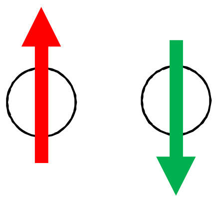
Nano-scale skyrmions and atomic-scale spin textures studied with STM

Kirsten von Bergmann
University of Hamburg

atomic-scale magnetic order: ingredients

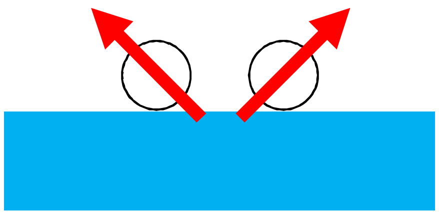
magnetic exchange interaction

$$E = -J\,(S_1 \cdot S_2)$$

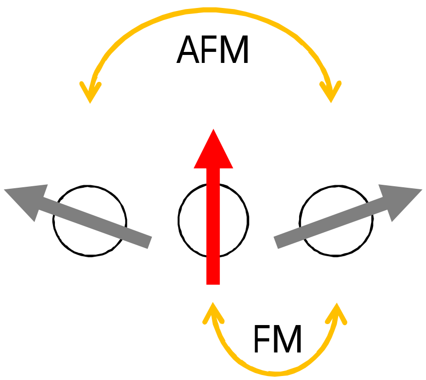


antisymmetric exchange (DMI)
Dzyaloshinskii-Moriya interaction
due to spin-orbit coupling
and broken inversion symmetry

$$E = -D\,(S_1 \times S_2)$$



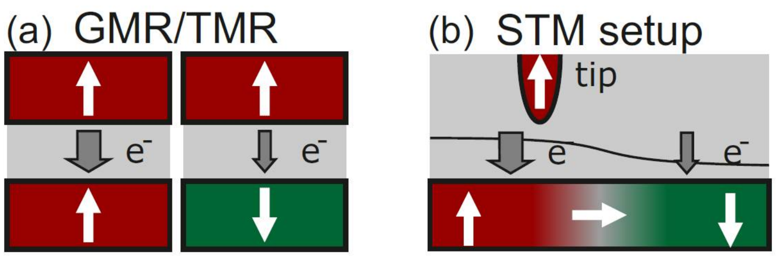
exchange frustration

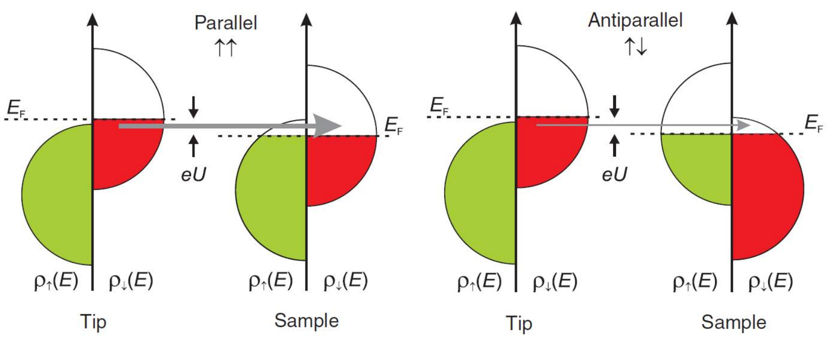


spin-polarized STM

M. Bode, Rep. Prog. Phys. **66**, 523 (2003).
R. Wiesendanger, Rev. Mod. Phys. **81** 1495 (2009).

TMR-effect
(tunnel magnetoresistance)
in STM geometry



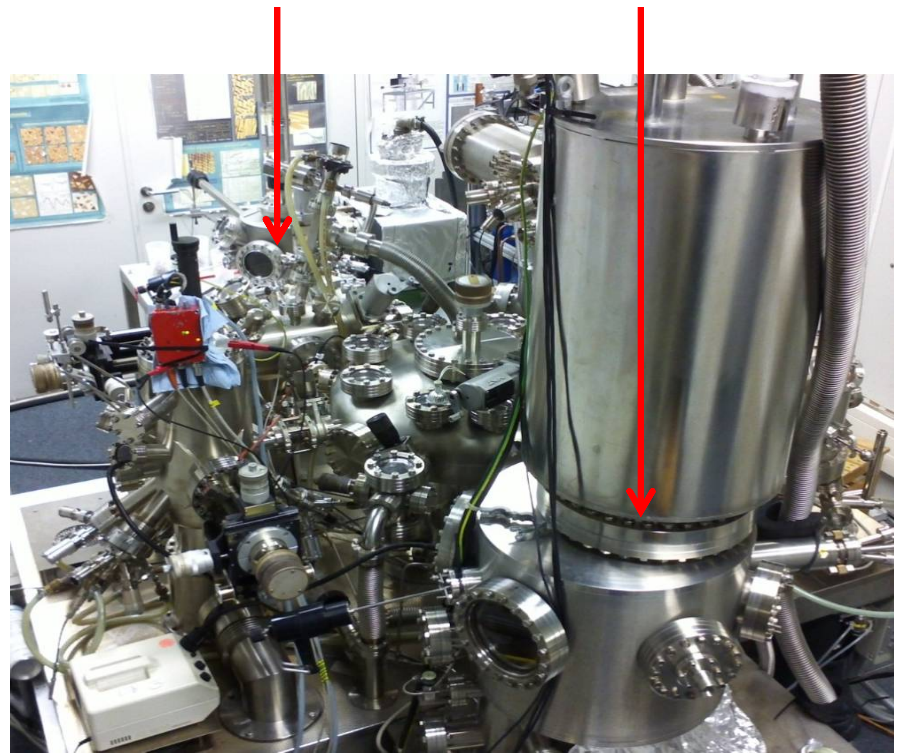


$$I_{\rm SP}(U_0) = I_0[1 + P_{\rm s} \cdot P_{\rm t} \cdot \cos(\vec{M}_{\rm s}, \vec{M}_{\rm t})]$$

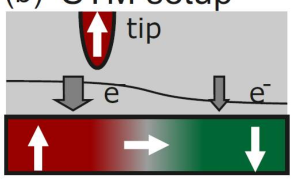
in-situ tip
and sample
preparation

STM
T = 1.3 - 4.2 K
$B_\perp$ < 9 T

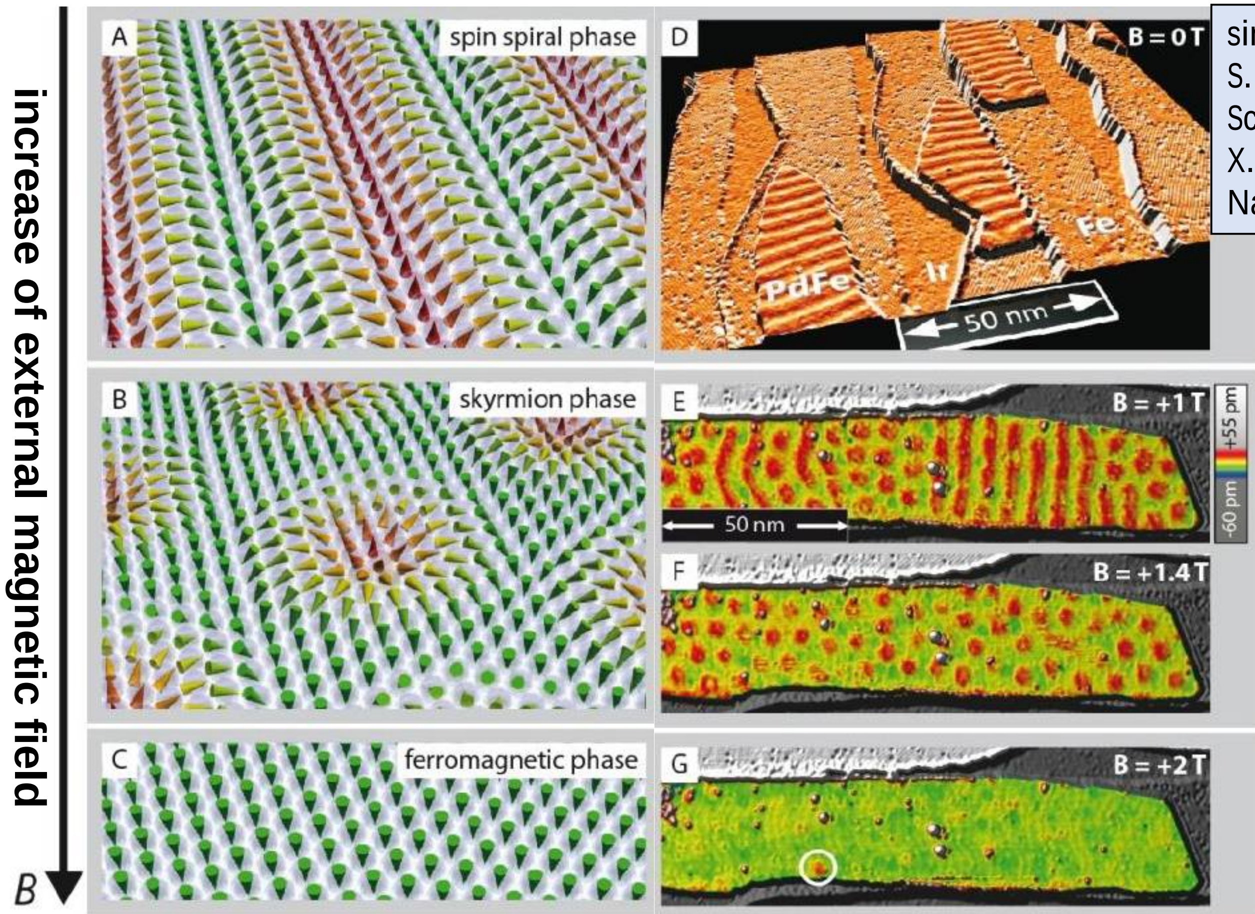
STM
T = 8 - 13 K
$B_\perp$ < 2.5 T



SP-STM on Pd/Fe/Ir(111)



Cr-tip (AFM:
no change in *B*)



similar to:
S. Mühlbauer et al.,
Science **323**, 915 (2009).
X.Z. Yu et al.,
Nature **465**, 901 (2010).

spin spiral
due to
competition
of *J* and **D**

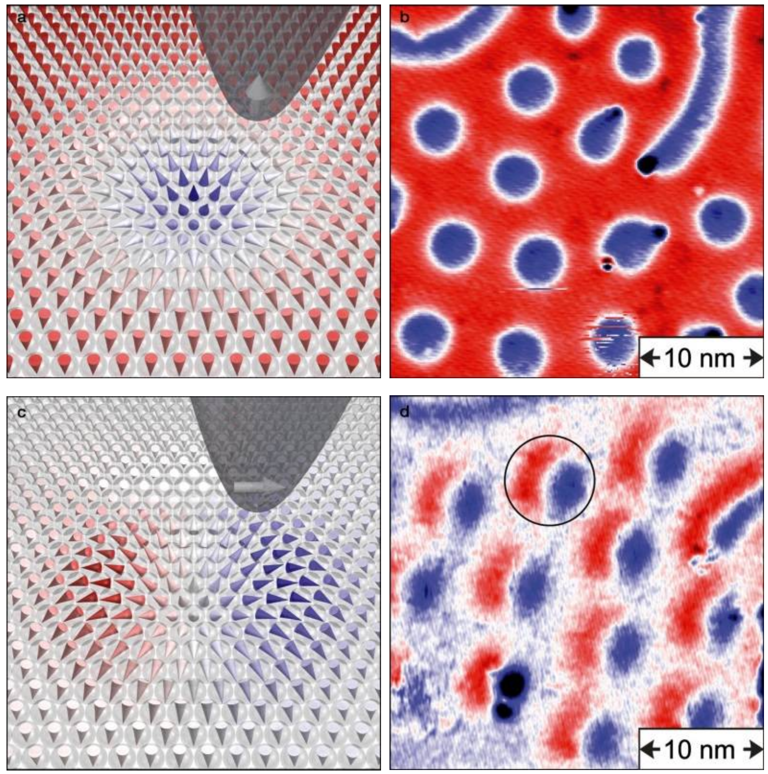
N. Romming, ...KvB et al., Science **341**, 636 (2013).

SP-STM and skyrmions

Pd/Fe/Ir(111)

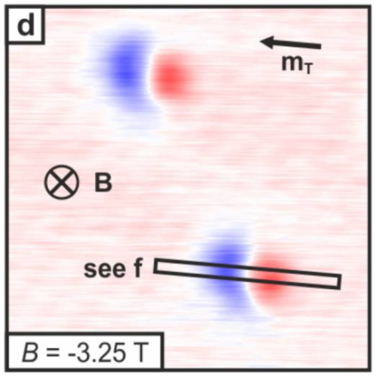
out-of-plane components

in-plane components



N. Romming, ...KvB et al., Science **341**, 636 (2013); Phys. Rev. Lett. **114**, 177203 (2015).

spin structure of an isolated skyrmion



two overlapping 180° domain walls

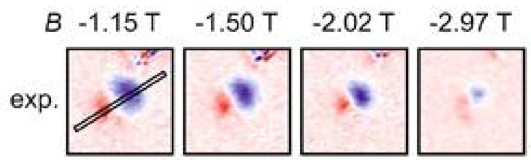
$$\theta(\rho, c, w) = \sum_{+,-} \left[\arcsin\left(\tanh\left(\frac{-\rho \pm c}{w/2} \right) \right) \right]$$

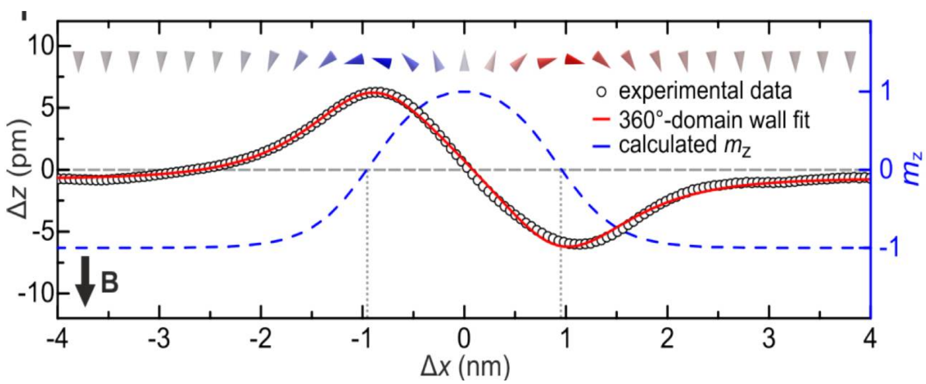
ρ position, c center, w width of wall

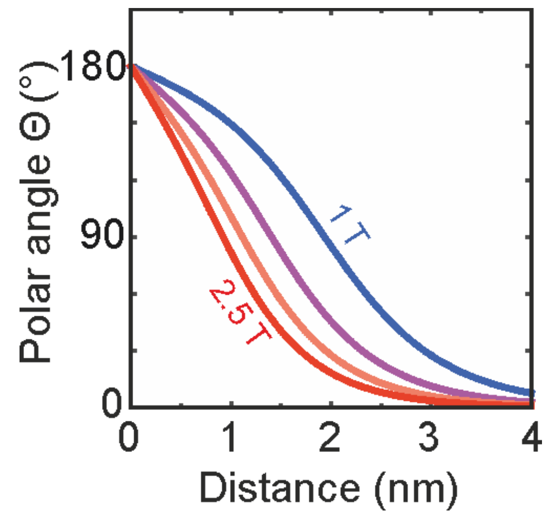
$$w_0 = 2\sqrt{\frac{A}{K_{\mathrm{eff}}}}.$$

exchange stiffness

effective anisotropy





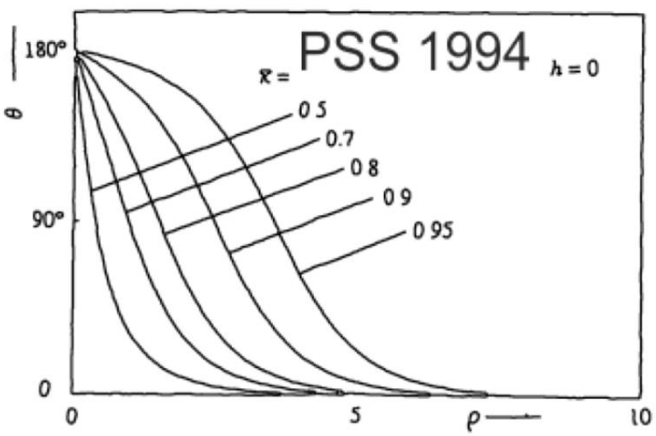


N. Romming, ...KvB et al.,
Phys. Rev. Lett. **114**, 177203 (2015).

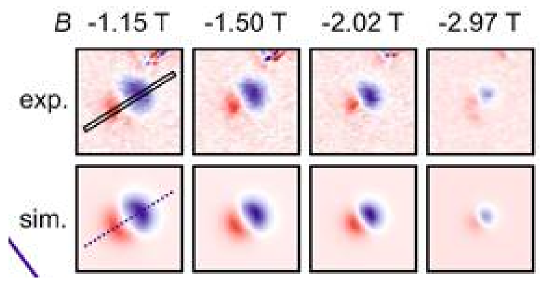
material parameters

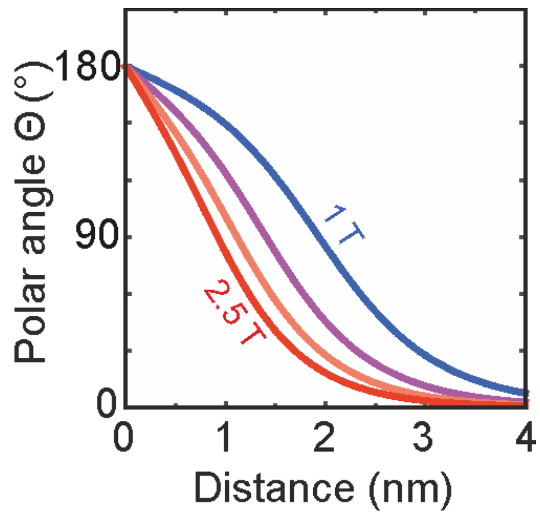
$$E(\theta(\rho)) = 2\pi t \int_0^\infty \left[A\left(\left(\frac{d\theta}{d\rho}\right)^2 + \frac{\sin^2\theta}{\rho^2} \right) - D\left(\frac{d\theta}{d\rho} + \frac{\sin\theta\cos\theta}{\rho} \right) - K\cos^2\theta - B_z M_S \cos\theta \right] \rho\, d\rho$$

A. Bogdanov, A. Hubert, J. Magn. Magn. Mater. **138**, 255 (1994), Phys. Status Solidi B **186**, 527 (1994)



A = 2.0 pJ/m $|D|$ = 3.9 mJ/m² K = 2.5 MJ/m³ M_S = 1.1 MA/m

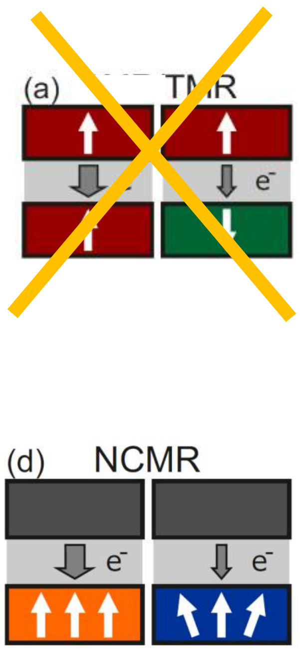


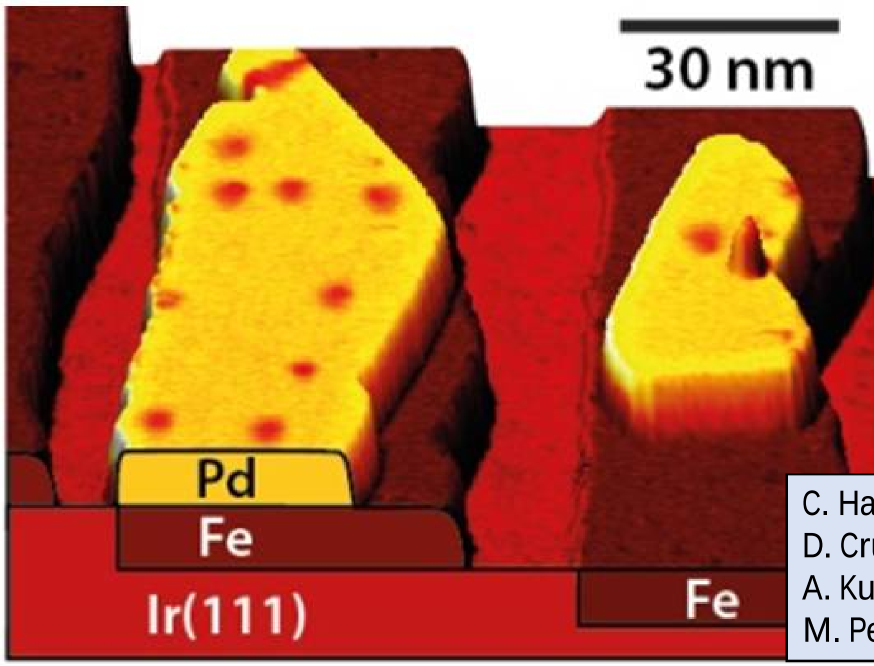


M_s from DFT, also good agreement with the other parameters.
B. Dupe et al., Nat. Commun. **5**, 4030 (2014).
E. Simon et al., Phys. Rev. B **90**, 094410 (2014).

N. Romming, ...KvB et al., Phys. Rev. Lett. **114**, 177203 (2015).

STM with non-magnetic tip: electronic properties



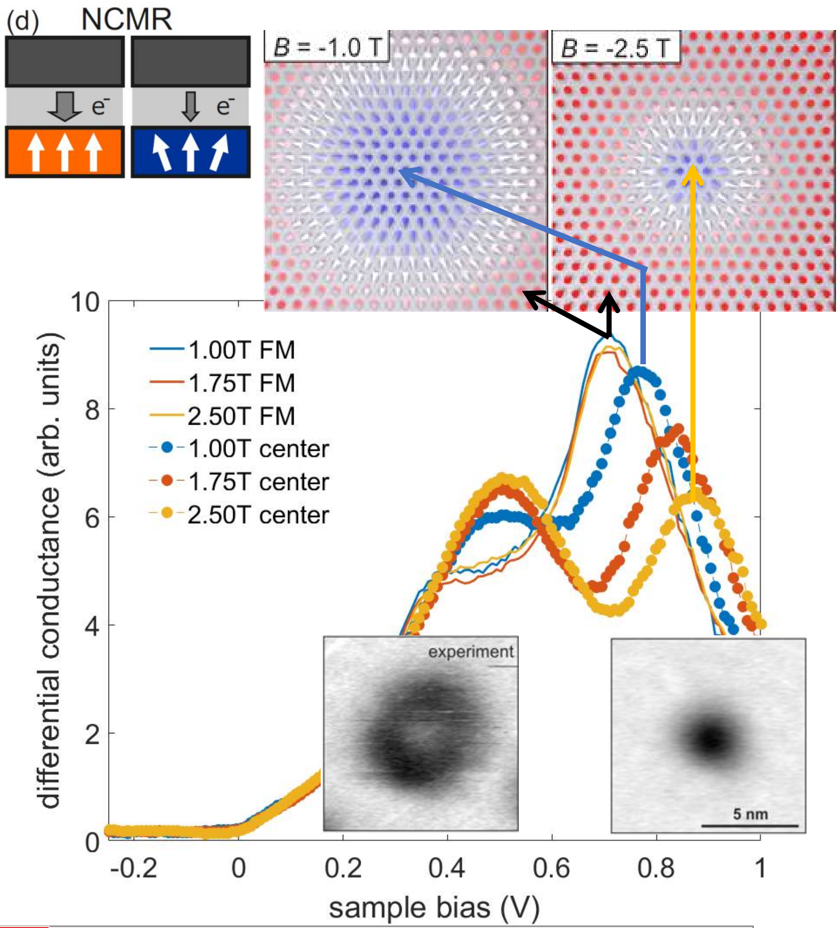


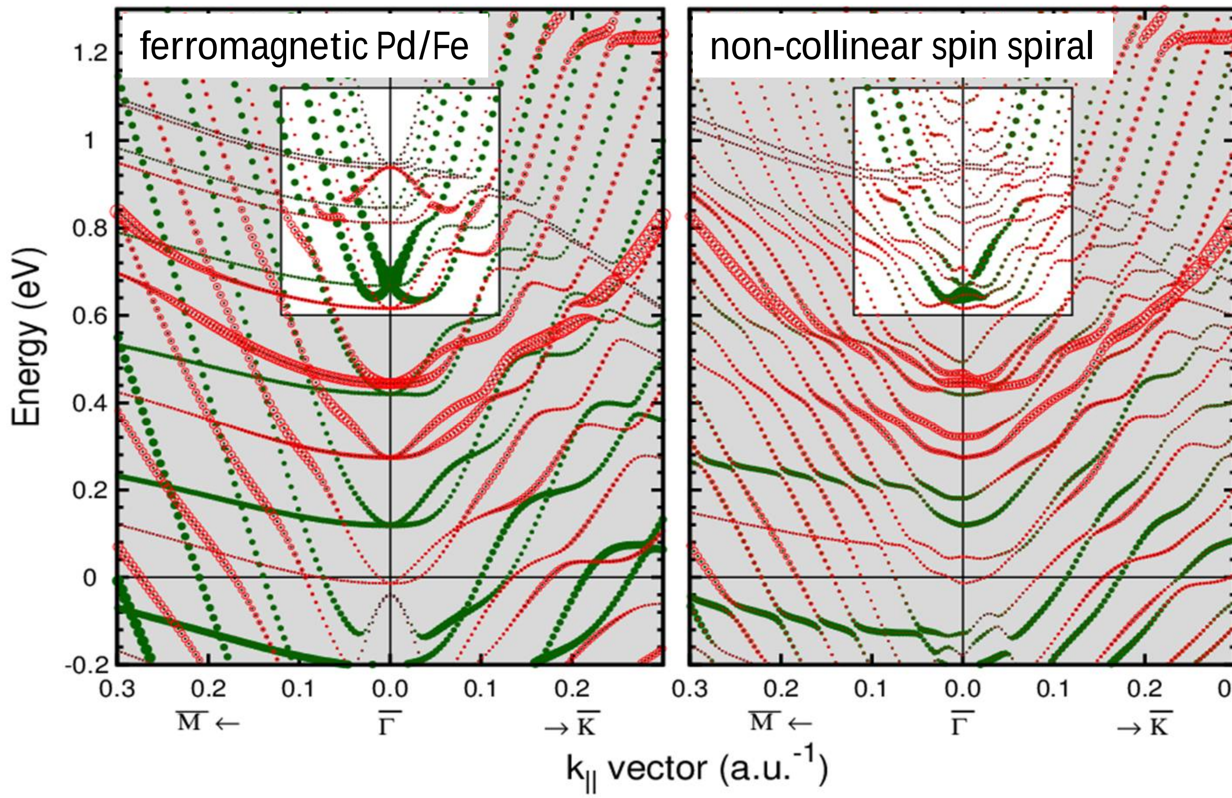
when the magnetic state
is non-collinear
there is a different
electronic structure
due to mixing of spin-up
and spin-down bands

C. Hanneken, ..., KvB et al., Nature Nano. **10**, 1039 (2015).
D. Crum et al., Nature Commun. **6**, 8541 (2015).
A. Kubetzka, ..., KvB, Phys. Rev. B **95**, 104433 (2017).
M. Perini, ..., KvB, Phys. Rev. Lett. **123**, 237205 (2019).

topography colorized with differential conductance signal:
we 'see' the skyrmions also with non-spin-polarized STM tip,
due to the non-collinear magnetoresistance effect

spectroscopy and DFT





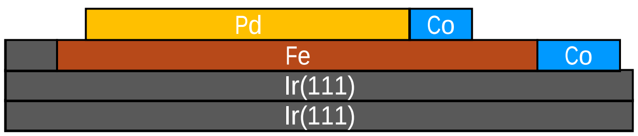
changes of the band structure everywhere in the Brillouin zone !!!
not limited to tunnel experiments, relevant for all transport (see E_F)

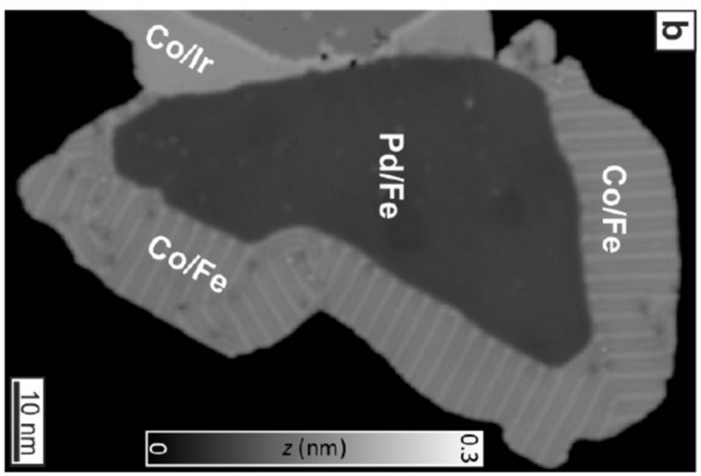
C. Hanneken, ..., KvB et al., Nature Nano. **10**, 1039 (2015).

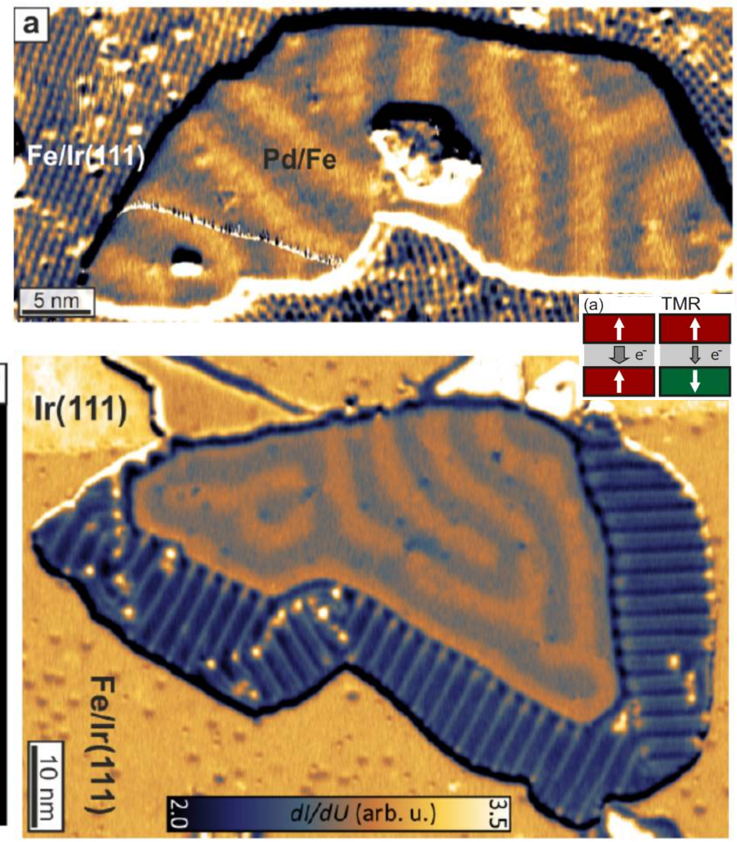
spin spirals in Pd/Fe with modified rim

J. Spethmann, ..., KvB, arXiv:2108.06223

the Co/Fe areas are in-plane



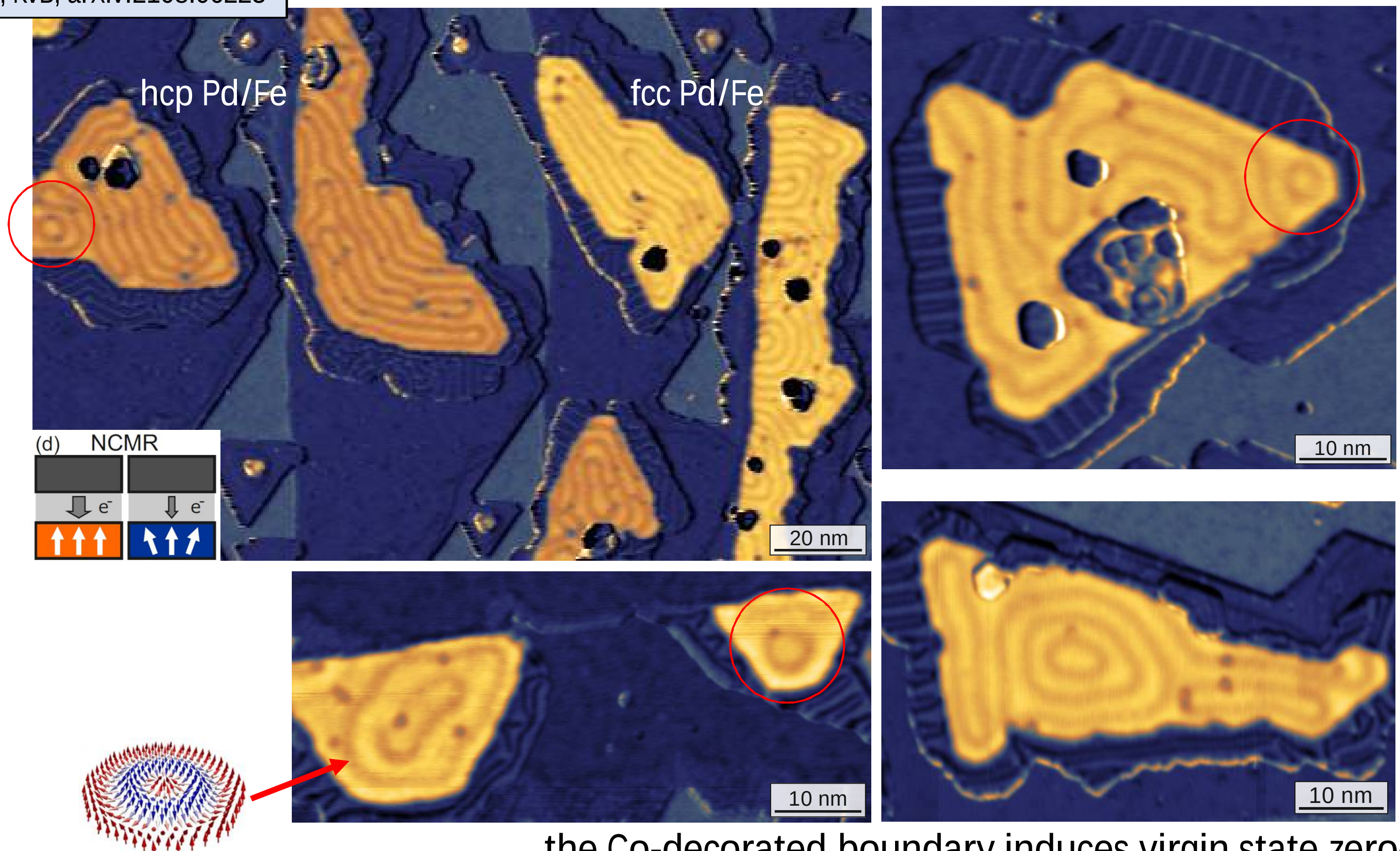




the spin spiral material Pd/Fe is surrounded by Co/Fe (in-plane);
now the spirals orient differently with respect to the island boundary

virgin state: Co/Fe next to Pd/Fe/Ir(111)

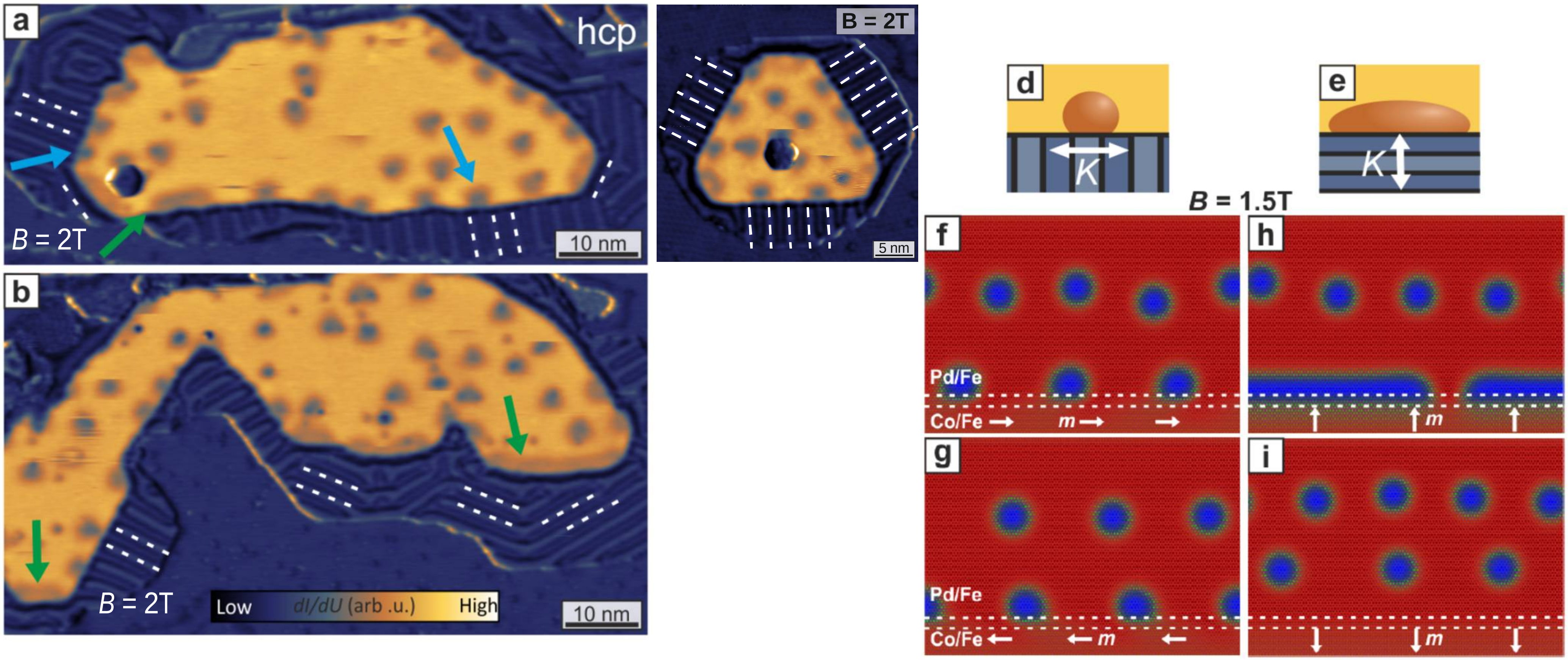
J. Spethmann, ..., KvB, arXiv:2108.06223



the Co-decorated boundary induces virgin state zero-field skyrmions, target states (skyrmionium), multi-π states

skyrmions at the edge

J. Spethmann, ..., KvB, arXiv:2108.06223



boundary magnetization direction leads to either localized or stripped-out skyrmions

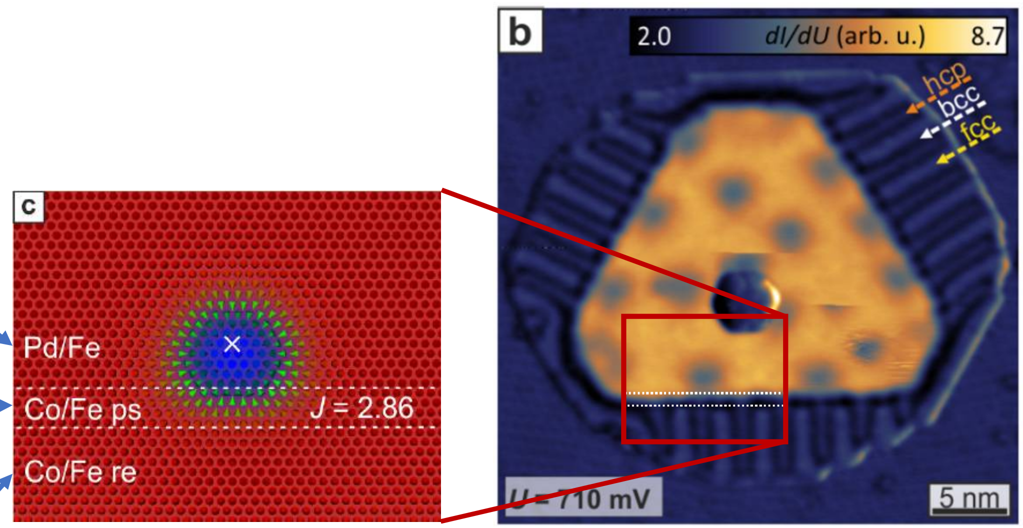
LLG atomistic simulations

J. Spethmann, ..., KvB, arXiv:2108.06223

Pd/Fe: exp. determined parameters
$J = 2.86$, $D = 0.76$, $K_z = 0.4$ meV/atom

pseudomorphic transition regime:
$J = J$, $D = D$, $K_z = -0.25$

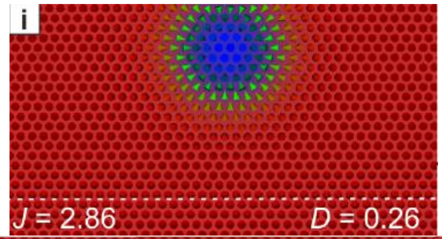
uniaxial reconstruction: random parameters
$J = 7.86$ (to mimic larger magnetic moment)
$D = D$, $K_x = 0.65$, $K_z = 0.4$



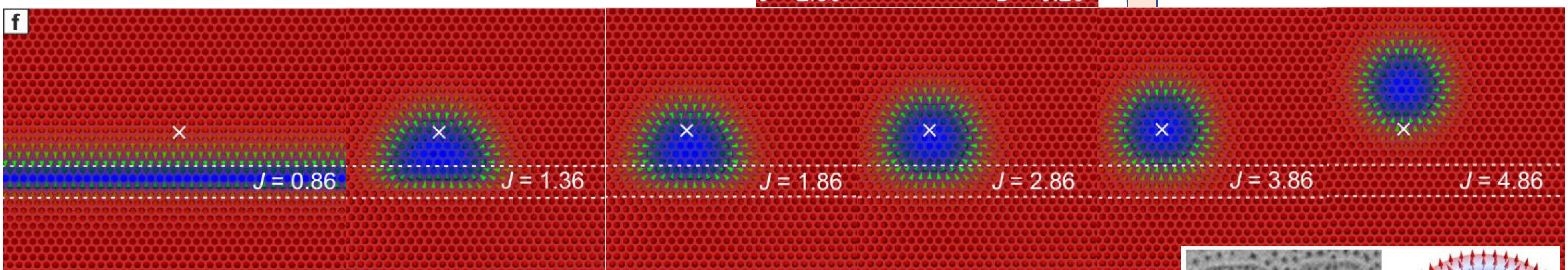
LLG atomistic simulations

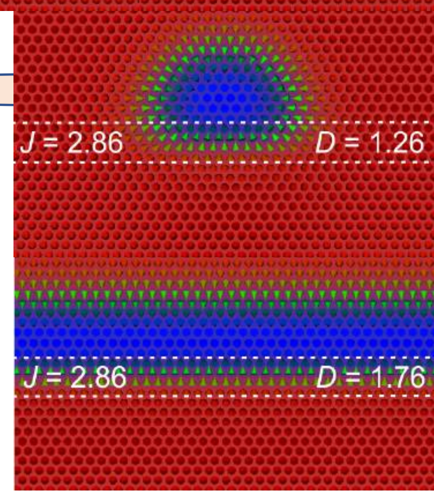
J. Spethmann, ..., KvB, arXiv:2108.06223

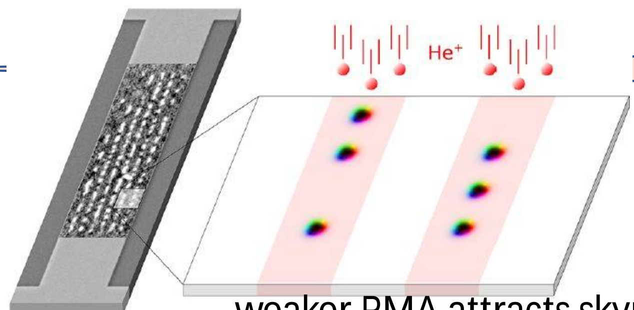
skyrmions can be pinned/repelled at the edges, depending on material parameters *J*,*D*,*K*



D

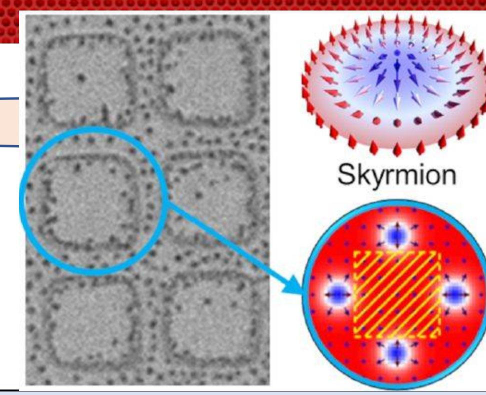






weaker PMA attracts skyrmions

R. Juge et al., Nano Lett. **21**, 2989 (2021).

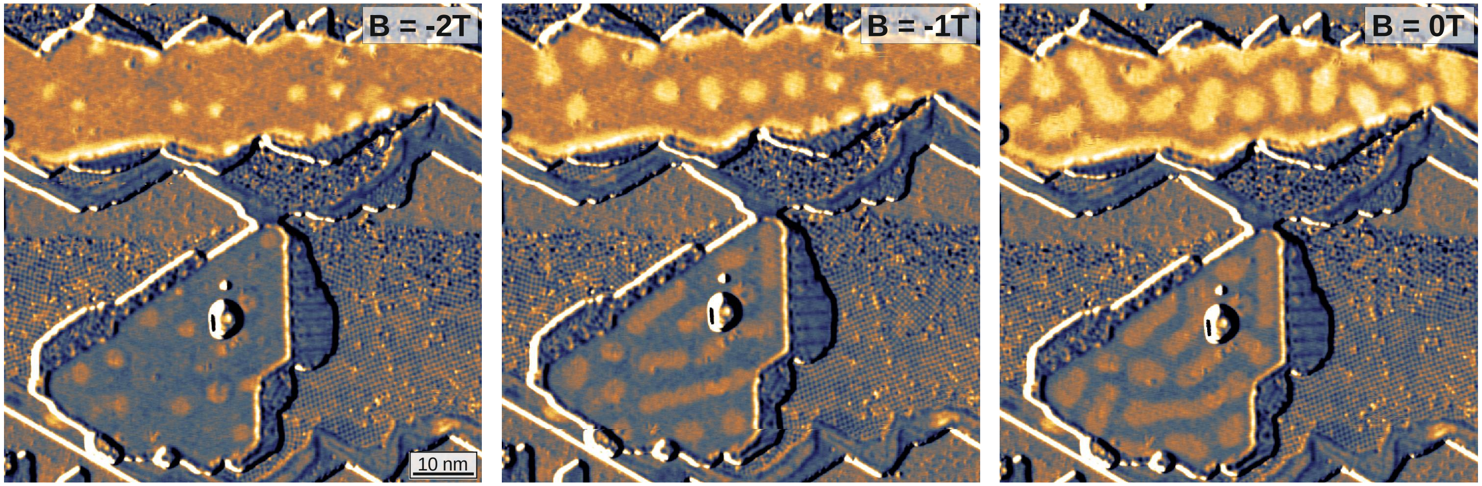


K. Ohara et al., Nano Lett. **21**, 4320 (2021).

higher PMA repells skyrmions

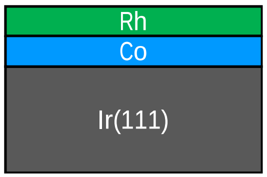
remanent zero-field skyrmions

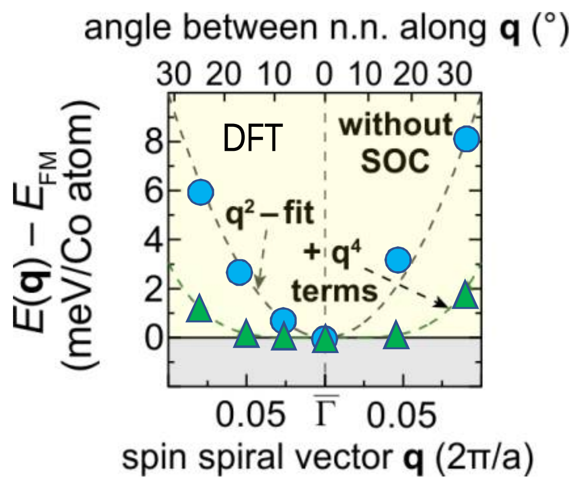
J. Spethmann, ..., KvB, arXiv:2108.06223



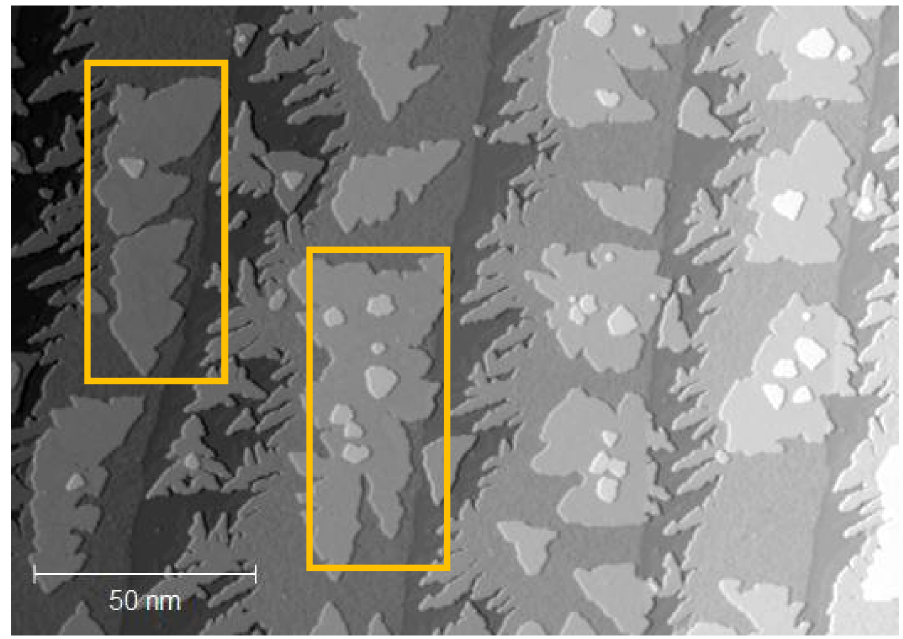
in the remament state Pd/Fe islands with a Co/Fe rim
exhibit many zero-field skyrmions

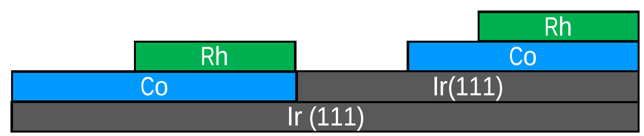
Rh/Co/Ir(111) – metastable zero-field skyrmios





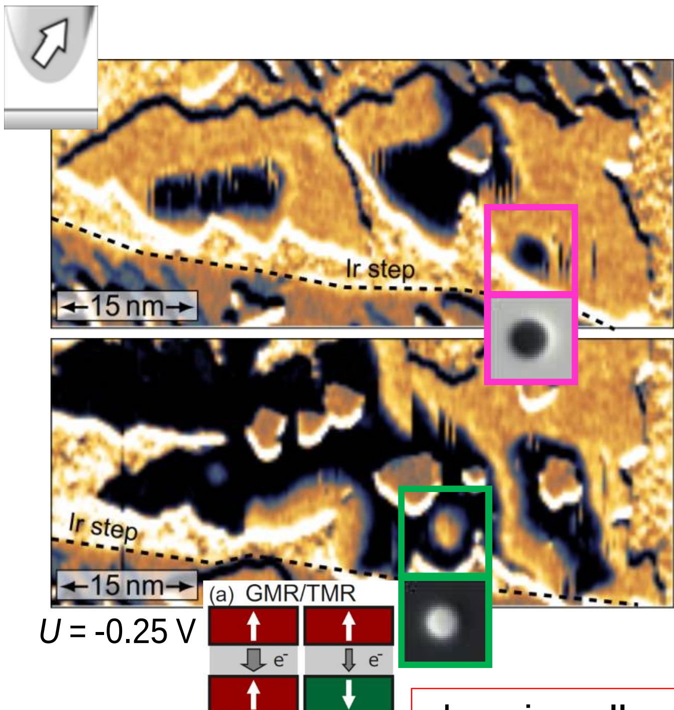
Rh/Co has a ferromagnetic ground state
strong exchange frustration
small energy cost for spin rotation up to ~15°

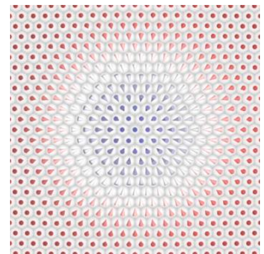




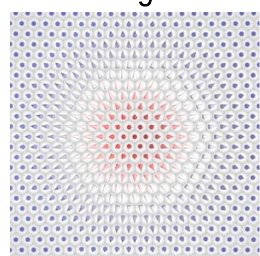
S. Meyer, ..., KvB, S. Heinze, Nature Commun. **10**, 3823 (2019).
M. Perini, ..., KvB, Phys. Rev. Lett. **123**, 237205 (2019).

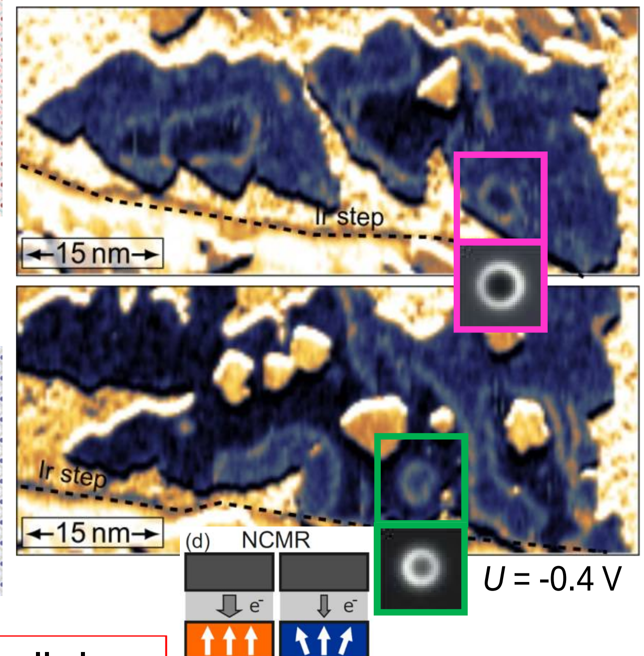
skyrmions in hcp-Rh/Co/Ir(111)





skyrmions
(up and down)
in the virgin state





domain walls are thin and unusually long
they have unique rotational sense

wall width w of 180° domain wall: $\cos\theta = \tanh\left(\frac{x}{w/2}\right)$

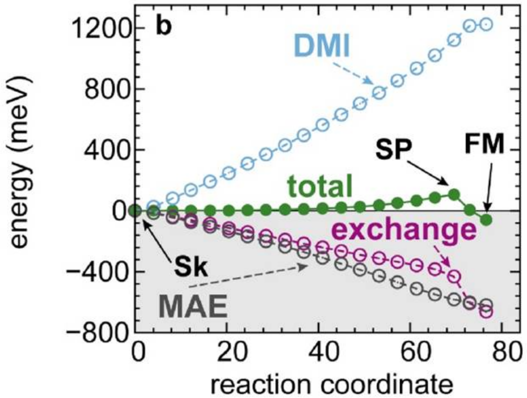
skyrmion diameter ($m_z = 0$) d

upper sk: d = 4.3 nm, w = 0.9 nm
lower sk: d = 3.5 nm, w = 1.0 nm

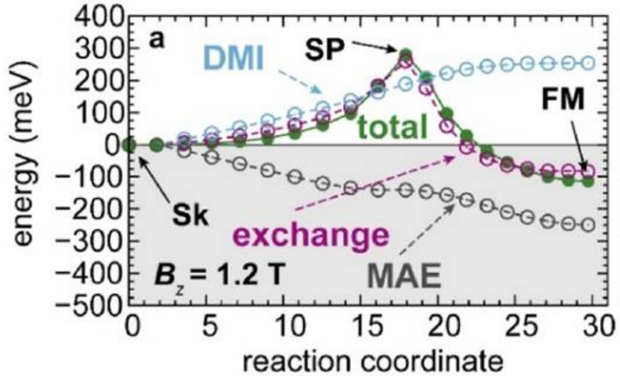
Energy barrier calculations with GNEB

GNEB = geodesic nudged elastic band

effective model

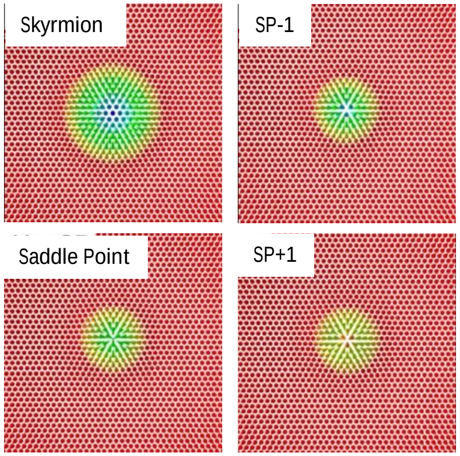


Rh/Co/Ir(111)



Typical collapse mechanism: shrinking

P.F. Bessarab et al., Comp. Phys. Comm. **196**, 335 (2015).
S. Rohart et al., Phys. Rev. B **93**, 214412 (2016).

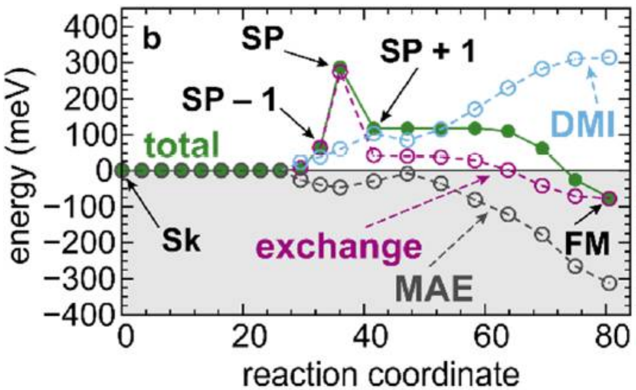


exchange frustration enhances skyrmion stability

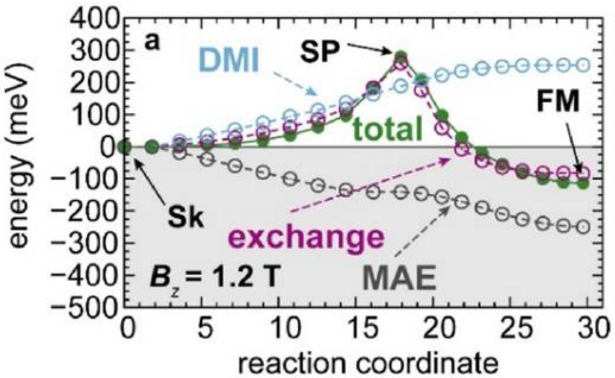
S. von Malottki et al., Sci. Rep. **7**, 12299 (2017).

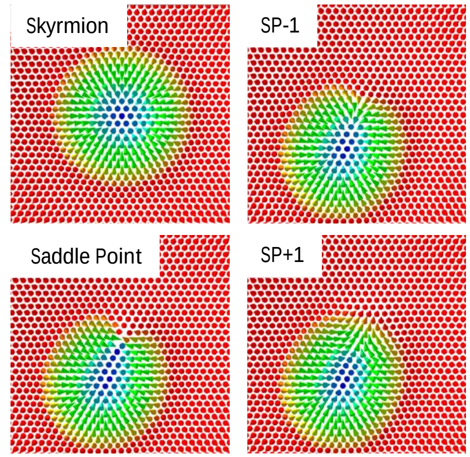
isolated zero-field skyrmion due to exch. frustration

Rh/Co/Ir(111) $B = 0$ T



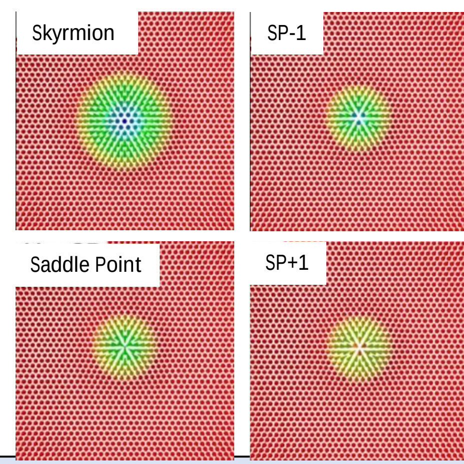
Rh/Co/Ir(111) $B = 1.2$ T





this chimera collapse also in canted fields for Pd/Fe

F. Muckel et al., Nature Phys. **17**, 395 (2021).



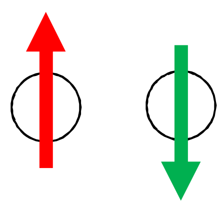
isolated zero-field magnetic skyrmions due to strong exchange frustration

S. Meyer, ..., KvB, S. Heinze, Nature Commun. **10**, 3823 (2019).

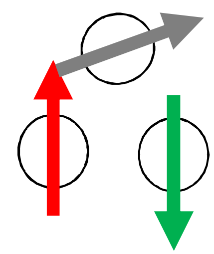
atomic-scale magnetic order: ingredients

magnetic exchange interaction

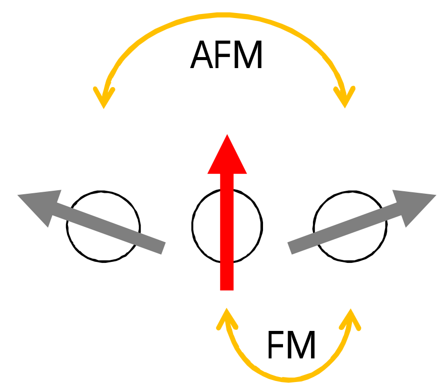
$$E = -J\,(S_1 \cdot S_2)$$



geometric frustration



exchange frustration



antisymmetric exchange (DMI)
Dzyaloshinskii-Moriya interaction
due to spin-orbit coupling
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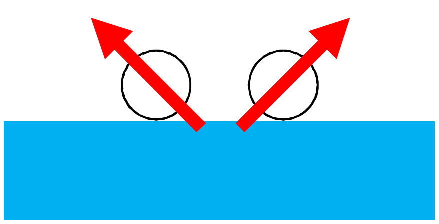
$$E = -D\,(S_1 \times S_2)$$



higher-order interactions

$$H_{\mathrm{HO}} = -\sum_{<ij>} B(\boldsymbol{m}_i\boldsymbol{m}_j)^2 - 2\sum_{<ijk>} Y_3[(\boldsymbol{m}_i\boldsymbol{m}_j)(\boldsymbol{m}_j\boldsymbol{m}_k) + (\boldsymbol{m}_j\boldsymbol{m}_k)(\boldsymbol{m}_k\boldsymbol{m}_i) + (\boldsymbol{m}_k\boldsymbol{m}_i)(\boldsymbol{m}_i\boldsymbol{m}_j)] - \sum_{<ijkl>} K_4[(\boldsymbol{m}_i\boldsymbol{m}_j)(\boldsymbol{m}_k\boldsymbol{m}_l) + (\boldsymbol{m}_i\boldsymbol{m}_l)(\boldsymbol{m}_j\boldsymbol{m}_k) - (\boldsymbol{m}_i\boldsymbol{m}_k)(\boldsymbol{m}_j\boldsymbol{m}_l)]$$

M. Hoffmann and S. Blügel, Phys. Rev. B **101**, 024418 (2020).

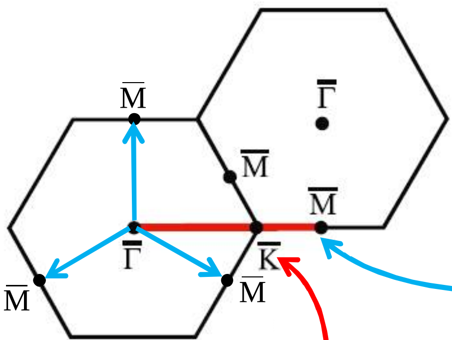
atomic-scale magnetic order

hexagonal monolayer:
afm nearest neighbor interaction J_1 → Néel state (120° coplanar)
competition afm J_1 and afm J_2 → RW-AFM (180° collinear)

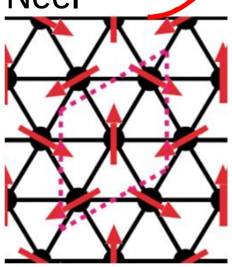
1-q state superposition multi-q state

uniaxial
3 rotational domains

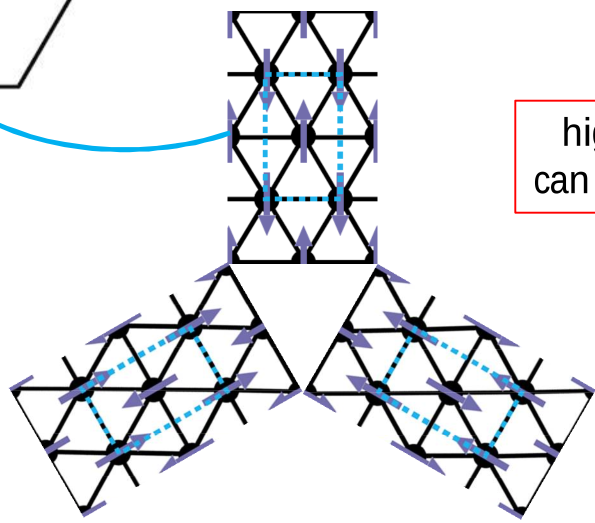
2-dimensionally modulated
3-dimensional spin structure



Néel

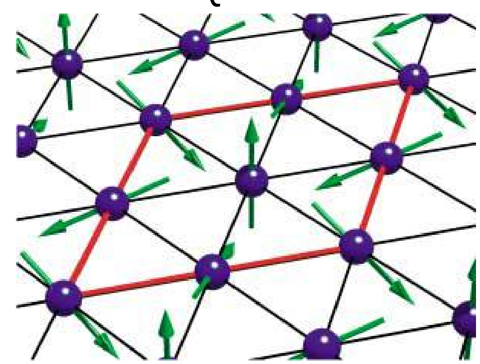


RW-AFM



higher-order interactions
can favor one over the other

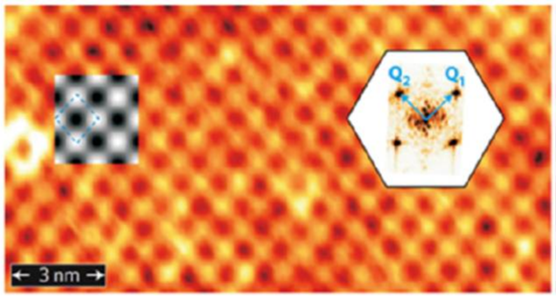
3Q-state

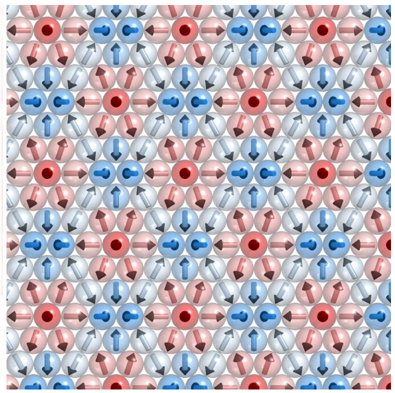


predicted for Mn/Cu(111)

P. Kurz, et al.,
Phys. Rev. Lett. **86**, 1106 (2001).

higher-order interactions

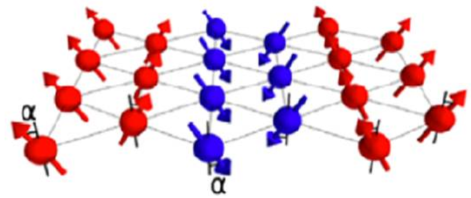




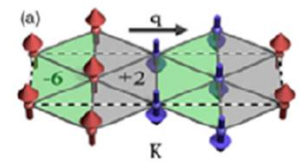
Fe/Ir(111) nanoskyrmion lattice
2-dimensional state

KvB, S. Heinze et al., Phys. Rev. Lett. **96**, 167203 (2006).
S. Heinze, KvB et al., Nature Phys. **7**, 718 (2011).

Rh/Fe/Ir(111) canted uudd

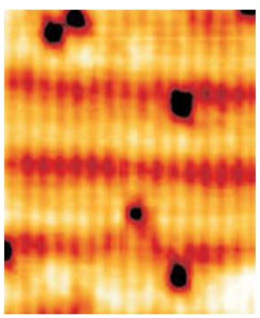


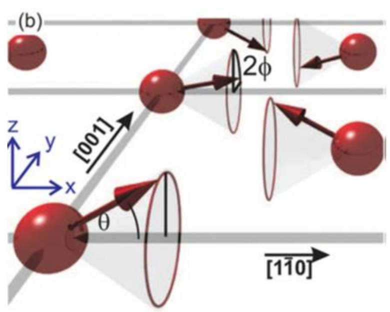
Fe/Rh(111): uudd



N. Romming, ..., KvB, Phys. Rev. Lett. **120**, 207201 (2018).
A. Krönlein et. al, Phys. Rev. Lett. **120**, 207202 (2018).

Mn-DL/W(110)
conical
antiferromag
spin spiral





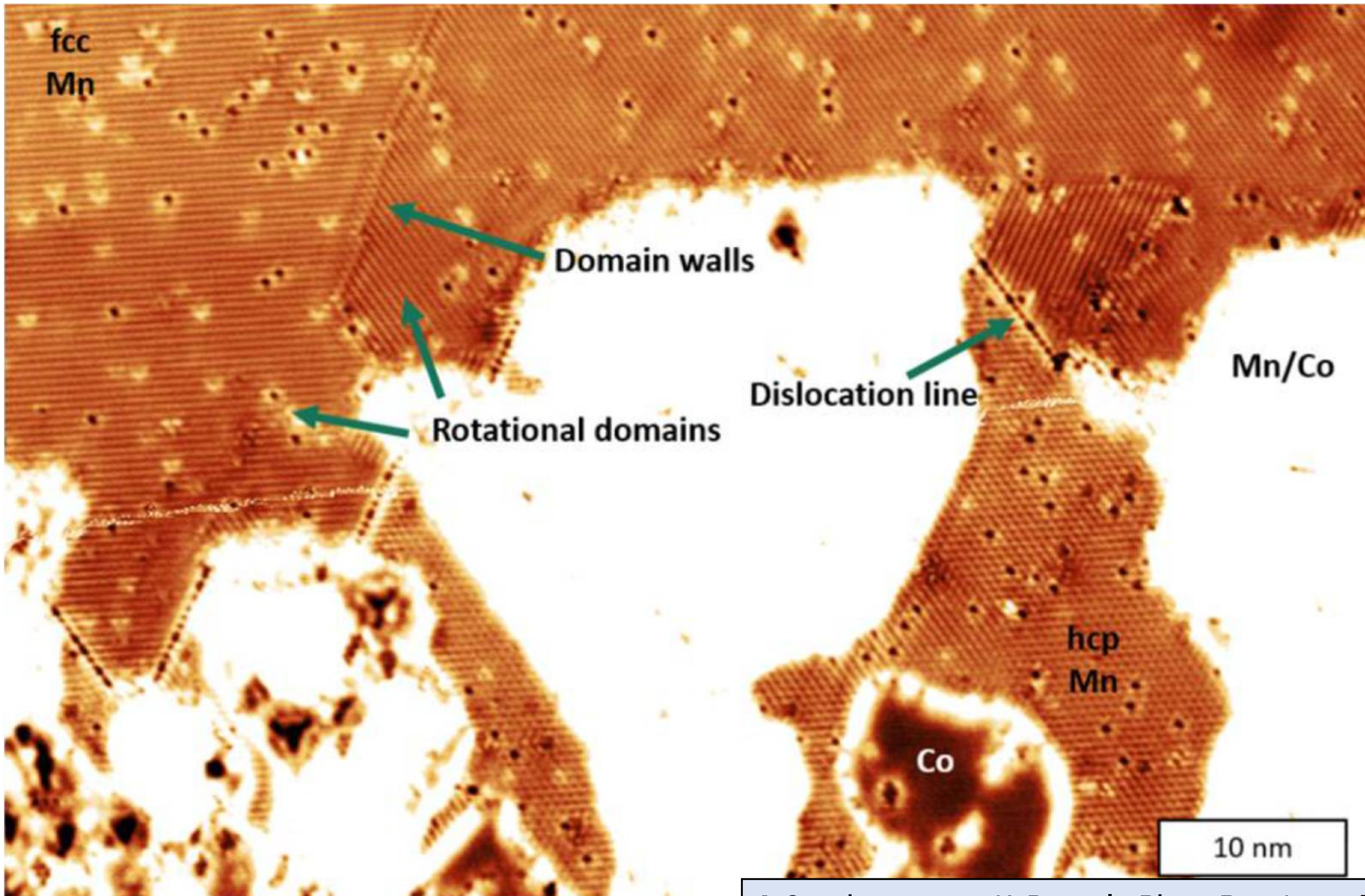
Y. Yoshida, ..., KvB et al, Phys. Rev. Lett. **108**, 087205 (2012).

More theoretical investigations,
including further phenomena and impact on transport

P. Ferriani et al, Phys. Rev. Lett. 99, 187203 (2007).
A. Al-Zubi et al., Phys. Status Solidi B 248, 2242 (2011).
M. Hoffmann et al, Phys. Rev. B **92**, 020401 (2015).
F.R. Lux et al, Communications Physics **1**, 60 (2018)
M. Hoffmann and S. Blügel, Phys. Rev. B **101**, 024418 (2020).
S. Grytsiuk et al, Nature Commun. 11, 1 (2020).
S. Paul et al, Nature Commun. 11, 4756 (2020).
.....

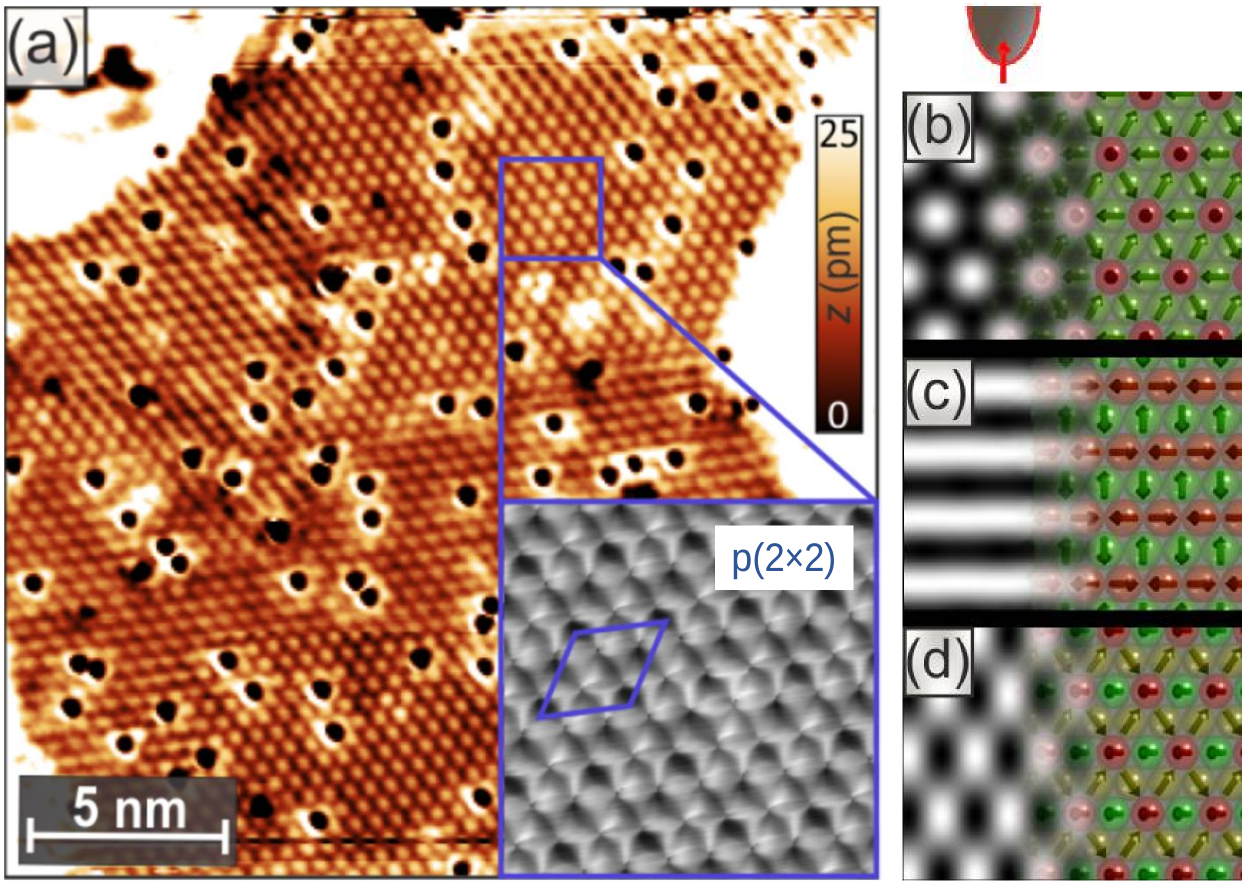
Mn monolayer on Re(0001)

fcc-Mn in SP-STM: stripes along the close-packed atomic rows, every other row → RW-AFM



J. Spethmann, ... KvB et al., Phys. Rev. Lett. **124**, 227203 (2020).
J. Spethmann, ... KvB et al., Nature Commun. **12**, 3488 (2021).

hcp-Mn/Re(0001): the 3Q-state



areas of hexagonal p(2×2) pattern
→ 3Q state
(superposition of 3 rotational domains of the RW-AFM state due to higher-order interactions)

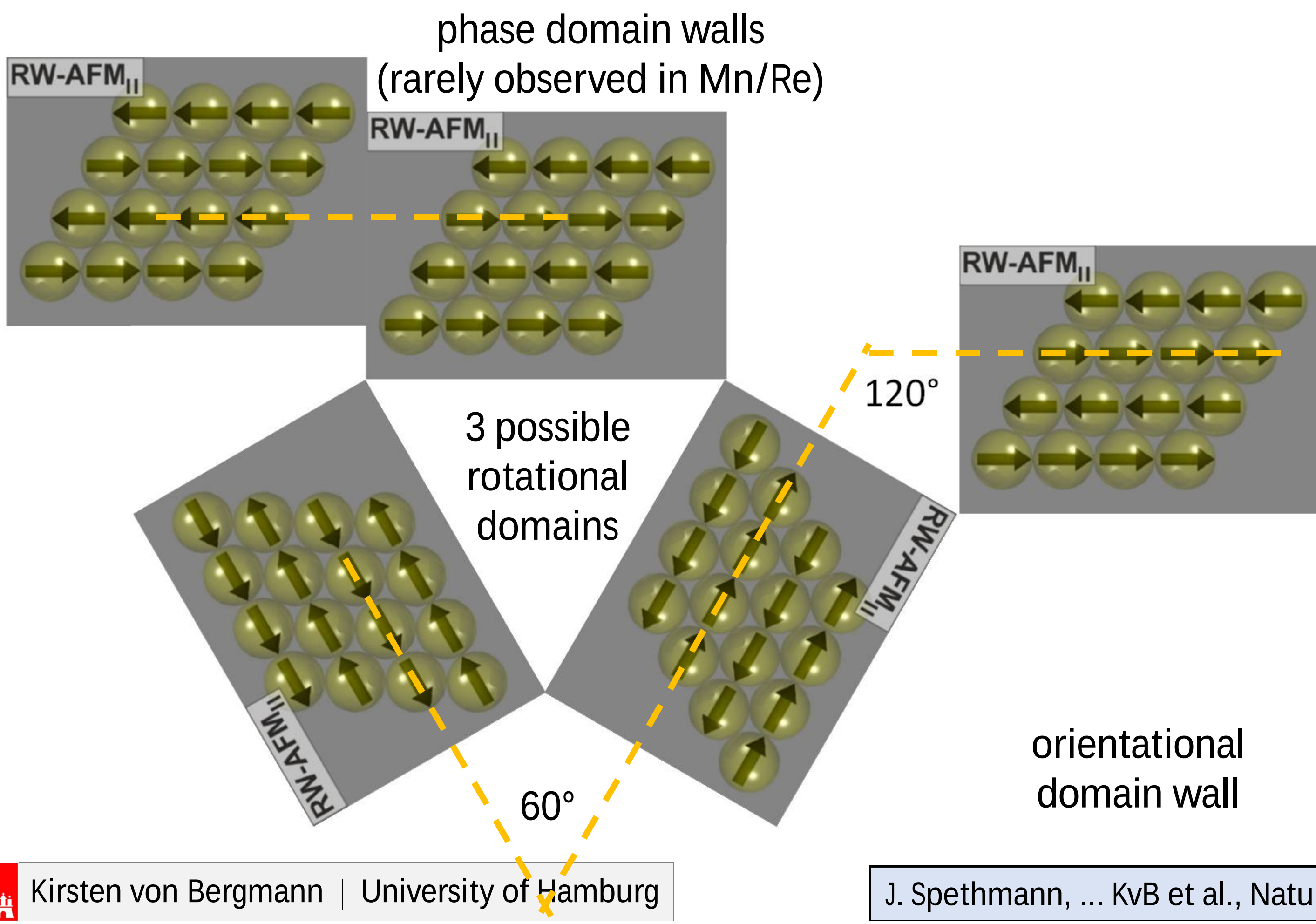
HOI

... looks slightly different in different sample areas, it must couple to the lattice ...

S. Haldar et al, arXiv.2106.08622

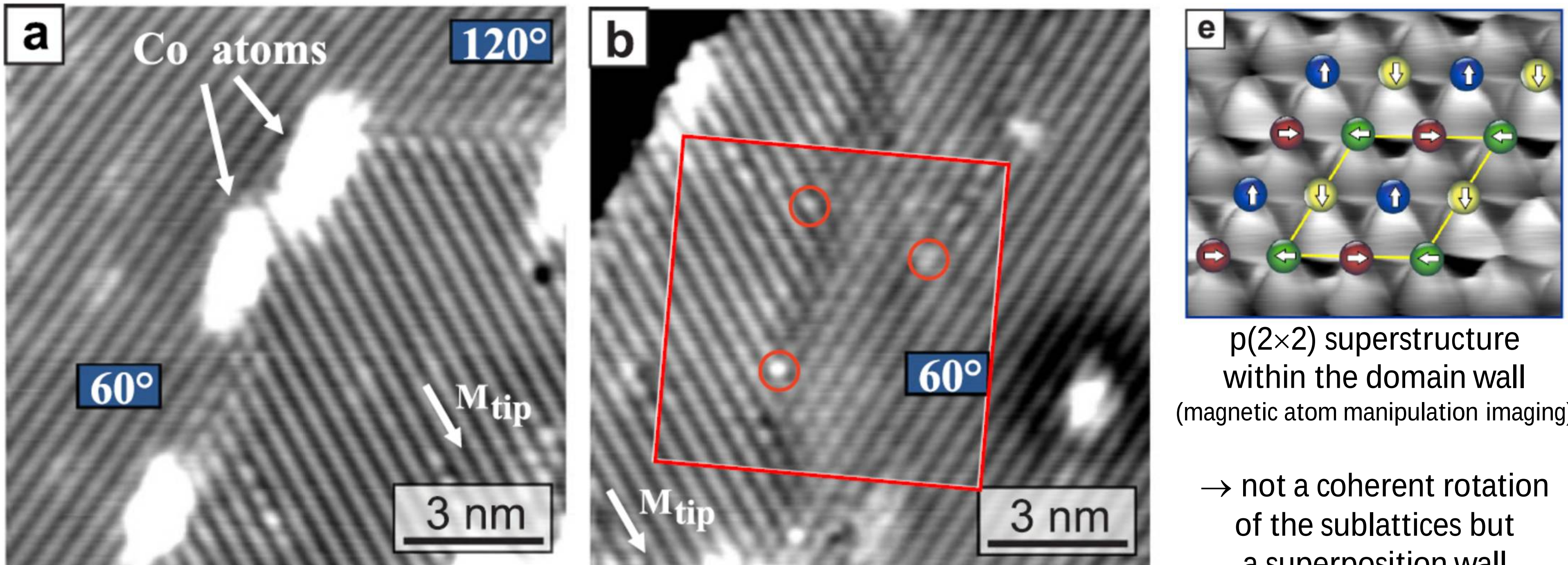
J. Spethmann, ... KvB et al., Phys. Rev. Lett. **124**, 227203 (2020).

RW-AFM domain walls



J. Spethmann, ... KvB et al., Nature Commun. **12**, 3488 (2021).

RW-AFM domain walls

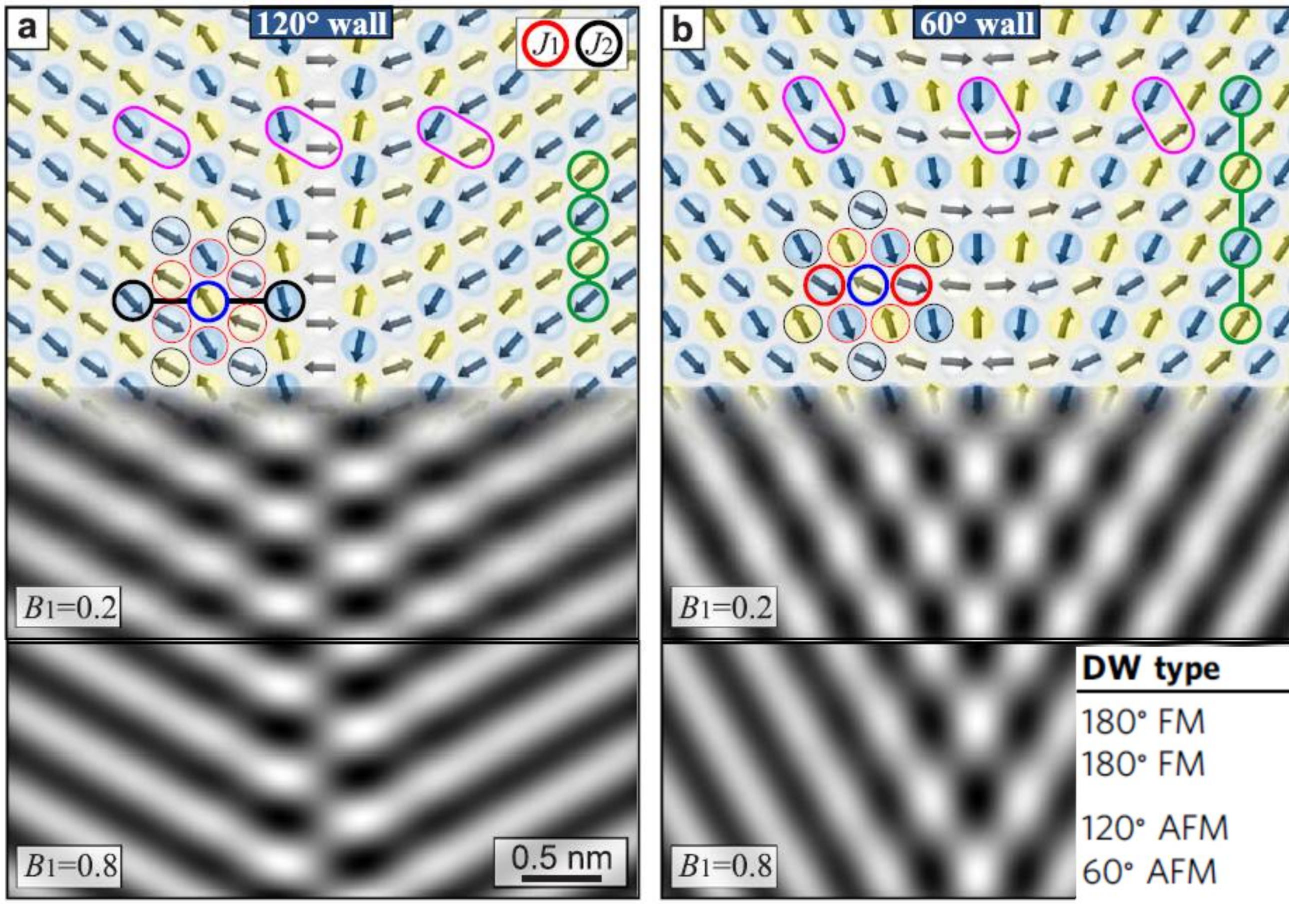


p(2×2) superstructure within the domain wall
(magnetic atom manipulation imaging)

→ not a coherent rotation of the sublattices but a superposition wall

J. Spethmann, ... KvB et al., Nature Commun. **12**, 3488 (2021).

superposition domain walls



$$H = -J_1(\mathbf{S}_i \cdot \mathbf{S}_j) - J_2(\mathbf{S}_i \cdot \mathbf{S}_j) - K(S_z)^2$$
$$- J_{\mathrm{ASE}}(\mathbf{S}_i \cdot \mathbf{d}_{ij})(\mathbf{S}_j \cdot \mathbf{d}_{ij}) - B_1(\mathbf{S}_i \cdot \mathbf{S}_j)^2$$

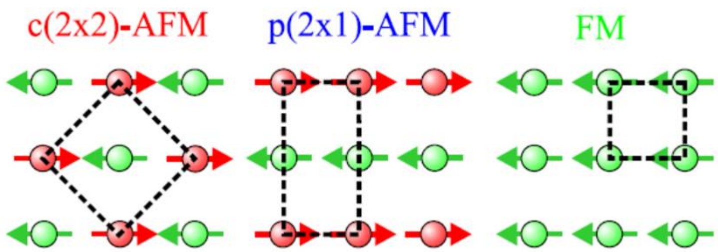
a set of simplified DFT parameters (in meV/atom)
$J_1 = -25$, $J_2 = -5$, $J_{\mathrm{ASE}} = +0.025$, $K = -1$, and B_1

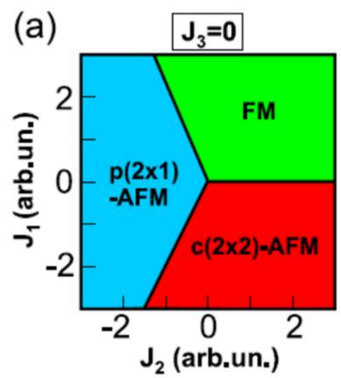
analytical formulas for these superposition domain walls: HOIs determine width and E

DW type	Model	Width	Energy
180° FM	A, K (continuum)	$2\sqrt{A/K}$	$4\sqrt{AK}$
180° FM	$J_1 > 0$, $K > 0$	$2a\sqrt{\frac{3}{2}J_1/K}$	$\frac{4}{a}\sqrt{2J_1K}$
120° AFM	$J_1, J_2 < 0$, $B_1 > 0$	$\frac{a}{2}\sqrt{3\lvert J_2\rvert/B_1}$	$\frac{8}{a}\sqrt{\lvert J_2\rvert B_1}$
60° AFM	$J_1, J_2 < 0$, $B_1 > 0$	$\frac{a}{2}\sqrt{\lvert J_1\rvert/B_1}$	$\frac{8}{a}\sqrt{\frac{1}{3}\lvert J_1\rvert B_1}$

J. Spethmann, ... KvB et al., Nature Commun. **12**, 3488 (2021).

superposition walls in other systems





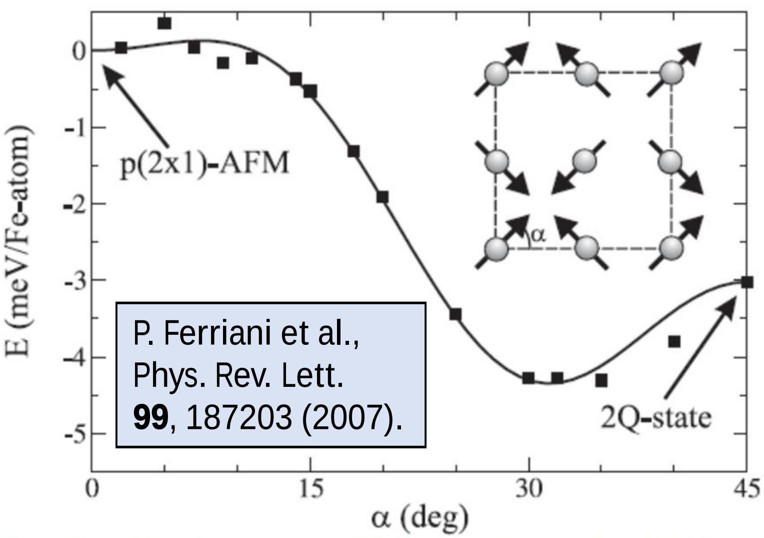
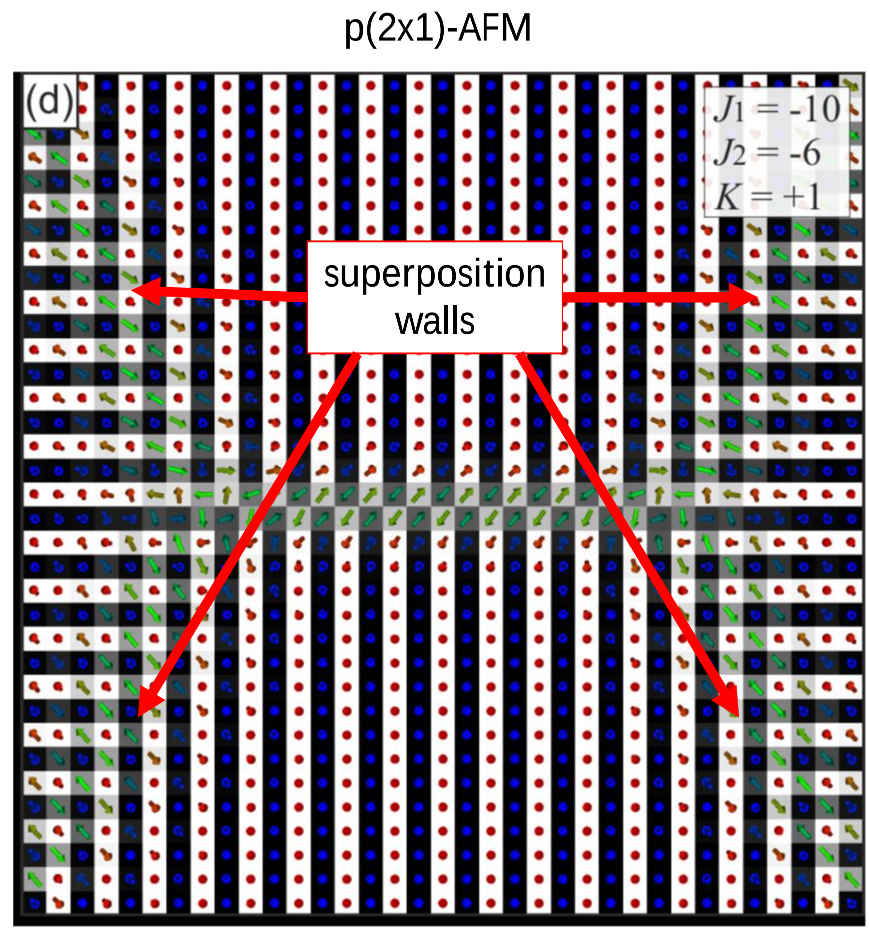


FIG. 4. Total energy of the configuration depicted in the inset for 1 ML Fe/$Ta_{0.42}W_{0.58}$ (001), as a function of the angle α.

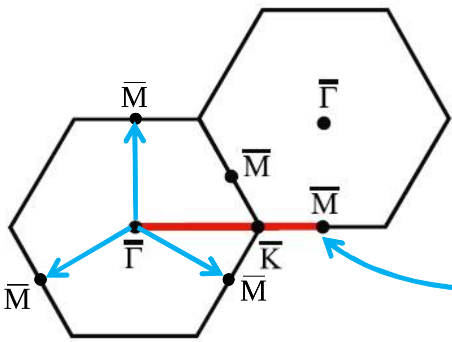


single-q to multi-q

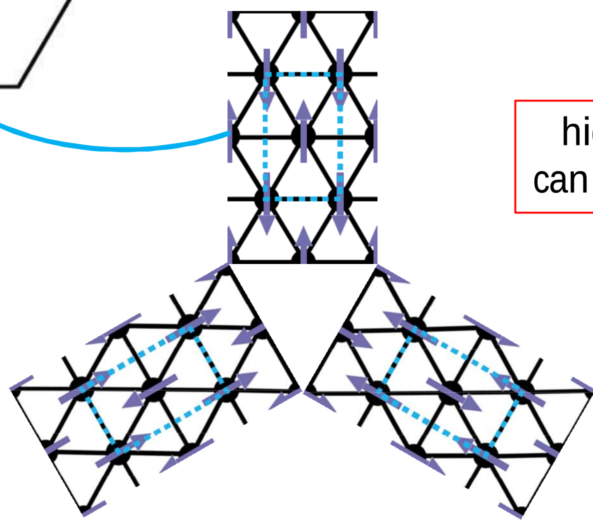
1-q state superposition multi-q state

uniaxial
3 rotational domains

2-dimensionally modulated
3-dimensional spin structure



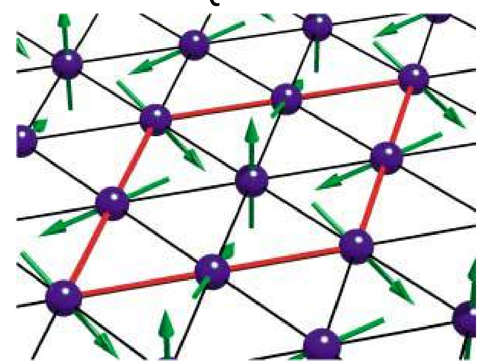
RW-AFM



higher-order interactions
can favor one over the other

**constraint of
constant magnetic moment
in the resulting
multi-q superposition**

3Q-state



predicted for Mn/Cu(111)

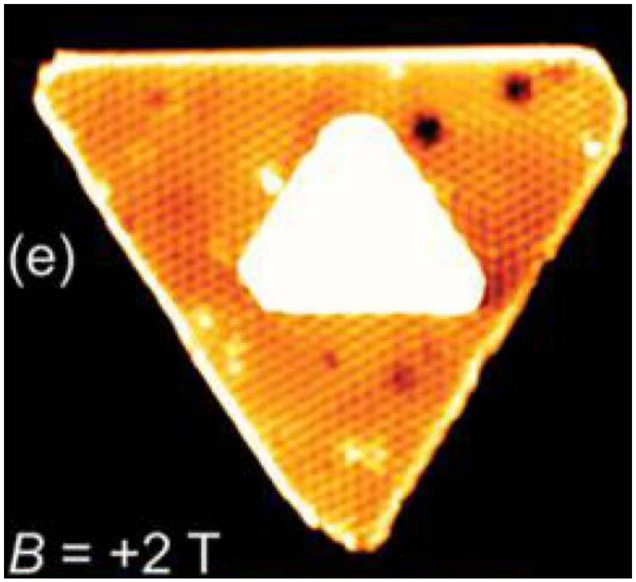
P. Kurz, et al.,
Phys. Rev. Lett. **86**, 1106 (2001).

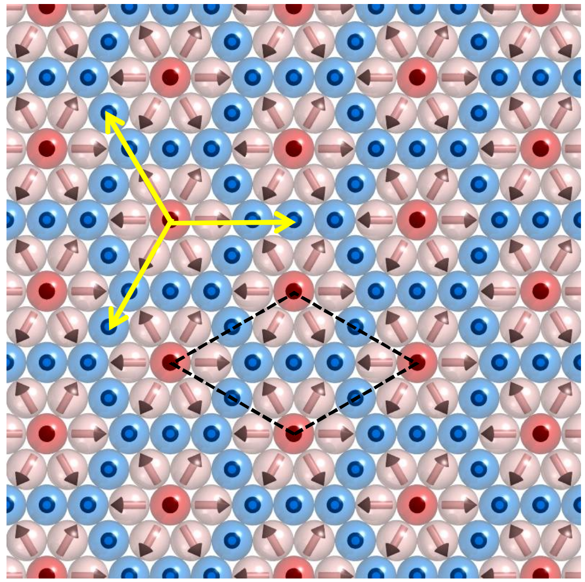
found in Mn/Re(0001)

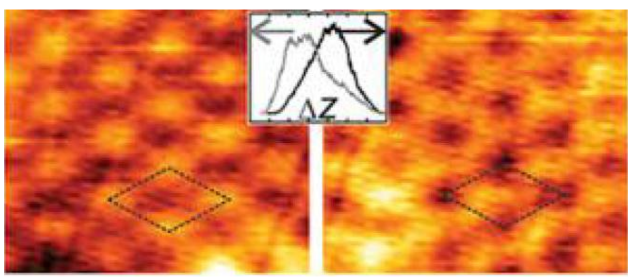
J. Spethmann, ... KvB et al., Phys. Rev. Lett. **124**, 227203 (2020).

larger magnetic unit cells ?

constraint of constant magnetic moment usually not possible

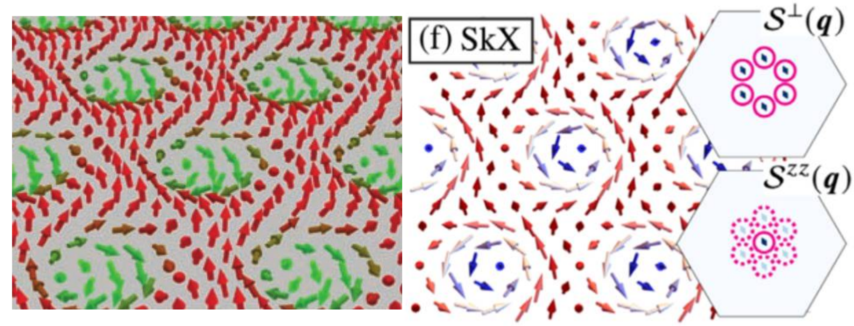


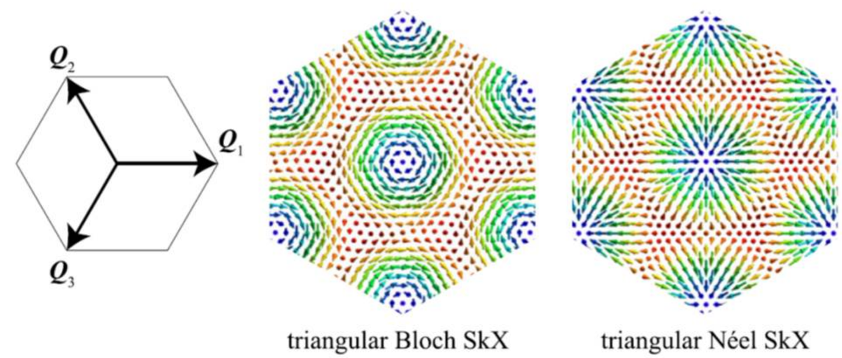




after the superposition we adjust the Fe magnetic moment to be constant (large intra-atomic exchange)

KvB, et. al, Nano Lett. **15**, 3280 (2015).

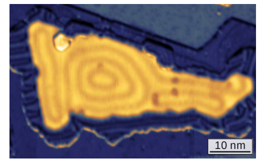




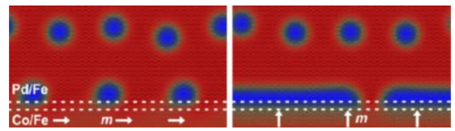
S. Mühlbauer et al., Science **323**, 915 (2009).
A.O. Leonov, M. Mostovoy, Nat. Commun. 6, 8275 (2015).
T. Kurumaji et al., Science 365, 6456 (2019).
S. Gao et al., Nature 586, 37 (2020).
N. D. Khanh et al., Nat. Nanotechnol. 15, 444 (2020).
Z. Wang et. al, Phys. Rev. Lett. **124**, 207201 (2020).
S. Hayami and Y. Motome, J. Phys.: Condens. Matter **33**, 443001 (2021), Topical Review.

summary

nano-scale skyrmions

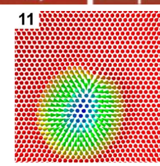


SP-STM and NCMR-imaging useful to characterize skyrmions
the rim can be utilized to modify the spin texture
zero-field skyrmions, target states, multi-π
localized or stripped-out skyrmions at the boundary



J. Spethmann, ..., KvB, arXiv:2108.06223

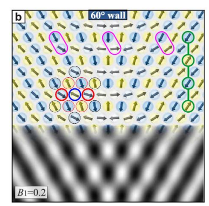
frustrated exchange can stablize isolated virgin state skyrmions



S. Meyer, ..., KvB, S. Heinze, Nature Commun. **10**, 3823 (2019).
M. Perini, ..., KvB, Phys. Rev. Lett. **123**, 237205 (2019).

higher-order interactions

HOIs can couple the RW-AFM on a hexagonal lattice to form the 3Q state
HOIs can lead to superposition walls between afm rotational domain walls
HOIs have a direct impact on the width and energy of superposition walls



J. Spethmann, ... KvB et al., Phys. Rev. Lett. **124**, 227203 (2020).
J. Spethmann, ... KvB et al., Nature Commun. **12**, 3488 (2021).

experimental screening is ... interesting ... always good for a surprise
Fe/Ir and Fe/Rh interfaces seem to promote atomic-scale magnetic order induced by HOIs
several square/hexagonal magnetic states (multi-q?) of different size have been identified

André Kubetzka
Jonas Spethmann
Marco Perini
Roland Wiesendanger

Stefan Heinze + group
(Theory, Univ. Kiel)

Deutsche Forschungsgemeinschaft DFG
MAGic Sky
Funded by the Horizon2020 Framework Programme of the European Union
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EU-FET-OPEN: MagicSky