Surface and Interface Magnetism

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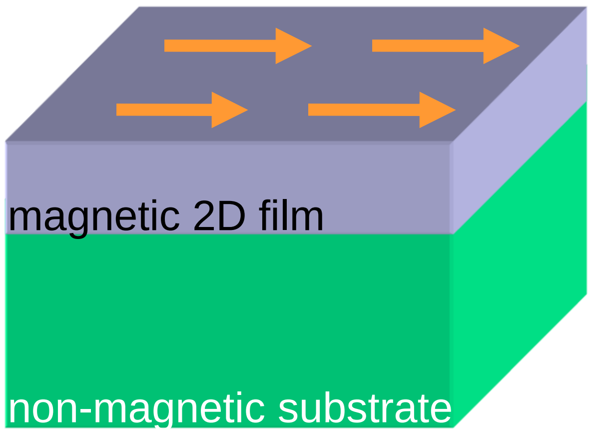
Forschungszentrum Jülich and JARA

SURFACE MAGNETISM: THREE FUNDAMENTAL QUESTIONS

Typical Energies: ≈1 eV



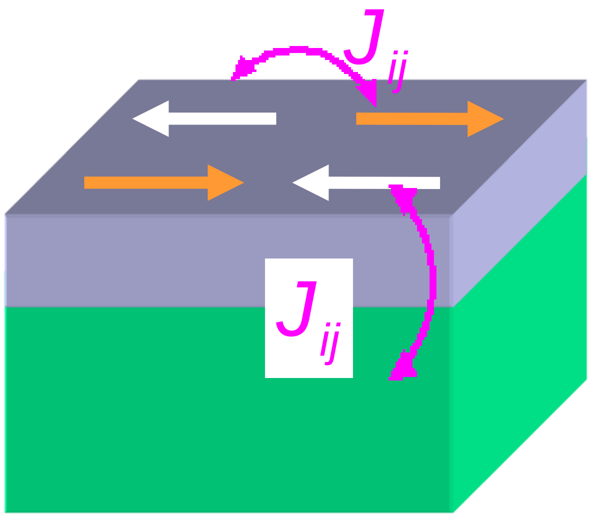
Magnetic Moments

Magnetism: Yes or No?

Intra-atomic Exchange

$$H = -\frac{1}{2}\sum_{i} I_i m_i^2$$

≈0.2 eV



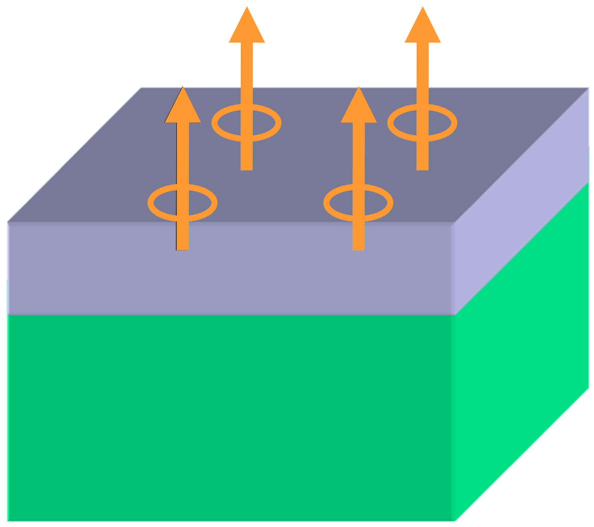
Magnetic Order

Ferro ⟺ Antiferro

Inter-atomic Exchange

$$H = -\frac{1}{2}\sum_{i,j} J_{i,j}\, \vec{m}_i \vec{m}_j$$

≈0.0005 eV



Magnetic Orientation

In-plane ⟺ Out-of-plane

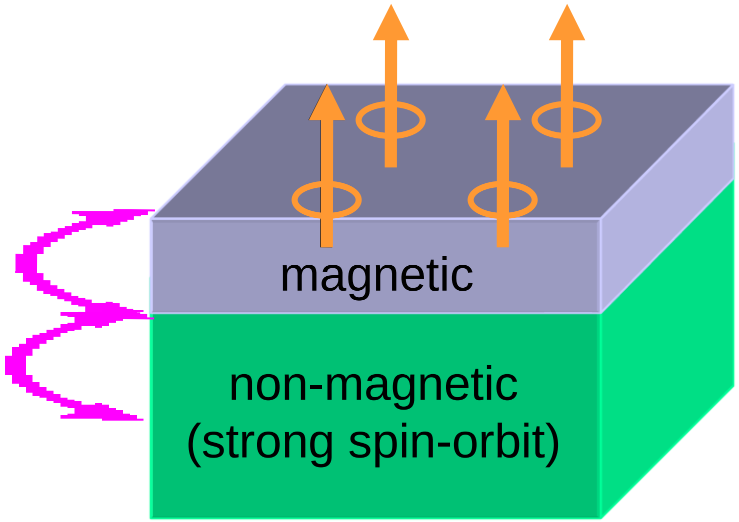
Spin-Orbit + Dipole-Dip

$$H = \sum_{i} K_i (\vec{m}_i\, \vec{e}_i)^2 + \sum_{i,j} \frac{1}{r_{i,j}^3}[\cdots]$$

BREAK OF INVERSION SYMMETRY

Break of inversion symmetry

P(z) 1 P(-z)



$$H_{\mathrm{DM}} = \sum_{ij} \mathbf{D}_{ij} \underbrace{\mathbf{m}_i \times \mathbf{m}_j}_{\mathbf{c}_{ij}}$$

Dzyaloshinskii-Moriya Interaction
Antisymmetric Exchange
Chiral magnetic interaction

E. Dzyaloshinskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **19**, 960 (1964) ; I. E. Dzyaloshinskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **20**, 665 (1965). T. Moriya, PRL **4**, 228 (1960) ; T. Moriya, PR **120**, 91 (1960)

Reminder bulk

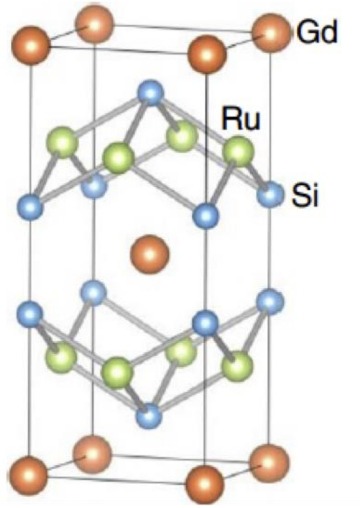
REMINDER 1: MAGNETIC MATERIALS

- Almost all magnetic materials contain 3d or 4f metal ions
- We have many more antiferromagnets than ferromagnets

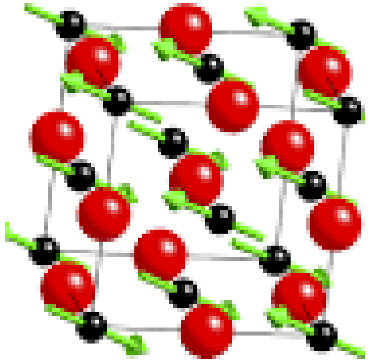
Example:

- Metallic magnetism: 3d metal compounds and 4f intermetallics
- Ionic magnetism: transition metal and 4f metal oxides
- Covalent magnetism: 2D van der Waals materials

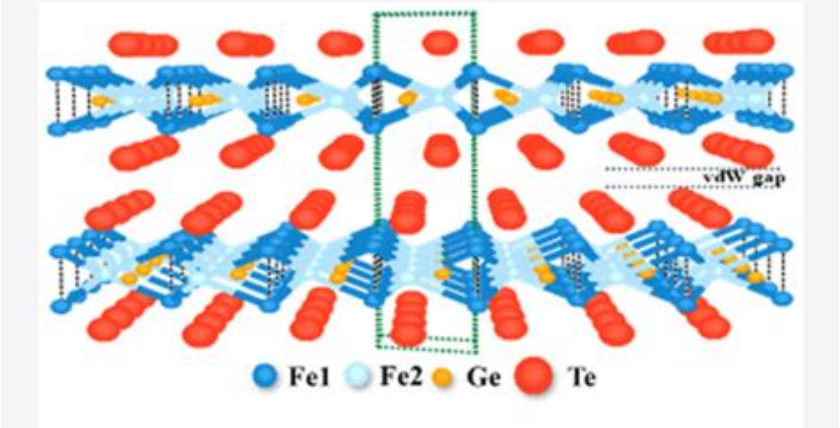
$GdRu_2Si_2$



NiO

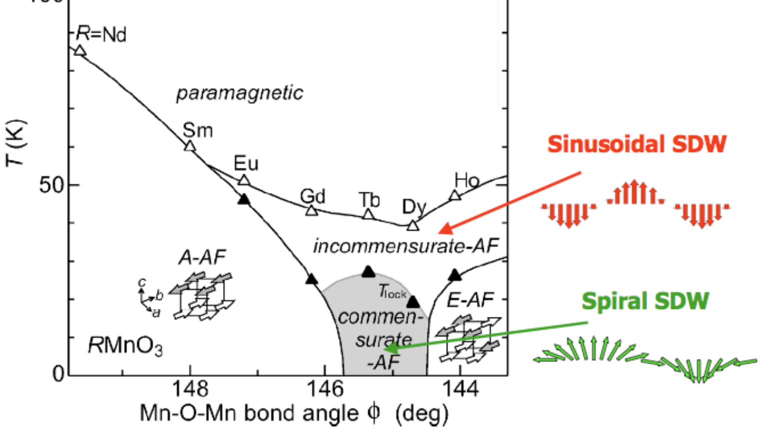


Bilayer of Fe_3GeTe_2



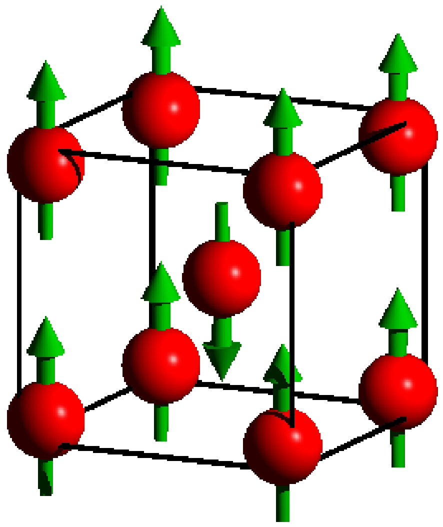
Orthorombic $RMnO_3$

T. Kimura et al PRB 68,060403 (2003)



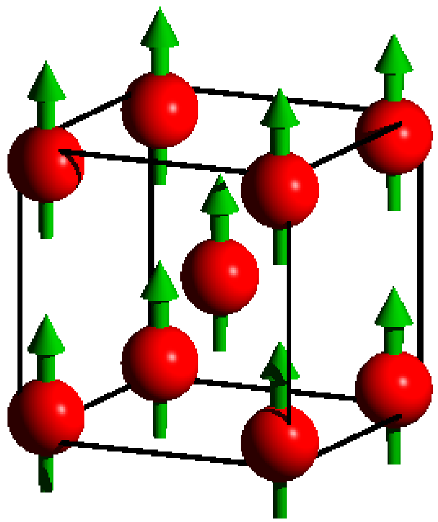
REMINDER 2: BULK MAGNETISM

- Itinerant magnets (metals)
- Collinear magnetic structure
  (quantization axis the same at each atom)



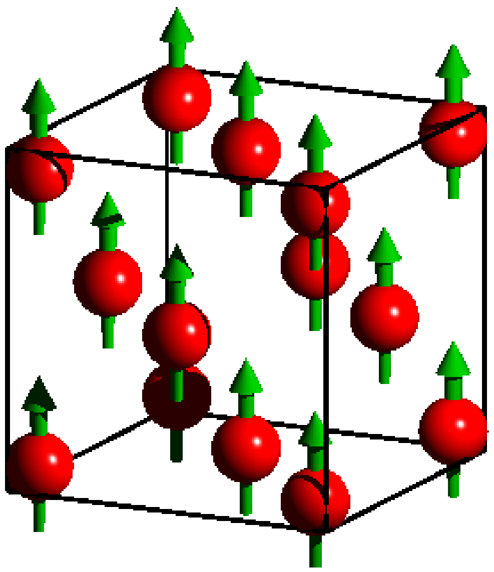
bcc-Cr:

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



bcc-Fe:

$M = 2.12\ \mu_B$

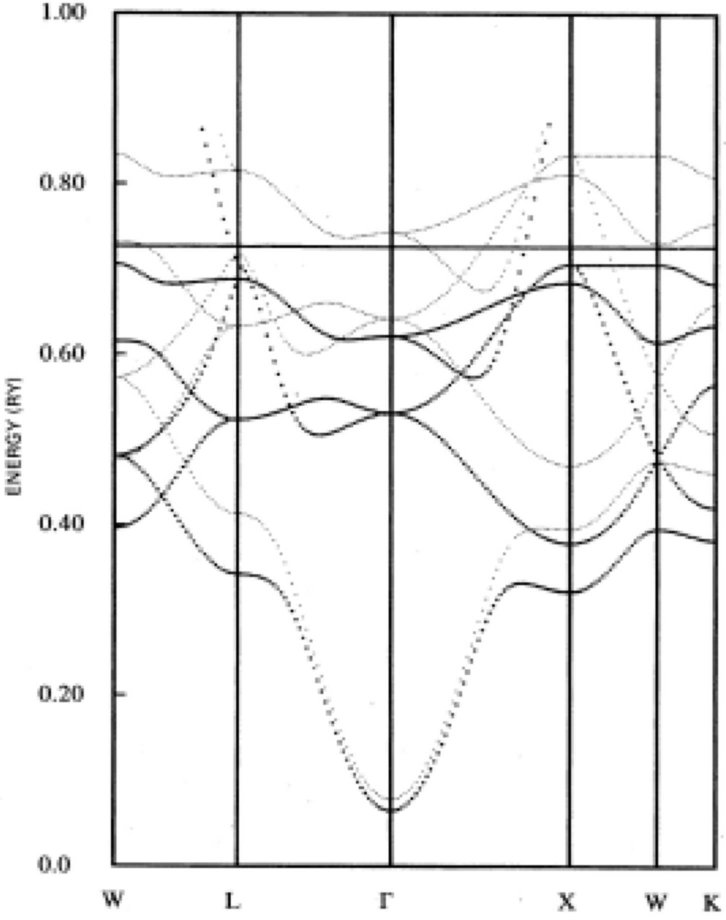


fcc-Ni:

$M = 0.55\ \mu_B$

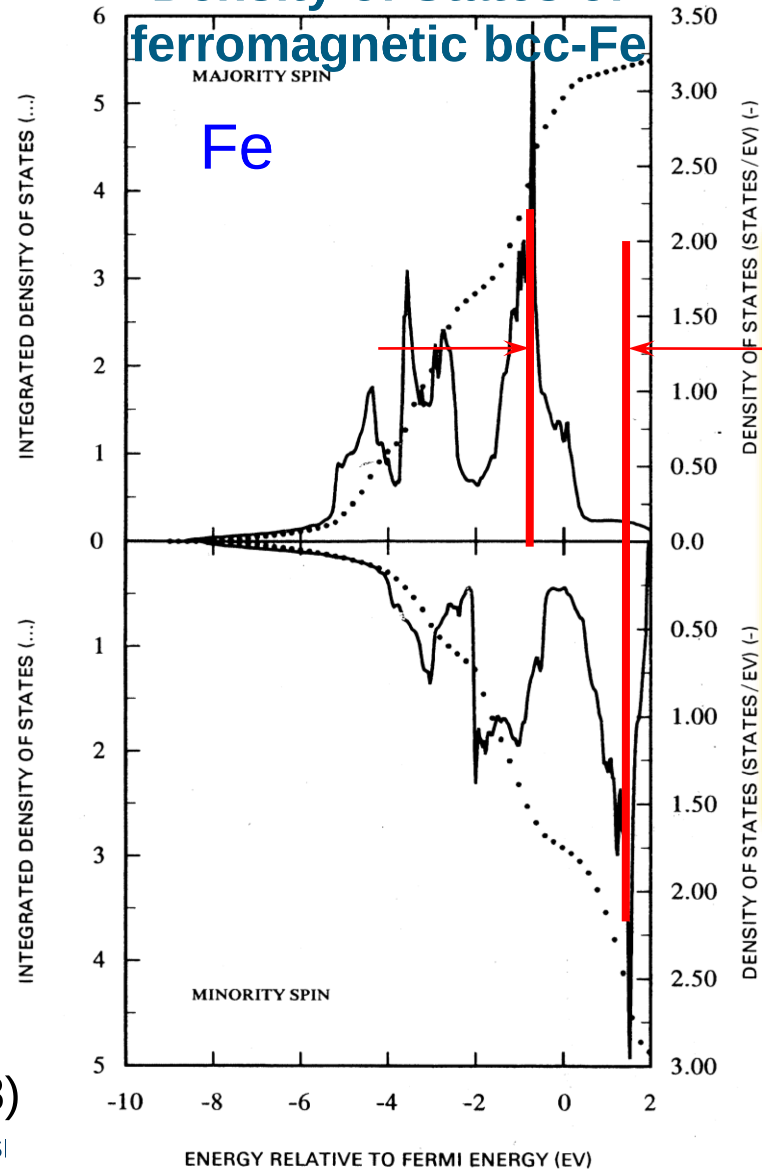
SPIN DEPENDENT ELECTRONIC STRUCTURE

Band structure of ferromagnetic fcc-Co

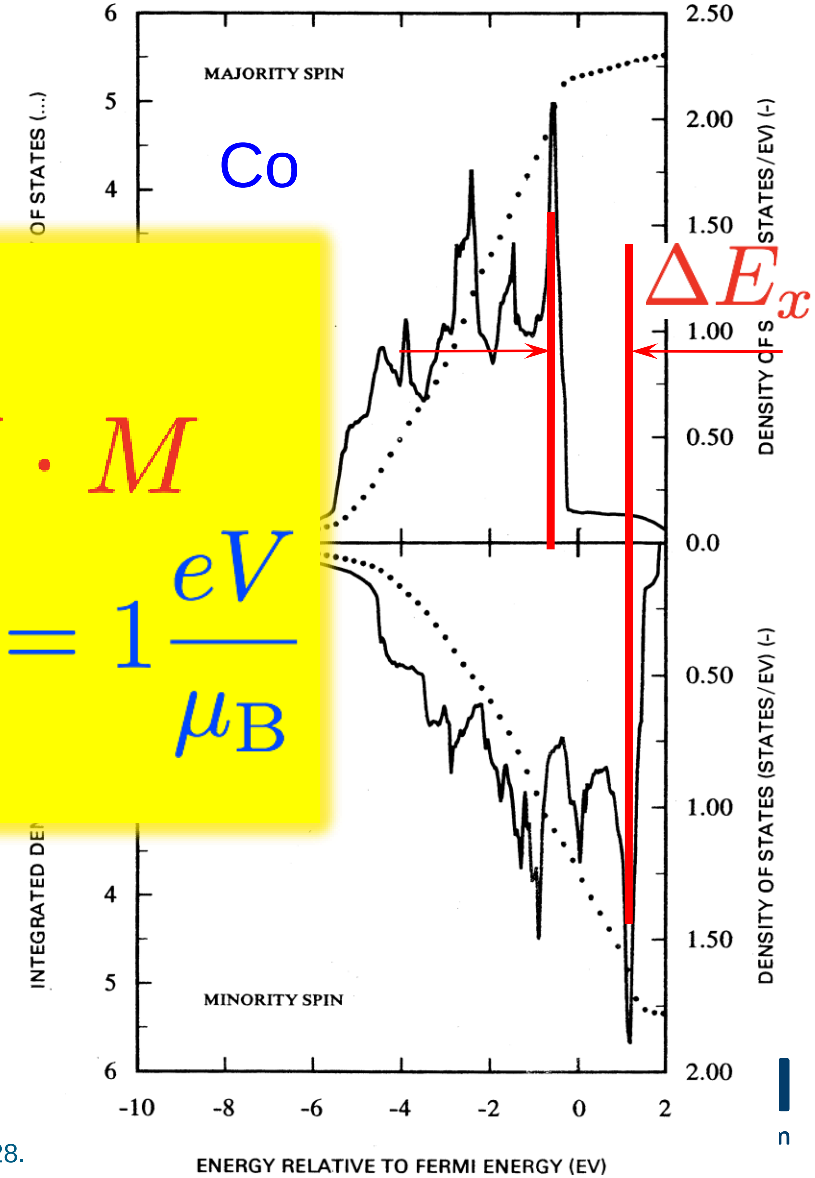


Taken from:
Moruzzi, Janak and Williams (1978)

Density of States of ferromagnetic bcc-Fe



DOS of fcc-Co



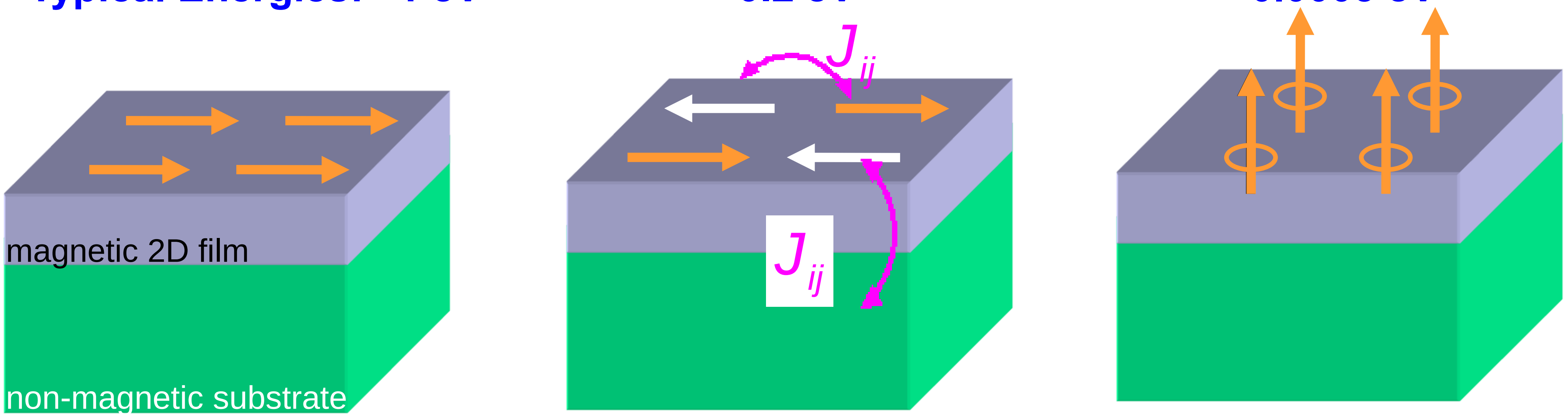
$$\Delta E_x = I \cdot M$$

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

Some basics of surfaces and interfaces

SURFACE MAGNETISM:
THREE FUNDAMENTAL QUESTIONS

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



Magnetic Moments

Magnetism: Yes or No?

Intra-atomic Exchange

$$H = -\frac{1}{2}\sum_i I_i m_i^2$$

Magnetic Order

Ferro ⟺ Antiferro

Inter-atomic Exchange

$$H = -\frac{1}{2}\sum_{i,j} J_{i,j}\,\vec{m}_i\vec{m}_j$$

Magnetic Orientation

In-plane ⟺ Out-of-plane

Spin-Orbit + Dipole-Dip

$$H = \sum_i K_i(\vec{m}_i\,\vec{e}_i)^2 + \sum_{i,j}\frac{1}{r_{i,j}^3}[\cdots])$$

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TYPICAL GROUND STATE ENERGIES

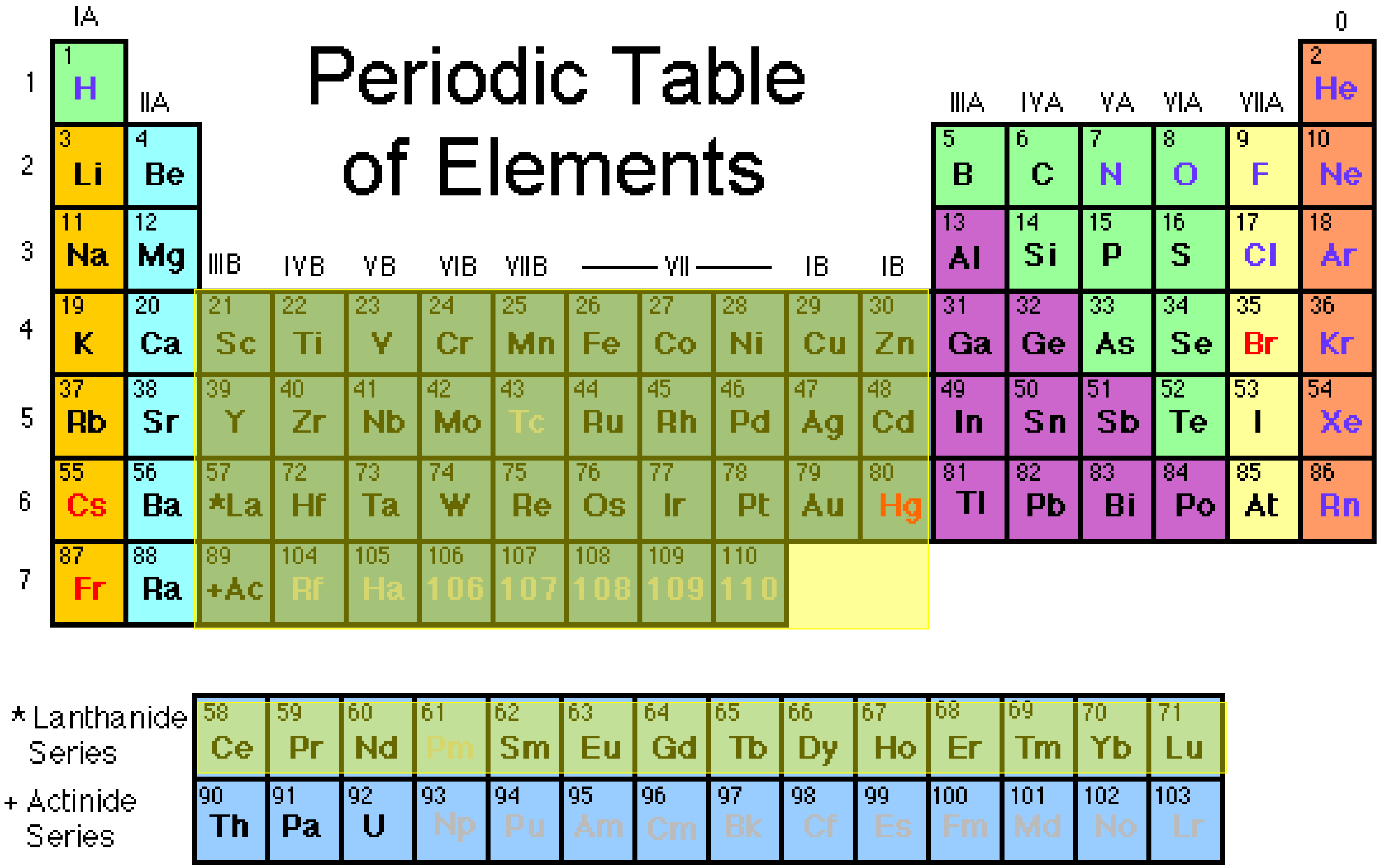
	E(eV/atom)
• Cohesive energy	5.5
• Local moment formation	1.0
• Alloy formation	0.5
• Magnetic order	0.2
• Structural relaxation	0.05
• Magnetic anisotropy	0.0005

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

MAGNETISM OF ATOMS

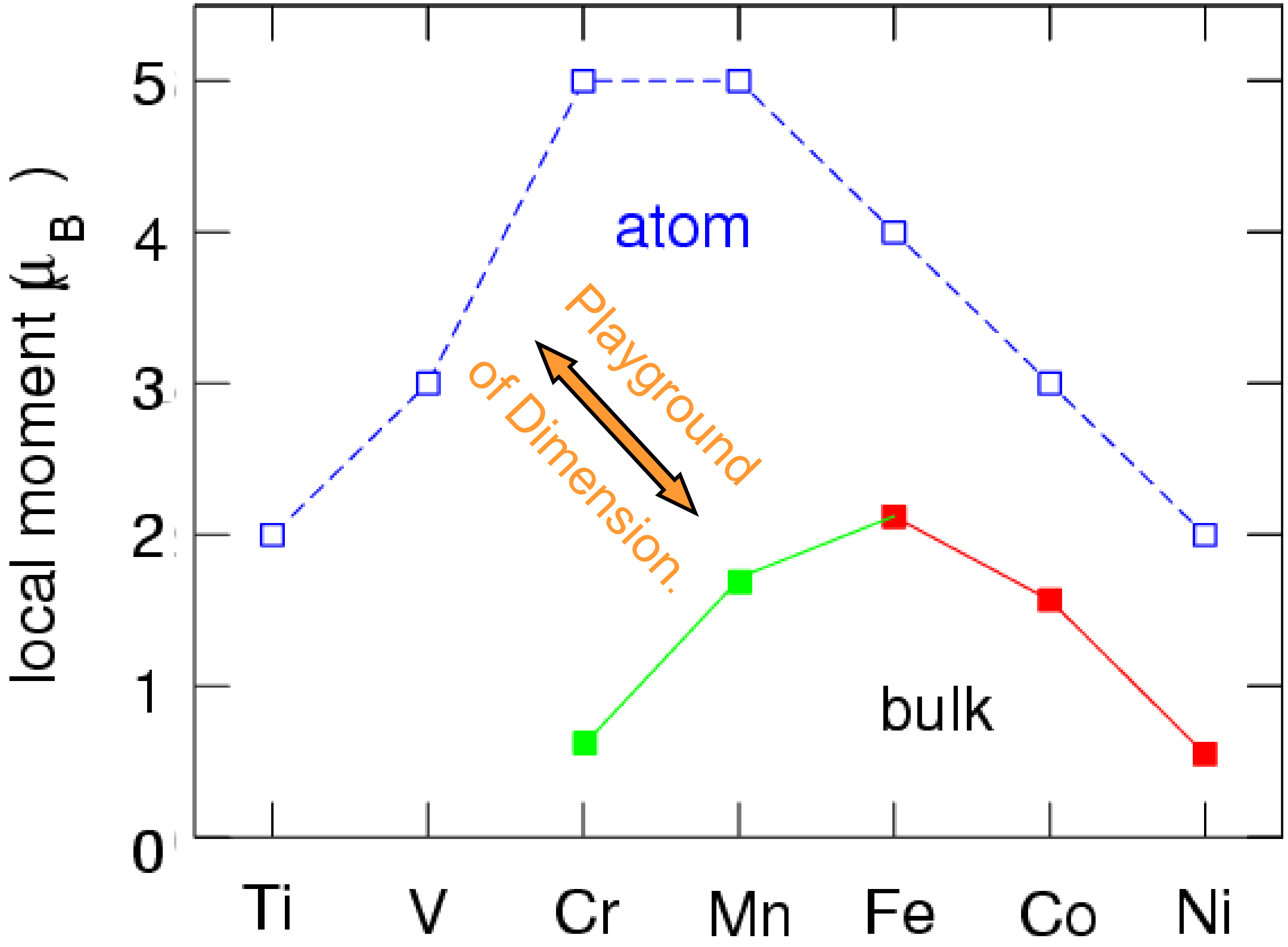
TRANSITION-METALS AND RARE EARTHS

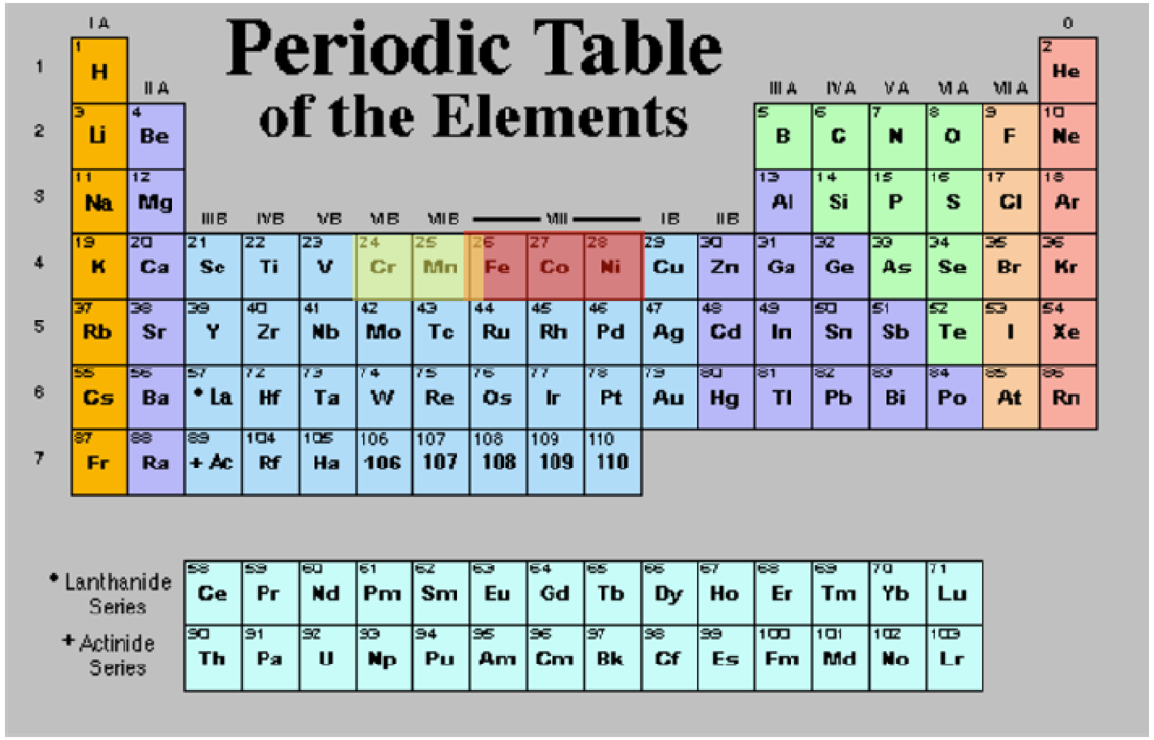
“almost all” atoms are “magnetic” (open shell atoms)



MAGNETISM IN REDUCED DIMENSION: ATOM VS BULK

"New Magnets" in reduced dimensions





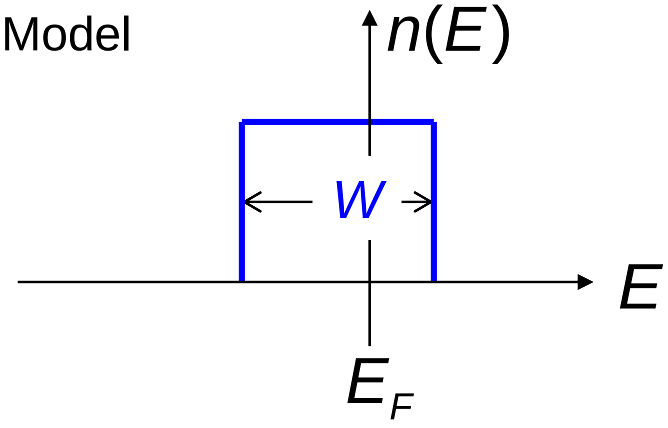
(i) Evaluation of Stoner Model for bulk materials

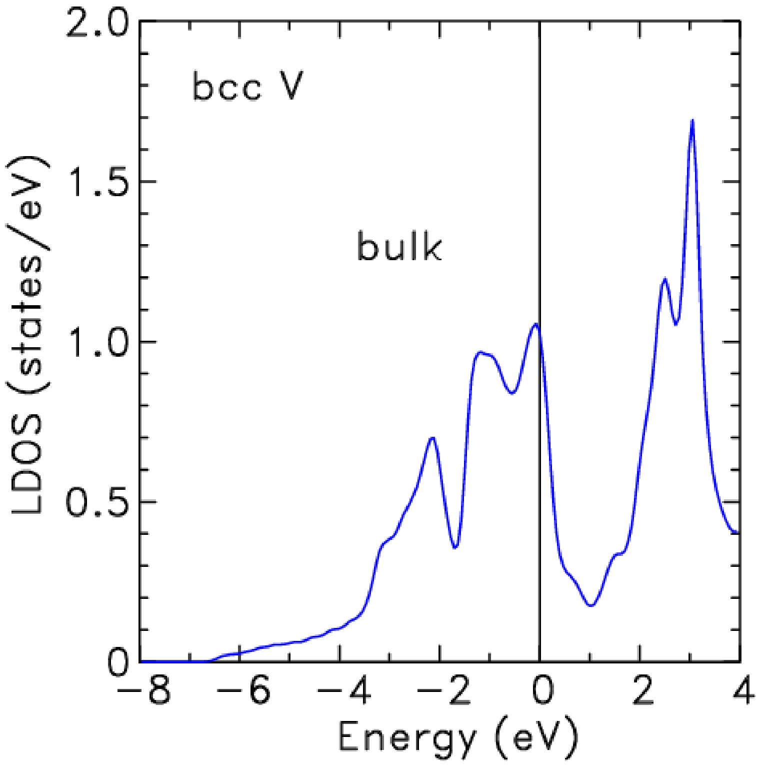
Stoner Model for Ferromagnetism

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

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

Model





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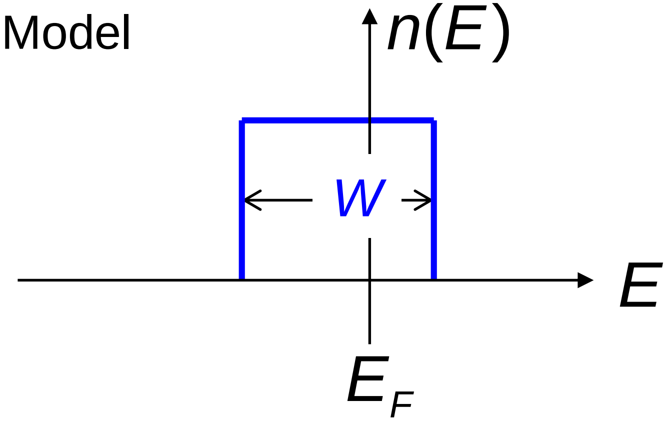
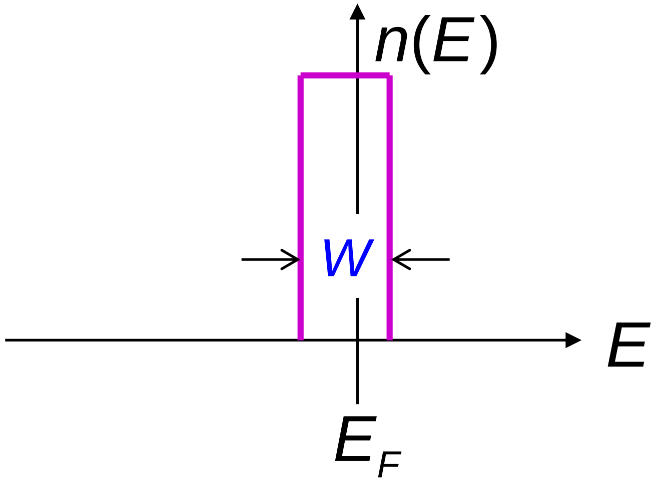
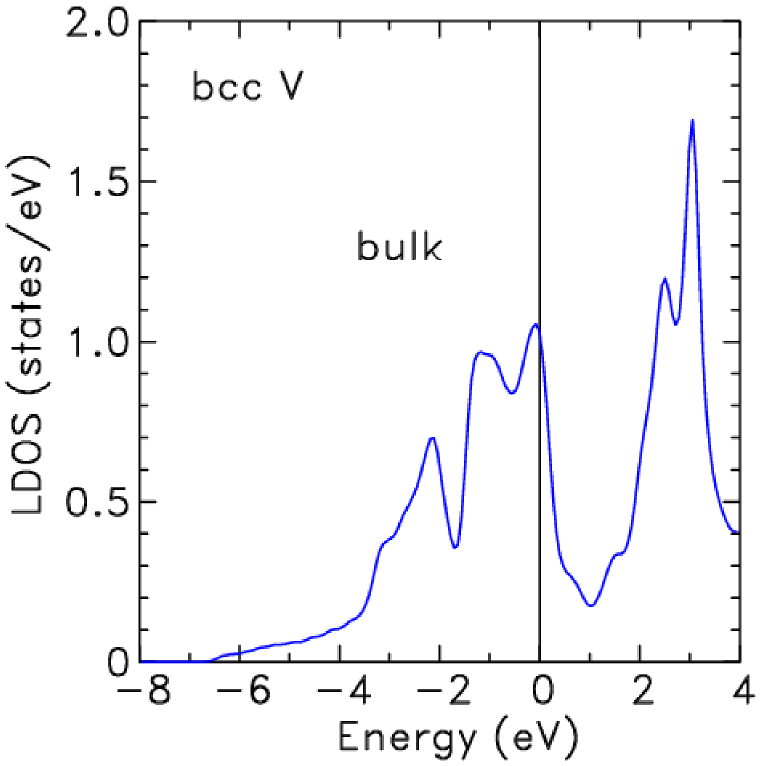
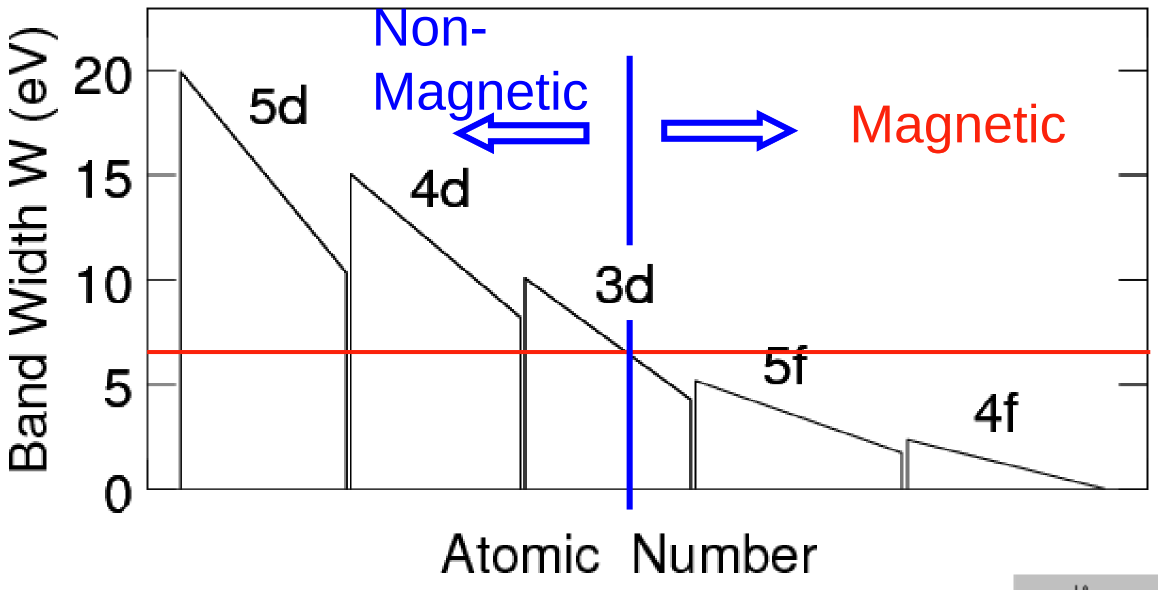
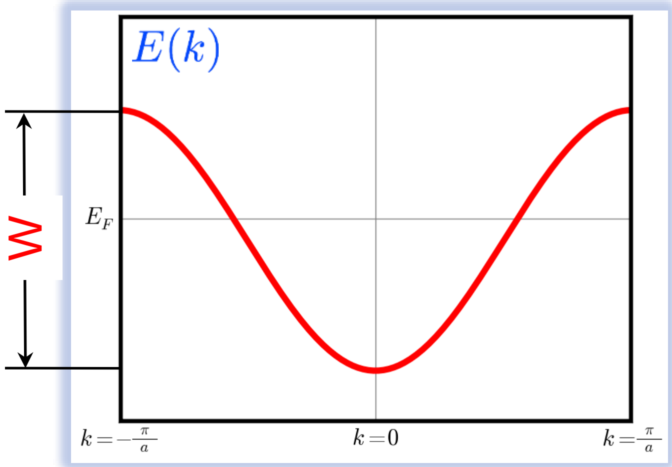


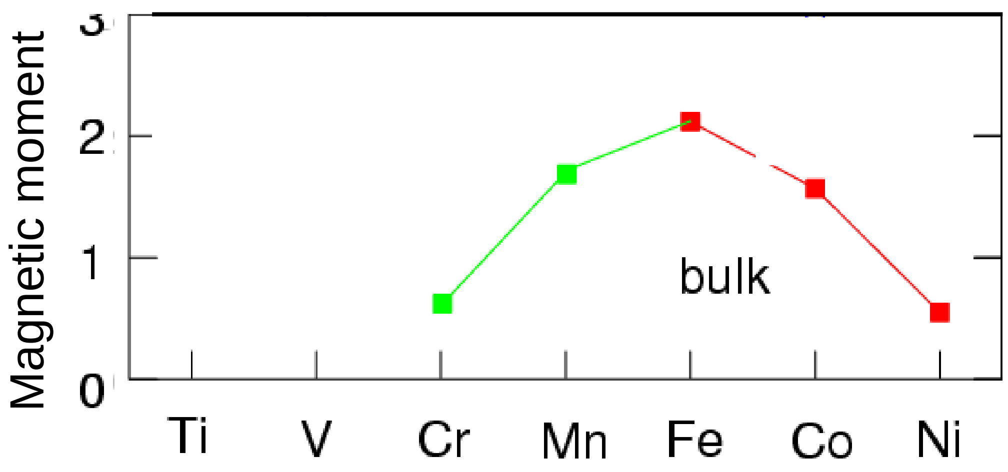


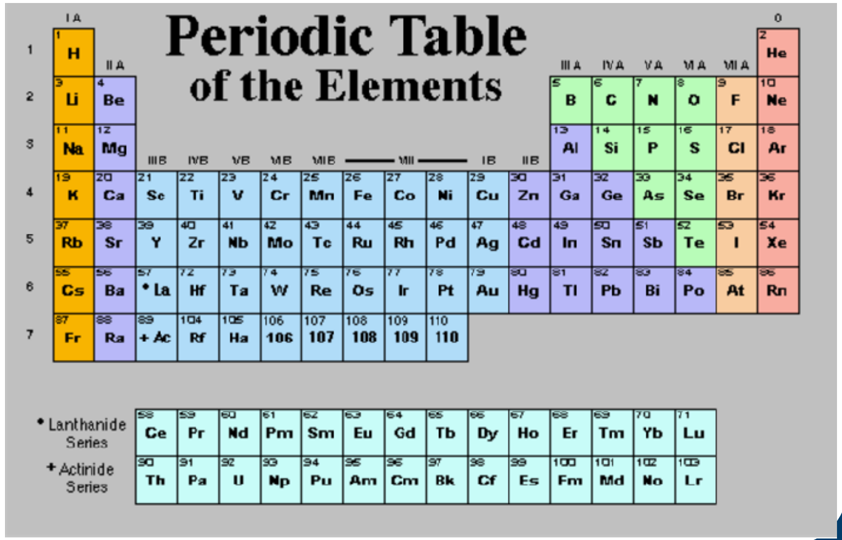


Bandwidths of metals









(ii) Magnetism in reduced dimension

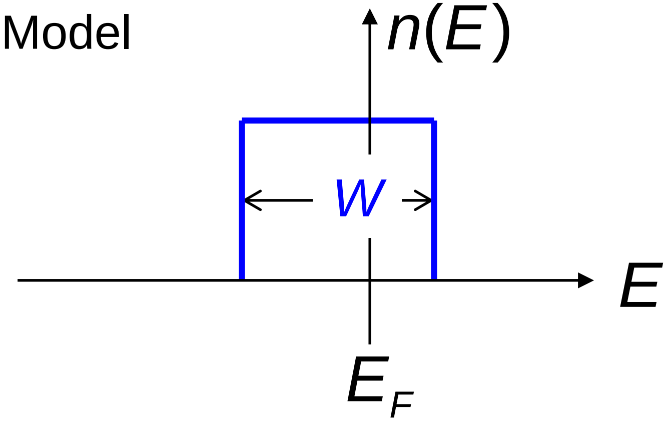
Ferromagnetic surfaces & thin films

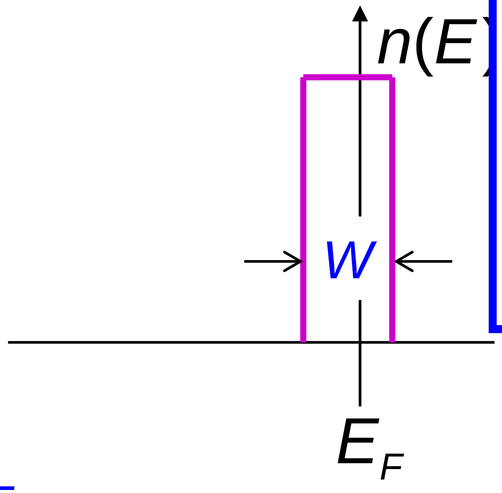
- Stoner criterion: $I \cdot n(E_F) \geq 1$

  (for d-electrons)

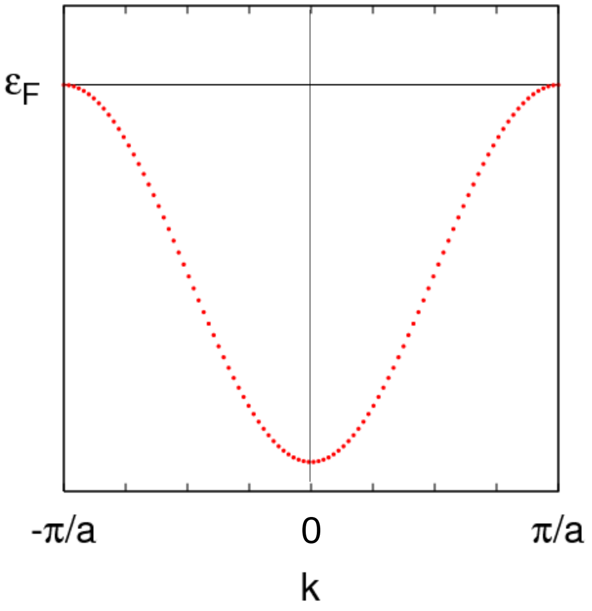
- Density of states: $n(E_F) \sim \frac{1}{W}$ $\quad [\; n \cdot W = 5 \;]$

Model

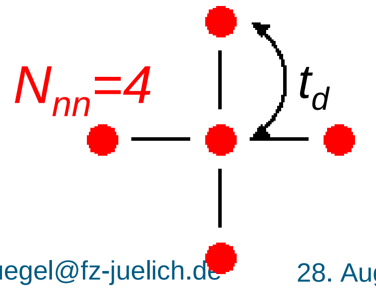




$$\varepsilon([0,0,k]) = \varepsilon_0 + 2\sqrt{N_{nn}}\, t_d \cos(ka)$$



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



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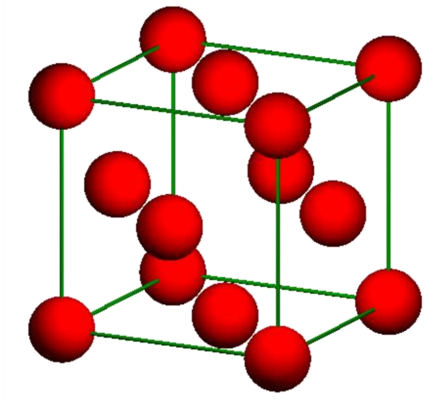
Role of Coordination Number

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

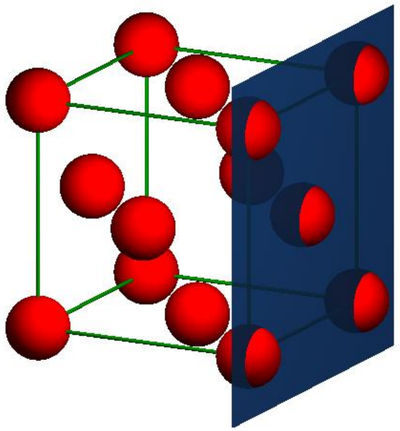


fcc-bulk:

$N_{fcc}=12$

$W_{fcc}:=1$

$n_{fcc}:=1$

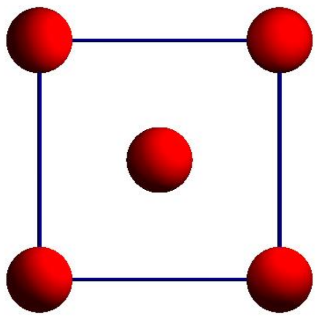


(100)-surface:

$N_{(100)}=8$

$W_{(100)}=0.82$

$n_{(100)}=1.22$



(100)-monolayer:

$N_{ML}=4$

$W_{ML}=0.58$

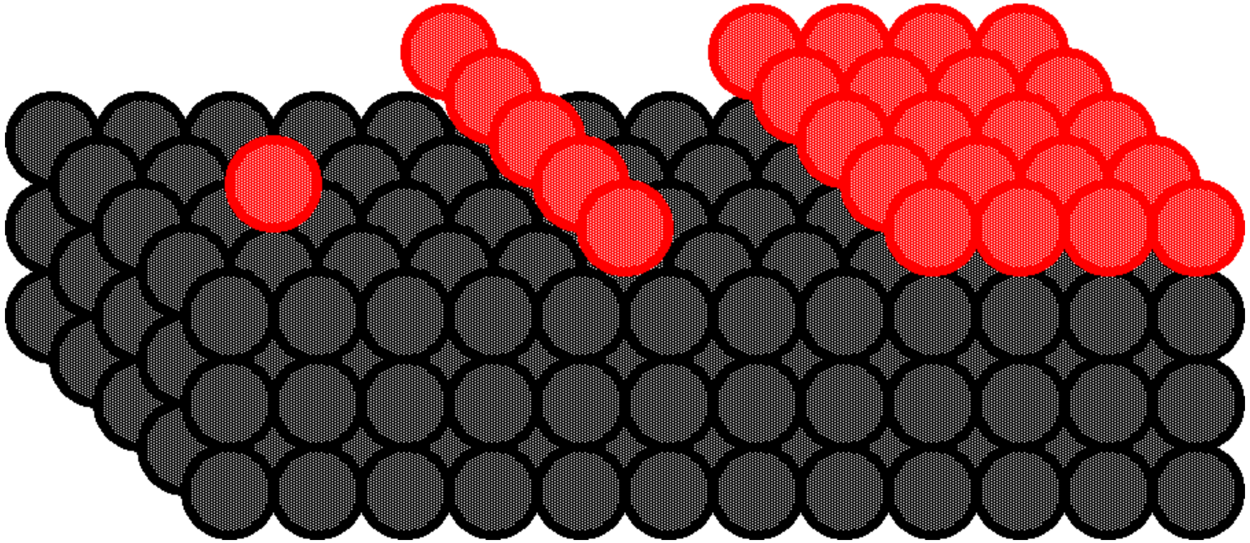
$n_{ML}=1.73$

SYSTEMS IN REDUCED DIMENSIONS

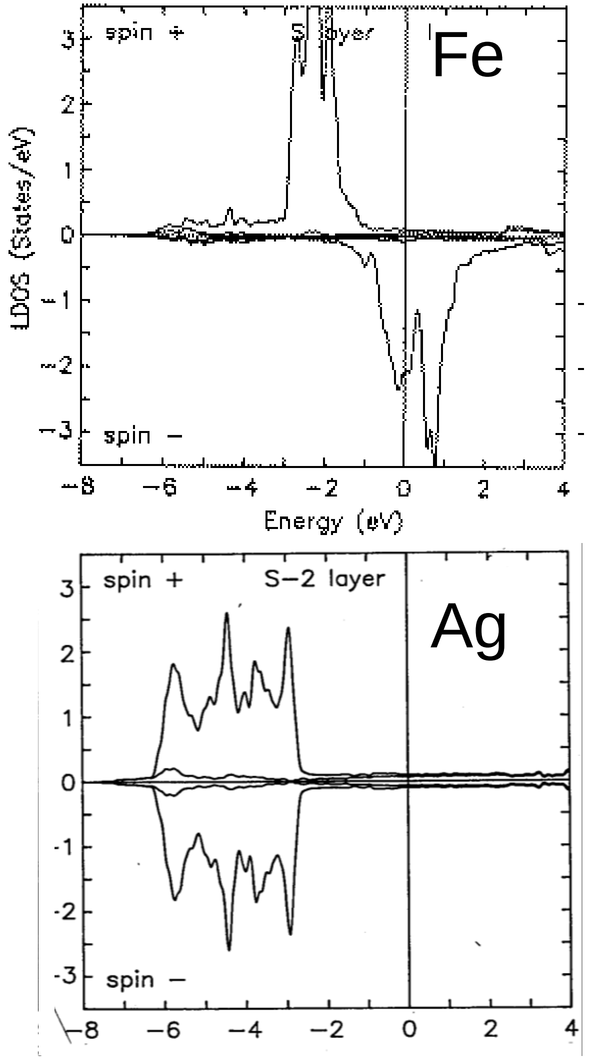
Reduced Dim.: Restrict hopping $t_{\parallel}$

Restrict exchange interaction $J_{\parallel}$

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

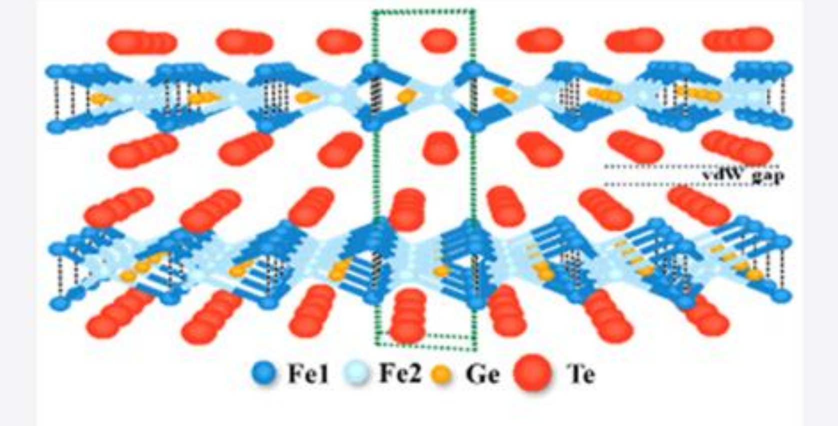


Example: Fe on Ag(100)

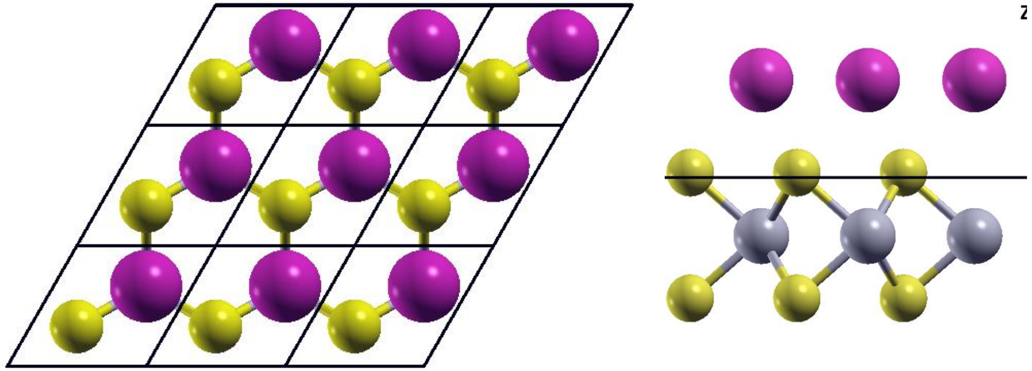


MAGNETIC 2D VAN DER WAALS MATERIALS

Bilayer of Fe_3GeTe_2



Eu on WSe_2



What is new:

- Covalent (i.e. directional) bond between spin-polarized 3d or 4f orbital and 4p or 5p chalcogenide atom
- p-orbital have a strong spin-orbit interaction => orbital texture
- Low-point symmetry ➔ various anisotropies :
  1. Magnetic Anisotropy
  2. Dzyaloshinskii-Moriya Interaction
  3. Kitaev Interaction

Surfaces

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

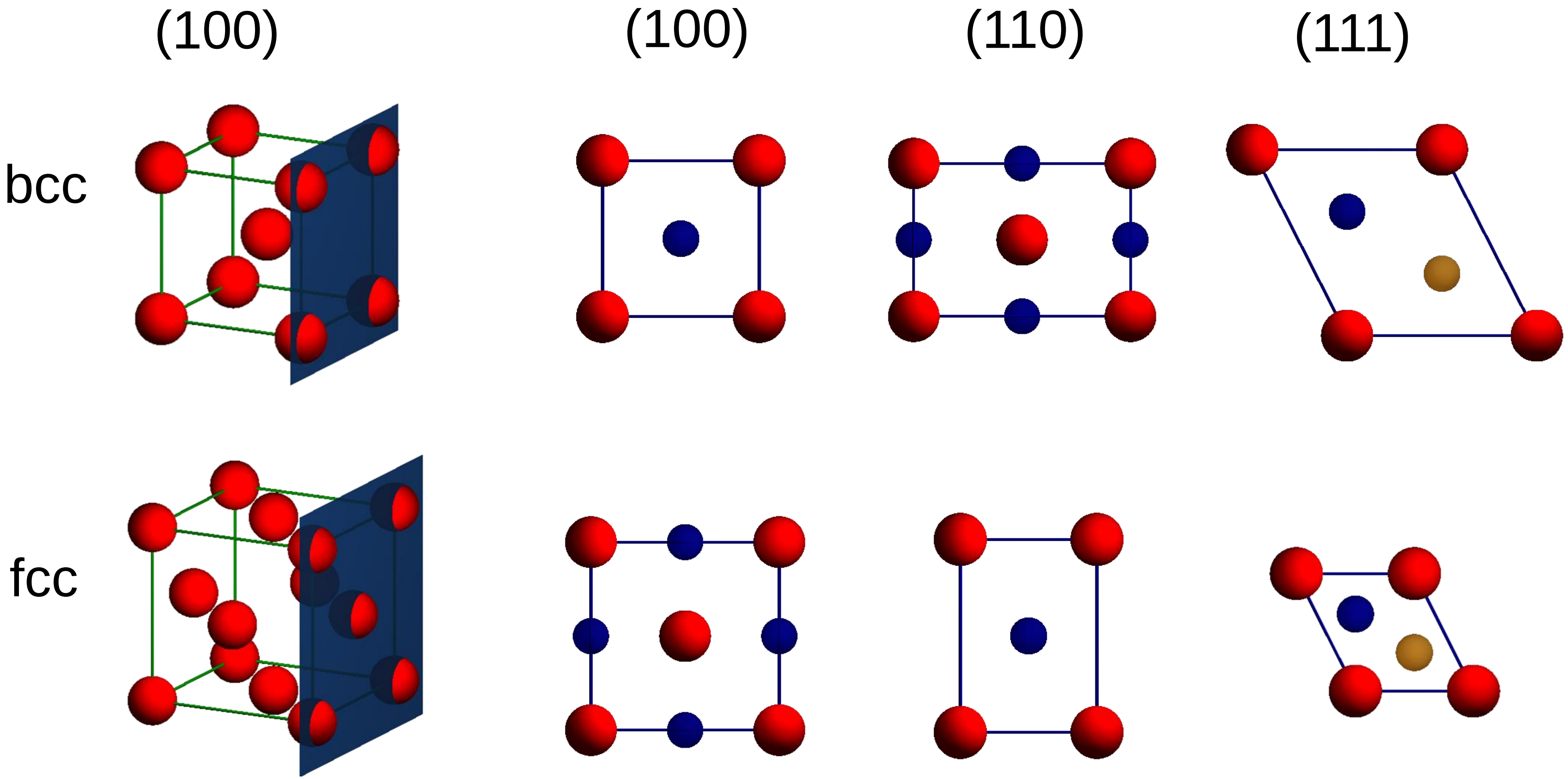
Surfaces: Magnetic Moments

(DFT results)

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

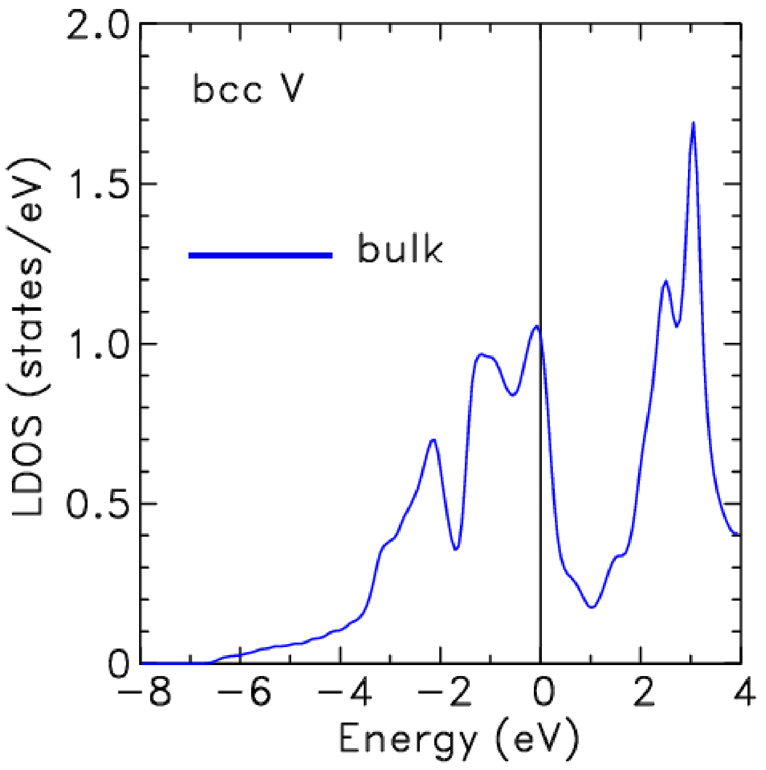


Surfaces: Magnetic Moments

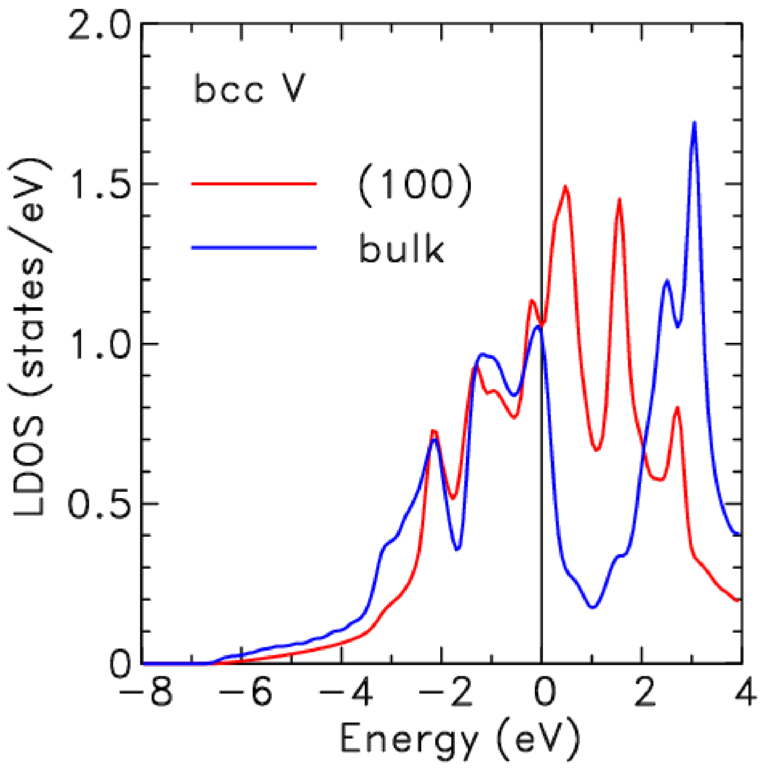
M [μ_B]	Cr (bcc)	Fe (bcc)	Co (hcp)	Ni (fcc)
(100)	2.55	2.88	1.85	0.68
(110)	—	2.43	—	0.74
(111) (0001)	—	2.48	1.70	0.63
Bulk	±0.60	2.13	1.62	0.61

Local Density of States (LDOS) of V(100)

Local Density of States
bulk V



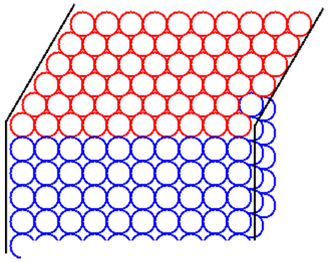
Local Density of States
bulk V
surface V(100)



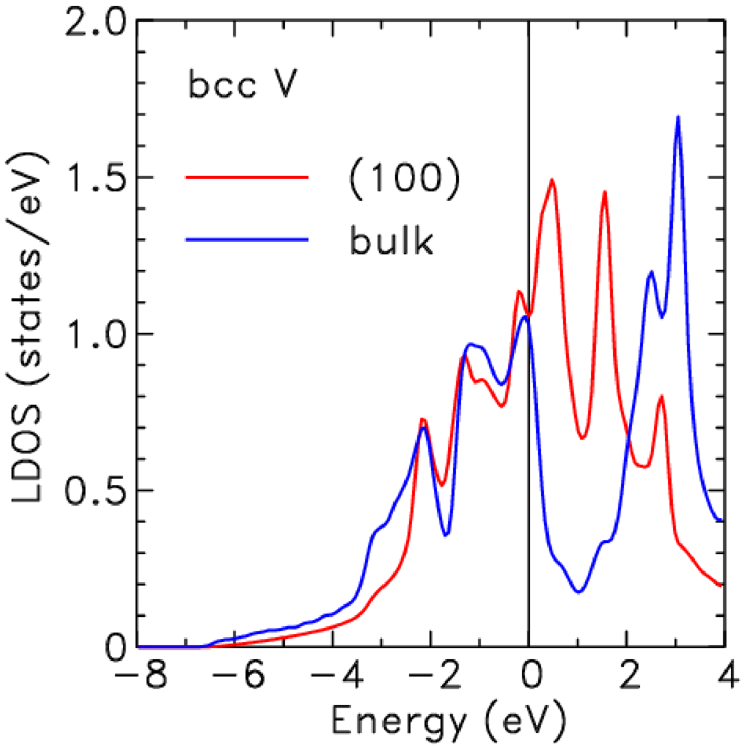
V bulk and surface (100) : nonmagnetic

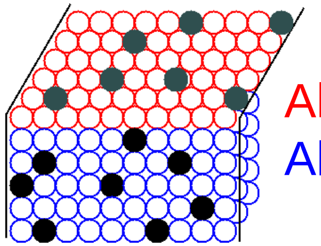
(100) SURFACES OF VRu, VRh, VPd ALLOYS

Local Density of States

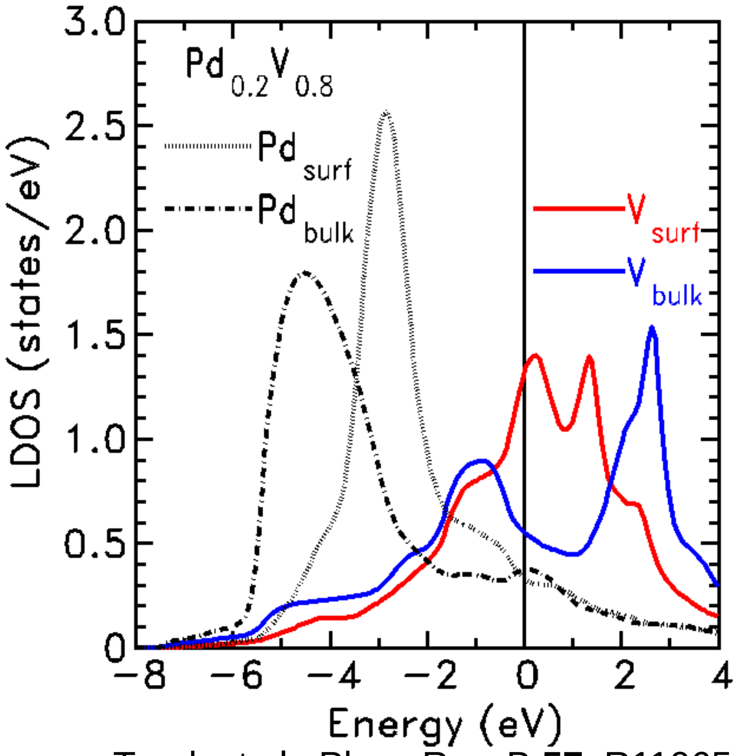


Clean surface V(100)
bulk V





Alloyed surface VPd(100)
Alloyed bulk VPd

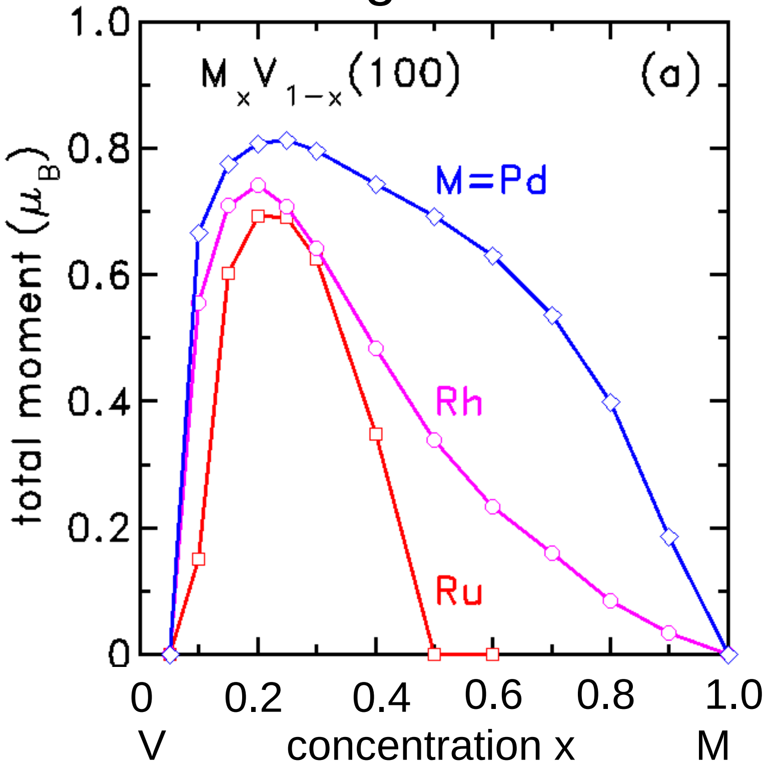


Turek et al, Phys. Rev. B **57**, R11065 (1998)

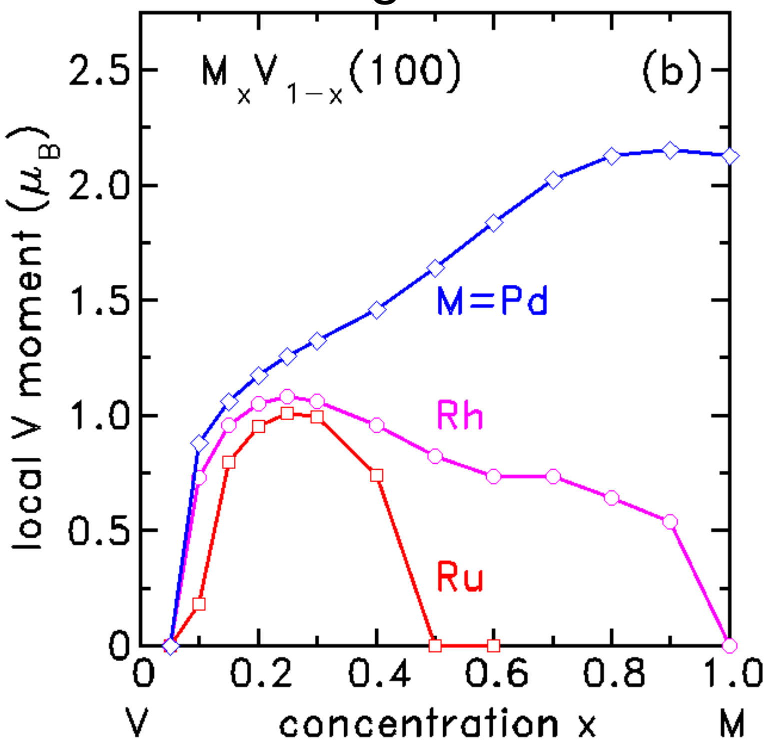
(100) SURFACES OF VRu, VRh, VPd ALLOYS

Magnetic Moment

Total magnetic moment



Local magnetic moment V

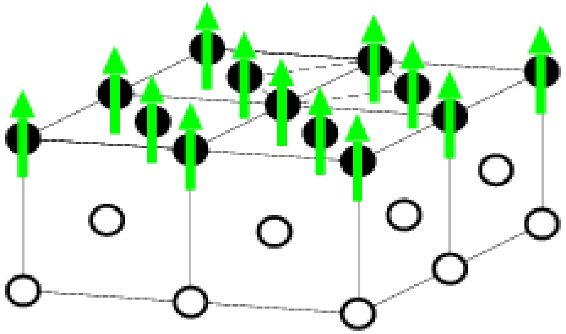


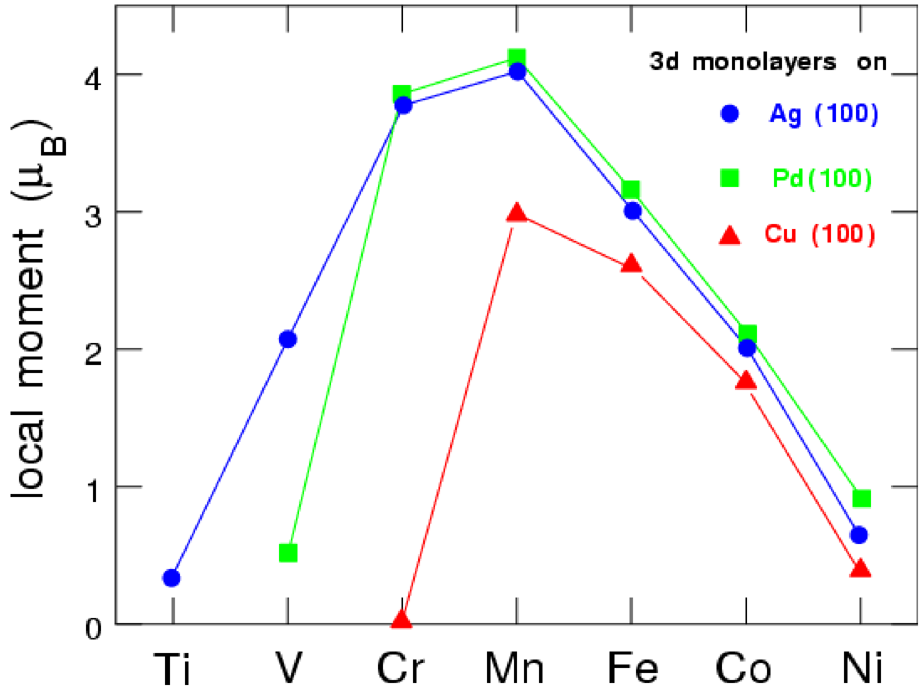
Turek et al, Phys. Rev. B **57**, R11065 (1998)

Ultrathin Films

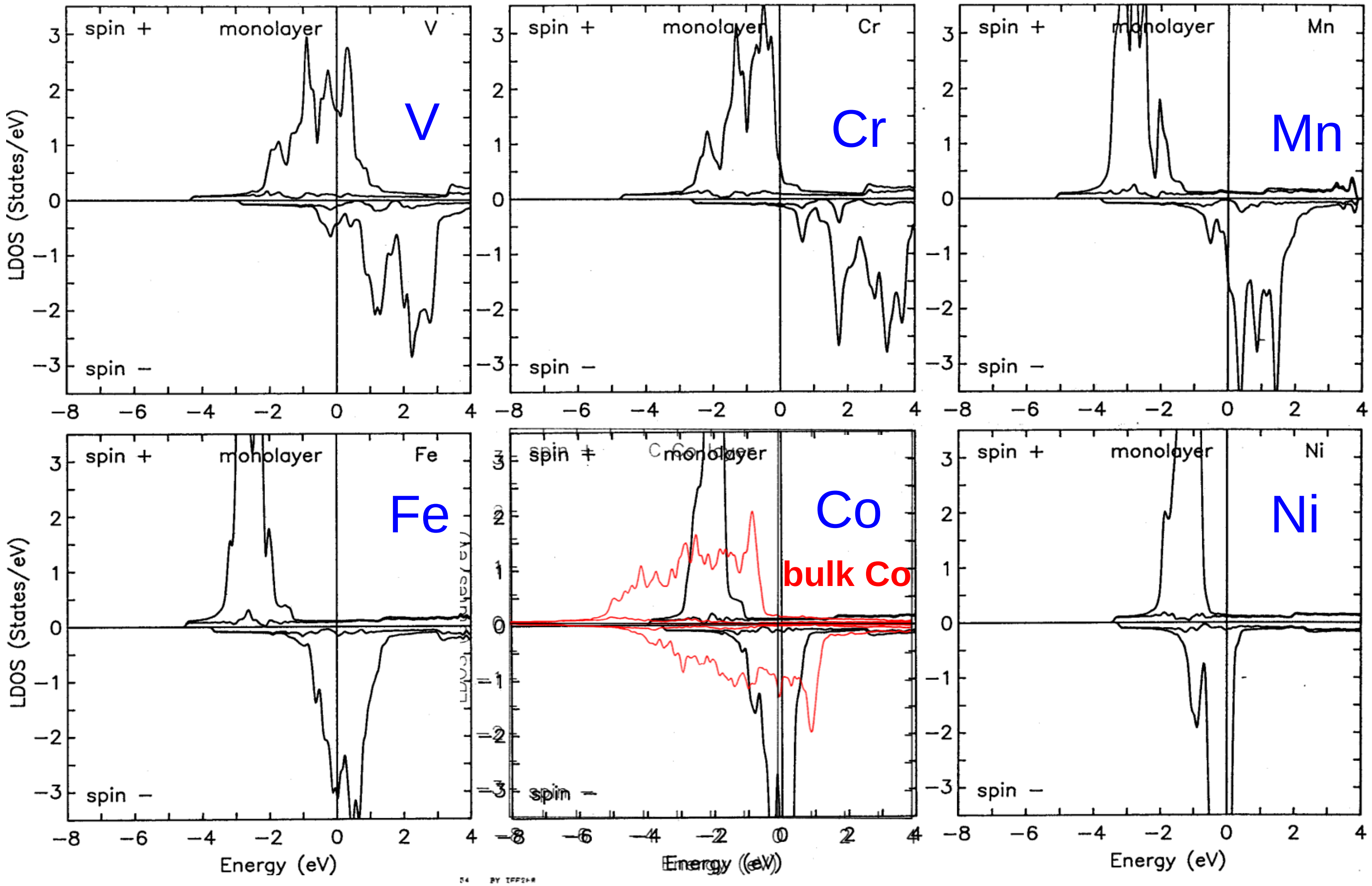
Realization on Noble Metal substrates
e.g. 3d on Ag(100)

2D-FERROMAGNETISM OF 3d-MONOLAYERS ON NOBEL METAL (100) SUBSTRATE





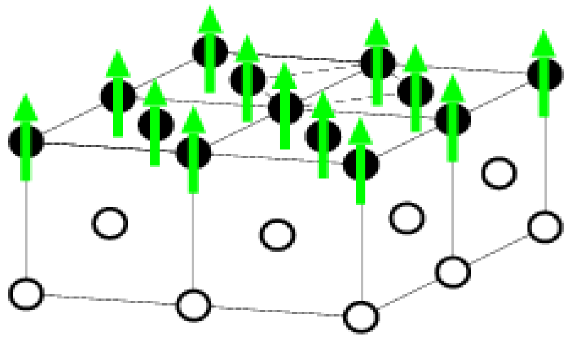
LDOS of Ferromagnetic 3d-metal/Ag(100)

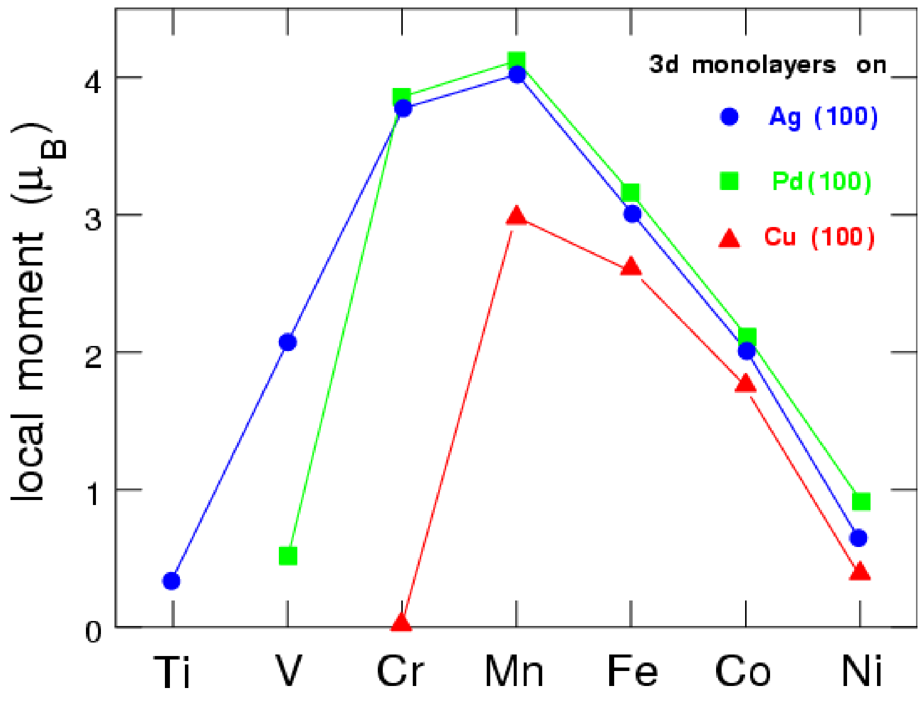


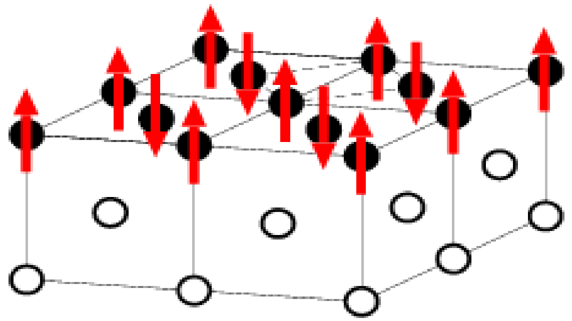
S. Blügel, D. Drittler, R. Zeller, and P.H. Dederichs, Appl. Phys. A **49**, 547 (1989)

Antiferromagnetism

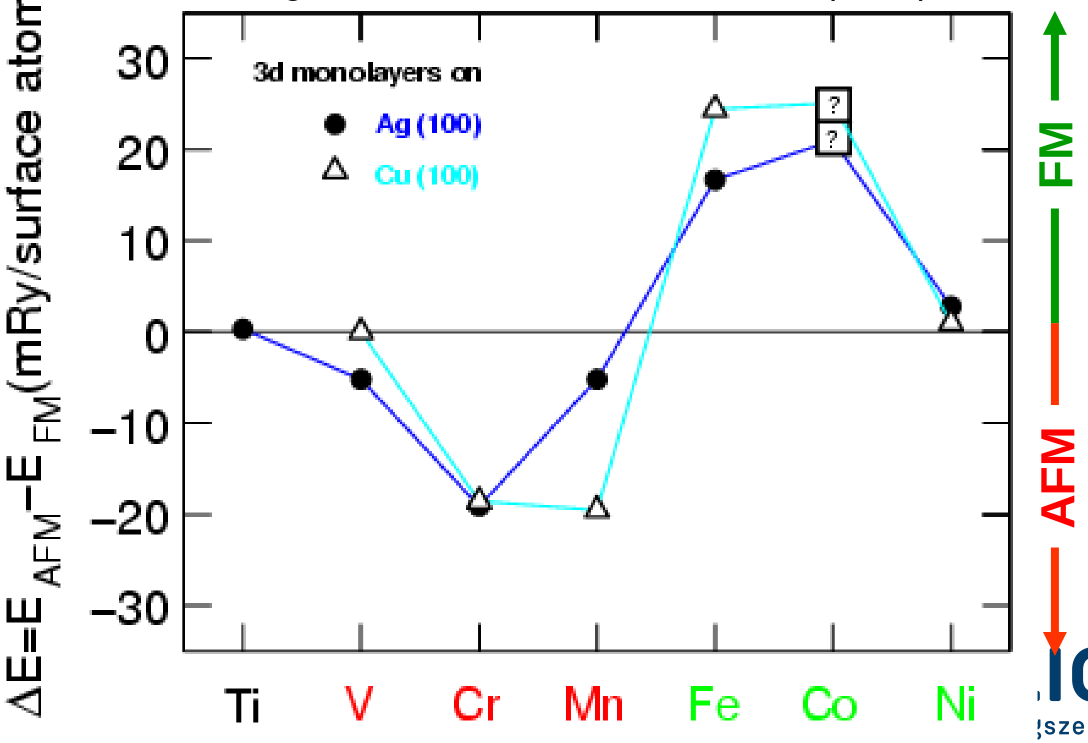
2D-ANTIFERROMAGNETISM OF MONOLAYERS ON NM(100)







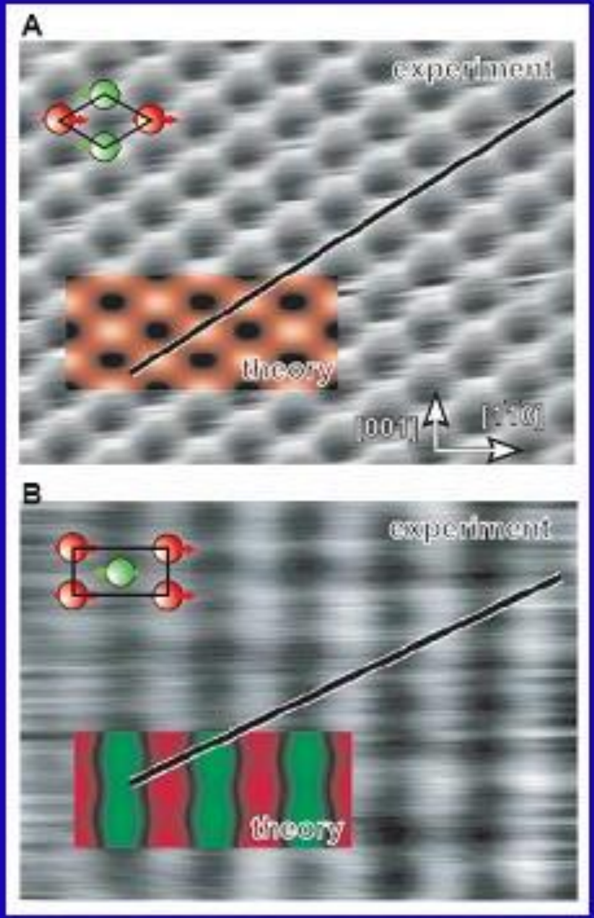
Blügel, Weinert, Dederichs, PRL **60** (1988)



SPIN-POLARIZED SCANNING TUNNELING MICROSCOPY EXPERIMENT

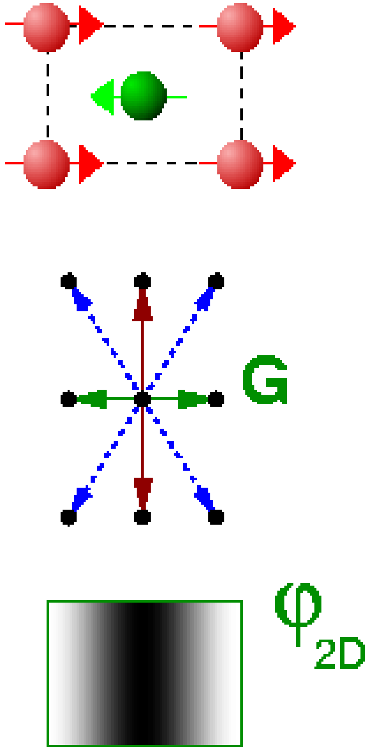
Mn on W(110)

- line contrast with magnetic tip
- ➢ Mn/W(110) is a collinear antiferromagnet

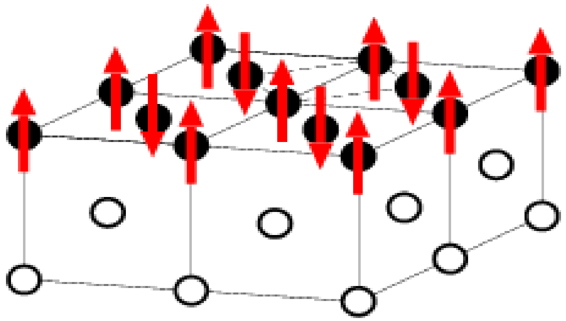


tip:	W or Fe/W
sample:	0.7 ML Mn/W(110)
STM:	U_{bias} = -3 mV
	I_{tun} = 40 nA
	T = 13 K

🗎 S. Heinze *et al.*, Science **288**, 1805 (2000)

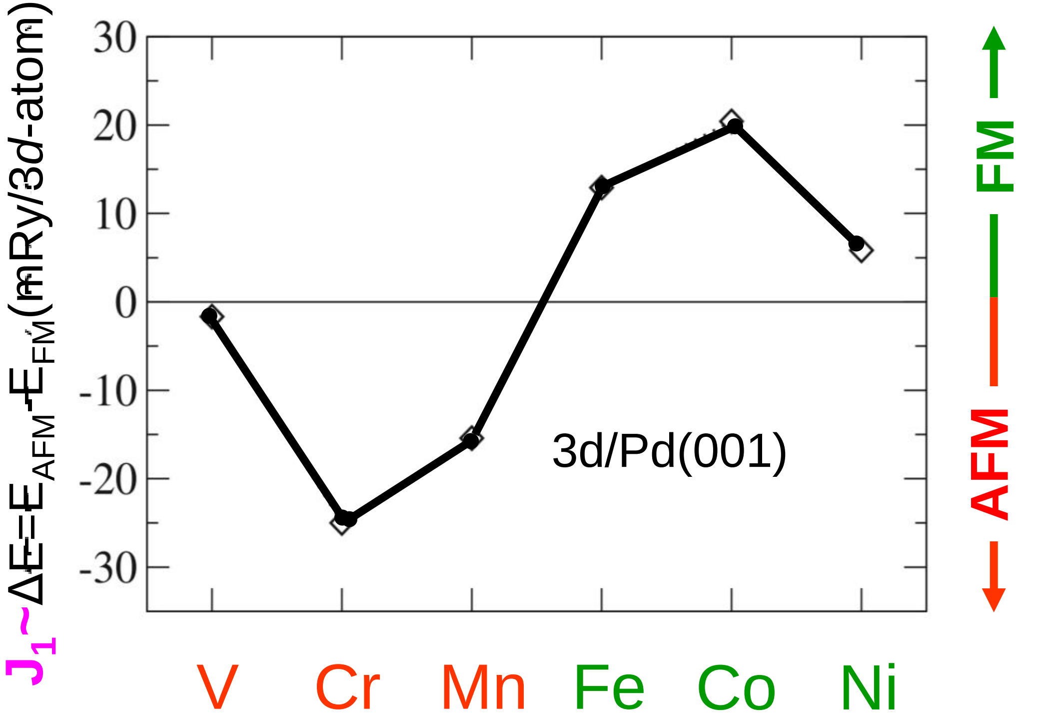


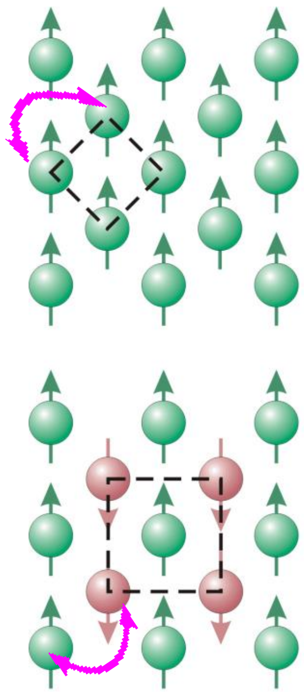
NEAREST NEIGHBOR HEISENBERG MODEL



$$E = -\frac{1}{2}\sum_{ij} J_{ij}\, \mathbf{M}_i \cdot \mathbf{M}_j$$

Nearest neighbor: $J_{ij} \approx J_1$

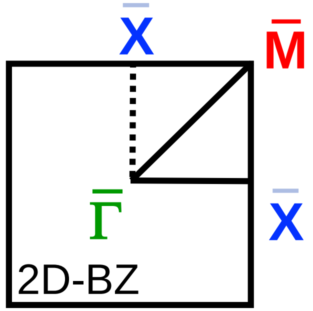


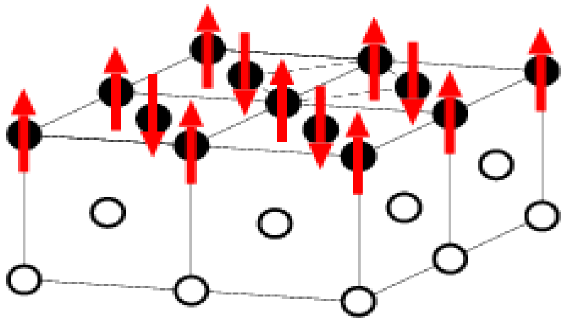


Blügel, Weinert, Dederichs, PRL **60** (1988)

BEYOND NEAREST NEIGHBOR HEISENBERG MODEL

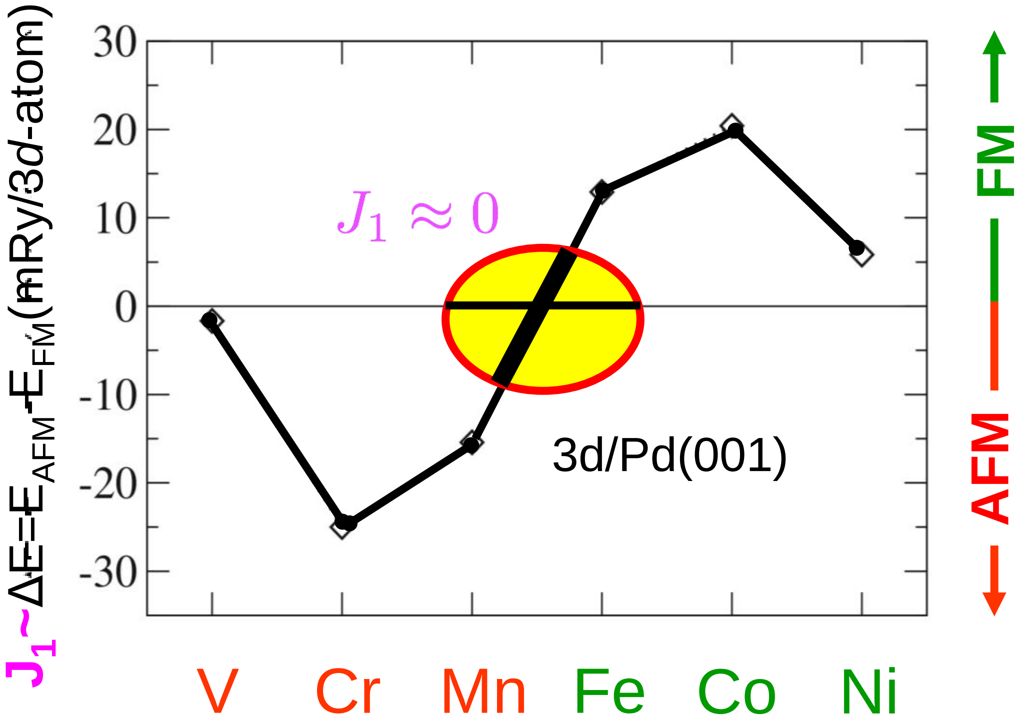
Spin spirals

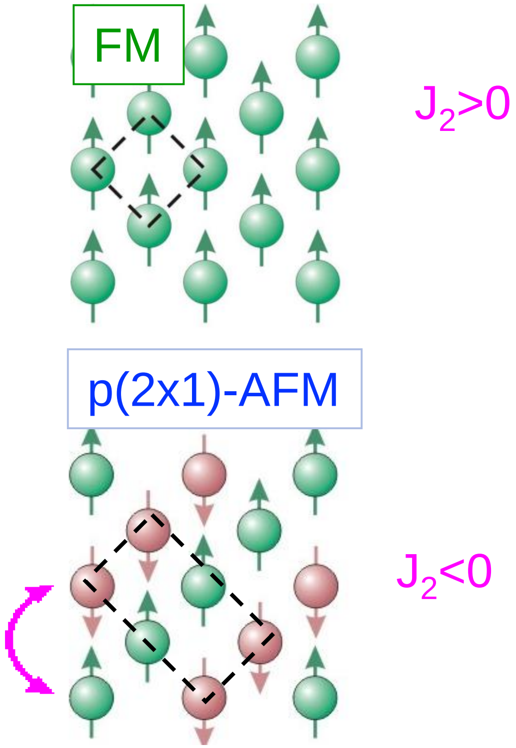


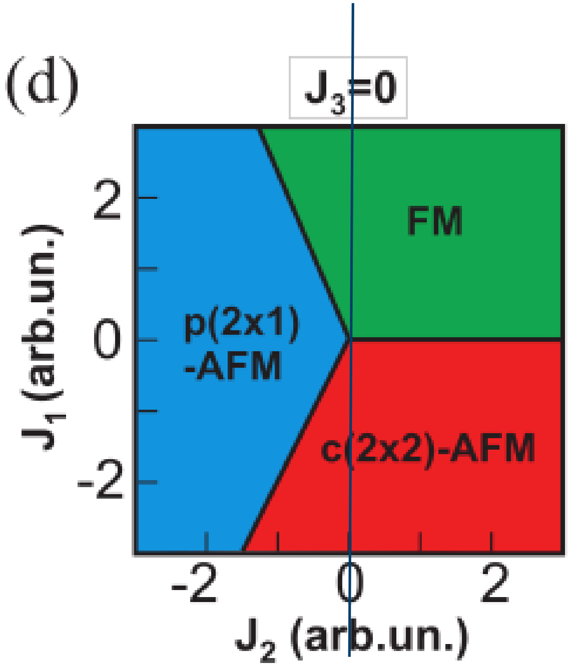


$$E = -\frac{1}{2}\sum_{ij} J_{ij}\, \mathbf{M}_i \cdot \mathbf{M}_j$$

Next nearest neighbor: $J_{ij} \approx J_1, J_2$

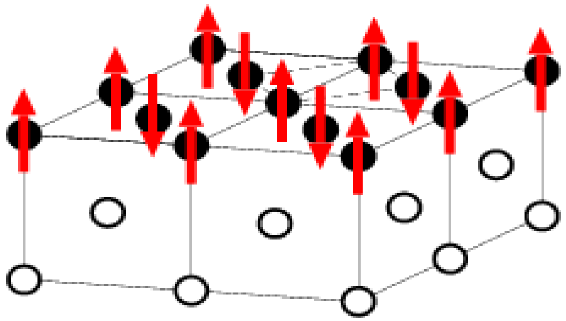






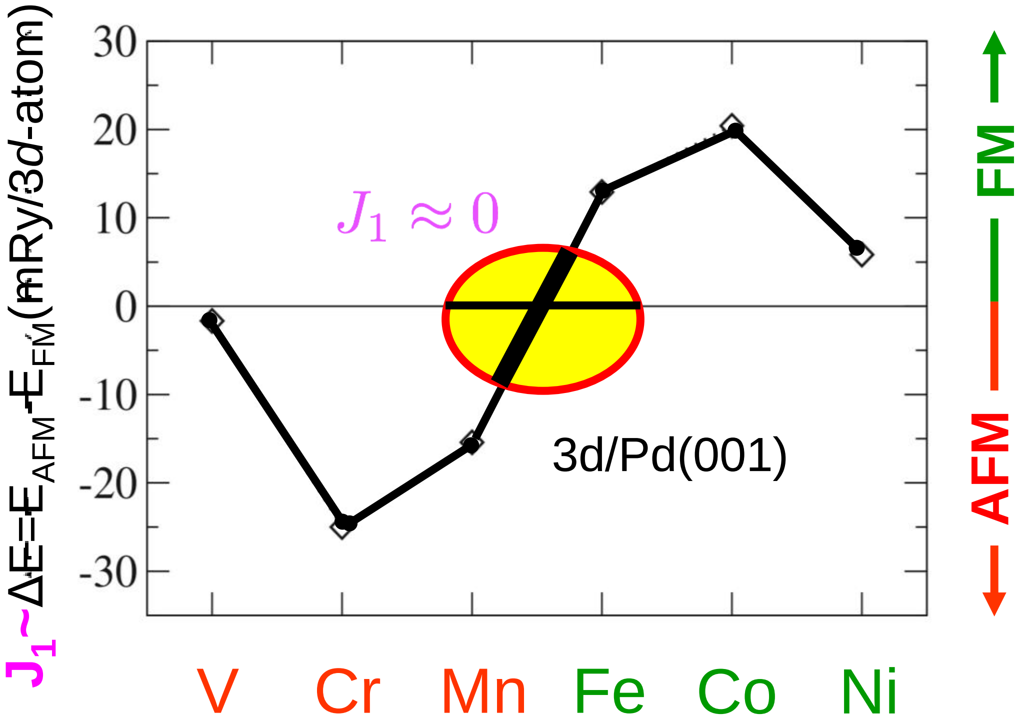
Blügel, Weinert, Dederichs, PRL **60** (1988)

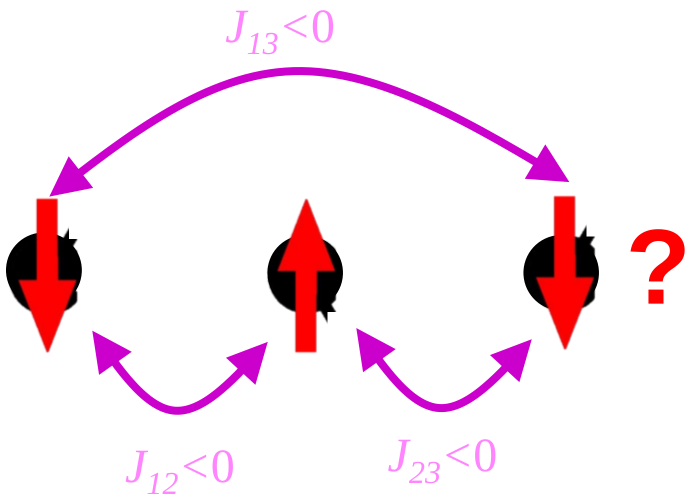
BEYOND NEAREST NEIGHBOR HEISENBERG MODEL

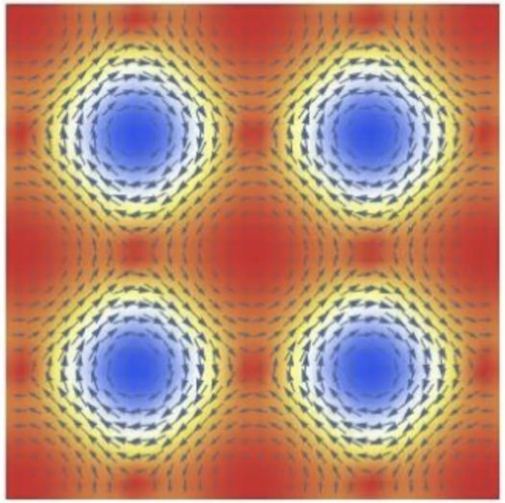


$$E = -\frac{1}{2}\sum_{ij} J_{ij}\,\mathbf{M}_i \cdot \mathbf{M}_j$$

- Magnetic exchange frustration



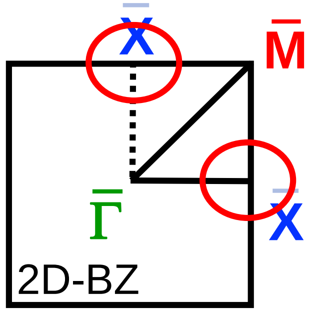


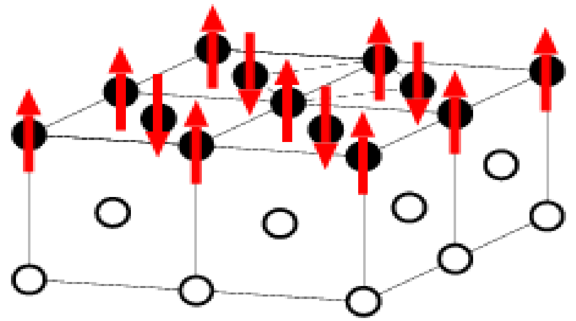


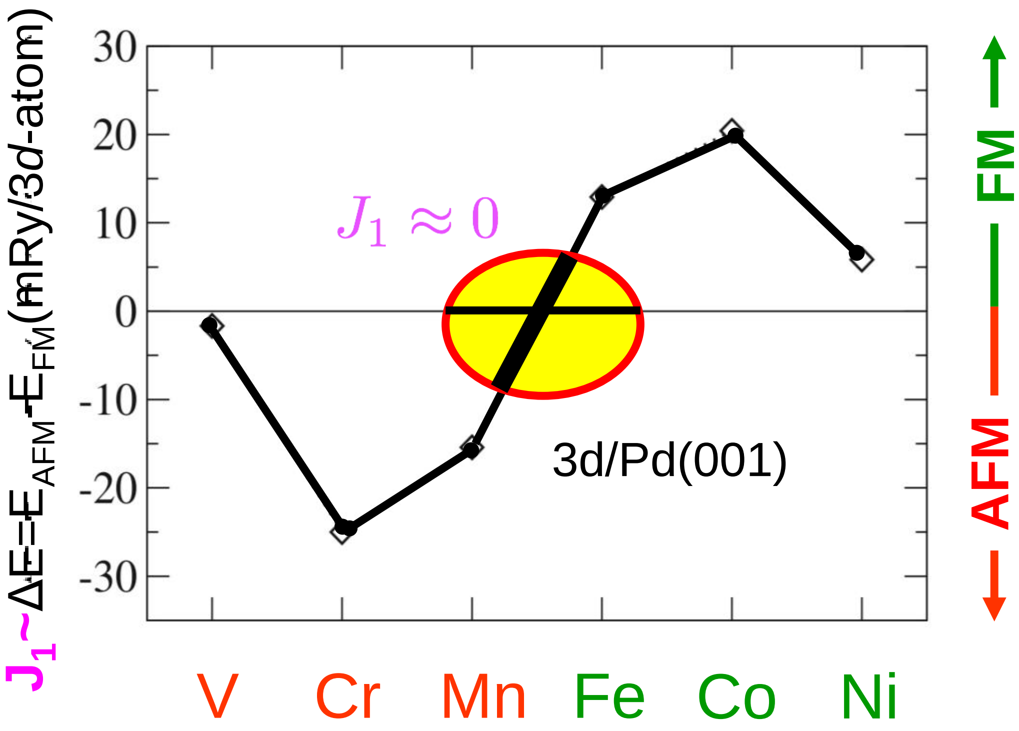
N. D. Khanh *et al.*, Nature Nanotech. **15**, 444 (2020)

BEYOND HEISENBERG MODEL

Spin spirals





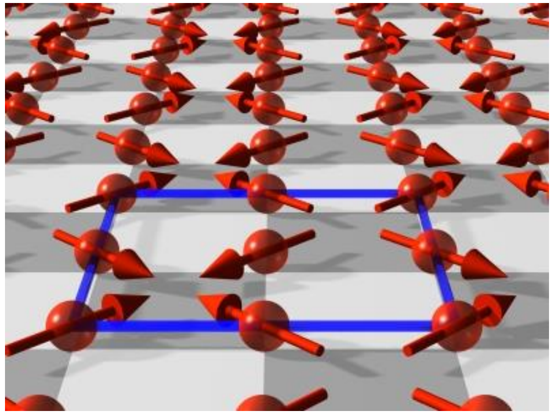


Beyond Heisenberg:

e.g. biquadratic interaction:

$$E_{\mathrm{biq}} = -\frac{1}{2}\sum_{ij} B_{ij}\,(\mathbf{M}_i \cdot \mathbf{M}_j)^2$$

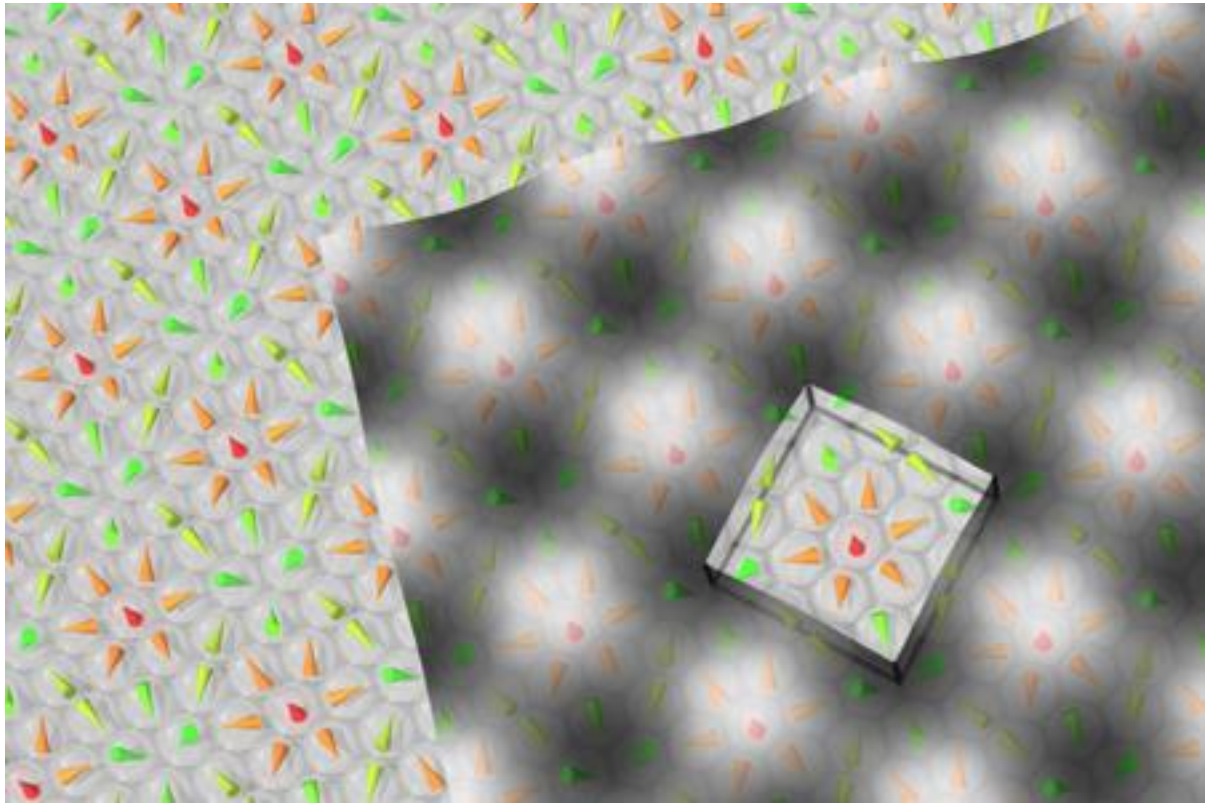
$$\mathbf{S}_n \sim \left(\mathbf{S}_{(\pi,0)} e^{i(\pi,0)\mathbf{R}_n} + cc\right) + \left(\mathbf{S}_{(0,\pi)} e^{i(0,\pi)\mathbf{R}_n} + cc\right)$$



P.Ferriani, I.Turek, S.Heinze, G.Bihlmayer, & S.Blügel, PRL (2007).

ATOMIC SCALE MAGNETIC SKYRMION LATTICE FE ON IR(111)

Beyond Heisenberg interaction



S. Heinze, K. von Bergmann, M. Menzel, J. Brede, A. Kubetzka, R. Wiesendanger, G. Bihlmayer and S. Blügel, Nat. Phys. **7**, 713 (2011)

$$H = -\sum_{ij} J_{ij}\,(\mathbf{S}_i \cdot \mathbf{S}_j)$$ exchange interaction

$$-\sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$ DM interaction

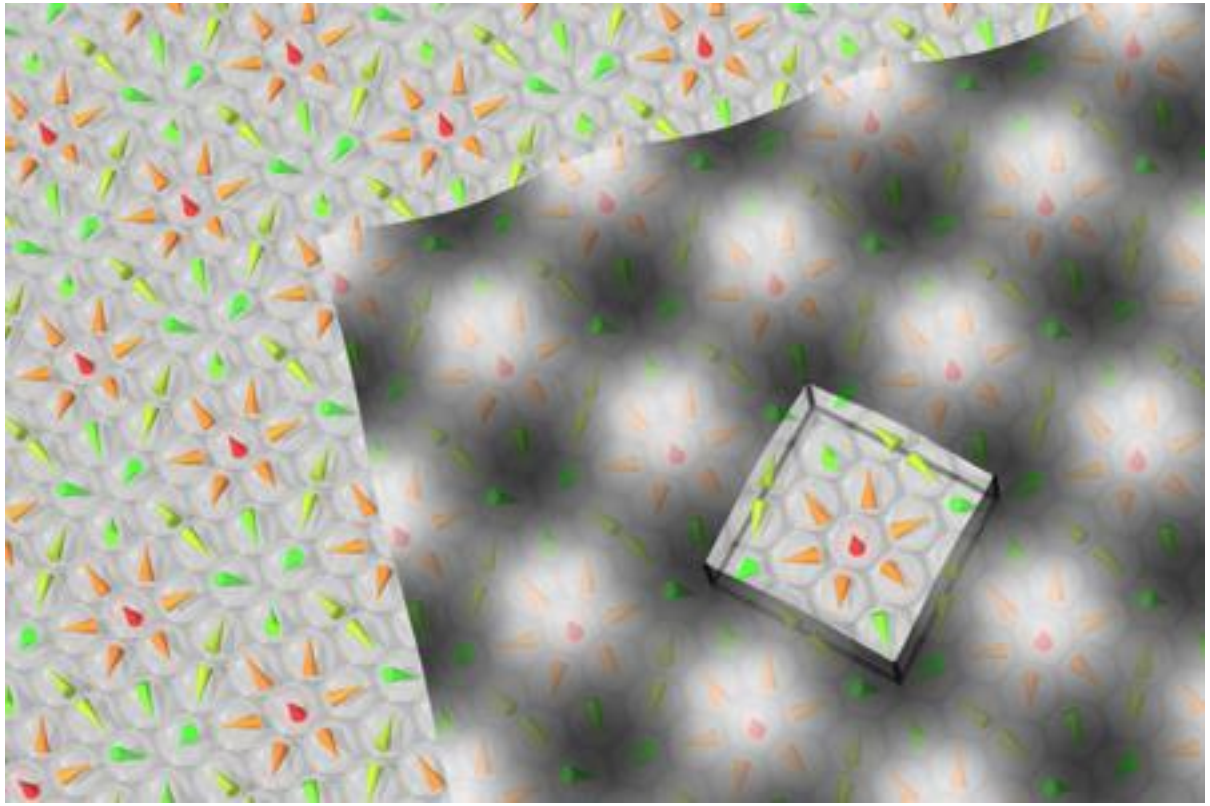
$$-\sum_{ijkl} K_{ijkl}\,[\,(\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) + (\mathbf{S}_i \cdot \mathbf{S}_l)(\mathbf{S}_j \cdot \mathbf{S}_k) - (\mathbf{S}_i \cdot \mathbf{S}_k)(\mathbf{S}_j \cdot \mathbf{S}_l)]$$ 4-spin interaction

$$-\sum_{ij} B_{ij}\,(\mathbf{S}_i \cdot \mathbf{S}_j)^2$$ biquadratic interaction

$$-\sum_{i} K_i\, S_i^2\, sin^2\phi_i$$ anisotropy

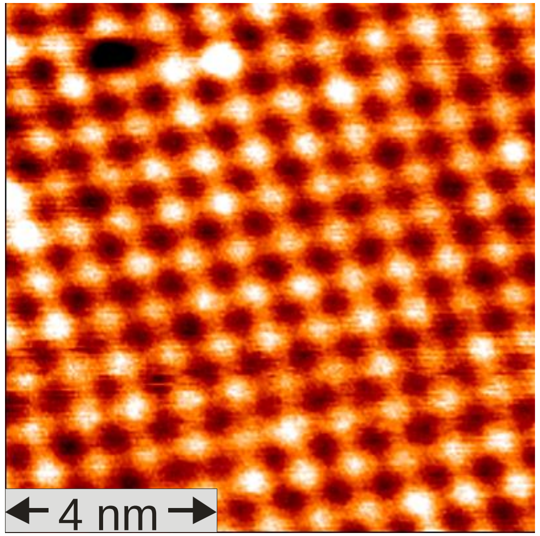
ATOMIC SCALE MAGNETIC SKYRMION LATTICE FE ON IR(111)

Beyond Heisenberg interaction



S. Heinze, K. von Bergmann, M. Menzel, J. Brede, A. Kubetzka, R. Wiesendanger, G. Bihlmayer and S. Blügel, Nat. Phys. **7**, 713 (2011)

SP-STM Topo Image



4-spin interaction

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

M. Takahashi, J. Phys. C **10**, 1289 (1977)

PROPOSED EXCHANGE INTERACTIONS OF LAST YEARS

- Biquadratic Exchange: $H_{\text{4-spin; 2-sites}} = -\sum_{ij} B_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right)^2$ Example: bcc Fe

- Four-Spin Three-Site Interaction:

Example: Fe/Rh(111) $H_{\text{4-spin; 3-sites}} = -\sum_{ijk} Y_{ijk} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right) \left(\mathbf{S}_i \cdot \mathbf{S}_k\right)$

Al-Zubi *et al.*, Phys. Status Solidi B **248**, 2242 (2011)
A. Krönlein *et al*, PRL **120**, 207202 (2018)

- Four-Spin Four-Site (“Ring-Exchange”) Interaction:

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

Example: Mn/Cu(111), Fe/Ir(111), 2Mn/W(110), Mn/Re(0001)

Ph. Kurz *et al.*, PRL **86**, 1106 (2001)
S. Heinze *et al.*, Nature Physics **7,** 713 (2011)
Y. Yoshida *et al.,* PRL **108**, 087205 (2012)
J. Spethmann, *et al* , PRL **124**, 227203 (2020)

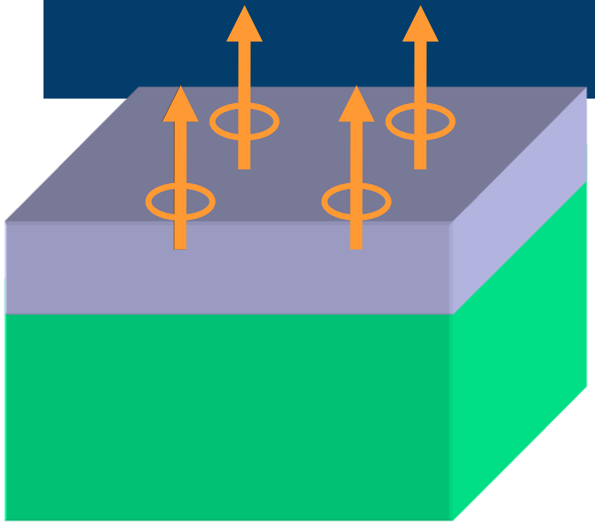
- Topological Chiral-Chiral Interaction (CCI):

$$H_{\text{6-spin; 6-sites}} = -\frac{1}{2} \sum_{ijki'j'k'} \left[\mathbf{S}_i \cdot \left(\mathbf{S}_j \times \mathbf{S}_k\right)\right] \boldsymbol{\tau}^{\dagger}_{ijk} \underline{\underline{\varkappa}}^{\text{CC}}_{ii'} \boldsymbol{\tau}_{i'j'k'} \left[\mathbf{S}_{i'} \cdot \left(\mathbf{S}_{j'} \times \mathbf{S}_{k'}\right)\right]$$

S. Grytsiuk, *et al.* Nat. Comm. **11**, 511 (2020)

Example: B20 MnGe

Magnetic Anisotropy



Magnetic Orientation

In-plane ⟺ Out-of-plane

Spin-Orbit + Dipole-Dip

$$H = \sum_i K_i(\vec{m}_i \vec{e}_i)^2 + \sum_{i,j} \frac{1}{r_{i,j}^3}[\cdots]$$

UNQUENCHING THE ORBITAL MOMENT BY SPIN-ORBIT INTERACTION

The spin-orbit interaction is in the wave function!

1st order perturbation theory:

$$|o\rangle^{(1)} = |o\rangle + \sum_u \frac{\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle}{(\epsilon_u - \epsilon_o)}|o\rangle$$

Orbital moment:

$$^{(1)}\langle o|\vec{L}|o\rangle^{(1)} \propto -\sum_{u(u\neq o)} \frac{\langle o|\vec{L}|u\rangle\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle}{(\epsilon_u - \epsilon_o)}|o\rangle$$

MAE due to MCA:

(2nd order perturbation)

$$E_{\mathrm{MCA}} \propto \langle H_{\mathrm{SO}}\rangle \quad \propto \quad \xi\,\langle o|\vec{L}|o\rangle^{(1)}\langle\vec{S}\rangle$$

$$\propto \quad -\sum_{u(u\neq o)} \frac{|\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle|^2}{(\epsilon_u - \epsilon_o)}$$

$|o\rangle$:= occupied, ground states

$|u\rangle$:= unoccupied, excited states

For d-states $|o\rangle, |u\rangle \in (|xy;\uparrow\rangle, |xz;\uparrow\rangle, |yz;\uparrow\rangle, |x^2-y^2;\uparrow\rangle, |3z^2-r^2;\uparrow\rangle$
$|xy;\downarrow\rangle, |xz;\downarrow\rangle, |yz;\downarrow\rangle, |x^2-y^2;\downarrow\rangle, |3z^2-r^2;\downarrow\rangle)$

UNQUENCHING THE ORBITAL MOMENT BY SPIN-ORBIT INTERACTION

The spin-orbit interaction is in the wave function!

1st order perturbation theory:

$$|o\rangle^{(1)} = |o\rangle - \sum_{u(u\neq o)} \frac{\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle}{(\epsilon_u - \epsilon_o)}|o\rangle$$

Symmetry-dependence
E.g. uniaxial symmetry

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

2nd 4th

$$G^V_{\text{cryst}}(\hat{M}) = K_1(\alpha_1^2 + \alpha_2^2) + K_2(\alpha_1^2 + \alpha_2^2)^2$$

$$\alpha_1^4 \propto \widehat{M}\cdot\widehat{M}\cdot\widehat{M}\cdot\widehat{M}$$

$$\propto \langle\vec{S}\rangle^4$$

MAE due to MCA:

(2nth order perturbation)

$$K_n \propto \langle H_{\text{SO}}\rangle \propto -\sum_{u(u\neq o)} \frac{|\langle u|\xi\vec{L}\cdot\vec{S}|o\rangle|^{2n}}{|(\epsilon_u - \epsilon_o)|^{(2n-1)}}$$

JÜLICH Forschungszentrum

FINITE CURIE TEMPERATURE IN 2D

Magnetization in *d* dimensions

- Spin stiffness $E(q)=Dq^2$
- Magnetization $M(T)-M(0) \propto \int_0^\infty \frac{q^{d-1}}{e^{Dq^2/k_B T}-1} dq$

small wave vectors

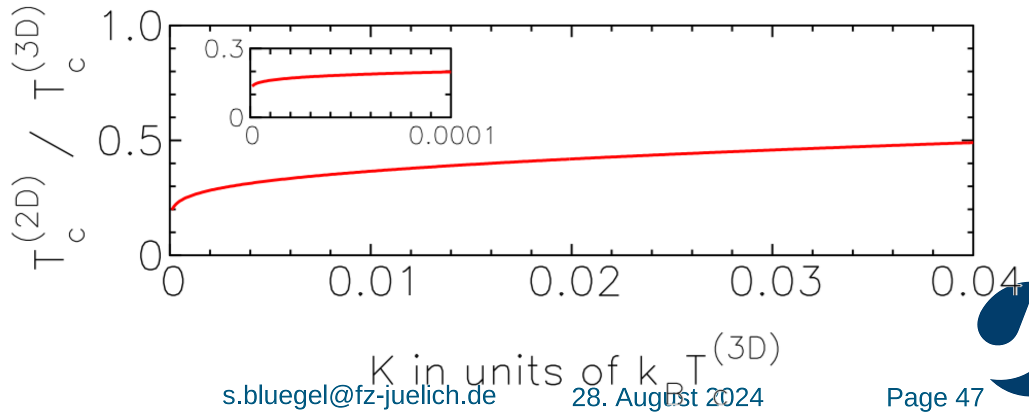
$$\frac{q^{d-1}}{e^{Dq^2/k_B T}-1} \approx \frac{q^{d-1}}{Dq^2/k_B T} \propto q^{d-3}$$

$d = 3$: finite magnetization
$d \leq 2$: divergent

Mermin-Wagner theorem:
The isotropic Heisenberg model with short-range interaction in one or two dimensions has no spontaneous magnetization at finite temperature.

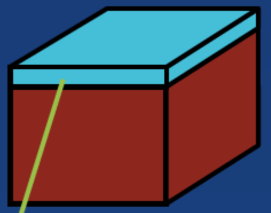
- Anisotropy (spin-orbit coupling) ⇒ energy gap in spin wave spectrum for q=0

- $$T_C^{(2D)} = T_C^{(3D)} \frac{2}{\ln\left(\frac{3\pi}{4}\frac{k_B T_C^{(3D)}}{K}\right)}$$



Erickson and Mills, PRB **43**, 11527 (1991)

Curie temperature (RPA): $$\frac{1}{k_B T_C^{RPA}} = \frac{6\mu_B}{m_s} \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{E(\mathbf{q})}$$



spin-wave energy: $$E(\mathbf{q}) = \Delta_{anis} + \frac{4\mu_B}{m_s} \sum_{j \neq 0} J_{0,j} \left(1 - \exp\left(i\mathbf{q} \cdot \mathbf{R}_{0,j}\right)\right)$$

$$T_C^{2D} \propto \frac{J}{\ln(J/\Delta_{anis})}$$

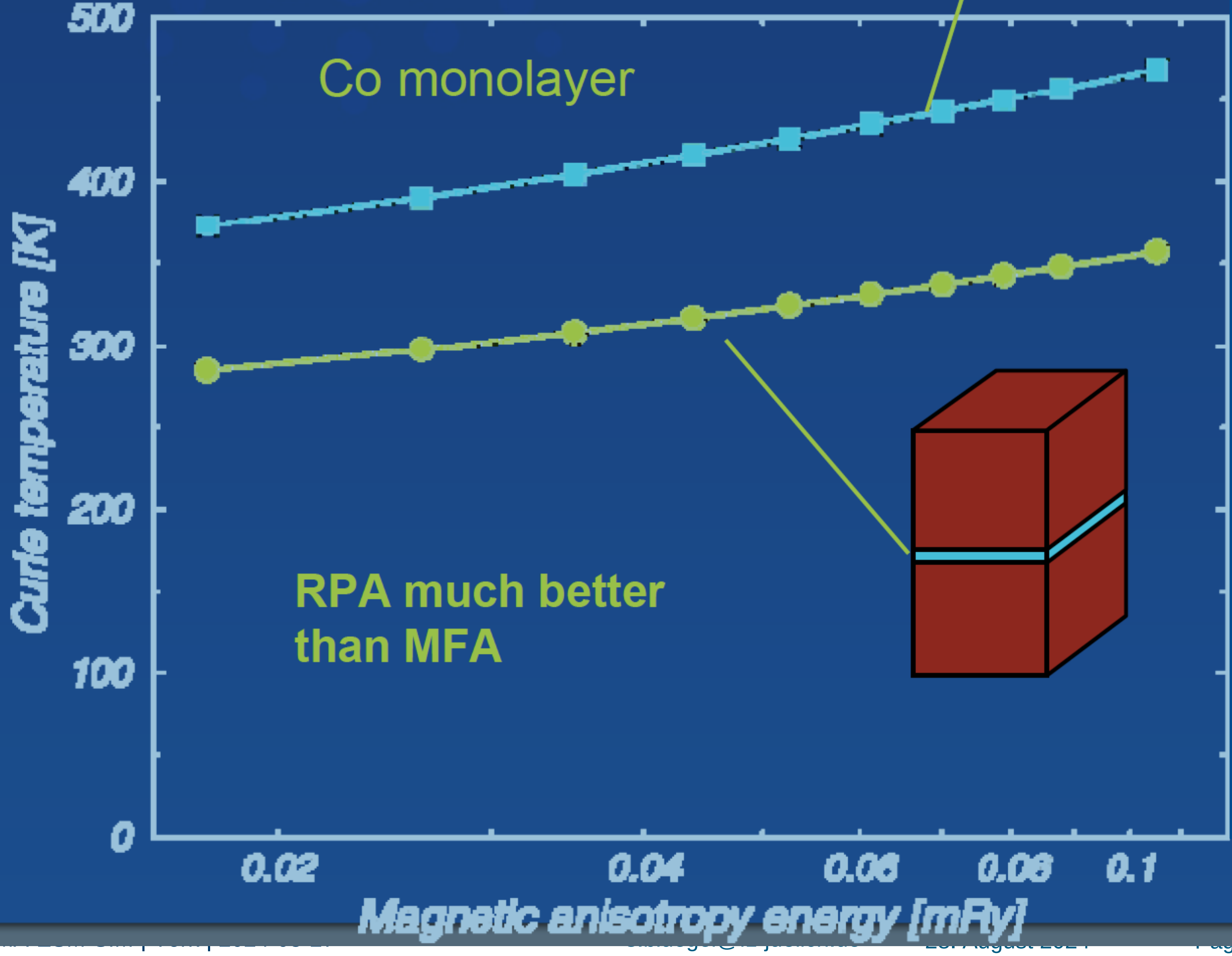
$T_C^{RPA} \rightarrow 0$

for $\Delta_{anis} \rightarrow 0$

(Mermin-Wagner)

typical order of magnitude of the anisotropy:

$$\Delta_{anis} \approx \frac{2\pi \quad M^2}{V}$$



Taken from P. Bruno

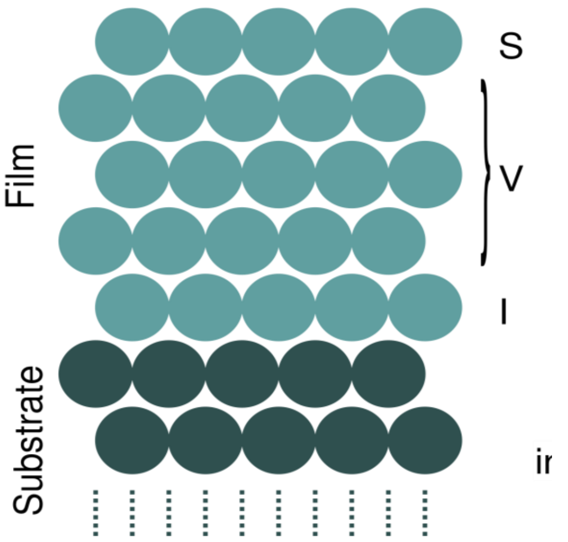
JÜLICH Forschungszentrum

Reorientation transition

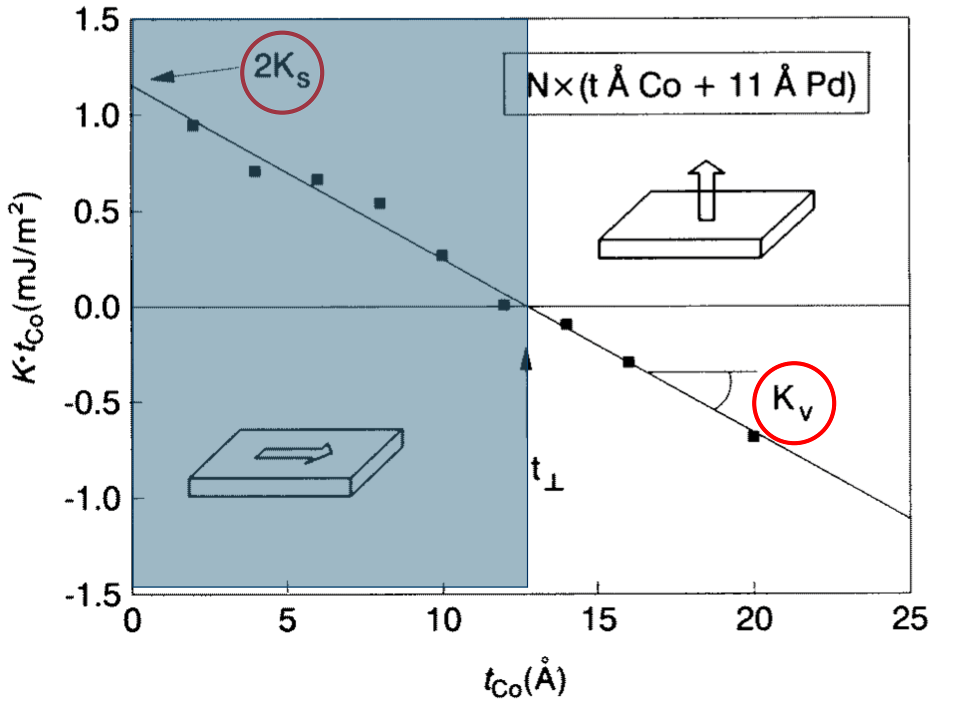
SPIN REORIENTATION TRANSITIONS AS FUNCTION OF LAYER THICKNESS t

$$\mathcal{G}(\widehat{M}) = \int_V dV\ G^V(\widehat{M}) + \int_S ds\ G^S(\widehat{M})$$

$\sim$ layer thickness t (for $\mathcal{G}(\widehat{M})$) $\qquad \sim t$ (for $G^V(\widehat{M})$) $\qquad \neq f(t)$ (for $G^S(\widehat{M})$)



$$K_{\text{eff}} \cdot t = K^V \cdot t + 2K^S$$

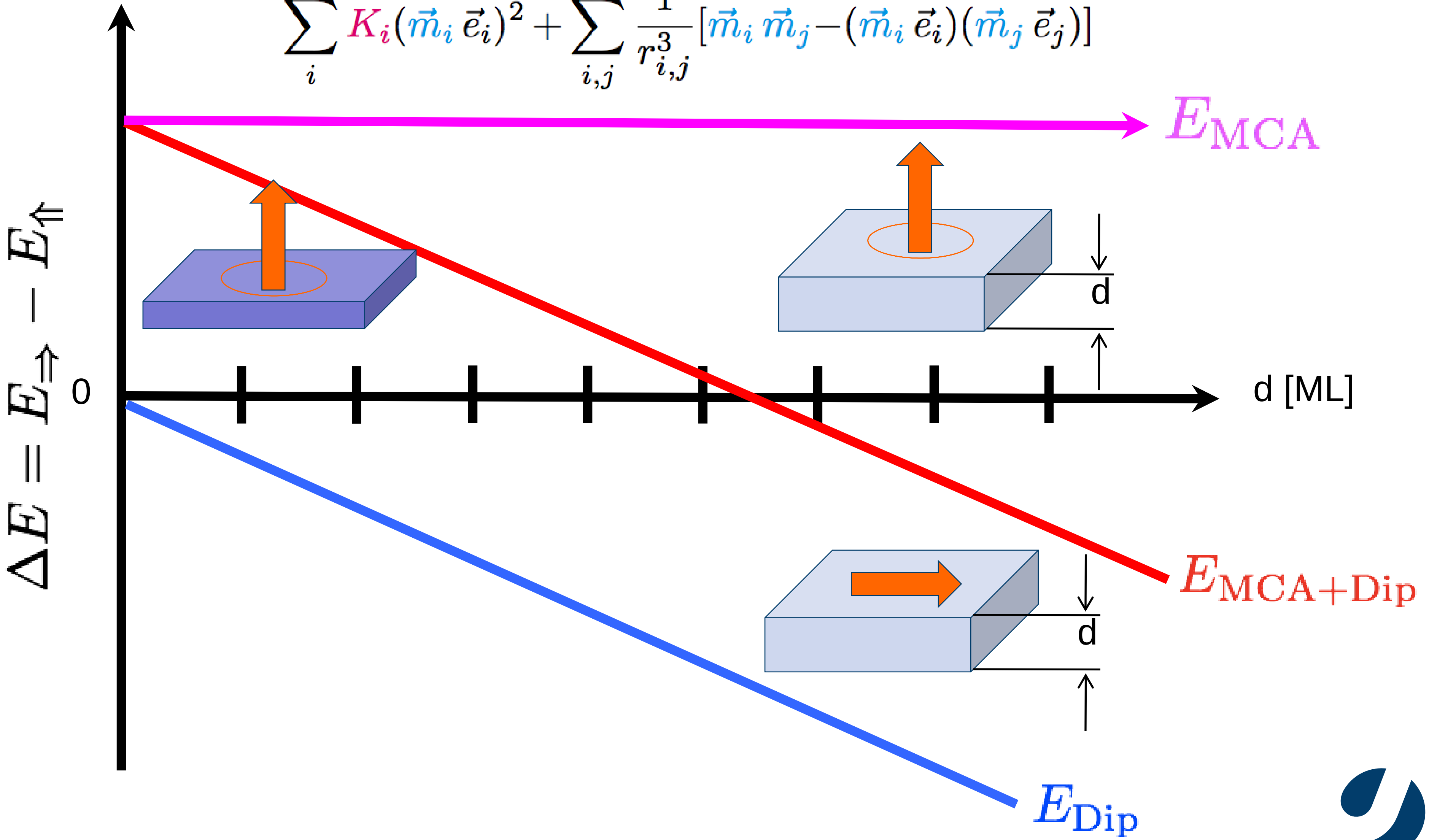


JÜLICH Forschungszentrum

SCHEMATIC DEPENDENCE OF ANISOTROPY ON THICKNESS

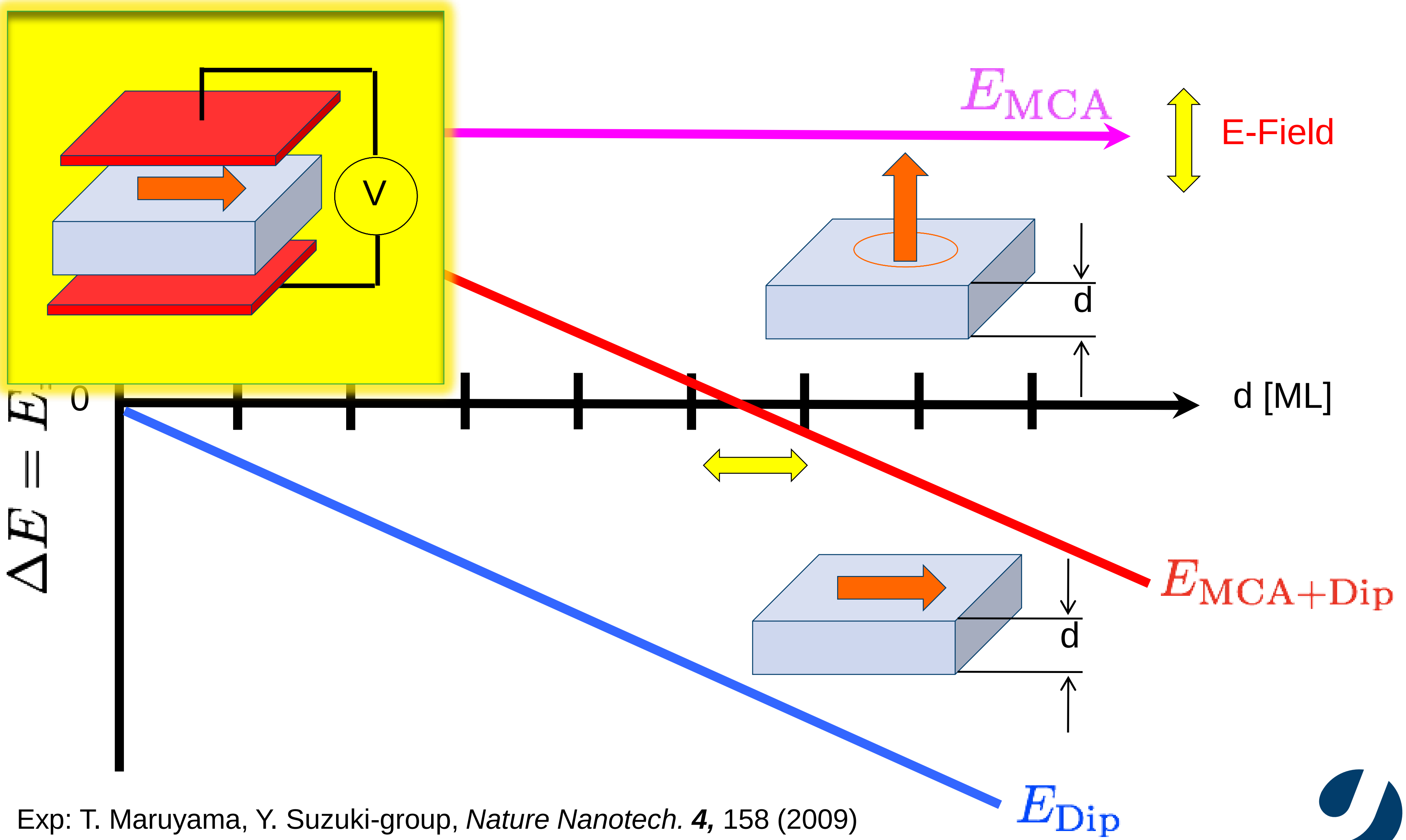
X. Nie & S. Blügel, European Patent Nr. 1099217

$$\sum_i K_i(\vec{m}_i\,\vec{e}_i)^2 + \sum_{i,j} \frac{1}{r_{i,j}^3}[\vec{m}_i\,\vec{m}_j - (\vec{m}_i\,\vec{e}_i)(\vec{m}_j\,\vec{e}_j)]$$



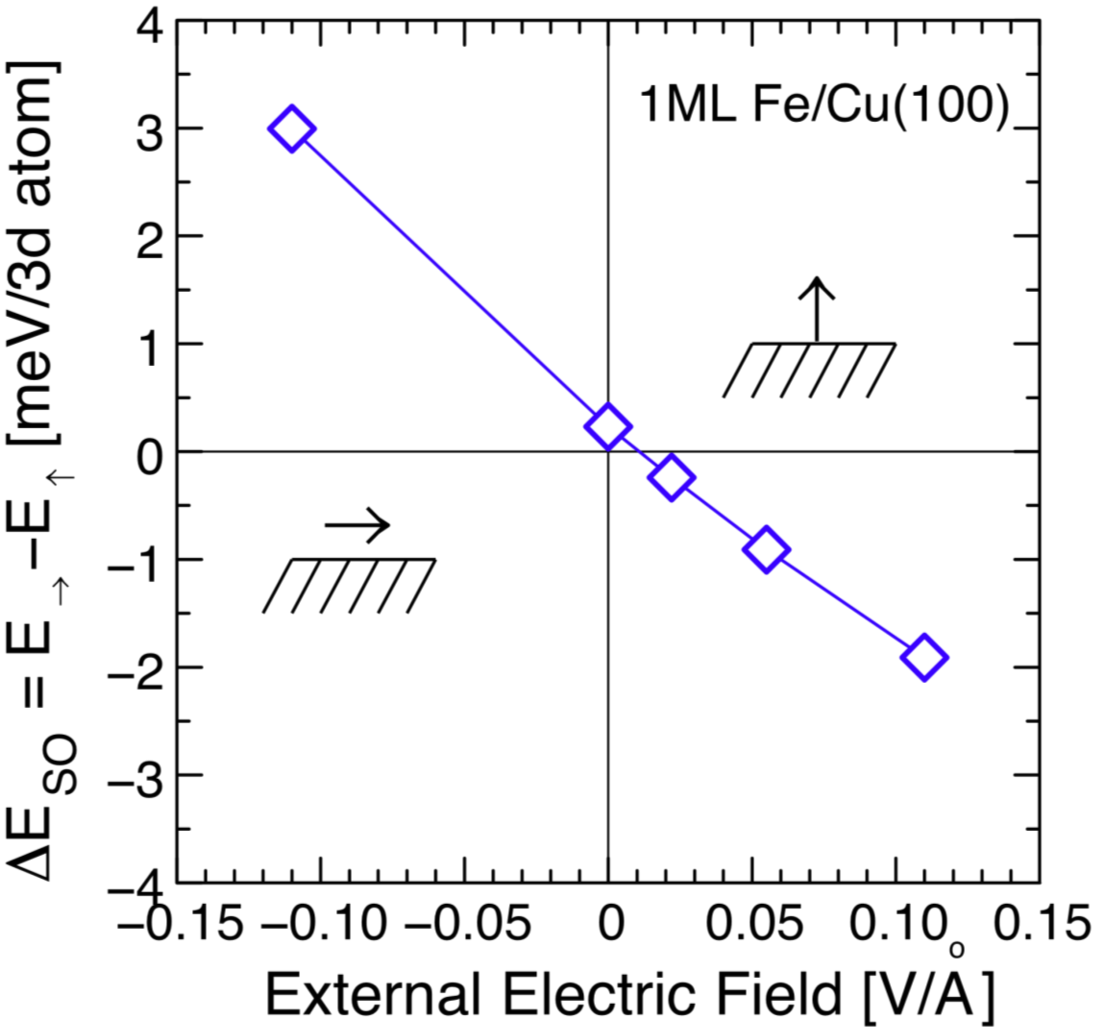
VOLTAGE CONTROL OF MAGNETIC ANISOTROPY

X. Nie & S. Blügel, European Patent Nr. 1099217



Exp: T. Maruyama, Y. Suzuki-group, *Nature Nanotech.* ***4,*** 158 (2009)

VOLTAGE CONTROL : 1 ML Fe ON Cu(100)



X. Nie & S. Blügel, European Patent Nr. 1099217

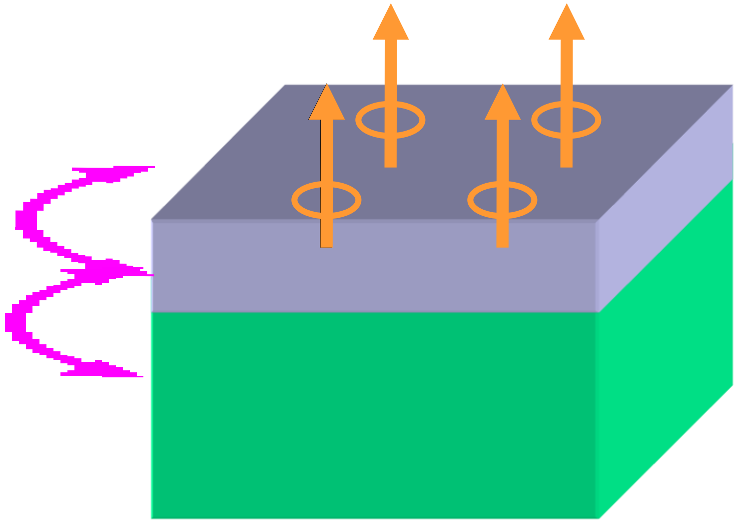
Dzyaloshinskii-Moriya Interaction (DMI)

DZYALOSHINSKII-MORIYA INTERACTION

E. Dzyaloshinskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **19**, 960 (1964) ; I. E. Dzyaloshinskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **20**, 665 (1965)\
T. Moriya, PRL **4**, 228 (1960) ; T. Moriya, PR **120**, 91 (1960)

Break of inversion symmetry

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



Chiral magnetic interaction
(Dzyaloshinskii-Moriya)

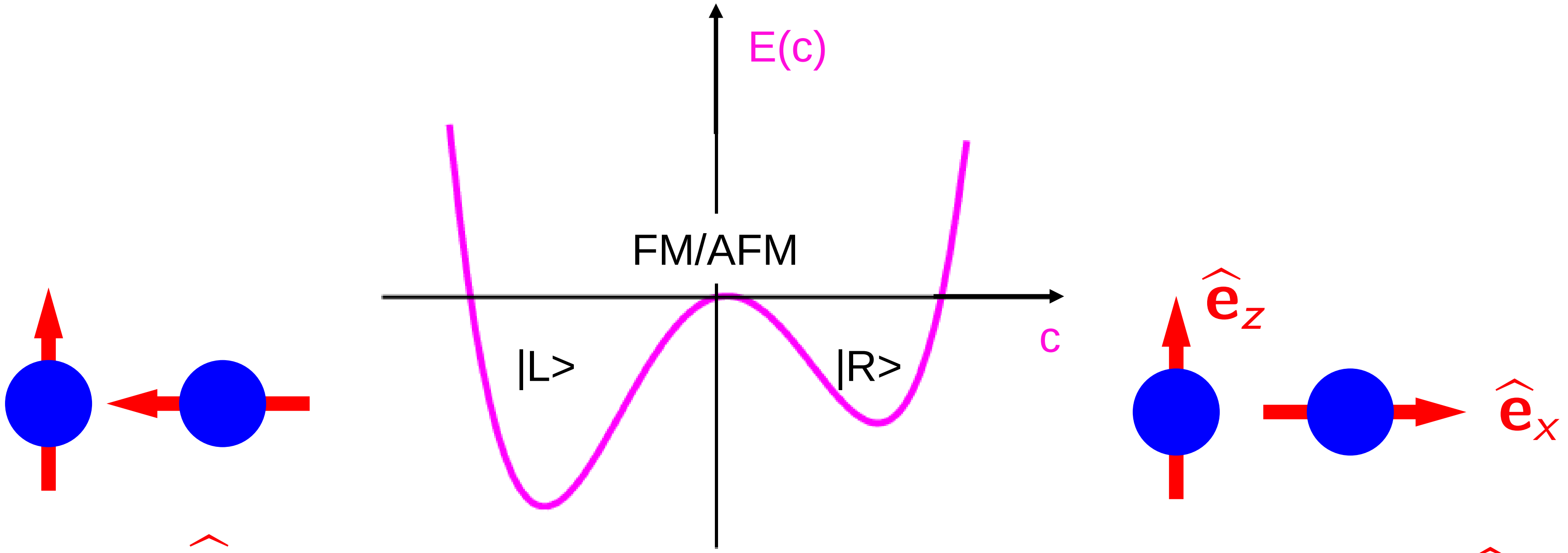
Magnetic Orientation

In-plane ⟺ Out-of-plane

JÜLICH Forschungszentrum

CHIRALITY OF DZYALOSHINSKII-MORIYA INTERACTION

I. E. Dzialoshinskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **5,** 1259 (1957); J. Phys. and Chem. Sol. **4**, 241 (1958)



$\mathbf{c} = -\hat{\mathbf{e}}_y$

$\mathbf{c} = \mathbf{m}_i \times \mathbf{m}_j = \hat{\mathbf{e}}_y$

$$\mathcal{H}_{\mathrm{DM}} = -\sum_{ij} \mathbf{D}_{ij} \underbrace{(\mathbf{S}_i \times \mathbf{S}_j)}_{\mathbf{c}}$$

DZYALOSHINSKII-MORIYA INTERACTION

$$\mathcal{H}_{\mathrm{DM}} = -\mathbf{D}_{12} \underbrace{(\mathbf{S}_1 \times \mathbf{S}_2)}_{\mathbf{c}} \quad / \quad e_{\mathrm{DM}}(\underline{\mathbf{D}};\mathbf{m}) = \underline{\mathbf{D}} : (\nabla \mathbf{m} \times \mathbf{m})$$

- DMI in centro-symmetric systems: $\sum_{ij} \mathbf{D}_{ij} = \mathbf{0}$

  I. E. Dzialoshinskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **5**, 1259 (1957), J. Phys. and Chem. Sol. **4**, 241 (1958)
  (nowadays popular in 2D systems , sometimes also termed hidden DMI)

- DMI in **non-**centro-symmetric systems $\sum_{ij} \mathbf{D}_{ij} \neq \mathbf{0}$

  J. Exptl. Theoret. Phys. (U.S.S.R.) **19**, 960 (1964); J. Exptl. Theoret. Phys. (U.S.S.R.) **20**, 665 (1965)
  ➔ leads to ordered structure with spatial modulation

MAGNETIC INTERACTIONS

$$H = \sum_{i,j} J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j + \sum_i \mathbf{S}_i^{T} \cdot \underline{K}_i \cdot \mathbf{S}_i \;\mathbf{S}_j)$$

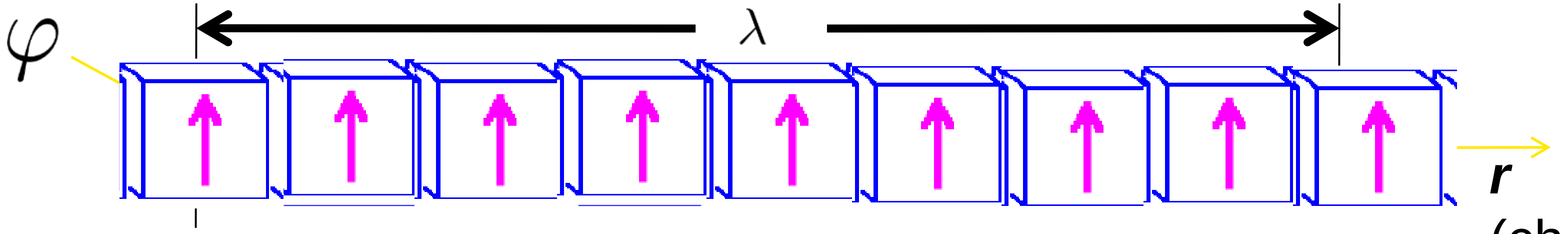
Isotropic symmetric exchange

Magnetic Anisotropy Energy

ge oriya

- Heisenberg-type interaction
- relativistic correction (SOC)
- surfaces and chains (breaking of inv. symmetry)

SOC effects



r
(chain direction)

- now: homogeneous flat spiral: $\frac{d\varphi}{dr} = 2\pi/\lambda = \text{const.}$

$$\Rightarrow E(\lambda) = A\lambda^{-2} + D\lambda^{-1} + \overline{K}$$

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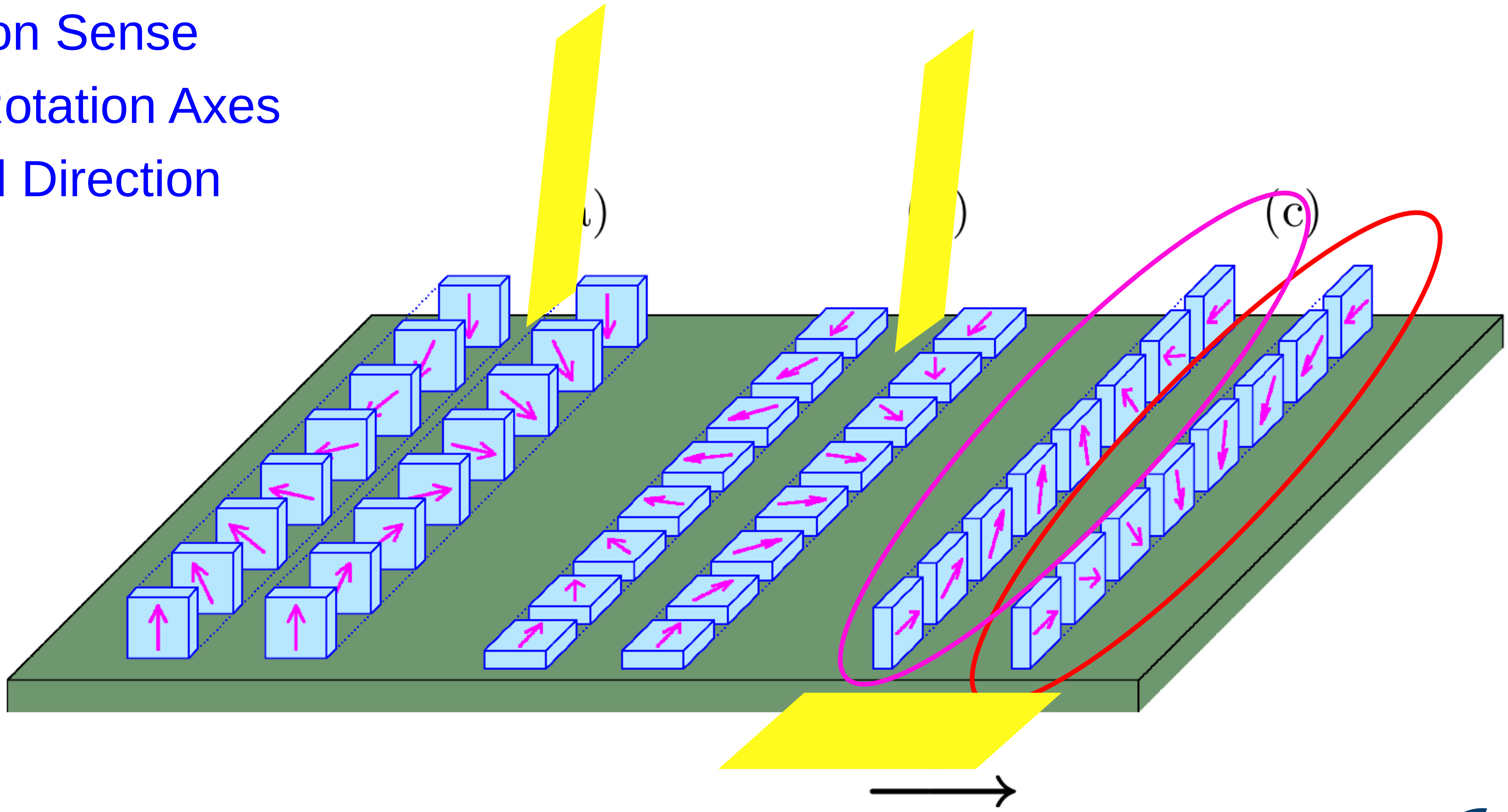
SPIN-SPIRALS IN MAGNETIC WIRES

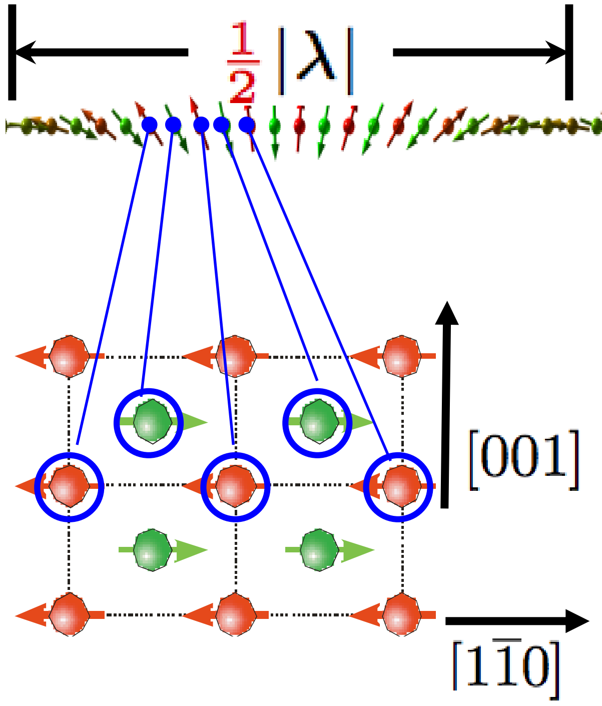
- Rotation Sense
- Spin Rotation Axes
- Spatial Direction



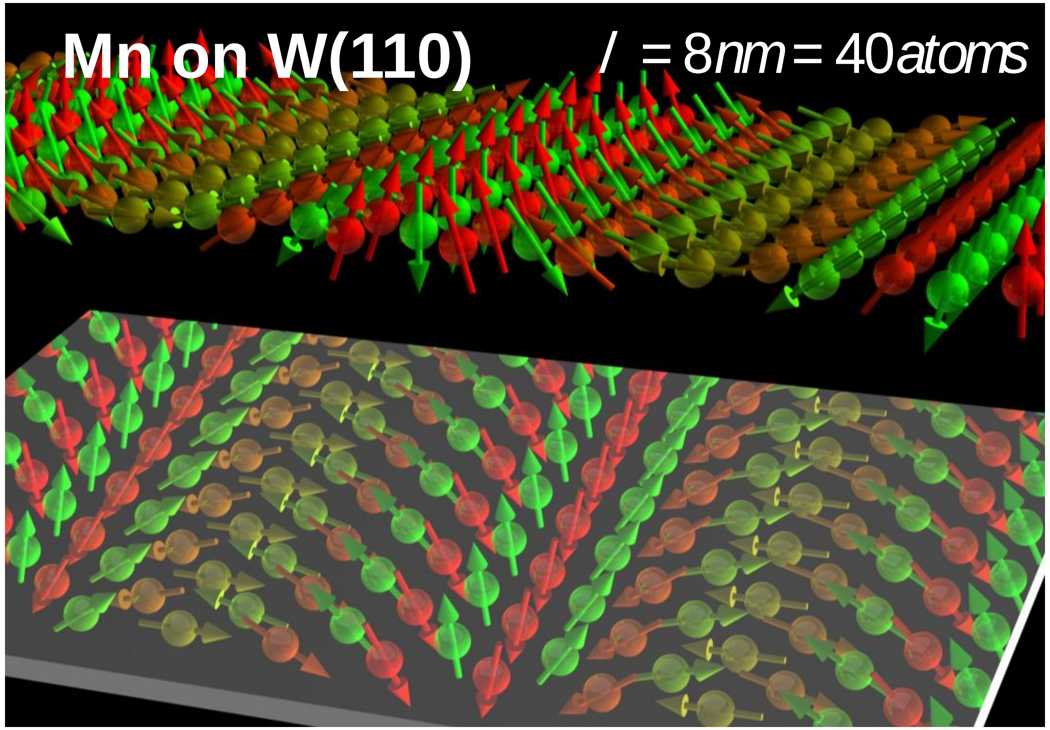
HOMOCHIRAL MAGNETIC SPIRAL: 1ML Mn on W(110)

Bode, Heide, von Bergmann, Ferriani, Heinze, Bihlmayer, Kubetzka, Pietzsch, Blügel, Wiesendanger, Nature **447,** 190 (2007)

Magnetic Configuration:



homochiral magnetism



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HOMOCHIRAL MAGNETIC SPIRAL: 1ML Mn on W(110)

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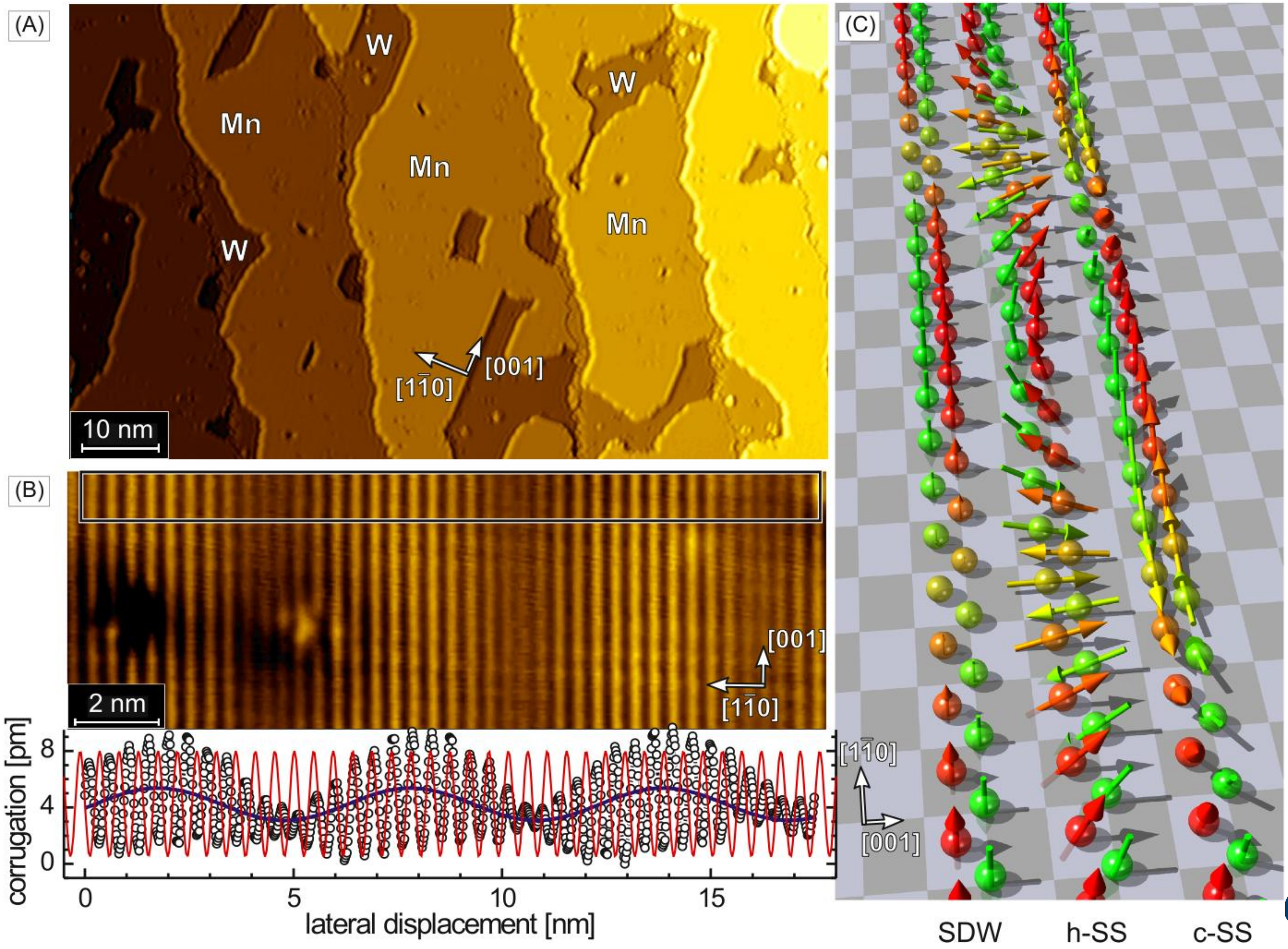
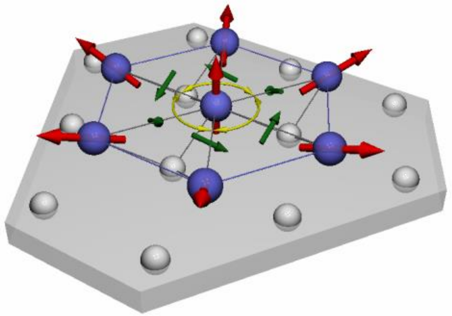


SUMMARY



❖ Atomistic Spin-Lattice Model (extended classical Heisenberg):

$$H = \frac{1}{2}\sum_{ij} J_{ij}\,\mathbf{S}_i\cdot\mathbf{S}_j + \sum_{ij}\mathbf{D}_{ij}\,\overbrace{\mathbf{S}_i\times\mathbf{S}_j}^{\mathbf{c}} + \sum_i \mathbf{S}_i\,\underline{\mathbf{K}}\,\mathbf{S}_i + \sum_{ij}\frac{1}{r_{ij}^3}\left[\mathbf{S}_i\cdot\mathbf{S}_j - (\mathbf{S}_i\cdot\hat{\mathbf{e}}_i)(\mathbf{S}_j\cdot\hat{\mathbf{e}}_i)\right] + \mathbf{B}_{\mathrm{ext}}\sum_i \mathbf{S}_i$$

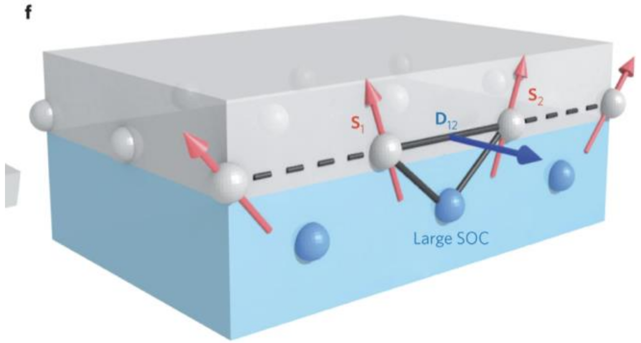
- $\mathbf{S}_i \in \mathbb{R}^3; \mathbf{S}_i \propto \mathbf{m}_i$ typically classical vector
- J_{ij}, D_{ij} i-j long range for metals ; n.N. for insulators

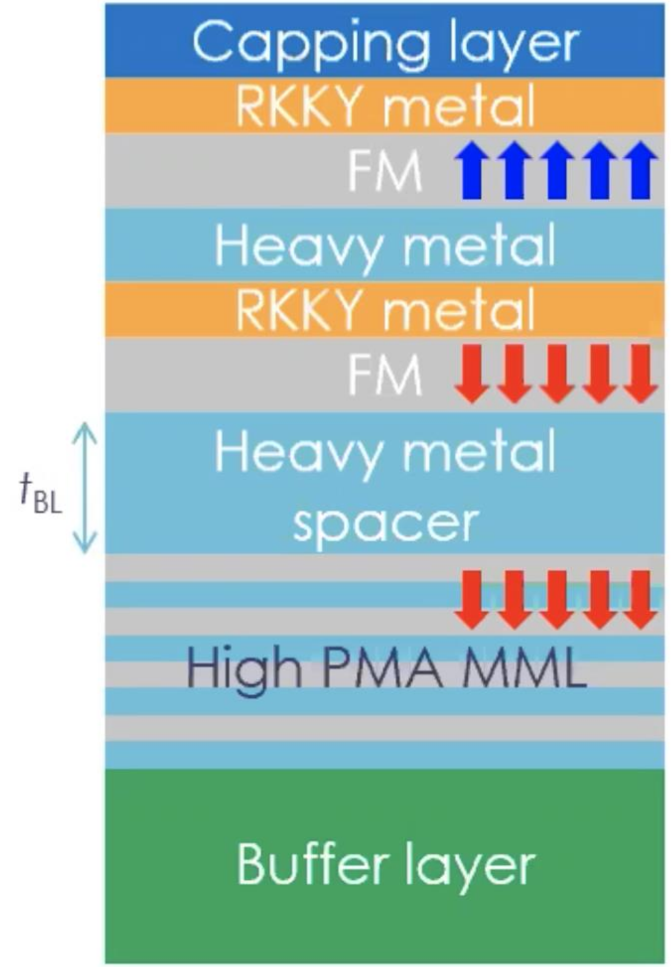
❖ Model parameters are changed at interfaces and surfaces:

- Reduction of coordination number leads to larger moments
- but smaller interatomic exchange and more complex magnetism
- Larger moments increases the role of higher order Interactions
- Lower symmetry leads to larger magnetocrystalline anisotropy dominating of dipol
- Broken symmetry +SOC leads to Dzyaloshinskii-Moriya interaction

MAGNETIC MULTILAYERS

A very tunable materials platform





- Choice of thickness
- Choice of layer composition
- Choice of growth conditions
- Choice of FM or AF coupling strength
- Possibility to modify DMI and PMA
- Possibility to use uncompensated structures
- Possibility to work with exchange bias field
- ……

W. Legrand *et al, Nature Materials* **19**, 34 (2020)

Thank you