 Phase Diagram
(J_1, J_2)-plane



1 Ferromagnetic
2 Néel State
3 Row-wise AFM
4 Spin-Spiral $(0,k_y)$

SSDW E(q): UML Cr and Mn on Cu (111)





Ph. Kurz, G. Bihlmayer, S. Blügel, J. Appl. Phys. **87**, 6101 (2000)

S. Heinze, Ph. Kurz, D. Wortmann, G. Bihlmayer, and S. Blügel, Appl. Phys. A **75**, 25 (2002).

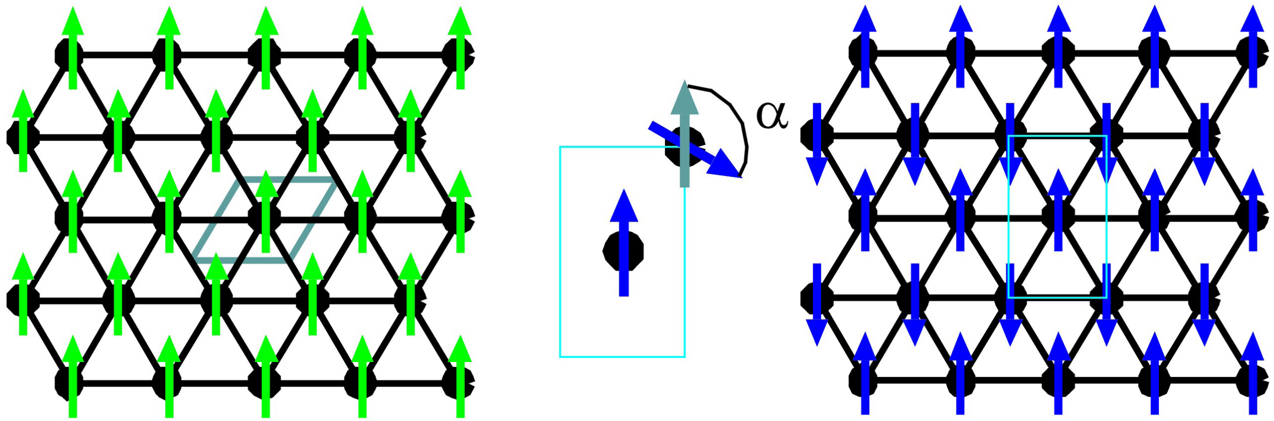
Spin configurations

$$H_{2-spin} = -\sum_{ij} J_{ij} S_i S_j$$

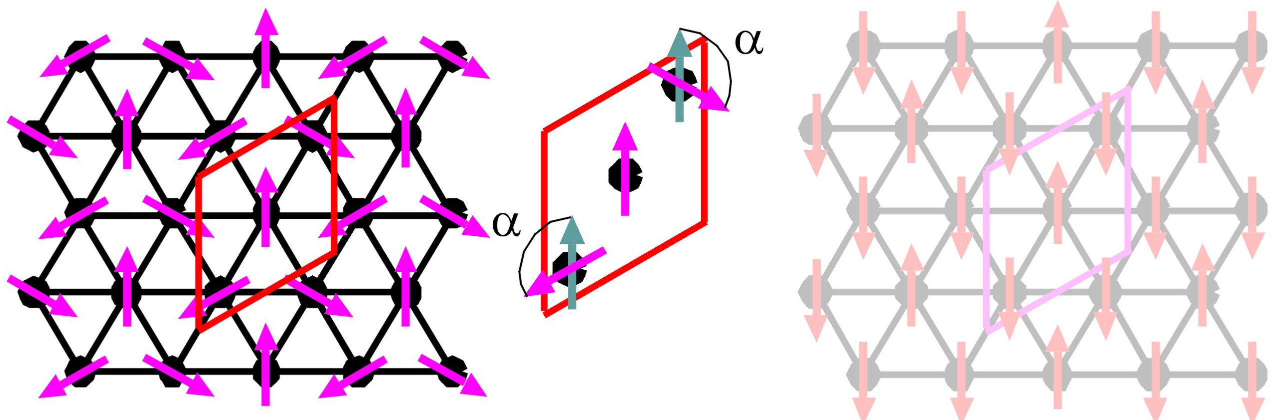
www.fz-juelich.de/iff/e_th1

Itinerant Antiferromagn.

Only n.n. interaction: Beyond n.n. interaction:



J_1>0: FM $E(\alpha) = -2J_1(1 + 2\cos\alpha)$ c(2x2)AFM



J_1<0: Neel State $(\sqrt{3} \times \sqrt{3})\ 180^\circ$

Heisenberg: $E(\alpha) = -J_1(4\cos\alpha + 2\cos 2\alpha)$

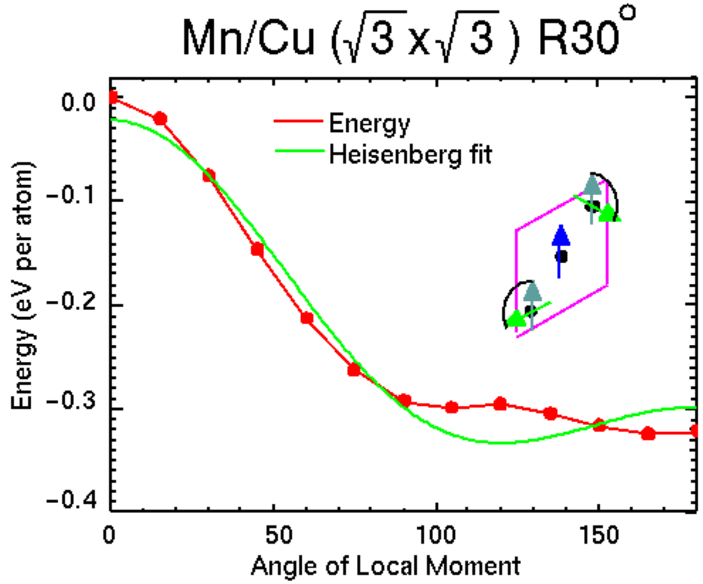
Heisenberg-Fit

www.fz-juelich.de/iff/e_th1

Heisenberg fit:

$$H_{2-spin} = -\sum_{ij} J_{ij} \vec{S}_i \vec{S}_j$$

$$E(\alpha) = -J_1(4\cos\alpha + 2\cos 2\alpha) + 6J_2$$



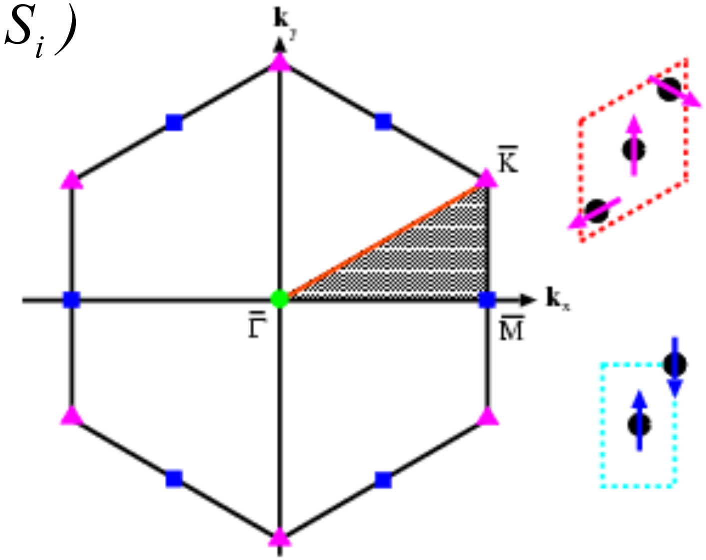
Missing Term $\propto \cos 3\alpha$

Four-Spin Interaction

4-spin interaction:

$$H_{4-spin} = -\sum_{ijkl} K_{ijkl} [(\vec{S}_i \vec{S}_j)(\vec{S}_k \vec{S}_l) + (\vec{S}_j \vec{S}_k)(\vec{S}_l \vec{S}_i) - (\vec{S}_i \vec{S}_k)(\vec{S}_j \vec{S}_l)]$$

$$(\boldsymbol{n.n.}) = -\boldsymbol{K_1}(\boldsymbol{4+8\cos 3\alpha})$$

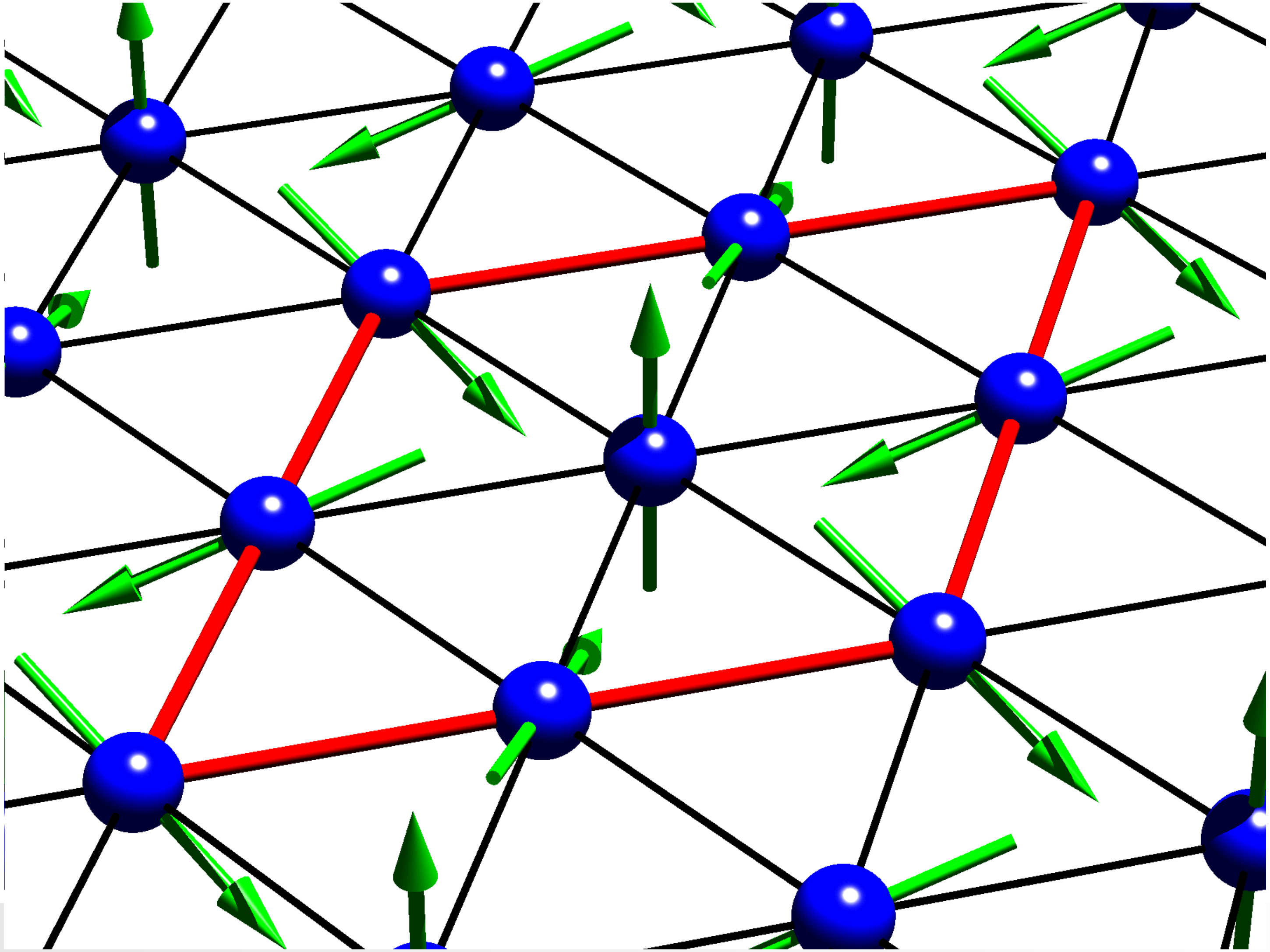


3Q vs 1Q State: $\boxed{\Delta E_{3Q-1Q} \approx K_1}$

$$\vec{m}(\vec{r}+\vec{R}_i) = m(\vec{r}) \times \frac{1}{\sqrt{3}} \sum_{k=1}^{3} exp(i\vec{Q}^{(k)}_{\bar{M}} \vec{R}_i)\, \hat{e}^{(k)}$$

3Q-Structure: 3D Spin Structure on a 2D Lattice

www.fz-juelich.de/iff/e_th1



Ph. Kurz, G. Bihlmayer, K.Hirai and S. Blügel, PRL **86**, 1106 (2001)

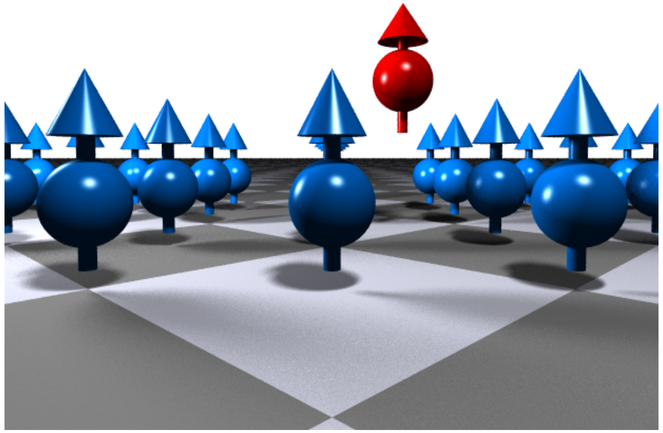
5. Finiteness: Nanowires

Non-collinear magnetism

Mn on Ni(001)

collinear result:

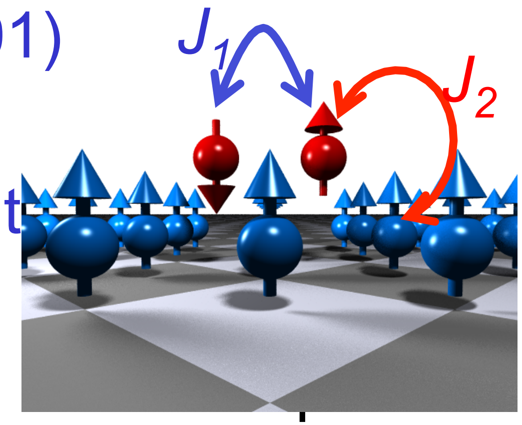
Saddle point



Non-collinear magnetism:

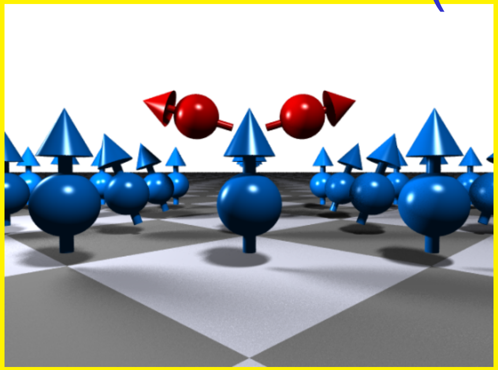
Mn on Ni(001)

collinear result



$H(ferri) = J_1$

Total E minimum (–13meV)

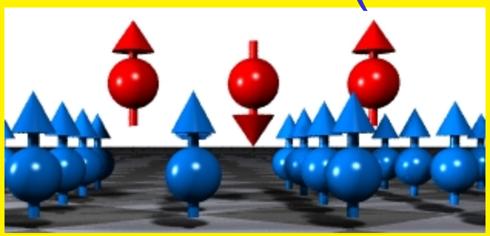


θ=72.5°

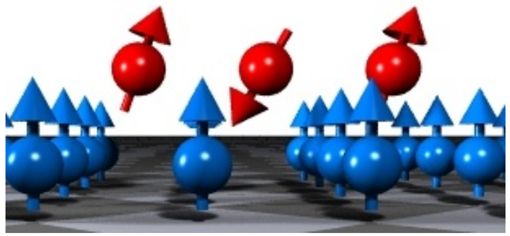
$H(ncol) = -J_1 cos(2\theta) - J_2\ cos(\theta)$

Total E minimum (–9meV)

col



$H(ferri) = 2J_1 - J_2$

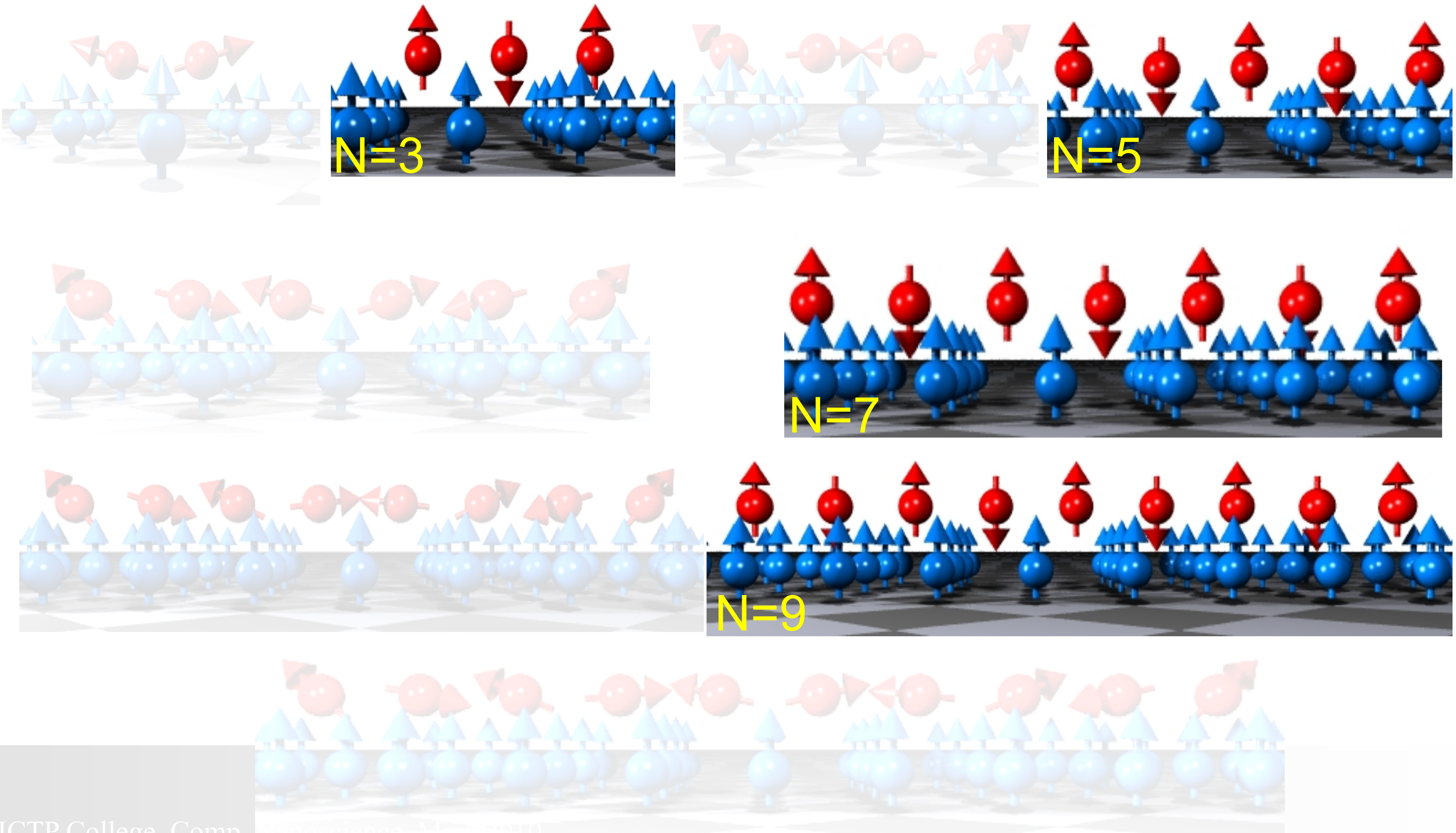


ncol

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

Odd numbered wires: antiparallel

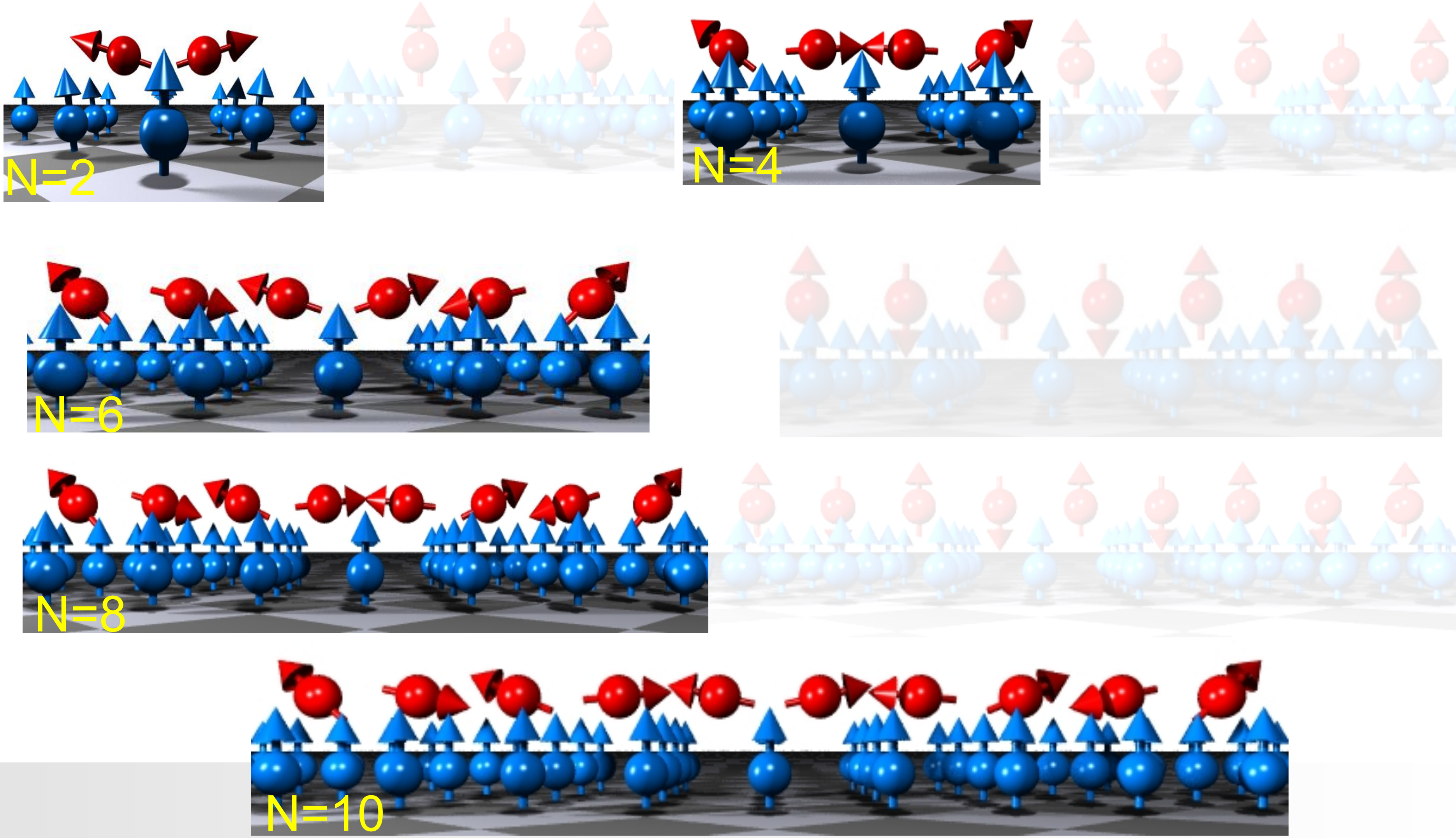
www.fz-juelich.de/iff/e_th1



Even-numbered wires: Frustration

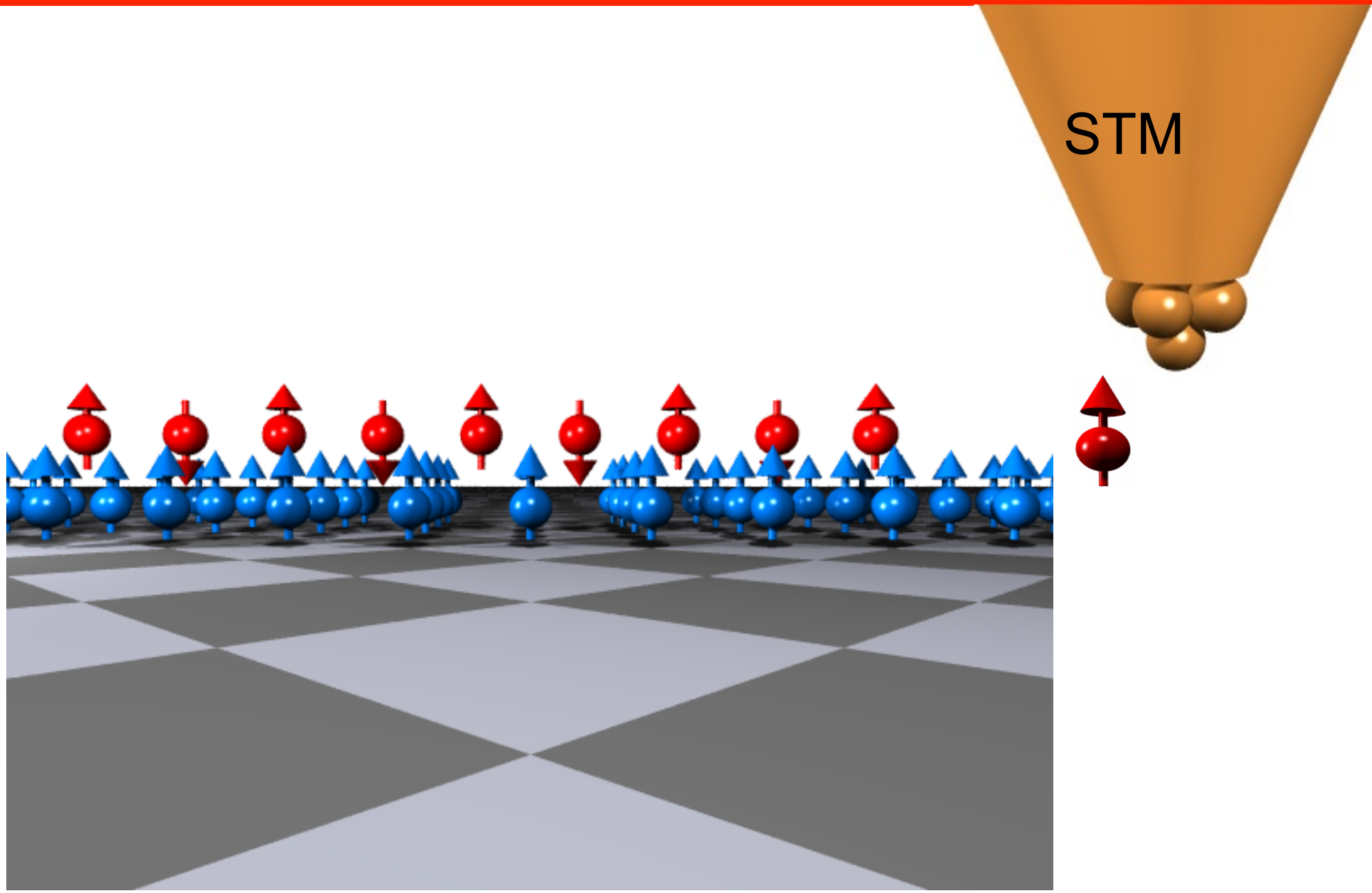
www.fz-juelich.de/iff/e_th1

even = non-collinear



Domino Effect

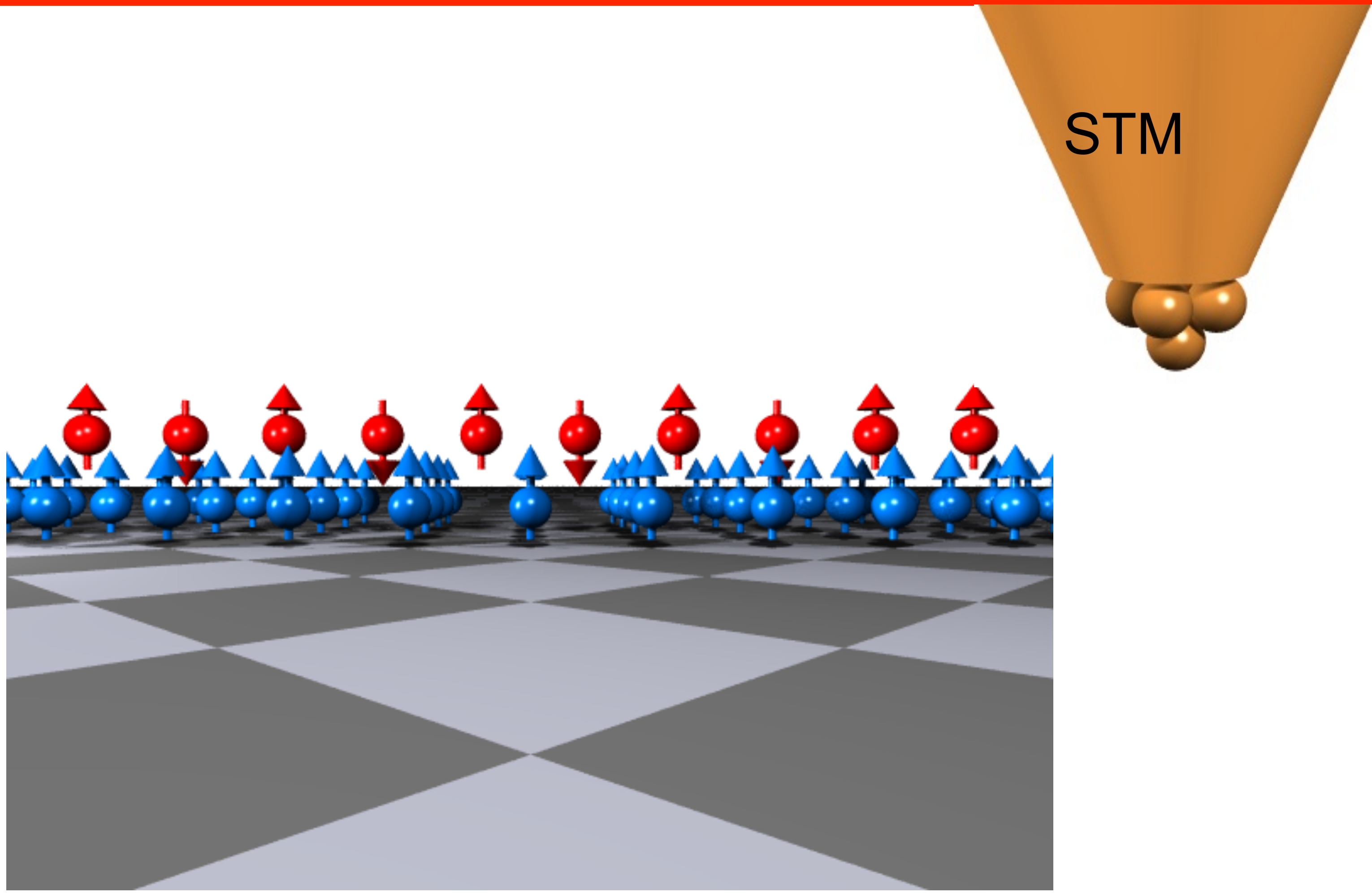
www.fz-juelich.de/iff/e_th1



Initial state

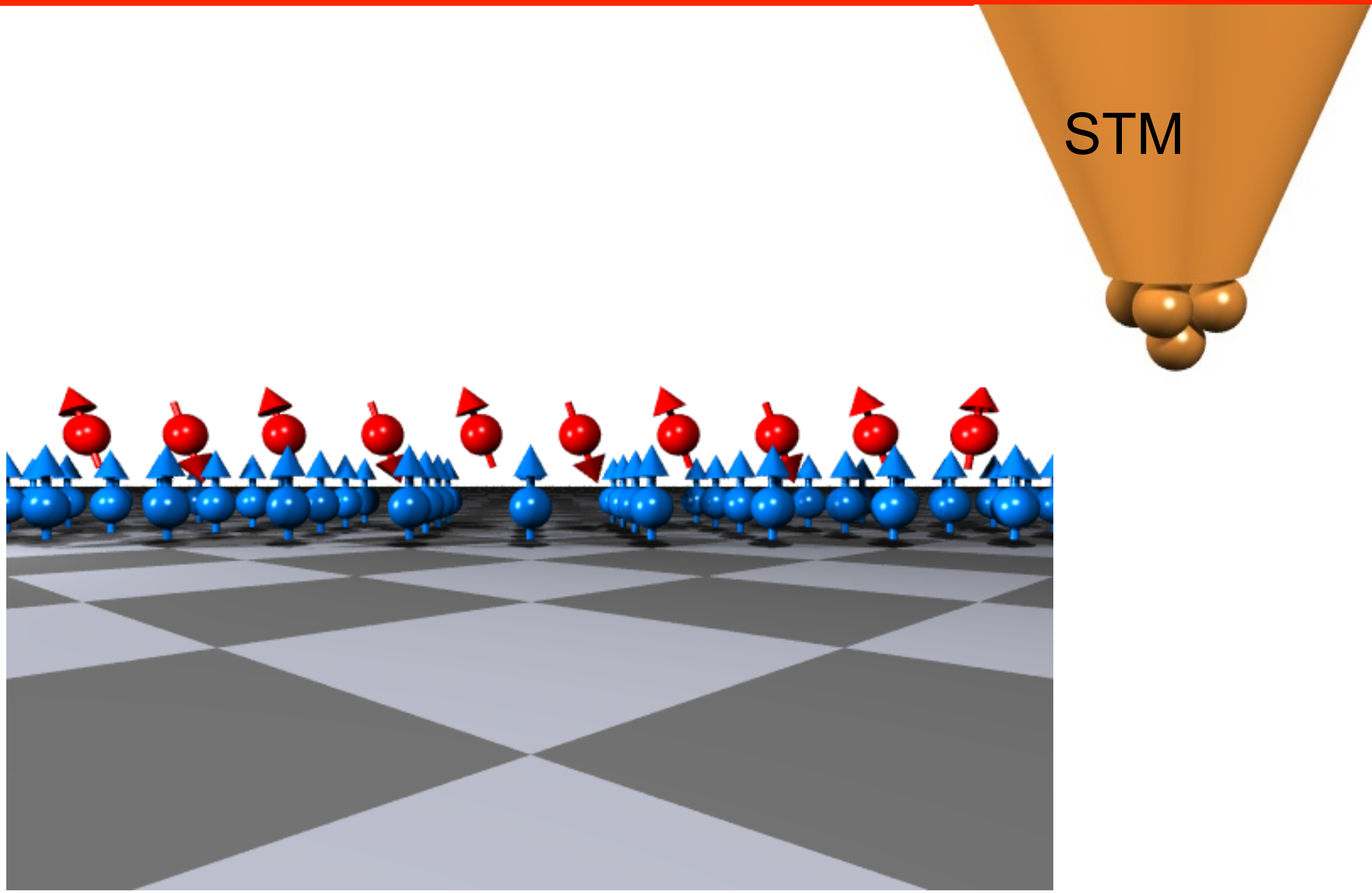
Domino Effect

www.fz-juelich.de/iff/e_th1

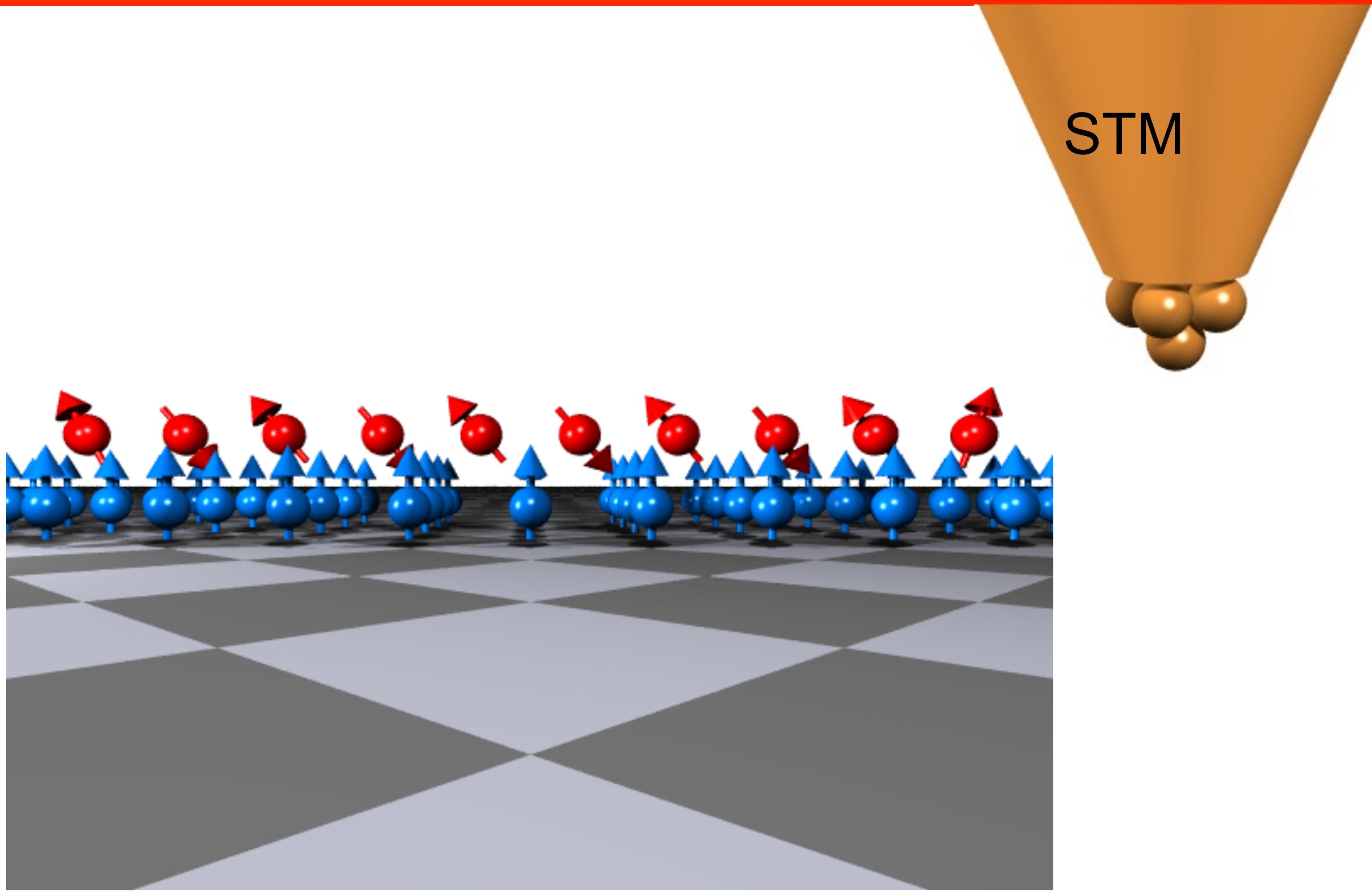


Domino Effect

www.fz-juelich.de/iff/e_th1

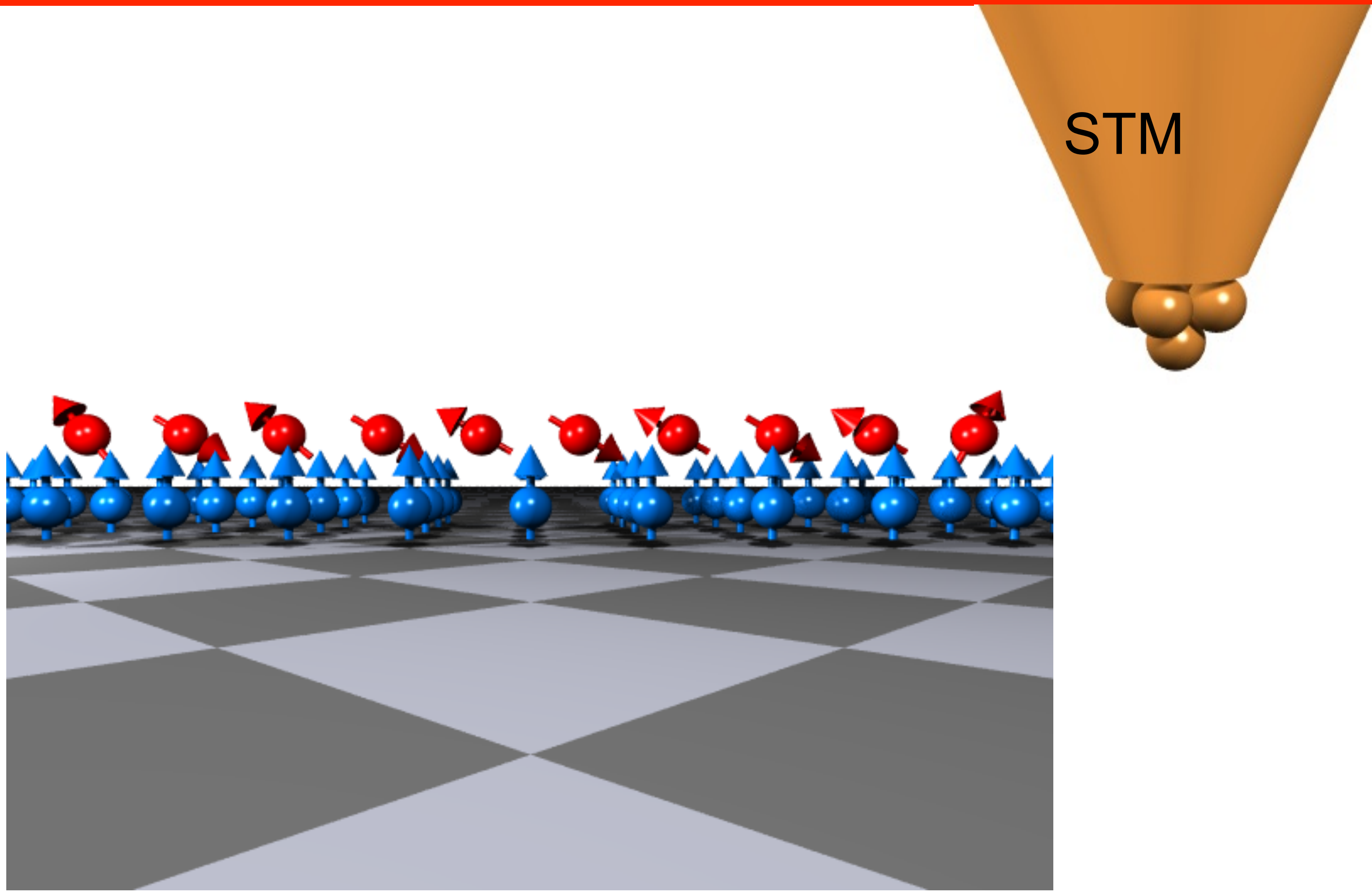


Domino Effect



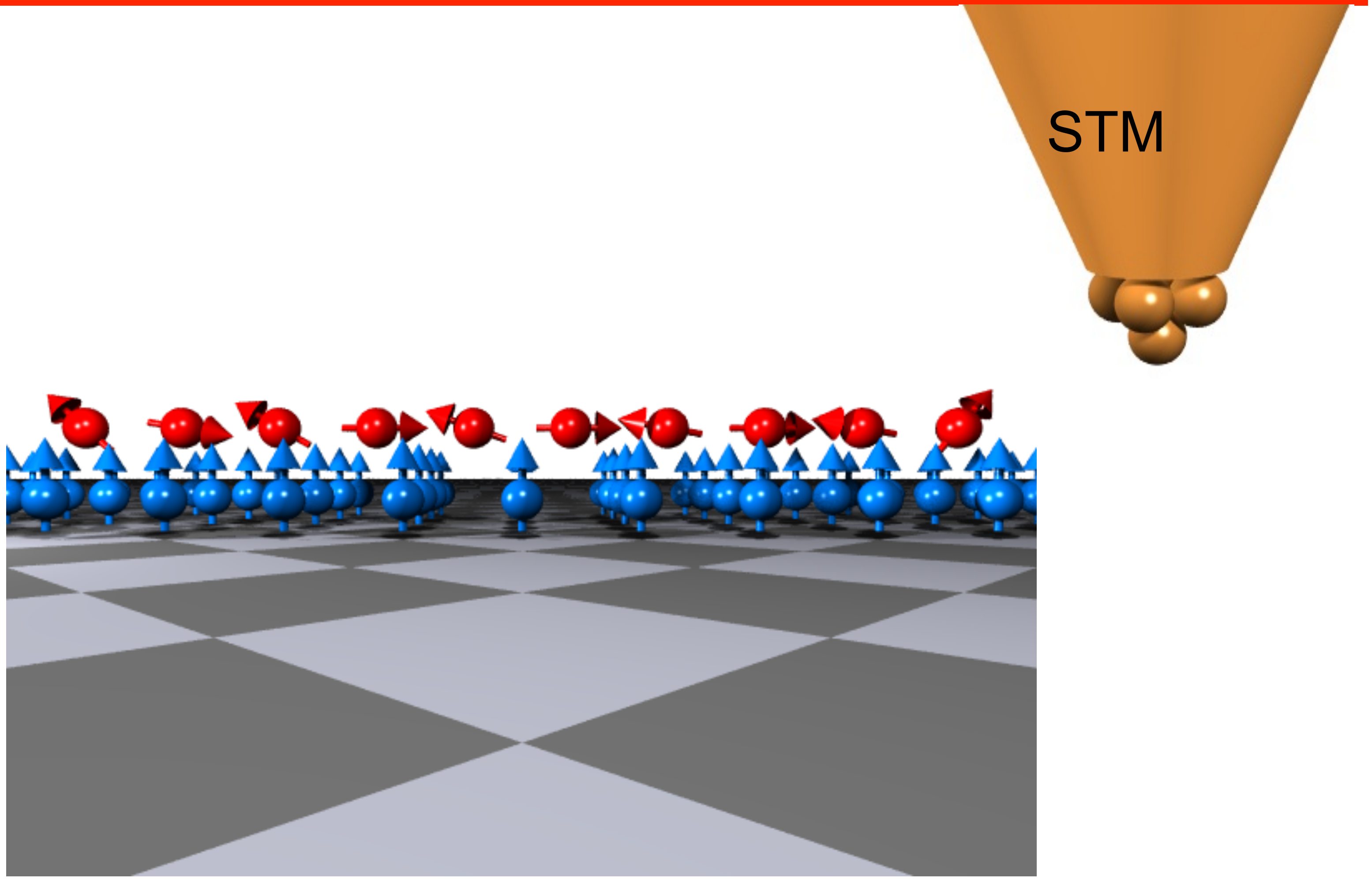
Domino Effect

www.fz-juelich.de/iff/e_th1



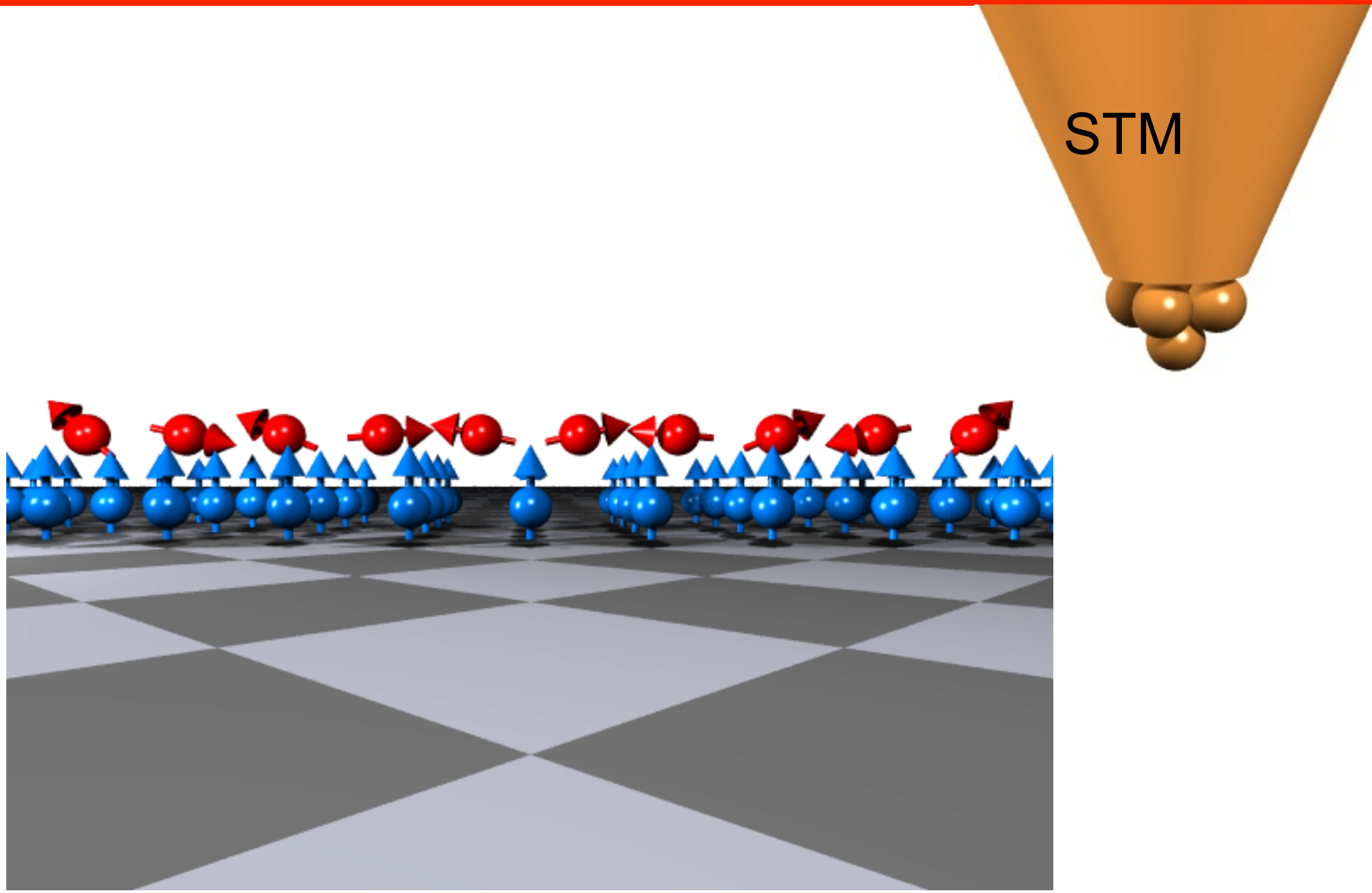
Domino Effect

www.fz-juelich.de/iff/e_th1



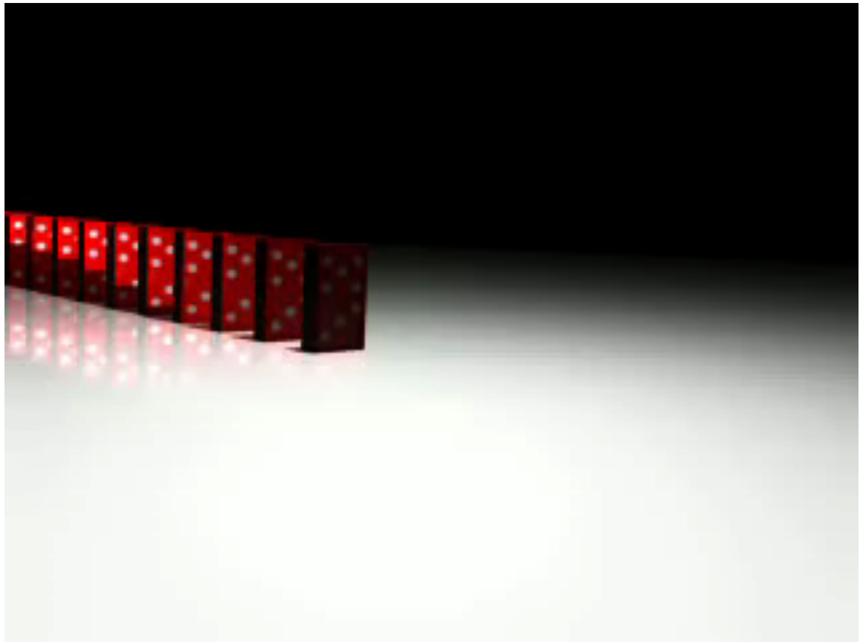
Domino Effect

www.fz-juelich.de/iff/e_th1



Final state

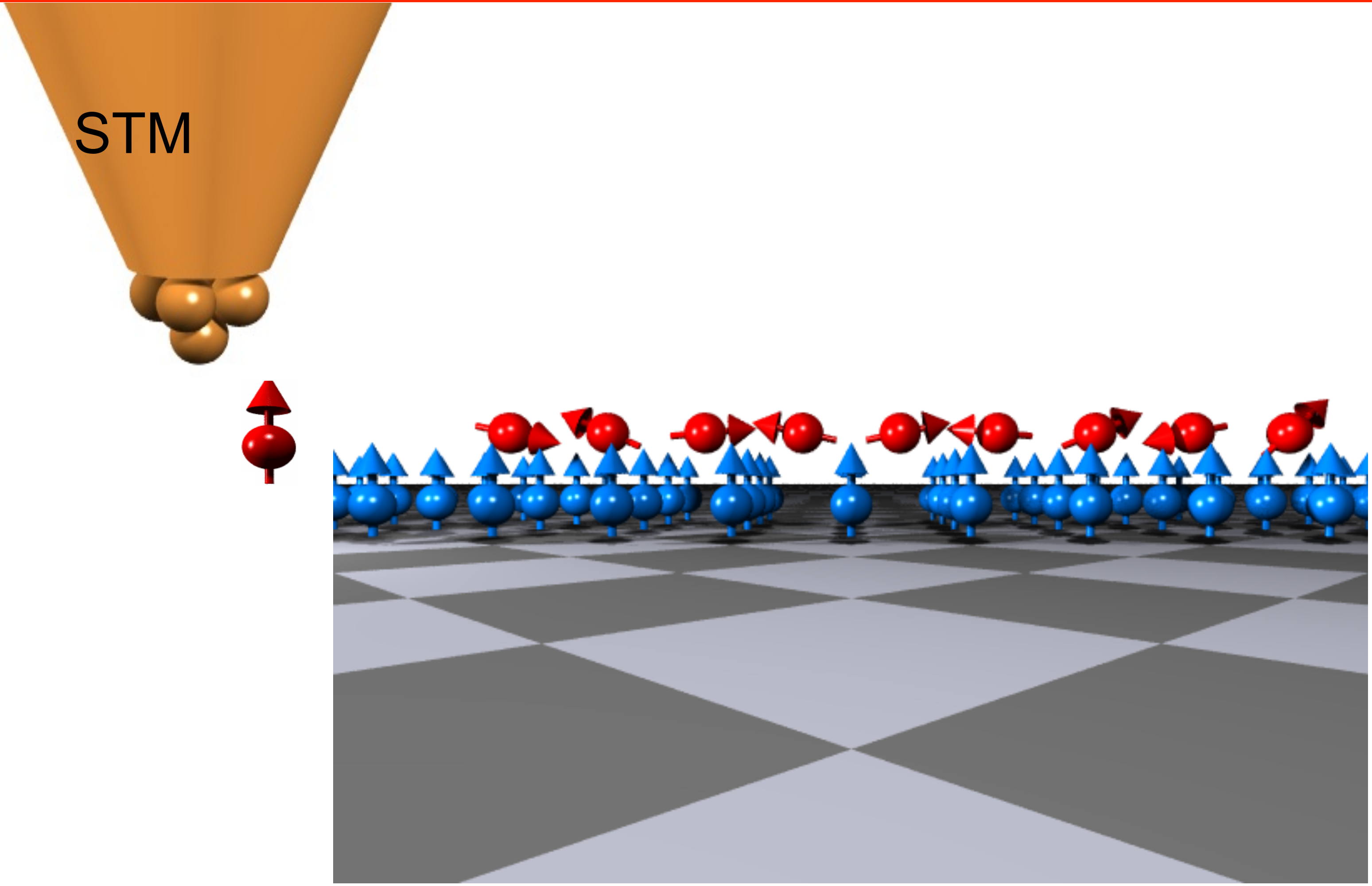
Domino Effect



From youtube.com: look at Domino effects!

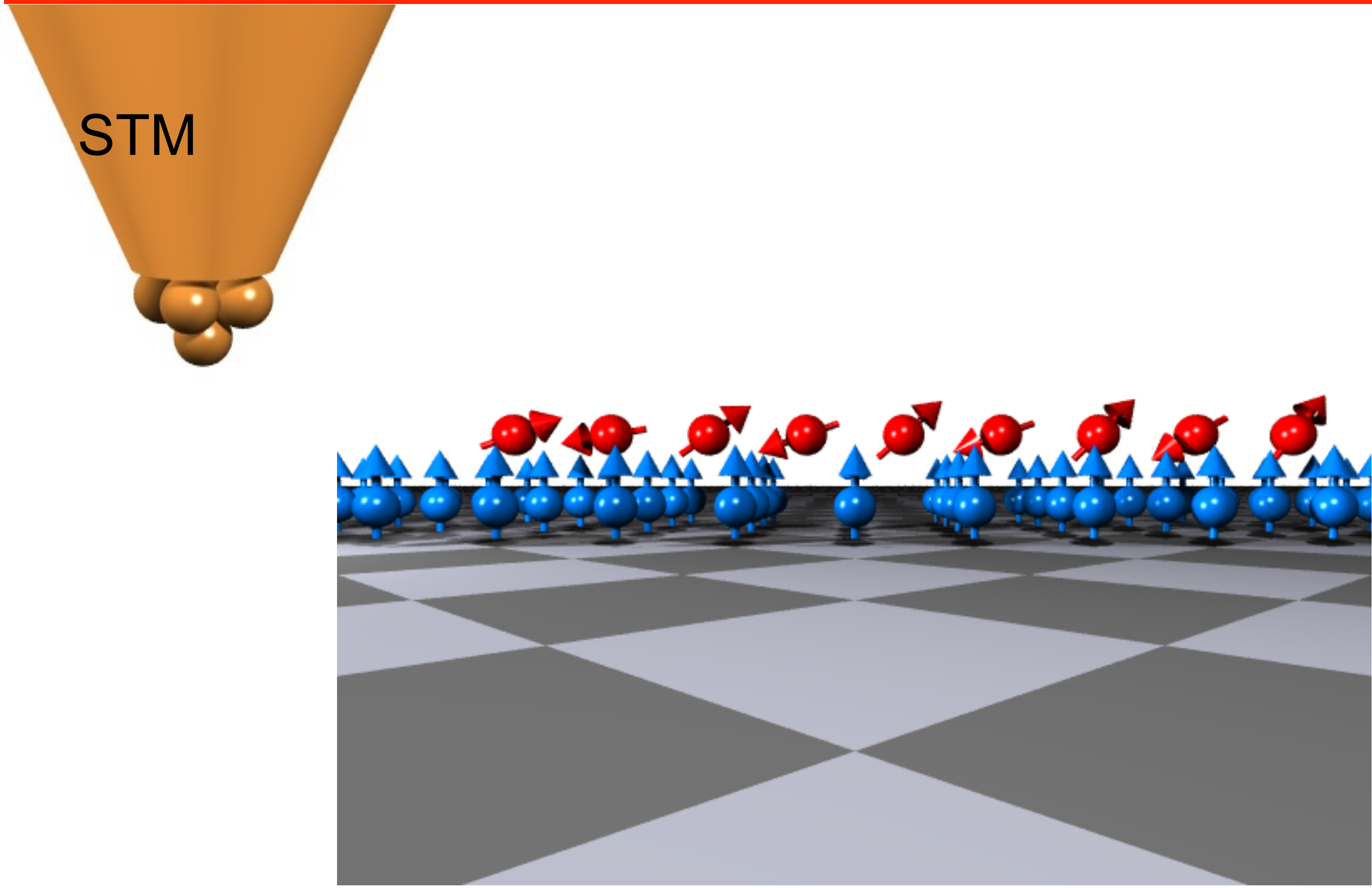
Domino Effect

www.fz-juelich.de/iff/e_th1

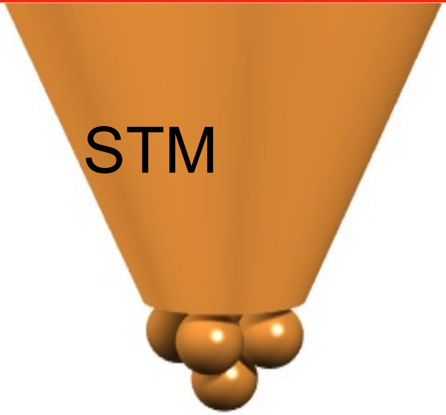


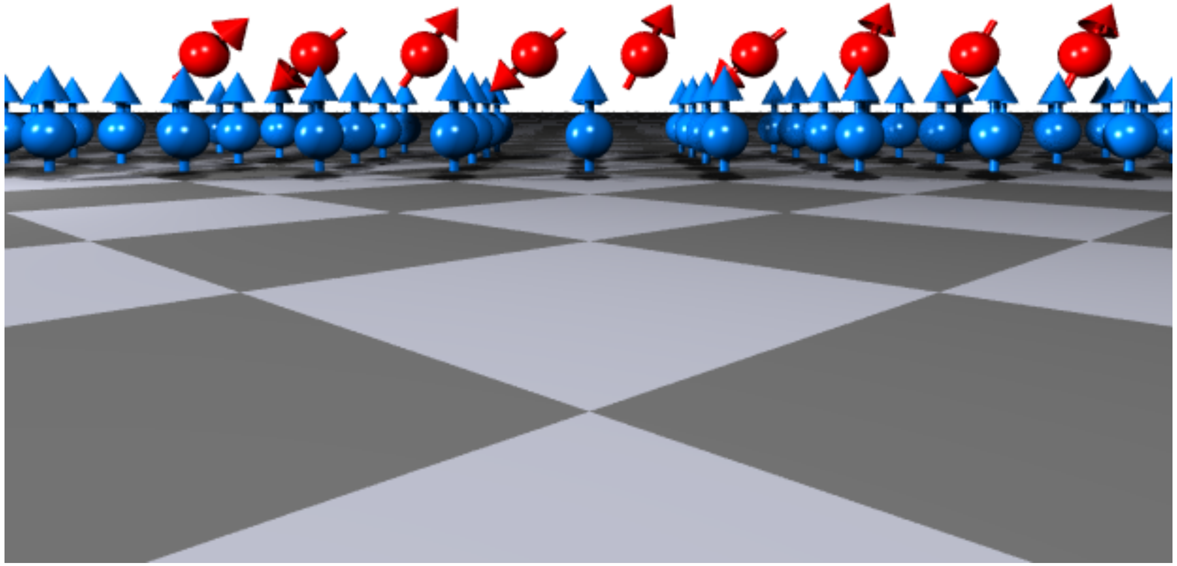
Domino Effect

www.fz-juelich.de/iff/e_th1



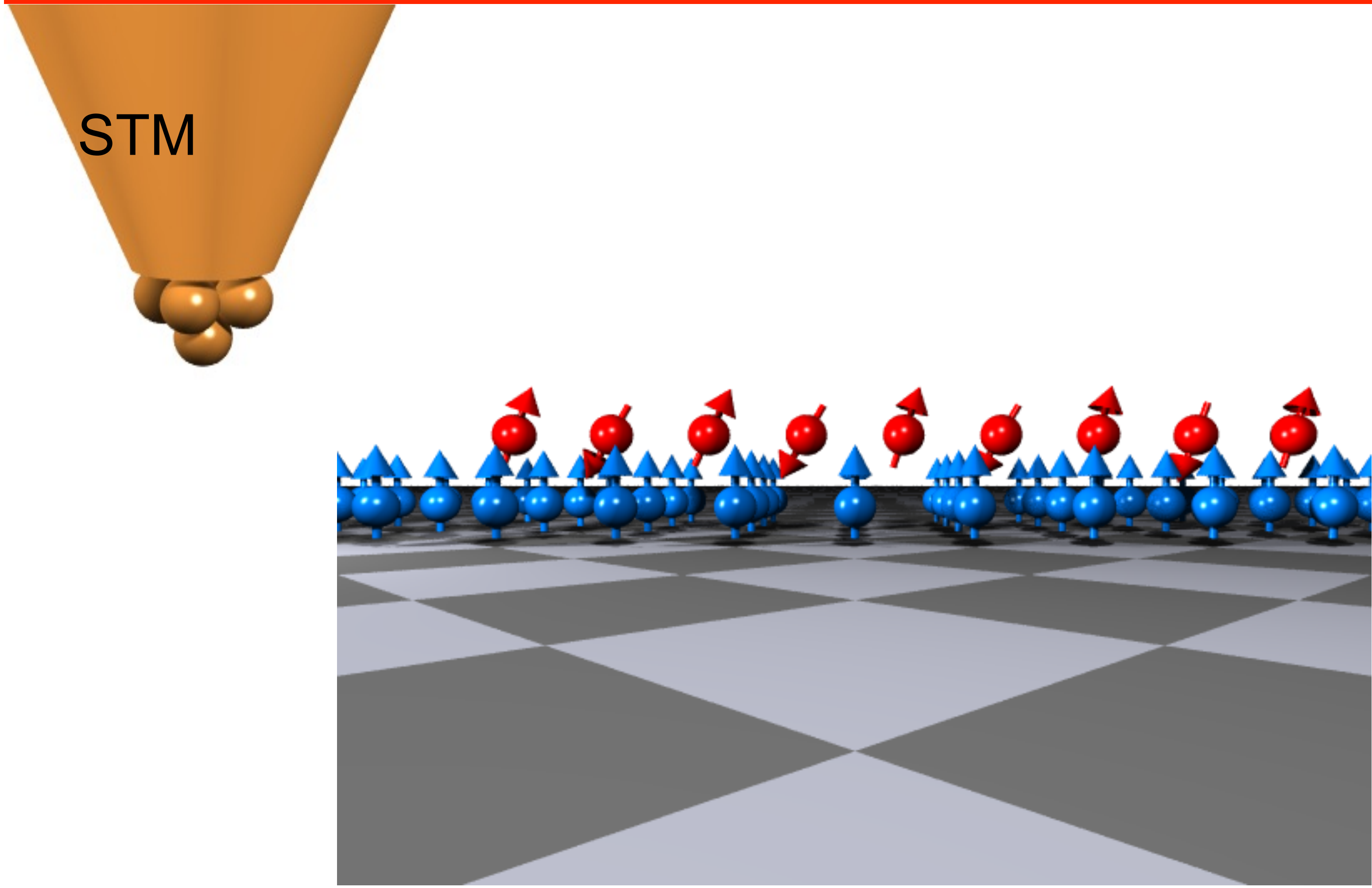
Domino Effect



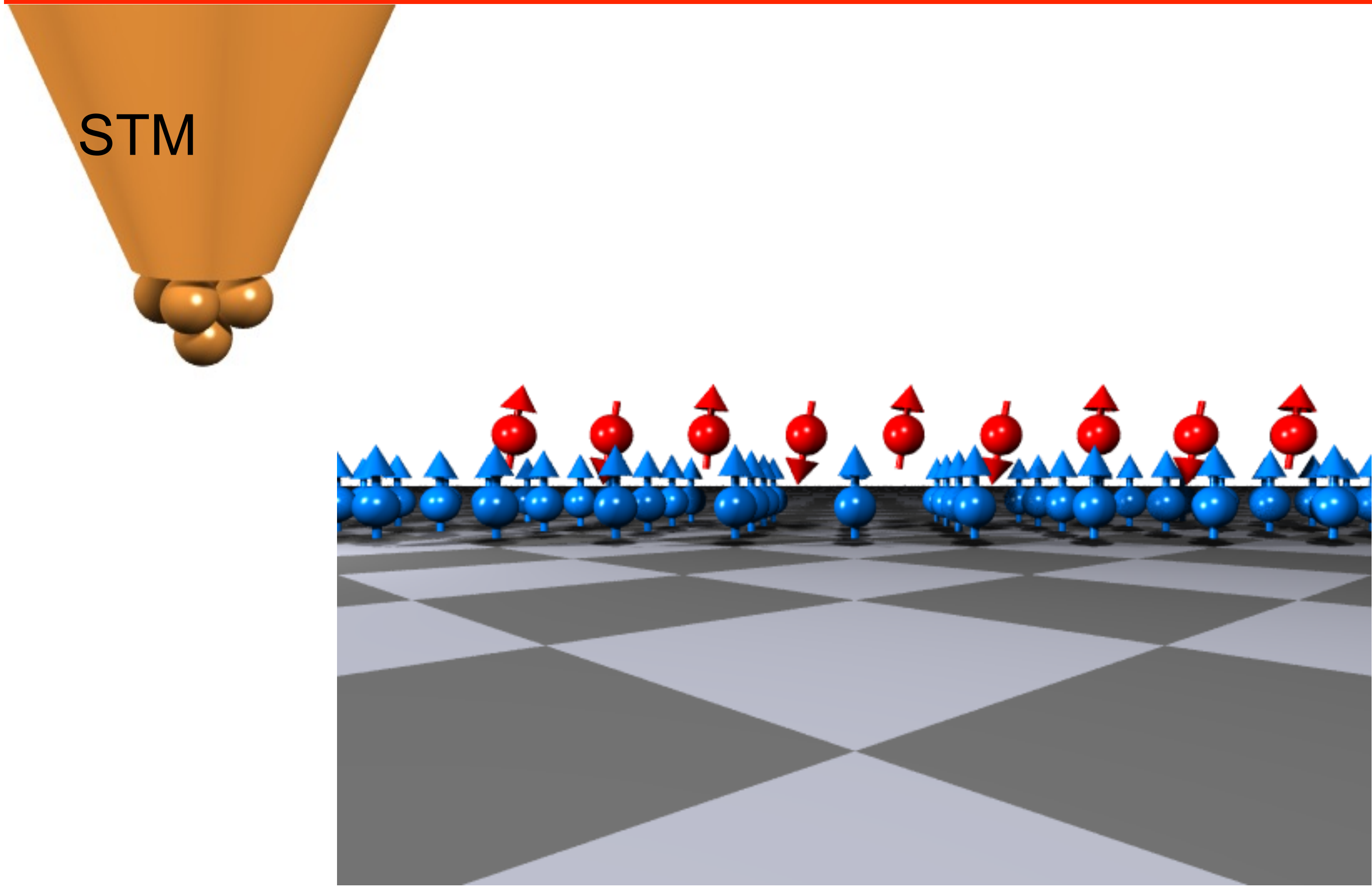


Domino Effect

www.fz-juelich.de/iff/e_th1

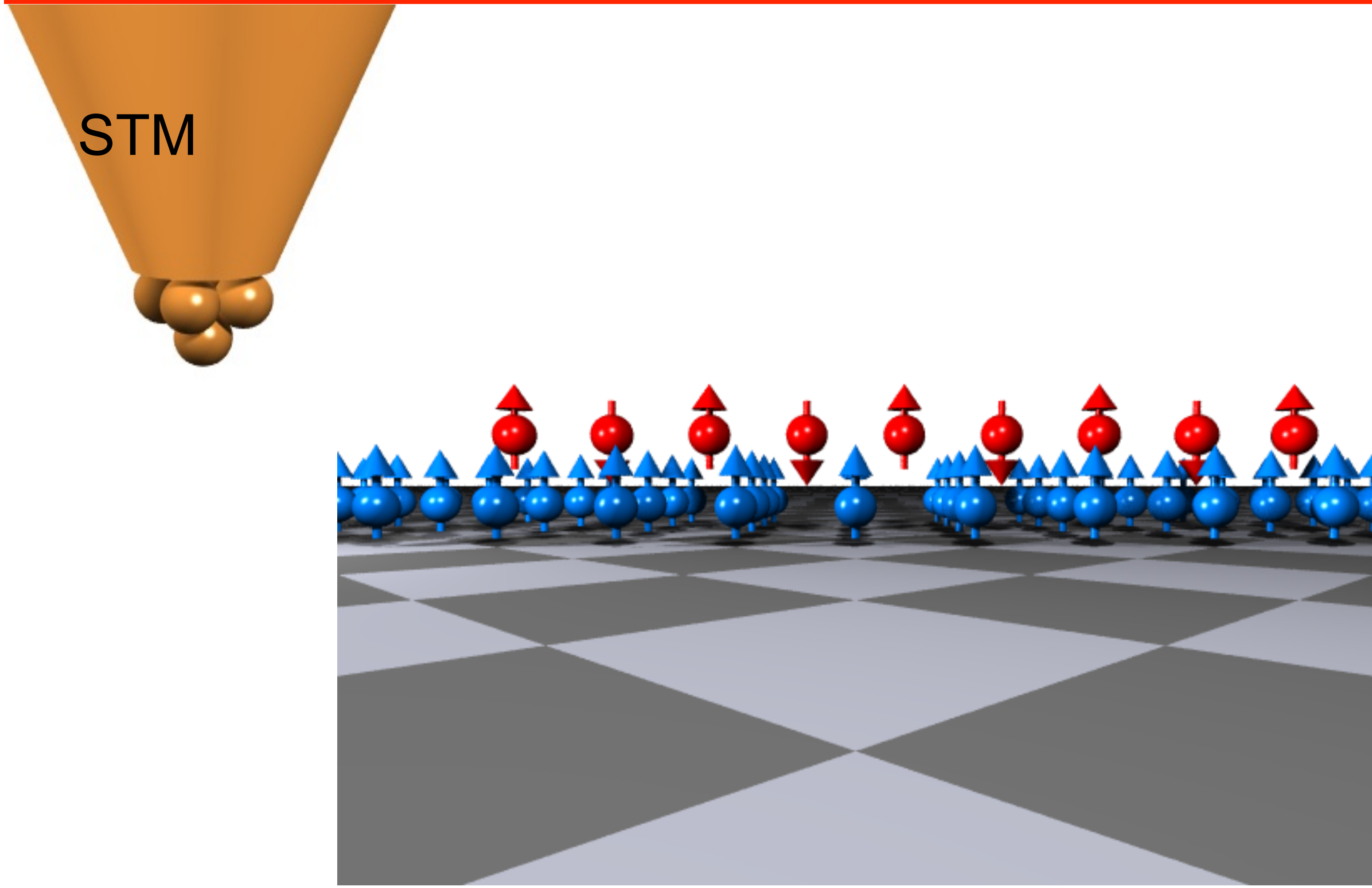


Domino Effect



Domino Effect

www.fz-juelich.de/iff/e_th1

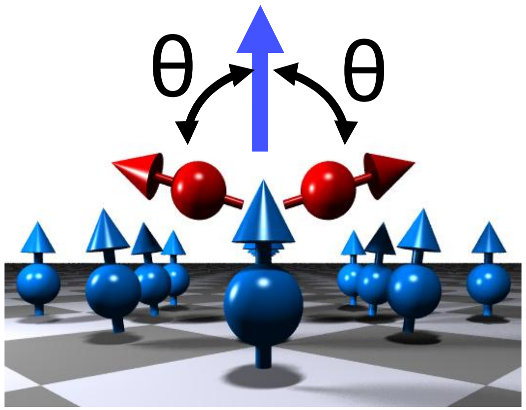


Final state 2

Multi-scale modelling: Map DFT to Classical Heisenberg

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

$$H = -J_1\sum_{i=2}^{N}\cos(\theta_i - \theta_{i-1}) - J_2\sum_{i=1}^{N}\cos(\theta_i)$$



Magnetic exchange interactions J extracted from ab-initio calculations:

1- Using total energy differences

2- Using infinitesimal rotations

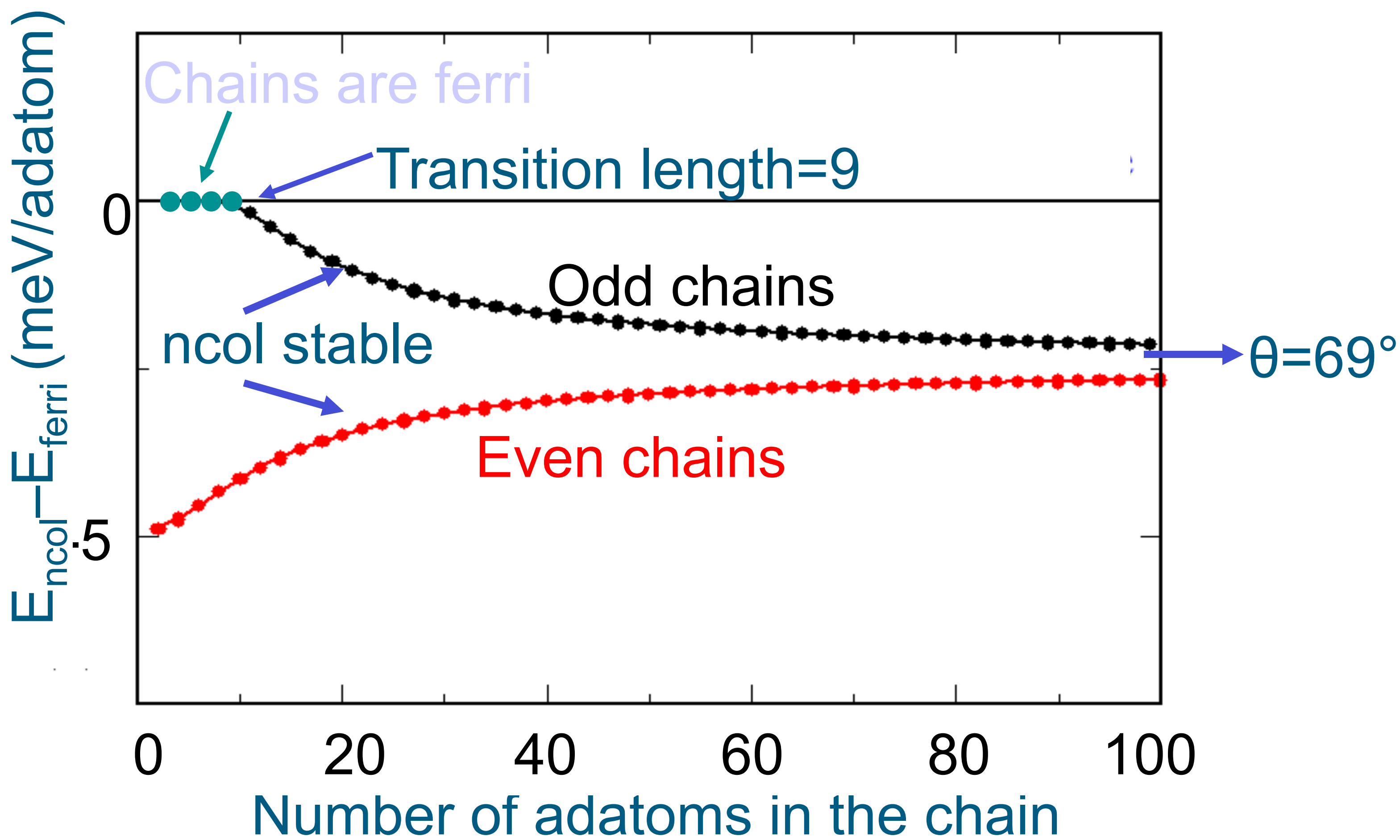
(Lichtenstein, Katsnelson, Antropov, Gubanov, JMMM, 67, 65 1987)

J_1 = J(Mn-Mn) = –138 meV

J_2 = J(Mn-Ni) = 4x13 meV

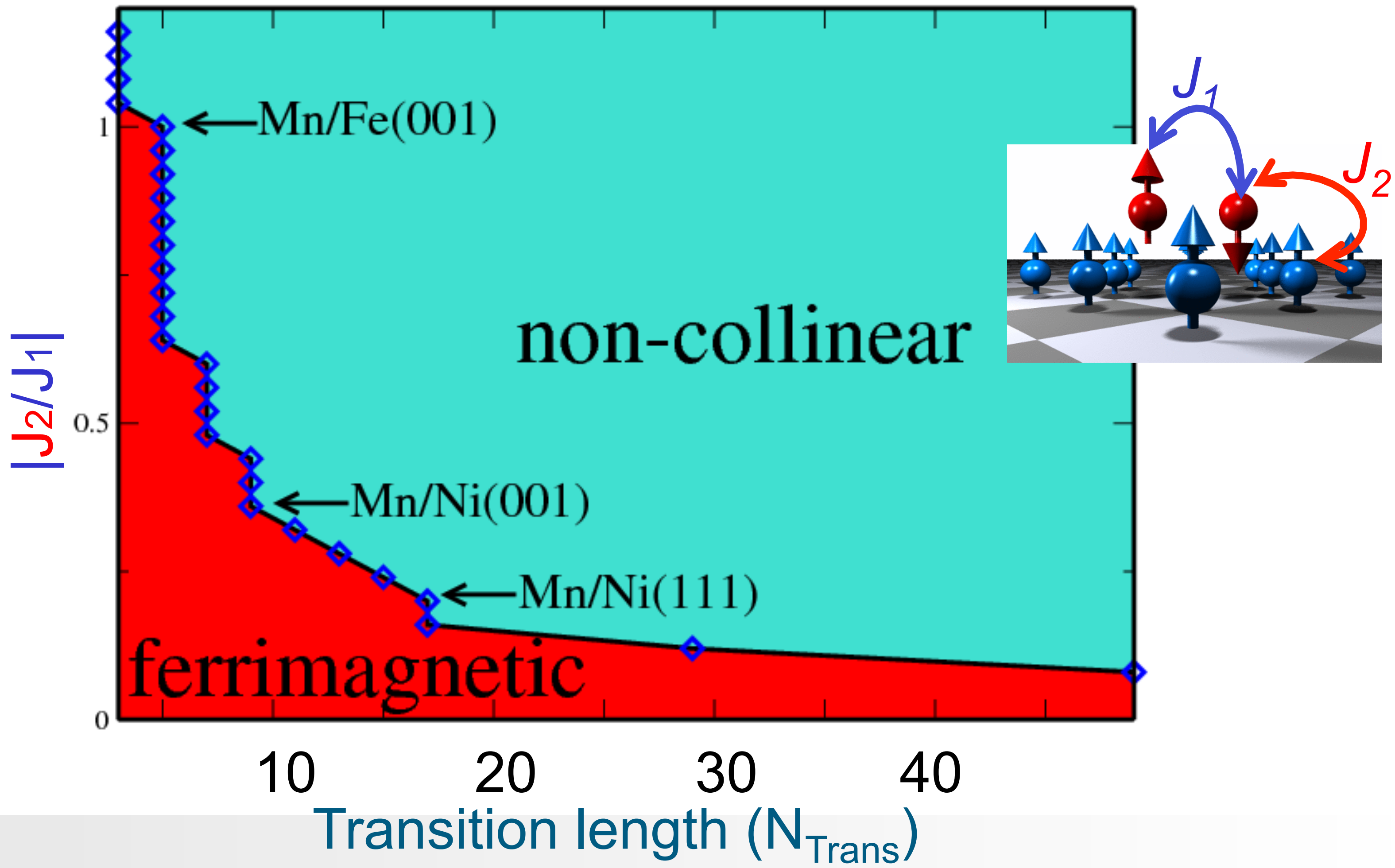
See also Mills, PRL, 20, 18 (1968), Politi & Pini, PRB 79, 12405 (2009)

Multi-scale modelling: Map DFT to Classical Heisenberg



Multi-scale modelling: Odd chains

If length > N_{Trans} : Ncol ground state



Samir Lounis et al, Phys. Rev. Lett. 101, 107204 (2008)

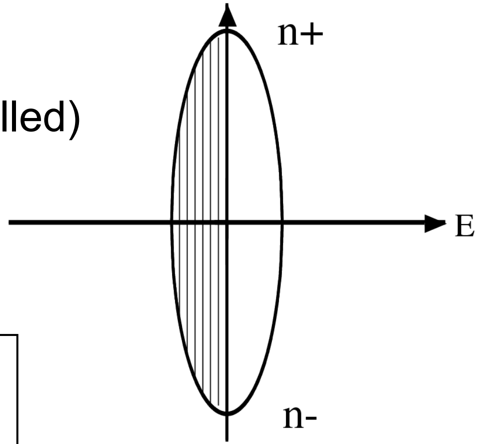
6. Magneto-volume effect

Relation: Magnetism — Relaxation

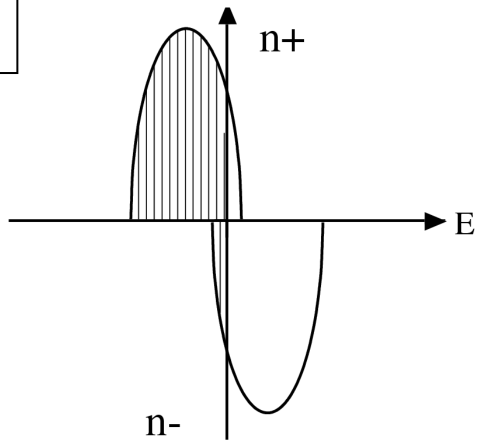
www.fz-juelich.de/iff/e_th1

Example Mn/Ag(100): Half-filled d-band

non-magnetic
(all bonding states filled)

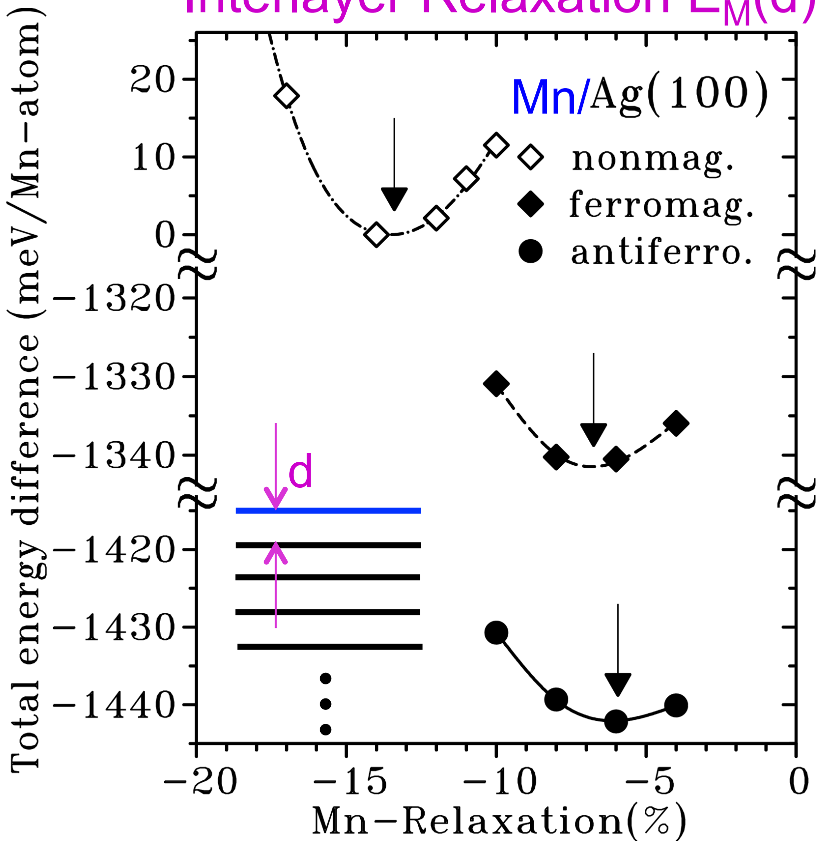


DOS



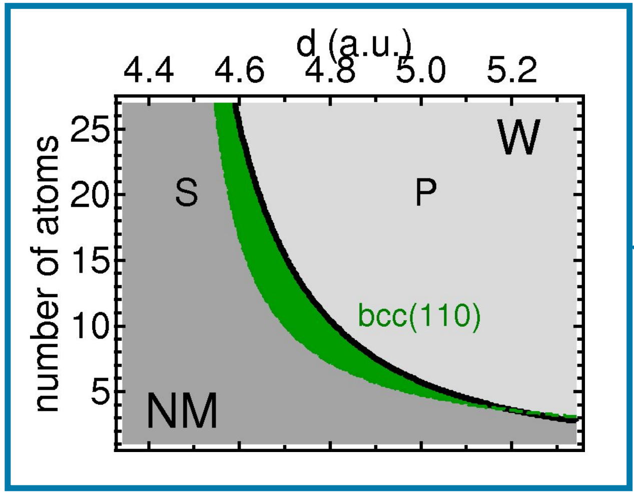
Magnetic
(large exch. splitt'g, bond+antibond'g states Filled)

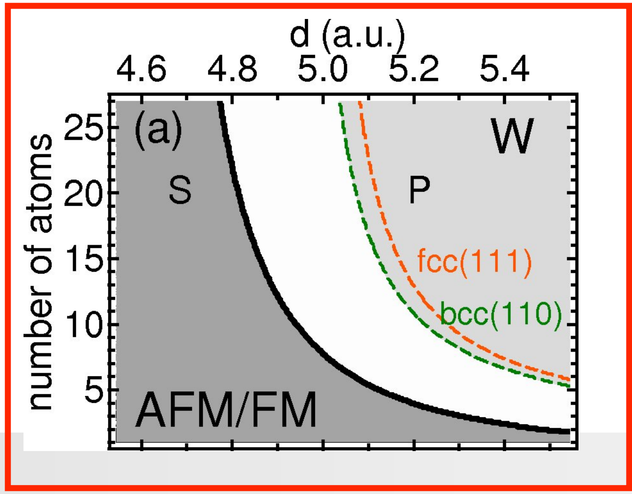
Interlayer Relaxation $E_M(d)$

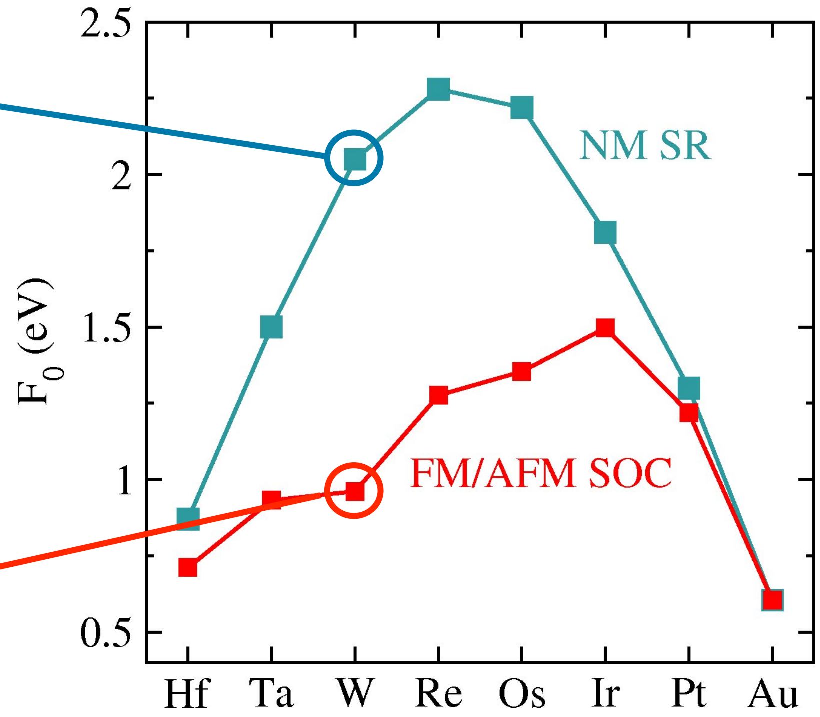


Magnetically hindered chain formation

www.fz-juelich.de/iff/e_th1







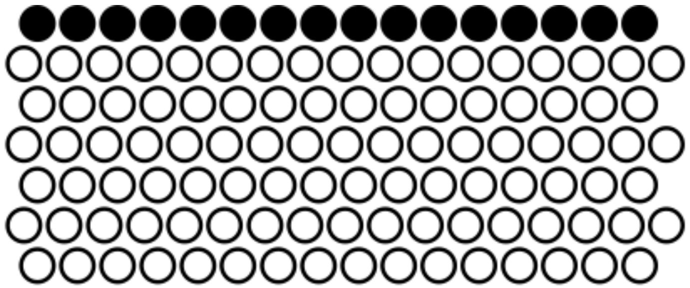
A. Thiess *et al.*, Nano Letters **8** , 2144 (2008)
A. Thiess *et al.*, Phys. Rev. Lett. **103**, 217201 (2009)

7. Magneto-Alloying effect

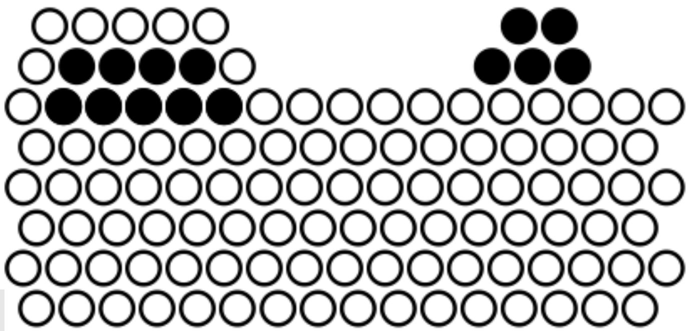
S. Blügel, Appl. Phys. A **63**, 595 (1996).

Stability of magnetic film at surface

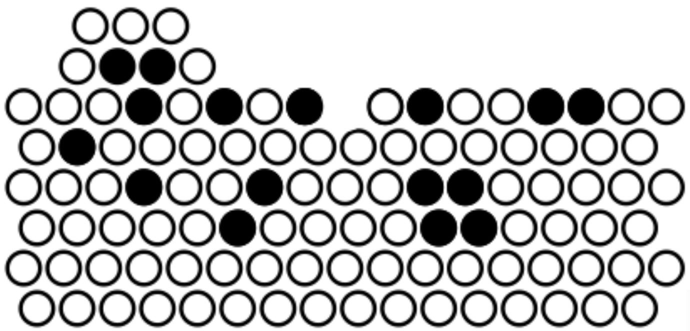
$$\Delta E_{\mathrm{I}\to\mathrm{F}} = -\frac{1}{2} I (M_{\mathrm{F}}^2 - M_{\mathrm{I}}^2)$$



perfect monolayer film



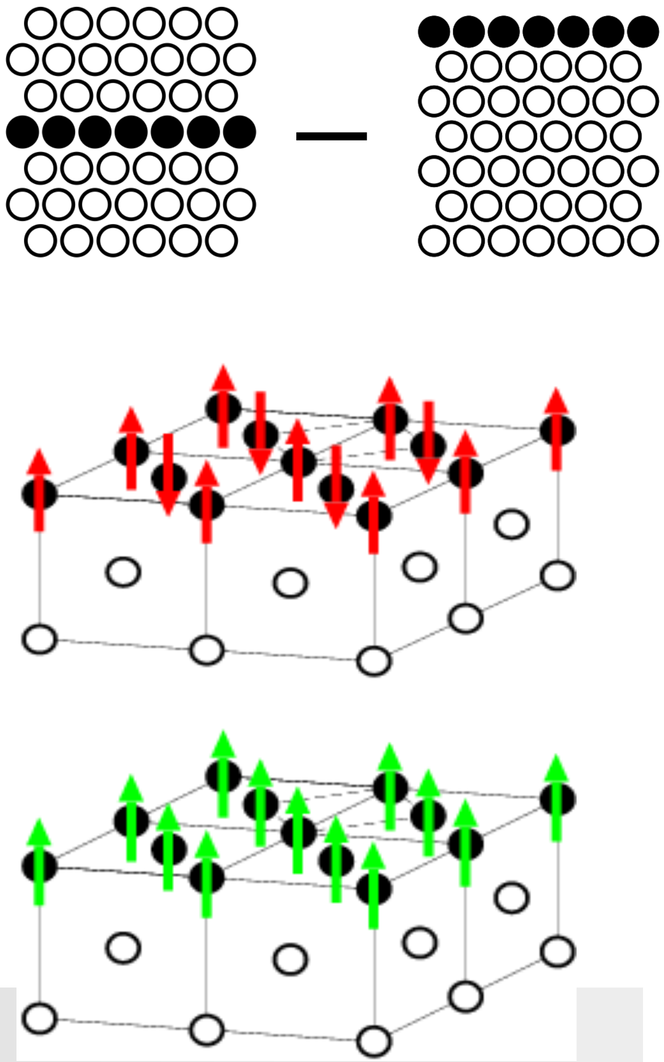
cluster formation

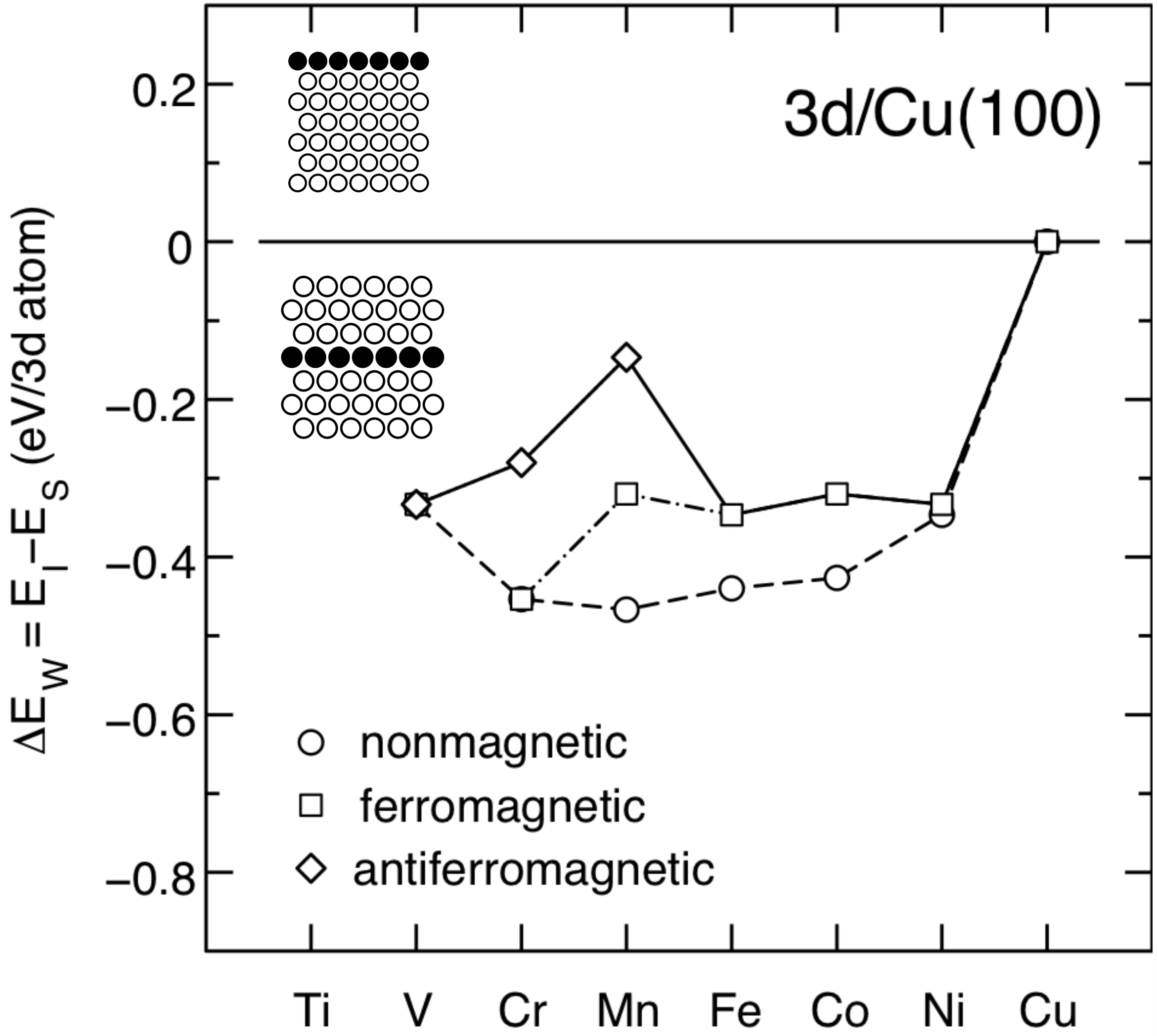


interdiffusion

Stability of film against interdiffusion

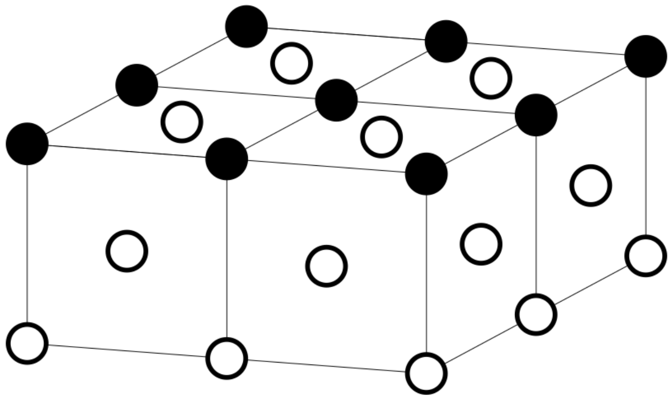
www.fz-juelich.de/iff/e_th1

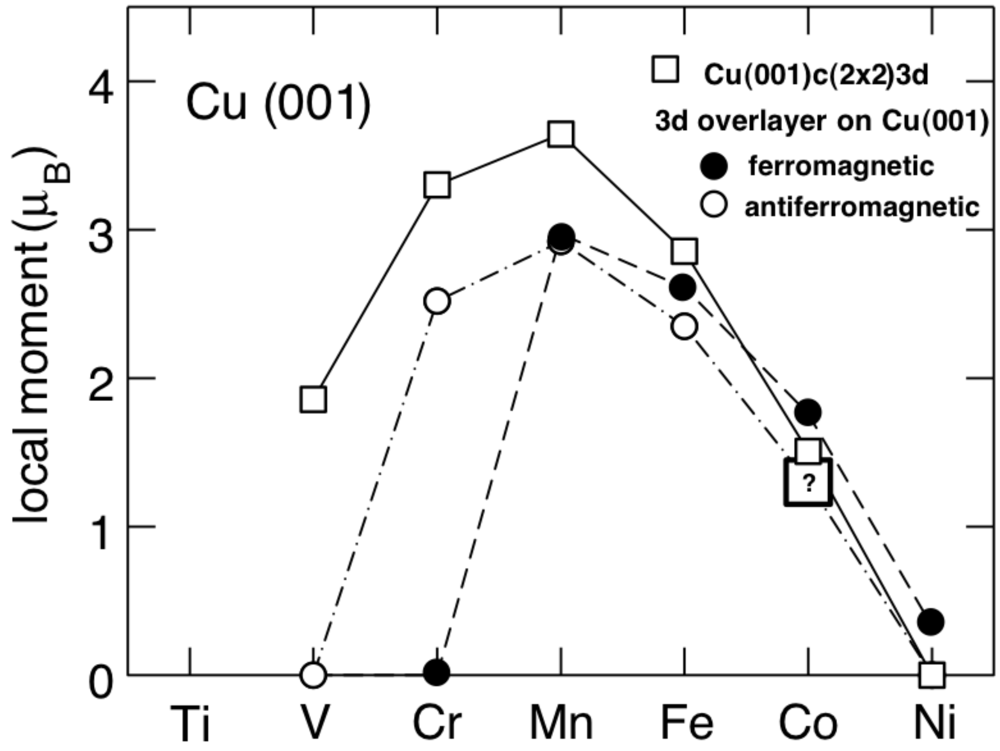


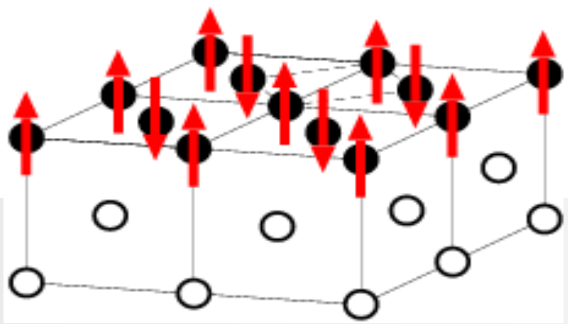


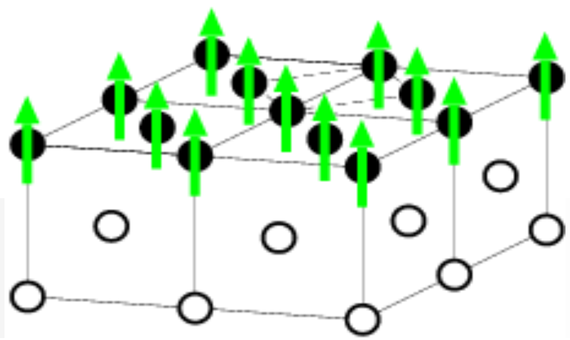
Magnetic moments of c(2x2) alloy

www.fz-juelich.de/iff/e_th1

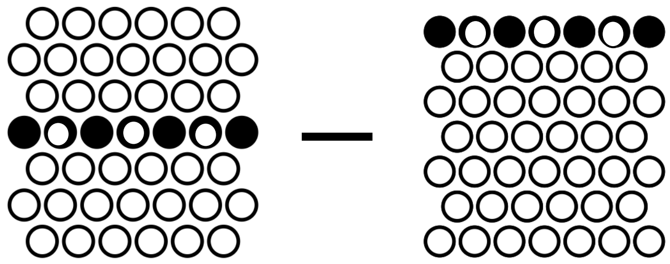


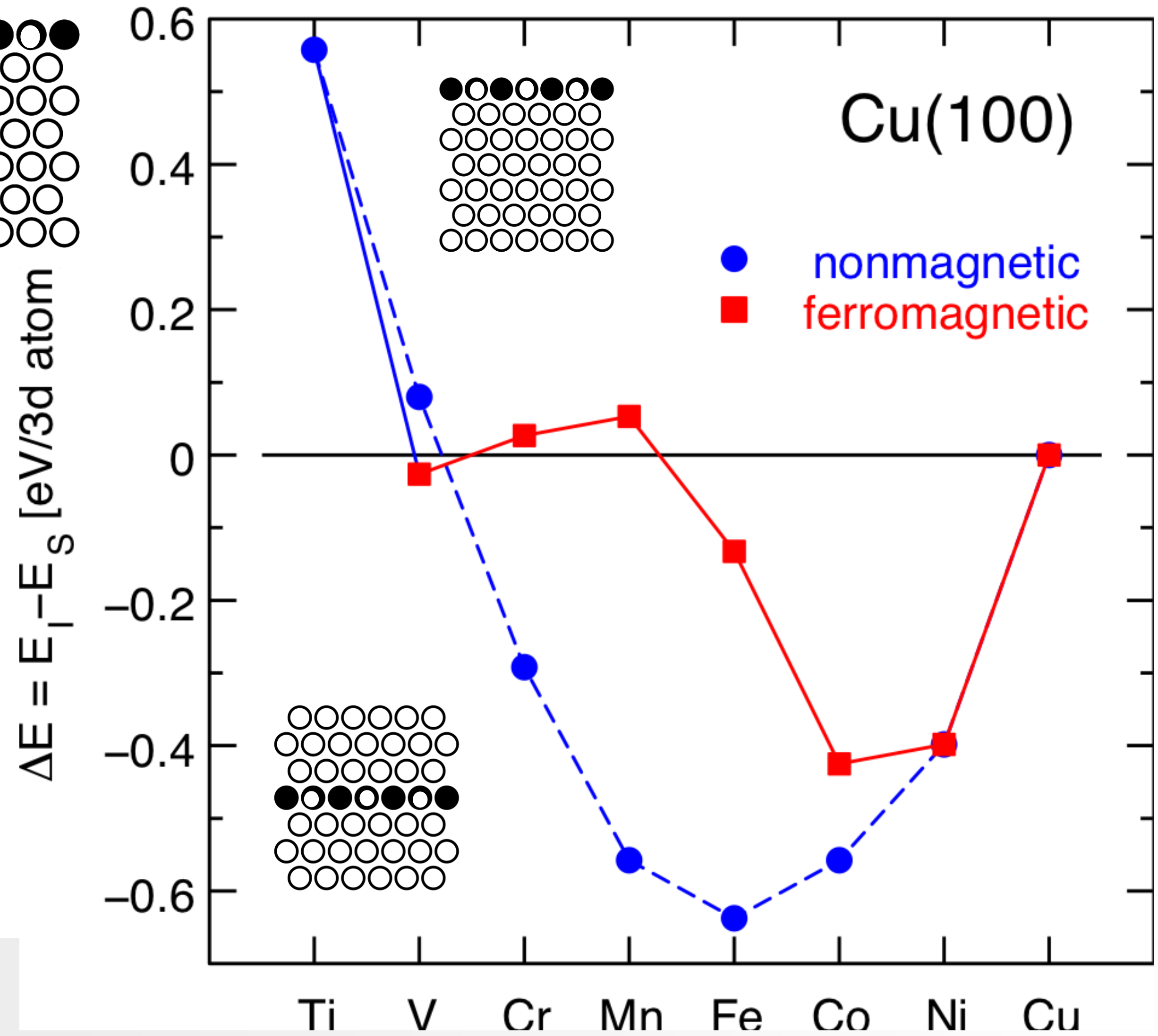






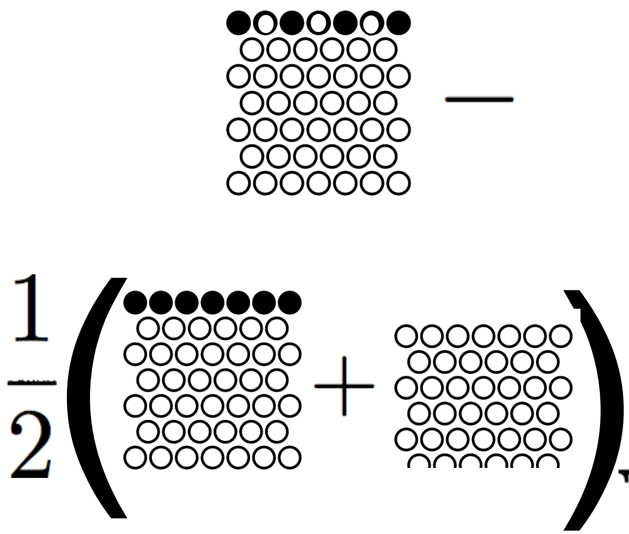
c(2x2)3dCu/Cu100: Stability against interdiffusion

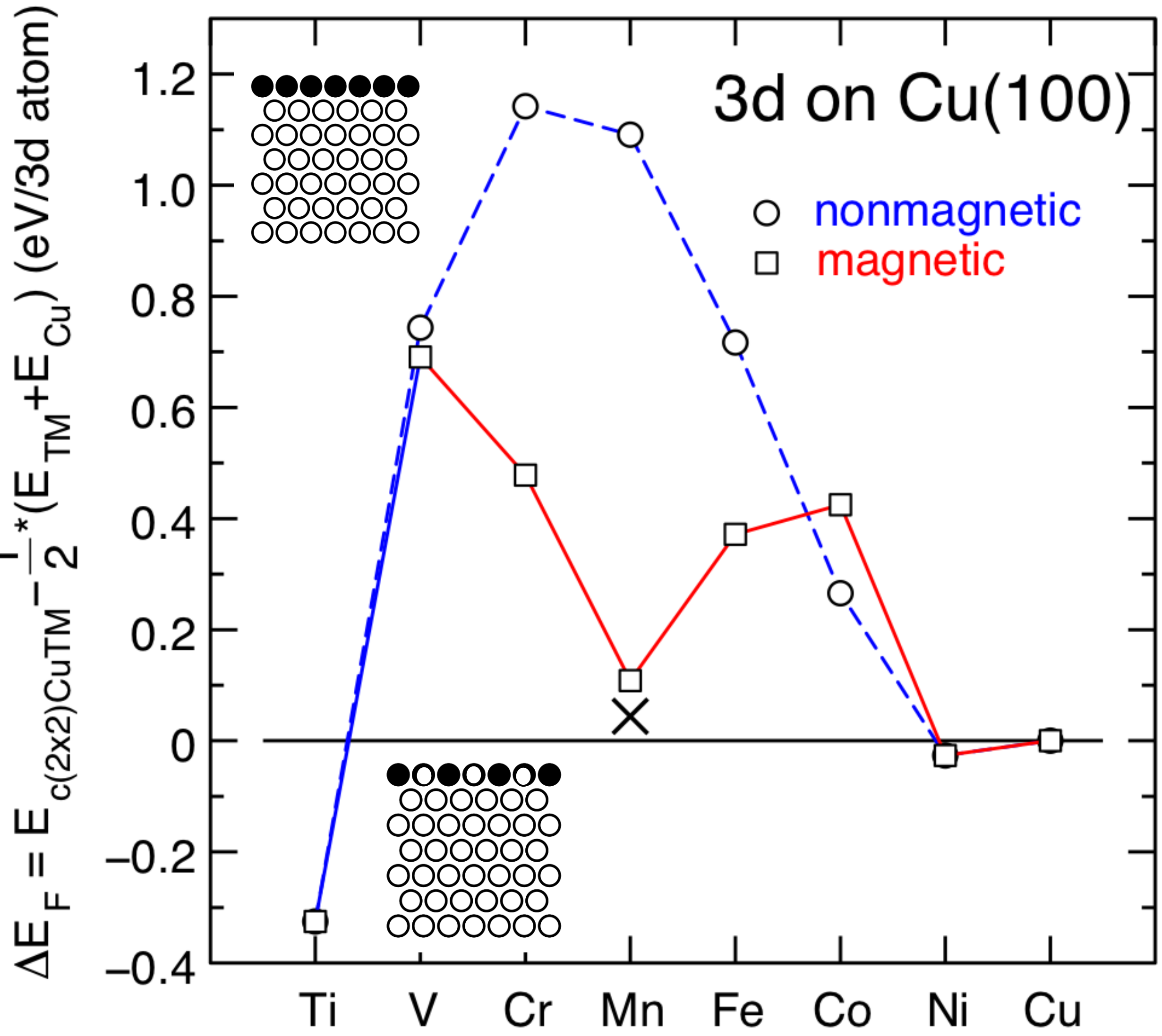




c(2x2)3dCu/Cu100: Alloy Formation

Formation energy:





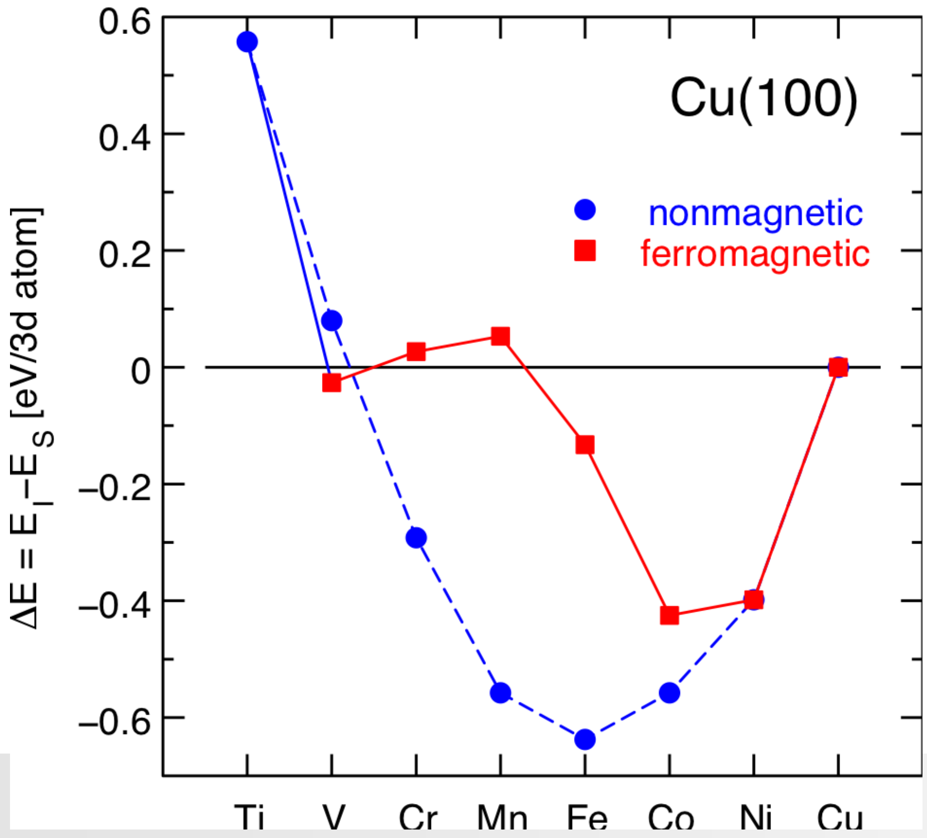
c(2x2)MnCu/Cu(100) Surface Alloy

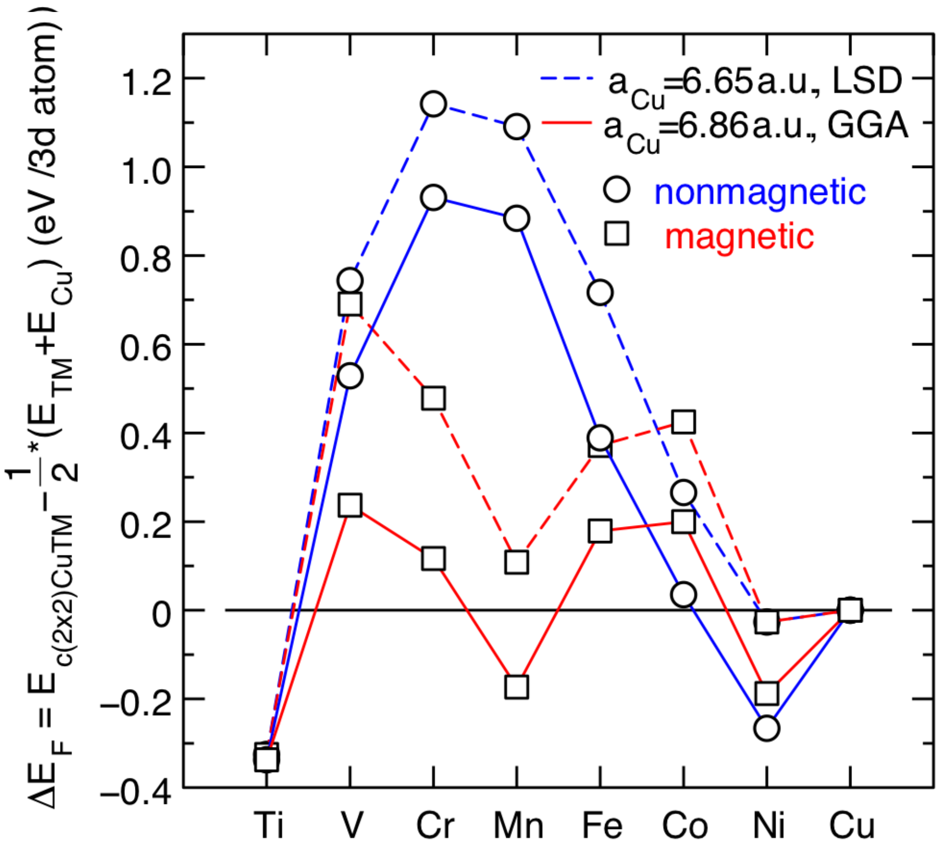
www.fz-juelich.de/iff/e_th1

2 Surface Alloys expected:

o magnetically stabilized : c(2x2)MnCu/Cu(100)

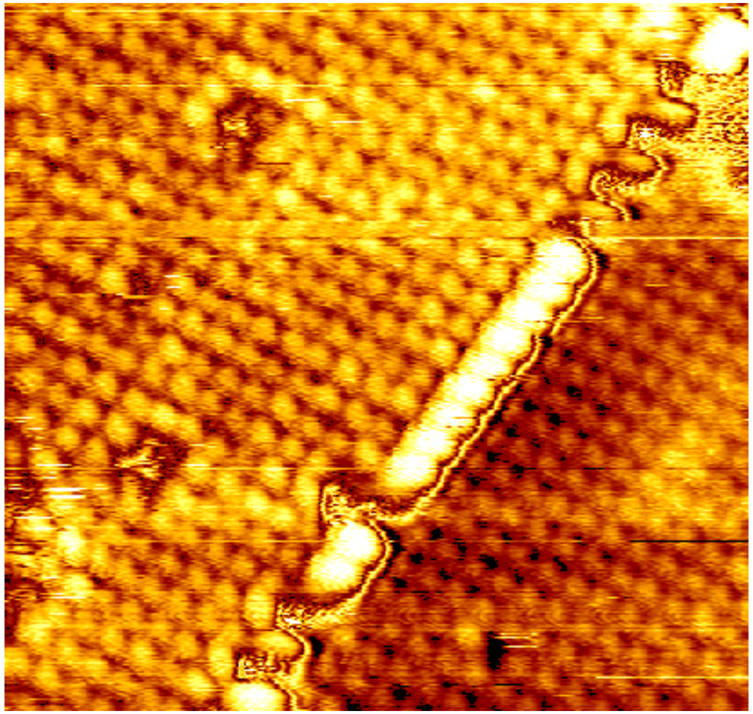
o nonmagnetic c(2x2)TiCu/Cu(100)



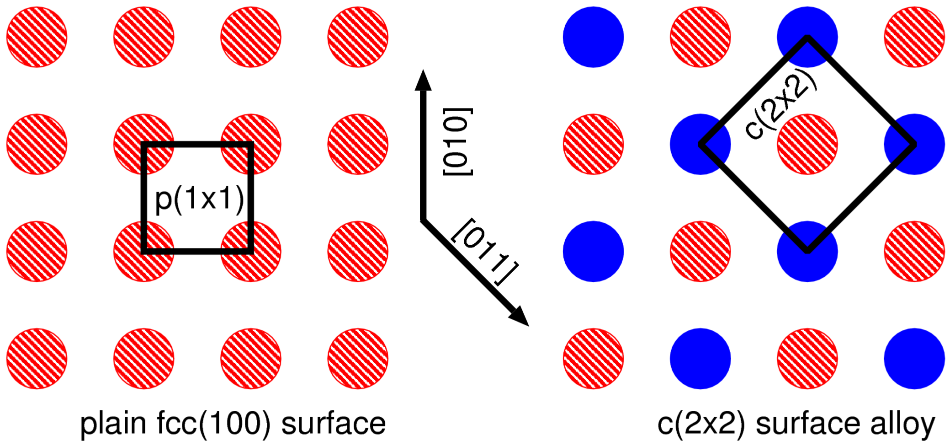


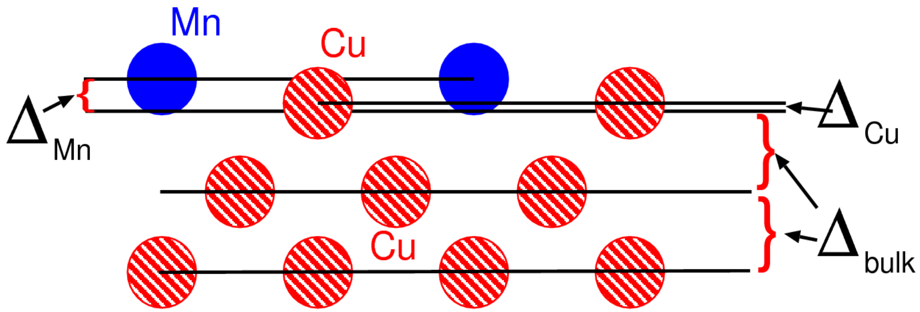
S. Blügel, Appl. Phys. A 63, 595 (1996)

STM of MnCu(100) c(2x2) surface alloy



R.G.P van der Kraan and H. van Kempen, Surf.Sci 338, 19 (1995)

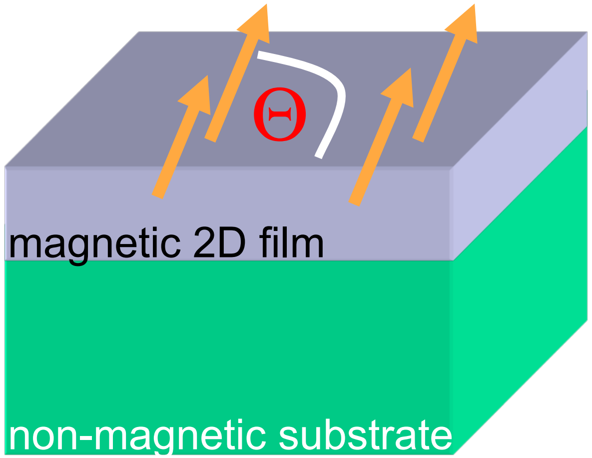




M. Wuttig, Y. Gauthier,, S. Blügel, PRL **70**, 3619 (1993).

8. Magnetic Anisotropy

Magnetic anisotropy

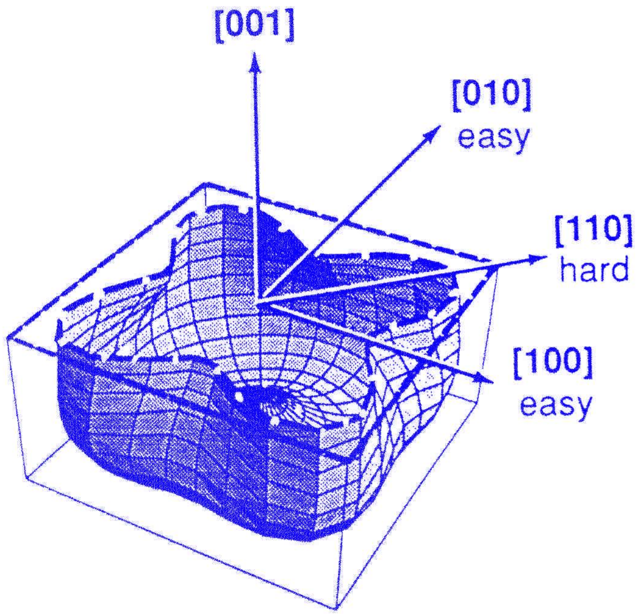


Magnetic Moments

Magnetism: Yes or No?

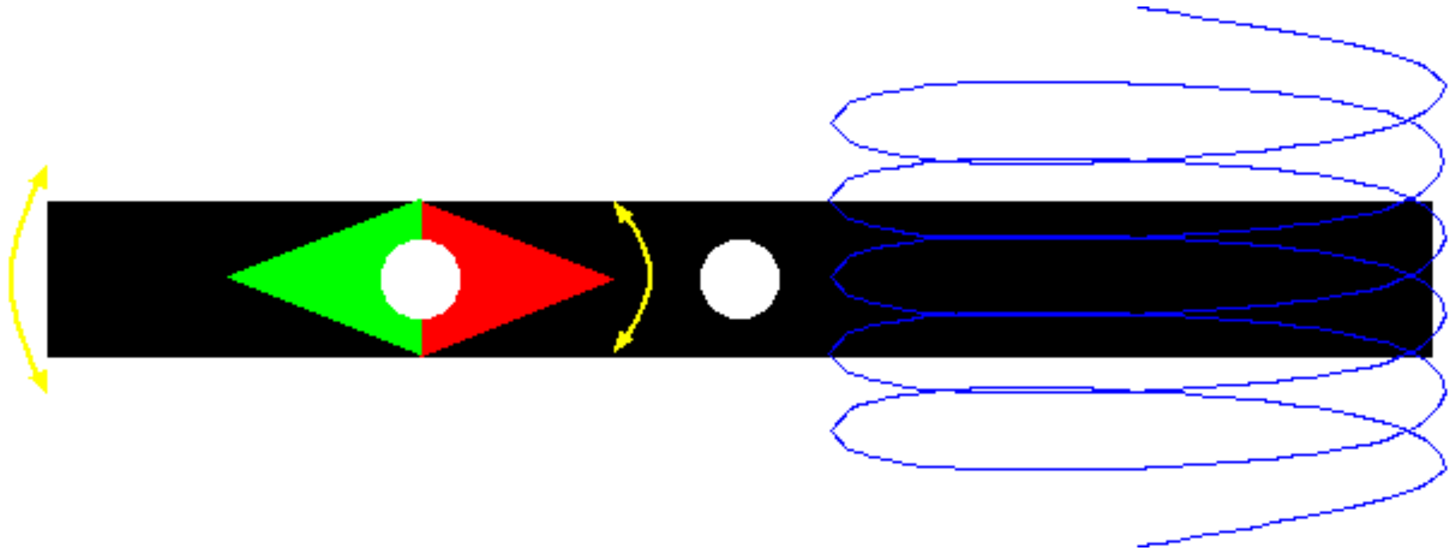
Exchange: $E(\Theta) = const$

Magnetic Anisotropy:

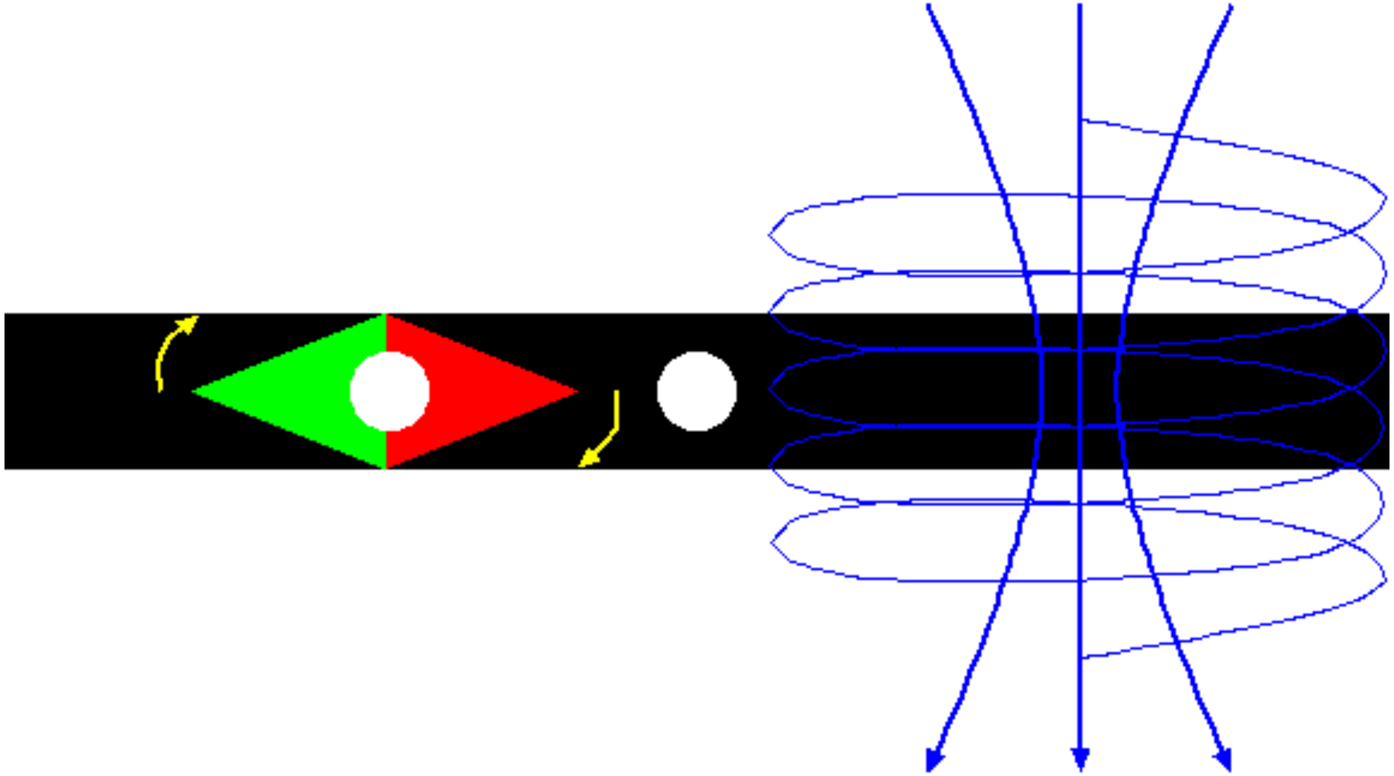


$$E(\Theta) = K_0 + K_1 \sin^2 \Theta + K_2 \sin^4 \Theta$$

Isotropic versus Anisotropic Interaction

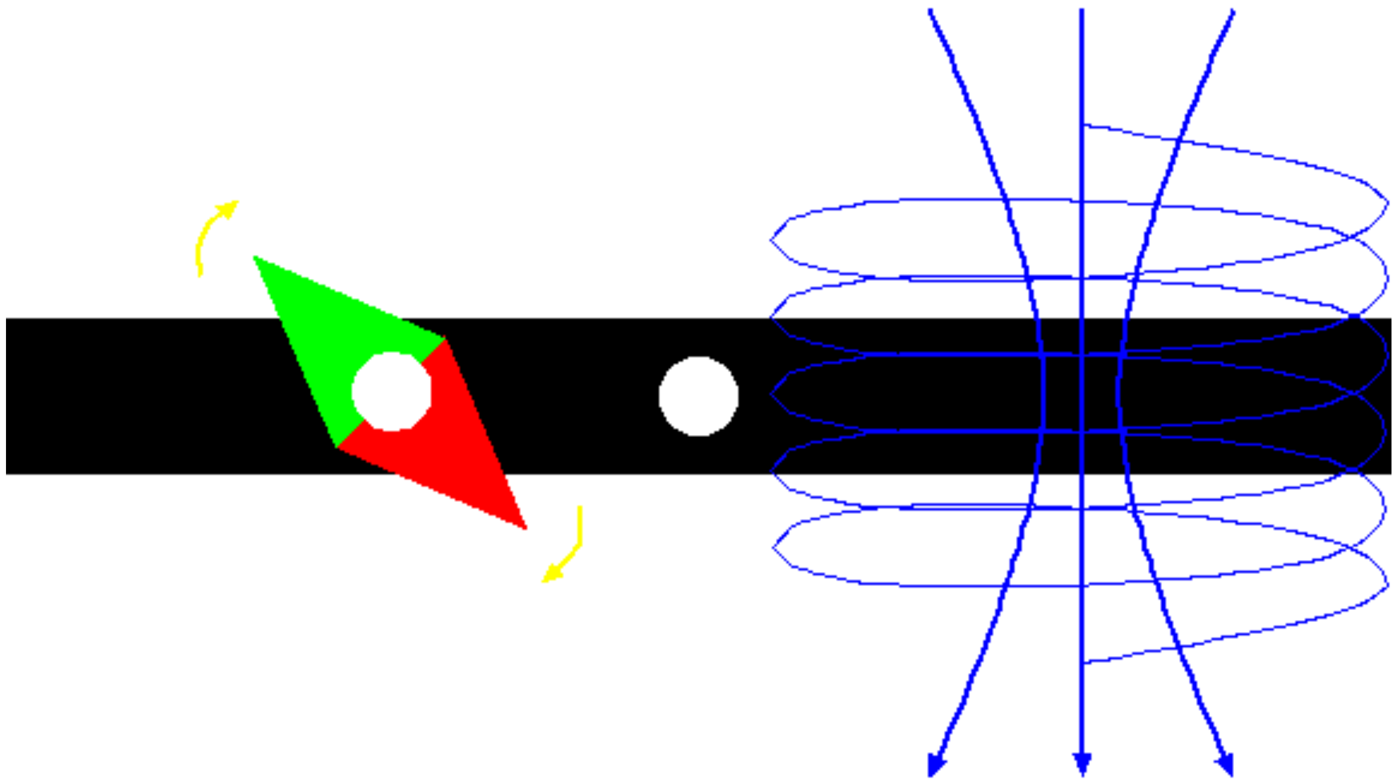


Isotropic versus Anisotropic Interaction



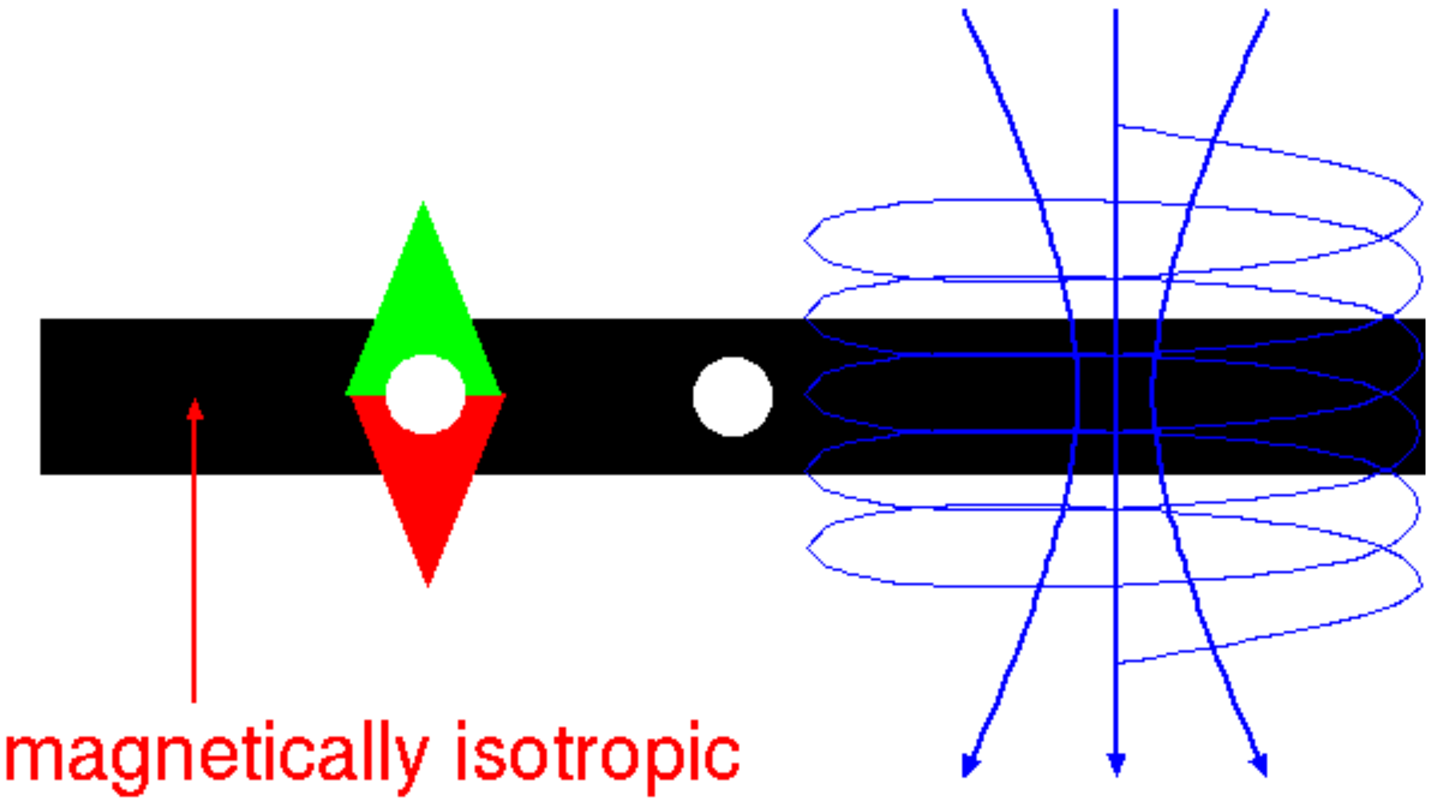
Isotropic versus Anisotropic Interaction

www.fz-juelich.de/iff/e_th1

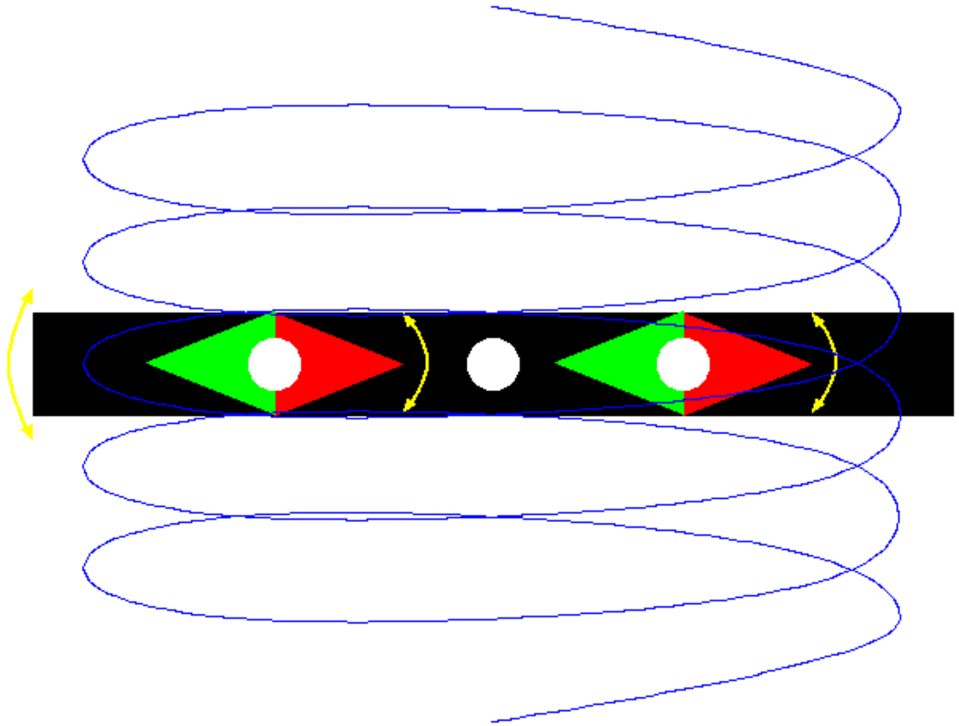


Isotropic versus Anisotropic Interaction

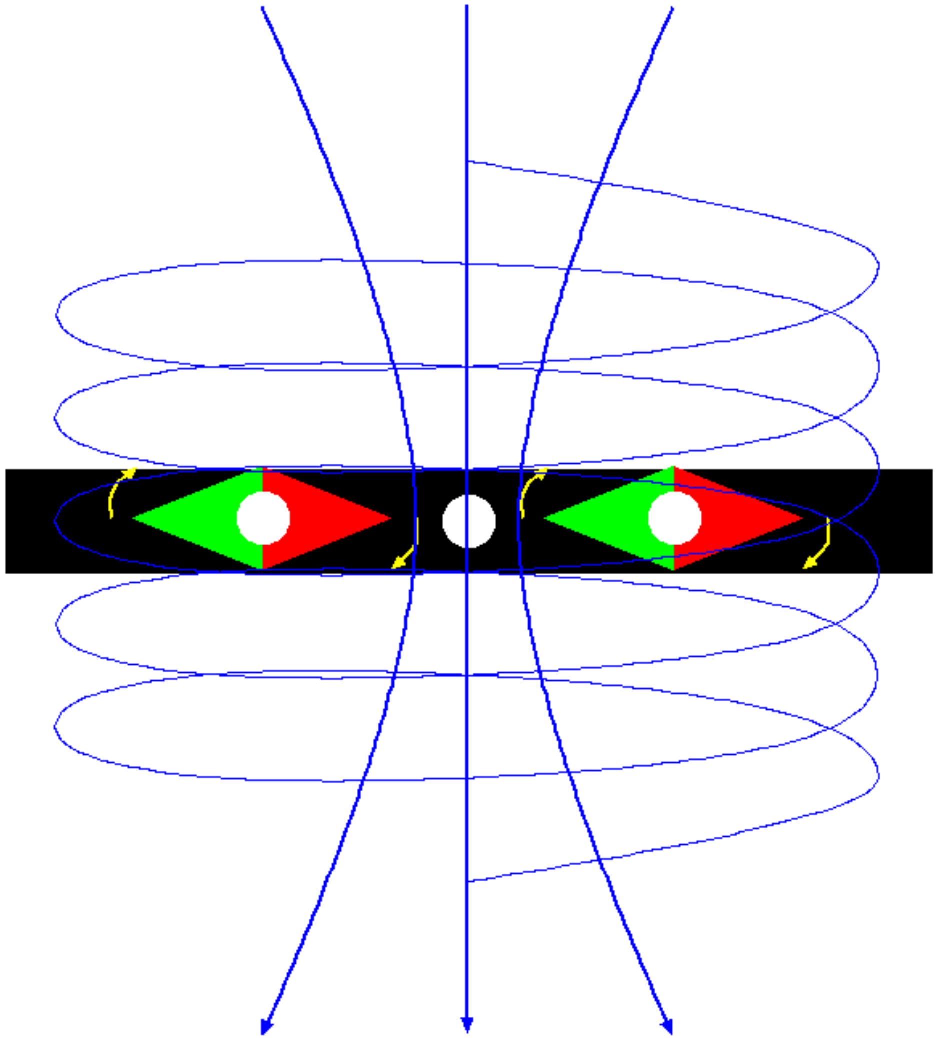
www.fz-juelich.de/iff/e_th1



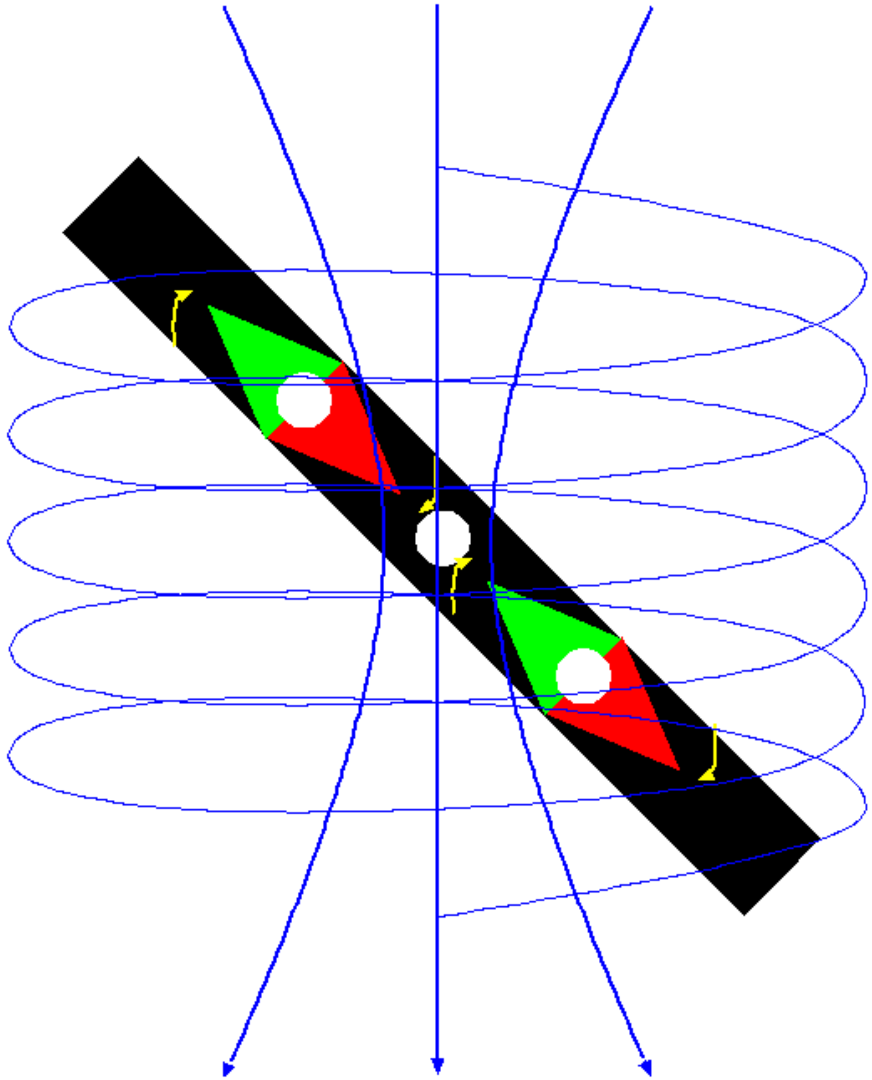
Isotropic versus Anisotropic Interaction



Isotropic versus Anisotropic Interaction

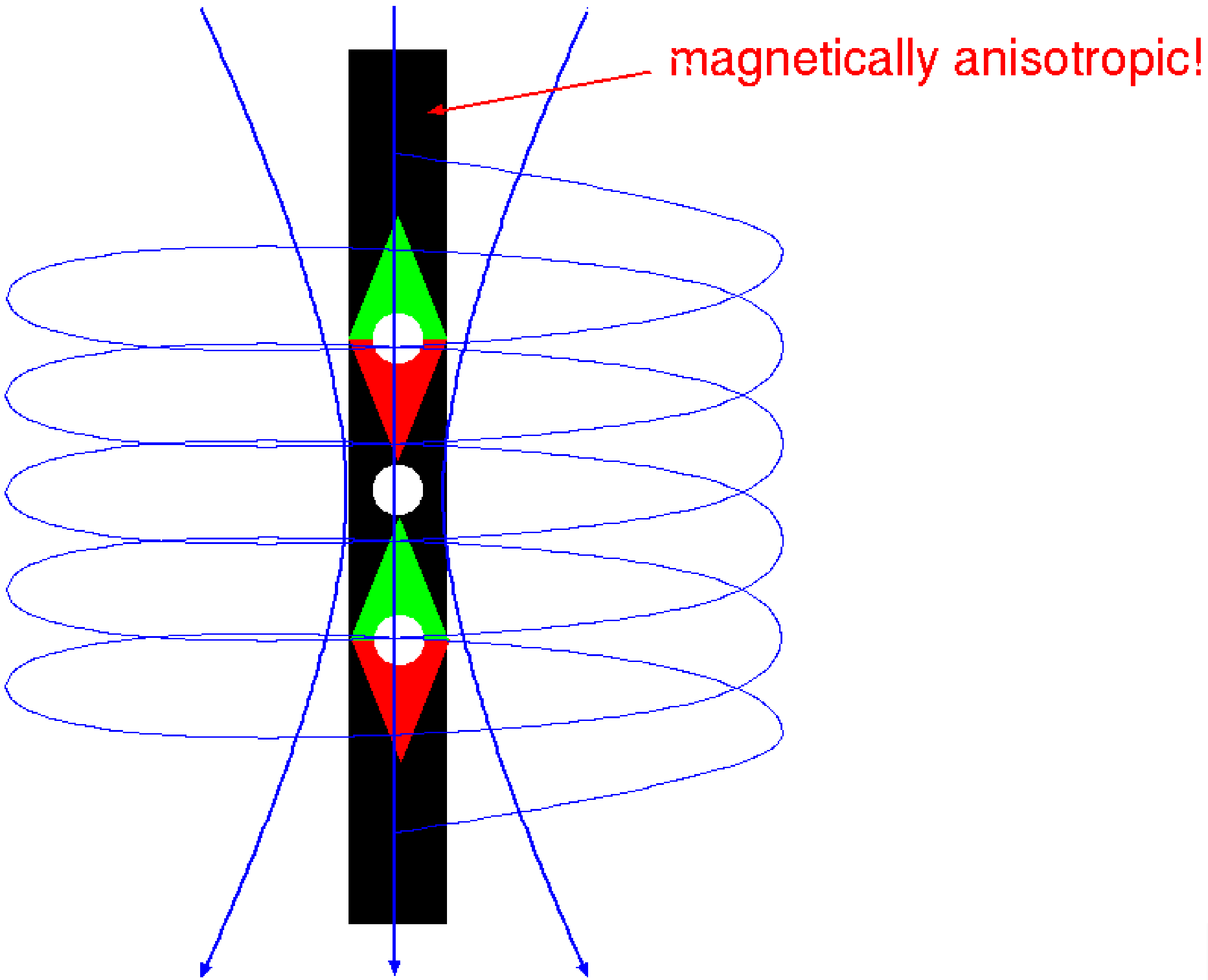


Isotropic versus Anisotropic Interaction



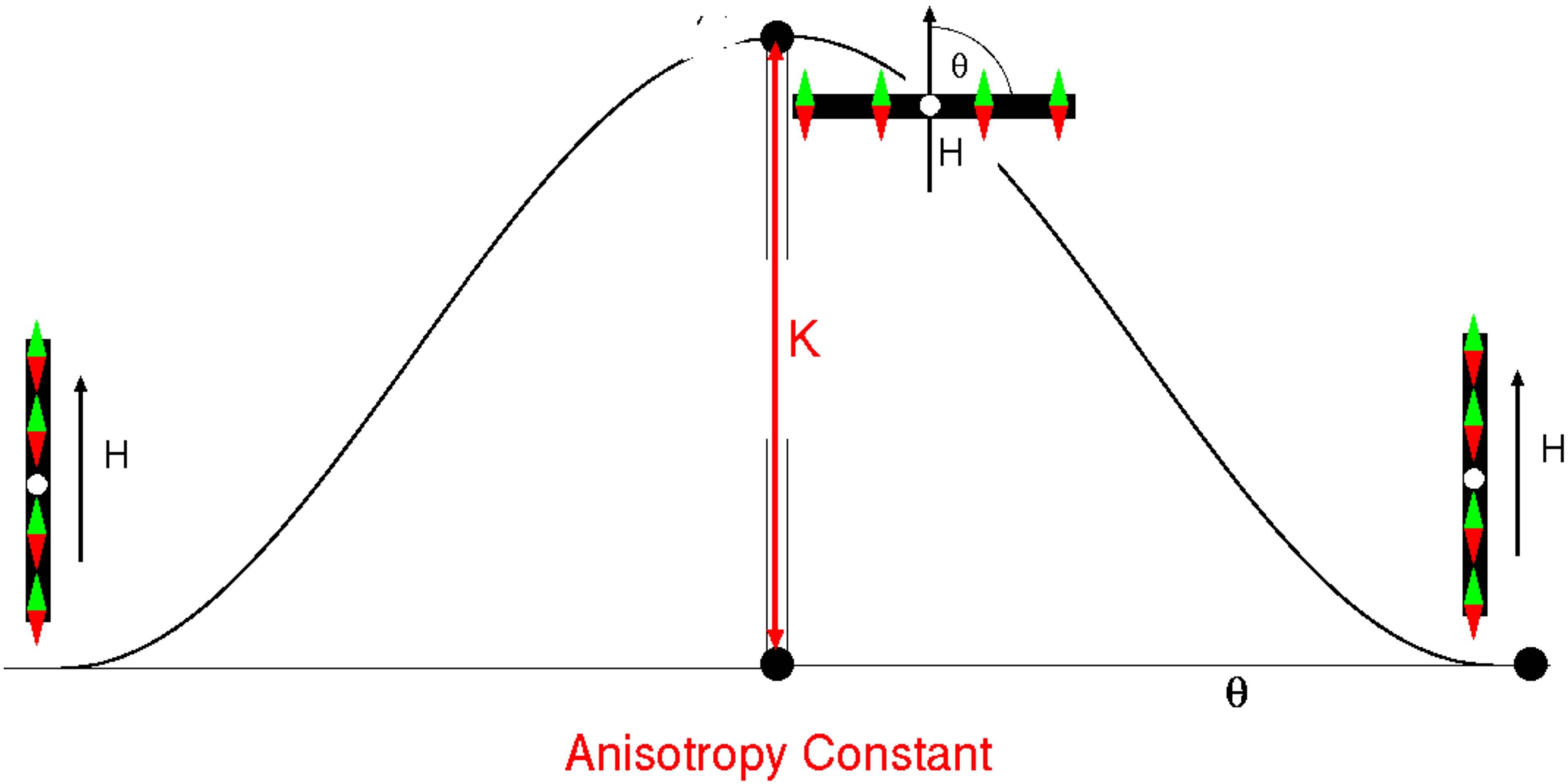
Isotropic versus Anisotropic Interaction

www.fz-juelich.de/iff/e_th1



Anisotropy Energy

www.fz-juelich.de/iff/e_th1



Anisotropy constants Fe, Co, Ni

www.fz-juelich.de/iff/e_th1

T=4.2K		Fe (bcc)	Co (hcp)	Ni (fcc)
K_1	[erg/cm^3]	$5.48\times10^{5(a)}$	$7.66\times10^{6(b)}$	$-12.63\times10^{5(a)}$
	[meV/atom]	4.02×10^{-3}	5.33×10^{-2}	-8.63×10^{-3}
K_2	[erg/cm^3]	$1.96\times10^{3(a)}$	$1.05\times10^{6(b)}$	$5.78\times10^{5(a)}$
	[meV/atom]	1.44×10^{-5}	7.31×10^{-3}	3.95×10^{-3}
K_3	[erg/cm^3]	$0.9\times10^{3(a)}$	–	$3.48\times10^{4(a)}$
	[meV/atom]	6.6×10^{6}	–	2.38×10^{-4}
K_4	[erg/cm^3]	–	$1.2\times10^{5(c)}$	–
	[meV/atom]	–	8.4×10^{-4}	6.9×10^{-4}
M_0	[G]	$1749.7\quad\times10^{0(b)}$	$1459.5\quad\times10^{0(d)}$	$524.8\quad\times10^{0(b)}$
	[μ_B/atom]	2.215×10^{0}	1.729×10^{0}	0.615×10^{0}
M_1	[G]	$-4.3\times10^{-1(a)}$	$-6.75\times10^{0(d)}$	$5.1\times10^{-1(a)}$
	[μ_B/atom]	-5.4×10^{-4}	$-8.0\ \times10^{-3}$	6.0×10^{-4}

Comparison of magn. Anisotropy energies

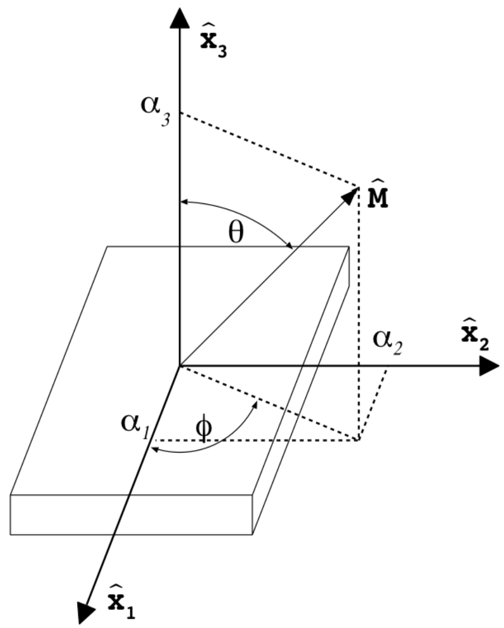
System		MAE [MJ/m^3]	MAE [$\mu eV/TM$ atom]
Bulk	Fe	0.017	1.4
	Co	0.042	2.7
	Ni	0.85	65
Multilagen	Co/Ni	2	
	Co/Pd, Co/Pt	5	300
Permanentmagnete	YCo_5	7	760
	$Nd_2Fe_{14}B$	12	
	$SmCo_5$	30	

Magnetic Anisotropy

www.fz-juelich.de/iff/e_th1

$$E = \sum_i \vec{S}_i \cdot \vec{\vec{K}}_i \cdot \vec{S}_i$$

$$\boxed{\xi_{nl} \approx Z \bullet \left(\frac{Z^3}{a_B^3}\right) \bullet \frac{1}{n^3 l^2}}$$



Spin-Orbit Interaction: $H_{SO} \propto \frac{1}{r}\frac{dV}{dr} L \bullet S = \xi_{nl} L \bullet S$

(Magneto-crystalline)

Dipol Interaction: $E_d(\Theta) = \frac{\mu_B^2}{2} \sum_{i,j,i \neq j} \frac{m_i m_j}{R_{i,j}^3} \left(1 - 3\cos^2 \Theta_{ij}\right)$

(Shape anisotropy)

Symmetry-dependence

E.g. Uniaxial Symmetry $E(\Theta) = K_0 + K_1 \sin^2 \Theta + K_2 \sin^4 \Theta$

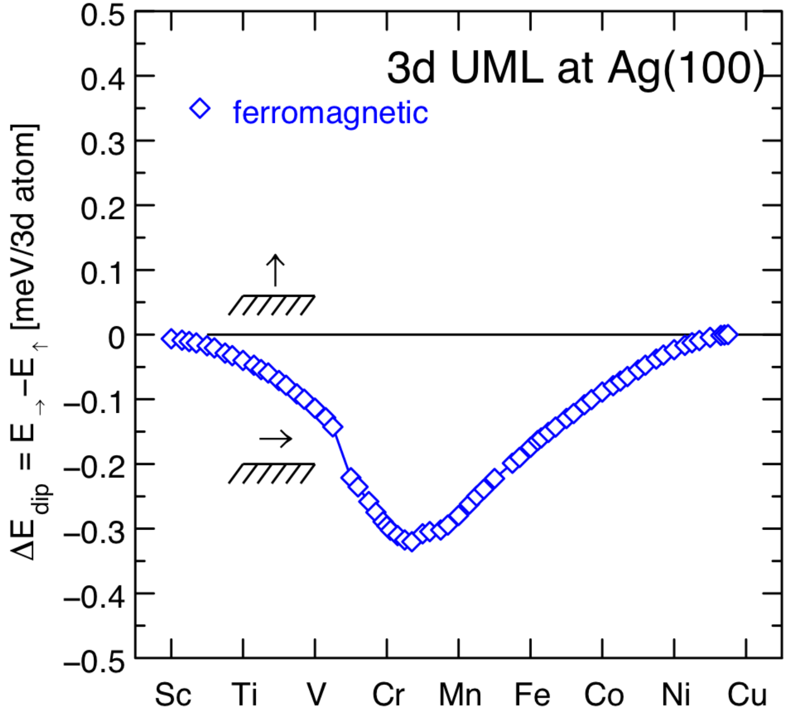
$$n - th = \sum \frac{|\langle u | H_{SO} | o \rangle|^n}{(\varepsilon_u - \varepsilon_o)^{n-1}}$$

2nd 4th

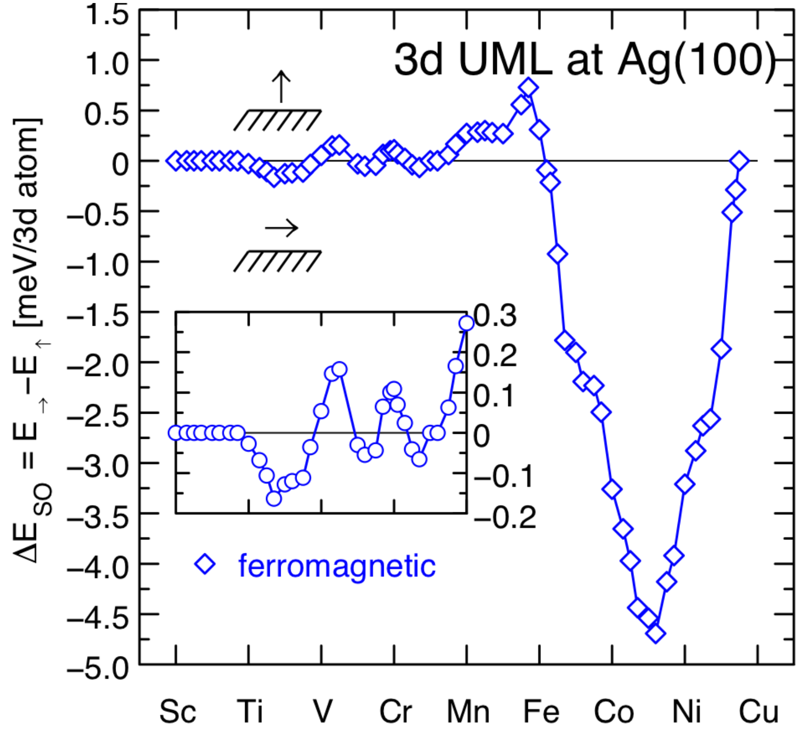
Example: unsupported 3d ML

www.fz-juelich.de/iff/e_th1

Dipol energy $\propto M^2$

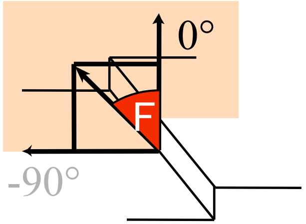


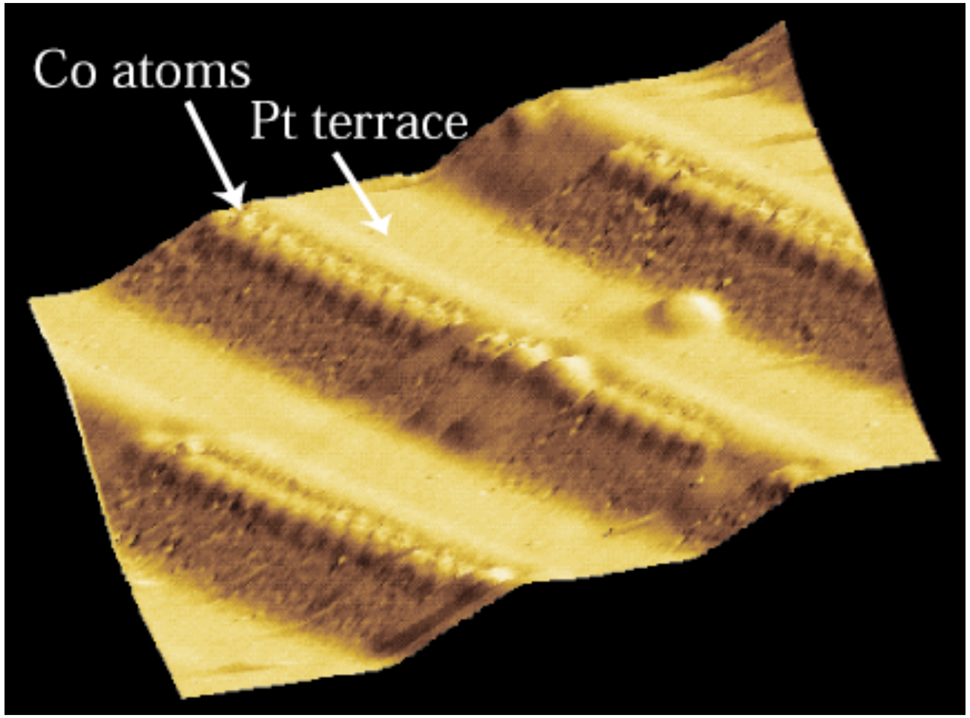
MCA (SO)

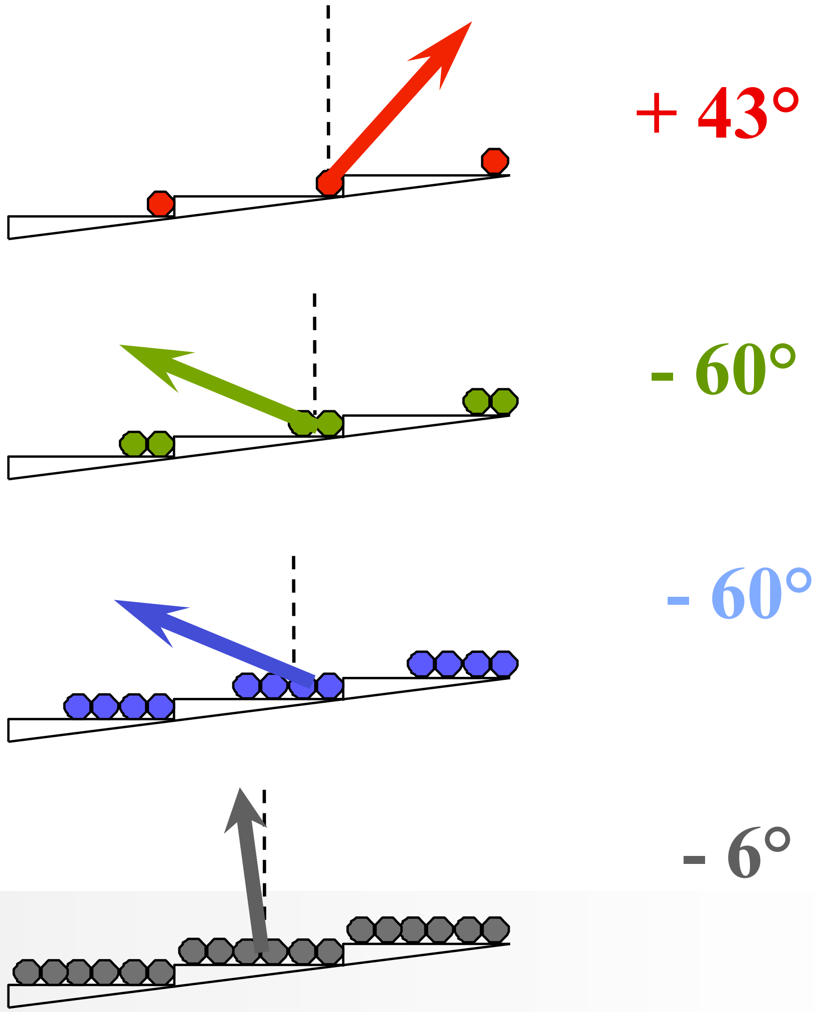


6. Chains

Magnetic Chains: Co on Pt(997)

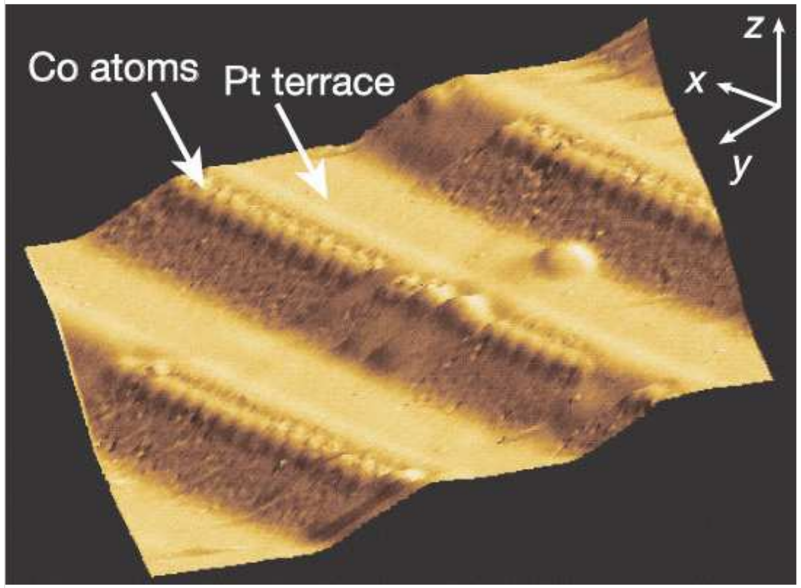


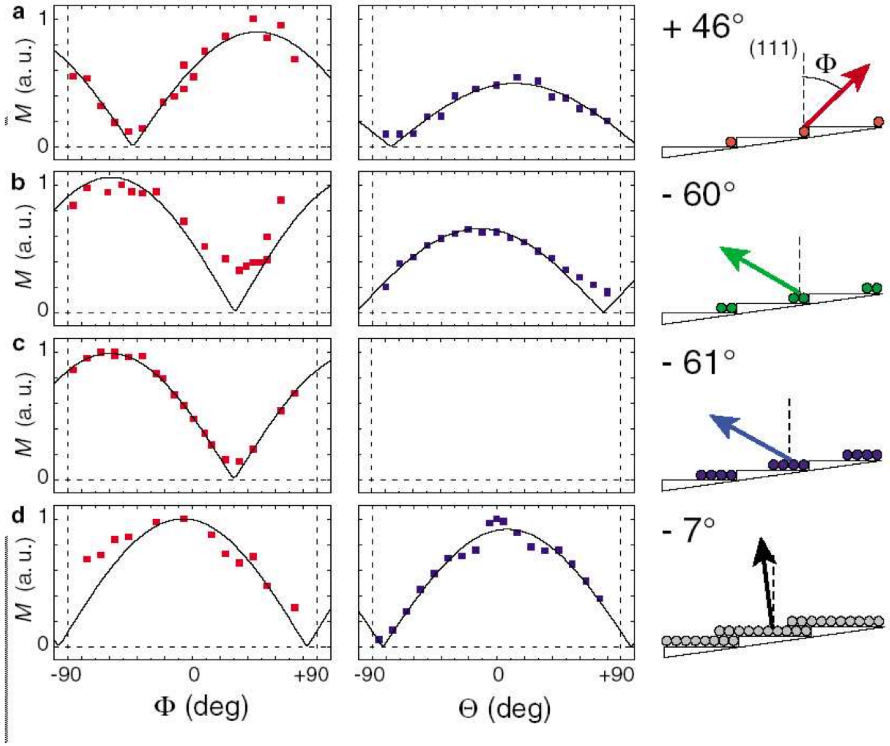




Gambardella, Carbone, Brune, Kern,
Nature **416**, 301 (2002)
Phys. Rev. Lett. **93,** 077203 (2004)

Experimental situation



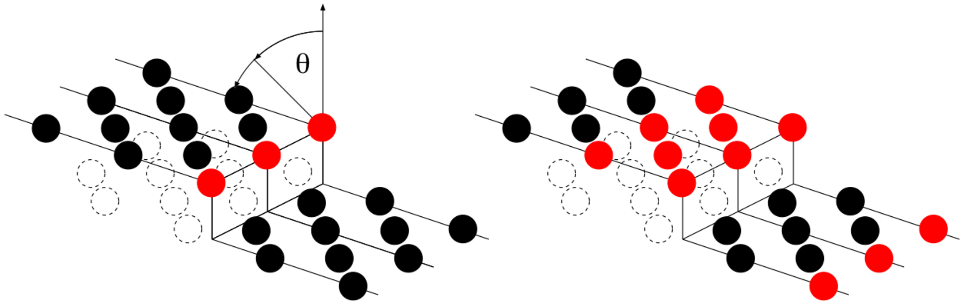


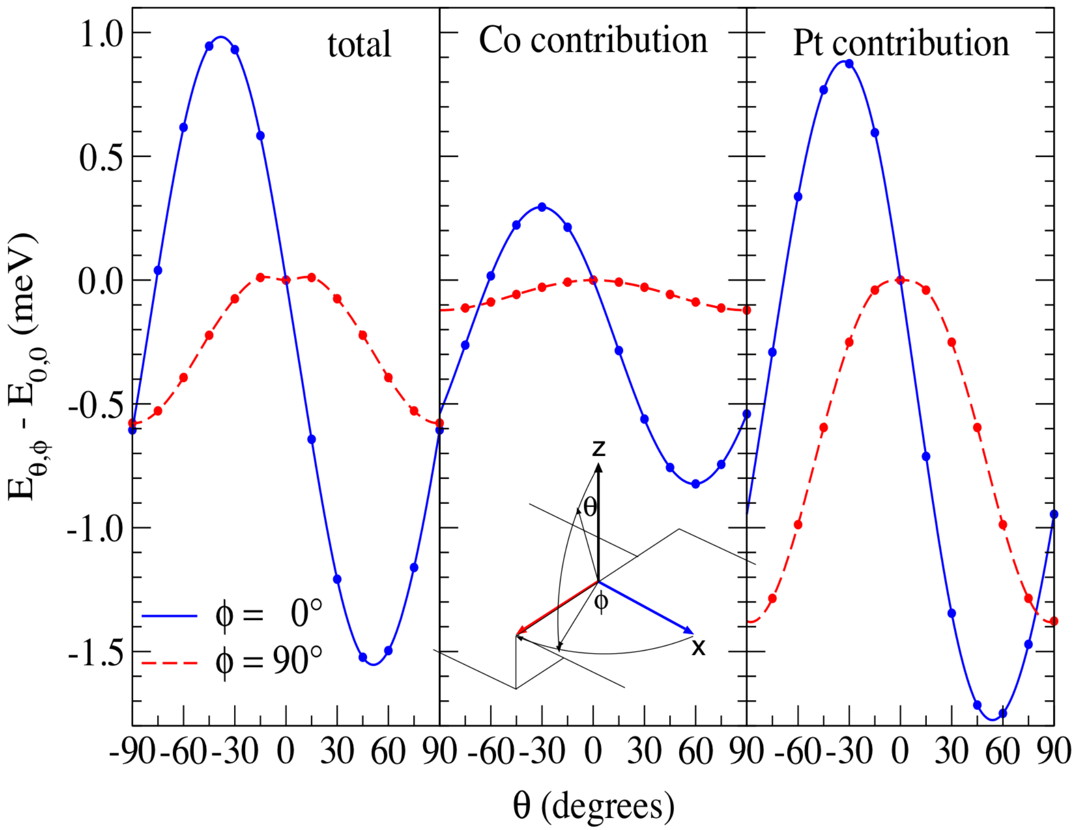
Co wire(s) on Pt(997)

[1] P.Gambardella et al.
Nature 416, 301 (2002); Phys. Rev. Lett. 93 077203 (2004)

- magnetic anisotropy & easy axis measured under applied field
- easy axis perpendicular to wire, oscillates with wire-width
- MAE: large for 1-wire, small for 2-wire, larger for thicker wires

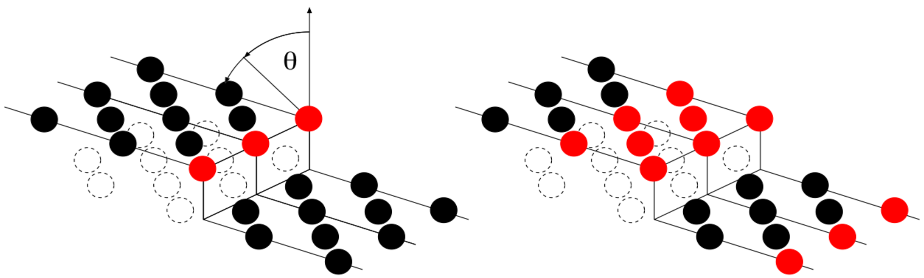
Co chain on Pt(667)

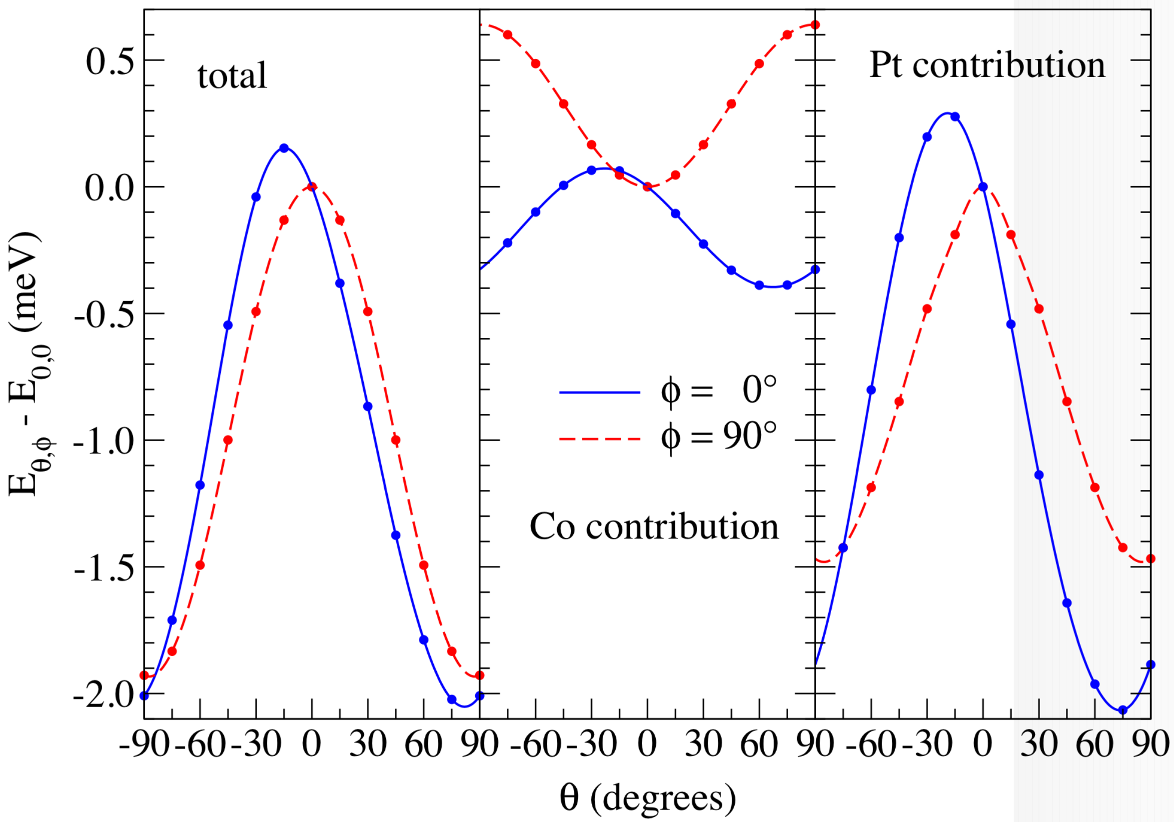




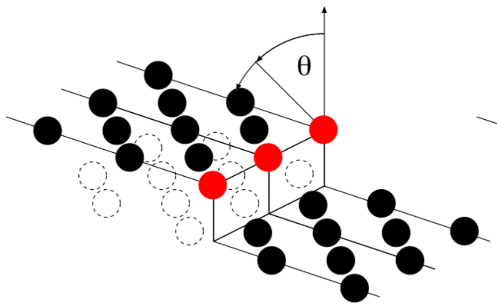
S. Baud, Ch. Ramseyer, G. Bihlmayer, S. Blügel, PRB **73**, 104427 (2006).

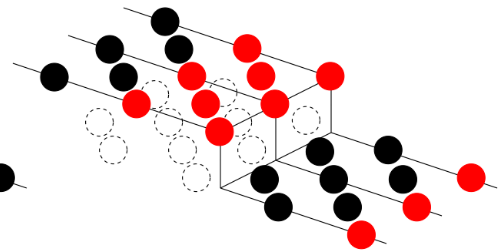
Co chain on Pt(667) : relaxed

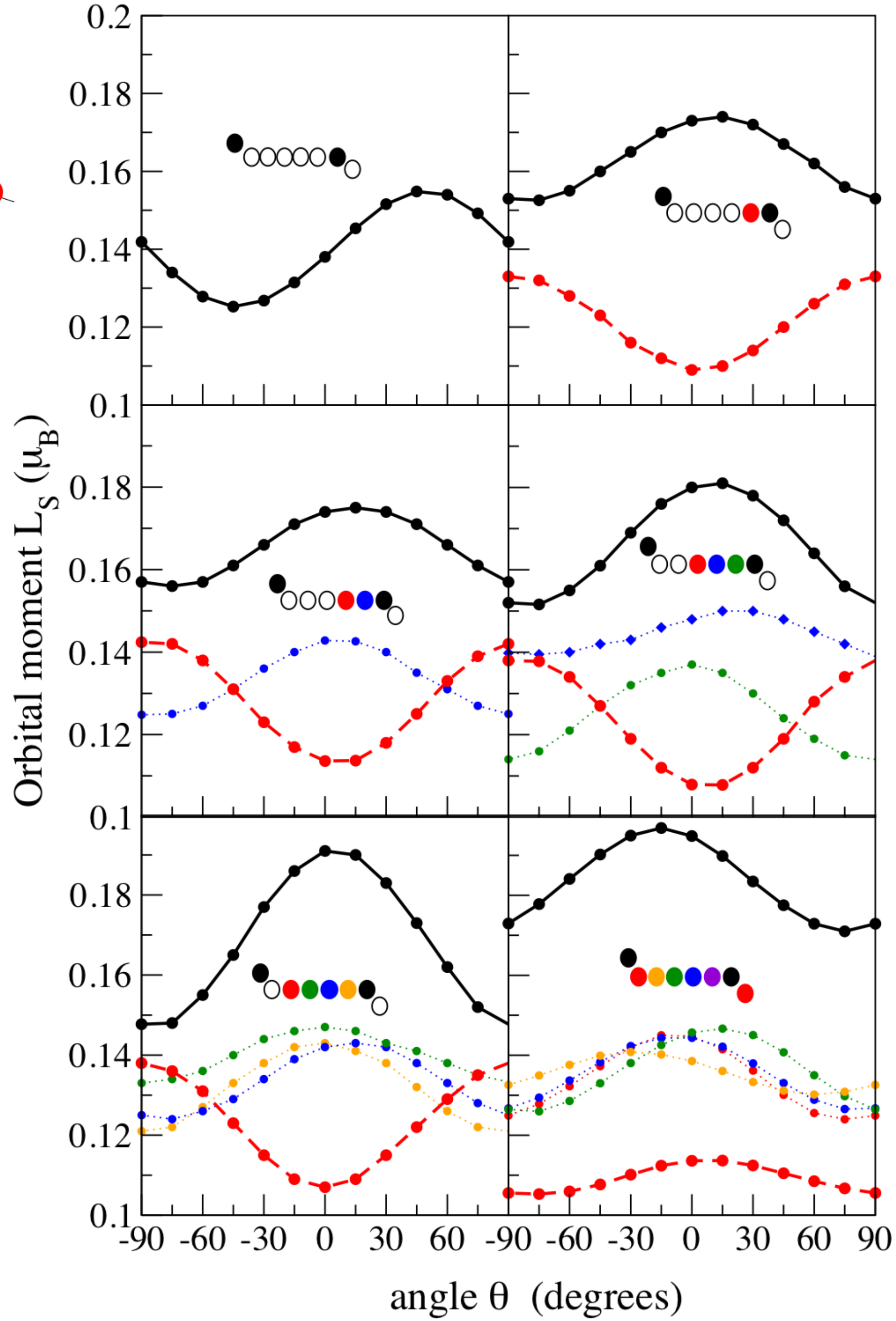


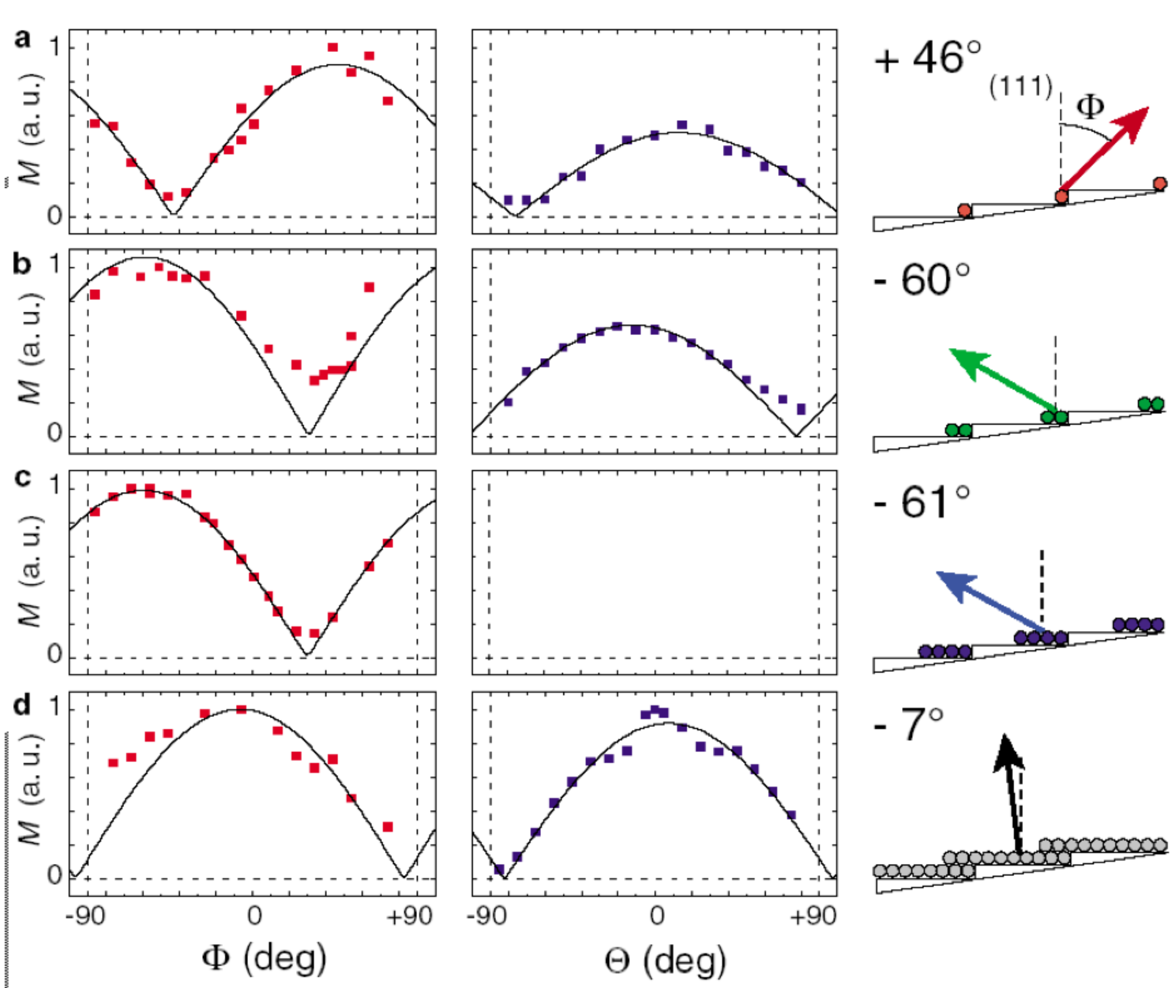


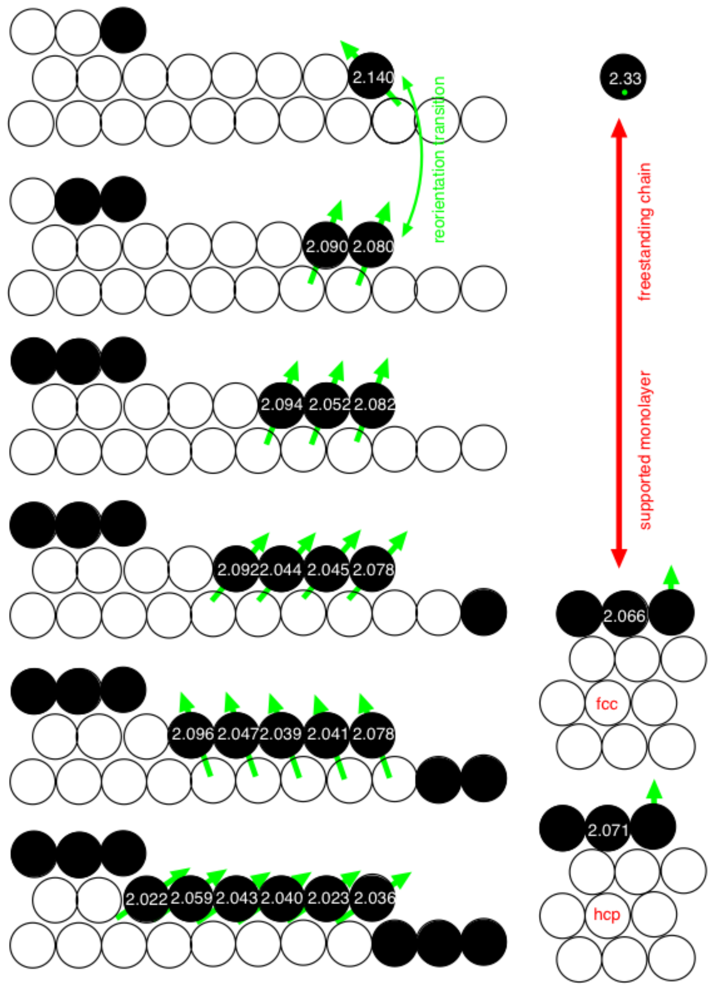
S. Baud, Ch. Ramseyer, G. Bihlmayer, S. Blügel, PRB **73**, 104427 (2006).


θ




Orbital moment L_S (μ_B)
angle θ (degrees)





P.Gambardella PRL 93, 077203 (2004)

S. Baud, Thesis (2004)

Summary

- Enhanced magnetism in reduced dimension
- Many different phases
- Competition due to competing interactions
- New physics due to symmetry breaking and finiteness