# Beyond Heisenberg Solids: From Multi-Spin Interactions to Novel Chiral Particles

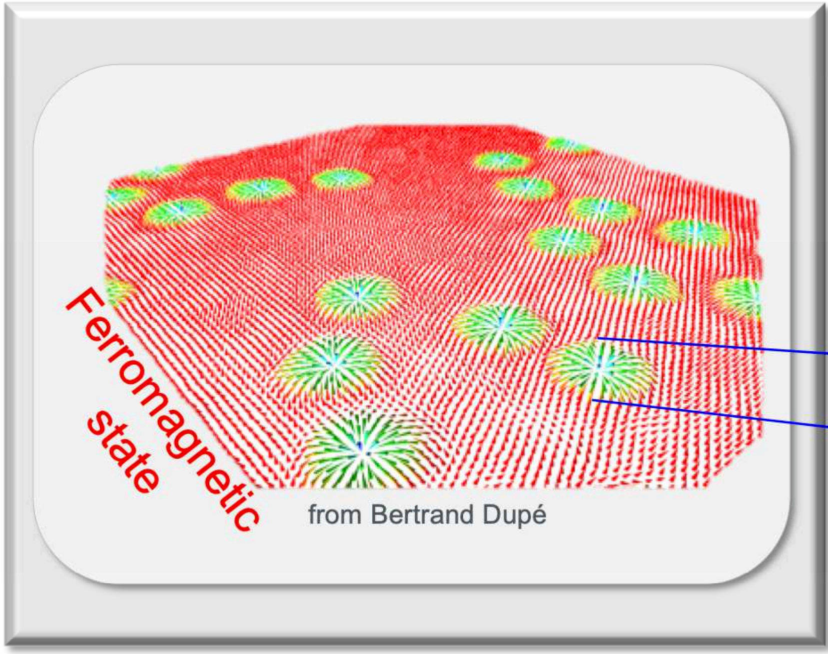
Stefan Blügel

*Peter Grünberg Institut and Institute for Advanced Simulation,*
*Forschungszentrum Jülich and JARA*

JÜLICH
Forschungszentrum

# SINGLE SMOOTH LOCALIZED MAGNETIZATION TEXTURES

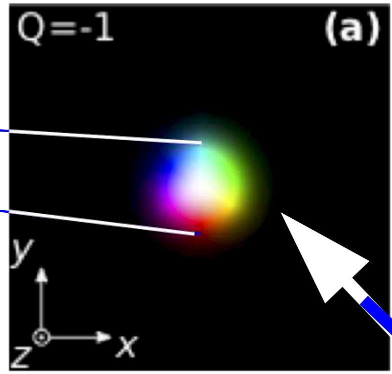
**Isolated Skyrmion**
**(topological solitons)**




- Micromagnetic energy functional **2D**:

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[ A|\nabla \mathbf{m}|^2 + \underline{\mathbf{D}} : (\nabla \mathbf{m} \times \mathbf{m}) + \mathbf{m} \cdot \underline{\mathbf{K}} \cdot \mathbf{m} - B\,\mathbf{m} \cdot \hat{\mathbf{e}}_z \right] dr^2$$

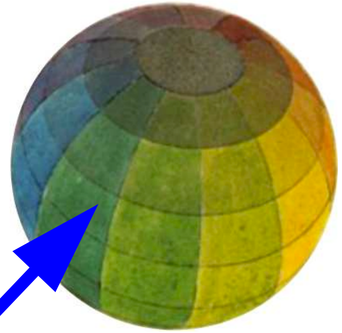
exchange interaction | Dzyaloshinskii-Moriya | magnetic anisotropy | Zeeman (magn. field)




from Vlad Kuchkin

$\mathbf{m} : \mathbb{R}^2 \rightarrow \mathbb{S}^2$

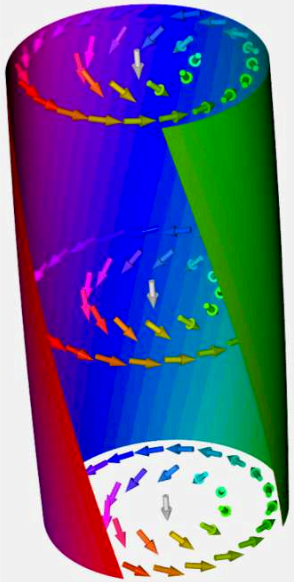
Smooth mapping
Here **d=2**,



$$Q = \frac{1}{4\pi} \int_{\mathbb{R}^2} \mathbf{m} \cdot \left( \frac{\partial \mathbf{m}}{\partial x} \times \frac{\partial \mathbf{m}}{\partial y} \right) dxdy$$

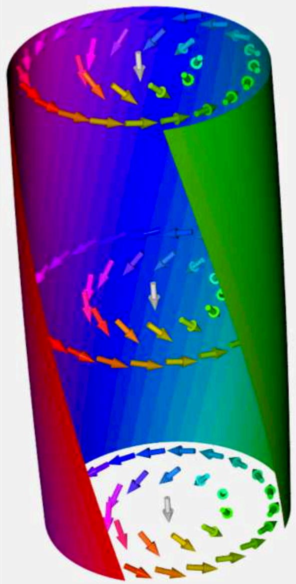
# LOCALIZED 3D MAGNETIZATION TEXTURES

## Skyrmion

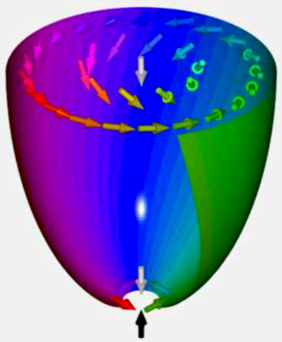


# LOCALIZED 3D MAGNETIZATION TEXTURES

**Skyrmion**

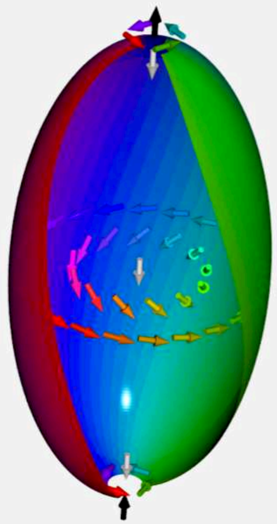


**Chiral bobber**



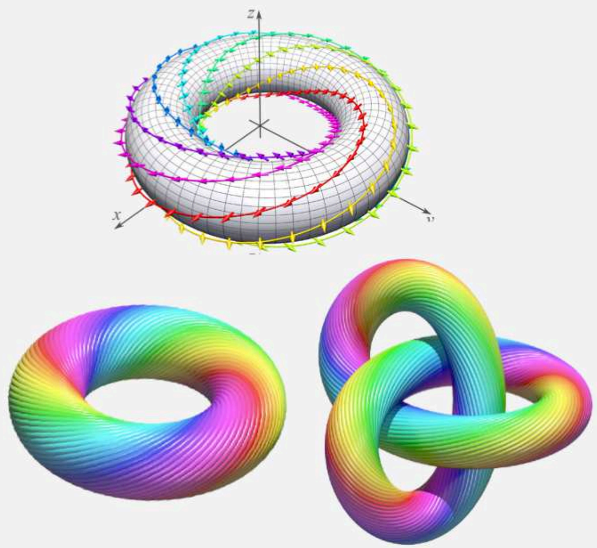
F.N. Rybakov, *et al.*,
PRB **87**, 094424 (2013);
PRL **115**, 117301 (2015);
NJP **18**, 045002 (2016)

**Globule**
**Quanco ball**



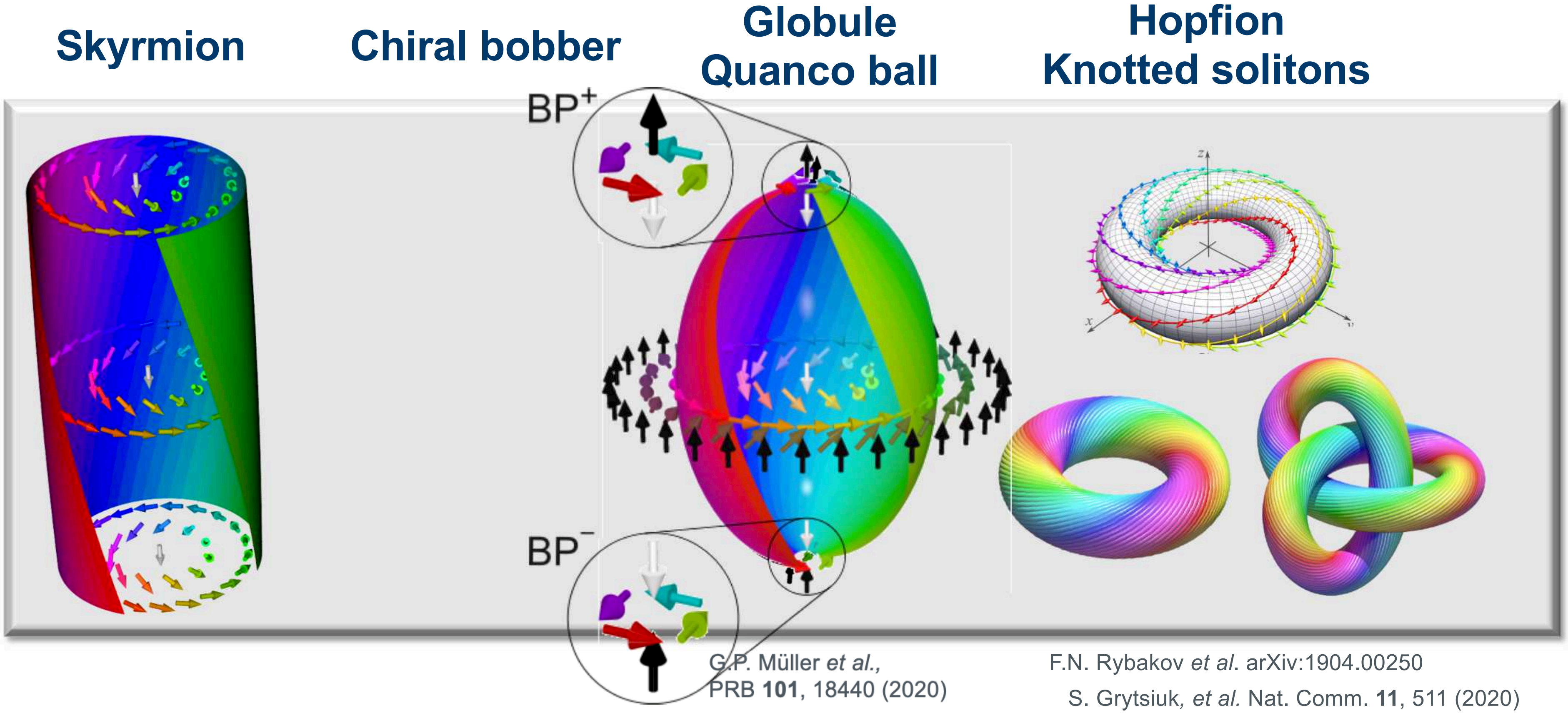
G.P. Müller *et al.*,
PRB **101**, 18440 (2020)

**Hopfion**
**Knotted solitons**




F.N. Rybakov *et al.* arXiv:1904.00250
S. Grytsiuk, *et al.* Nat. Comm. **11**, 511 (2020)

# LOCALIZED 3D MAGNETIZATION TEXTURES




G.P. Müller *et al.*, PRB **101**, 18440 (2020)

F.N. Rybakov *et al.* arXiv:1904.00250
S. Grytsiuk, *et al.* Nat. Comm. **11**, 511 (2020)

## Interesting electron transport properties

Redies, Lux, Hanke, Buhl, Müller, Kiselev, Blügel, Mokrousov, PRB **99**, 140407(R) (2019)



JÜLICH Forschungszentrum

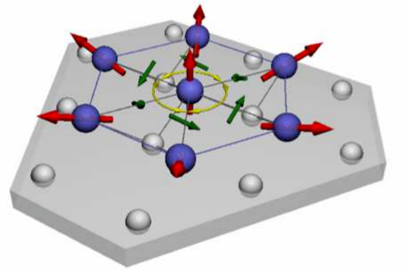
# MULTISCALE MODELING

❖ Micromagnetic-model:

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[ A\,|\nabla \mathbf{m}|^2 + \underline{\mathbf{D}} : (\nabla \mathbf{m} \times \mathbf{m}) + \mathbf{m} \cdot \underline{\mathbf{K}} \cdot \mathbf{m} - B\,\mathbf{m} \cdot \hat{\mathbf{e}}_z \right] dr$$

❖ Atomistic Spin-Lattice Model:

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

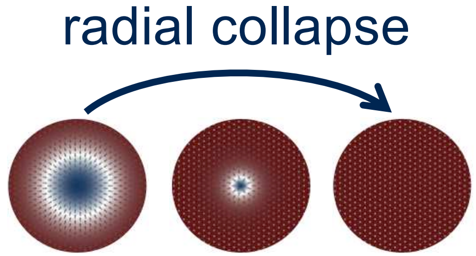


- Spin Stiffness:

$$A \propto \sum_{j>0} J_{0j} R_{0j}^2$$

- Spiralization (micromagnetic D)

$$\underline{\mathbf{D}} \propto \sum_{j>0} \mathbf{D}_{0j} \otimes \mathbf{R}_{0j}$$




**Conclusion: Limits to the micromagnetic model**
1) When skyrmions become small

Continuum approximation

$$\mathbf{m}(\mathbf{r} = \mathbf{R}_j) \approx \mathbf{m}(\mathbf{R}_i) + (\mathbf{R}_j - \mathbf{R}_i)\nabla \mathbf{m}(\mathbf{r}) \quad \Longleftarrow \quad \mathbf{m}_i = \mathbf{m}(\mathbf{R}_i)$$

# MULTISCALE MODELING

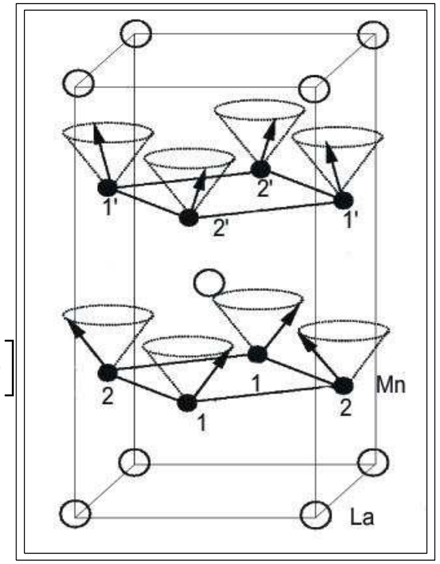
❖ Micromagnetic-model:

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[A\,|\nabla\mathbf{m}|^2 + \underline{\mathbf{D}} : (\nabla\mathbf{m} \times \mathbf{m}) + \mathbf{m}\cdot\underline{\mathbf{K}}\cdot\mathbf{m} - B\,\mathbf{m}\cdot\hat{\mathbf{e}}_z\right]\, d\mathbf{r}$$

❖ Atomistic Spin-Lattice Model:

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

$LaMn_2Ge_2$



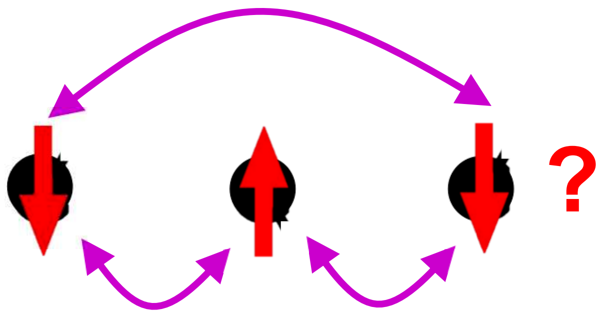

- Spin Stiffness:

$$A \propto \sum_{j>0} J_{0j} R_{0j}^2$$

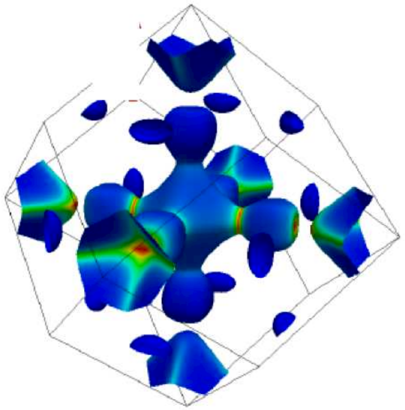
- Spiralization (micromagnetic D)

$$\underline{\mathbf{D}} \propto \sum_{j>0} \mathbf{D}_{0j} \otimes \mathbf{R}_{0j}$$

**Conclusion: Limits to the micromagnetic model**
1) When skyrmions become small
2) When competing exchange interaction

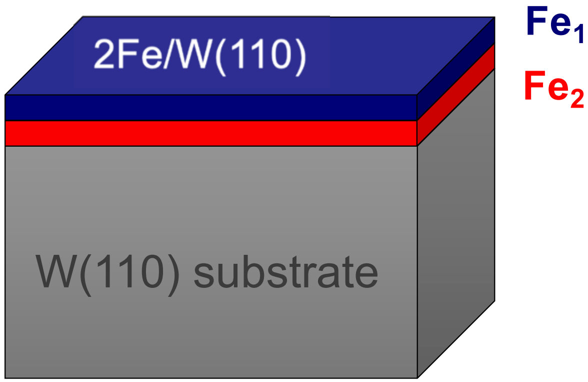


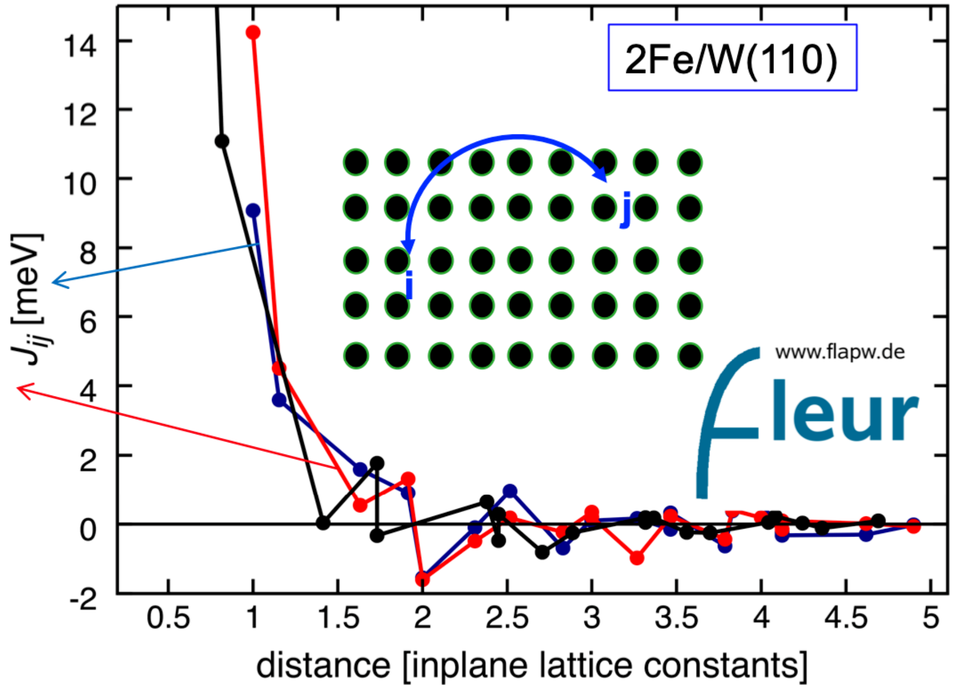
# FERMI SURFACE OF TRANSITION METALS



**bcc W** (Z=74)

Oscillatory behavior of $J_{ij}$




M. Hoffmann *et al*, Nat. Commun. **8**, 308 (2017)

**Metals:**
1) Long-ranged and competing interaction determined by Fermi Surface
2) Fermi Surface depends on magnetization direction and spin-state

# MULTISCALE MODELING

JÜLICH Forschungszentrum

❖ Micromagnetic-model:

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[ A\,|\nabla \mathbf{m}|^2 + \underline{\mathbf{D}} : (\nabla \mathbf{m} \times \mathbf{m}) + \mathbf{m} \cdot \underline{\mathbf{K}} \cdot \mathbf{m} - B\,\mathbf{m} \cdot \hat{\mathbf{e}}_z \right] dr$$

❖ Atomistic Spin-Lattice Model:

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

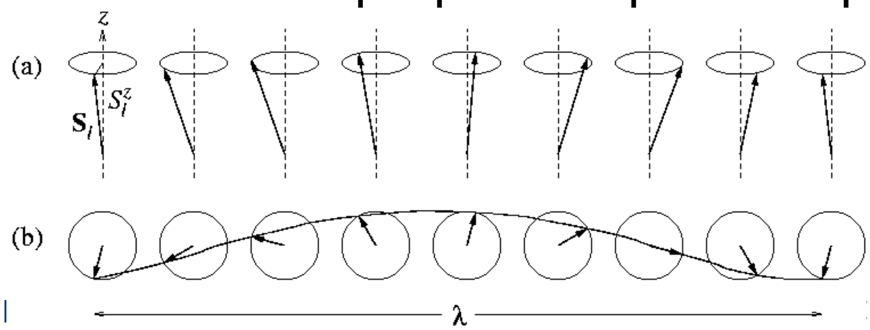
❖ DFT-model: *ab initio* total energy: $\mathbf{m}(\mathbf{r}) = \langle \Psi(\mathbf{r}) | \underline{\boldsymbol{\sigma}} | \Psi(\mathbf{r}) \rangle$

Basic idea: Compare the total energy landscape $E_{\mathrm{DFT}}\left([n], \{\mathbf{M}\}\right)$ to models

Note: Expansion of the energy has an initial state dependence $J_{ij}(\{\mathbf{M}\})$

Many tricks have been developed to determine purpose dependent parameter

- o Search of magnetic ground states
- o Thermodynamical properties
- o Magnetic excitations




$$\langle \mathbf{q} | \mathbf{S}_i^z | \mathbf{q} \rangle = \left( S - \frac{1}{N} \right) \hbar$$

# MULTISCALE MODELING

❖ Micromagnetic-model:

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[ A\,|\nabla\mathbf{m}|^2 + \underline{\mathbf{D}} : (\nabla\mathbf{m} \times \mathbf{m}) + \mathbf{m}\cdot\underline{\mathbf{K}}\cdot\mathbf{m} - B\,\mathbf{m}\cdot\hat{\mathbf{e}}_z \right] dr$$

spirit

Gideon P. Müller *et al.*
PRB **99**, 224414 (2019)

github.com/spirit-code

❖ Atomistic Spin-Lattice Model:

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

❖ DFT-model: From *ab initio* total energy: $\mathbf{m}(\mathbf{r}) = \langle \Psi(\mathbf{r}) | \underline{\boldsymbol{\sigma}} | \Psi(\mathbf{r}) \rangle$

$$E^{\mathrm{DFT}}_{\mathrm{tot}}(\mathbf{q}, \hat{e}_{\mathrm{rot}}) = E^{\mathrm{DFT}}_{\mathrm{noSOC}}(\mathbf{q}) + \Delta E^{\mathrm{DFT}}_{\mathrm{SOC}}(\mathbf{q}, \hat{e}_{\mathrm{rot}})$$

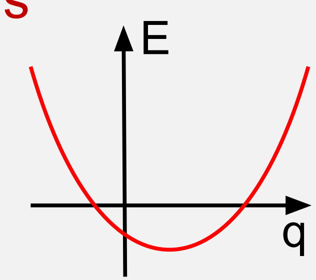
→ • $J_{ij}$, $D_{ij}$ $\underline{K}$

➢ Spin-spirals

$$E(q) = Aq^2 + Dq$$

$$\mathcal{A} = \left.\frac{d^2E(\mathbf{q})}{d\mathbf{q}\,d\mathbf{q}}\right|_{\mathbf{q}\to 0}$$

$$\mathcal{D} = \left.\frac{dE(\mathbf{q},\mathbf{e})}{d\mathbf{q}}\right|_{\mathbf{q}\to 0}$$




www.flapw.de
fleur

➢ Infinitesimal rotation

$$\{J_{ij}, \mathbf{D}_{ij}\} = -\frac{1}{\pi}\mathrm{Im}\int dE\,\mathrm{Tr}\left[\Delta V_i^{\alpha} G_{ij} \Delta V_j^{\alpha'} G_{ji}\right]$$

H. Ebert at el.,, PRB **79**, 045209 (2009).
A.I. Liechtenstein et al. J. Phys. F**14**, L125;
Solid State Com. **54**, 327 (1985)

JuKKR ($\delta E_{ij}$)

M. Heide, G. Bihlmayer, and S. Blügel, Physica B **404**, 2678 (2009)
B. Zimmermann, M. Heide, G. Bihlmayer, and S. Blügel, PRB **90**, 115427 (2014)
B. Schweflinghaus, B. Zimmermann, G. Bihlmayer and S. Blügel, PRB **94**, 024403 (2016)

# LARGE MAGNETIC MOMENTS OF METALS

- Typical metals have large local moment $m \in \{1, \ldots, 4\}\mu_B \quad \Leftrightarrow \quad \mathcal{S} \in \{1/2, \ldots, 2\}$
- Reminder Spin Algebra

$$\text{Spin} - \frac{1}{2}: \quad (\boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2})^2 = 3 - 2\boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2}$$

$$\text{Spin} - S: \quad (\boldsymbol{\sigma_1}(S) \cdot \boldsymbol{\sigma_2}(S))^{2S+1} = a_0 + a_1 (\boldsymbol{\sigma_1}(S) \cdot \boldsymbol{\sigma_2}(S)) + \cdots + a_{2S} (\boldsymbol{\sigma_1}(S) \cdot \boldsymbol{\sigma_2}(S))^{2S}$$

**4th-order exchange interactions**

$$H_4 = -\frac{1}{2}\sum_{ijkn} K_{ijkn}\left(\mathbf{S}_i \cdot \mathbf{S}_j\right)\left(\mathbf{S}_k \cdot \mathbf{S}_n\right)$$

M. Hoffmann *et al.*, PRB **101**, 024418 (2020)

**Message:**
1) For S>1/2 ➔ Higher-Order Spin Interaction

➡ **Beyond Heisenberg Solids** if this interaction becomes important

Invoke Skyrme Mechanism: T. Skyrme: *Proc. Roy. Soc. A* **260**, 127 (1961)

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[A\,|\nabla \mathbf{m}|^2 + S\,|\nabla \mathbf{m}|^{2+2n} + \mathbf{m} \cdot \underline{\mathbf{K}} \cdot \mathbf{m} - B\,\mathbf{m} \cdot \hat{\mathbf{e}}_z\right] dr^2$$

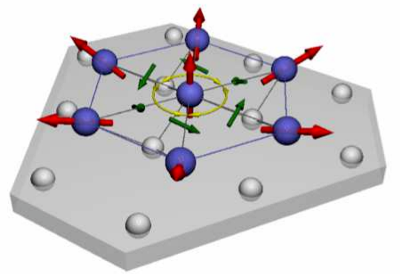
# MULTISCALE MODELING

- Micromagnetic-model:

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left[A\,|\nabla \mathbf{m}|^2 + \underline{\mathbf{D}} : (\nabla \mathbf{m} \times \mathbf{m}) + \mathbf{m}\cdot\underline{\mathbf{K}}\cdot\mathbf{m} - B\,\mathbf{m}\cdot\hat{\mathbf{e}}_z\right]\,d\mathbf{r}$$

- Atomistic Spin-Lattice Model:

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



- Spin Stiffness:

$$A \propto \sum_{j>0} J_{0j} R_{0j}^2$$

- Spiralization (micromagnetic D)

$$\underline{\mathbf{D}} \propto \sum_{j>0} \mathbf{D}_{0j} \otimes \mathbf{R}_{0j}$$

**Conclusion: Limits to the micromagnetic model**

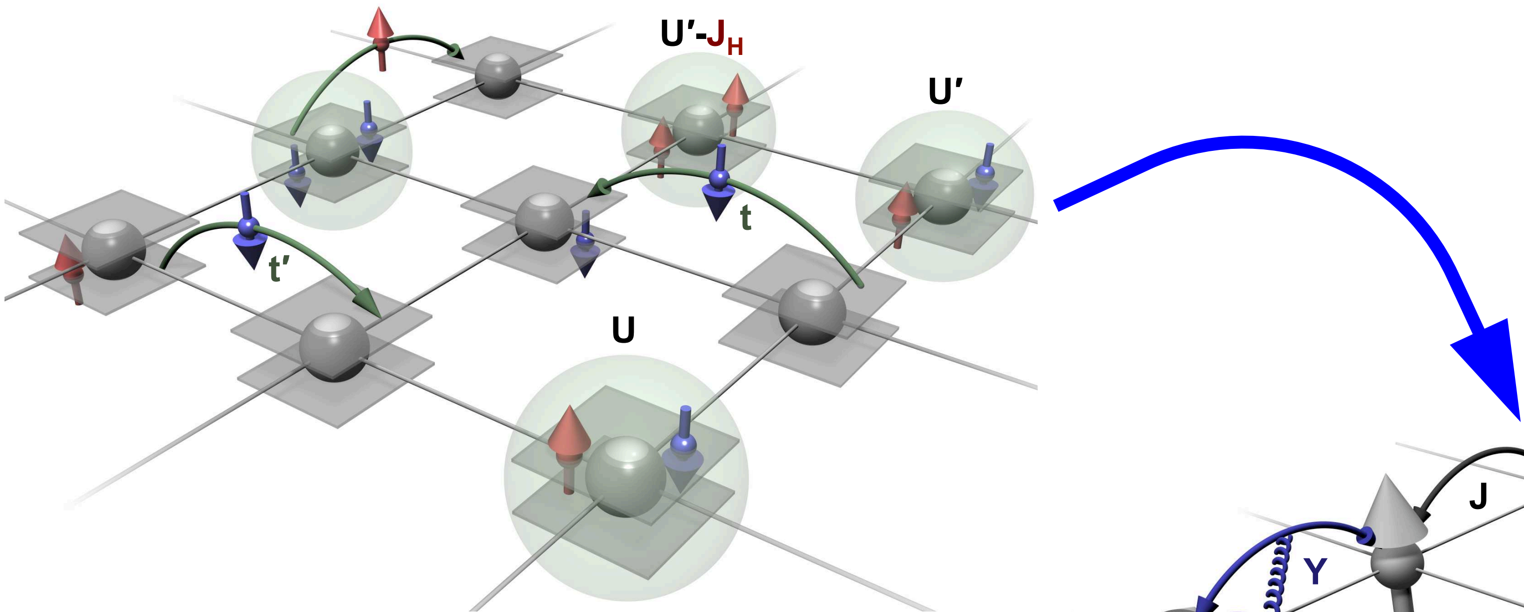
1) When skyrmions become small
2) When competing exchange interaction
3) When dealing with beyond Heisenberg solids

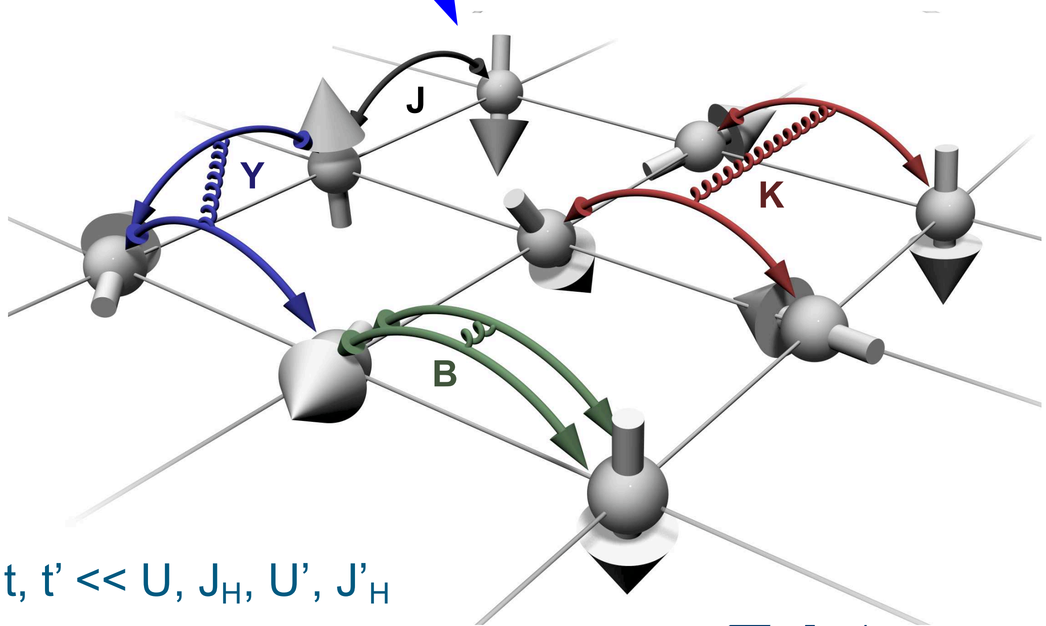
**4th-order exchange interactions**

$$H_4 = -\frac{1}{2}\sum_{ijkn} K_{ijkn}\left(\mathbf{S}_i\cdot\mathbf{S}_j\right)\left(\mathbf{S}_k\cdot\mathbf{S}_n\right)$$

M. Hoffmann *et al.*, PRB **101**, 024418 (2020)

# FROM MULTIBAND HUBBARD MODEL TO SPIN MODEL




By downfolding to

Low-energy subspace

- S=1/2: singly occupied states
- generally: Spin S at each side

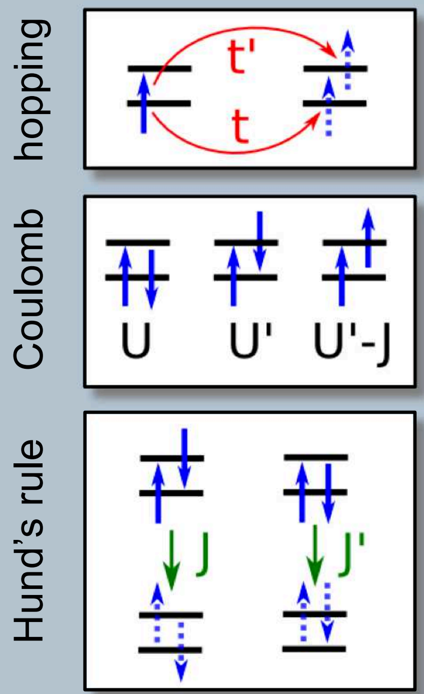
Löwdin's partitioning up to fourth order perturbation:

- canonical transformation $\tilde{H} = e^{-S}\, H\, e^{S}$ suitable for t, t' << U, $J_H$, U', $J'_H$

# Hubbard model

**Multi-band Hubbard model**

*electron*-Hamiltonian

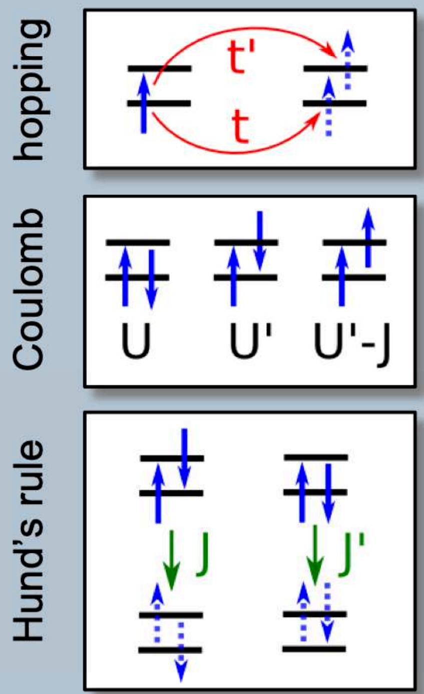


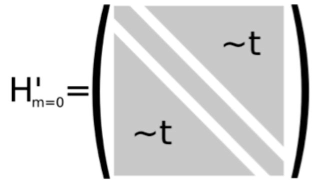

$$
\begin{aligned}
H = &- \sum_{i<j,\alpha,\sigma} t_{i,j,\alpha} \left( c^\dagger_{i,\alpha,\sigma} c_{j,\alpha,\sigma} + \text{h.c.} \right) \\
&- \sum_{\substack{i,j,\sigma \\ \alpha\neq\alpha'}} t'_{i,\alpha,j,\alpha'} \left( c^\dagger_{i,\alpha,\sigma} c_{j,\alpha',\sigma} + \text{h.c.} \right) \\
&+ \sum_{i,\alpha} U_{i,\alpha}\, n_{i,\alpha,\uparrow} n_{i,\alpha,\downarrow} \\
&+ \sum_{\substack{i,\sigma \\ \alpha<\alpha'}} U'_{i,\alpha,\alpha'} \left( n_{i,\alpha,\sigma} n_{i,\alpha',\sigma} + n_{i,\alpha,\sigma} n_{i,\alpha',\bar{\sigma}} \right) \\
&- \sum_{\substack{i,\sigma \\ \alpha<\alpha'}} J_{i,\alpha,\alpha'}\, n_{i,\alpha,\sigma} n_{i,\alpha',\sigma} \\
&- \sum_{i,\alpha<\alpha'} J_{i,\alpha,\alpha'} \left( c^\dagger_{i,\alpha,\uparrow} c_{i,\alpha,\downarrow} c^\dagger_{i,\alpha',\downarrow} c_{i,\alpha',\uparrow} + \text{h.c.} \right) \\
&- \sum_{i,\alpha<\alpha'} J'_{i,\alpha,\alpha'} \left( c^\dagger_{i,\alpha,\uparrow} c_{i,\alpha',\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\alpha',\downarrow} + \text{h.c.} \right)
\end{aligned}
$$

# Higher-order exchange interactions: Hubbard model

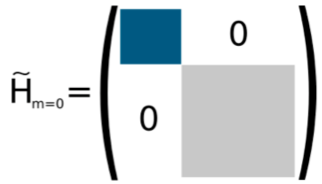
## Multi-band Hubbard model

*electron*-Hamiltonian



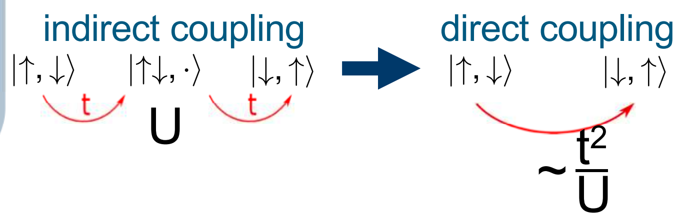




Downfolding




Mapping to spin Hamiltonian

$$H = J\,(\mathbf{S}_i \cdot \mathbf{S}_j) + \ldots$$




## Effective *spin* Hamiltonian

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

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

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

**Biquadratic = 4-spin–2-site**

$$-\sum_{ijk} Y_{ijk}\,(\mathbf{S}_i \cdot \mathbf{S}_j)\,(\mathbf{S}_i \cdot \mathbf{S}_k)$$

**4-spin–3-site**

$$-\sum_{ijkl} K_{ijkl}\,(\mathbf{S}_i \cdot \mathbf{S}_j)\,(\mathbf{S}_k \cdot \mathbf{S}_l)$$

**4-spin–4-site**

M. Hoffmann *et al.*, PRB **101**, 024418 (2020)

# EXAMPLE: FOUR-SPIN-TREE-SITE INTERACTION

M. Hoffmann *et al.*, PRB **101**, 024418 (2020)

❖ Four-spins-three-sites

$$H_3 = -\sum_{ijk} Y_{ijk} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right) \left(\mathbf{S}_i \cdot \mathbf{S}_k\right)$$

❖ Spin operators $n^{\dagger}_{3,1,\downarrow} n^{\dagger}_{1,2,\uparrow} c^{\dagger}_{3,2,\downarrow} c^{\dagger}_{2,2,\uparrow} c^{\dagger}_{2,1,\uparrow} c^{\dagger}_{1,1,\downarrow} c_{1,1,\uparrow} c_{2,1,\downarrow} c_{2,2,\downarrow} c_{3,2,\uparrow}$

❖ Parameter Four-spins-three-sites for 3 orbitals

$$\begin{aligned} Y_{3\times 3} = &+ (t-t')^2 \cdot (t^2 + 2tt' + 3t'^2) \cdot \Bigg[ -\frac{1}{(U+2J_H)^2} \cdot \left( \frac{16}{9(2U+3J_H+U')} + \frac{8}{9(2U+4J_H-U'+J'_H)} + \frac{16}{81 J_H} \right) \\ &\qquad + \frac{16}{243(U+2J_H)J_H^2} - \frac{16}{243(5J_H+U)J_H^2} \Bigg] \\ &+ \frac{1}{(U+2J_H)^2} \cdot \Bigg[ -\frac{8t^4 + 64t^2t'^2 + 32tt'^3 + 40t'^4}{9(2U+4J_H-U'-J'_H)} + \frac{16t'^2(t'+2t)^2}{9(U+2J_H-U'-J'_H)} \\ &\qquad + \frac{64t^4 + 384t^2t'^2 + 128tt'^3 + 288t'^4}{27(U+2J_H)} \Bigg] \end{aligned}$$

# HUBBARD MODEL + SPIN-ORBIT INTERACTION

$$H = \frac{1}{2}\sum_{ij} J_{ij}\, \mathbf{m}_i \cdot \mathbf{m}_j + \sum_{ij} \mathbf{D}_{ij}\, (\mathbf{m}_i \times \mathbf{m}_j) + \sum_{ij} \mathbf{C}_{ij}\, (\mathbf{m}_i \cdot \mathbf{m}_j)(\mathbf{m}_i \times \mathbf{m}_j) + \cdots$$

$2^{nd}$ – order perturbation

$4^{th}$ –order perturbation

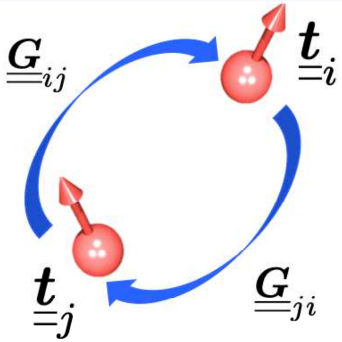
Lászlóffy, Rózsa, Palotás, Udvardi and Szunyogh, PRB **99** 184430 (2019)
Brinker, dos Santos Dias, Lounis, NJP **21** 083015 (2019)

# EXCHANGE INTERACTIONS FROM DFT MODEL

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

$$E_{\mathrm{DFT}}([n],\{\mathbf{M}\}) \longrightarrow E_{\mathrm{DFT}}([n],\{\mathbf{M}+\delta\mathbf{M}\}) = E_{\mathrm{DFT}}([n],\{\mathbf{M}\}) + \delta E_{\mathrm{sp}}(\{\mathbf{M}+\delta\mathbf{M}\}) + \mathcal{O}((\delta\mathbf{M})^2(\delta n)^2)$$

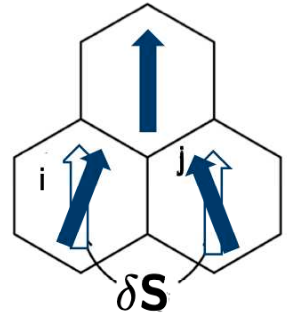
Single particle energy $\delta E_{\mathrm{sp}} = -\frac{1}{\pi}\mathrm{Im}\int_{-\infty}^{\epsilon_F} \mathrm{d}\epsilon\ \mathrm{Tr}\ln\left[1 - G(\epsilon)\delta t(\epsilon)\right]$




$$G_{ij} = A_{ij}\,\sigma_0 + \mathbf{B}_{ij}\cdot\boldsymbol{\sigma}$$

$$\delta t_i(\epsilon) = t_i^s(\epsilon)\,\delta\mathbf{S}_i\cdot\boldsymbol{\sigma}$$

$$\ln(1-x) = -x - \frac{x^2}{2} - \frac{x^3}{3} - \frac{x^4}{4} - \cdots$$




2nd – order term: $\delta E_{2\text{-spin}} = -\frac{1}{2\pi}\mathrm{Im}\ \mathrm{Tr}\int_{-\infty}^{\epsilon_F}\mathrm{d}\epsilon \sum_{ij} G_{ij}(\epsilon)\delta t_j(\epsilon)G_{ji}(\epsilon)\delta t_i(\epsilon)$

Collecting $\propto \delta t_j \delta t_i \rightarrow \mathbf{S}_i \star \mathbf{S}_j := \sum_{ij}\left[J_{ij}^{\mathrm{iso}}\,\delta\mathbf{S}_i\cdot\delta\mathbf{S}_j + \mathbf{D}_{ij}\cdot\left(\delta\mathbf{S}_i\times\delta\mathbf{S}_j + \delta\mathbf{S}_i\cdot\underline{\mathbf{J}}_{ij}^{\mathrm{ani}}\,\delta\mathbf{S}_j\right)\right]$ terms

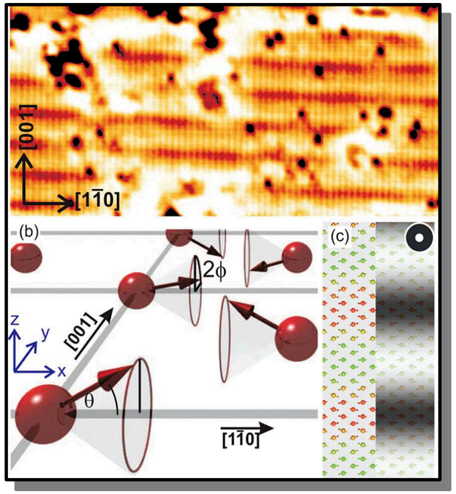
with

$$J_{ij}^{\mathrm{iso}} = -\frac{1}{\pi}\mathrm{Im}\ \mathrm{Tr}\int_{-\infty}^{\epsilon_F}\mathrm{d}\epsilon\left\{A_{ij}(\epsilon)t_j^s(\epsilon)A_{ji}(\epsilon)t_i^s(\epsilon) + \left[\mathbf{B}_{ij}(\epsilon)t_j^s(\epsilon)\right]\cdot\left[\mathbf{B}_{ji}(\epsilon)t_i^s(\epsilon)\right]\right\}$$

$$\mathbf{D}_{ij} = -\frac{1}{\pi}\mathrm{Re}\ \mathrm{Tr}\int_{-\infty}^{\epsilon_F}\mathrm{d}\epsilon\left\{A_{ij}(\epsilon)t_j^s(\epsilon)\mathbf{B}_{ji}(\epsilon)t_i^s(\epsilon) - \mathbf{B}_{ij}(\epsilon)t_j^s(\epsilon)A_{ji}(\epsilon)t_i^s(\epsilon)\right\}$$

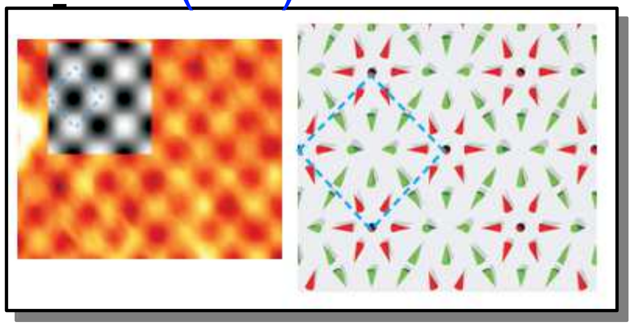
# Examples of 4 spin-interactions

_2Mn/W(110)




Yoshida *et al.*,PRL 108, 087205 (2012)

_Fe/Ir(111)



Heinze *et al.*, Nature Physics 7, 713 (2011)

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

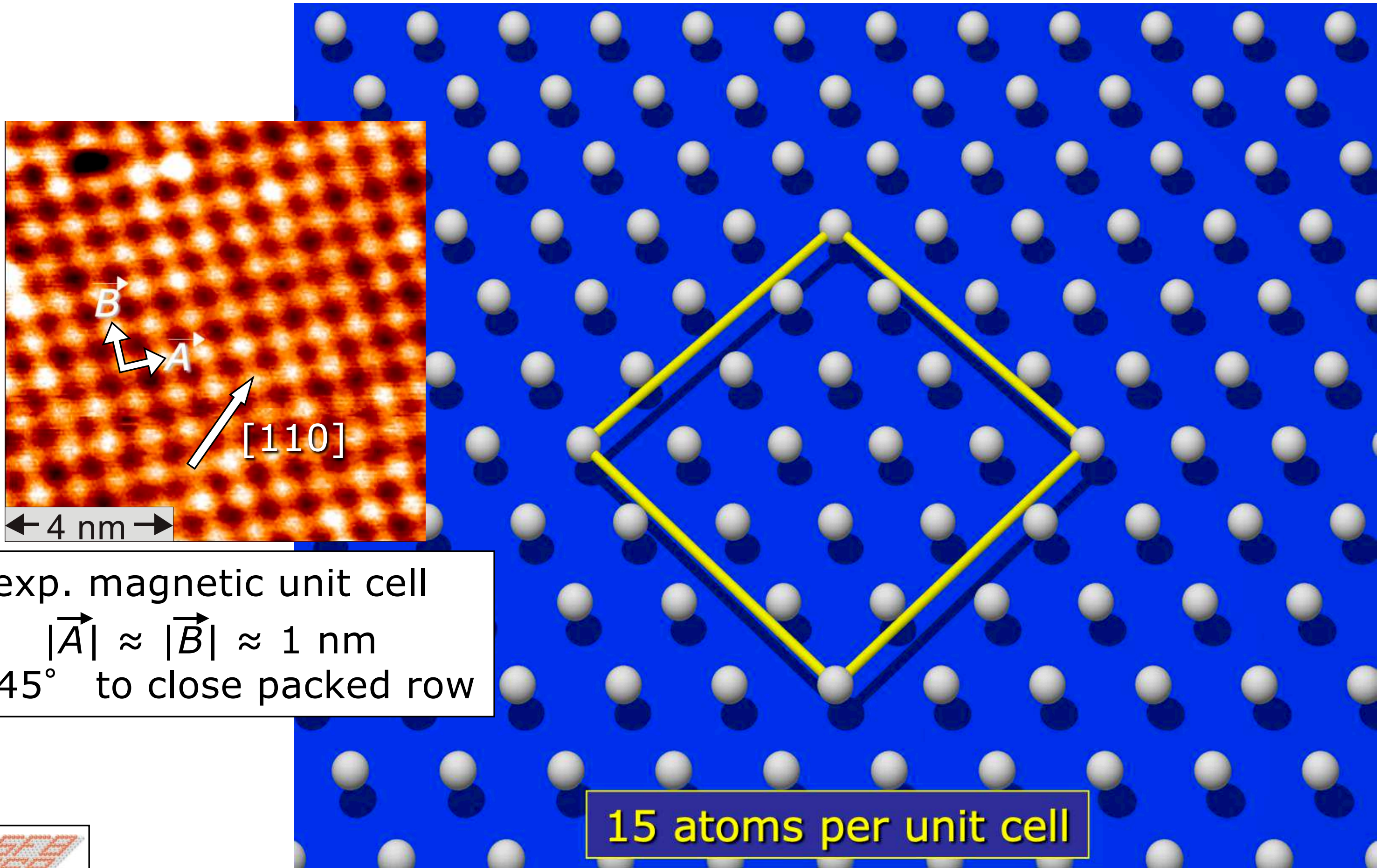
$$-\sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$ DM interaction

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

# FE MONOLAYER ON IR(111): MAGNETIC UNIT CELL



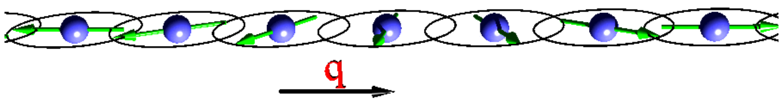

exp. magnetic unit cell
$|\vec{A}| \approx |\vec{B}| \approx 1$ nm
$\pm 45^\circ$ to close packed row

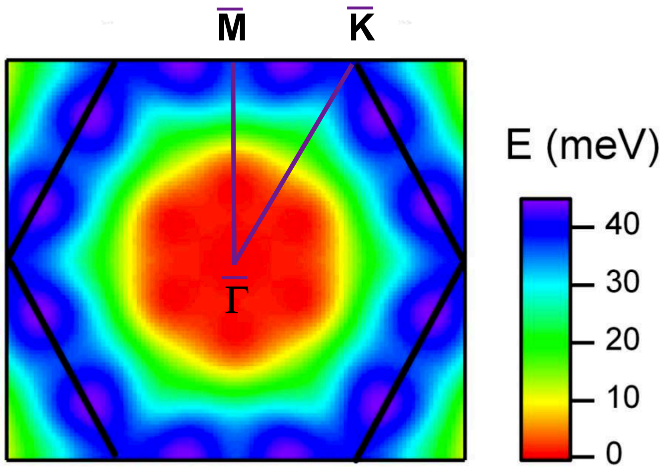
K. von Bergmann
University of Hamburg

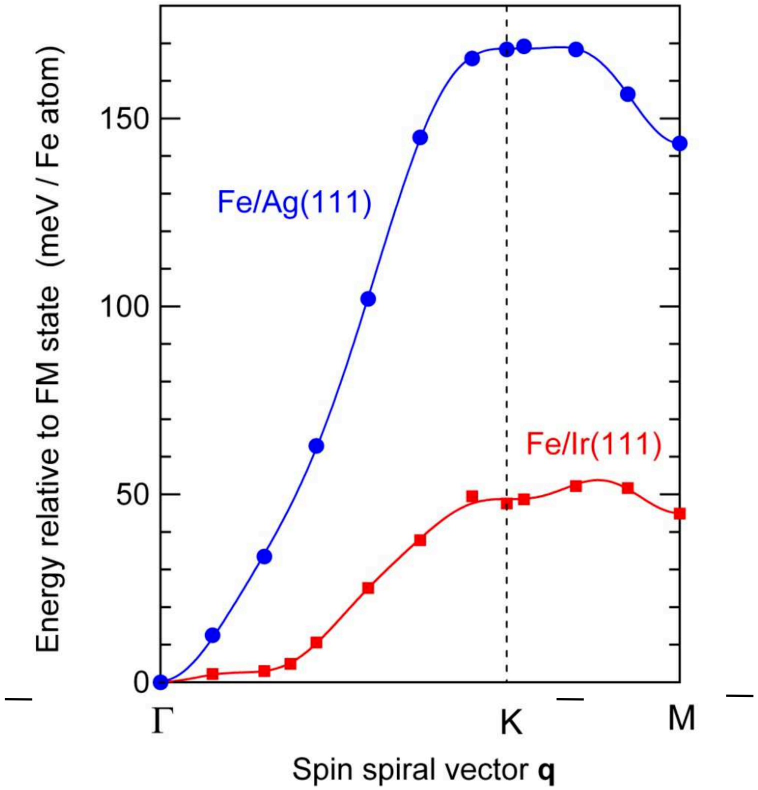
# SPIN SPIRAL CALCULATIONS FOR FE/IR(111)

Heisenberg model : $H = -\sum_{ij} J_{ij} (\mathbf{S}_i \cdot \mathbf{S}_j)$

Spin spiral:



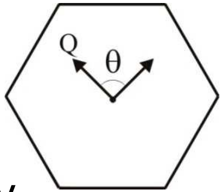





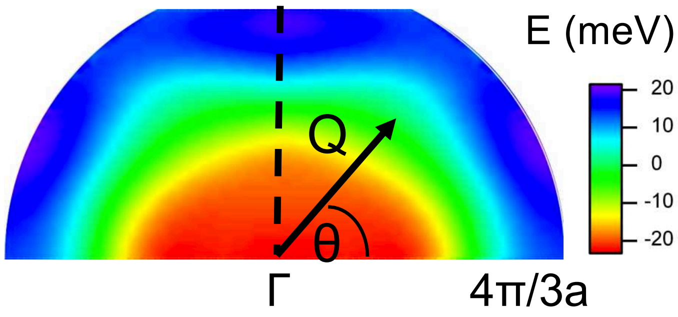
JÜLICH Forschungszentrum

# ENERGY CONTRIBUTIONS TO THE SKYRMION LATTICE

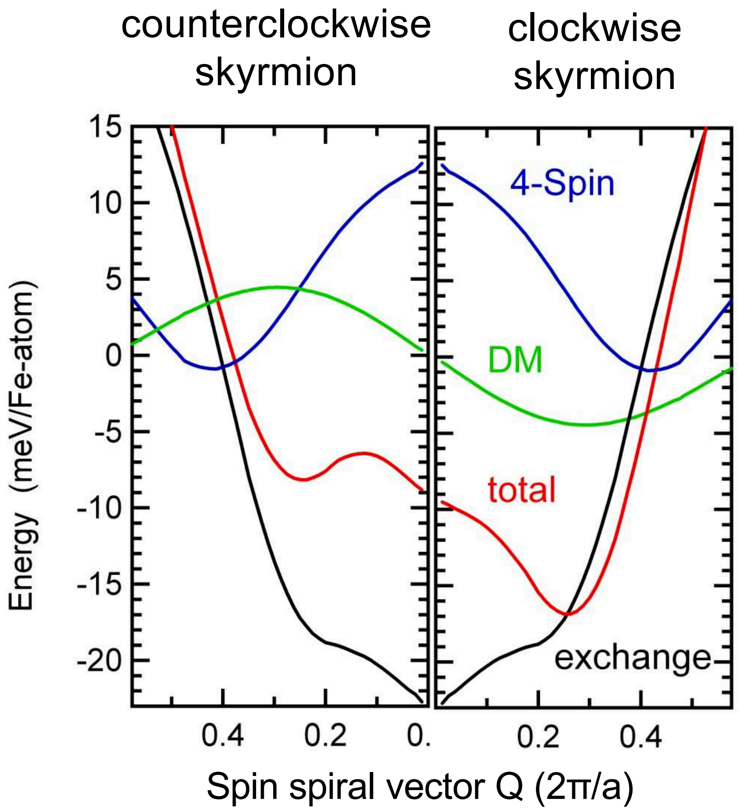
skyrmion lattice
defined by *Q* & *θ*



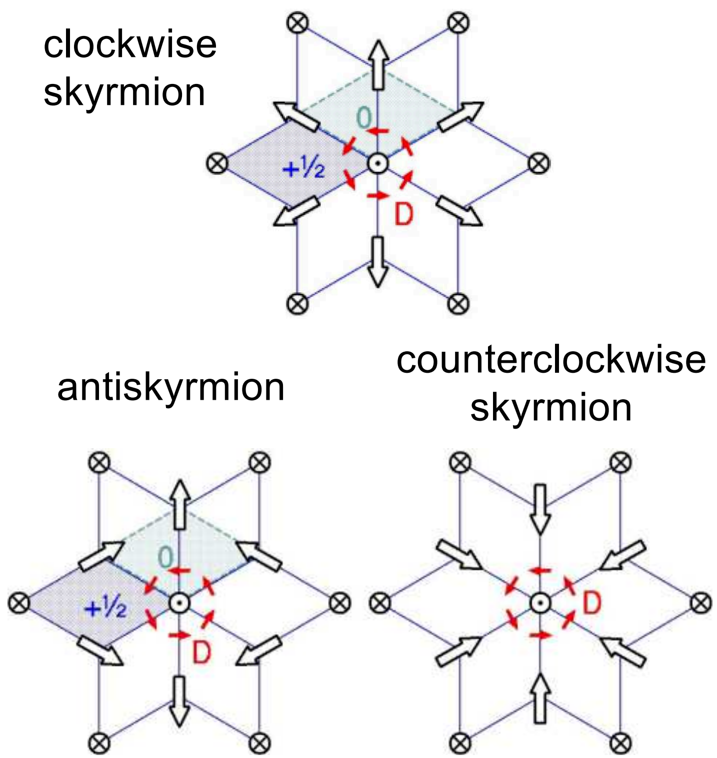

exchange energy



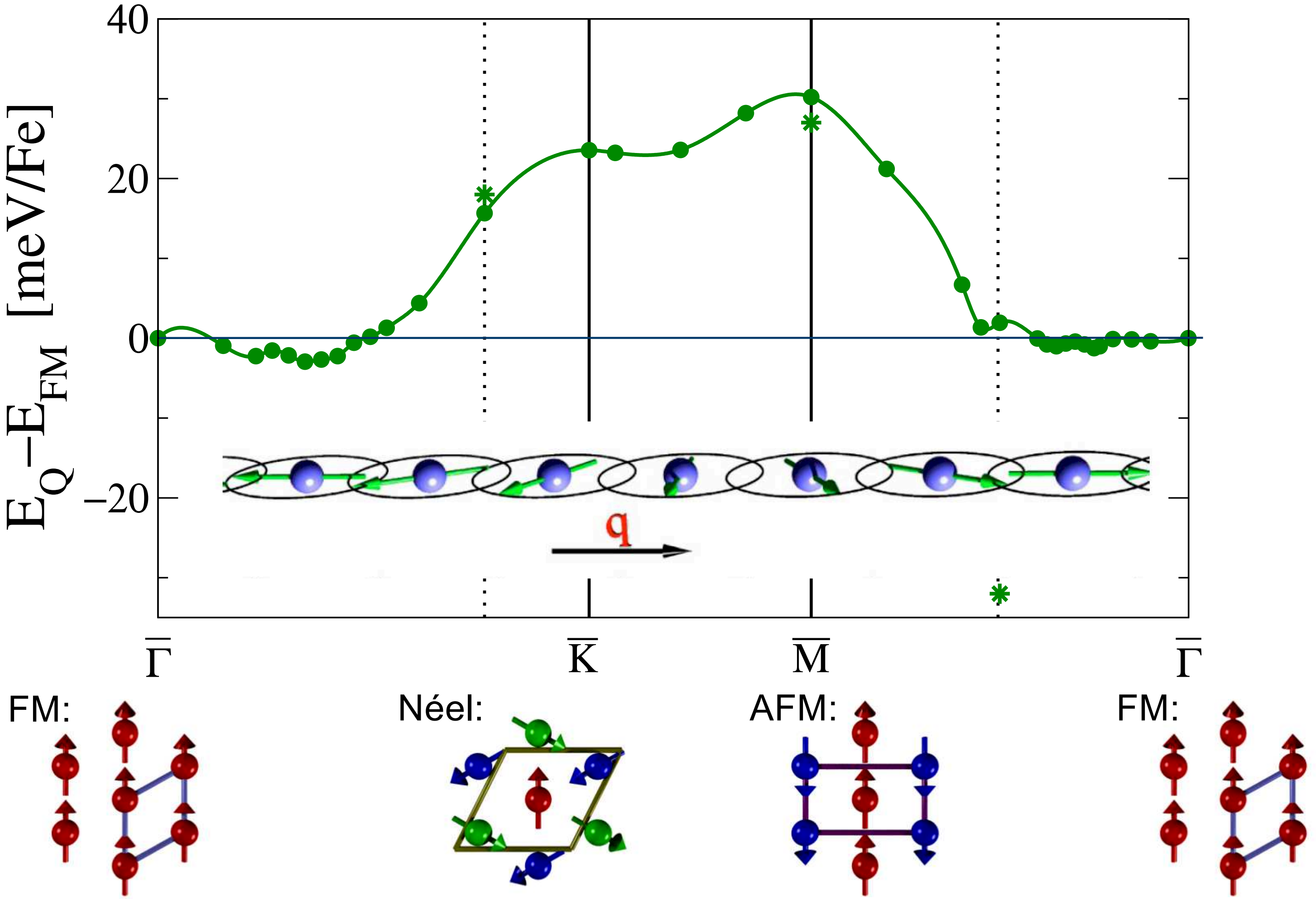
# ROLE OF DZYALOSHINSKII-MORIYA INT.




$$H_{\mathrm{DM}} = -\sum_{ij} \mathbf{D}(\mathbf{S}_i \times \mathbf{S}_j)$$

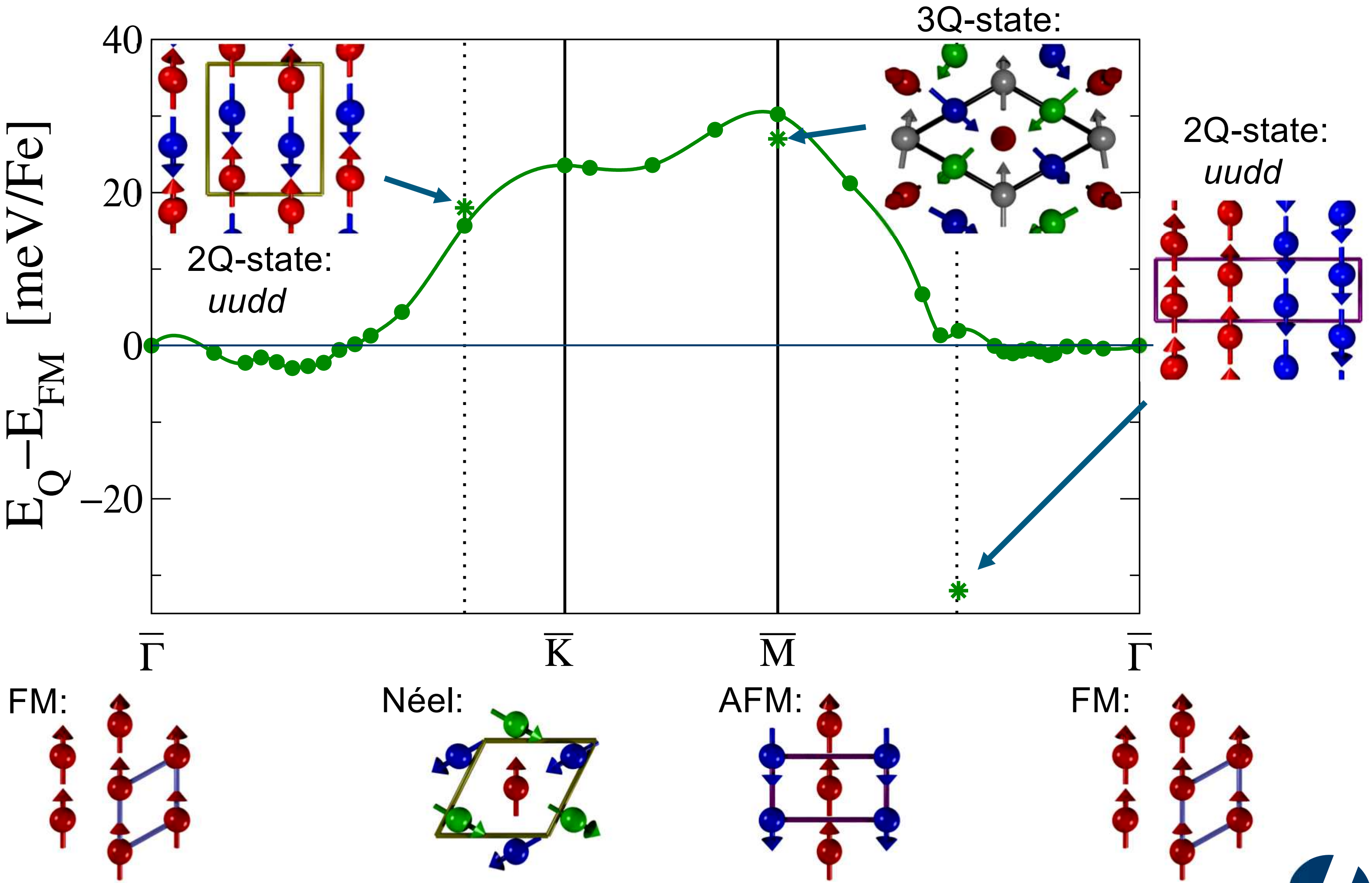


# Example – Fe monolayer on Rh(111): Fe/Rh(111)



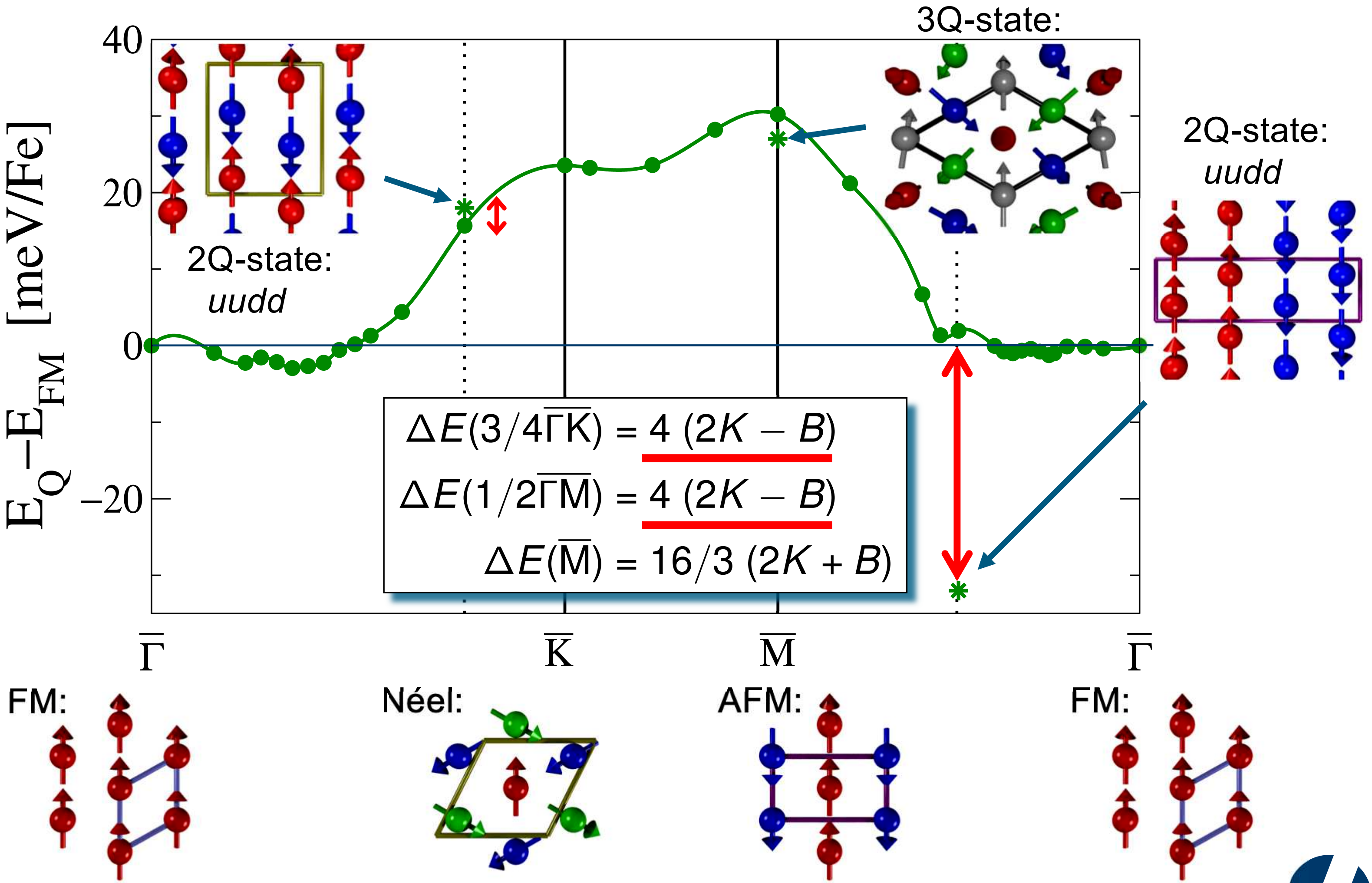

Al-Zubi *et al.*, Phys. Status Solidi B **248**, 2242 (2011)

# Example – Fe monolayer on Rh(111): Fe/Rh(111)



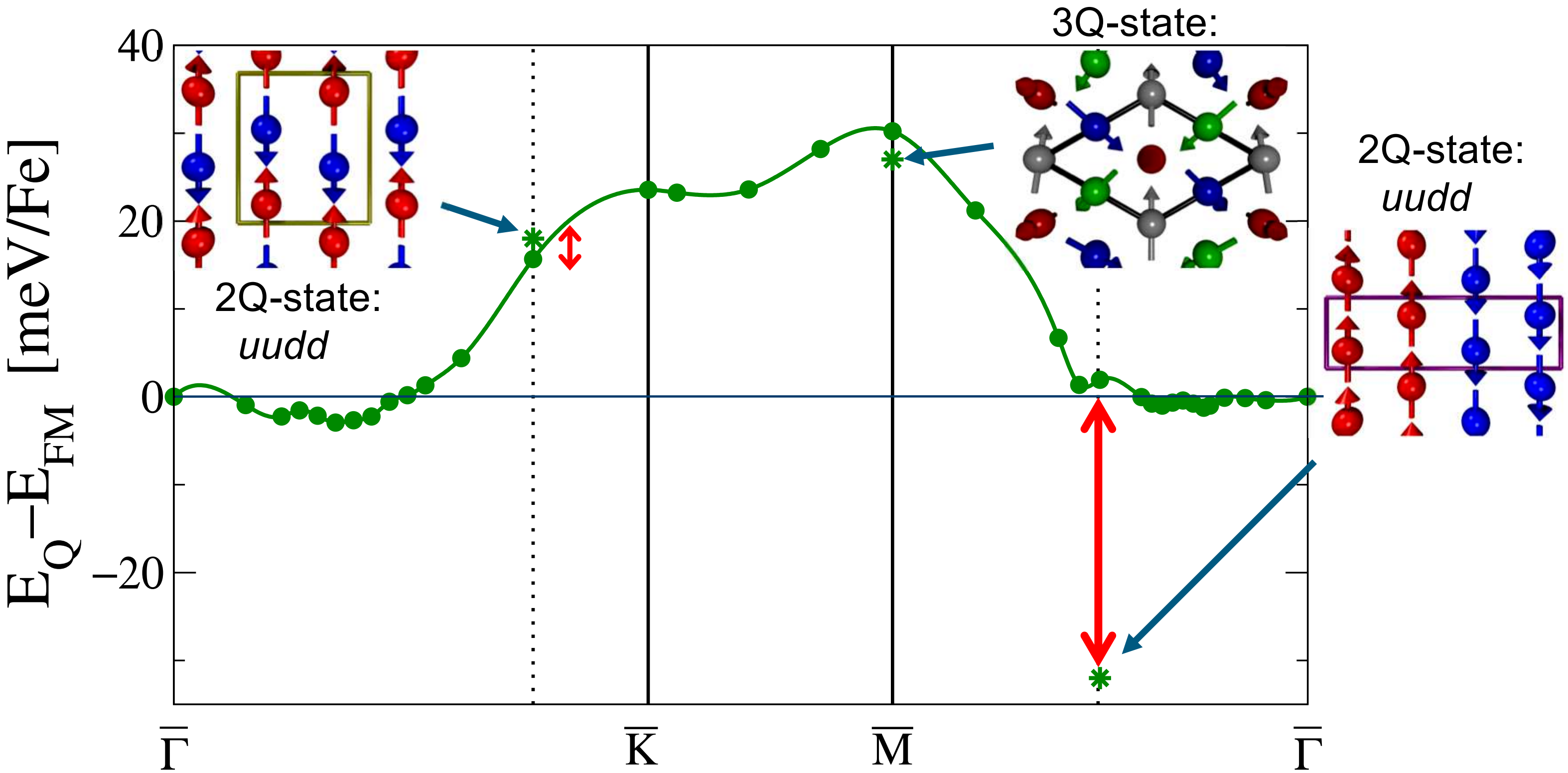

Al-Zubi *et al.*, Phys. Status Solidi B **248**, 2242 (2011)

# Example – Fe monolayer on Rh(111): Fe/Rh(111)




Al-Zubi *et al.*, Phys. Status Solidi B **248**, 2242 (2011)

# Example – Fe monolayer on Rh(111): Fe/Rh(111)




$$\Delta E(3/4\overline{\Gamma K}) = 4\,(2K - B) + 4\,Y_{3spin}$$
$$\Delta E(1/2\overline{\Gamma M}) = 4\,(2K - B) - 4\,Y_{3spin}$$
$$\Delta E(\overline{M}) = 16/3\,(2K + B) - 16/3\,Y_{3spin}$$

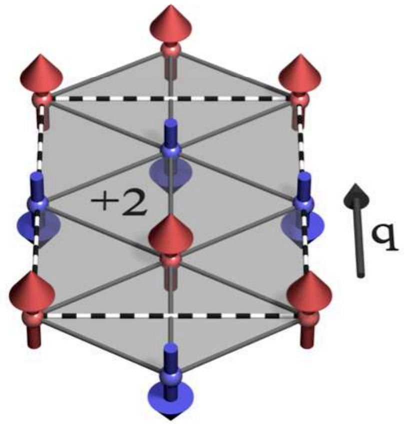
$J_1$ = 3.80 meV
$B$ = 3.39 meV
$K$ = 0.07 meV
$Y_{3spin}$ = 4.00 meV

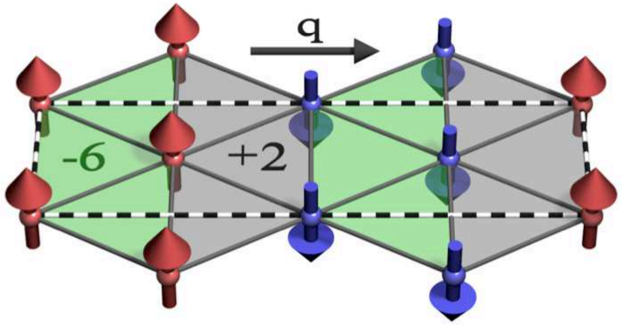

Al-Zubi *et al.*, Phys. Status Solidi B **248**, 2242 (2011)

JÜLICH Forschungszentrum

# CONVINCING EXPERIMENTALIST

# Higher-order exchange interactions

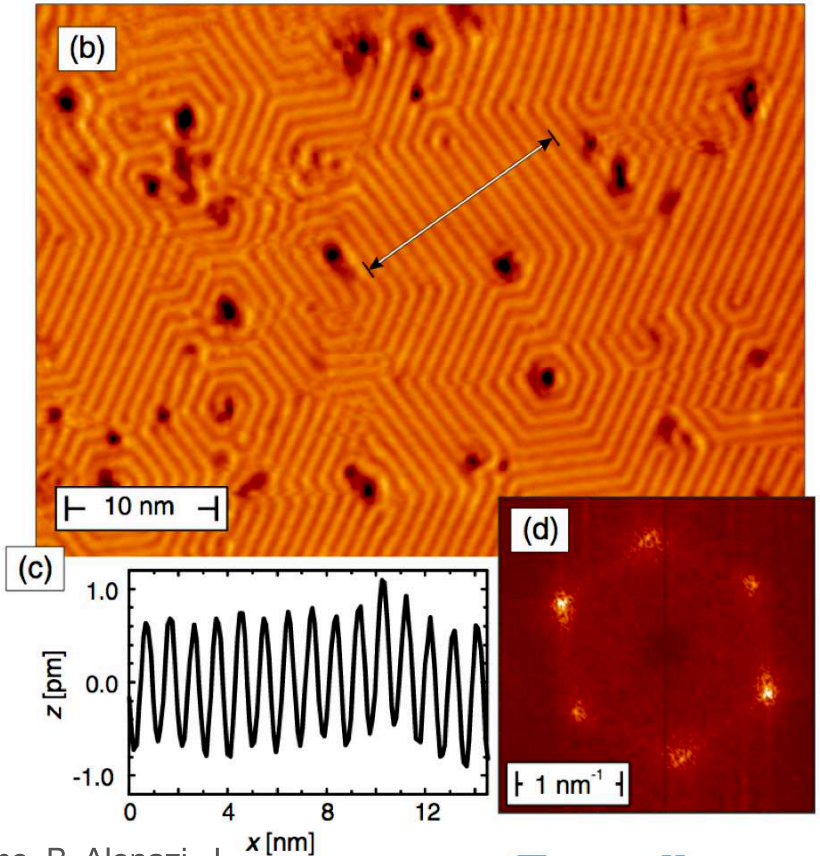



$$\Delta E(3/4\overline{\Gamma\mathrm{K}}) = 4\,(2K - B) + 4\,Y_{3spin}$$

$$\Delta E(1/2\overline{\Gamma\mathrm{M}}) = 4\,(2K - B) - 4\,Y_{3spin}$$

**Fe/Rh(111)**
uudd state stabilized by
4-spin–3-site interaction




higher-order exchange interactions can be calculated by performing DFT calculations for single-Q (spin-spirals) and multi-Q (uudd, 3Q, …) states from their energy differences

A. Krönlein, M. Schmitt, M. Hoffmann, J. Kemmer, N. Seubert, M. Vogt, J. Küspert, M. Böhme, B. Alonazi, J. Kügel, H. A. Albrithen, M. Bode, G. Bihlmayer, and S. Blügel PRL **120**, 207202 (2018)

# Example 3D

## FeGe

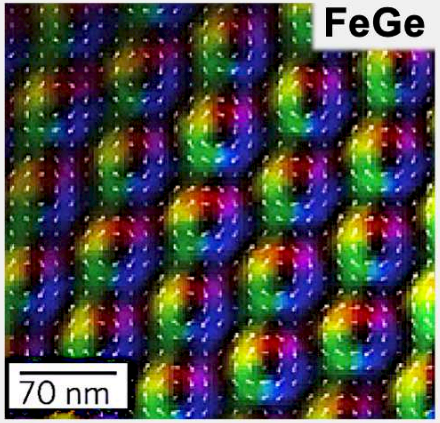
Qualitatively understood
Quantitatively something missing

## MnGe

not understood

**Complex magnetic textures from exotic interactions**

Yu *et al*. Nat. Mater. **10**, 106 (2011)



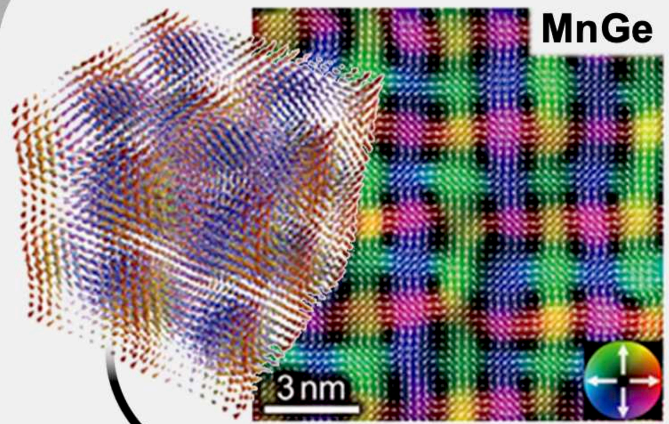

**2D skyrmions**

**Chiral exchange interaction**

$$\boldsymbol{D}_{ij} \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_j)$$

*+ external magnetic field*

Tanigaki *et al*. Nano Lett. **15**, 5438 (2015)




**3D spin texture**

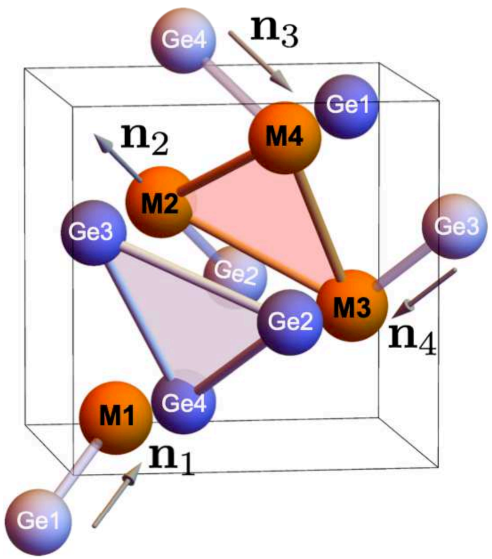
**Unknown interactions**

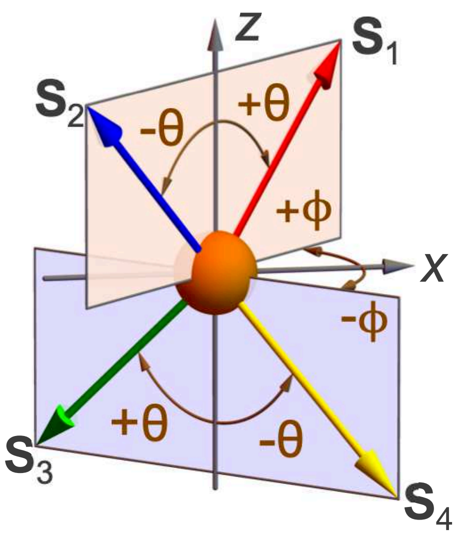
We cannot explain this so far

Beyond Heisenberg Interactions

# MAGNETIC INTERACTIONS IN B20 COMPOUNDS

## Crystal and magnetic structure




**Unit Cell:**
4 magnetic (Fe/Mn) & 4 Ge atoms.

$\mathbf{n}_i$ – 3-fold rot. axis on $i^{\text{th}}$ magn. atom.

**Particular AFM order:** the angles of each spin are referred to the symmetry direction $\mathbf{n}_i$ is the same:

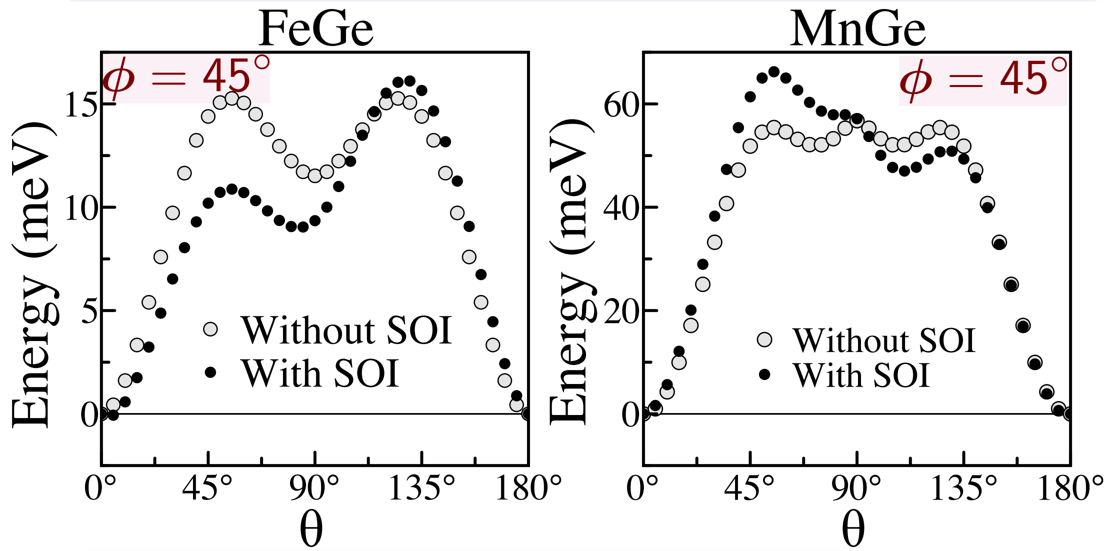
$$\mathbf{S}_i(\theta,\phi) = \begin{pmatrix} n_{ix}\sin(\theta)\cos(\phi) \\ n_{iy}\sin(\theta)\sin(\phi) \\ n_{iz}\cos(\theta) \end{pmatrix}$$

controls non-coplanarity

## The energy of Heisenberg interaction

$$E^{\text{ex}} = -\frac{1}{2}\sum_{ij} J_{ij}\,\mathbf{S}_i\cdot\mathbf{S}_j = \text{const}$$

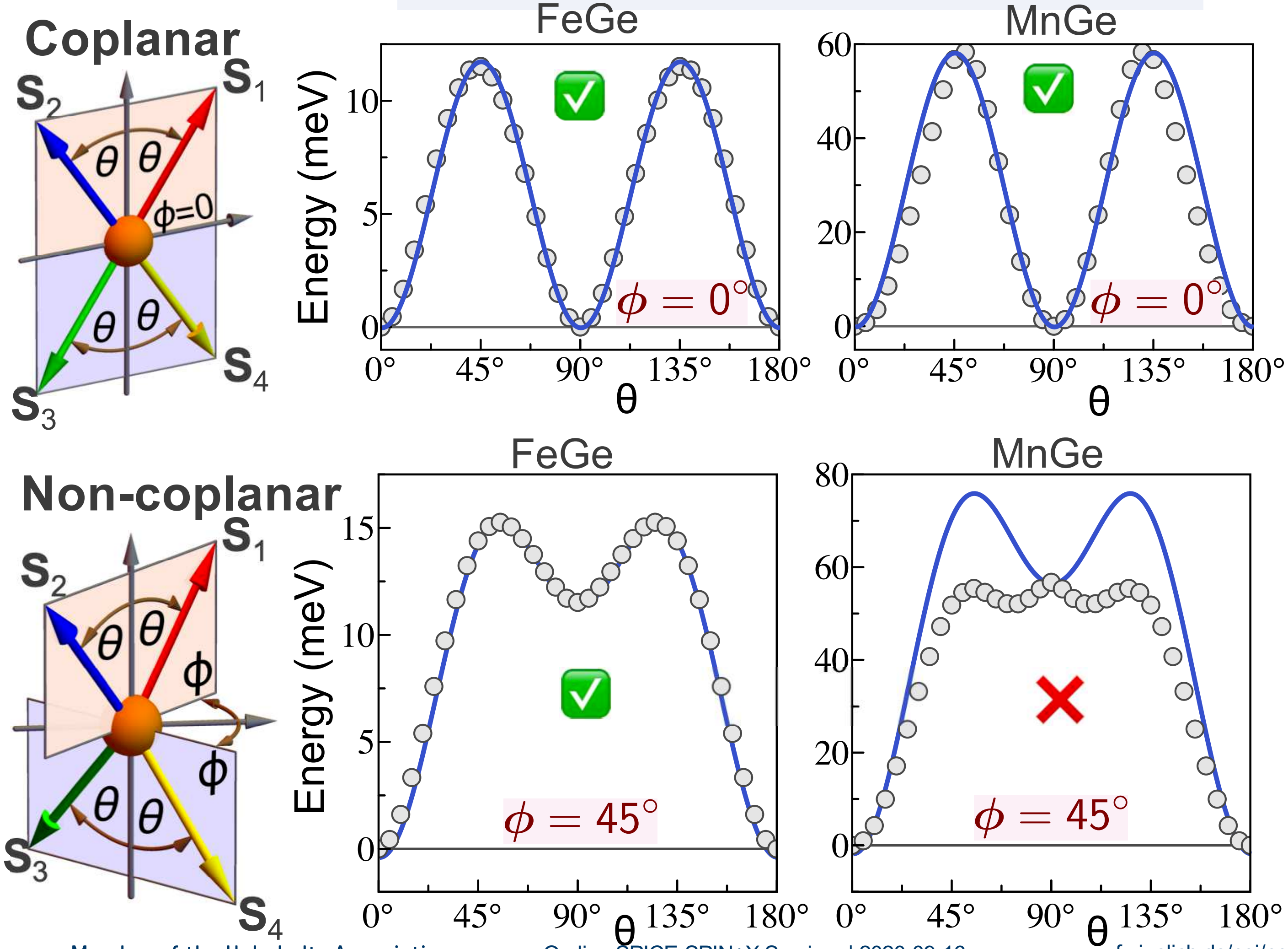
## First-principles (DFT) results




- Energy difference to Heisenberg large
- Energy change indicates the higher-order magnetic interactions.
- What are those magnetic interactions?

# SYMMETRIC HIGHER-ORDER EXCHANGE

DFT results without Spin-Orbit Interaction




**4th-order exchange interactions**

$$E_4 = -\frac{1}{2}\sum_{ijkn} k_{ijkn}\left(\mathbf{S}_i \cdot \mathbf{S}_j\right)\left(\mathbf{S}_k \cdot \mathbf{S}_n\right)$$

M. Hoffmann *et al.*, PRB **101**, 024418 (2020)

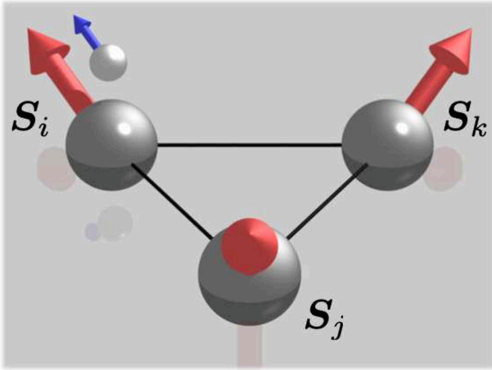
- 4th-order Ex. describe the energy variation with θ well in FeGe.
- Energy scale for MnGe larger than for FeGe.
- Model-fit **deviates** strongly from the calculated curve in **MnGe** if the spins are **non-coplanar.**

**Novel interaction is needed.**

# CONCEPT OF NEW INTERACTION

- Introduction of new chiral interaction :
  **topological-chiral interaction**
  - Chiral-Chiral Interaction (CCI)
  - Spin-chiral Interaction (SCI)
- Phenomenological introduction
- Investigation of B20-FeGe, MnGe
- Sketch of more rigorous derivation

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




**Orbital effect:** hopping in noncollinear background generates emergent "magnetic field"

**TOM: Topological Orbital Moment**

*skyrmions...*

$$\mathbf{L}_\triangle^{\mathrm{TO}} = \kappa_\triangle^{\mathrm{TO}} \mathbf{B}_\triangle^{\mathrm{eff}} \longleftarrow B^{\mathrm{eff}} \propto \hat{\mathbf{n}} \cdot (\partial_x \hat{\mathbf{n}} \times \partial_y \hat{\mathbf{n}}) \xleftarrow{\text{``slow''}} \chi_\triangle = \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$$

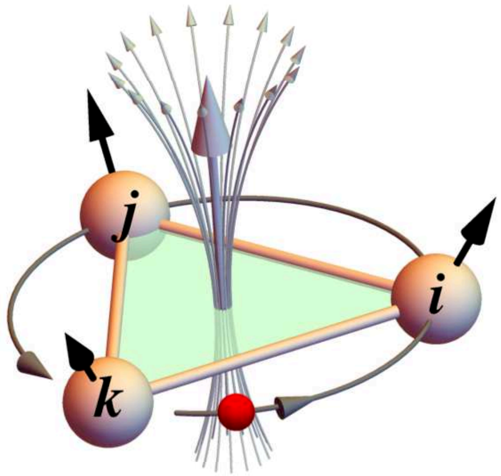
*scalar spin chirality*

$\kappa^{\mathrm{TO}}$ : topological orbital susceptibility

Hanke *et al.*, PRB **94**, 121114(R) (2016); Sci. Rep. **7**, 41078 (2017)

Taguchi *et al.*, Science **291**, 2573 (2001)
Shindou, Nagaosa, PRL **87**, 116801 (2001)

# EMERGENT FIELD AND TOPOLOGICAL ORBITAL MOMENT




## Spin-Chirality

$$\chi_{ijk} = \mathbf{S}_i \cdot [\mathbf{S}_j \times \mathbf{S}_k]$$

## Emergent B-field

$$\mathbf{B}^{\text{eff}} \sim \chi_{ijk}\,\boldsymbol{\tau}_{ijk} = \mathbf{S}_i \cdot [\mathbf{S}_j \times \mathbf{S}_k]$$

## Topological Orbital moment

$$\mathbf{L}_{ijk}^{\text{TO}} = \kappa_{ijk}^{\text{TO}}\,\mathbf{S}_i \cdot [\mathbf{S}_j \times \mathbf{S}_k]\,\boldsymbol{\tau}_{ijk}$$

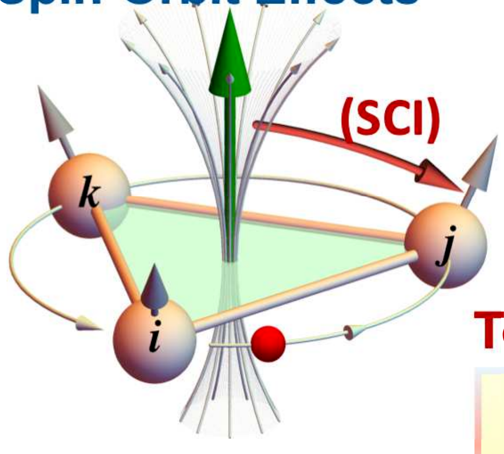
**The total TOM per atom site**

$$\mathbf{L}_i^{\text{TO}} = \sum_{j,k} \mathbf{L}_{ijk}^{\text{TO}} = \sum_{j,k} \kappa_{ijk}^{\text{TO}}\,\chi_{ijk}\,\boldsymbol{\tau}_{ijk}$$


J.-P. Hanke *et al.*, Sci. Rep. **7**, 41078 (2017)
F. R. Lux *et al.*, Commun. Phys. **1**, 60 (2018)

Y. Taguchi *et al.*, Science **291**, 2573 (2001)
M. Hoffmann *et al.*, Phys. Rev. B **92**, 020401(R) (2015)
M. d. S. Dias *et al.*, Nat. Commun. **7**, 13613 (2016)

# NEW: SPIN-CHIRAL INTERACTION (SCI)




**Spin-Chirality**

$$\chi_{ijk} = \mathbf{S}_i \cdot [\mathbf{S}_j \times \mathbf{S}_k]$$

**Emergent B-field**

$$\mathbf{B}^{\text{eff}} \sim \chi_{ijk}\,\boldsymbol{\tau}_{ijk} = \mathbf{S}_i \cdot [\mathbf{S}_j \times \mathbf{S}_k]$$

## New: Spin-chiral interaction (SCI)

$$E^{\text{SC}} = \varkappa^{\text{SC}} \sum_i \mathbf{L}_i^{\text{TO}} \cdot \mathbf{S}_i = \sum_{i(jk)} \varkappa_{ijk}^{\text{SC}} (\boldsymbol{\tau}_{ijk} \cdot \mathbf{S}_i)\, [\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)]$$

## Topological Orbital moment

$$\mathbf{L}_{ijk}^{\text{TO}} = \kappa_{ijk}^{\text{TO}}\, \mathbf{S}_i \cdot [\mathbf{S}_j \times \mathbf{S}_k]\, \boldsymbol{\tau}_{ijk}$$

- **SCI** is the 4-order 3-site interaction, arises as a result of a direct coupling between the **TOM** and local spins
- **SCI** depends on spin-orbit coupling (SOC)
- **SCI** is rotationally anisotropic interaction
- **SCI favours non-coplanar structures of scalar spin chirality of specific sign**

**The total TOM per atom site**

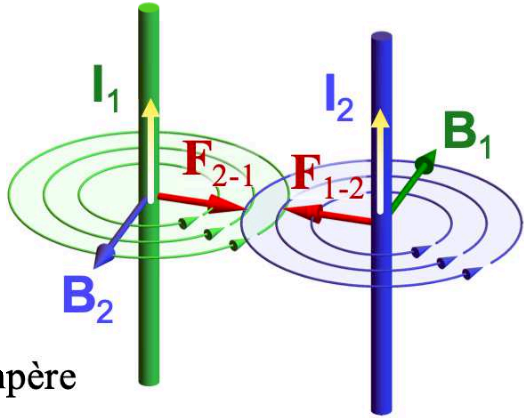
$$\mathbf{L}_i^{\text{TO}} = \sum_{j,k} \mathbf{L}_{ijk}^{\text{TO}} = \sum_{j,k} \kappa_{ijk}^{\text{TO}}\, \chi_{ijk}\, \boldsymbol{\tau}_{ijk}$$


J.-P. Hanke *et al.*, Sci. Rep. **7**, 41078 (2017)
F. R. Lux *et al.*, Commun. Phys. **1**, 60 (2018)

Y. Taguchi *et al.*, Science **291**, 2573 (2001)
M. Hoffmann *et al.*, Phys. Rev. B **92**, 020401(R) (2015)
M. d. S. Dias *et al.*, Nat. Commun. **7**, 13613 (2016)

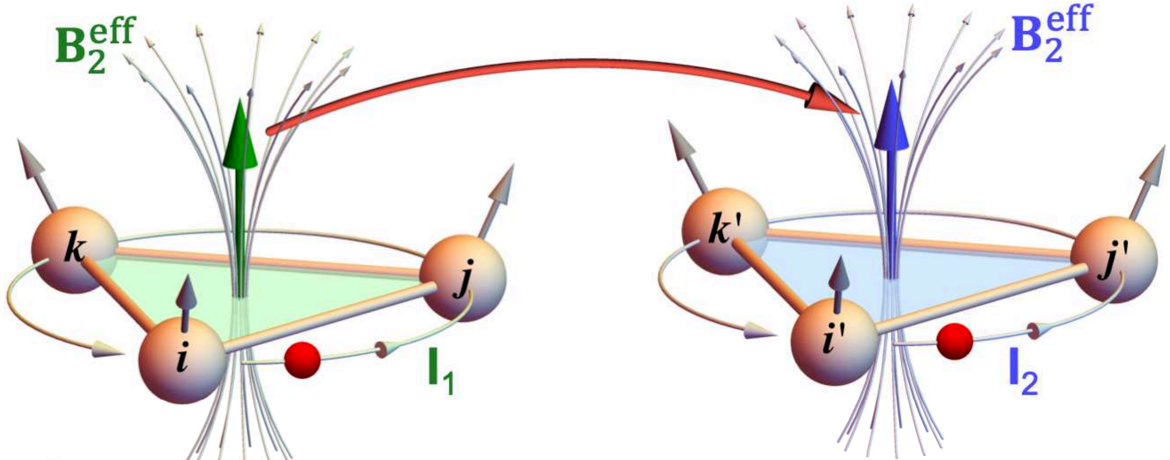
# NEW: CHIRAL-CHIRAL INTERACTION (CCI)

André-Marie Ampère




**Current-current interaction**

$$E_{12} \approx -\frac{1}{2} M_{12}\, \mathbf{I}_1 \cdot \mathbf{I}_2$$



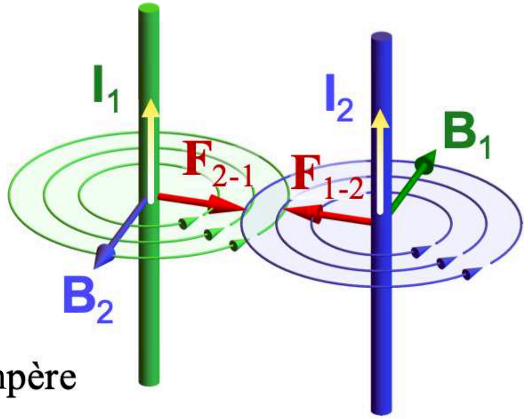

$$-\frac{1}{2}\left[\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)\right] \boldsymbol{\tau}^{\dagger}_{ijk}\, \underline{\underline{\varkappa}}^{\mathrm{CC}}_{ii'}\, \boldsymbol{\tau}_{i'j'k'} \left[\mathbf{S}_{i'} \cdot (\mathbf{S}_{j'} \times \mathbf{S}_{k'})\right]$$

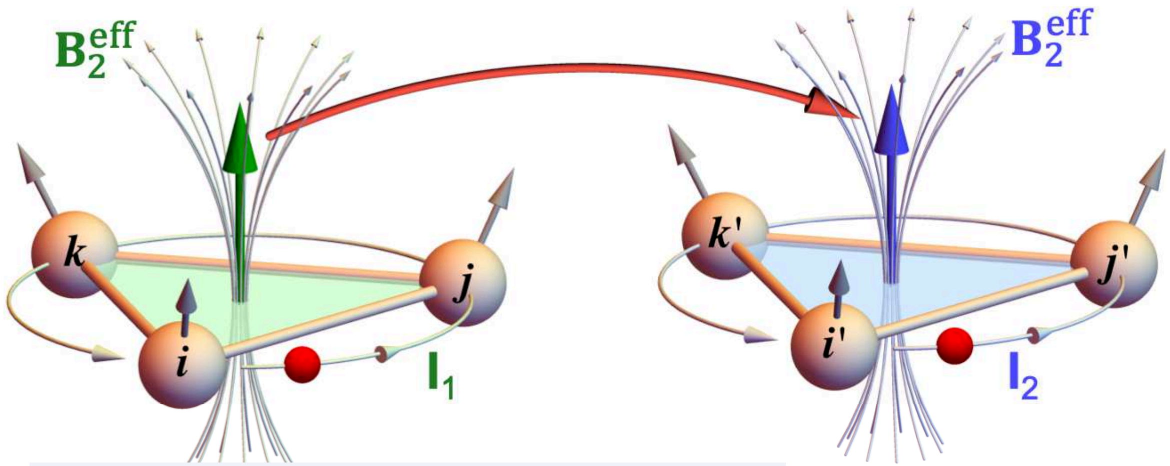
**Chiral-chiral interaction (CCI)**

- **CCI** is the 6-order 6-site interaction
- It is governed by a **TOM** and requires no SOI and no external B-field.
- It is rotationally invariant chiral interaction
- **Favours states with 3D magnetic texture**

# NEW: CHIRAL-CHIRAL INTERACTION (CCI)

André-Marie Ampère




## Current-current interaction

$$E_{12} \approx -\frac{1}{2} M_{12}\, \mathbf{I}_1 \cdot \mathbf{I}_2$$

Interaction of TOM with emergent field:

$$E^{\mathrm{CC}} \sim 1/2\, \varkappa^{\mathrm{TO}} \mathbf{L}^{\mathrm{TO}}_{\triangle} \cdot \mathbf{B}^{\mathrm{eff}}_{\triangle}$$

## Chiral-chiral interaction (CCI)

restriction to on-site triangular plaquette

$$E^{\mathrm{CC}} = -\frac{1}{2} \sum_{i(jk)} \varkappa^{\mathrm{CC}}_{ijk} \chi^2_{ijk} = -\frac{1}{2} \sum_{i(jk)} \varkappa^{\mathrm{CC}}_{ijk} \left[\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)\right]^2$$

- **CCI** is the 6-order 3-site interaction
- It is governed by a **TOM** and requires no SOI and no external B-field.
- It is rotationally invariant chiral interaction
- **Favours states with 3D magnetic texture**

# CONTINUUM DESCRIPTION OF MAGNETIZATION TWIST

continuum representation: $\mathbf{S}_i \to \mathbf{m}(\mathbf{r}) = (m_1, m_2, m_3) \, : \, \mathbb{R}^3 \to \mathbb{S}^2$ i.e. $|\mathbf{m}(\mathbf{r})| = 1$

$$\mathbf{m}(\mathbf{R}_j) = \mathbf{m}(\mathbf{R}_i + R_{ji}\,\widehat{\mathbf{e}}_{ji}) \simeq \mathbf{m}(\mathbf{R}_i) + R_{ji} \sum_{\alpha} \frac{\partial \mathbf{m}}{\partial r_\alpha} \widehat{\mathbf{e}}_{\alpha|ji} \qquad \alpha \in \{x, y, z\}$$

Scalar chirality $\quad \chi_\triangle = \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k) \longrightarrow \chi(\mathbf{r}) \propto \mathbf{F}(\mathbf{r}) \cdot \tau(\mathbf{r})$

solenoidal gyro-vector field
[induced Faddeev magnetic field]
[Berry curvarture]

$$\mathbf{F} = (F_x, F_y, F_z) \quad \text{with} \quad F_\alpha = \sum \varepsilon_{\alpha\beta\gamma} f_{\beta\gamma}$$

$$f_{\beta\gamma} = \mathbf{m} \cdot \left[ \frac{\partial \mathbf{m}}{\partial r_\beta} \times \frac{\partial \mathbf{m}}{\partial r_\gamma} \right] \quad \text{with} \quad \alpha,\ \beta,\ \gamma,\ \in \{x, y, z\}$$

Topo. orbital moment $\quad \mathbf{L}_i^{\mathrm{TO}} = \sum_{(jk)} \kappa_{jk}^{\mathrm{TO}} \chi_{ijk} \boldsymbol{\tau}_{ijk} \longrightarrow \ell^{\mathrm{TO}}(\mathbf{r}) = \underline{\kappa}^{\mathrm{TO}} \mathbf{F}(\mathbf{r})$

Reminder skyrmions (2D): $f_{\beta\gamma}(\mathbf{r}) \longrightarrow q(x, y) = \mathbf{m} \cdot \left[ \frac{\partial \mathbf{m}}{\partial x} \times \frac{\partial \mathbf{m}}{\partial y} \right] \quad \text{with} \quad Q = \int_{\mathbb{R}^2} dr\, q$
(topological charge)

# MICROMAGNETIC: TOPOLOGICAL-CHIRAL INTERACTION

**Chiral-chiral interaction (CCI)** $E^{\mathrm{CC}} = -\frac{1}{2}\sum_{i(jk)} \varkappa_{ijk}^{\mathrm{CC}} \chi_{ijk}^2 \longrightarrow$

$$E_{\mathrm{mm}}^{\mathrm{CC}} = -\frac{1}{2}\int \mathrm{d}\mathbf{r}\, \mathbf{F}(\mathbf{r}) \cdot \underline{\varkappa}^{\mathrm{CC}} \cdot \mathbf{F}(\mathbf{r})$$

**generalized Faddeev term**

Hopfion: Knotted magnetization soliton


For cubic system: $\underline{\varkappa}^{\mathrm{CC}} = \varkappa^{\mathrm{CC}} \underline{\mathbb{1}}$

$$E_{\mathrm{mm}}^{\mathrm{CC}} = -\frac{1}{2}\varkappa^{\mathrm{CC}} \int \mathrm{d}\mathbf{r}\, |\mathbf{F}(\mathbf{r})|^2$$

original Faddeev term

**Faddeev Model:** Heisenberg + Faddeev term

$$E(\mathbf{m}) = E_{\mathrm{mm}}^{\mathrm{Heis}} + E_{\mathrm{mm}}^{\mathrm{CC}} = -\frac{1}{2}\int_{\mathbb{R}^3} \mathrm{d}\mathbf{r}\, \left( A\,|\nabla \mathbf{m}(\mathbf{r})|^2 + \varkappa^{\mathrm{CC}}\,|\mathbf{F}(\mathbf{r})|^2 \right)$$

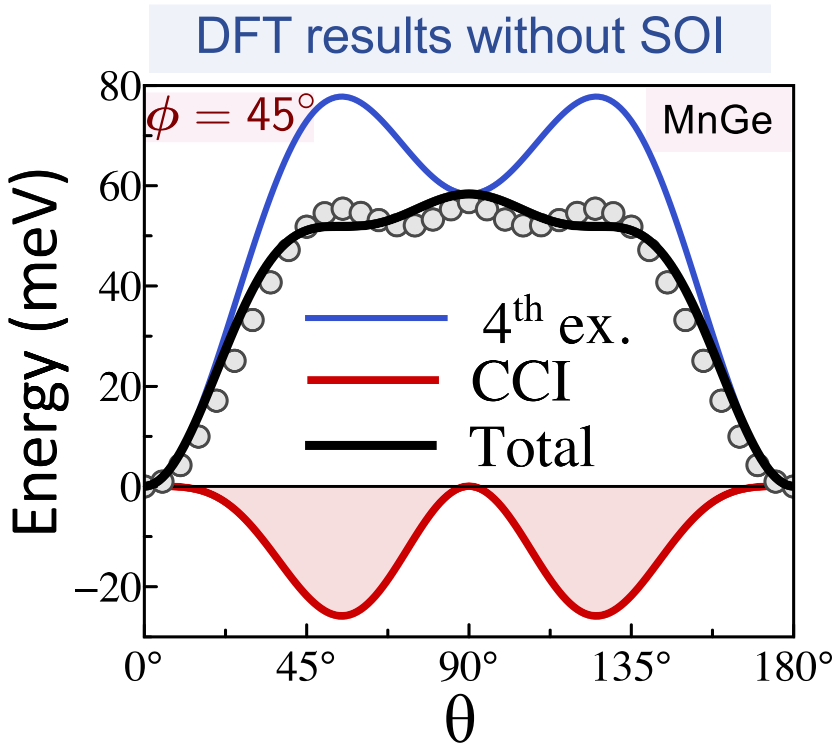
Faddeev, Lett. Math. Phys. **1**, 289 (1976)

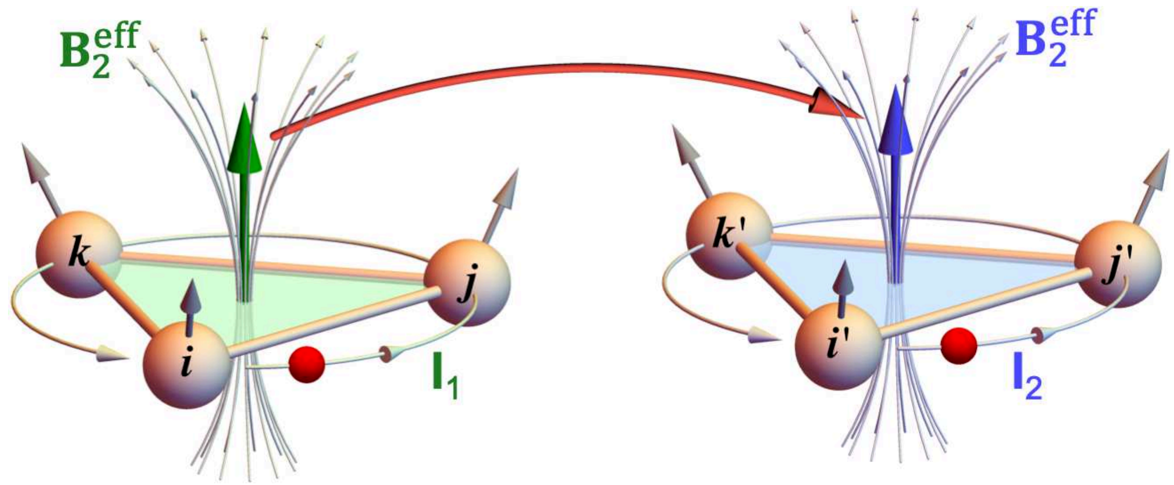
Solution: Hopfions with Hopf number $H(\mathbf{m}) = \left(\frac{1}{4\pi}\right)^2 \int_{\mathbb{R}^3} \mathrm{d}\mathbf{r}\, \mathbf{A} \cdot \mathbf{F}$ with $\mathbf{F} = \nabla \times \mathbf{A}$

vector potential to divergence-free F

**Spin-chiral interaction (SCI)** $E^{\mathrm{SC}} = \sum_i \varkappa_i^{\mathrm{SC}} \mathbf{L}_i^{\mathrm{TO}} \cdot \mathbf{S}_i \longrightarrow E_{\mathrm{mm}}^{\mathrm{SC}} = \int \mathrm{d}\mathbf{r}\, \mathbf{m}(\mathbf{r}) \cdot \underline{\varkappa}^{\mathrm{SC}} \cdot \mathbf{F}(\mathbf{r})$

# NEW: CHIRAL-CHIRAL INTERACTION (CCI)



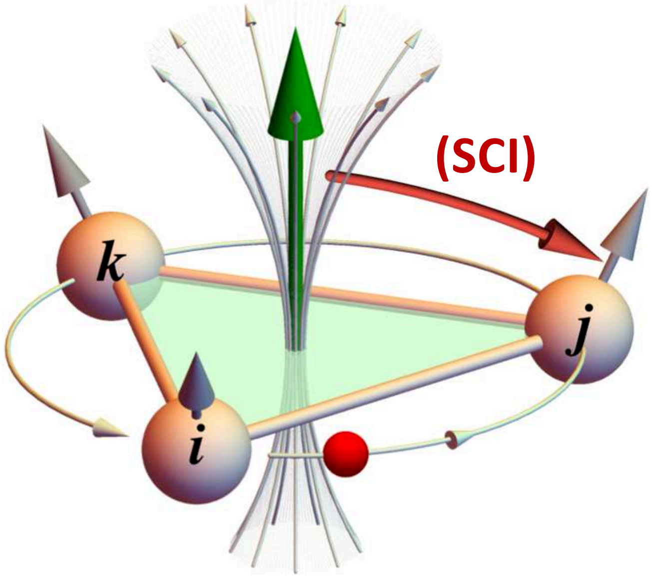

**Chiral-chiral interaction (CCI)**

restriction to on-site triangular plaquette

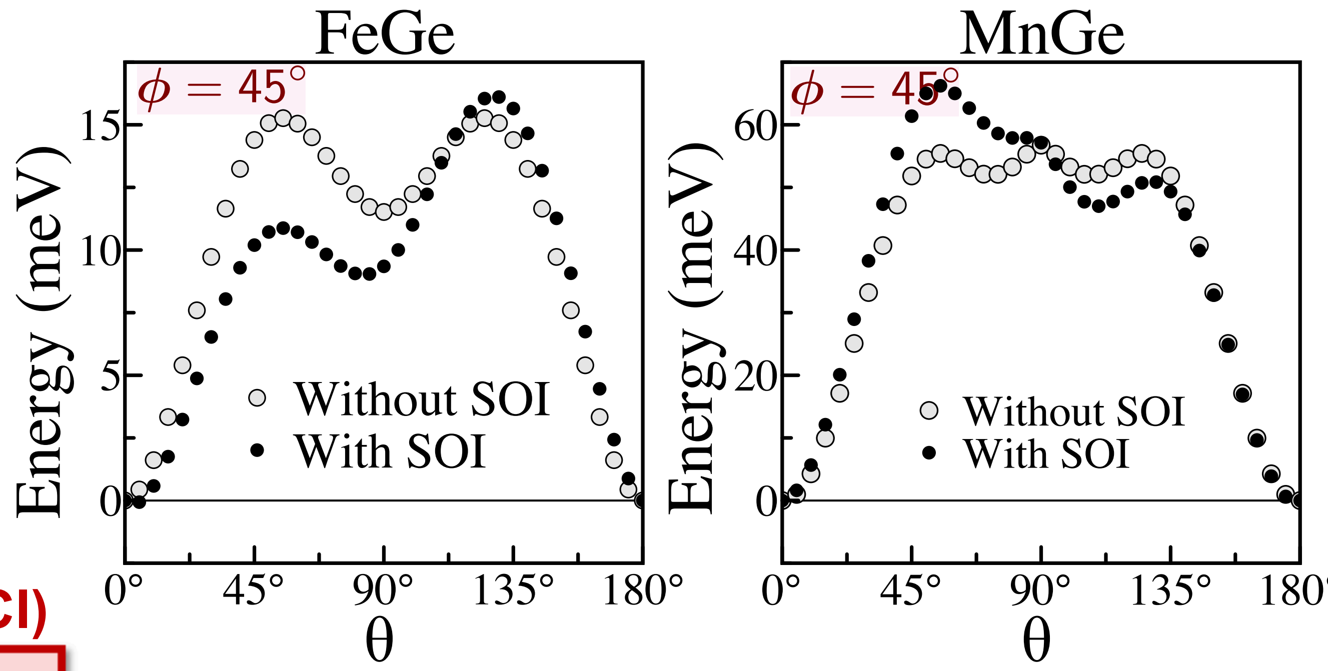
$$E^{CC} = -\frac{1}{2}\sum_{i(jk)} \varkappa_{ijk}^{CC} \chi_{ijk}^2 = -\frac{1}{2}\sum_{i(jk)} \varkappa_{ijk}^{CC} \left[\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)\right]^2$$

# NEW: SPIN-CHIRAL INTERACTION (SCI)

## Spin-Orbit Effects




Recall: DFT results



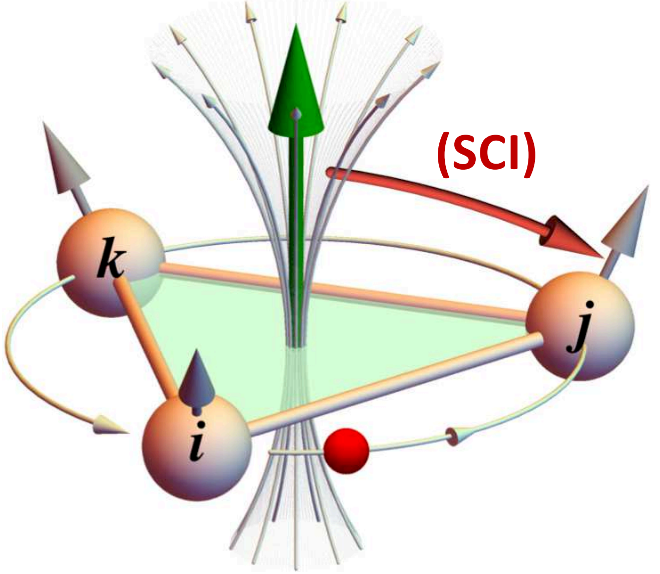

**New: Spin-chiral interaction (SCI)**

$$E^{\mathrm{SC}} = \varkappa^{\mathrm{SC}} \sum_i \mathbf{L}_i^{\mathrm{TO}} \cdot \mathbf{S}_i = \\ = \sum_{i(jk)} \varkappa_{ijk}^{\mathrm{SC}} \left(\boldsymbol{\tau}_{ijk} \cdot \mathbf{S}_i\right) \left[\mathbf{S}_i \cdot \left(\mathbf{S}_j \times \mathbf{S}_k\right)\right]$$

Take energy difference between results with and without SOI

# NEW: SPIN-CHIRAL INTERACTION (SCI)

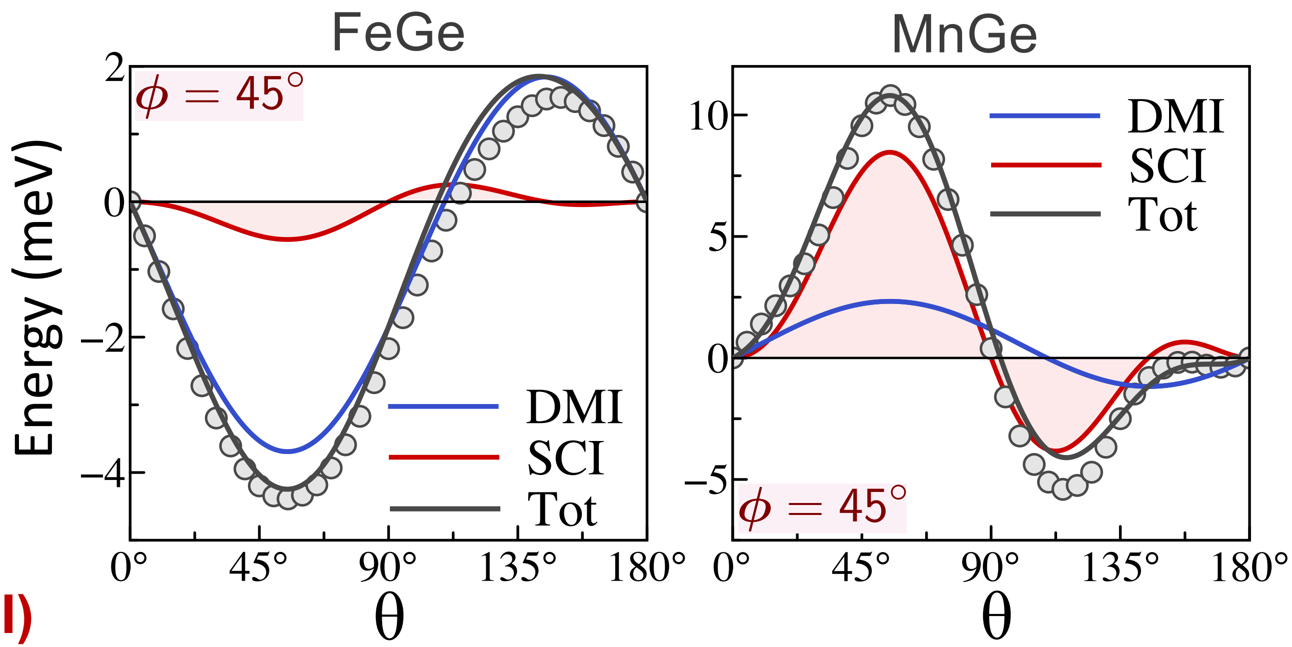
## Spin-Orbit Effects




## New: Spin-chiral interaction (SCI)

$$E^{\mathrm{SC}} = \varkappa^{\mathrm{SC}} \sum_i \mathbf{L}_i^{\mathrm{TO}} \cdot \mathbf{S}_i =$$
$$= \sum_{i(jk)} \varkappa_{ijk}^{\mathrm{SC}} \left(\boldsymbol{\tau}_{ijk} \cdot \mathbf{S}_i\right) \left[\mathbf{S}_i \cdot \left(\mathbf{S}_j \times \mathbf{S}_k\right)\right]$$

DFT results due to Spin-Orbit Interaction (SOI)



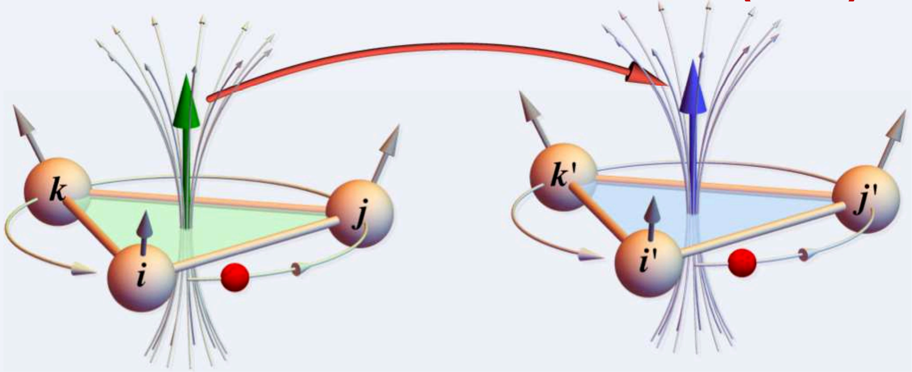

- **SCI** dominates DMI in MnGe
- DMI dominates **SCI** in FeGe
- **SCI** + DMI describe total contributions to SOI well.

JÜLICH Forschungszentrum

# CONCLUSIONS

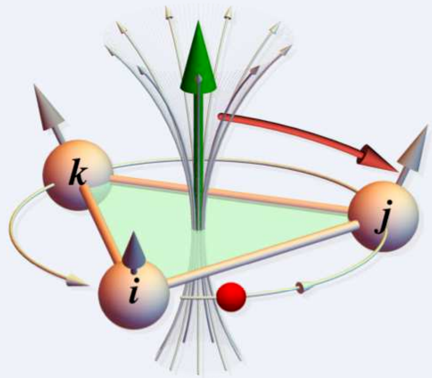
We have discovered two novel chiral 3-site magnetic interactions driven by topological orbital magnetism in B20 compounds:

## 1. Chiral-chiral interaction (CCI)




- **CCI** is the 6-order 3-site interaction rooting in the Zeeman interaction of the TOM with the emergent magnetic field due to the chirality
- It is **rotationally invariant** chiral interaction

## 2. Spin-chiral interaction (SCI)




- **SCI** is the 4-order 3-site interaction, arises as a result of a direct coupling between the **TOM** and local spins.
- It is **rotationally anisotropic** interaction, favours non-coplanar structures of scalar spin chirality of specific sign.
- It dominates DMI in MnGe

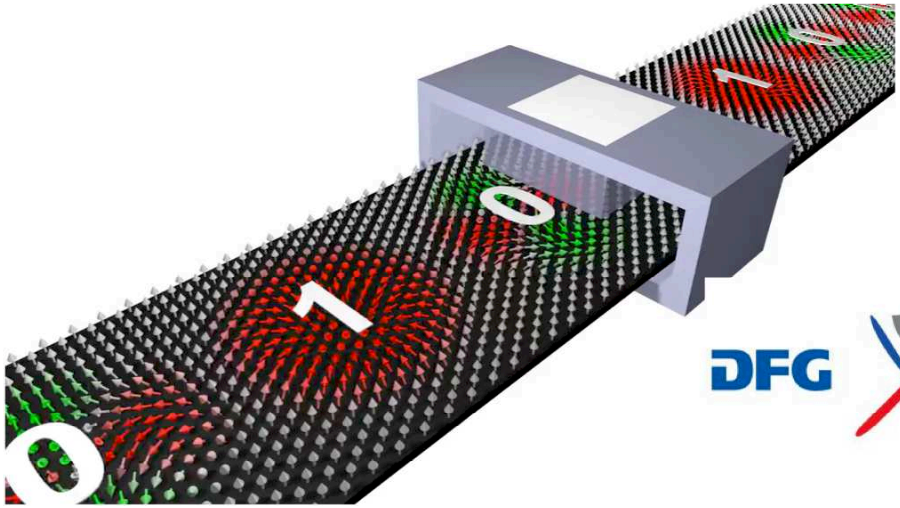
- Found interactions could be a key in resolving the pending puzzle of spin structure in MnGe.
- New Interactions may serve as a fruitful platform for promoting new classes of chiral magnetic materials and discovery of novel chiral phases with the prospect of Hopfions.
- B20-materials are beyond-Heisenberg solids with important 4-spin contributions.



JÜLICH Forschungszentrum

# ACKNOWLEDGEMENTS

Sergiy Grytsyuk | Jan-Philipp Hanke | Markus Hoffmann | Bernd Zimmermann | Gideon Müller | Juba Bouaziz | Nikolai Kiselev | Samir Lounis | Yuriy Mokrousov




rannís

MAGic Sky

Funded by the Horizon2020 Framework Programme of the European Union

DFG SPP 1666

SPP2137 Skyrmionics
Topological Spin Phenomena in Real-Space for Applications

HELMHOLTZ GEMEINSCHAFT 20 Jahre


CRC 1238
Control and Dynamics of Quantum Materials

DARPA
Topological Excitations in Electronics (TEE)

JARA

JÜLICH Forschungszentrum

# SUMMARY

- ❖ Brief introduction of spin-models
- ❖ Motivation higher-order interaction through Hubbard Model
- ❖ Sketch of more rigorous derivation from DFT
- ❖ Examples Multi-q states (e.g. Fe/Ir(111))
- ❖ Introduction of new chiral interaction :
  **topological-chiral interaction**
  - Chiral-Chiral Interaction (CCI)
  - Spin-chiral Interaction (SCI)
- ❖ Phenomenological introduction
- ❖ Investigation of B20-MnGe

*Thank you*