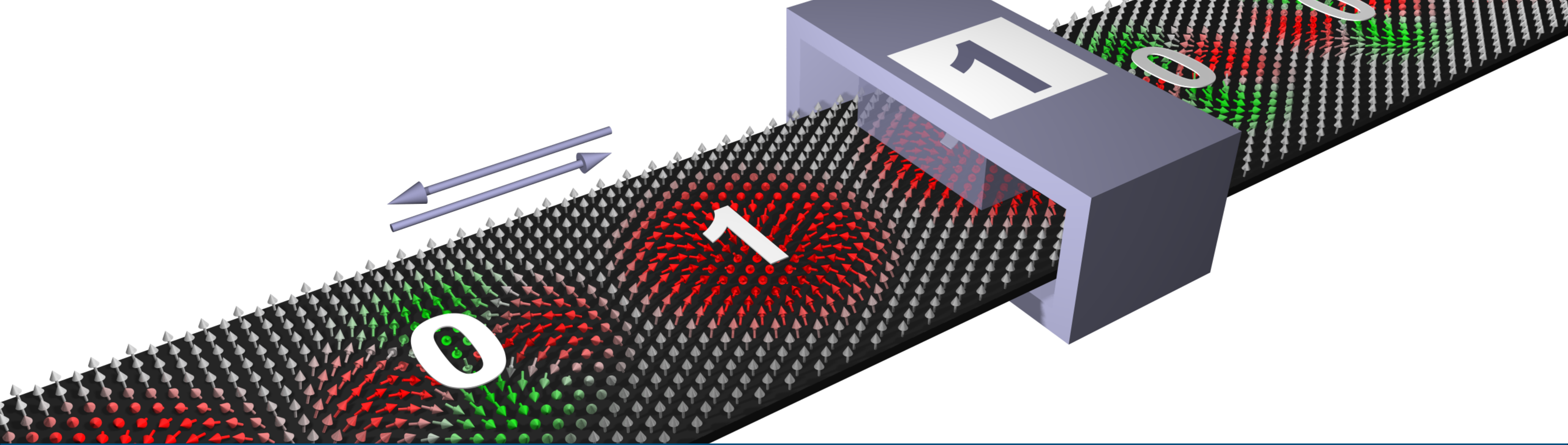


Advanced Magnetism

September 13, 2019 I **Markus Hoffmann**

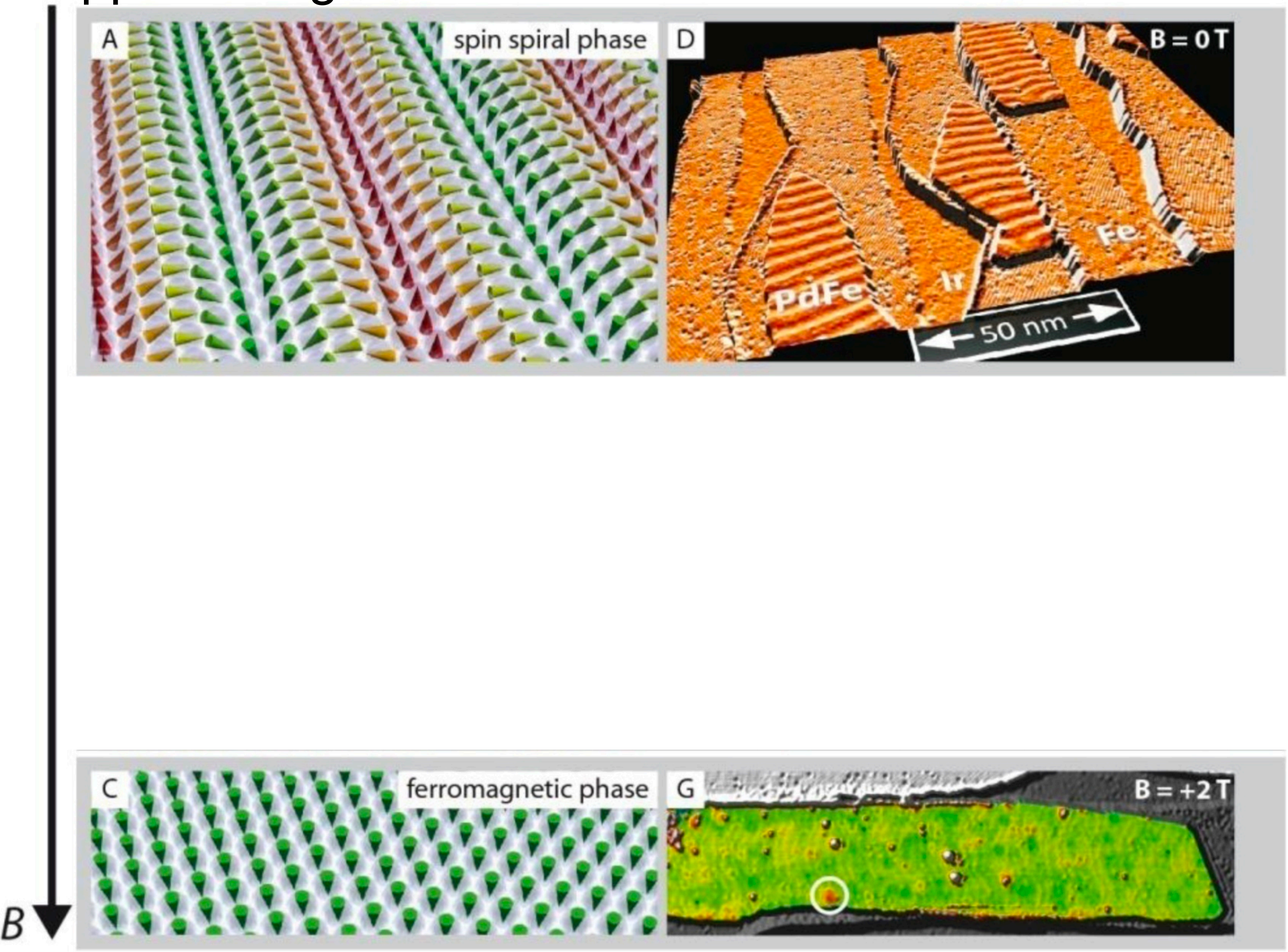
PGI-1 and IAS-1, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

MAX DRIVING THE EXASCALE TRANSITION

JÜLICH Forschungszentrum

Motivation

Pd/Fe/Ir(111): complex phase diagram under an applied magnetic field



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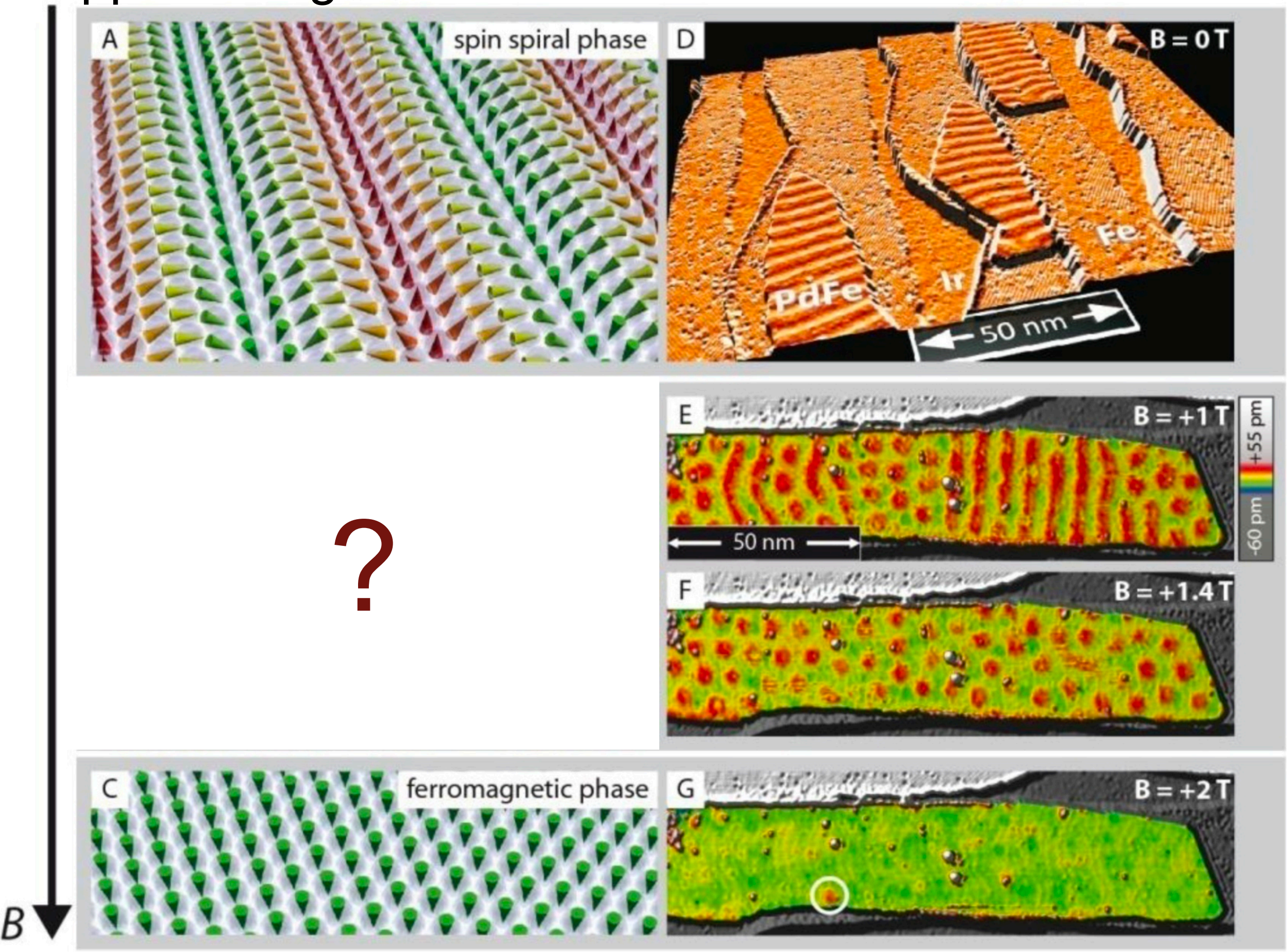

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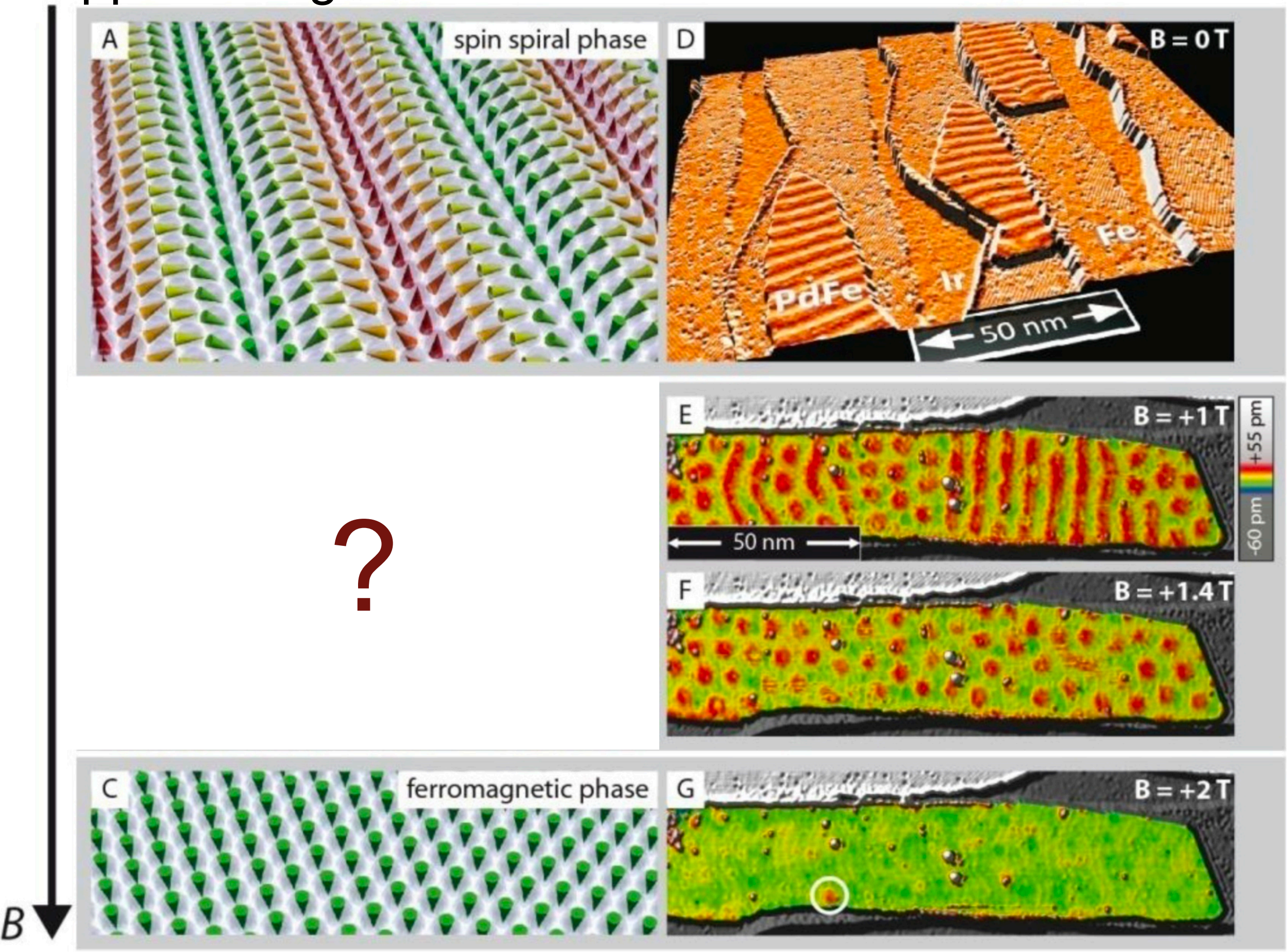

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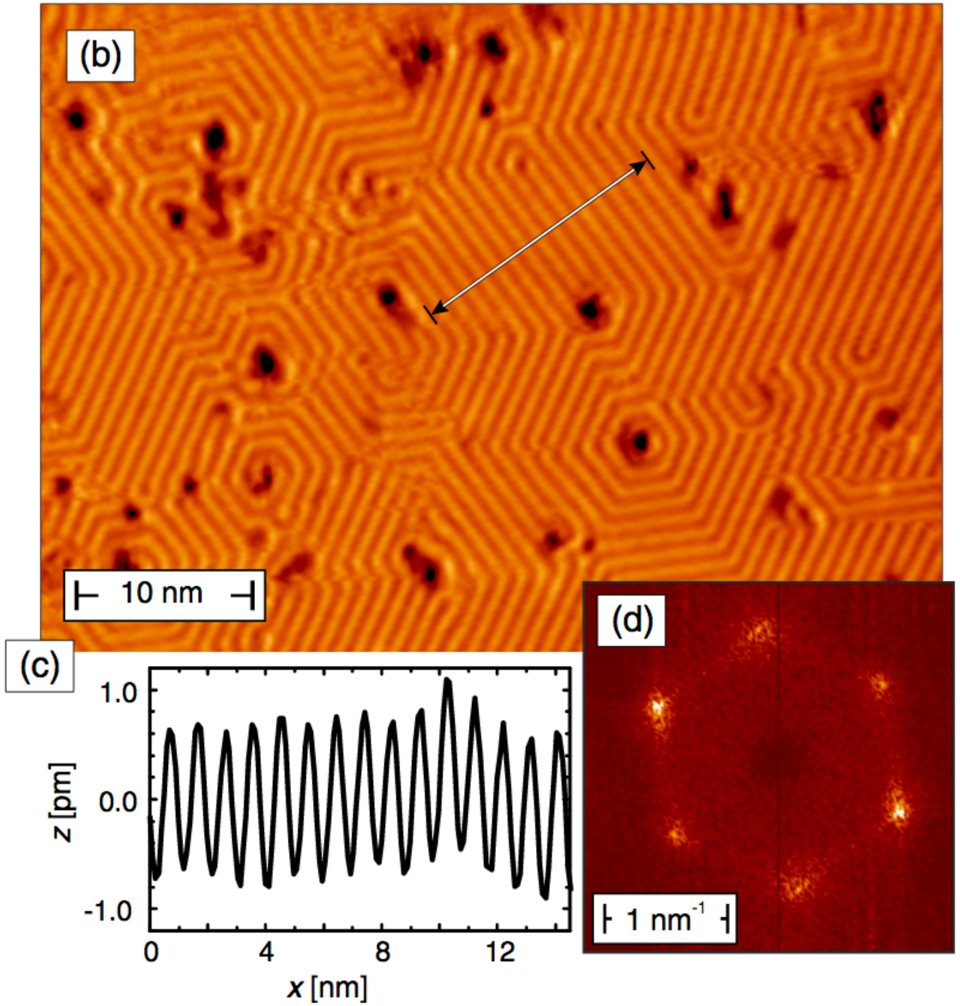
Fe/Rh(111): unconventional ground state



A. Krönlein, **MH** *et al.*, Phys. Rev. Let. **120**, 207202 (2018)

Outline

Higher order exchange interactions

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TRANSITION

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Dzyaloshinskii-Moriya interaction

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Skyrmionic magnetic textures

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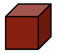
Summary & Conclusion

Multiscale modelling



1 nm

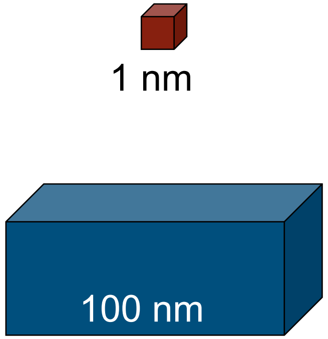
$|\psi_i\rangle$

Density functional theory

- material specific, predictive
- treats every electron
- fully quantum-mechanical

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Multiscale modelling



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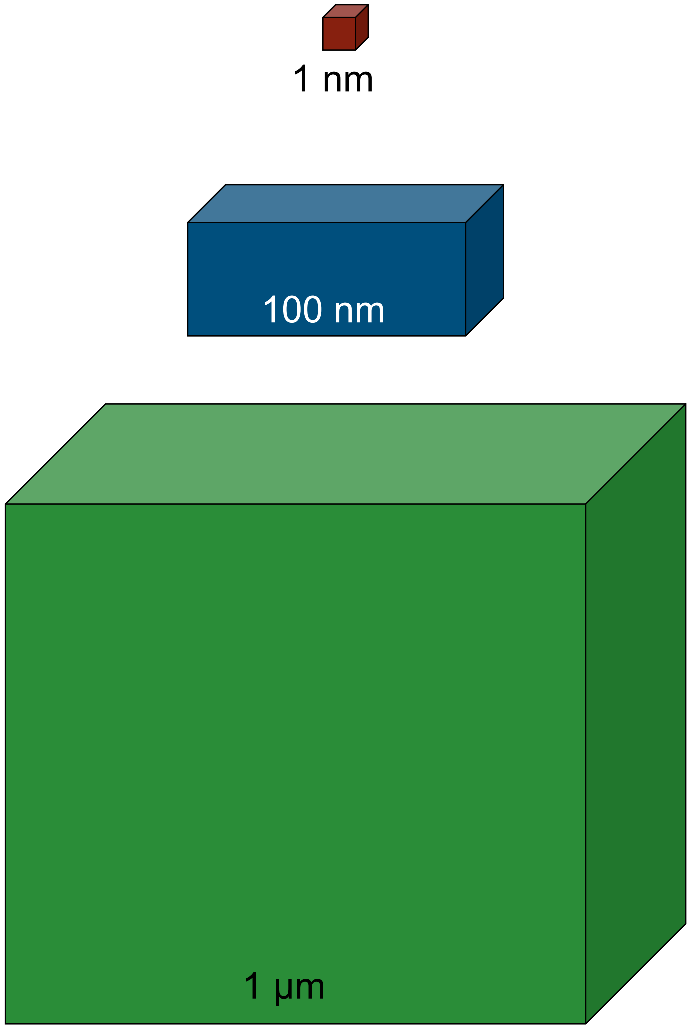
$\mathbf{S}_i$

Atomistic spin-lattice model

$$E = \sum_{ij} J_{ij}\left(\mathbf{S}_i \cdot \mathbf{S}_j\right) + \ldots$$

- crystal structure
- finite temperature (MC) & dynamics (LLG)

Multiscale modelling



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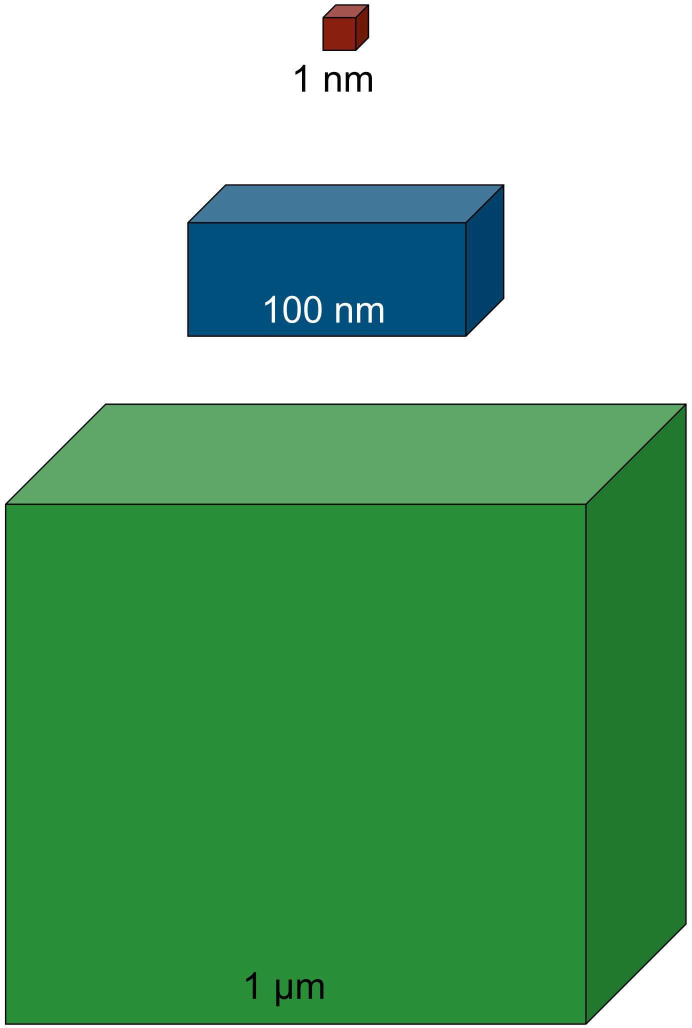
$\mathbf{m}(\mathbf{r})$

Micromagnetic model

- continuous magnetization
- analytical expressions

$$E = \int_V A\,(\nabla\mathbf{m})^2 + \ldots$$

Multiscale modelling



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realistic parameters from DFT!

Higher-order exchange interactions

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Extended Heisenberg Hamiltonian

Typically, DFT results are mapped to an effective (classical) spin Hamiltonian:

$$H = -\sum_{ij} J_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right) - \sum_{ij} \mathbf{D}_{ij} \cdot \left(\mathbf{S}_i \times \mathbf{S}_j\right) - \sum_i K_i \left(\mathbf{S}_i \cdot \hat{\mathbf{K}}_i\right)^2 - \sum_i \mathbf{B} \cdot \mathbf{S}_i$$

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exchange interaction

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exchange interaction

Dzyaloshinskii-Moriya interaction

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magnetocrystalline anisotropy

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Zeeman (magn. field)

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exchange interaction

Dzyaloshinskii-Moriya interaction

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Zeeman (magn. field)

two-site interactions

single-site interactions

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

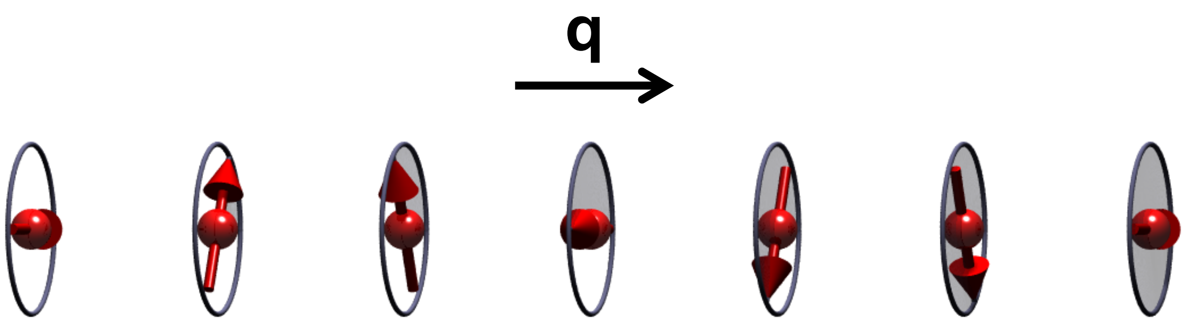
two-site interactions (exchange, Dzyaloshinskii-Moriya) | single-site interactions (anisotropy, Zeeman)

Natural questions:

- are there more possible single- and two-site interactions?
- how about interactions involving more than two sites, do they exist?

Spin-spirals: energy minimizers of the Heisenberg model

So far: exchange interaction stabilizes spin spiral ground state



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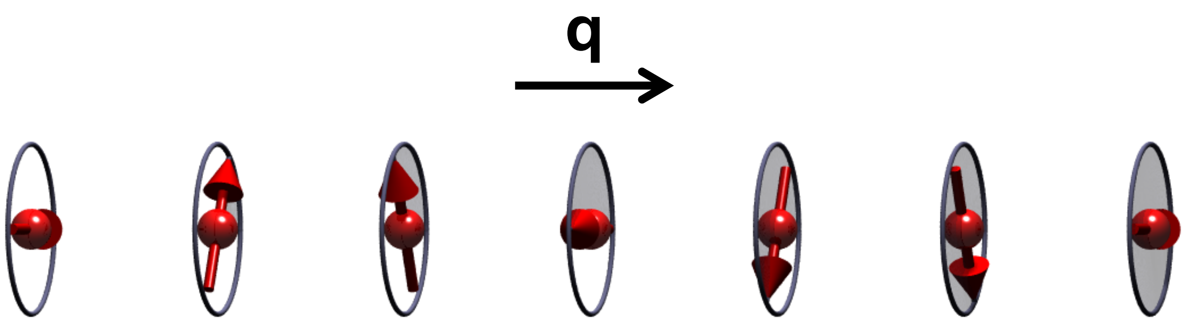

But: multiple energetically degenerated spirals might exist

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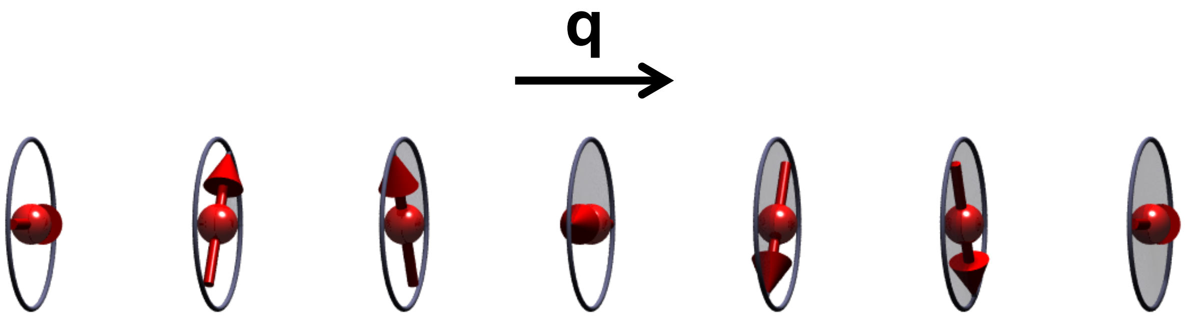

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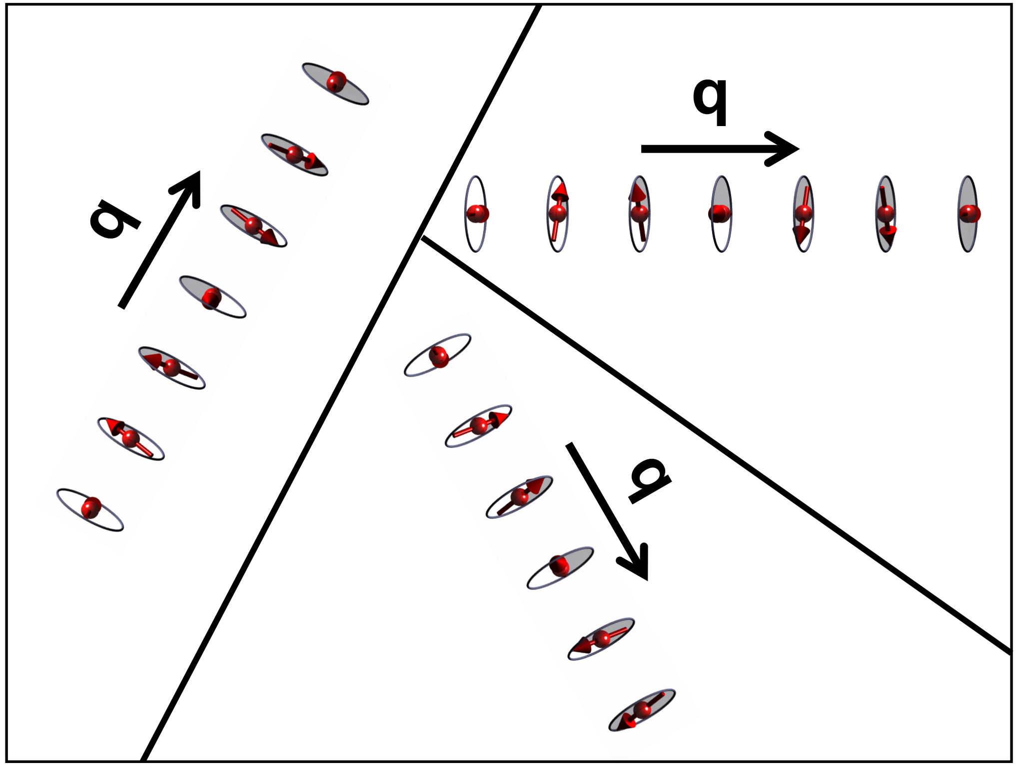
Option 1: Domains



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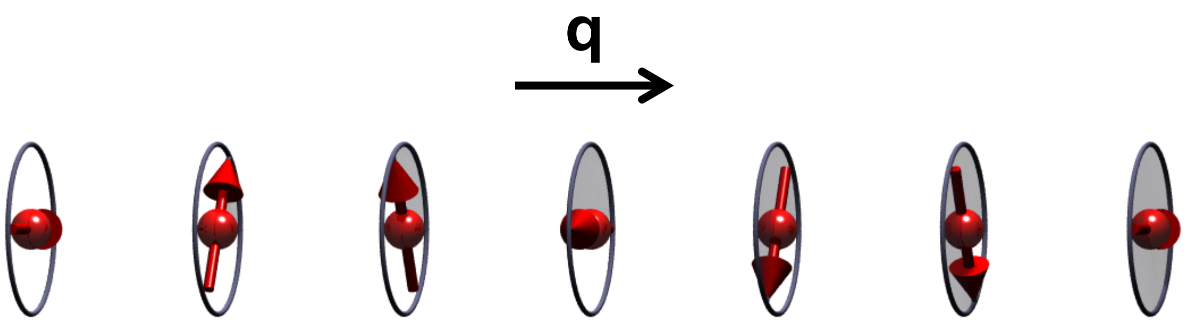

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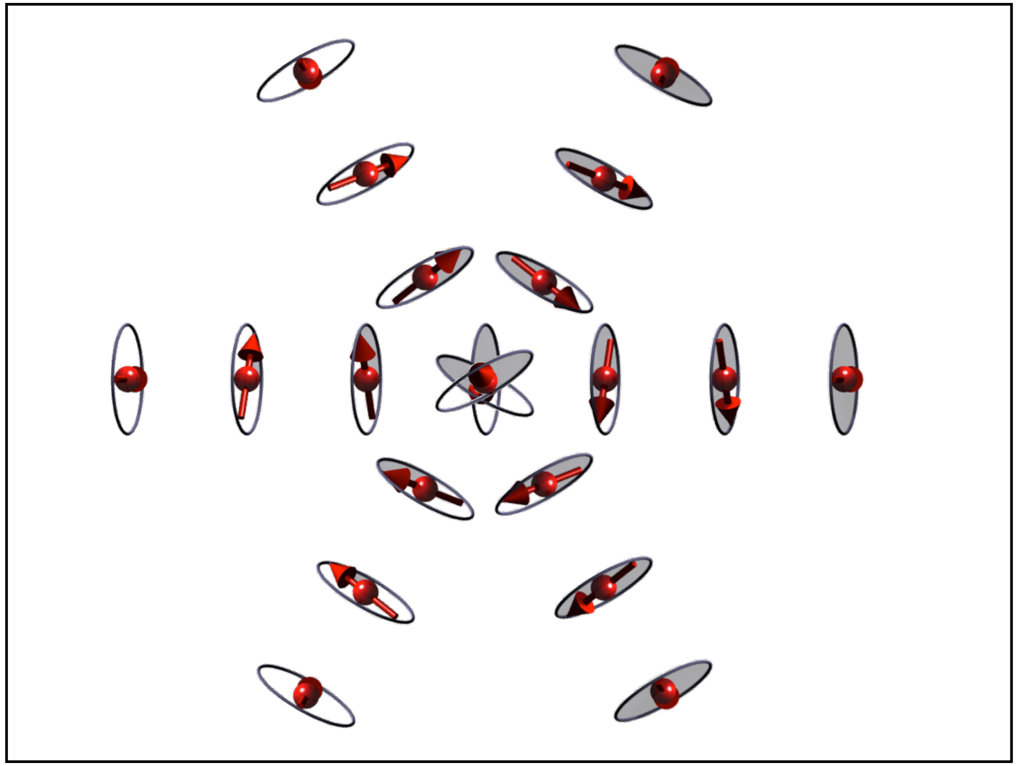
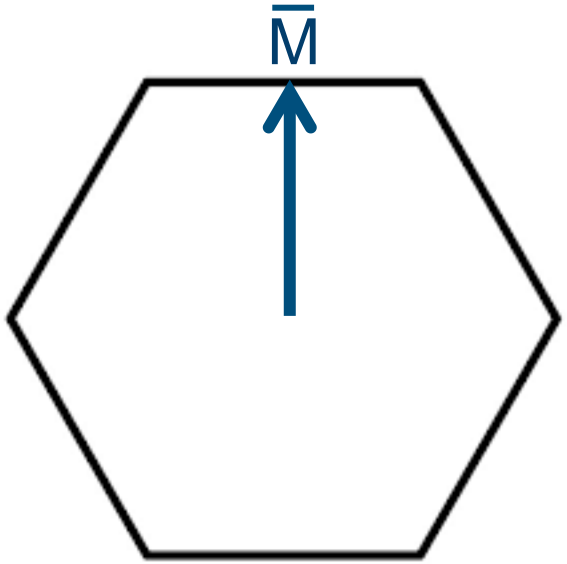
Option 2: Superposition



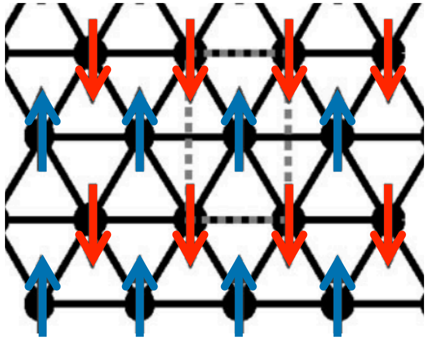
Multi-Q states

Example: 3Q-state on hexagonal lattice



energetically lowest spin-spiral: $\bar{M}$

row-wise antiferromagnet



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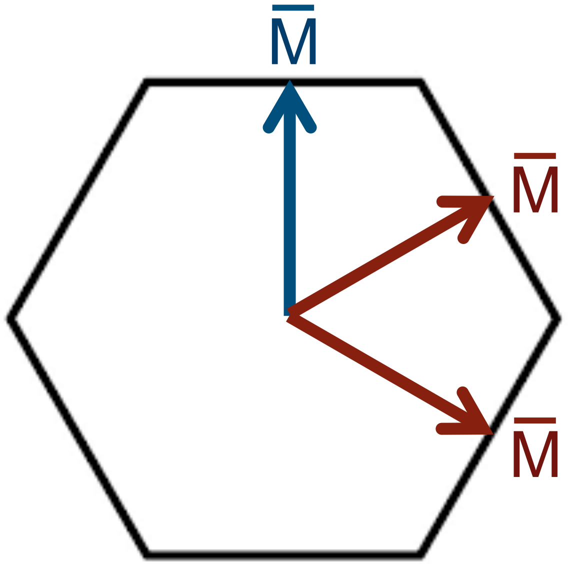
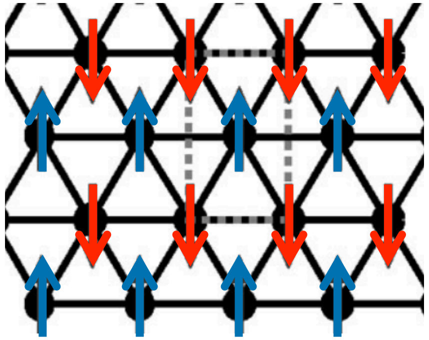


energetically lowest spin-spiral: M̄

row-wise
antiferromagnet



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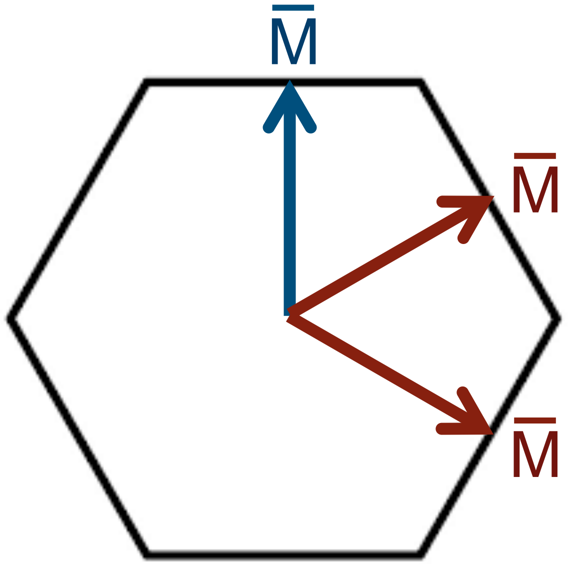

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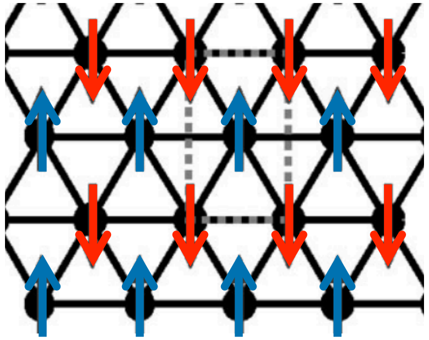
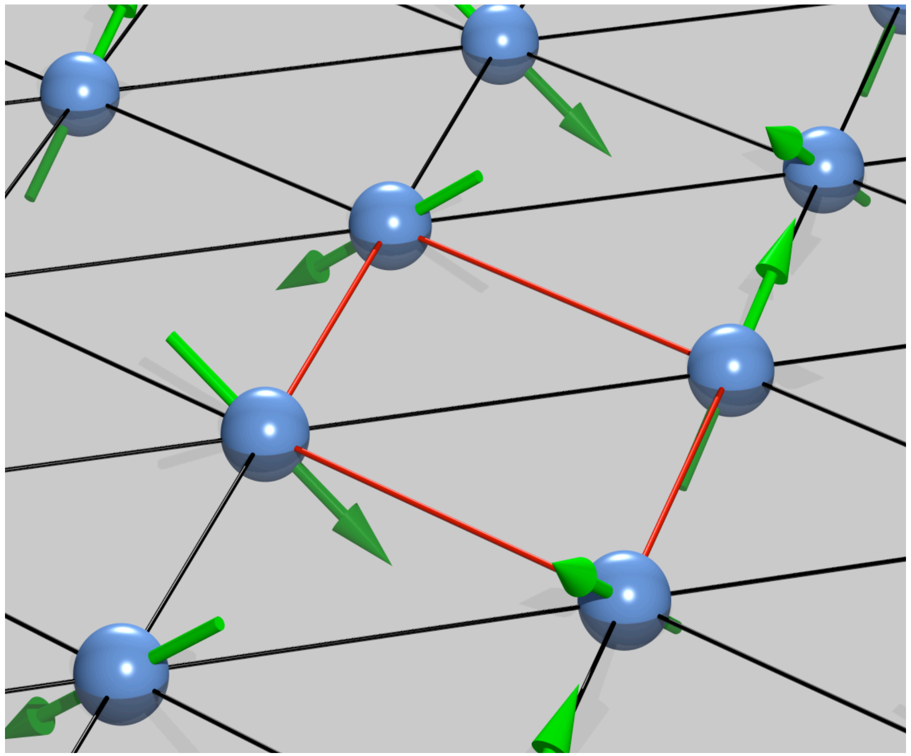




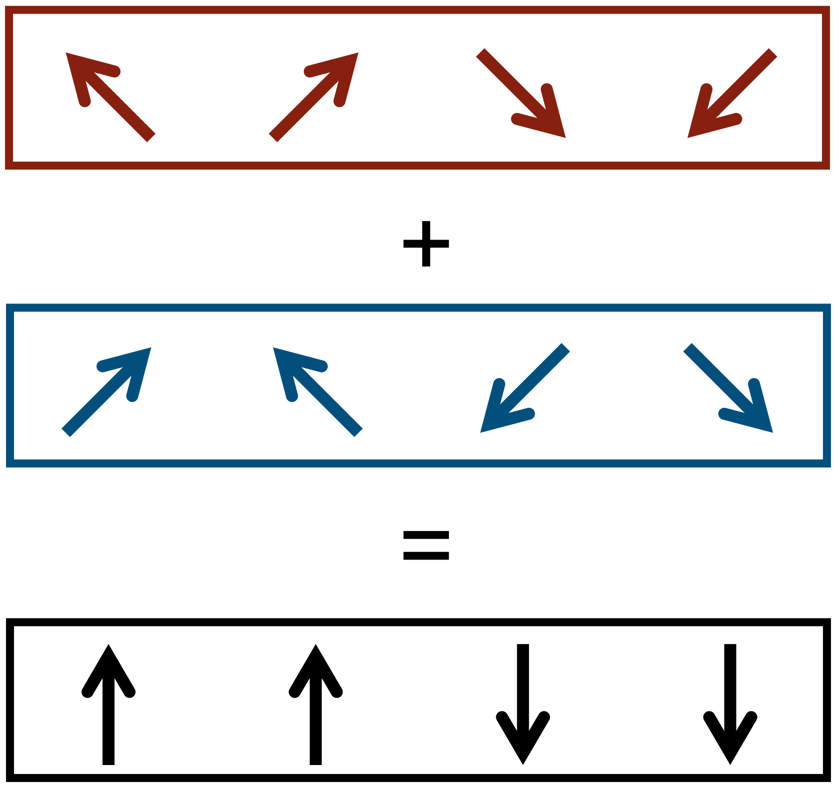
Picture: JP Hanke

Multi-Q states

Example: up-up-down-down states

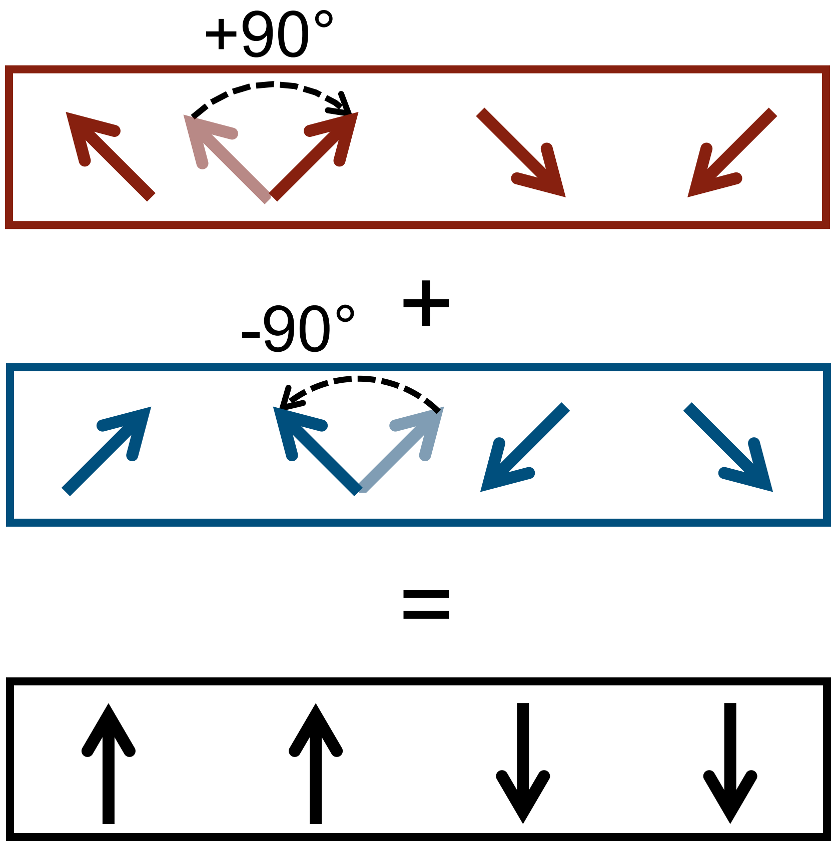
Multi-Q states

Example: up-up-down-down states



Multi-Q states

Example: up-up-down-down states



Multi-Q states

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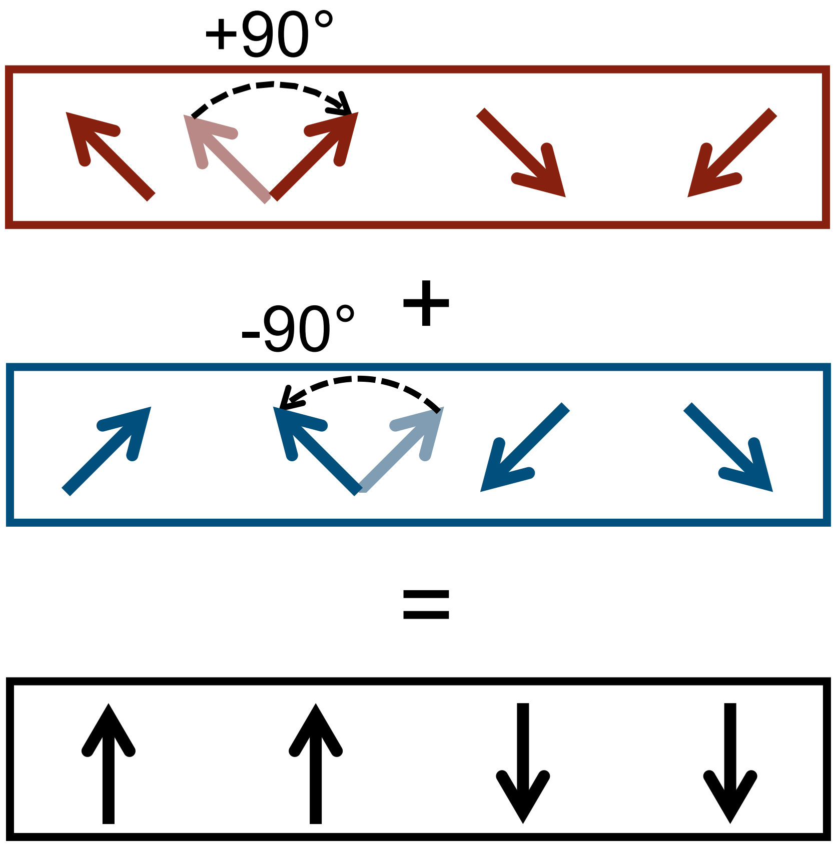

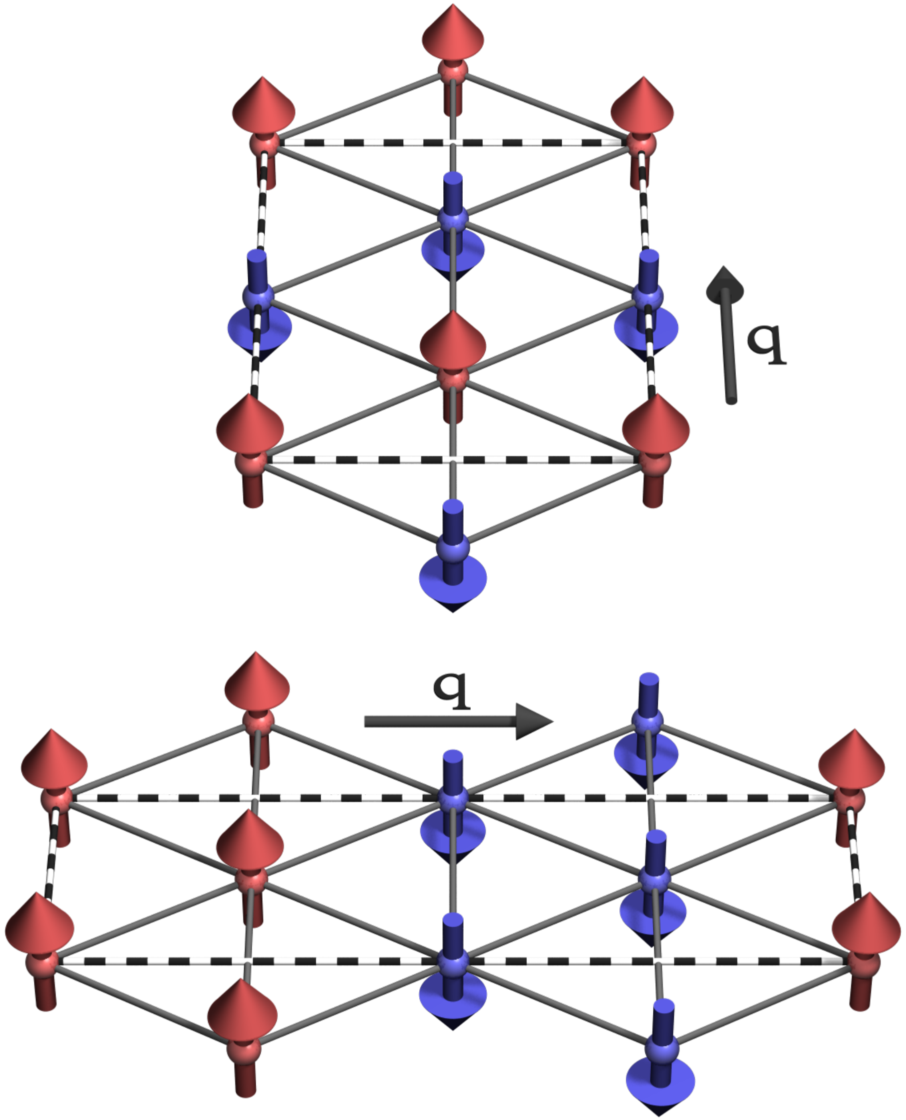

Higher-order exchange interactions

Extended Heisenberg Hamiltonian

$$
\begin{aligned}
H = &- \sum_{ij} J_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right) \\
&- \sum_{ij} \mathbf{D}_{ij} \cdot \left(\mathbf{S}_i \times \mathbf{S}_j\right) \\
&- \sum_{ijkl} B_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right)^2 \\
&- \sum_{ijk} Y_{ijk} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right)\left(\mathbf{S}_i \cdot \mathbf{S}_k\right) \\
&- \sum_{ijkl} K_{ijkl} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right)\left(\mathbf{S}_k \cdot \mathbf{S}_l\right)
\end{aligned}
$$

Higher-order exchange interactions

Extended Heisenberg Hamiltonian

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

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

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

biquadratic

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

4-spin–3-site

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

4-spin–4-site

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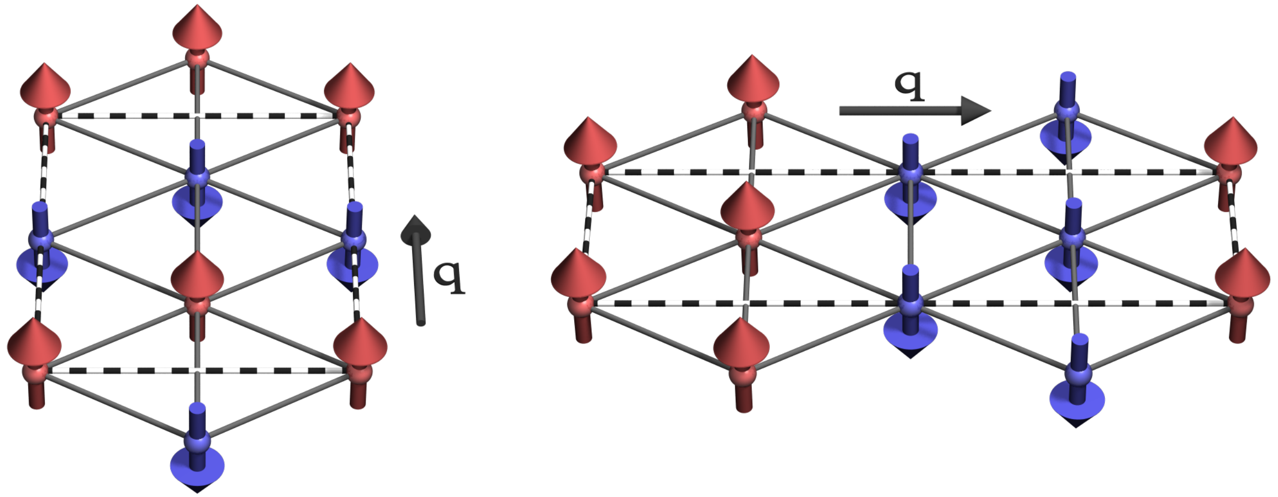
4-spin−4-site

- Higher-order interactions can be derived from a multi-band Hubbard model
- Hubbard model describes **electrons** on a lattice via **hopping** between different lattice sites as well as **on-site interactions** like Coulomb repulsion
- effective **spin** Hamiltonian can be obtained by downfolding fermionic degrees of freedom into low-energy spin sector
- see for example **arXiv:1803.01315** for a more detailed explanation

Higher-order exchange interactions



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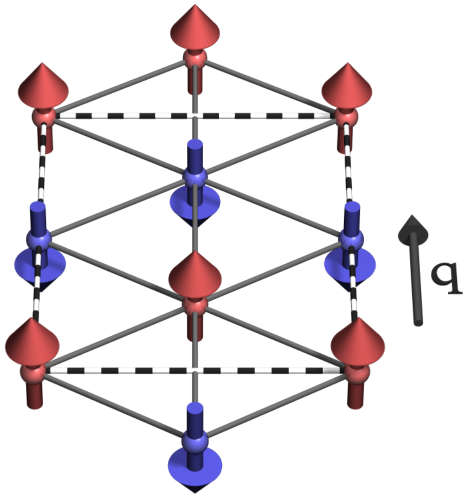
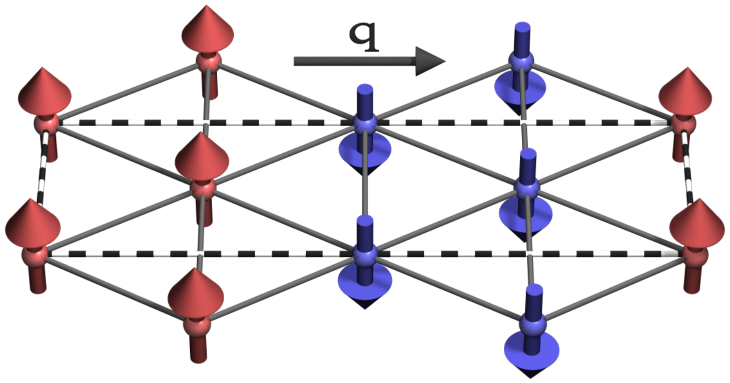
Higher-order exchange interactions





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

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

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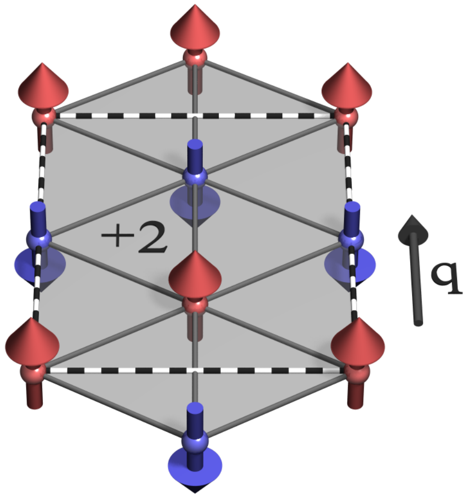
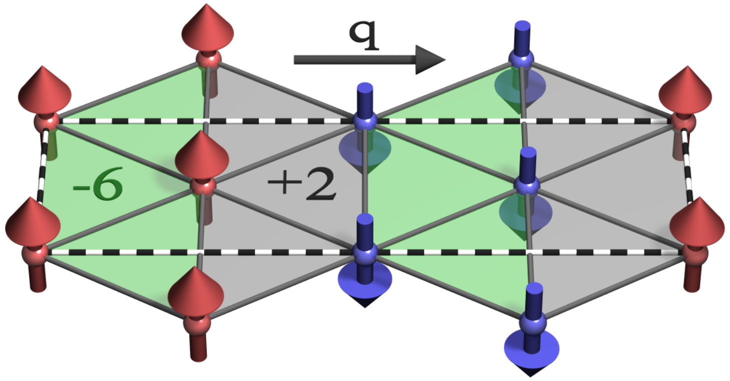


$\Delta E(3/4\overline{\Gamma K}) = 4\,(2K - B)$

$+ 4\ Y_{3spin}$



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

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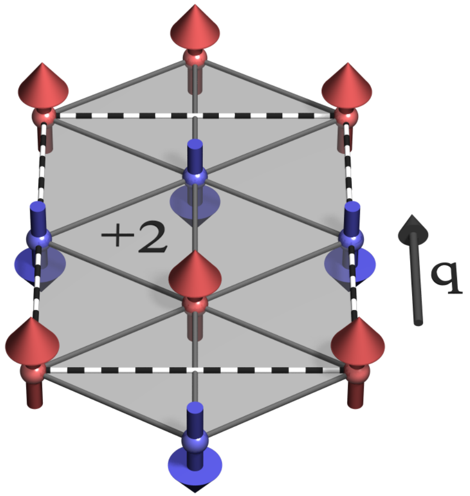
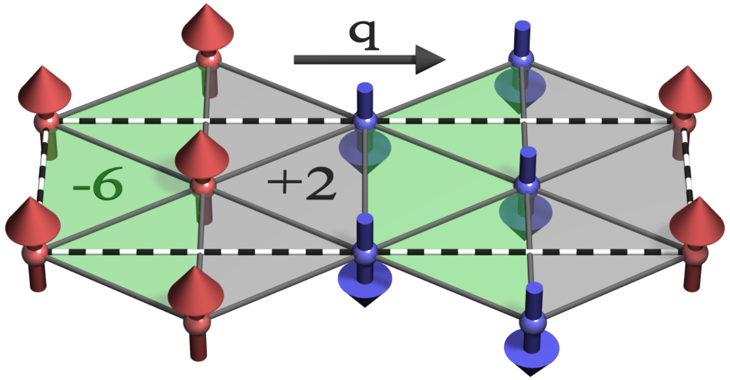
Higher-order exchange interactions





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$+\,4\,Y_{3spin}$

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

$-\,4\,Y_{3spin}$

→ 4-spin−3-site interaction favors one uudd state over the other

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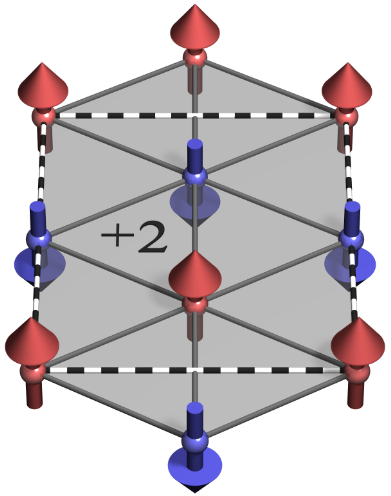
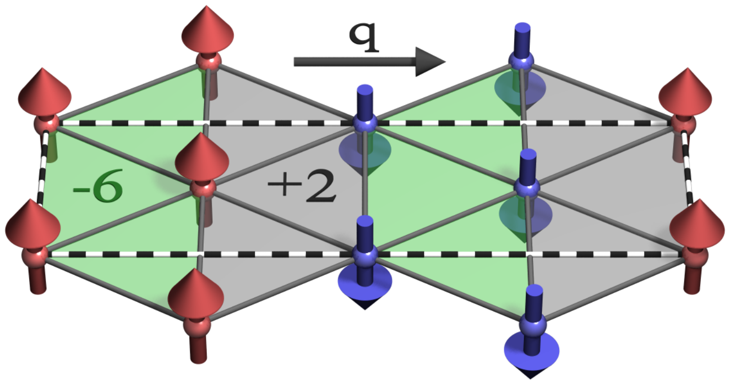


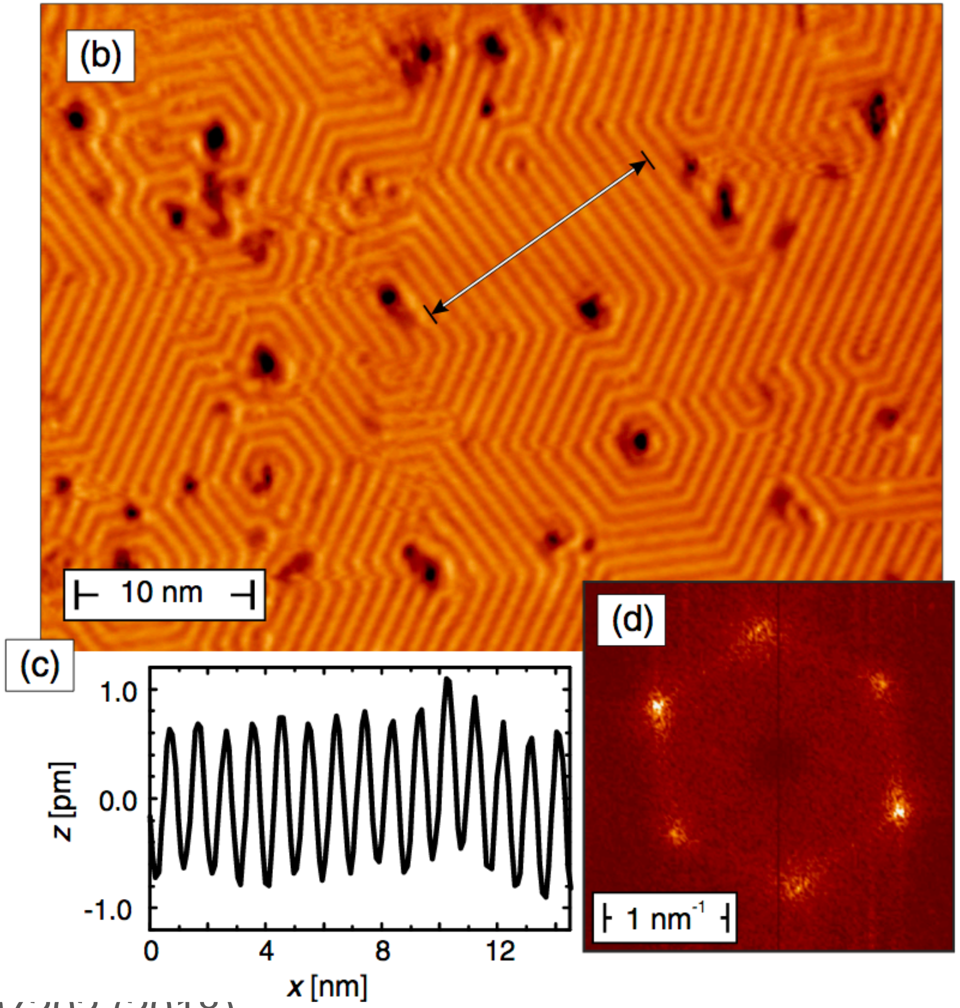


$$\Delta E(3/4\overline{\Gamma \mathrm{K}}) = 4\,(2K - B) + 4\,Y_{3spin}$$

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

→ 4-spin–3-site interaction favors one uudd state over the other

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



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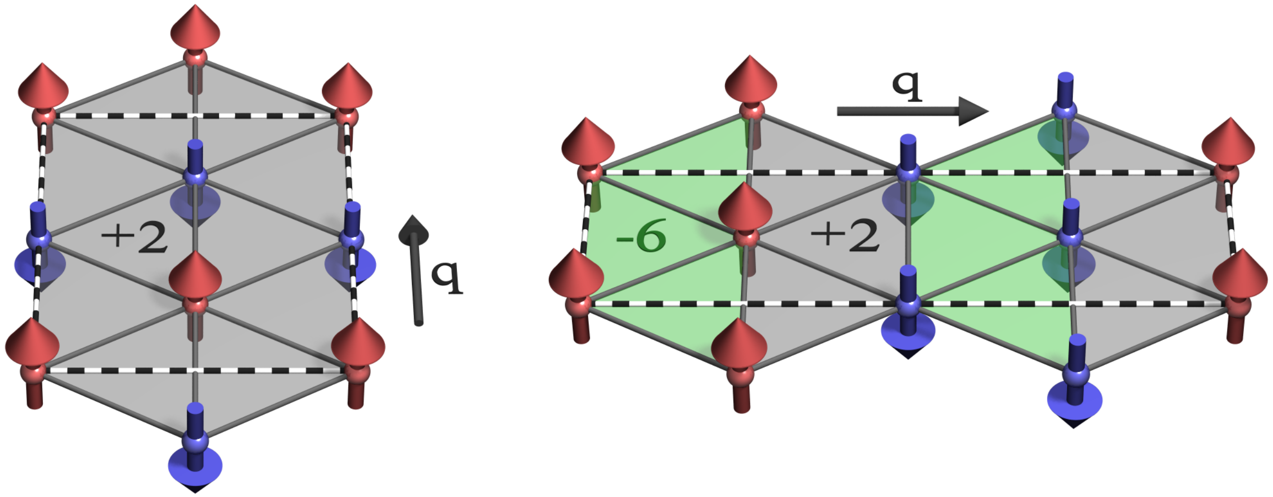

$\Delta E(3/4\overline{\Gamma \mathrm{K}}) = 4\,(2K - B)$ $+\, 4\, Y_{3spin}$

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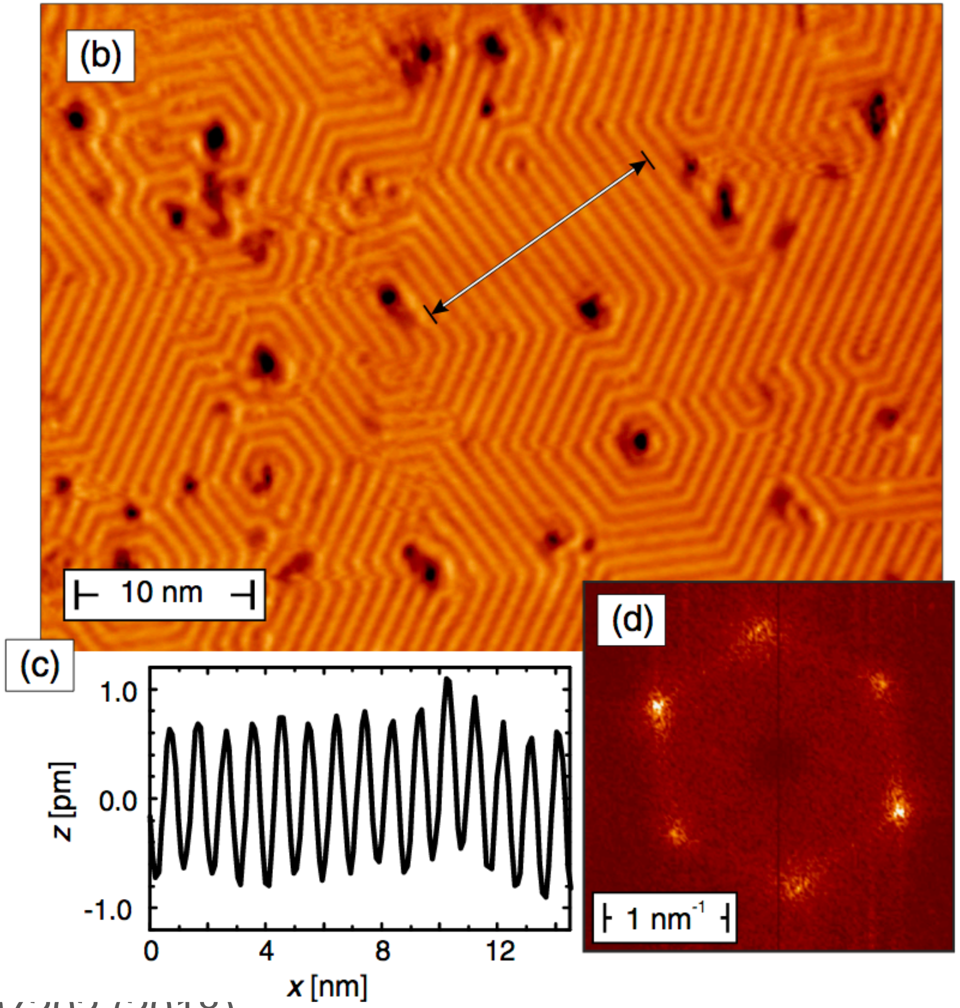
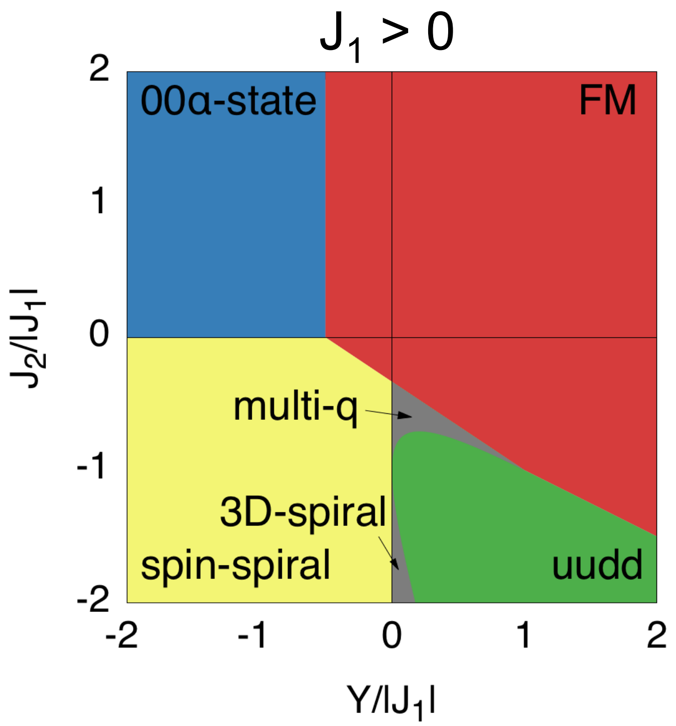
4-spin−3-site interaction

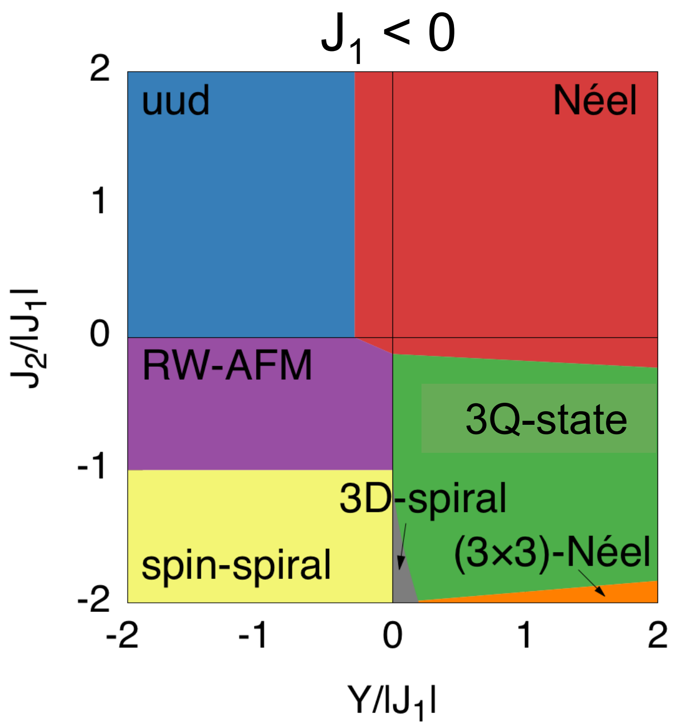


higher-order exchange interactions can be calculated by performing DFT calculations for single-Q (spin-spirals) and multi-Q (uudd, 3Q, ...) states from their energy differences

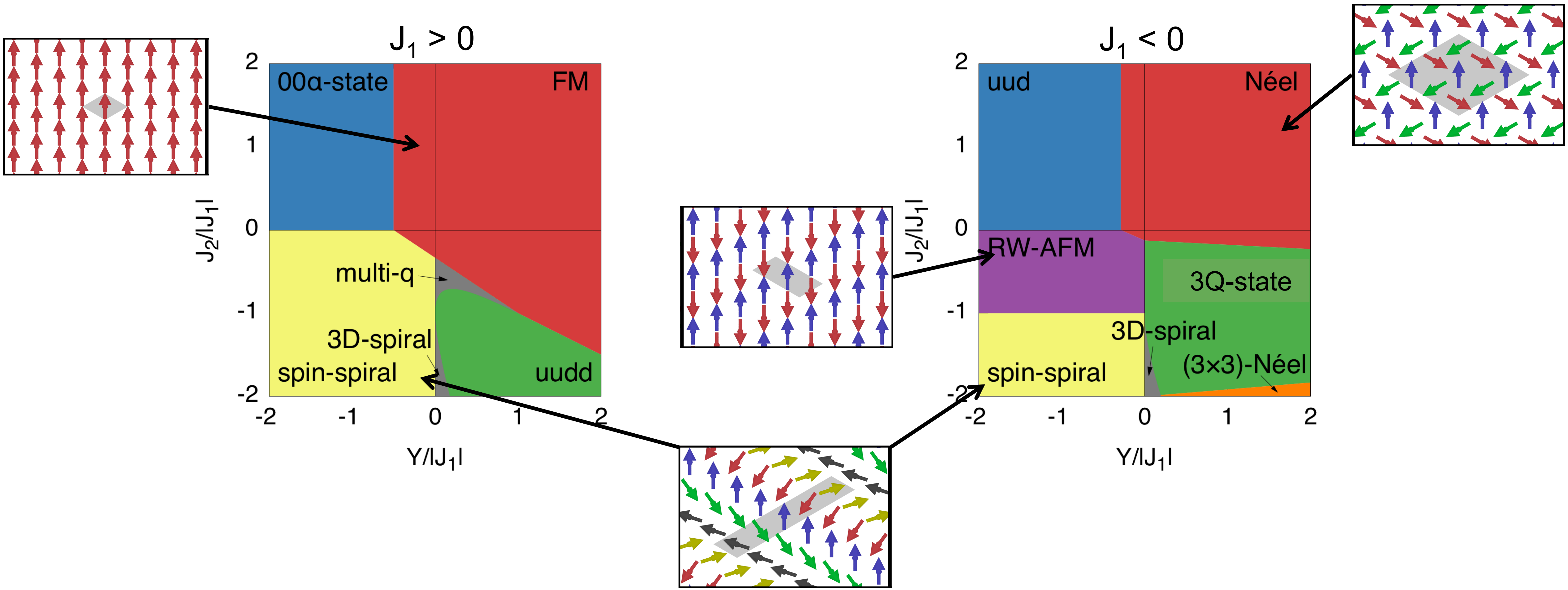
A. Krönlein, **MH** *et al.*, Phys. Rev. Let. **120**, 207202 (2018)

4-spin–3-site interaction: phase diagrams

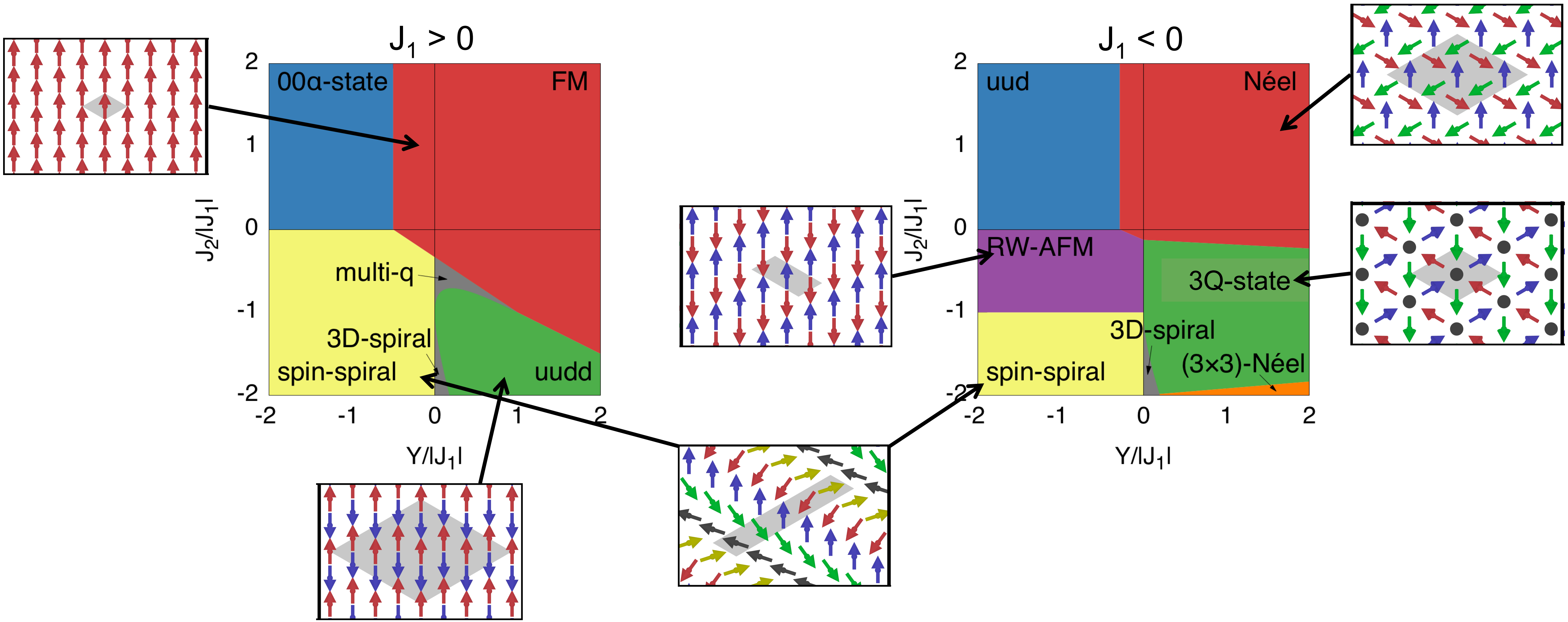




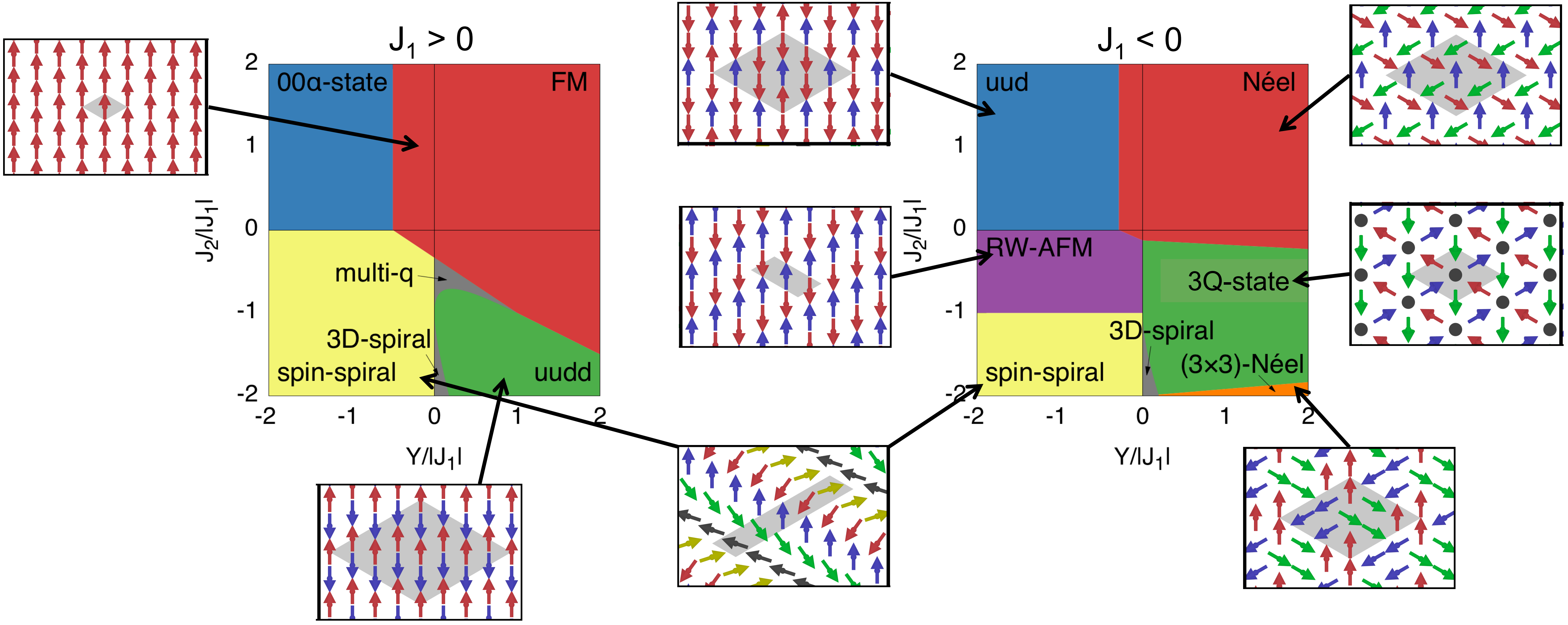
4-spin–3-site interaction: phase diagrams



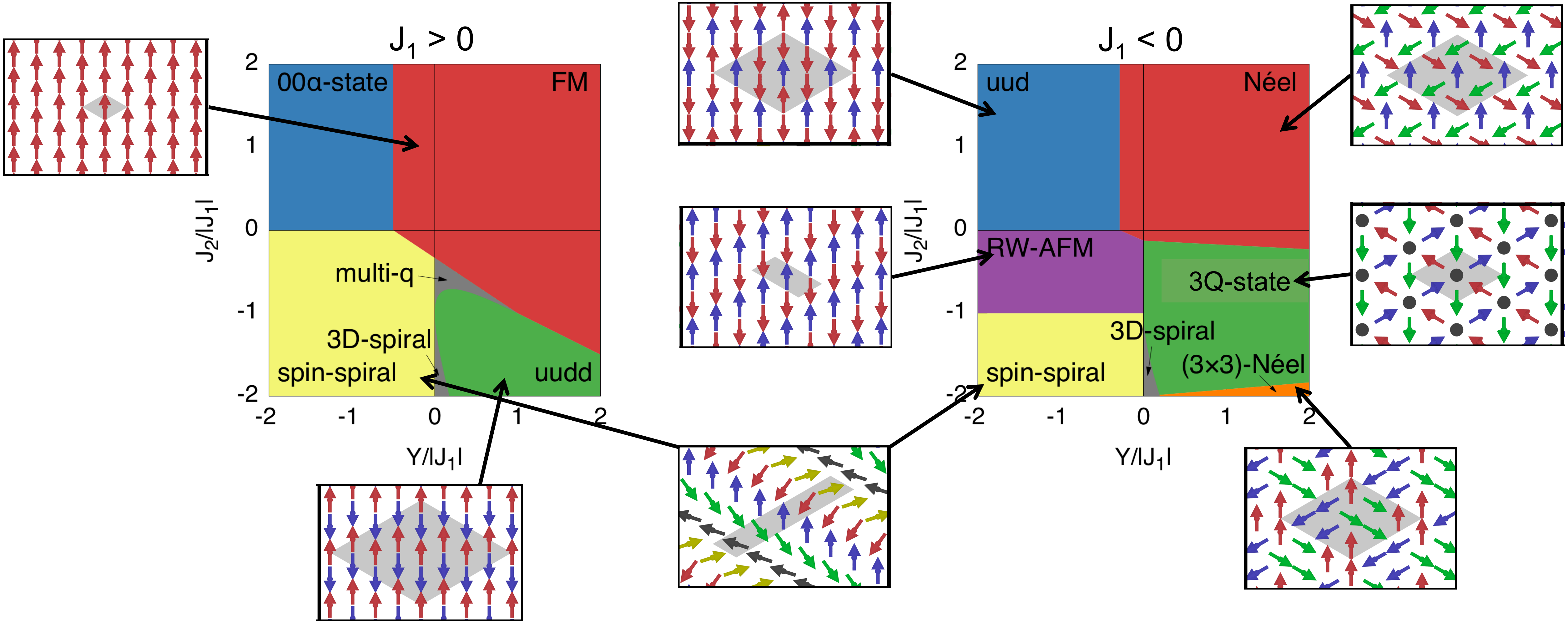
4-spin–3-site interaction: phase diagrams



4-spin–3-site interaction: phase diagrams



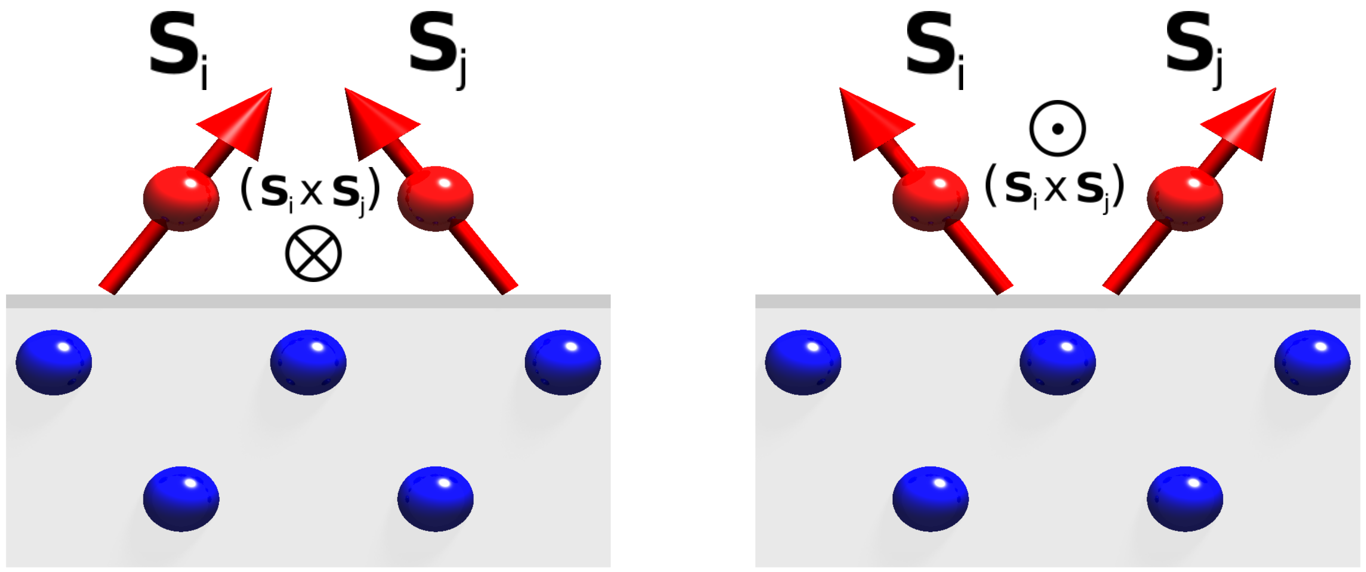
4-spin–3-site interaction: phase diagrams



→ • huge variety of possible collinear as well as non-collinear structures
• many of them **not yet** found in nature!

Dzyaloshinskii-Moriya interaction

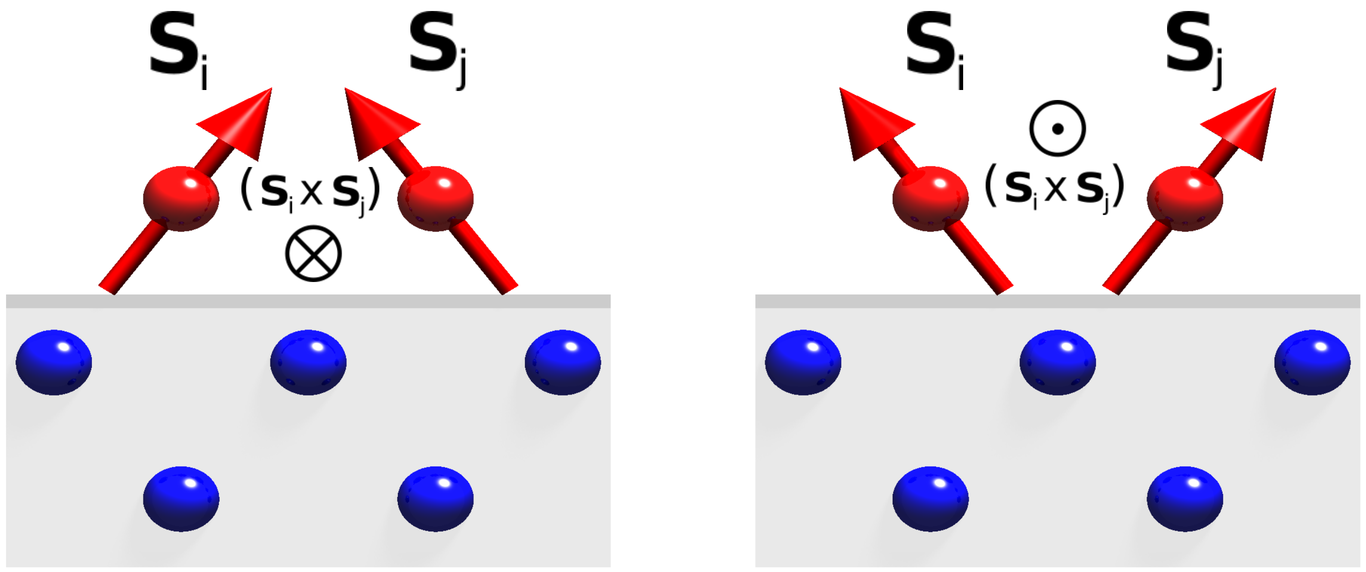
DMI in the atomistic model



Energy contribution due to DMI:

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

DMI in the atomistic model



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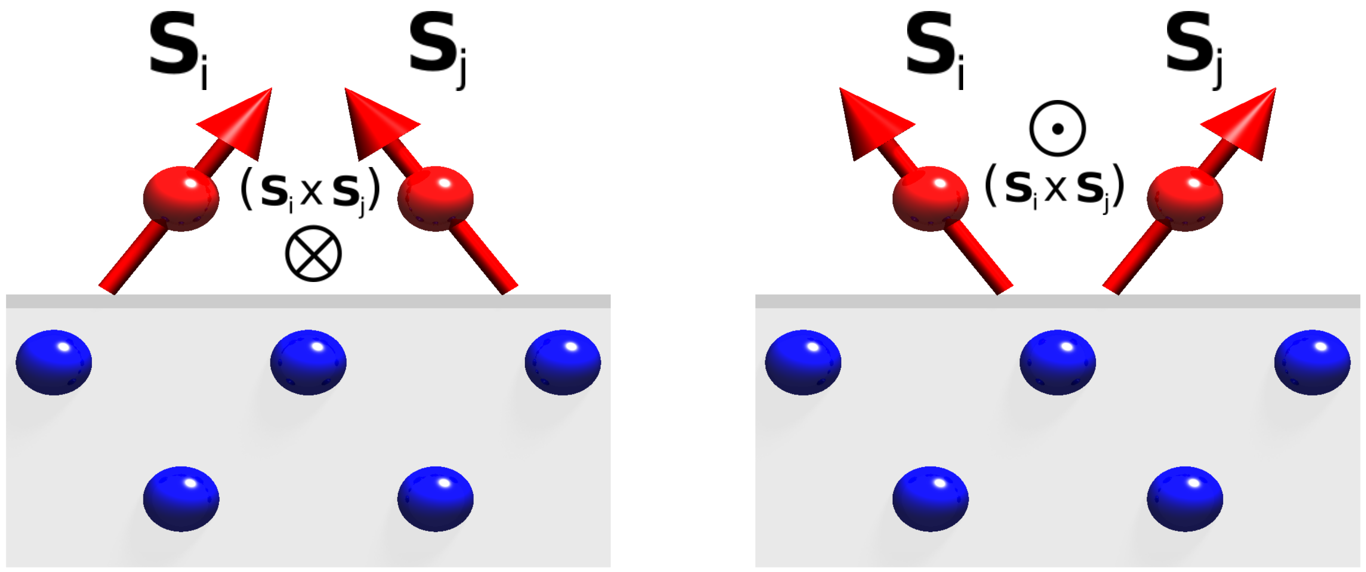
- caused by combination of
  - **spin-orbit coupling**
  - **broken inversion symmetry**
- prefers canting with **unique** rotational sense
- prefers rotation around unique **rotation axis**

DMI in the atomistic model



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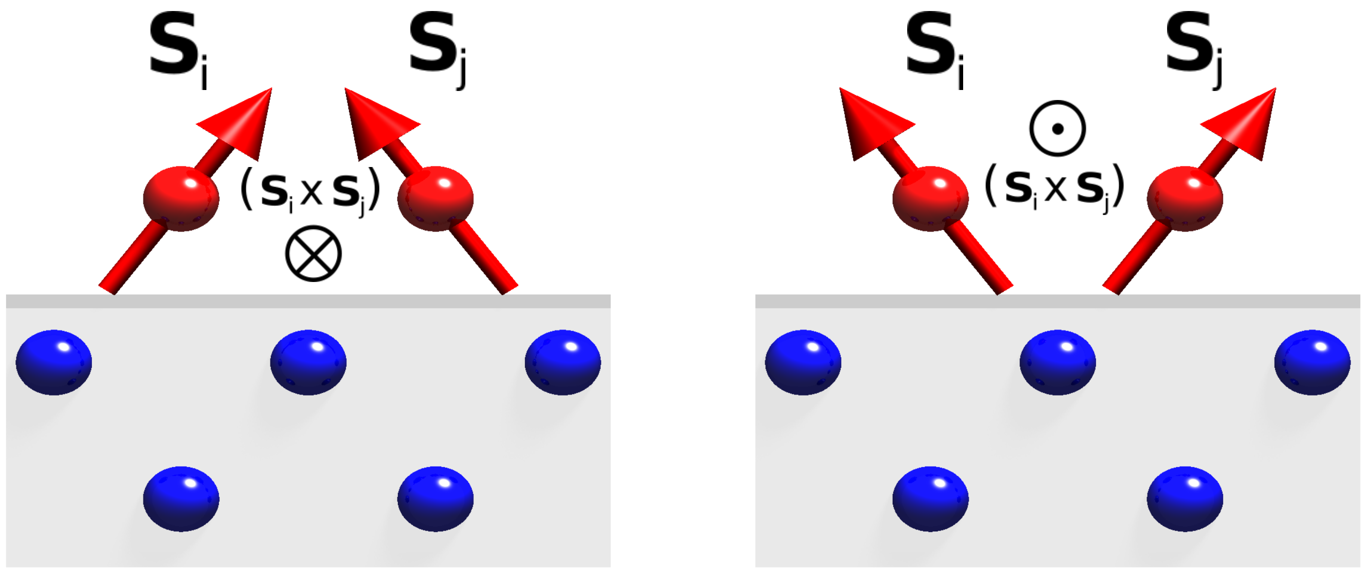

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vector quantity

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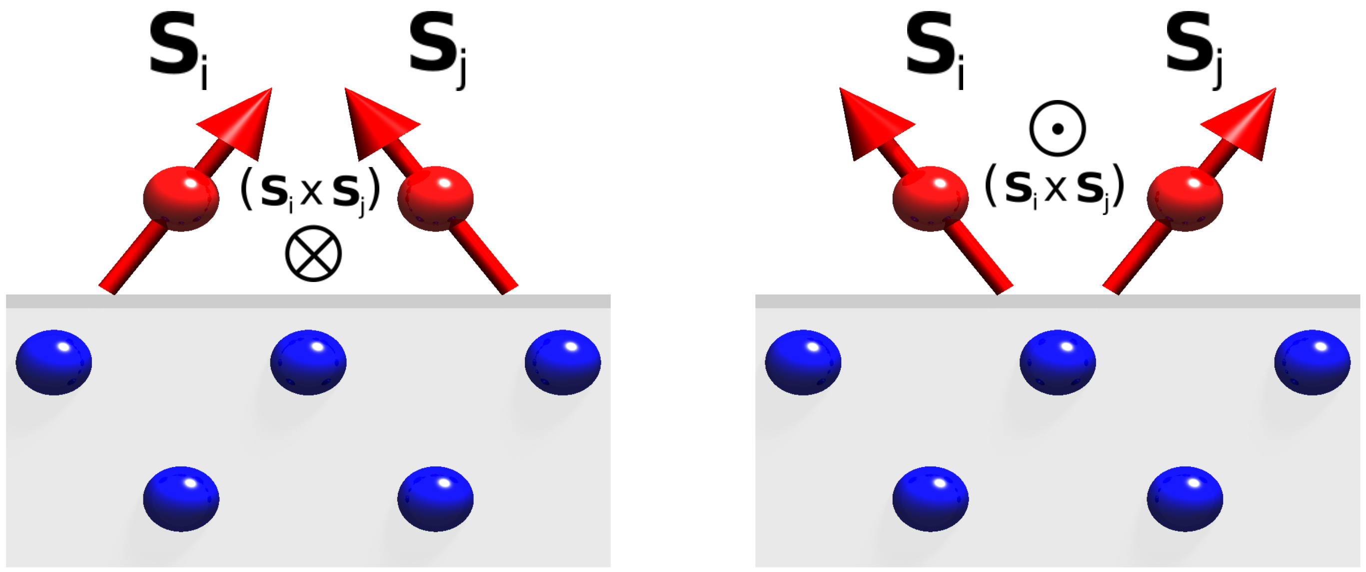
DMI in the atomistic model



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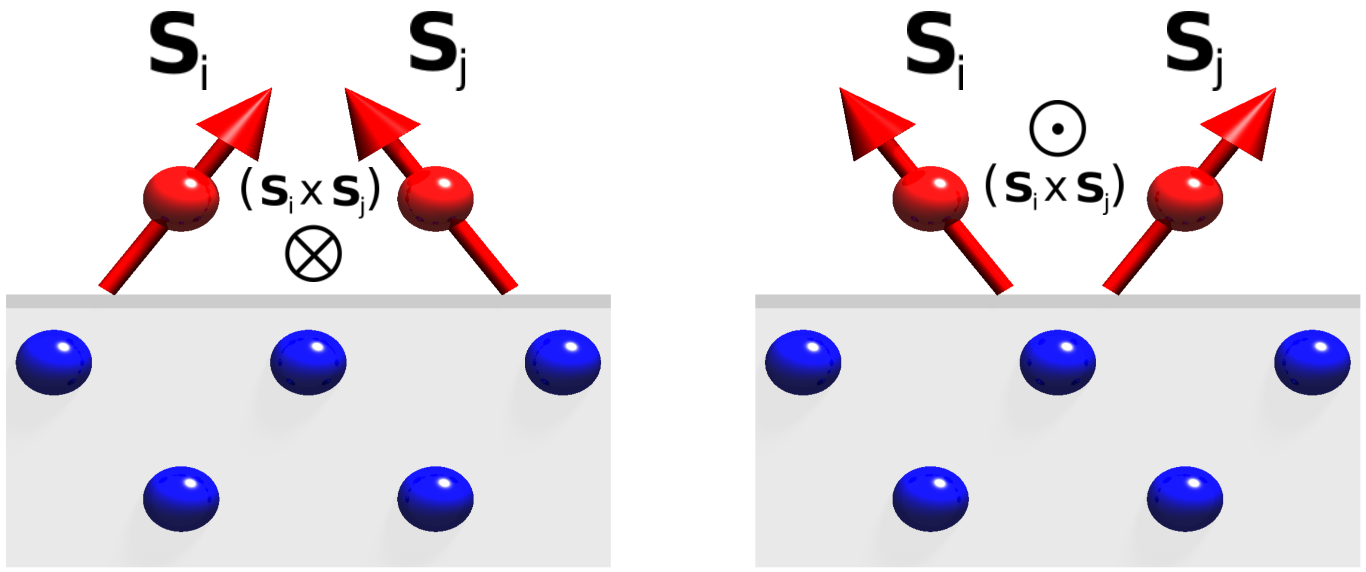

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vector quantity

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- prefers canting with **unique** rotational sense ← **scalar** parameter would be sufficient
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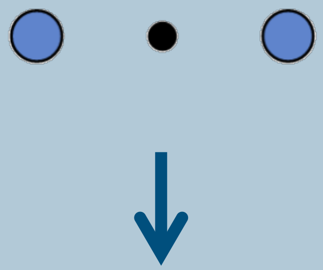
What defines direction of DM vectors?

Moriya rules: determining DMI vector orientation

Moriya rules: determining DMI vector orientation

center = inversion center



$\mathbf{D}_{ij} = 0$

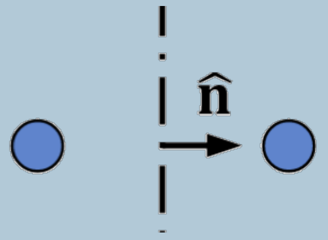
Illustrations taken from:
Brinker *et al* 2019
New J. Phys. **21** 083015

Moriya rules: determining DMI vector orientation

center = inversion center

$\mathbf{D}_{ij} = 0$

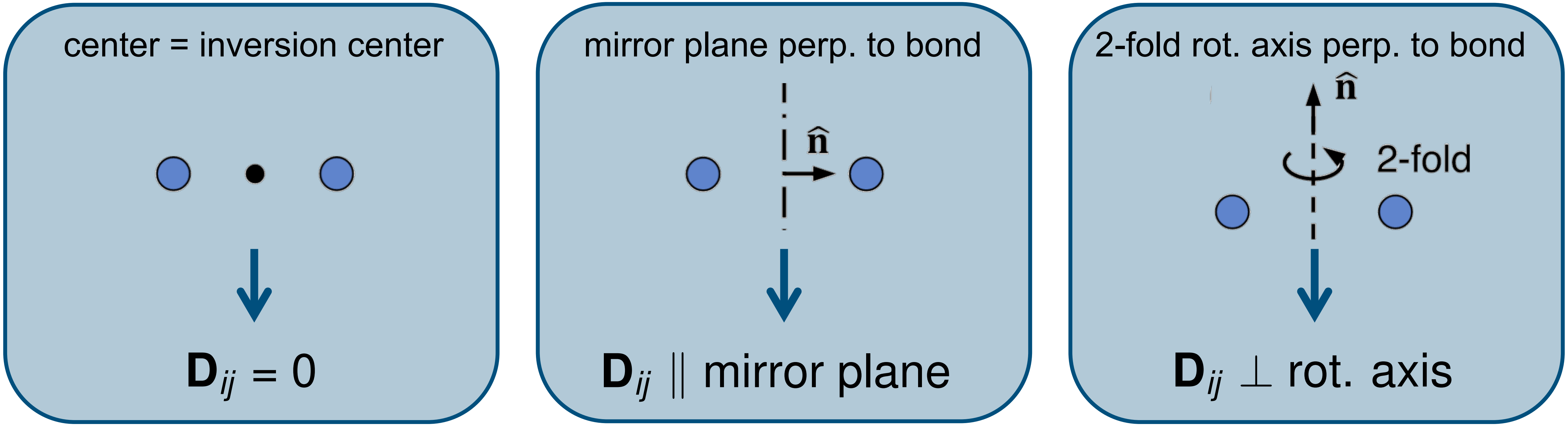
mirror plane perp. to bond



$\mathbf{D}_{ij} \parallel$ mirror plane

Illustrations taken from:
Brinker *et al* 2019
New J. Phys. **21** 083015

Moriya rules: determining DMI vector orientation



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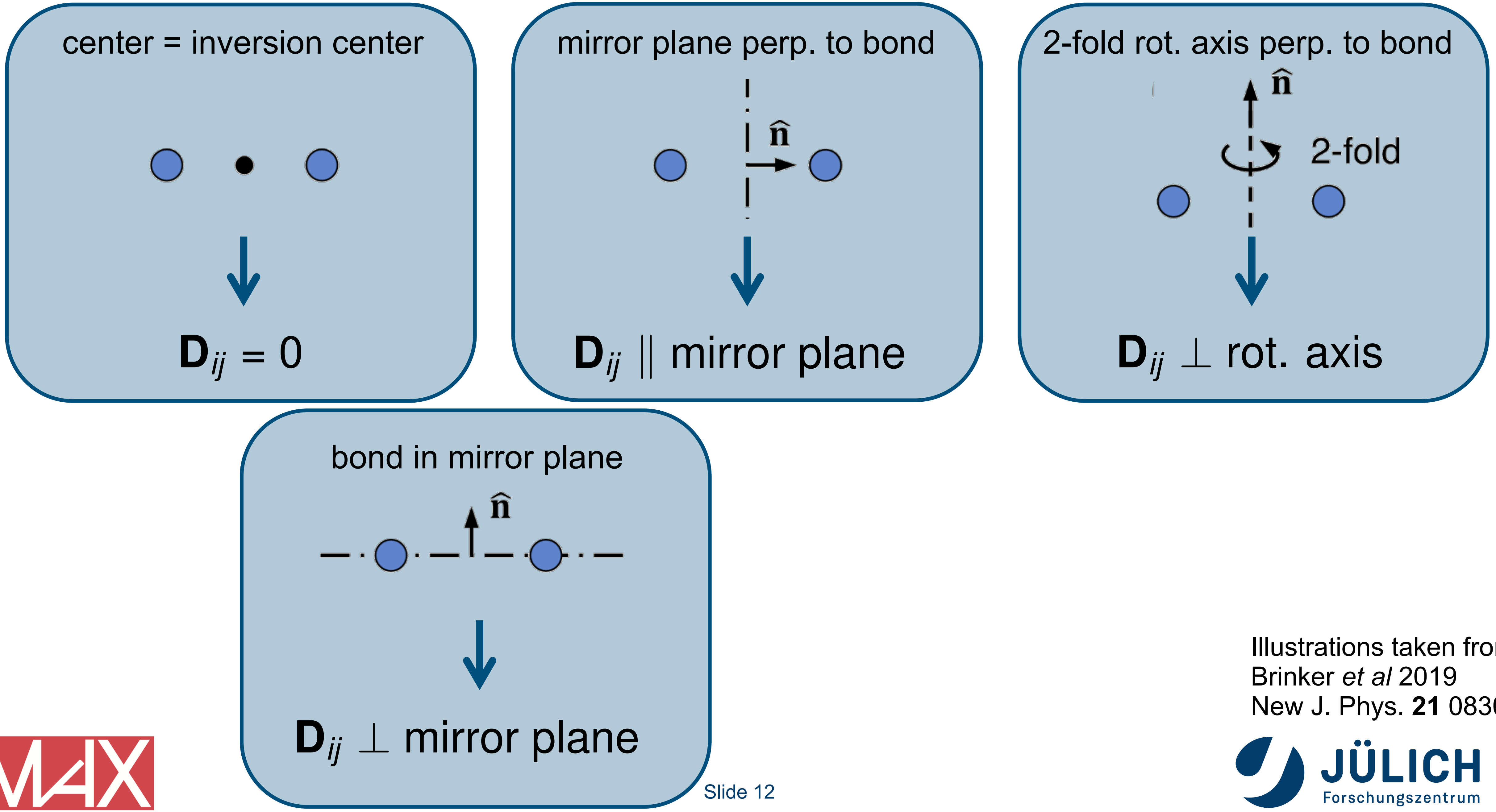
Moriya rules: determining DMI vector orientation



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Brinker *et al* 2019
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Moriya rules: determining DMI vector orientation

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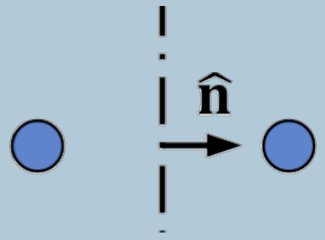
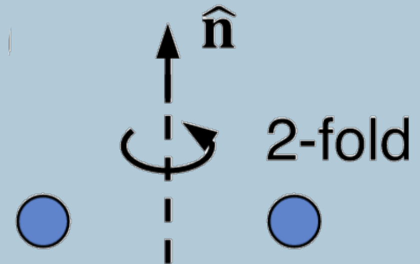
$\mathbf{D}_{ij} = 0$

mirror plane perp. to bond



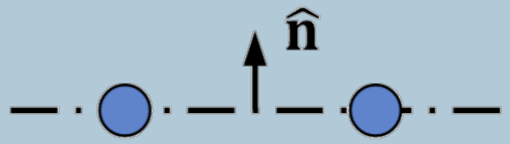
$\mathbf{D}_{ij} \parallel$ mirror plane

2-fold rot. axis perp. to bond



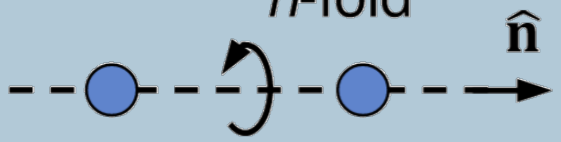
$\mathbf{D}_{ij} \perp$ rot. axis

bond in mirror plane



$\mathbf{D}_{ij} \perp$ mirror plane

bond = rotation axis

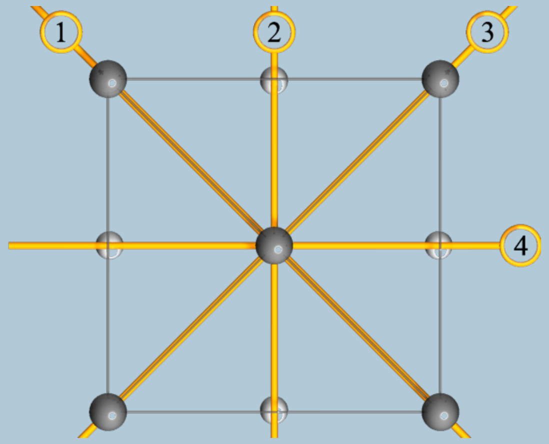


$\mathbf{D}_{ij} \parallel$ rot. axis

Illustrations taken from:
Brinker *et al* 2019
New J. Phys. **21** 083015

DM vectors in different symmetry classes

C_{4v} symmetry [e.g. fcc(100)]



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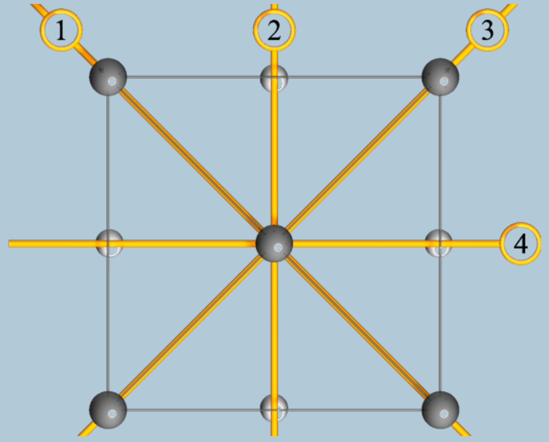

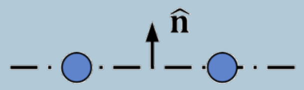

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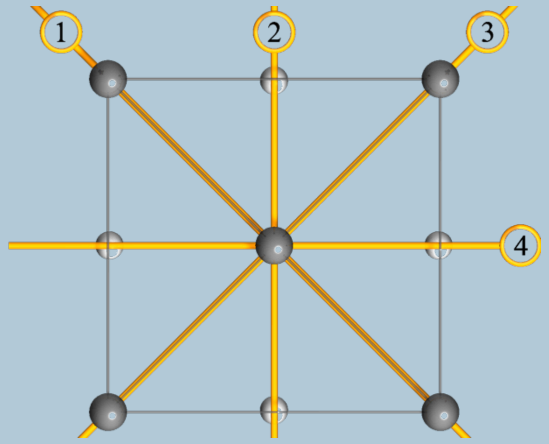
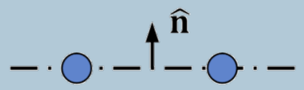


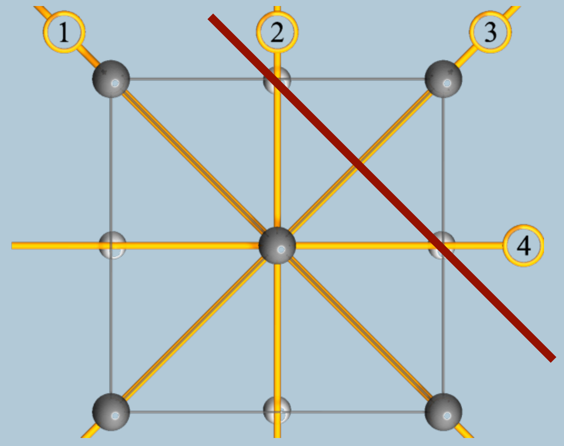


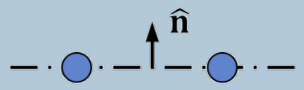
$\mathbf{D}_{ij}$ ⊥ mirror plane

→ inplane

DM vectors in different symmetry classes

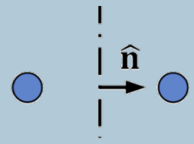
C_{4v} symmetry [e.g. fcc(100)]





$\mathbf{D}_{ij} \perp$ mirror plane

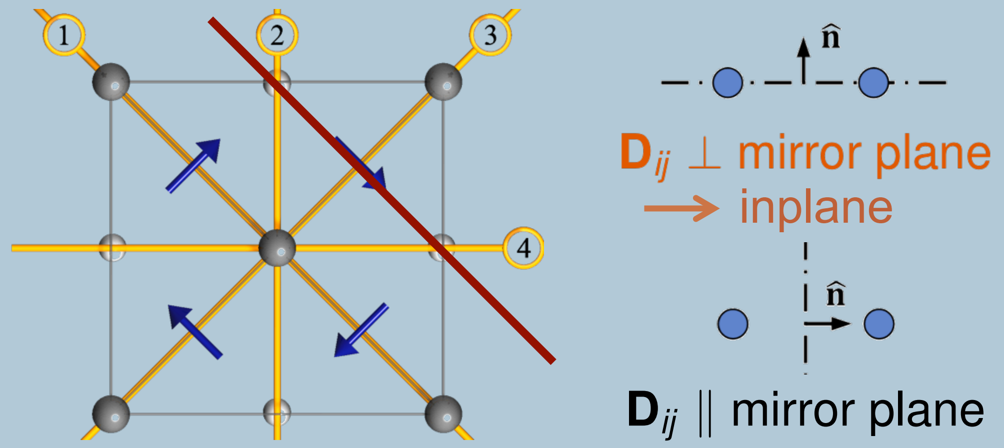
→ inplane



$\mathbf{D}_{ij} \parallel$ mirror plane

DM vectors in different symmetry classes

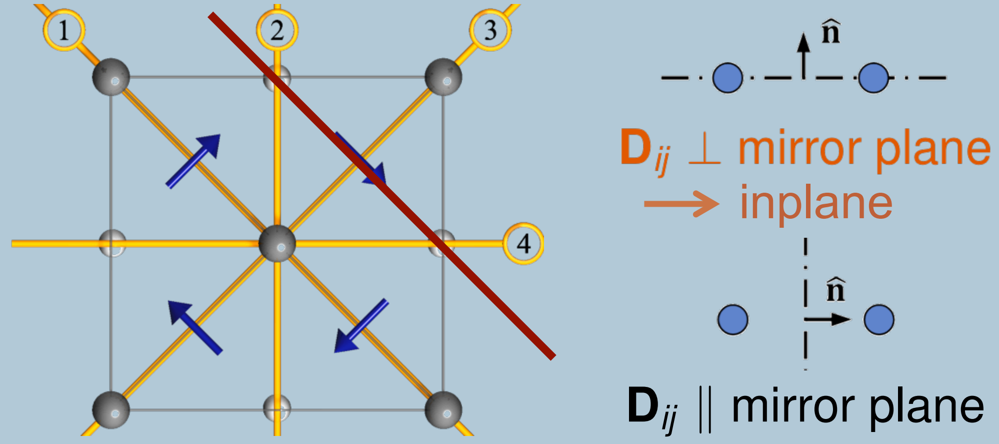
C_{4v} symmetry [e.g. fcc(100)]



atomistic $\mathbf{D}_{01}$: direction fixed

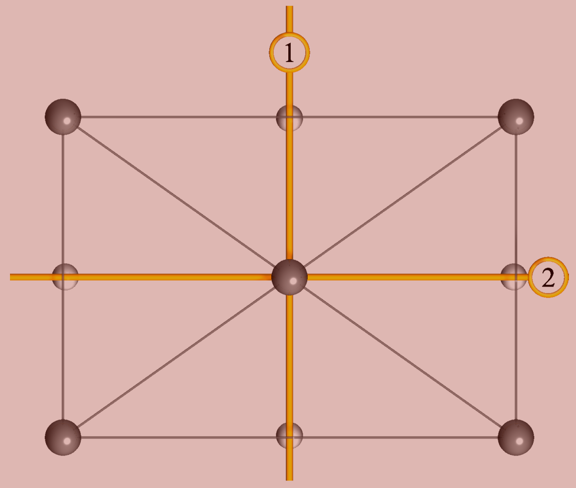
DM vectors in different symmetry classes

C_{4v} symmetry [e.g. fcc(100)]



atomistic $\mathbf{D}_{01}$: direction fixed

C_{2v} symmetry [e.g. bcc(110)]

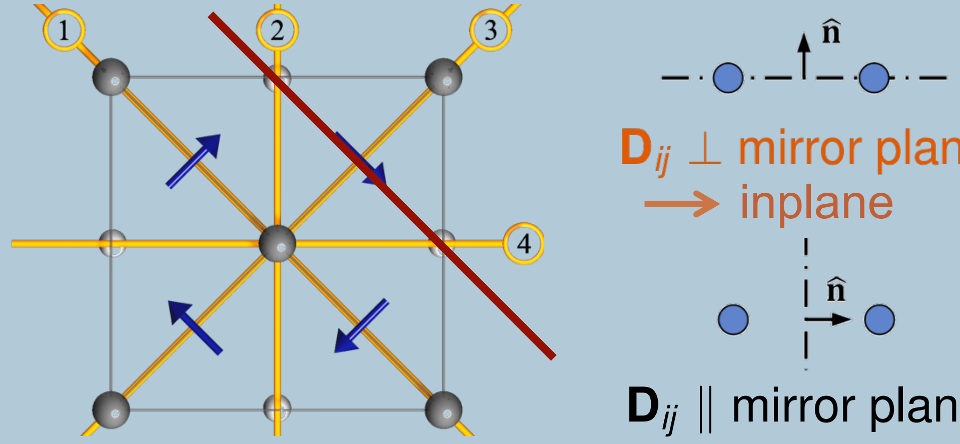


DRIVING THE EXASCALE TRANSITION

JÜLICH Forschungszentrum

DM vectors in different symmetry classes

C_{4v} symmetry [e.g. fcc(100)]

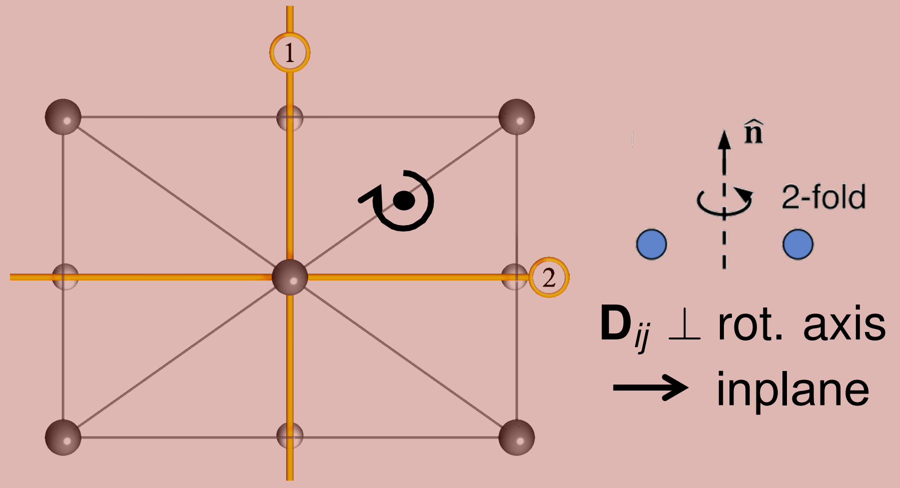


$\mathbf{D}_{ij} \perp$ mirror plane → inplane

$\mathbf{D}_{ij} \parallel$ mirror plane

atomistic $\mathbf{D}_{01}$: direction fixed

C_{2v} symmetry [e.g. bcc(110)]



$\mathbf{D}_{ij} \perp$ rot. axis → inplane

DRIVING THE EXASCALE TRANSITION

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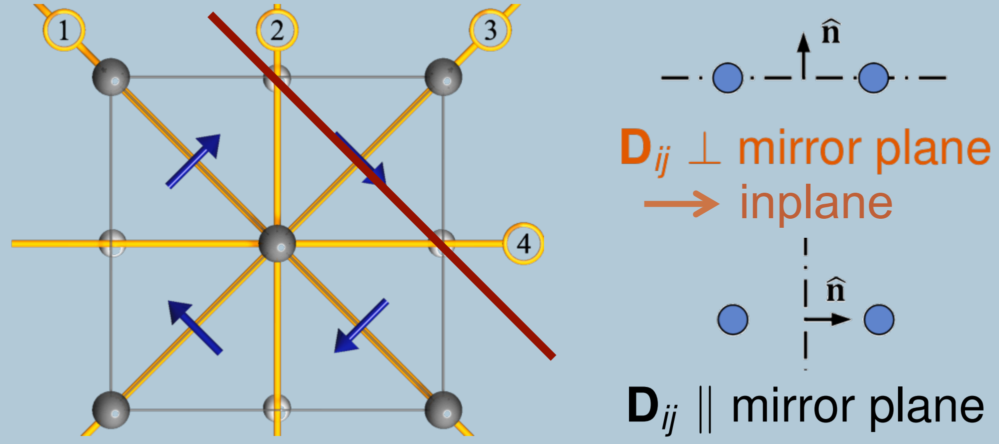

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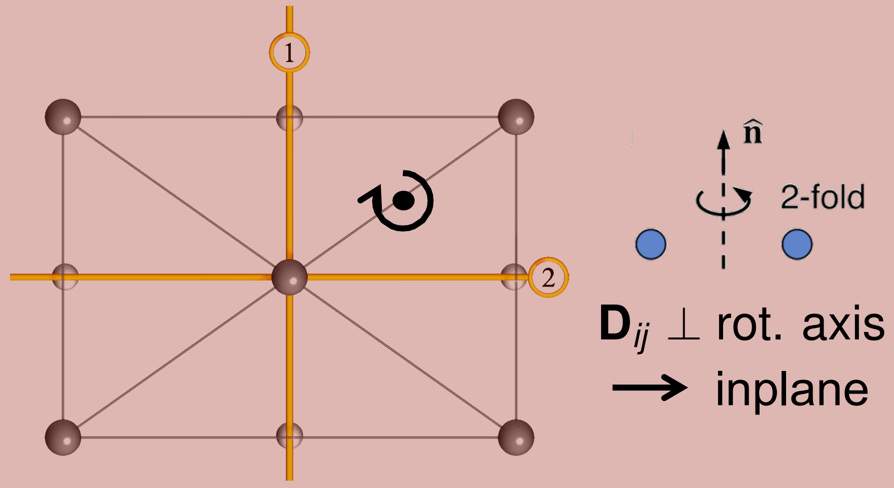
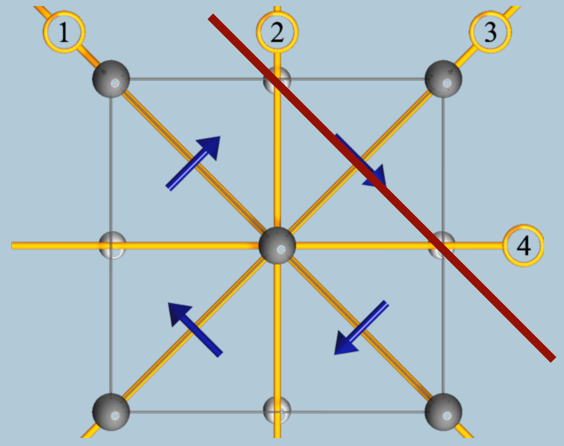


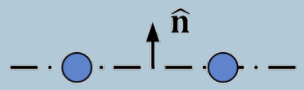
additional mirror planes:

couple D_{ij}'s

DM vectors in different symmetry classes

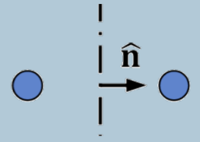
C_{4v} symmetry [e.g. fcc(100)]





$\mathbf{D}_{ij} \perp$ mirror plane

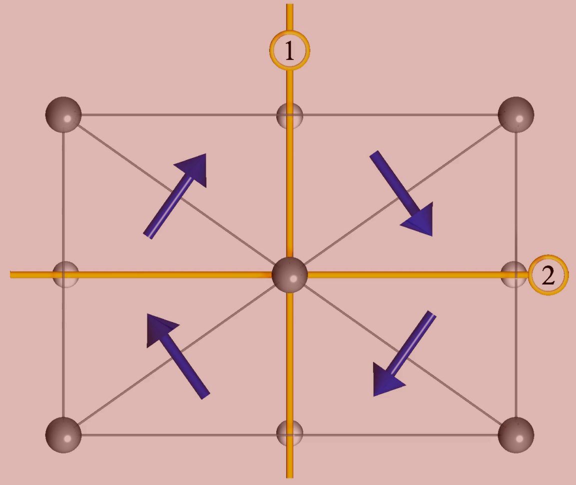
→ inplane

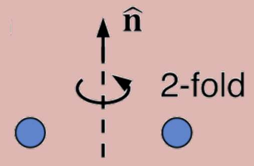


$\mathbf{D}_{ij} \parallel$ mirror plane

atomistic $\mathbf{D}_{01}$: direction fixed

C_{2v} symmetry [e.g. bcc(110)]





$\mathbf{D}_{ij} \perp$ rot. axis

→ inplane

additional mirror planes:

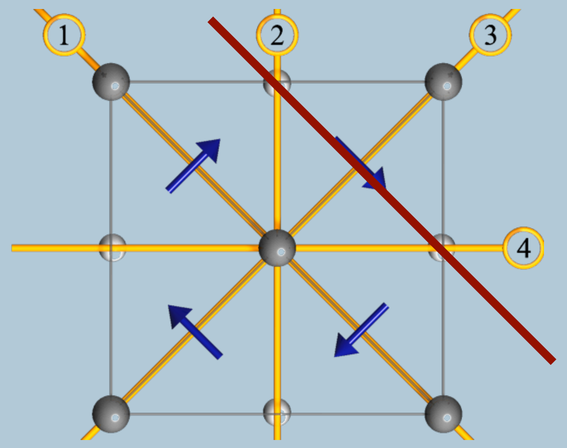
couple D_{ij}'s

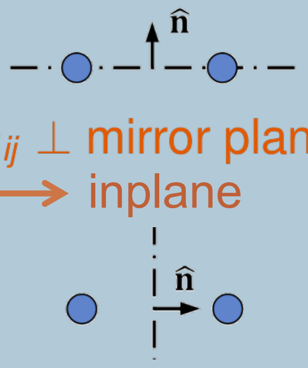
atomistic: any direction $\mathbf{D}_{01} = \begin{pmatrix} D_x \\ D_y \end{pmatrix}$

(electronic structure→DFT)

DM vectors in different symmetry classes

C_{4v} symmetry [e.g. fcc(100)]





$\mathbf{D}_{ij} \perp$ mirror plane → inplane

$\mathbf{D}_{ij} \parallel$ mirror plane

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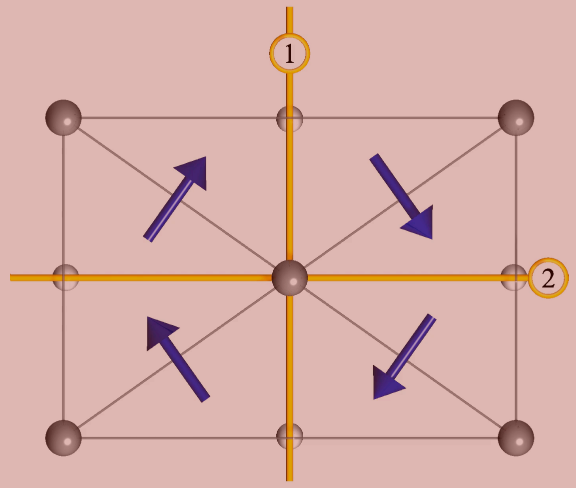

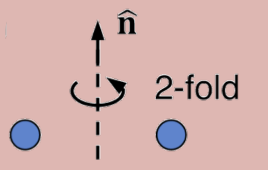

$\mathbf{D}_{ij} \perp$ rot. axis → inplane

additional mirror planes:

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atomistic: any direction $\mathbf{D}_{01} = \begin{pmatrix} D_x \\ D_y \end{pmatrix}$

(electronic structure→DFT)

Micromagnetic equivalent:

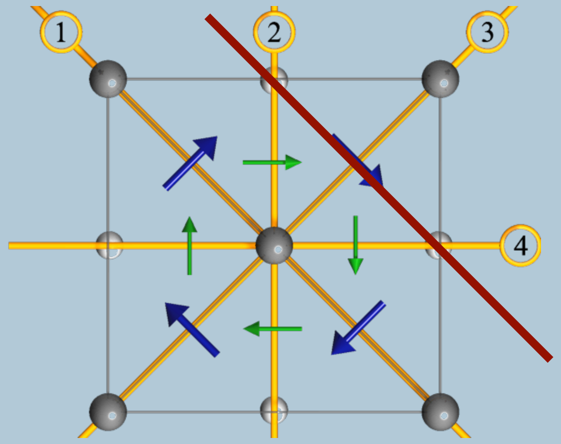
"spiralization" $$\boldsymbol{D} = \frac{1}{A_\Omega} \sum_j \mathbf{D}_{0j} \otimes \mathbf{R}_{0j}$$

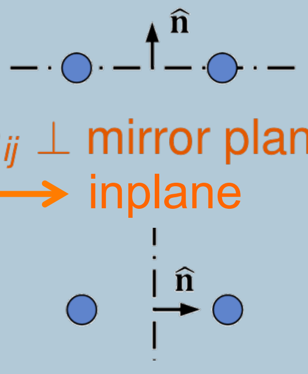
Direct access to preferred rotation axis $\hat{e}_{rot}$ for propagation along $\hat{e}_\rho$:

$$\hat{e}_{rot} \parallel \boldsymbol{D}\, \hat{e}_\rho$$

DM vectors in different symmetry classes

C_{4v} symmetry [e.g. fcc(100)]



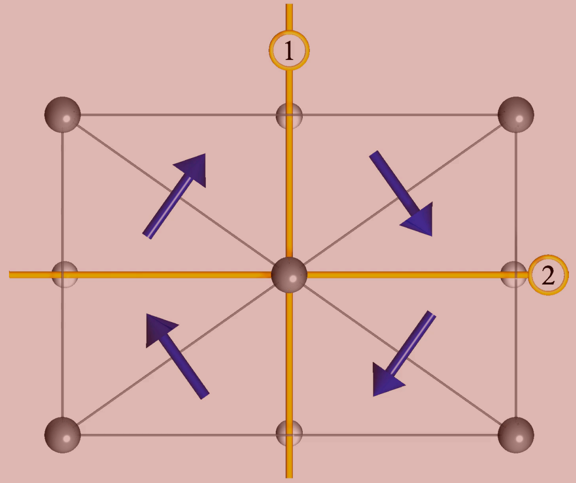


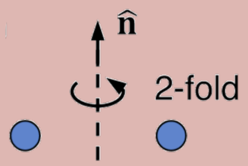
atomistic $\mathbf{D}_{01}$: direction fixed

⇕

micromag. $\mathcal{D} = D \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

C_{2v} symmetry [e.g. bcc(110)]





$\mathbf{D}_{ij} \perp$ rot. axis
→ inplane

additional mirror planes:

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(electronic structure→DFT)

DM vectors in different symmetry classes

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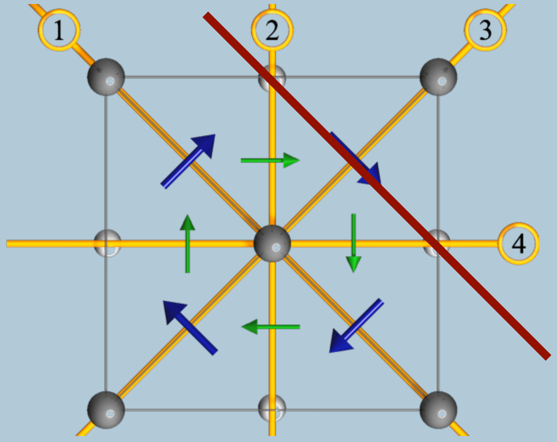
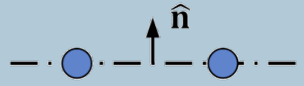
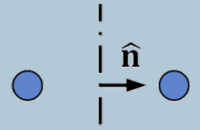




$\mathbf{D}_{ij} \perp$ mirror plane

→ inplane



$\mathbf{D}_{ij} \parallel$ mirror plane

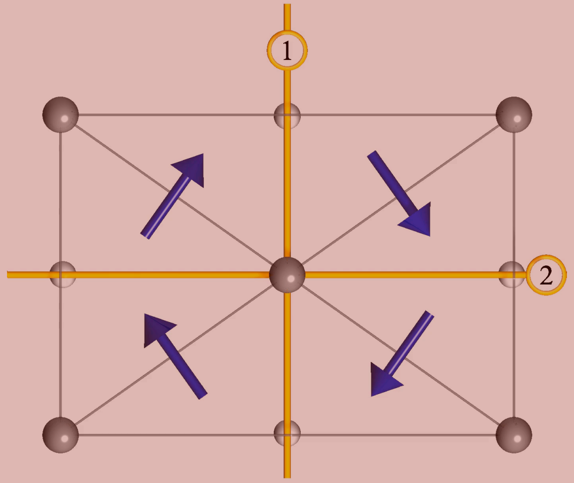
atomistic $\mathbf{D}_{01}$: direction fixed

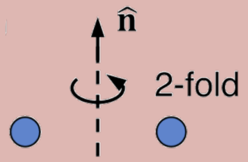
⇕

micromag. $\mathcal{D} = \boxed{D} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

one scalar degree of freedom:
- rotational sense
- rotational speed

C_{2v} symmetry [e.g. bcc(110)]





$\mathbf{D}_{ij} \perp$ rot. axis

→ inplane

additional mirror planes:

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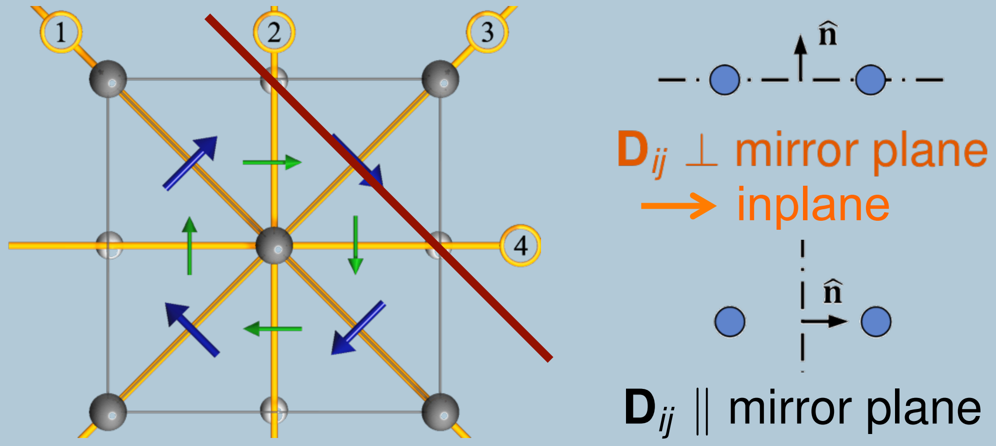
atomistic: any direction $\mathbf{D}_{01} = \begin{pmatrix} D_x \\ D_y \end{pmatrix}$

(electronic structure→DFT)

DM vectors in different symmetry classes

C_{4v} symmetry [e.g. fcc(100)]

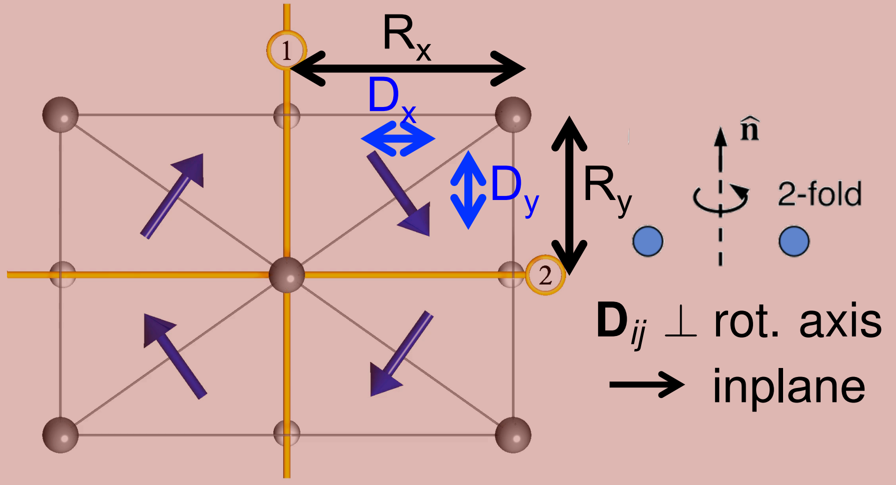


atomistic $\mathbf{D}_{01}$: direction fixed

micromag. $\mathcal{D} = D \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

one scalar degree of freedom:
- rotational sense
- rotational speed

C_{2v} symmetry [e.g. bcc(110)]



additional mirror planes:

couple D_{ij}'s

atomistic: any direction $\mathbf{D}_{01} = \begin{pmatrix} D_x \\ D_y \end{pmatrix}$

(electronic structure→DFT)

micromag. $\mathcal{D} = \begin{pmatrix} 0 & 4D_xR_y \\ 4D_yR_x & 0 \end{pmatrix}$

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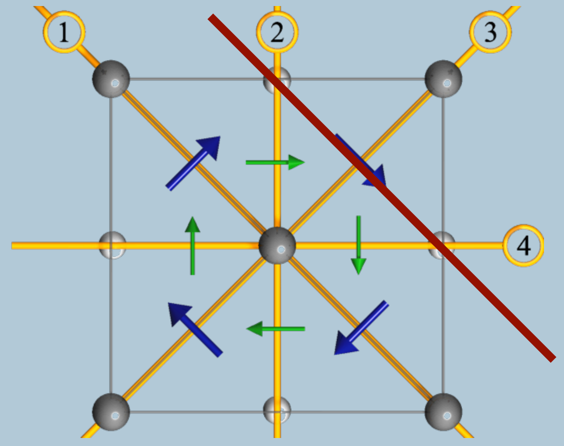
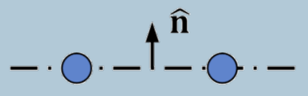
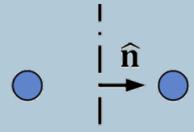




$\mathbf{D}_{ij} \perp$ mirror plane
→ inplane



$\mathbf{D}_{ij} \parallel$ mirror plane

atomistic $\mathbf{D}_{01}$: direction fixed

⇕

micromag. $\mathcal{D} = D \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

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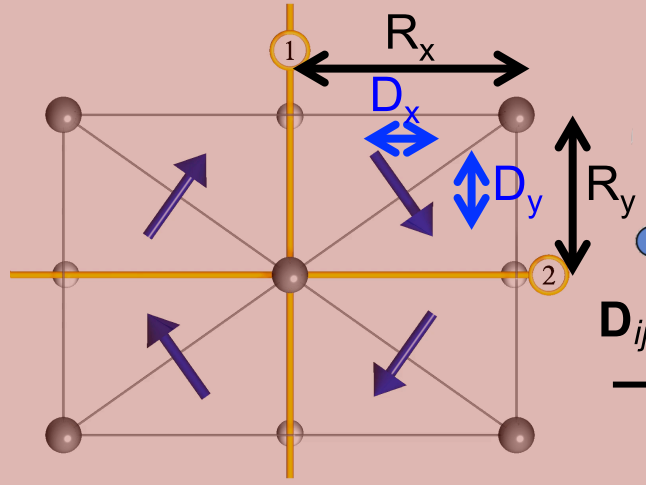
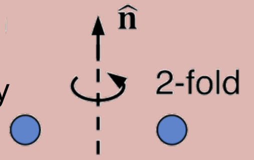
C_{2v} symmetry [e.g. bcc(110)]





$\mathbf{D}_{ij} \perp$ rot. axis
→ inplane

additional mirror planes:

couple D_{ij}'s

atomistic: any direction $\mathbf{D}_{01} = \begin{pmatrix} D_x \\ D_y \end{pmatrix}$
(electronic structure→DFT)

⇕

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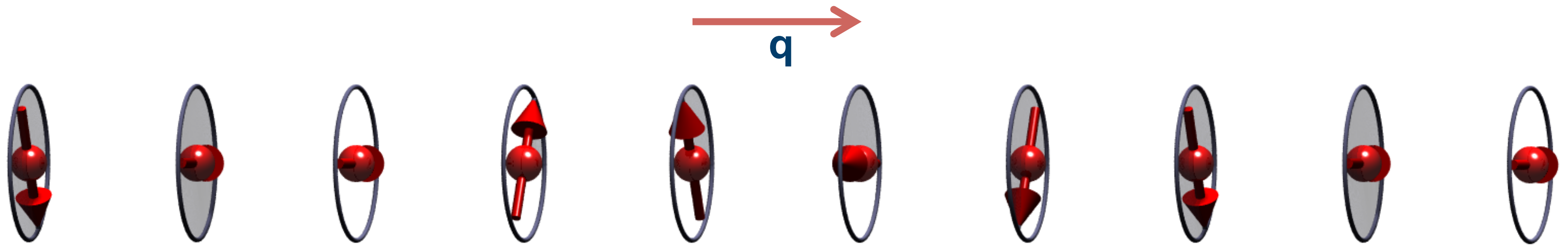
2 degrees of freedom

Calculation of DM interaction from DFT



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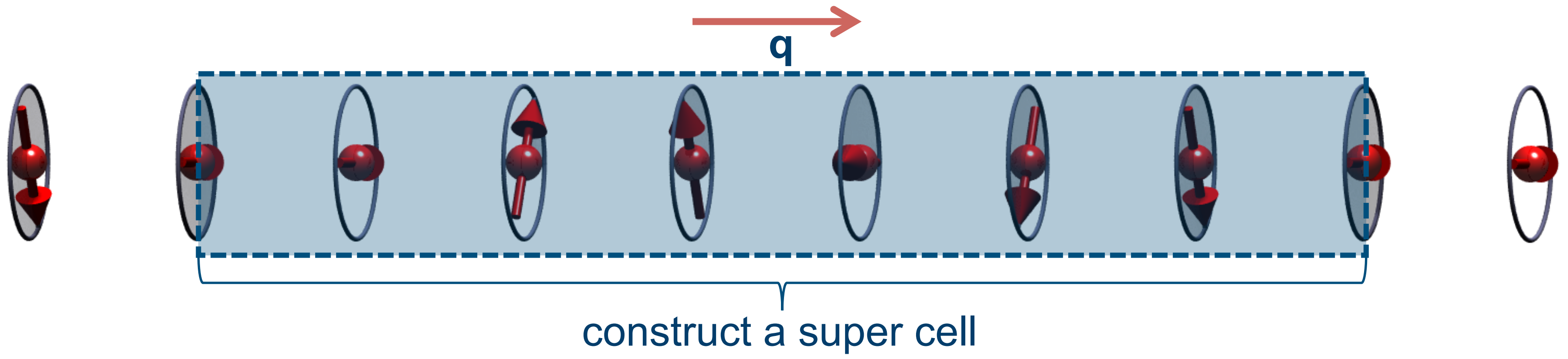

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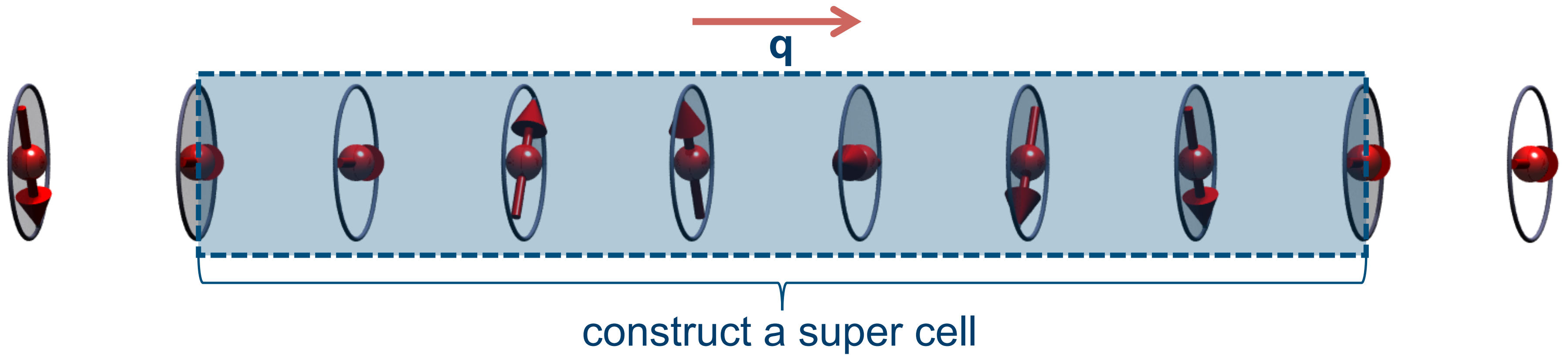
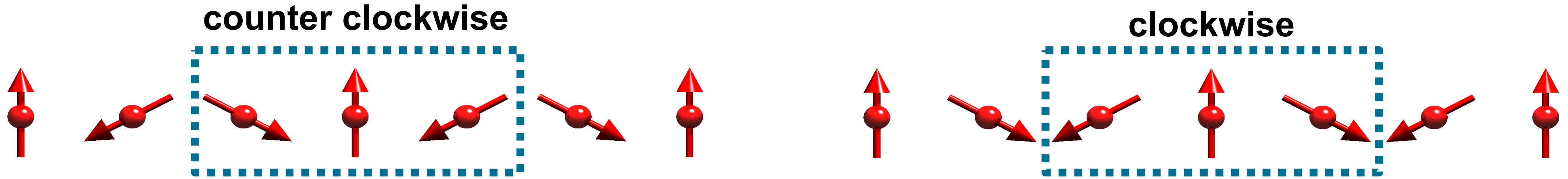
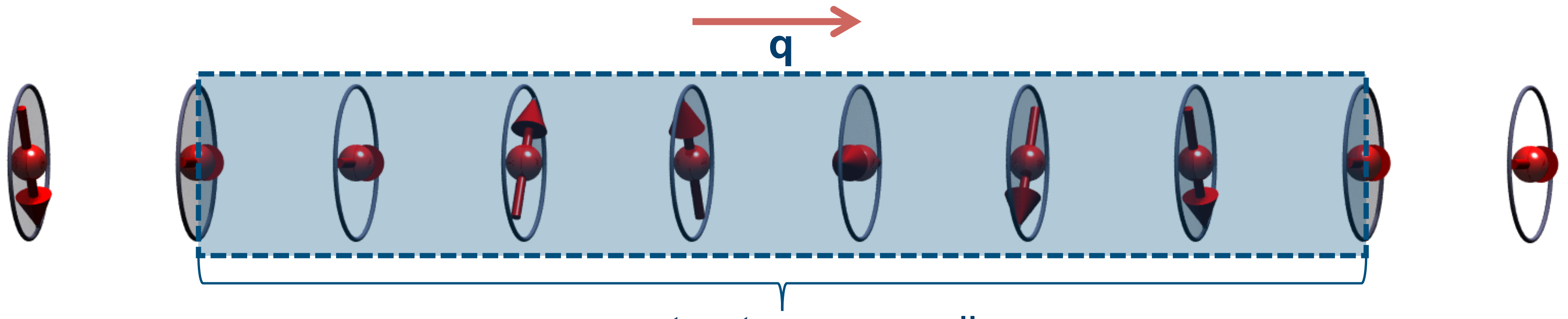


Calculate total energies (including SOC) for non-collinear structures with opposite rotational senses



MH *et al.*, PRB **92** , 020401(R) (2015)
H. Yang *et al.*, PRL **115**, 267210 (2015)

Calculation of DM interaction from DFT



Calculate total energies (including SOC) for non-collinear structures with opposite rotational senses

E_{ccw} E_{cw}

$$D \propto E_{soc} = \frac{1}{2}\left(E_{ccw} - E_{cw}\right)$$

MH *et al.*, PRB **92** , 020401(R) (2015)
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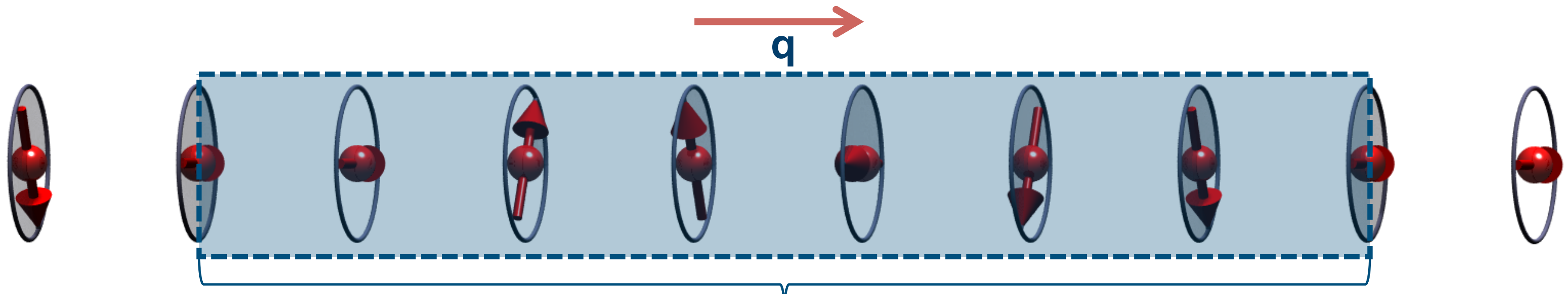

construct a super cell

Pros

- only few fast calculations
- easy to interpret

Calculate total energies (including SOC) for non-collinear structures with opposite rotational senses

counter clockwise | **clockwise**

E_{ccw} | E_{cw}

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MH *et al.*, PRB **92** , 020401(R) (2015)
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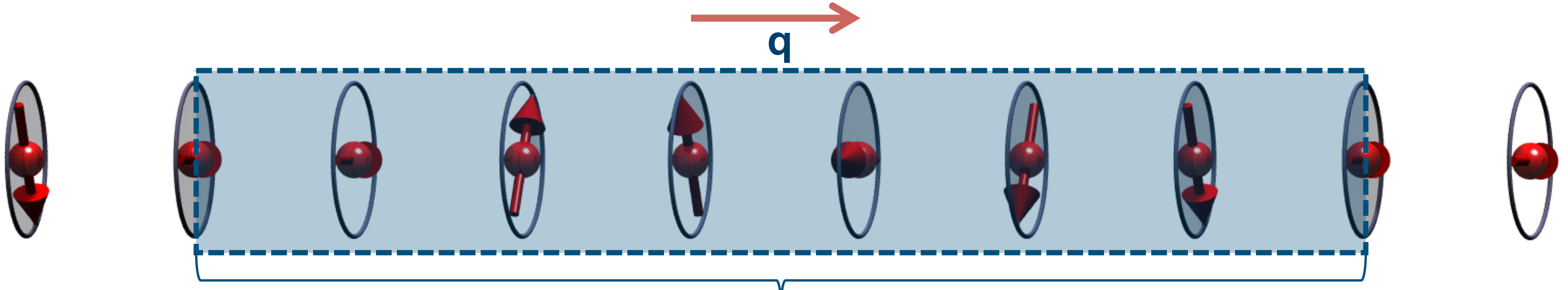


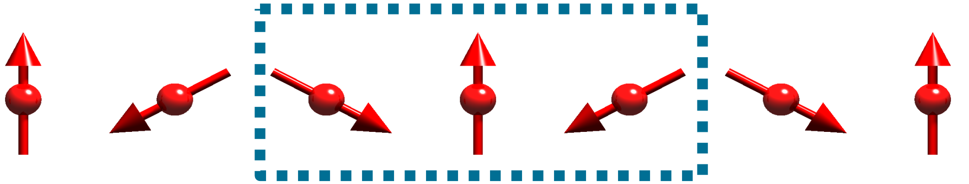
construct a super cell

Pros
- only few fast calculations
- easy to interpret

Cons
- q-dependence!
- large super cell might be needed

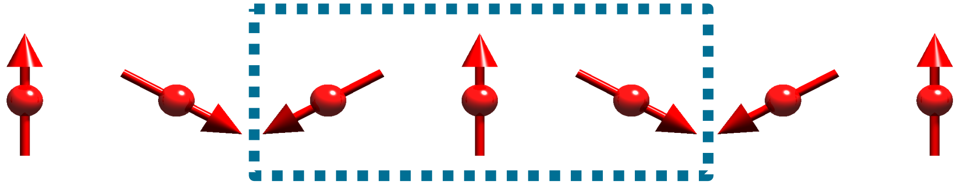
Calculate total energies (including SOC) for non-collinear structures with opposite rotational senses

counter clockwise



E_{ccw}

clockwise



E_{cw}

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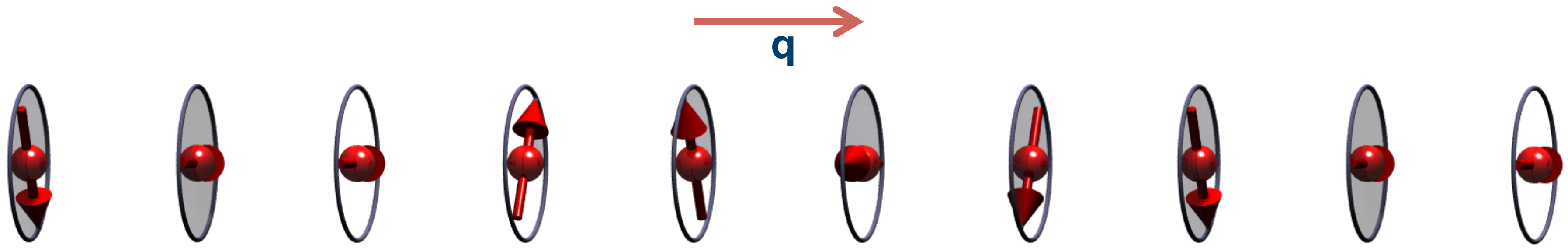

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Fleur

juDFT

Step 1: Absence of SOC: Generalized Bloch theorem

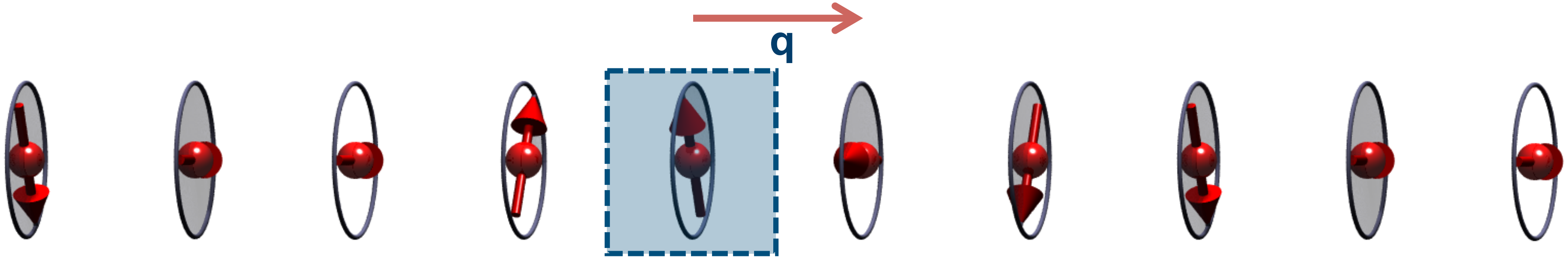
$$\Psi_{\mathbf{k}\nu} = \begin{pmatrix} e^{i(\mathbf{k}-\mathbf{q}/2)\cdot\mathbf{r}} & u^{\uparrow}_{\mathbf{k}\nu}(\mathbf{r}) \\ e^{i(\mathbf{k}+\mathbf{q}/2)\cdot\mathbf{r}} & u^{\downarrow}_{\mathbf{k}\nu}(\mathbf{r}) \end{pmatrix}$$

periodic in chemical lattice

- very efficient
- arbitrary **q**

L. M. Sandratskii, J. Phys.: Condens. Matter **3**, 8565 (1991)

Calculation of DM interaction from DFT



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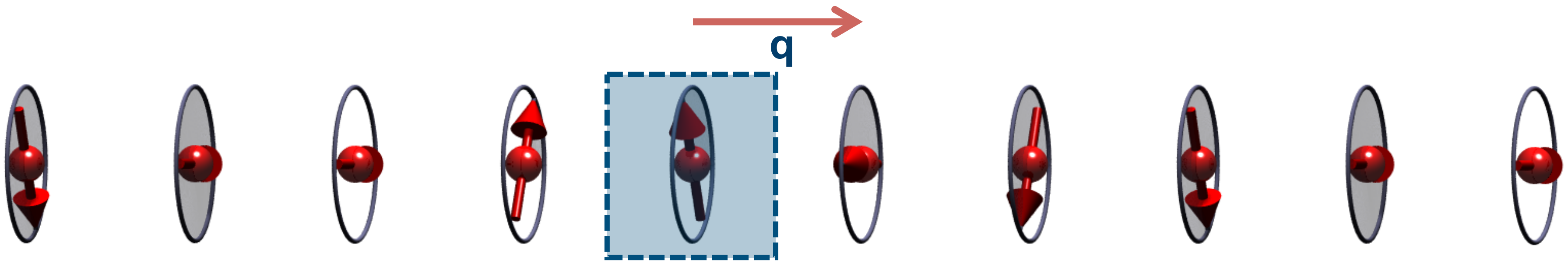

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periodic in chemical lattice

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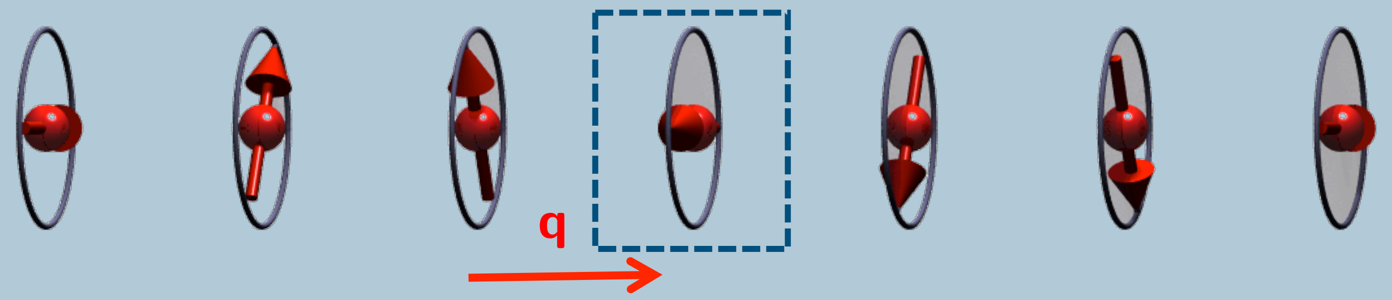
L. M. Sandratskii, J. Phys.: Condens. Matter **3**, 8565 (1991)

Step 2: Add SOC in 1st order perturbation theory

$$\delta\varepsilon_{\mathbf{k}\nu} = \langle u^{\uparrow}_{\mathbf{k}\nu}(\mathbf{r})|\mathcal{H}_{\mathrm{SOC}}|u^{\uparrow}_{\mathbf{k}\nu}(\mathbf{r})\rangle + \langle u^{\downarrow}_{\mathbf{k}\nu}(\mathbf{r})|\mathcal{H}_{\mathrm{SOC}}|u^{\downarrow}_{\mathbf{k}\nu}(\mathbf{r})\rangle$$

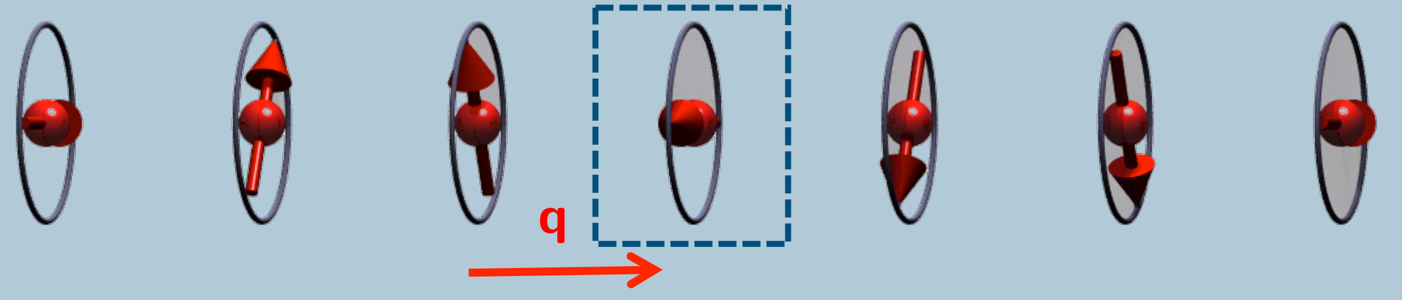
M. Heide, G. Bihlmayer and S. Blügel, Physica B **404,** 2678 (2009)

Calculation of DM interaction from DFT



DFT calculations $E_{\text{tot}}^{\text{DFT}}(\mathbf{q}, \hat{e}_{\text{rot}}) = E_{\text{noSOC}}^{\text{DFT}}(\mathbf{q})$

Calculation of DM interaction from DFT



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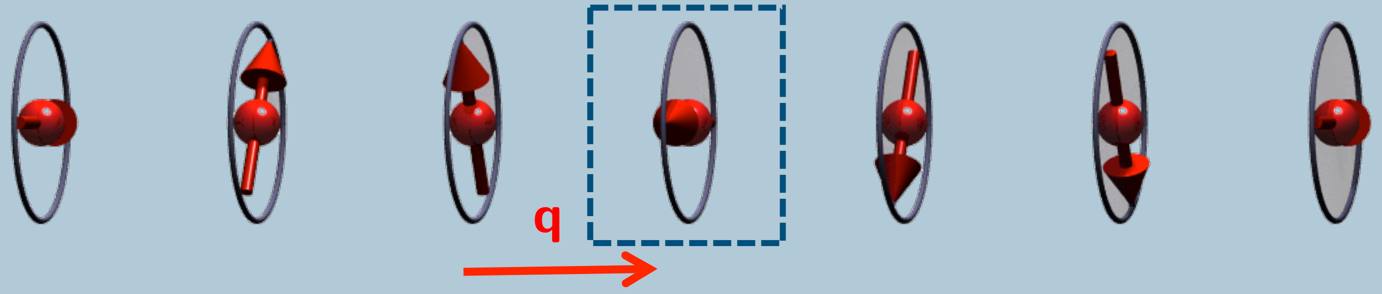

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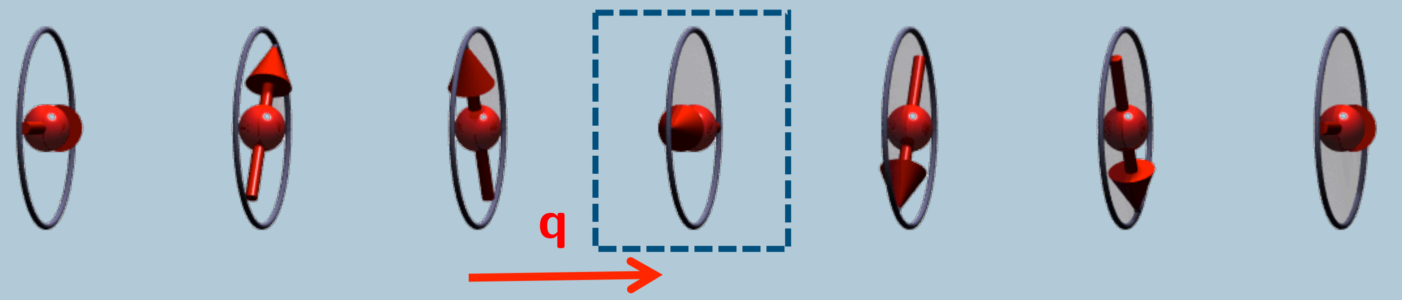

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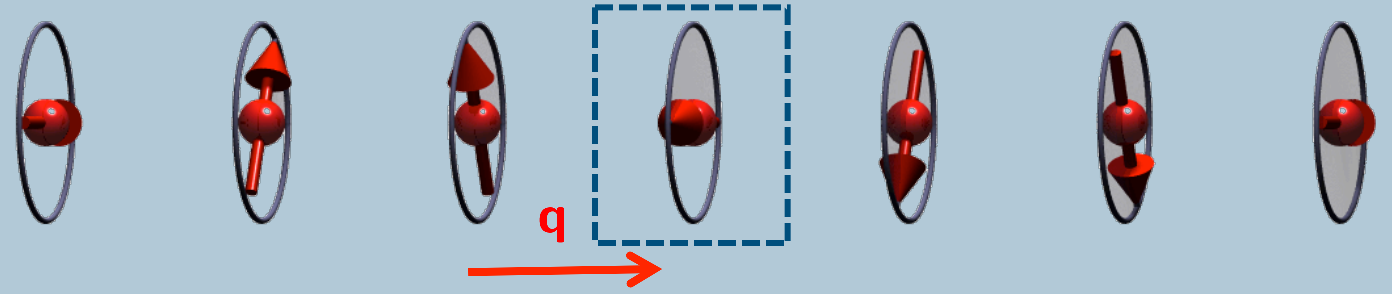
Micromagnetic model $\approx \delta\mathbf{q} \cdot \mathcal{A}|_{\mathbf{q}_0} \cdot \delta\mathbf{q}$ $\xrightarrow{\text{mapping}}$ $\mathcal{A}$

Calculation of DM interaction from DFT



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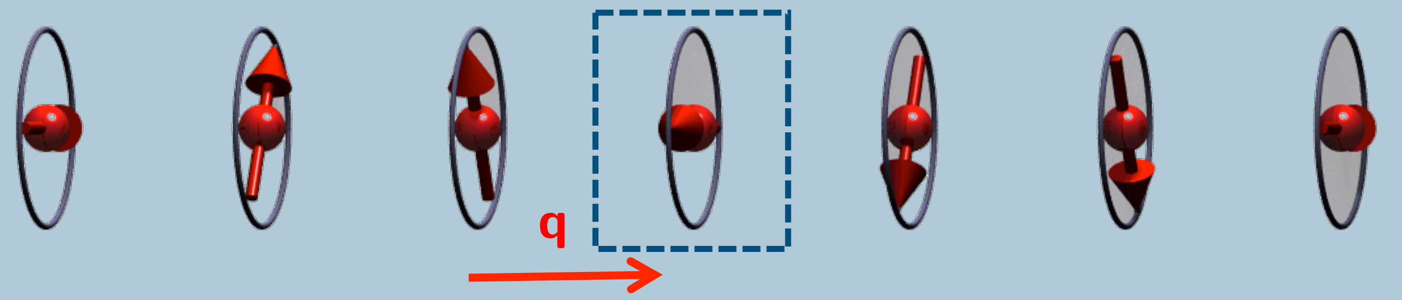

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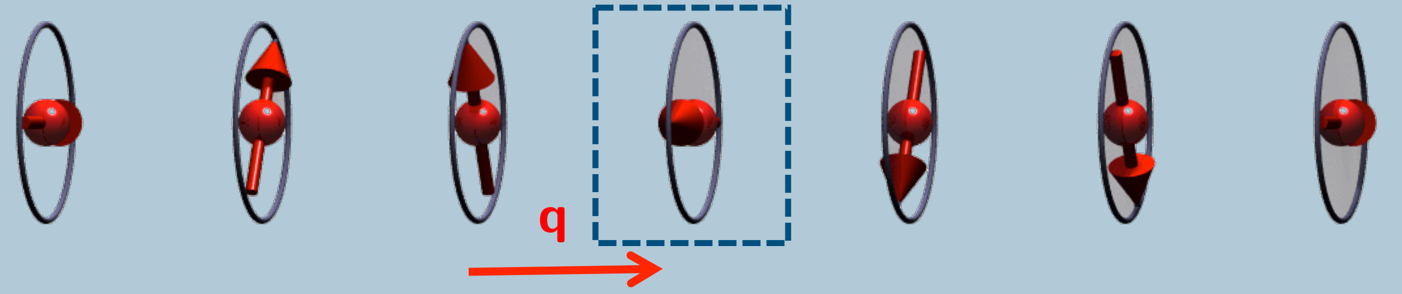
Calculation of DM interaction from DFT



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only component **parallel** to rotation axis

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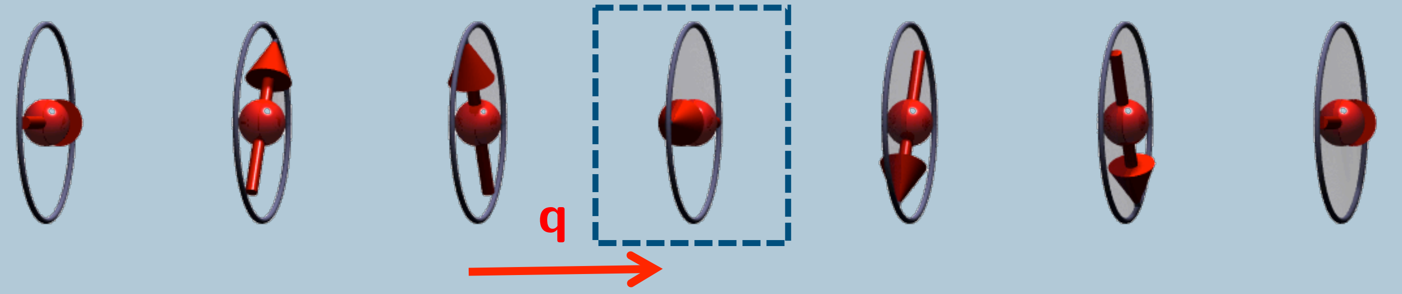

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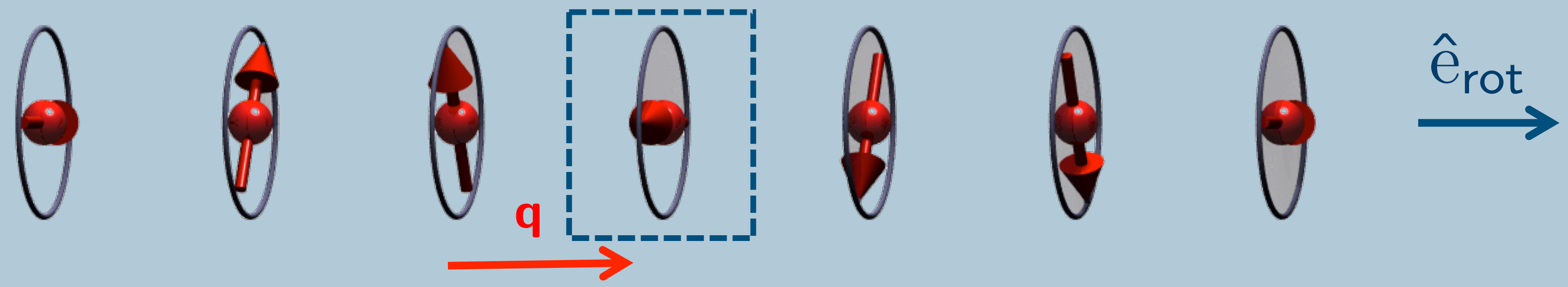
only one **row** of the tensor

DRIVING THE EXASCALE TRANSITION

JÜLICH Forschungszentrum

Calculation of DM interaction from DFT



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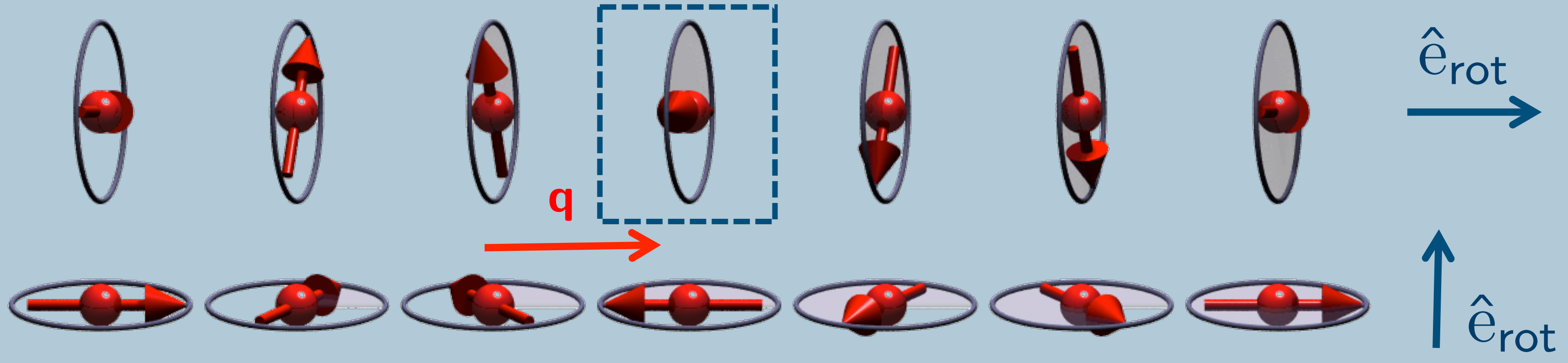

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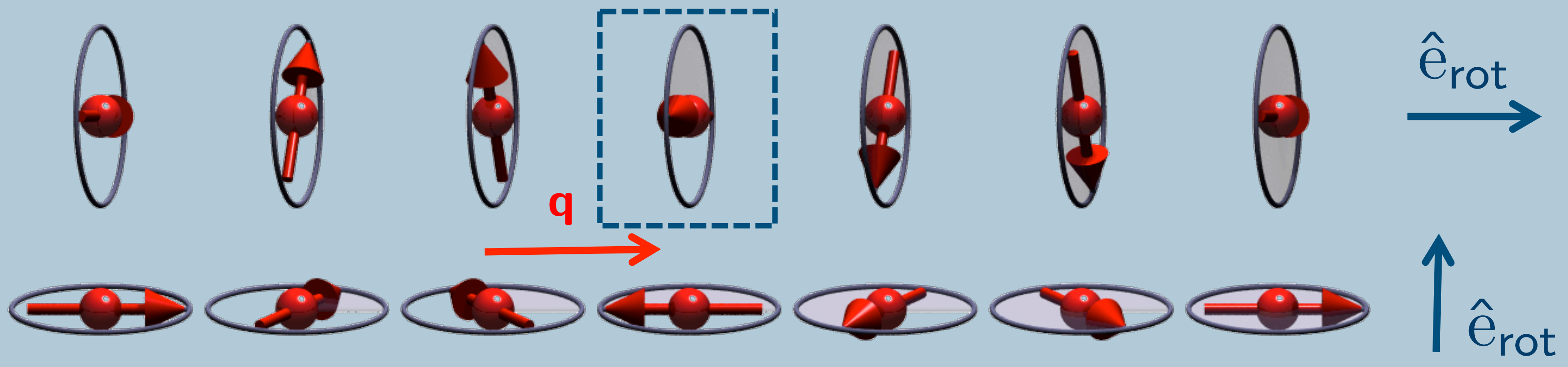

at least **three** sets of calculations needed to extract full DMI information from DFT

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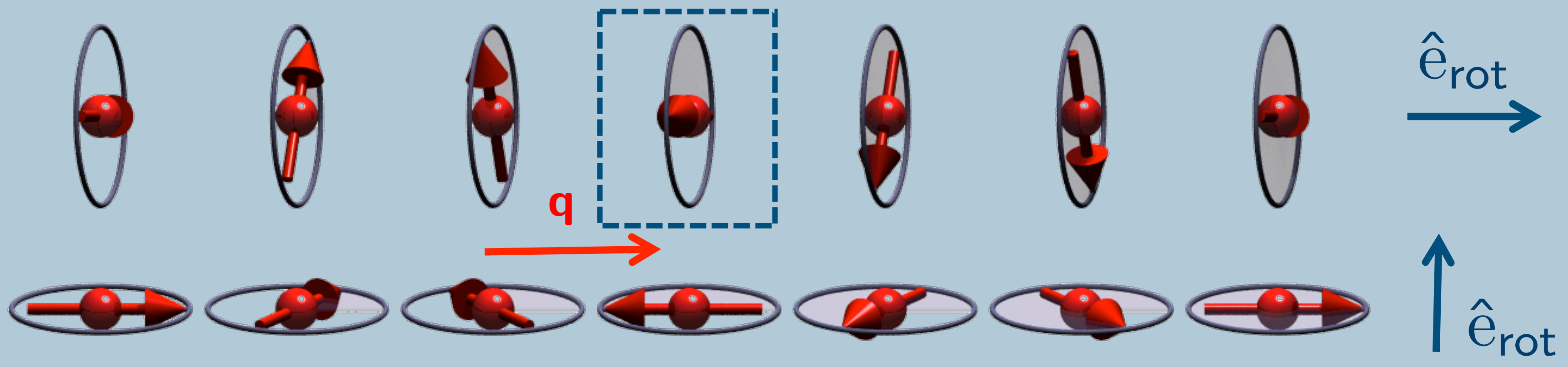

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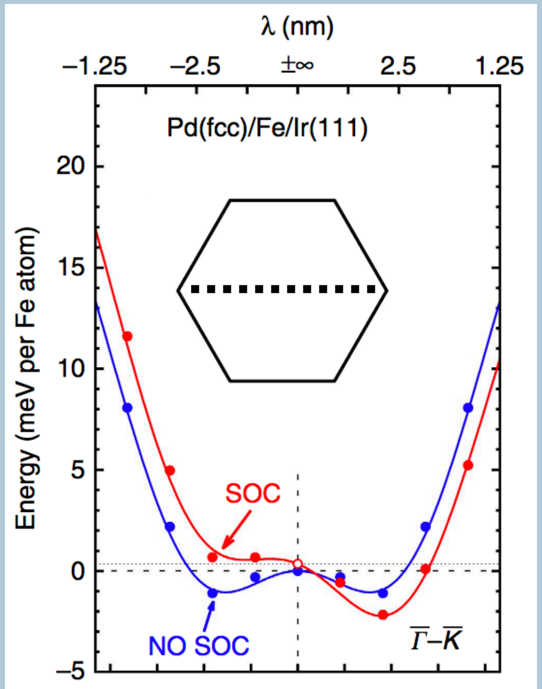
How does such a mapping look like?

Calculation of DM interaction from DFT

extraction of atomistic parameters via fit

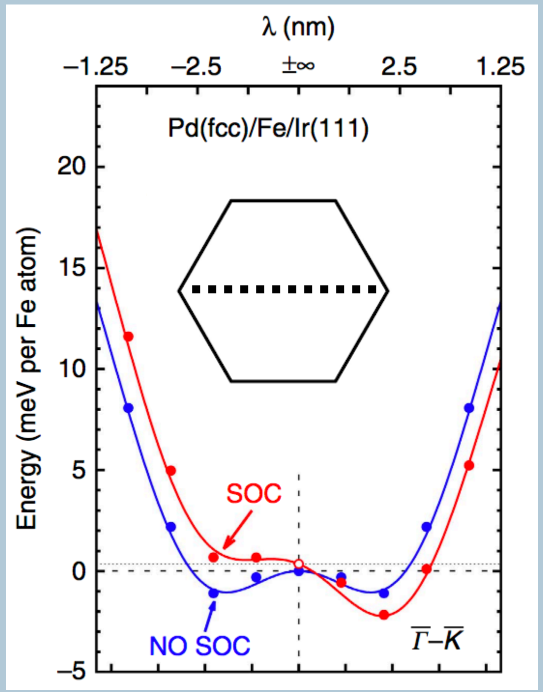


B. Dupé, **MH** *et al.*, Nature Commun. **5**, 4030 (2014)

- calculate spin-spirals along **particular** (high-sym.) **directions**
- **fit** energies to **analytical** formula (ie. first N neighbors)

Calculation of DM interaction from DFT

extraction of atomistic parameters via fit



B. Dupé, **MH** *et al.*, Nature Commun. **5**, 4030 (2014)

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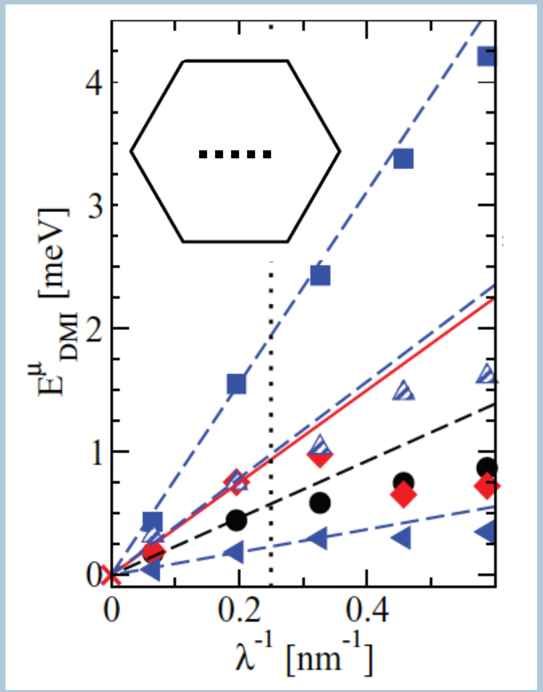
extraction of micromagnetic parameters

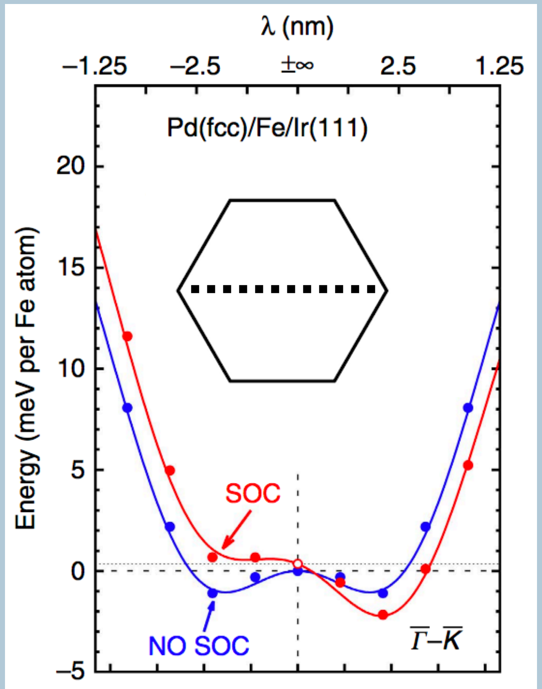


B. Zimmermann *et al.*, PRB **90**, 115427 (2014)

- **linear fit** close to collinear state → small q-vectors
- **layer resolved** information about contribution to DMI available

Calculation of DM interaction from DFT

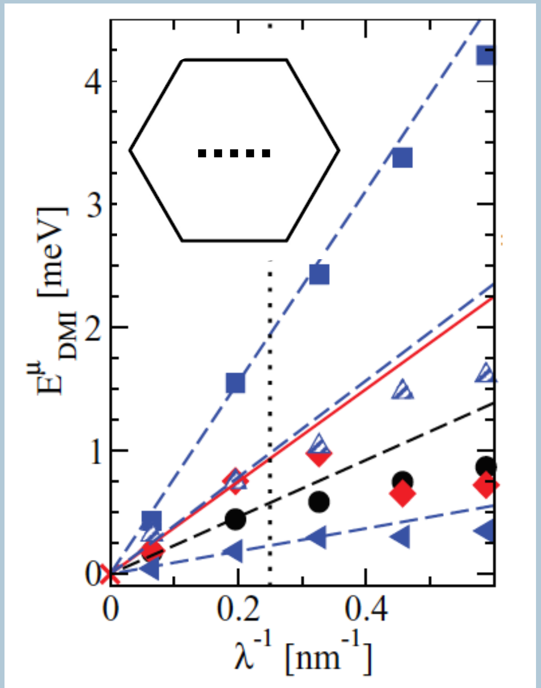
extraction of atomistic parameters via fit



B. Dupé, **MH** *et al.*, Nature Commun. **5**, 4030 (2014)

- calculate spin-spirals along **particular** (high-sym.) **directions**
- **fit** energies to **analytical** formula (ie. first N neighbors)

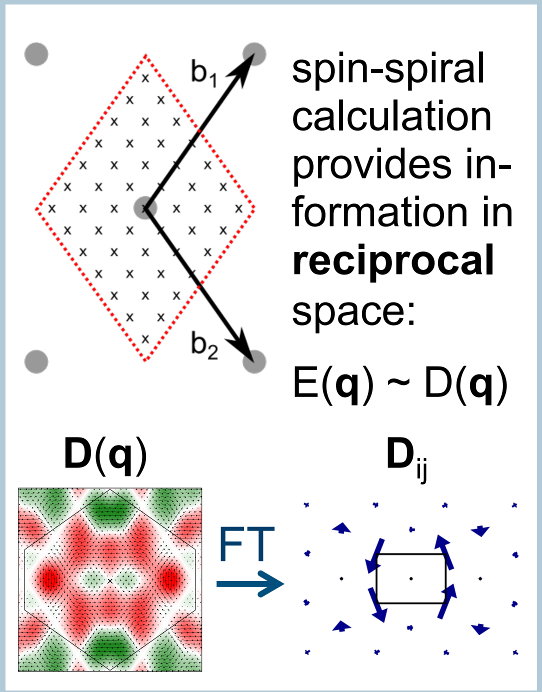
extraction of micromagnetic parameters



B. Zimmermann *et al.*, PRB **90**, 115427 (2014)

- **linear fit** close to collinear state → small q-vectors
- **layer resolved** information about contribution to DMI available

extraction of atomistic parameters via Fourier transform



MH *et al.*, Nature Commun. **8**, 308 (2017)

- calculate spin-spirals on discrete **mesh** in **full Brillouin zone**
- obtain $\mathbf{D}_{ij}$ from **D**(**q**) via Fourier transform

DRIVING THE EXASCALE TRANSITION

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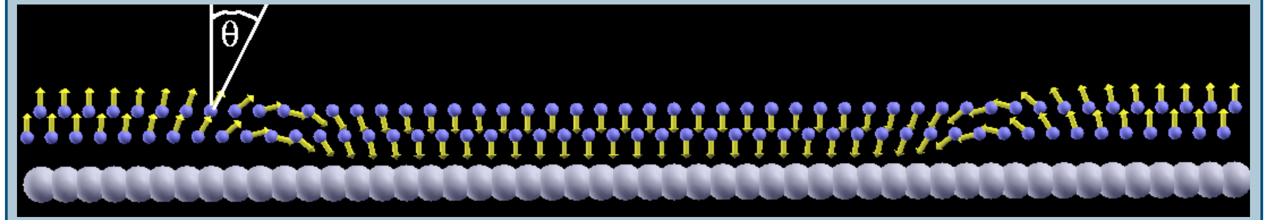
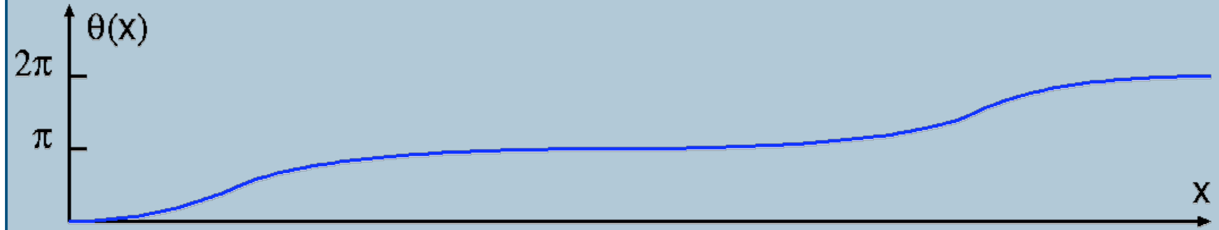
Skyrmionic magnetic textures

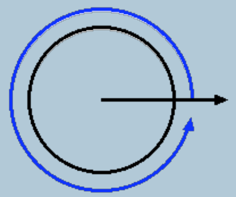
Topological charges

1D winding number

$$S = \frac{1}{2\pi}\int \frac{\partial\theta(x)}{\partial x}\,dx \;= 1$$







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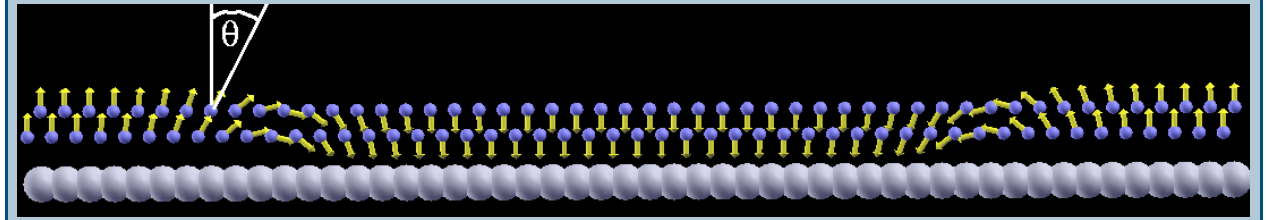
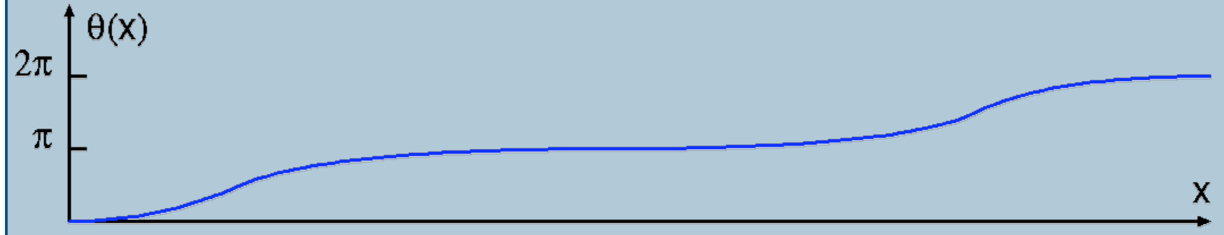
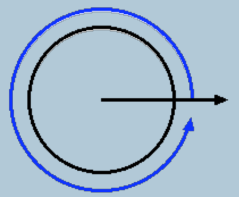
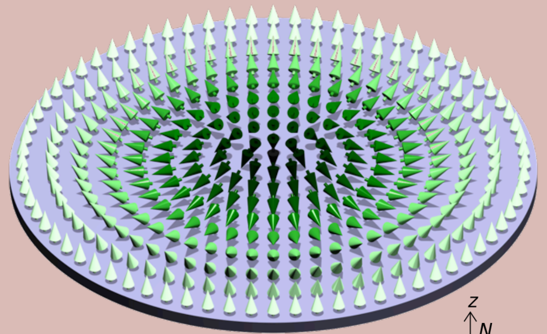






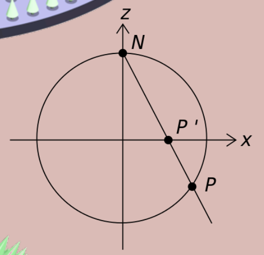
2D "winding number": topological charge

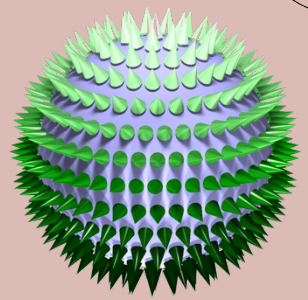
$$Q = \frac{1}{4\pi}\int \mathbf{m}\cdot(\partial_x\mathbf{m}\times\partial_y\mathbf{m})\,\mathrm{d}x\mathrm{d}y$$



"Skyrmion"

stereographic projection

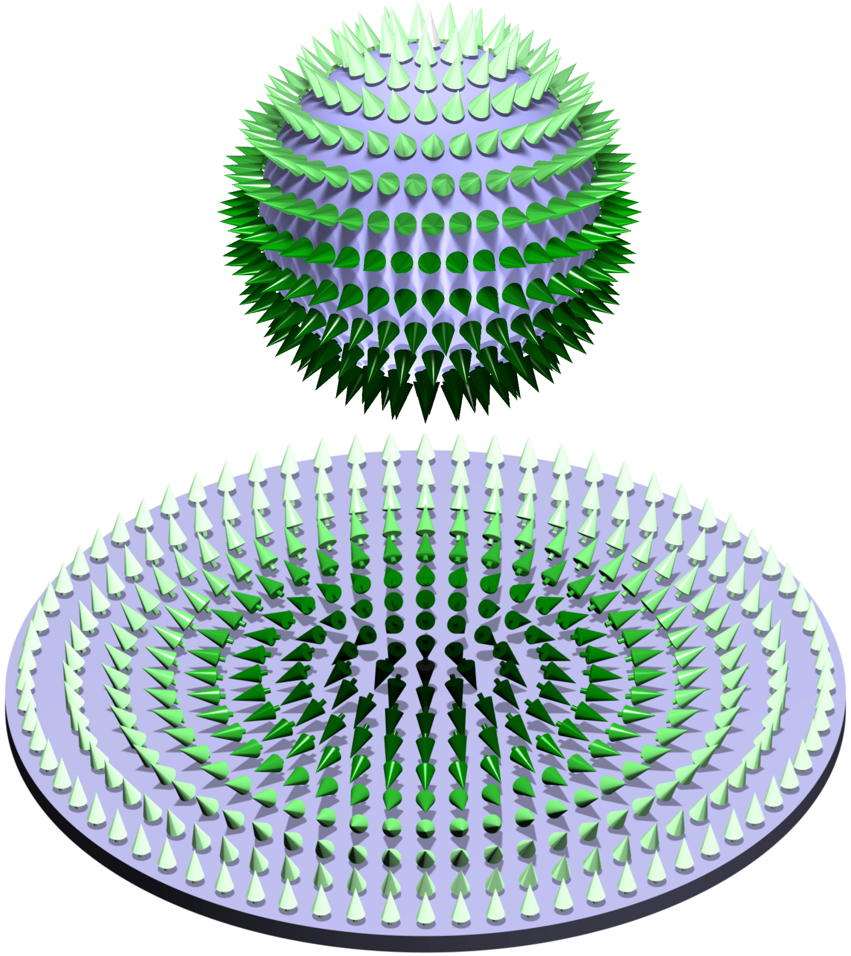




each orientation is obtained at least once in the structure

Skyrmionic structures

Néel-type (“Hedgehog”) Skyrmion



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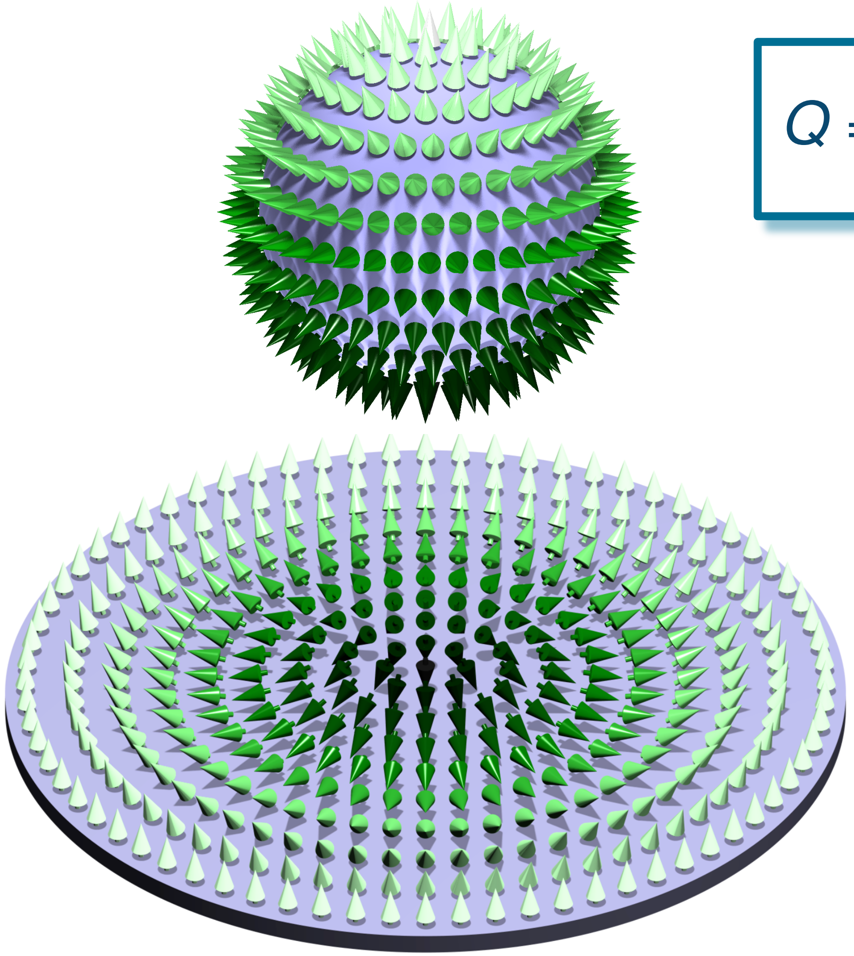

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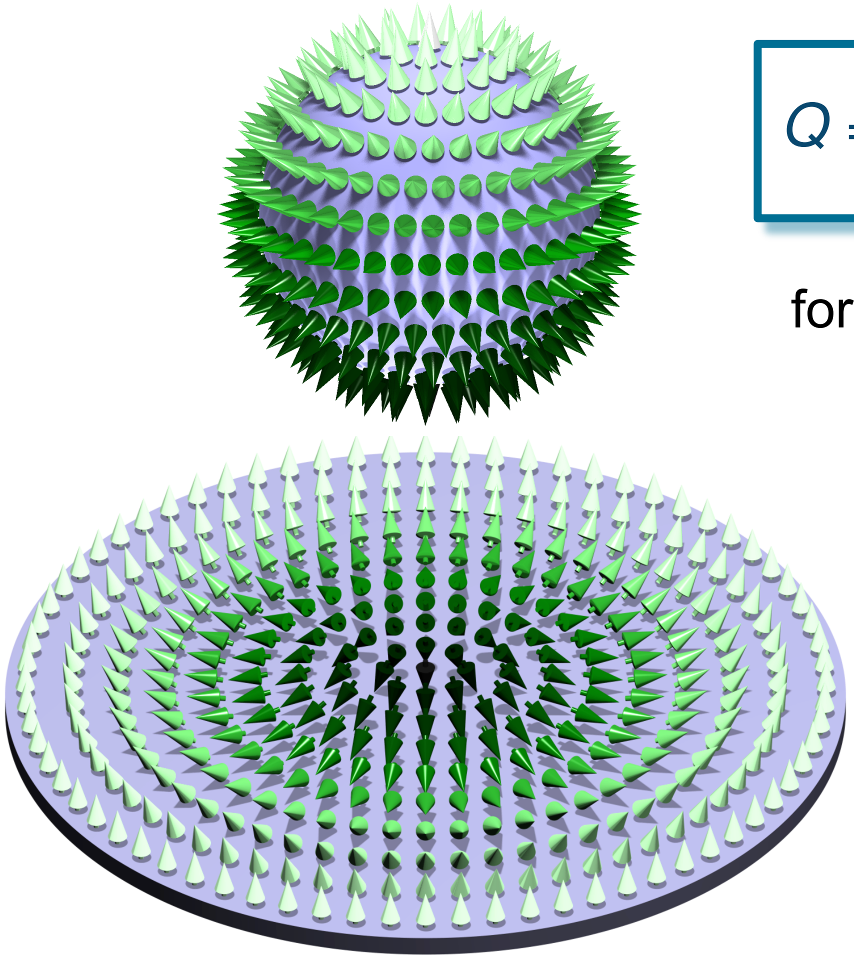

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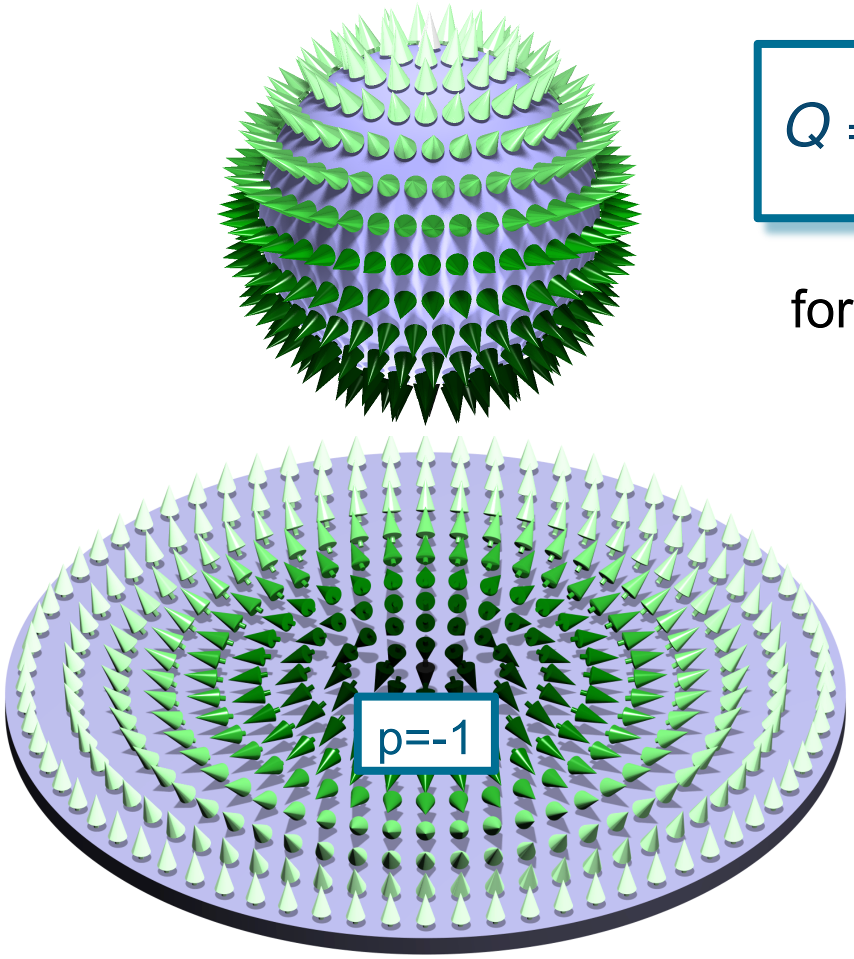

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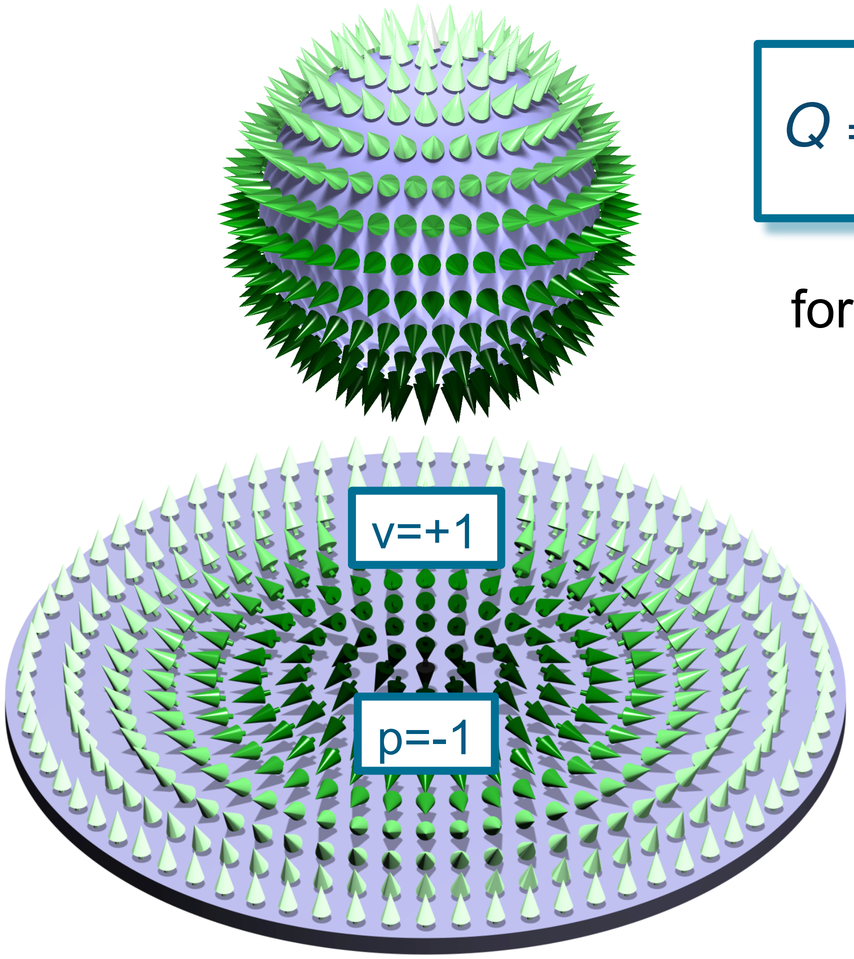

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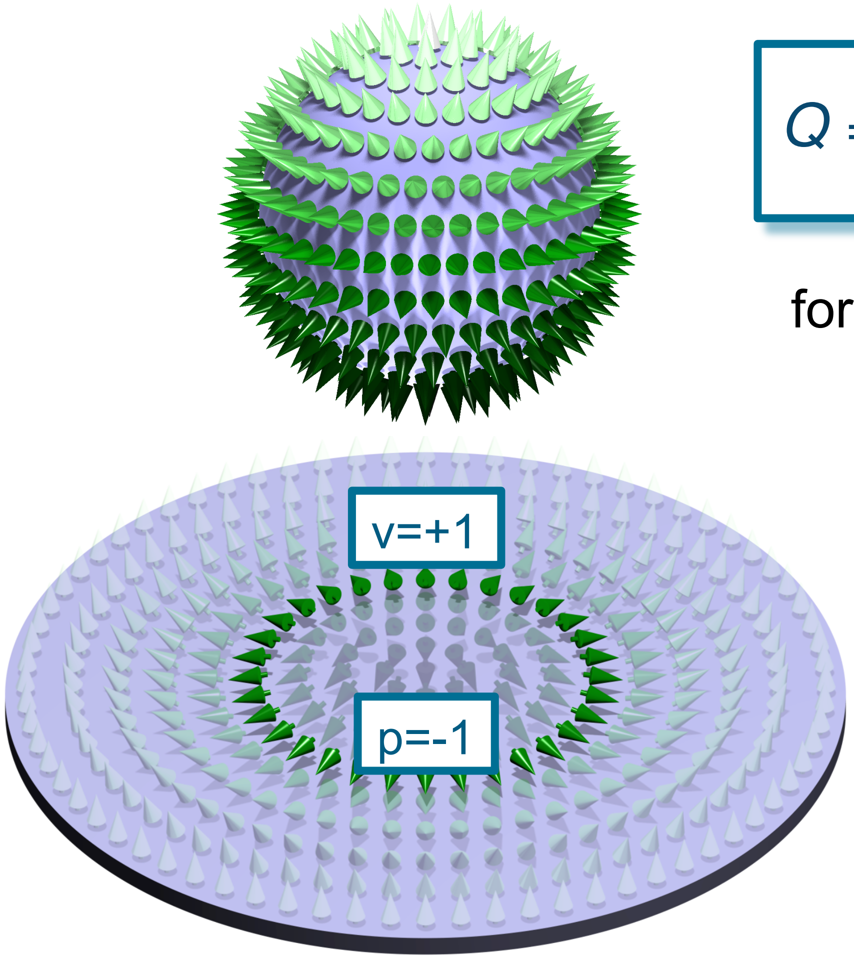

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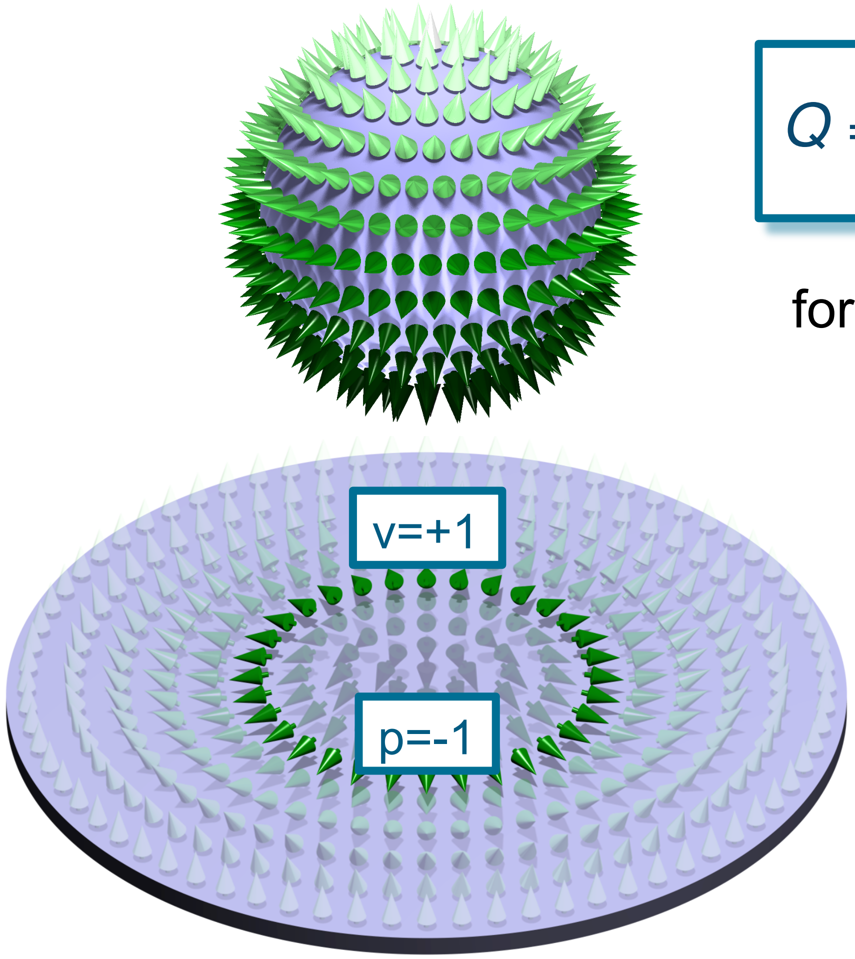

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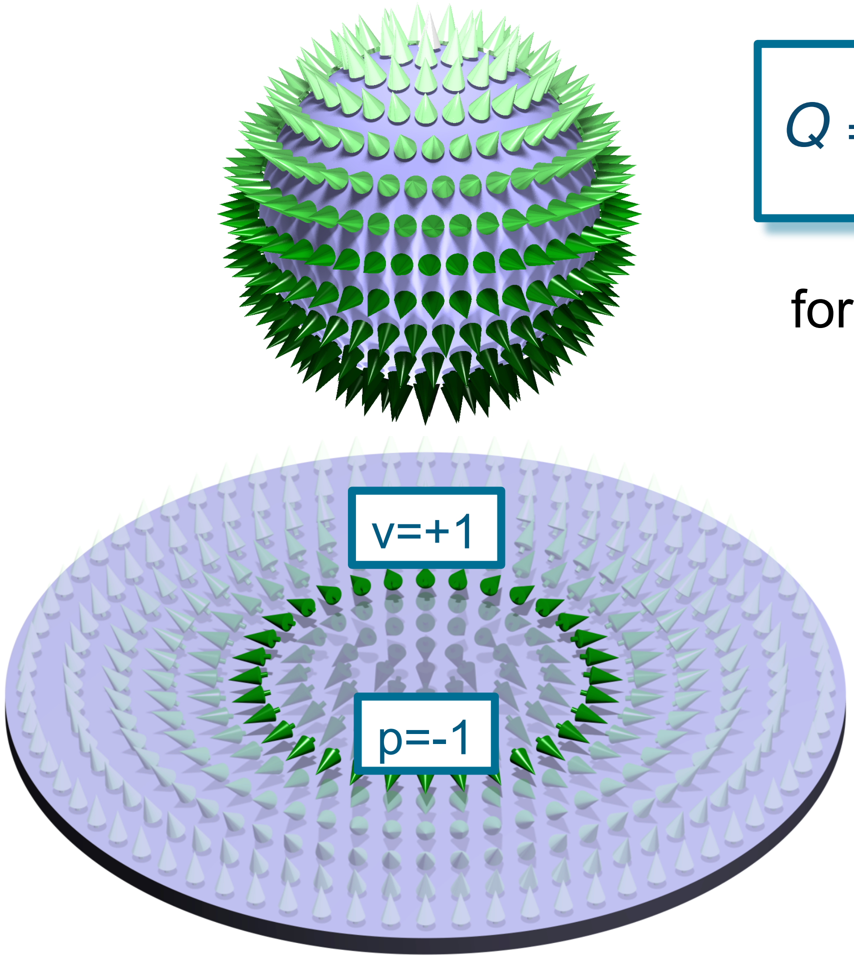

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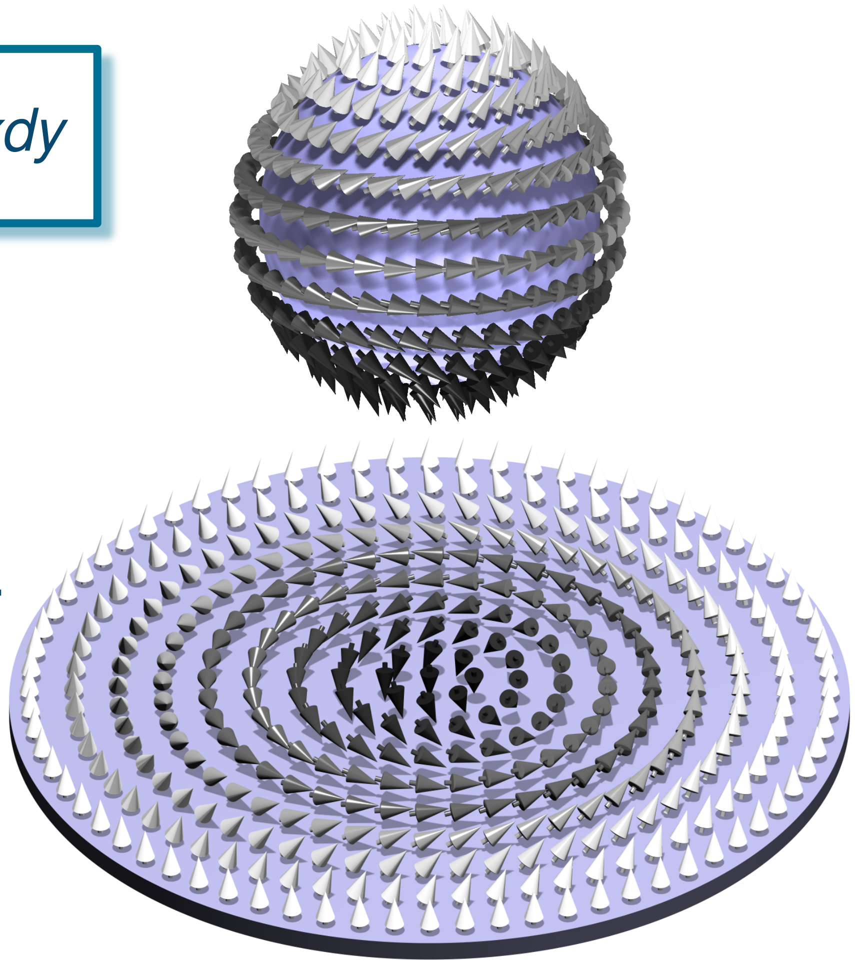

Skyrmionic structures

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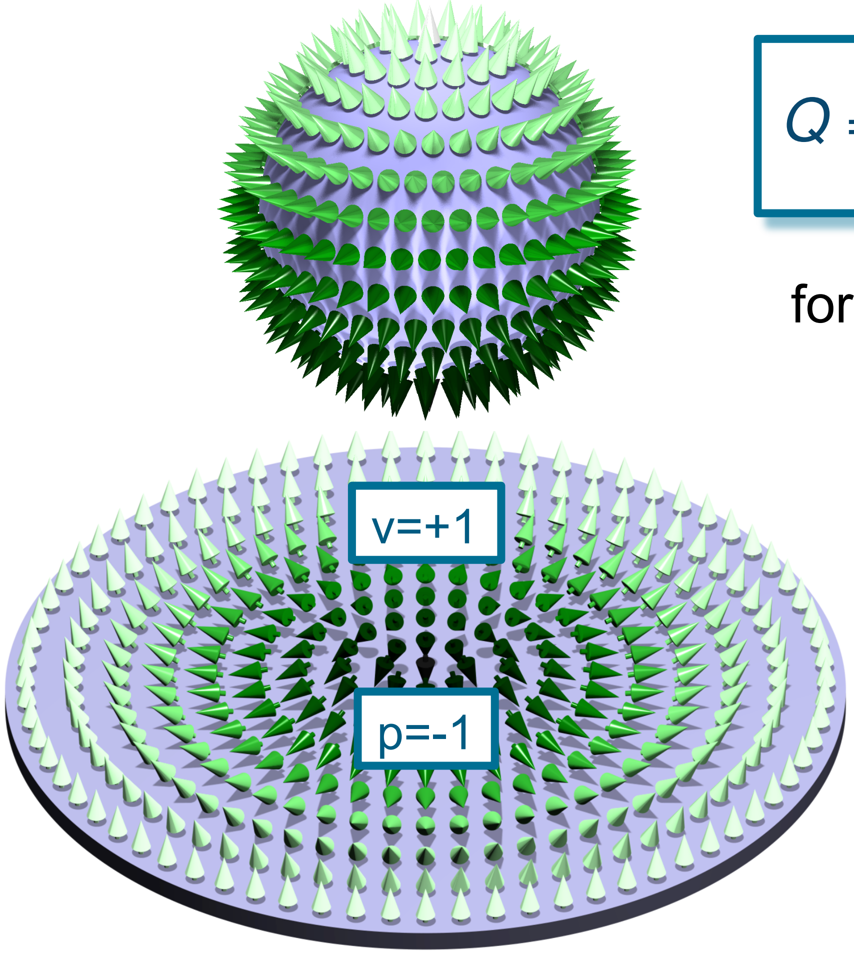

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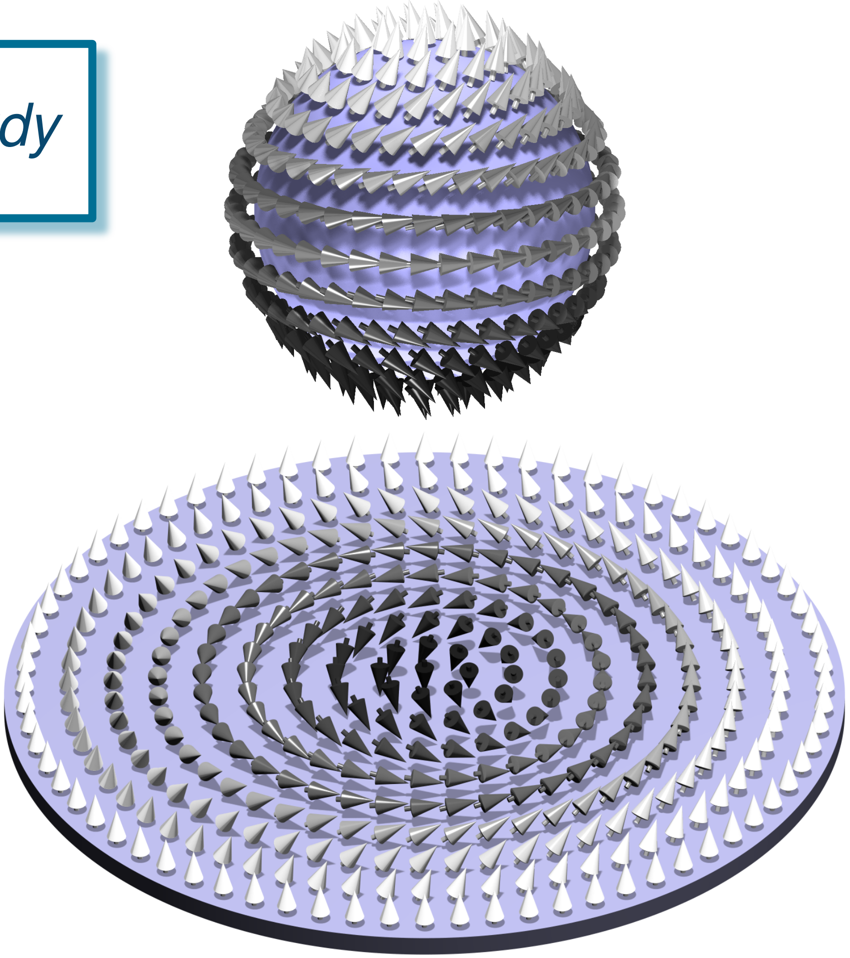

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Skyrmionic structures

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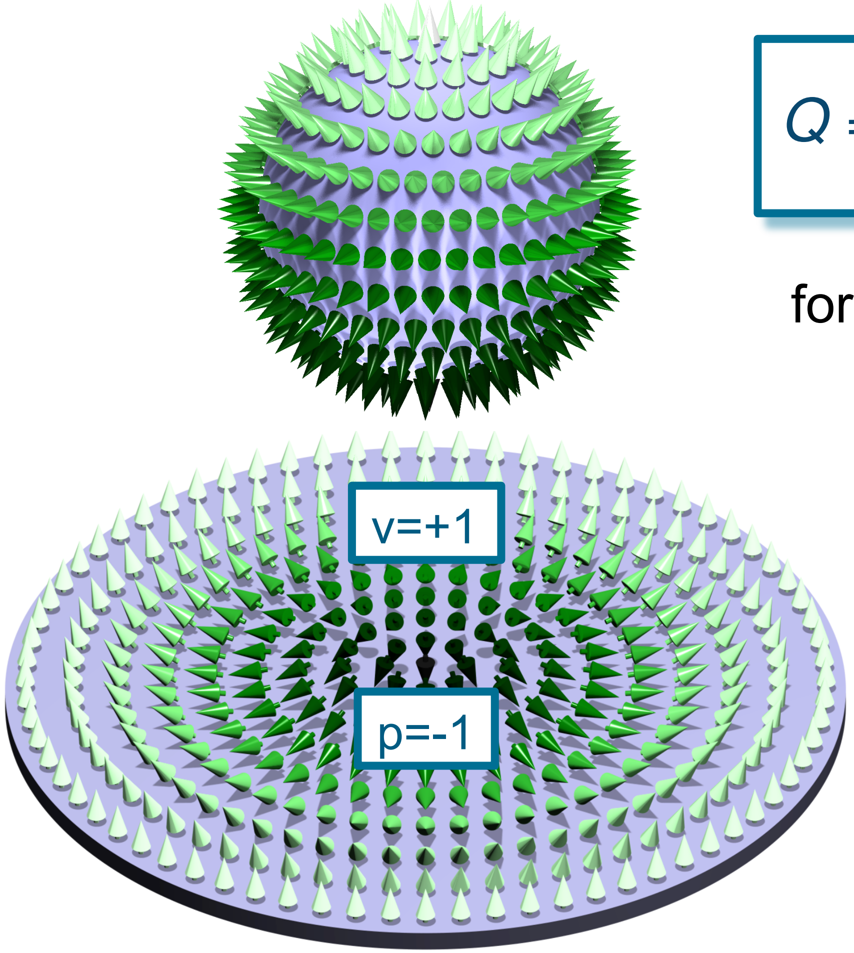

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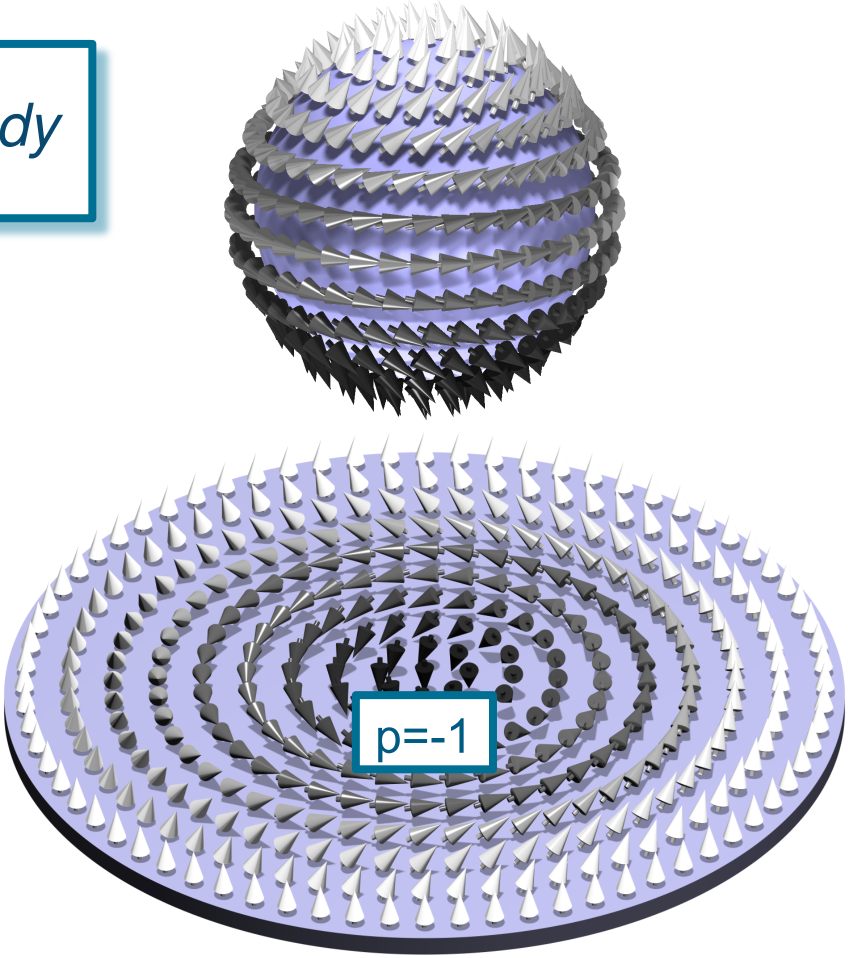

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Skyrmionic structures

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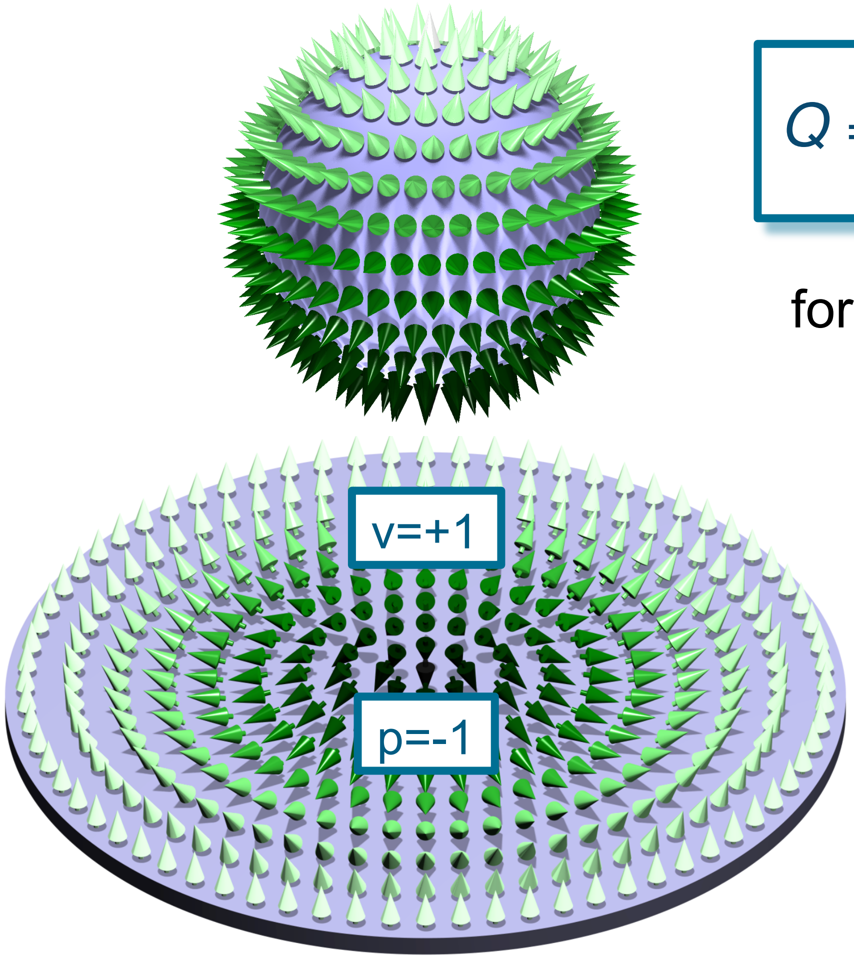

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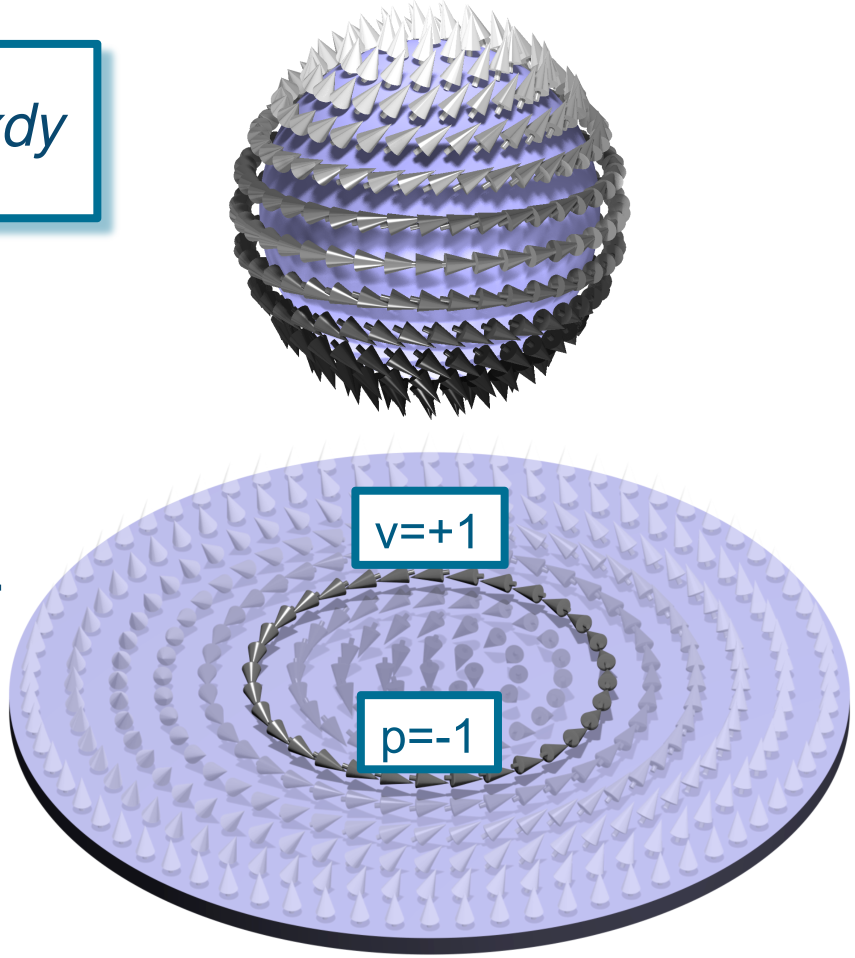

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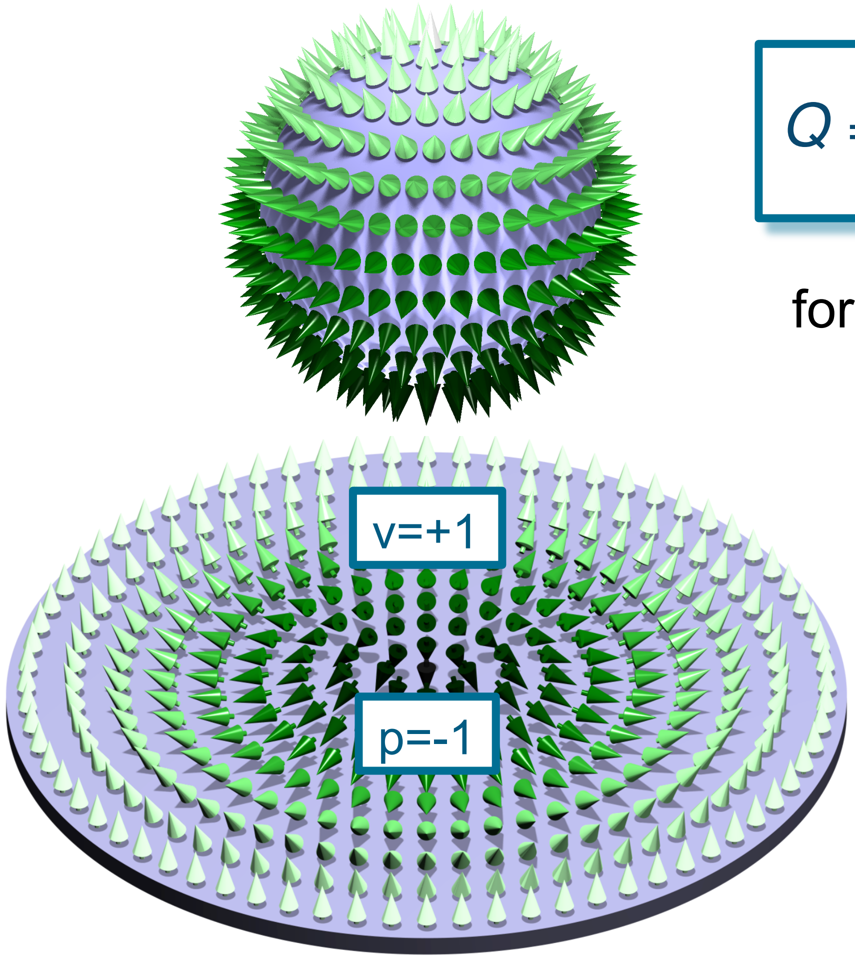

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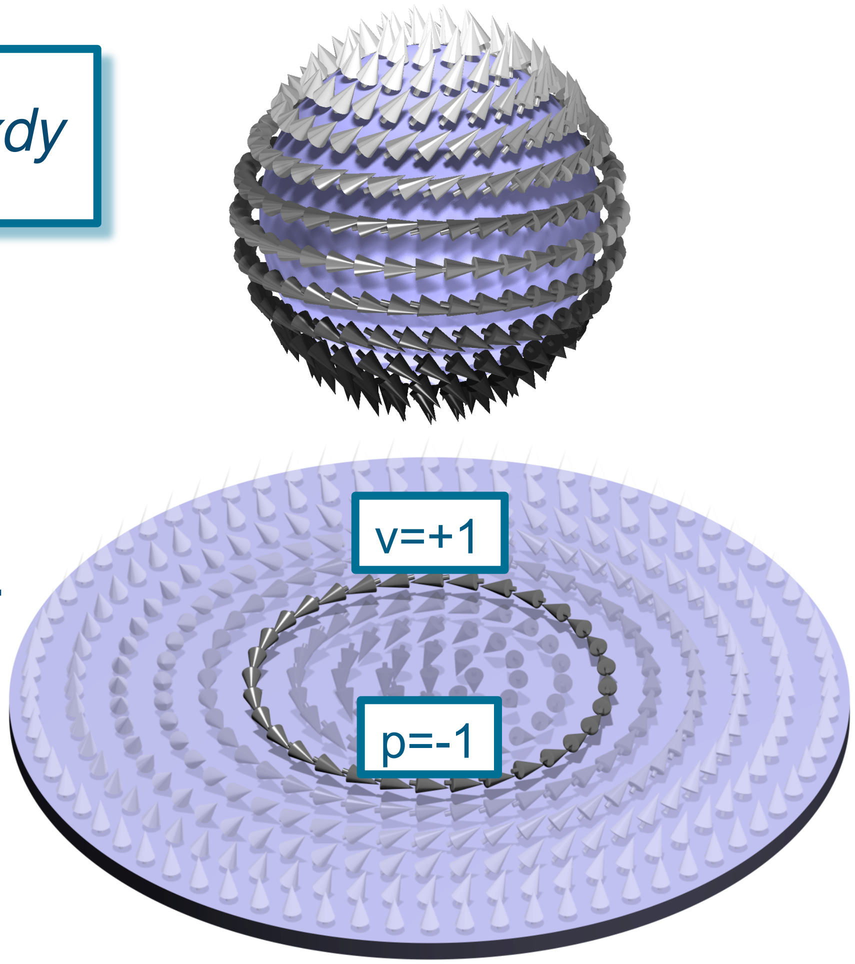

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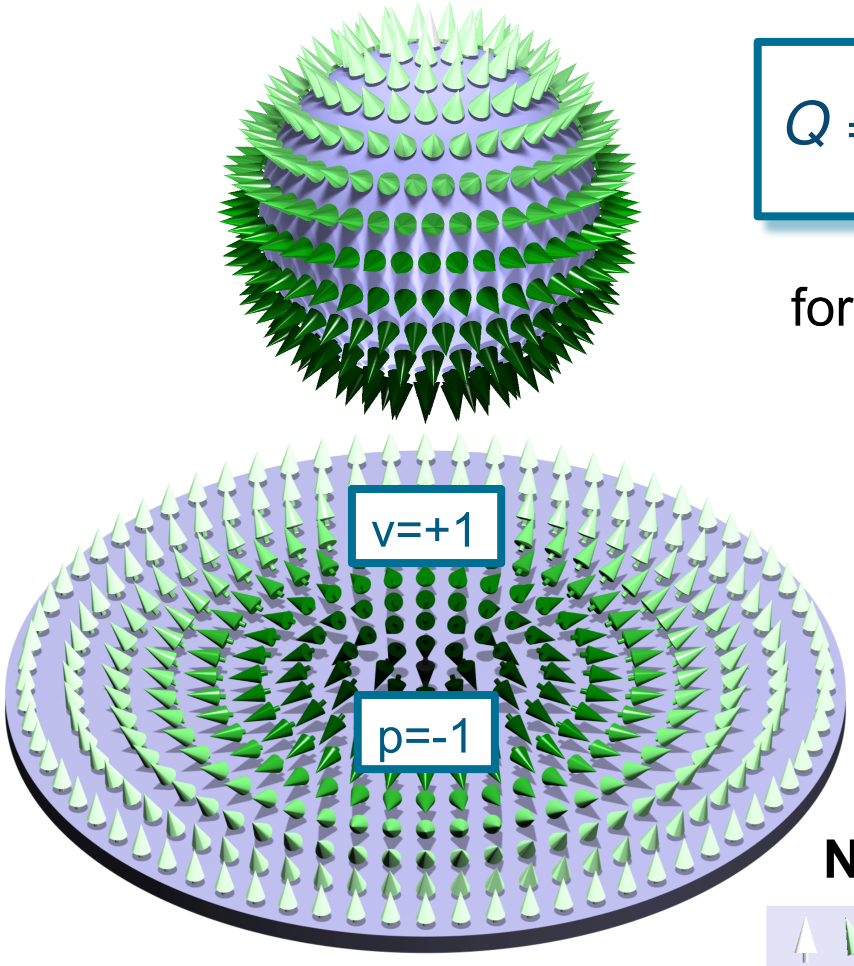

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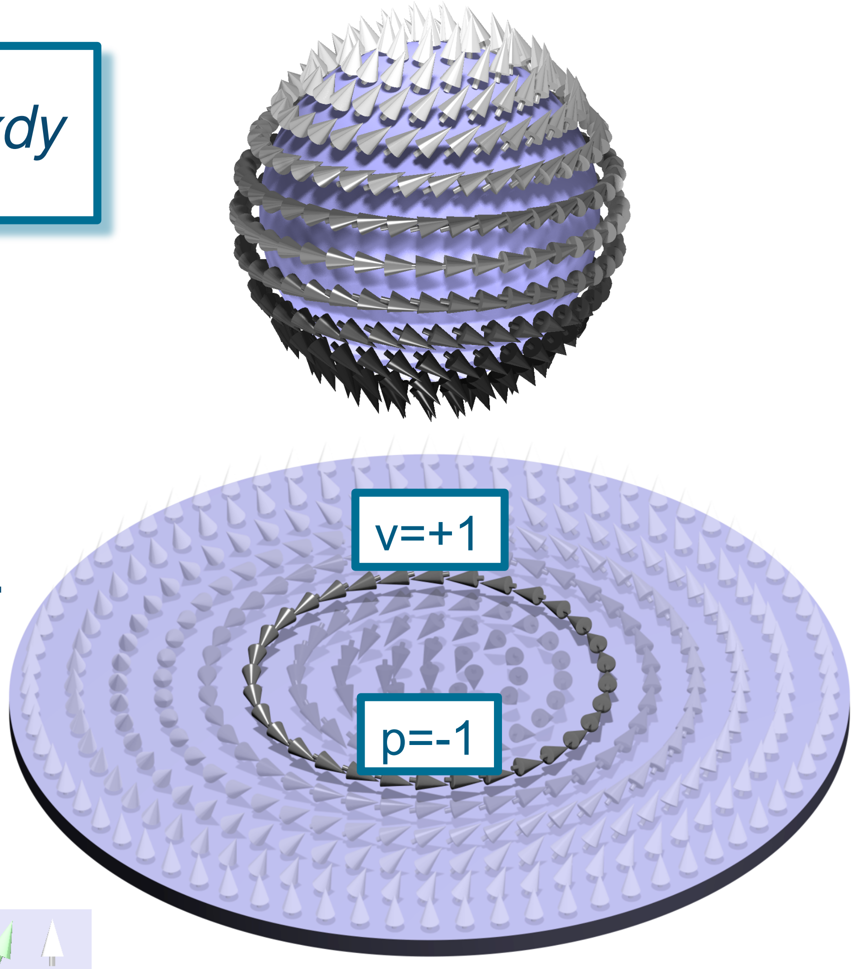

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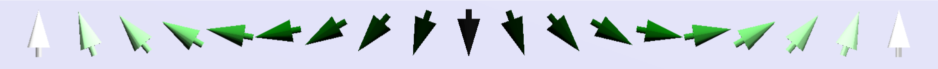
Néel-type rotation: rot axis $\otimes$ q $\longrightarrow$



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Skyrmionic structures

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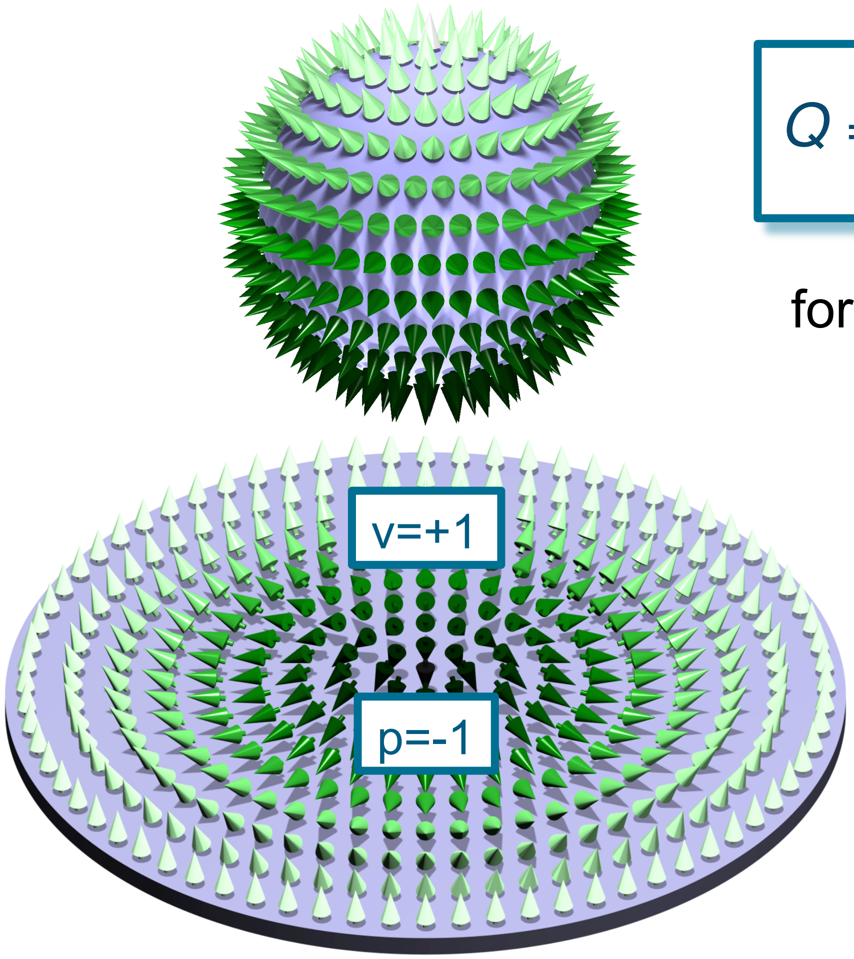

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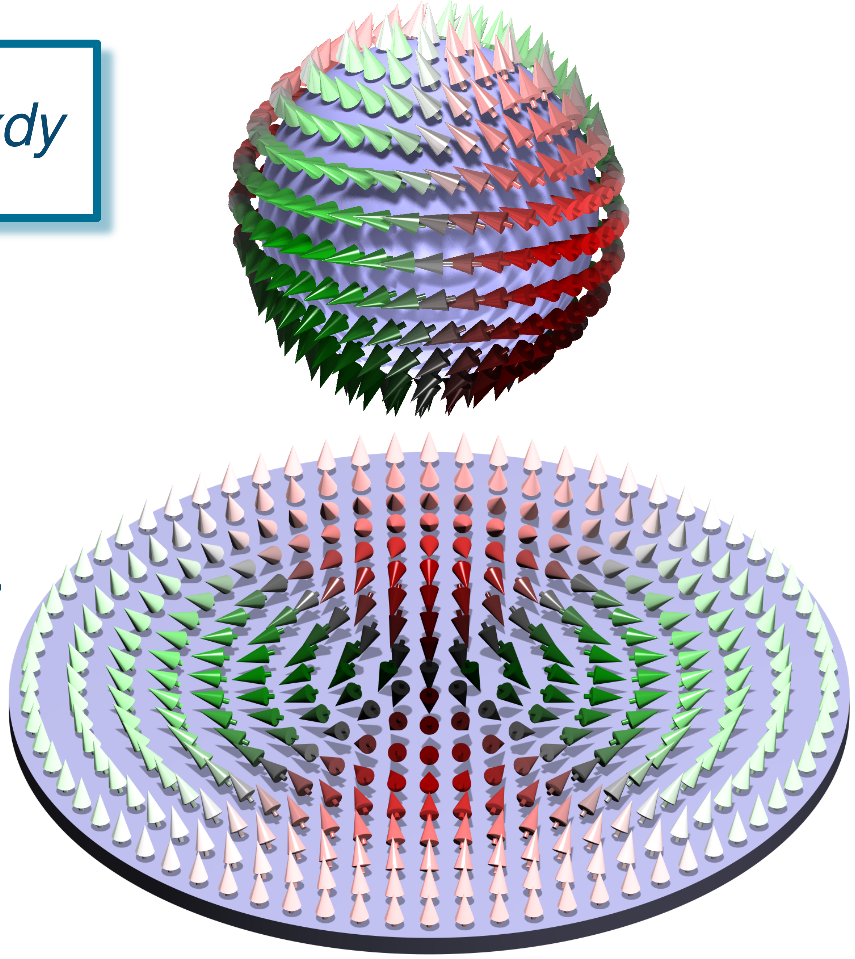
Antiskyrmion / "multichiral" skyrmion



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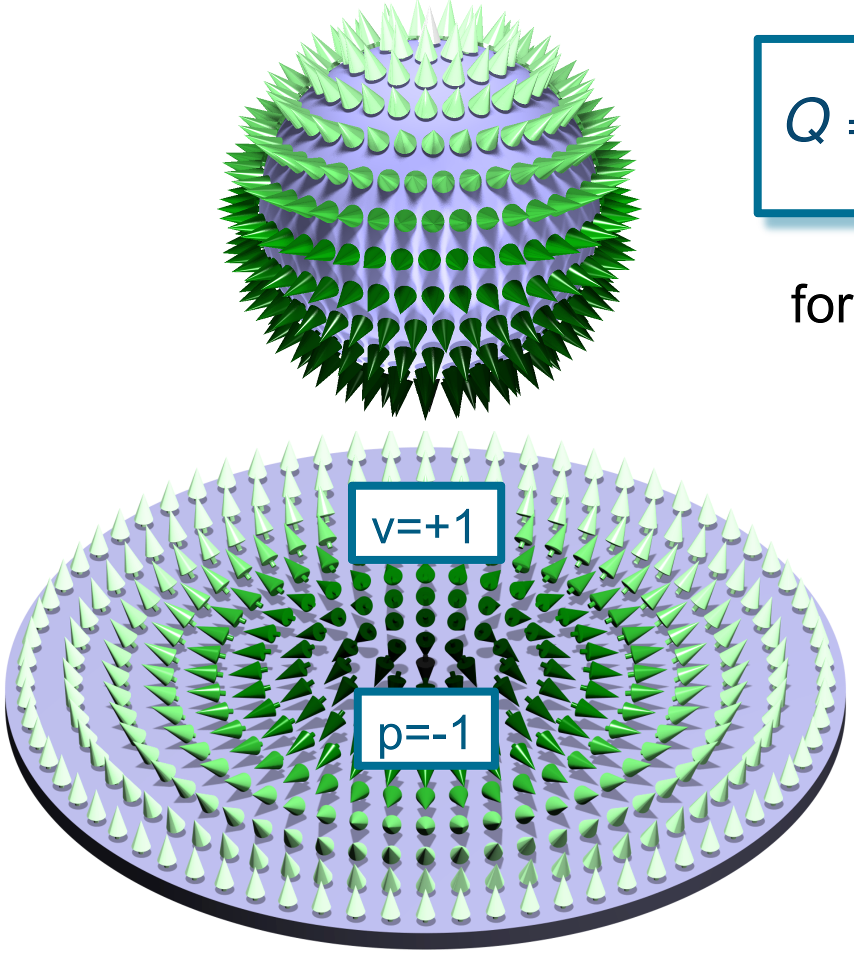
Skyrmionic structures

Néel-type (“Hedgehog”) Skyrmion



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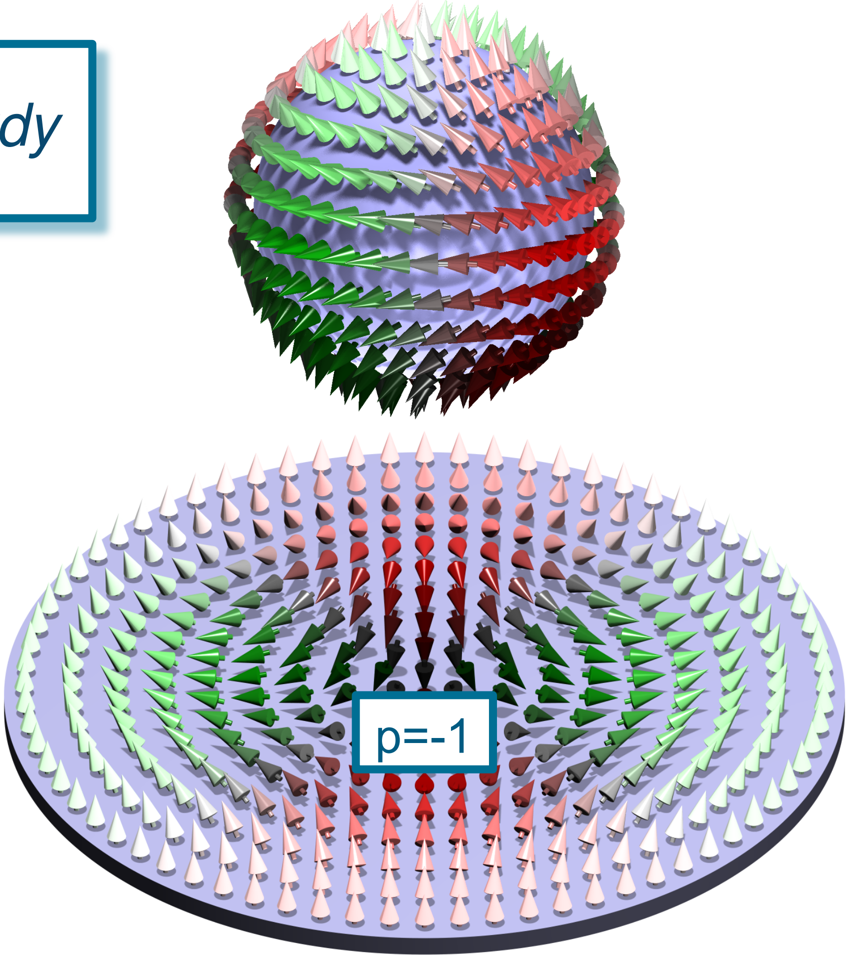

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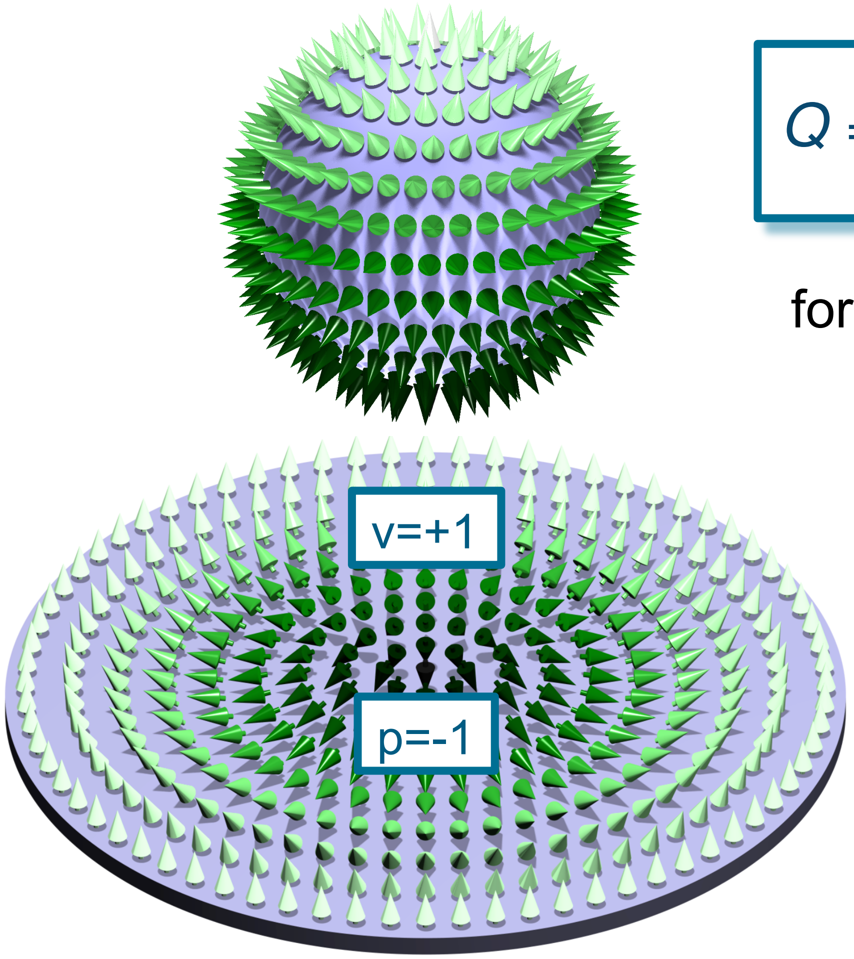

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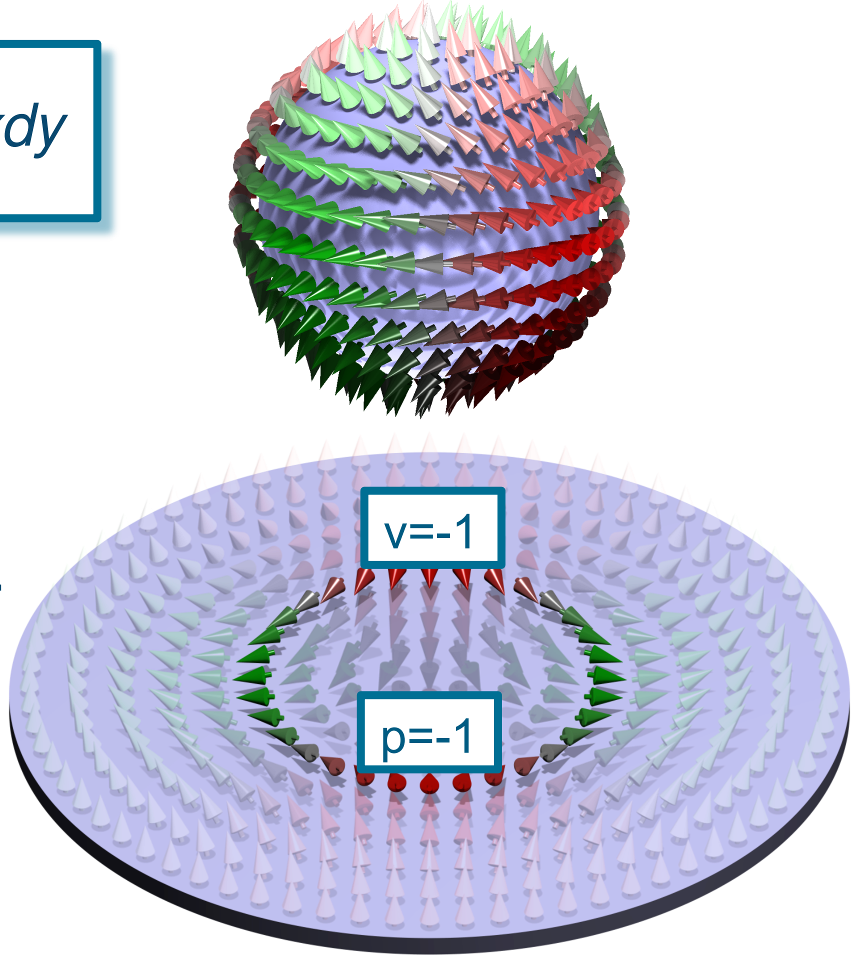

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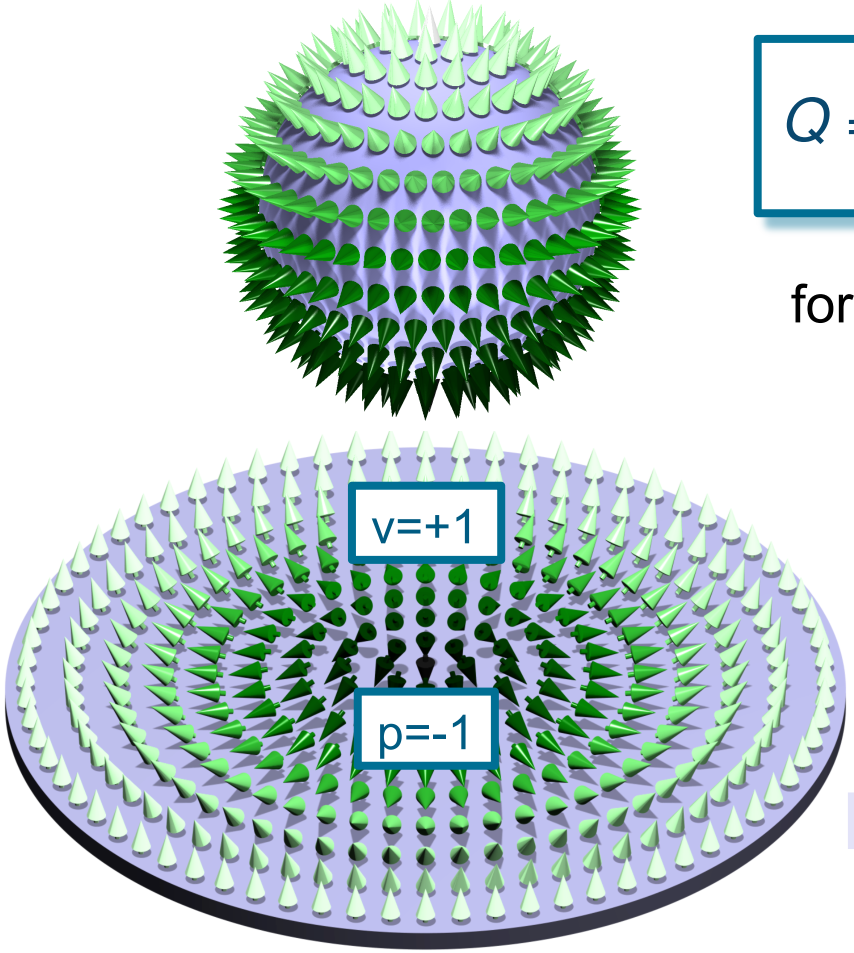

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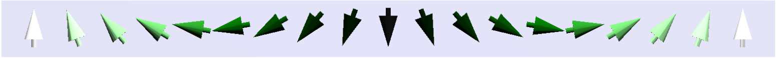

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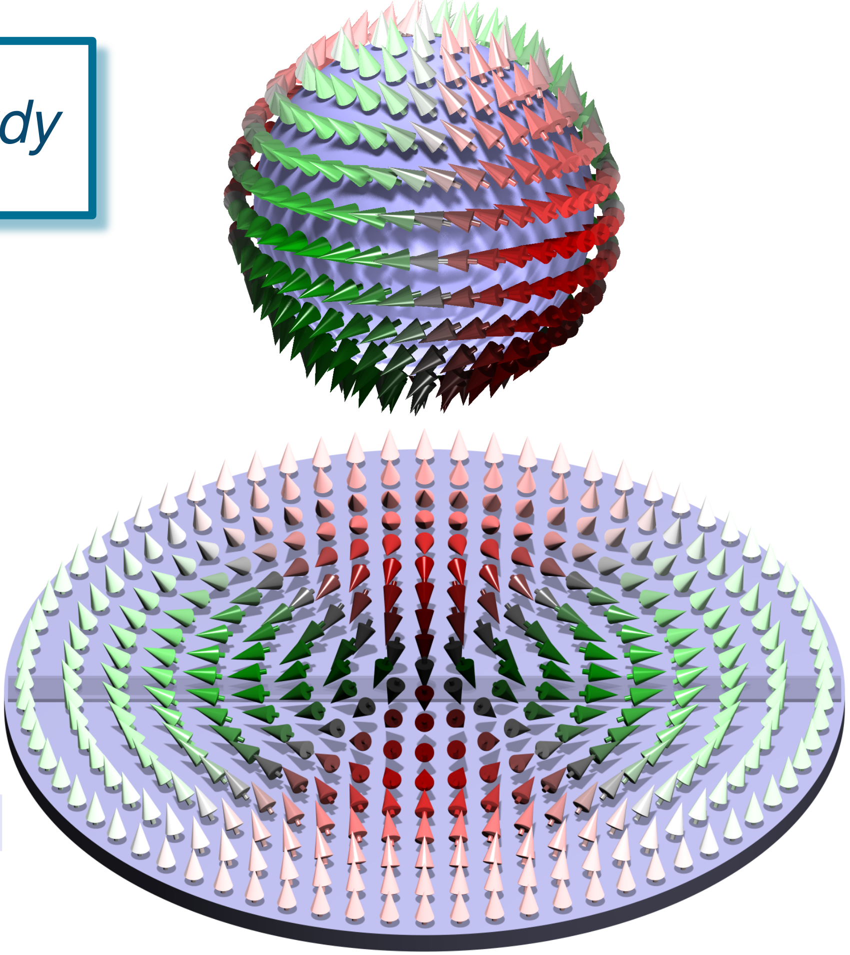

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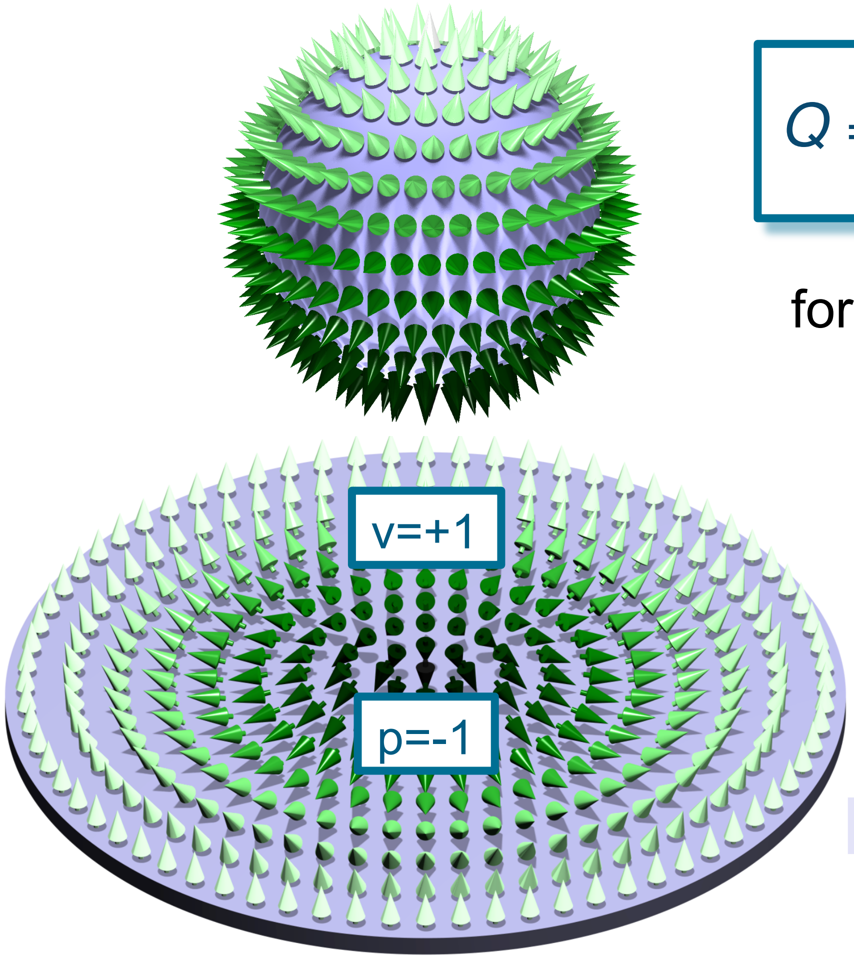

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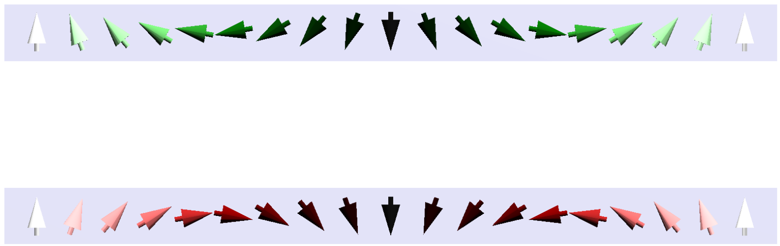
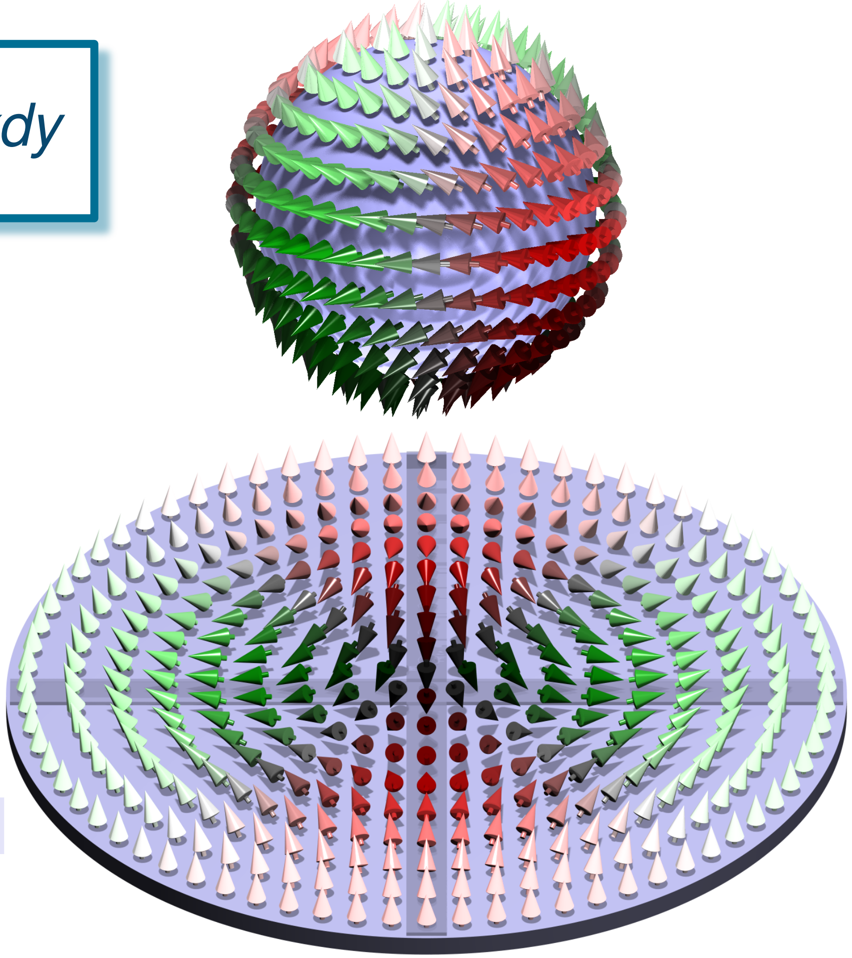


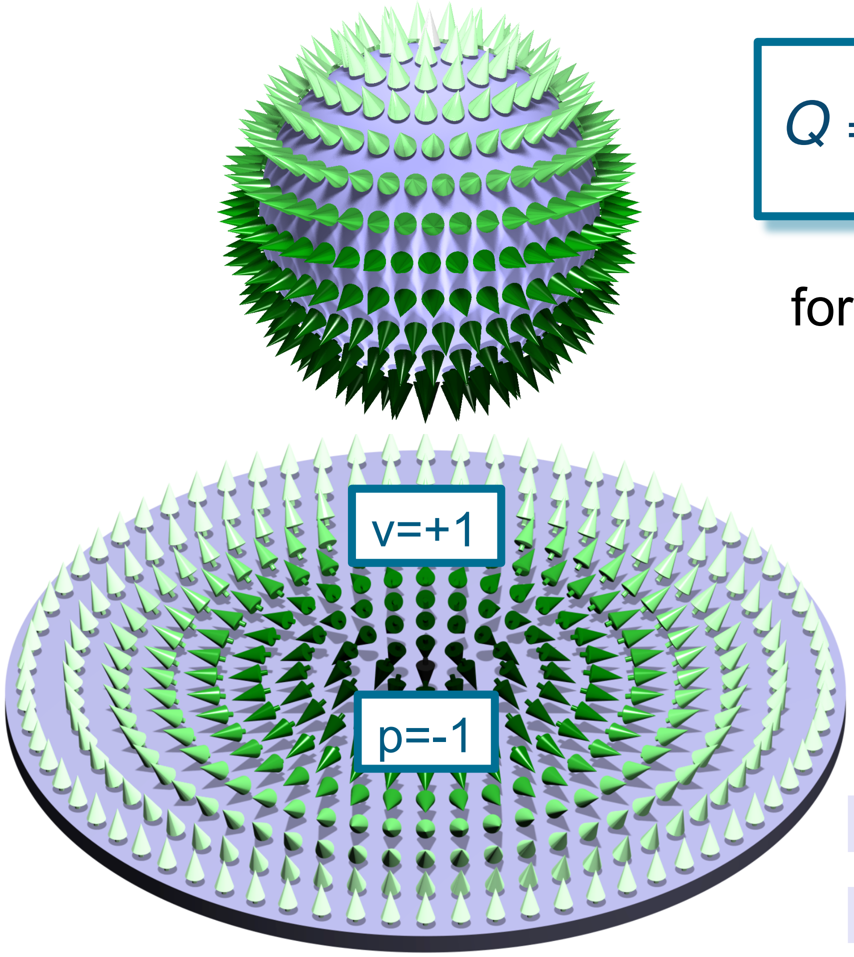
Antiskyrmion / “multichiral” skyrmion



$$Q = +1$$

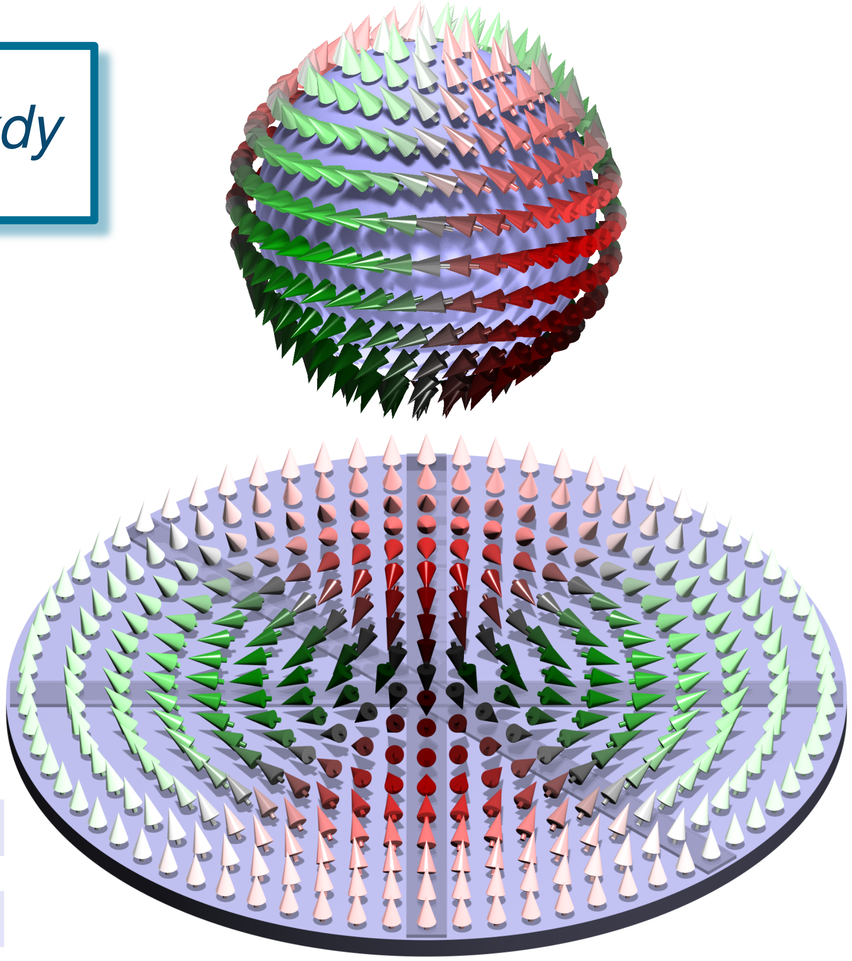
Skyrmionic structures

Néel-type (“Hedgehog”) Skyrmion



$Q = -1$

Antiskyrmion / “multichiral” skyrmion



$Q = +1$

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

for skyrmionic structure:

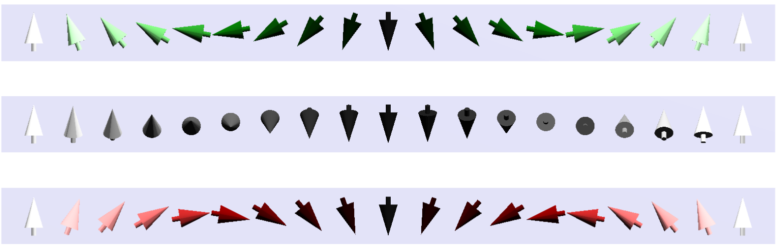
$$Q = p \cdot v$$

polarization

$p = m_z(\mathbf{r} = 0)$

“vorticity”

$$v = \frac{1}{2\pi} \oint_{\Gamma} \frac{m_{\parallel} \times \nabla m_{\parallel}}{1 - m_z^2} \cdot \mathbf{dr}$$



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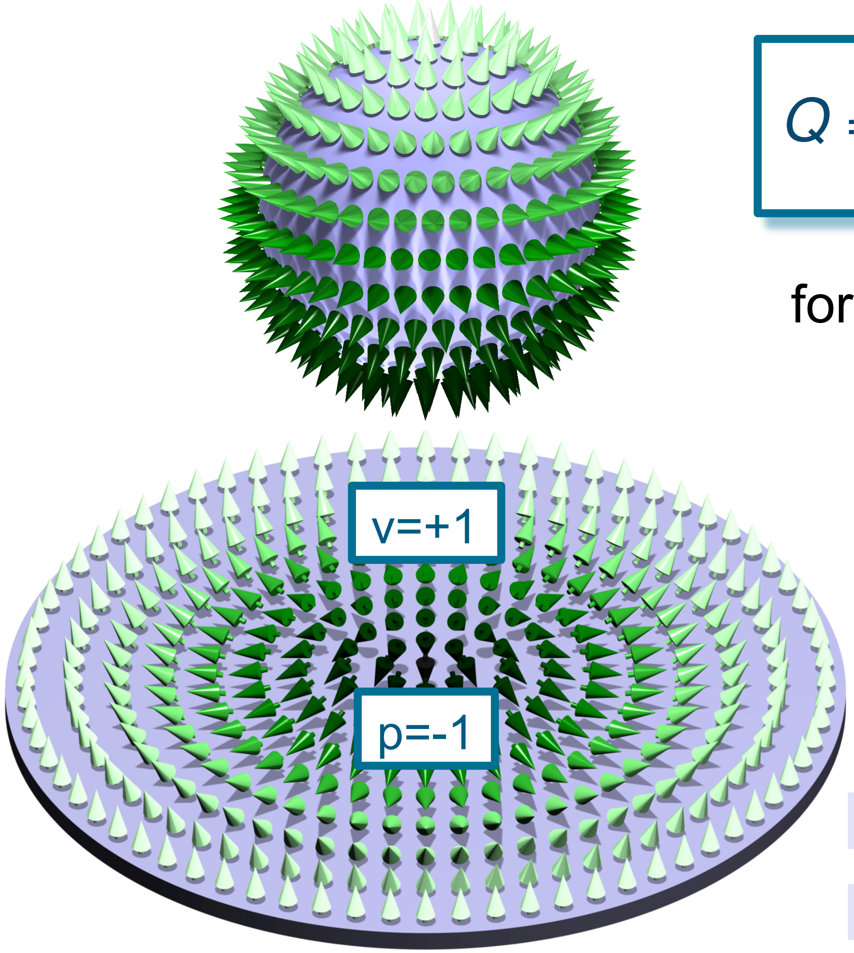
Skyrmionic structures

Néel-type ("Hedgehog") Skyrmion



$$Q = -1$$

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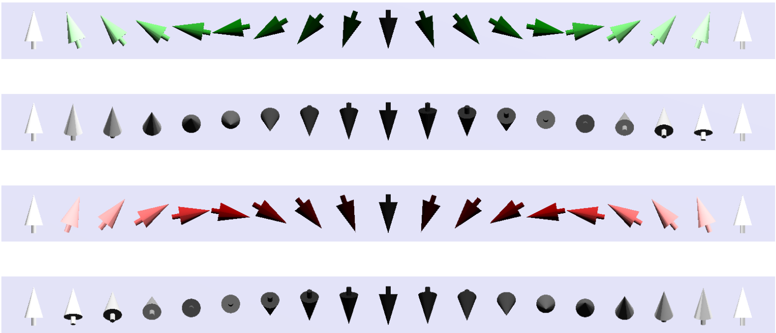

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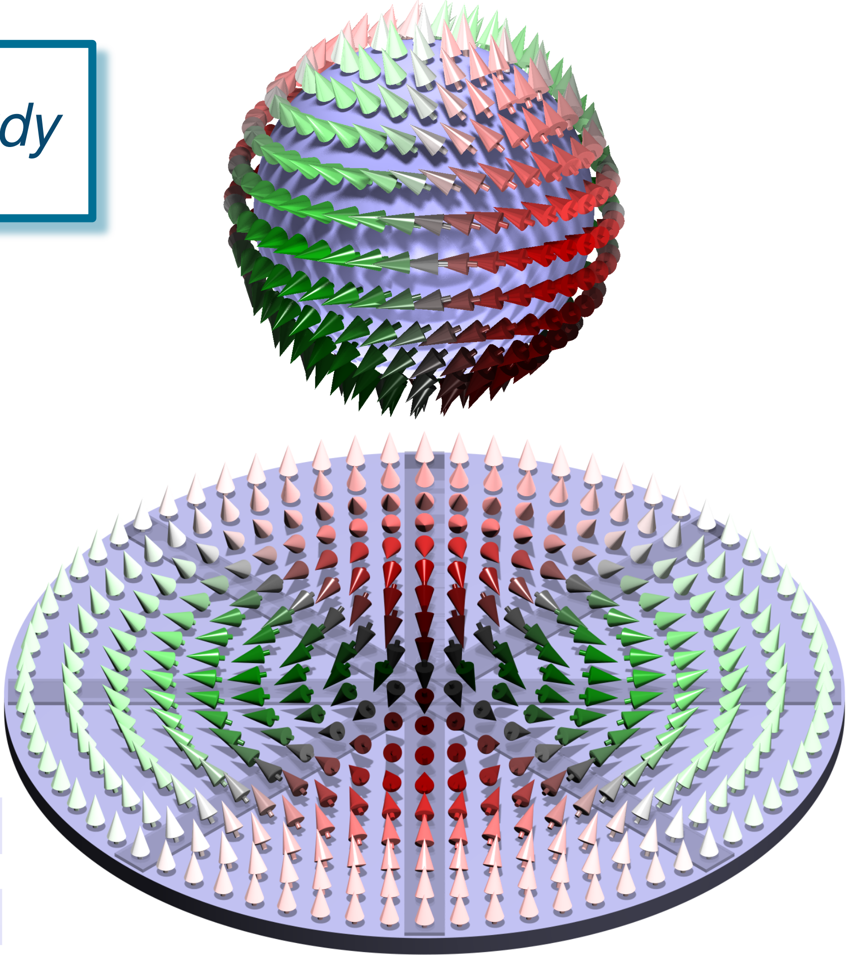

$$Q = +1$$

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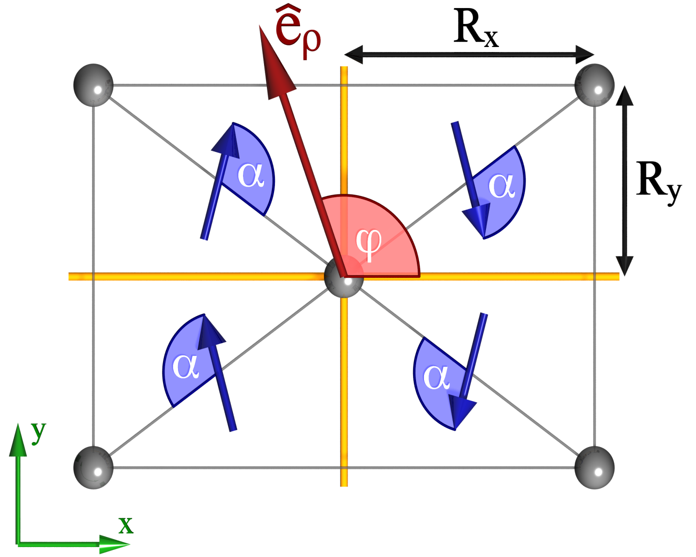
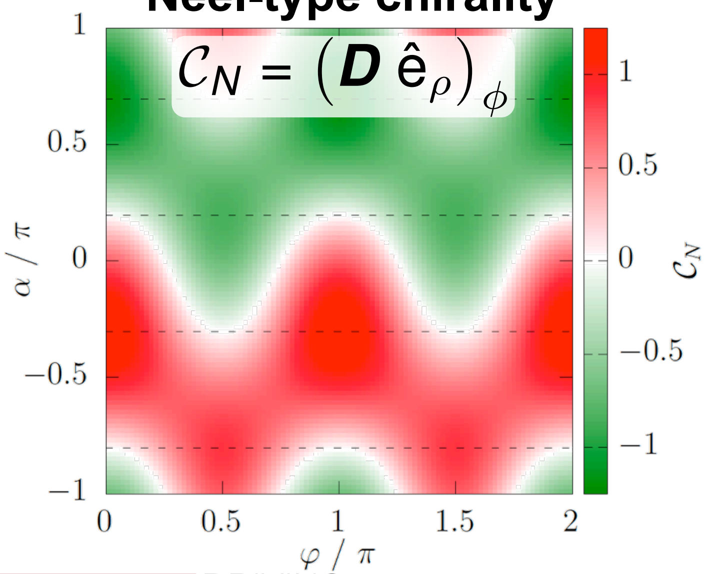
Magnetic structures in C_{2v} symmetry class



Néel-type chirality



MAX DRIVING THE EXASCALE TRANSITION

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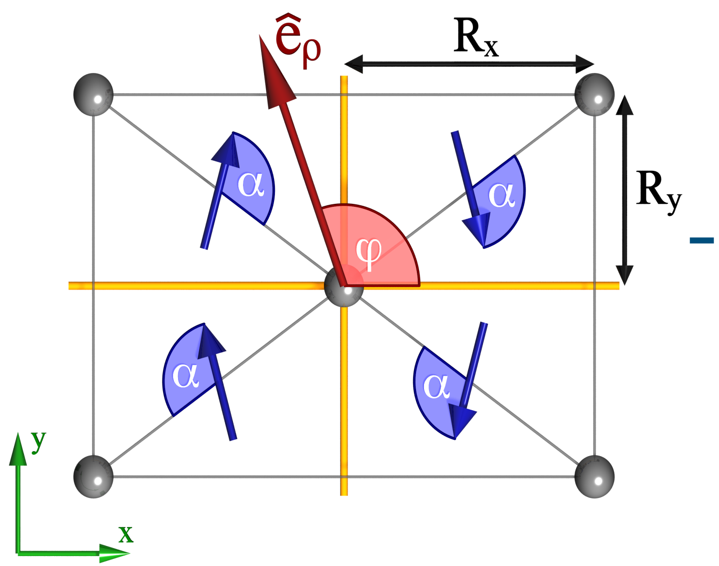
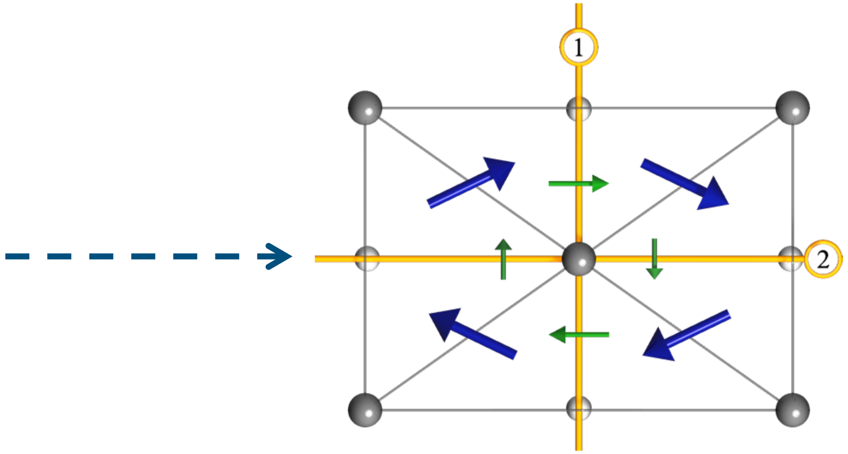
Magnetic structures in C_{2v} symmetry class





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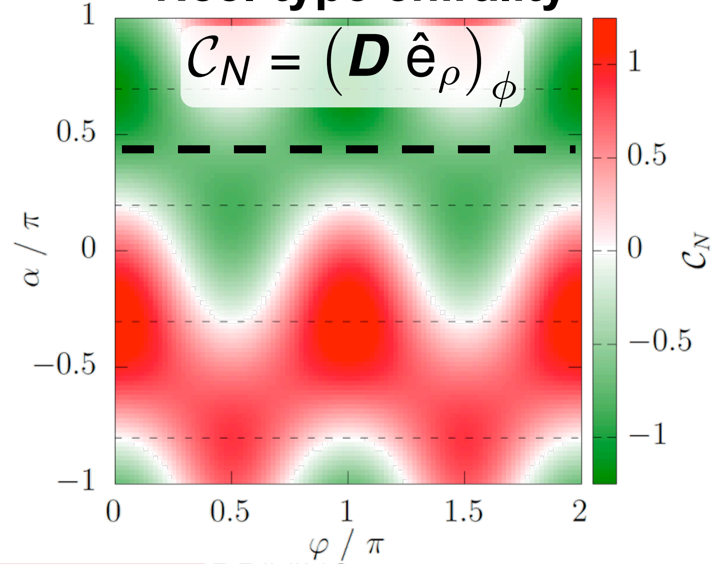

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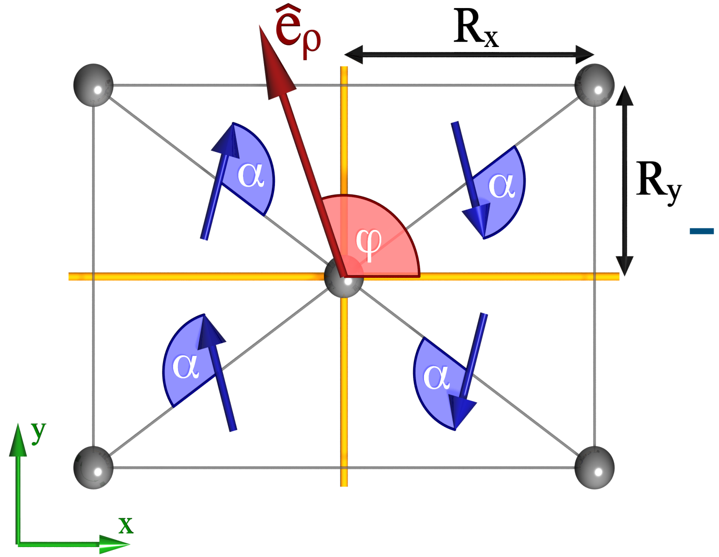

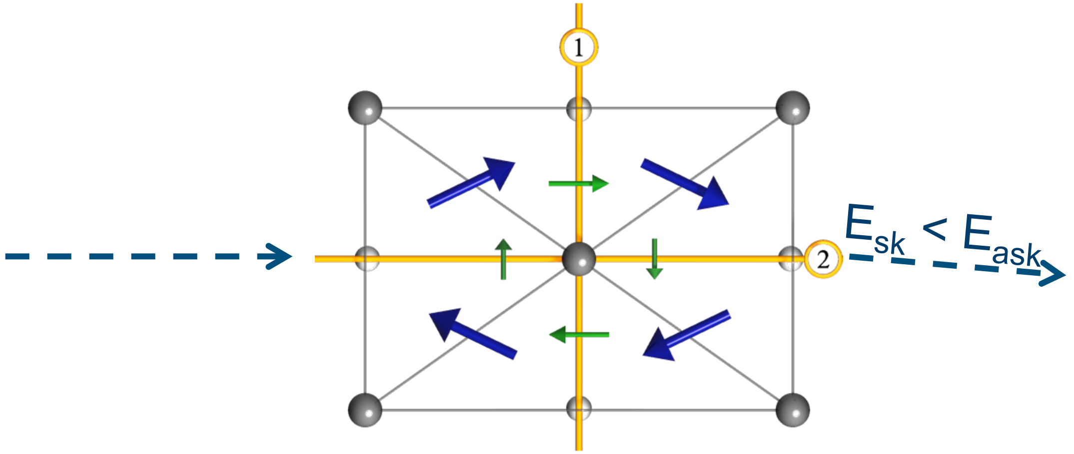

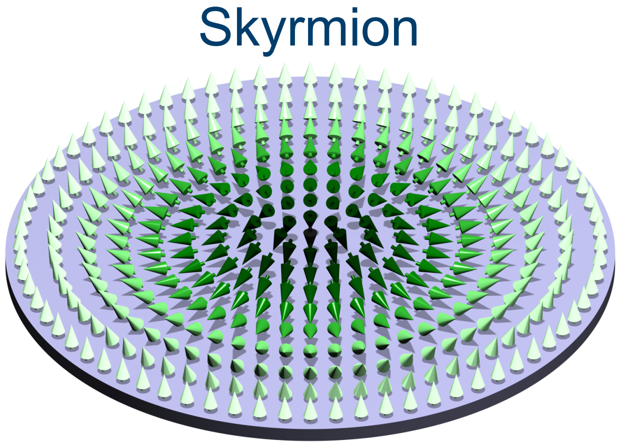

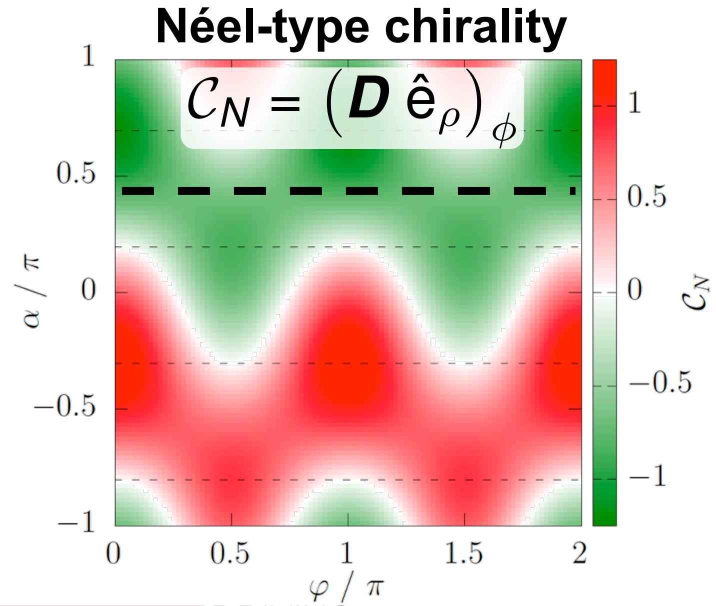

MAX DRIVING THE EXASCALE TRANSITION

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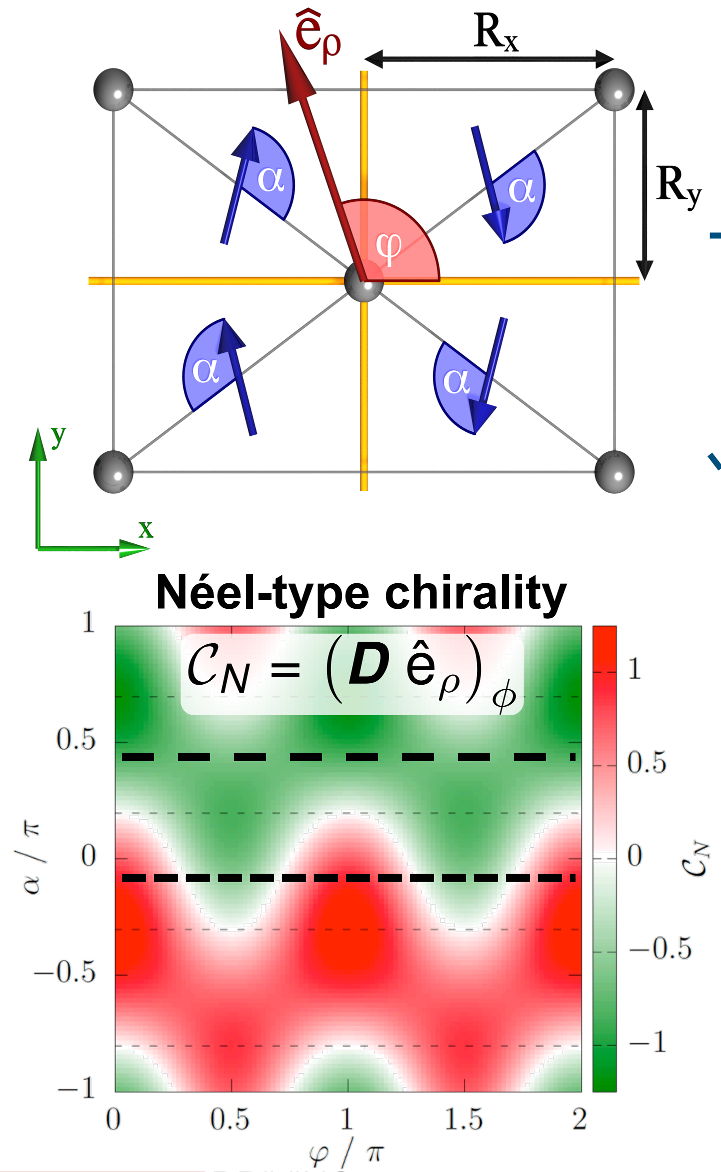
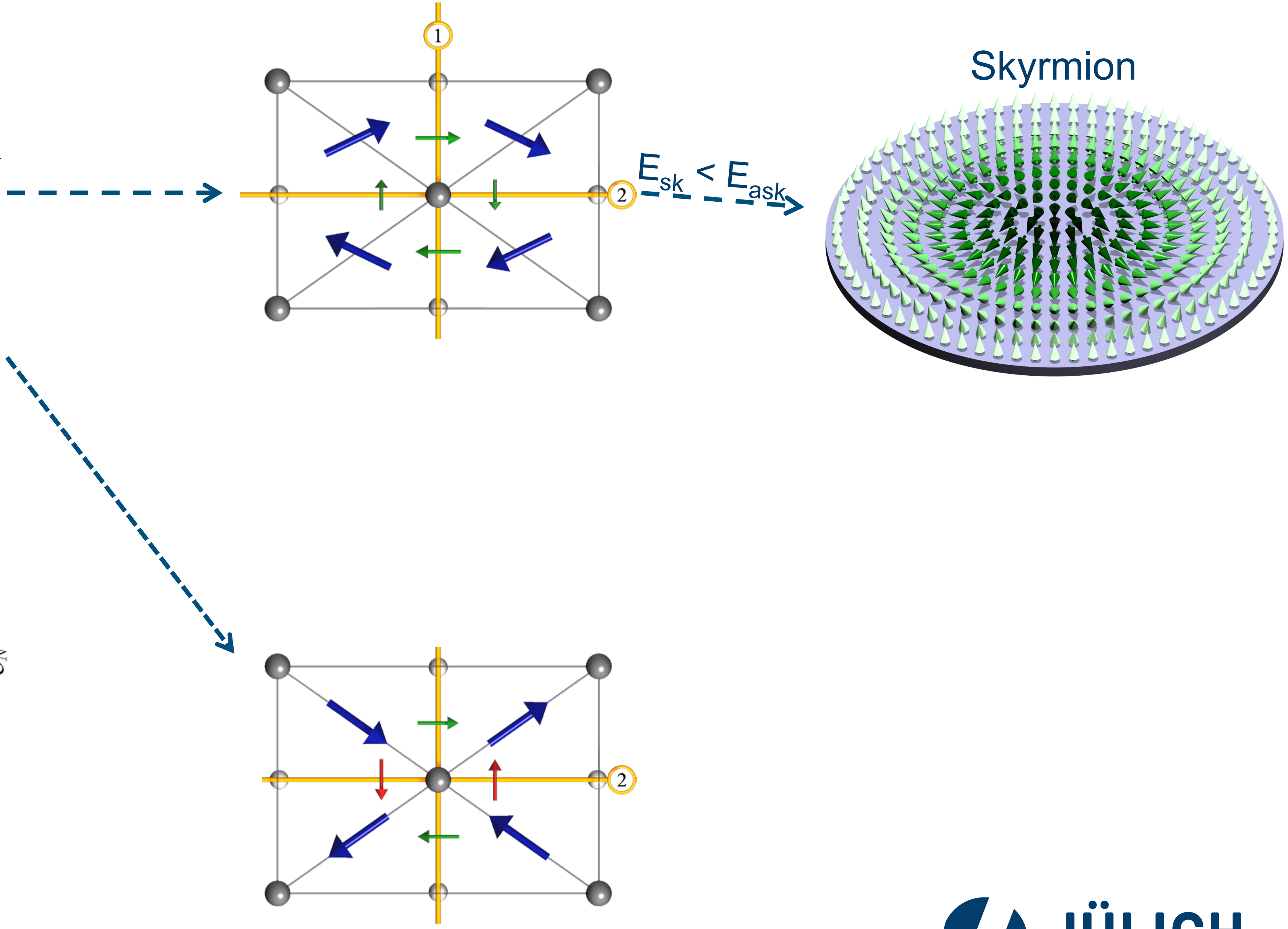
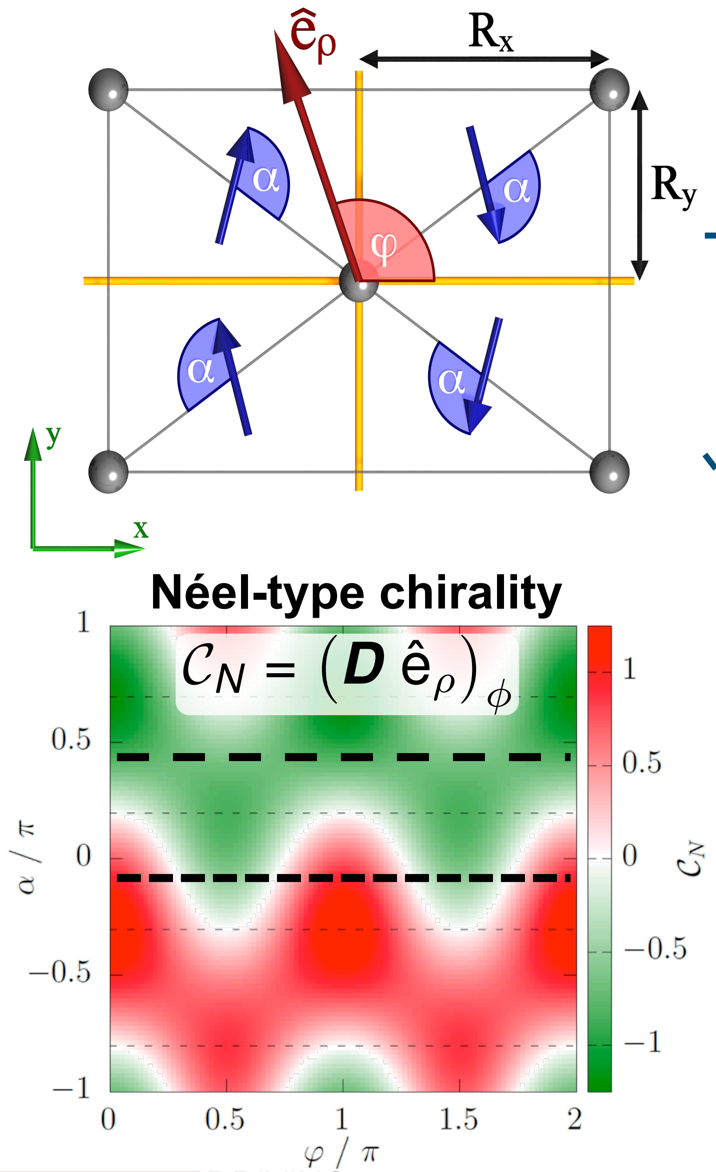
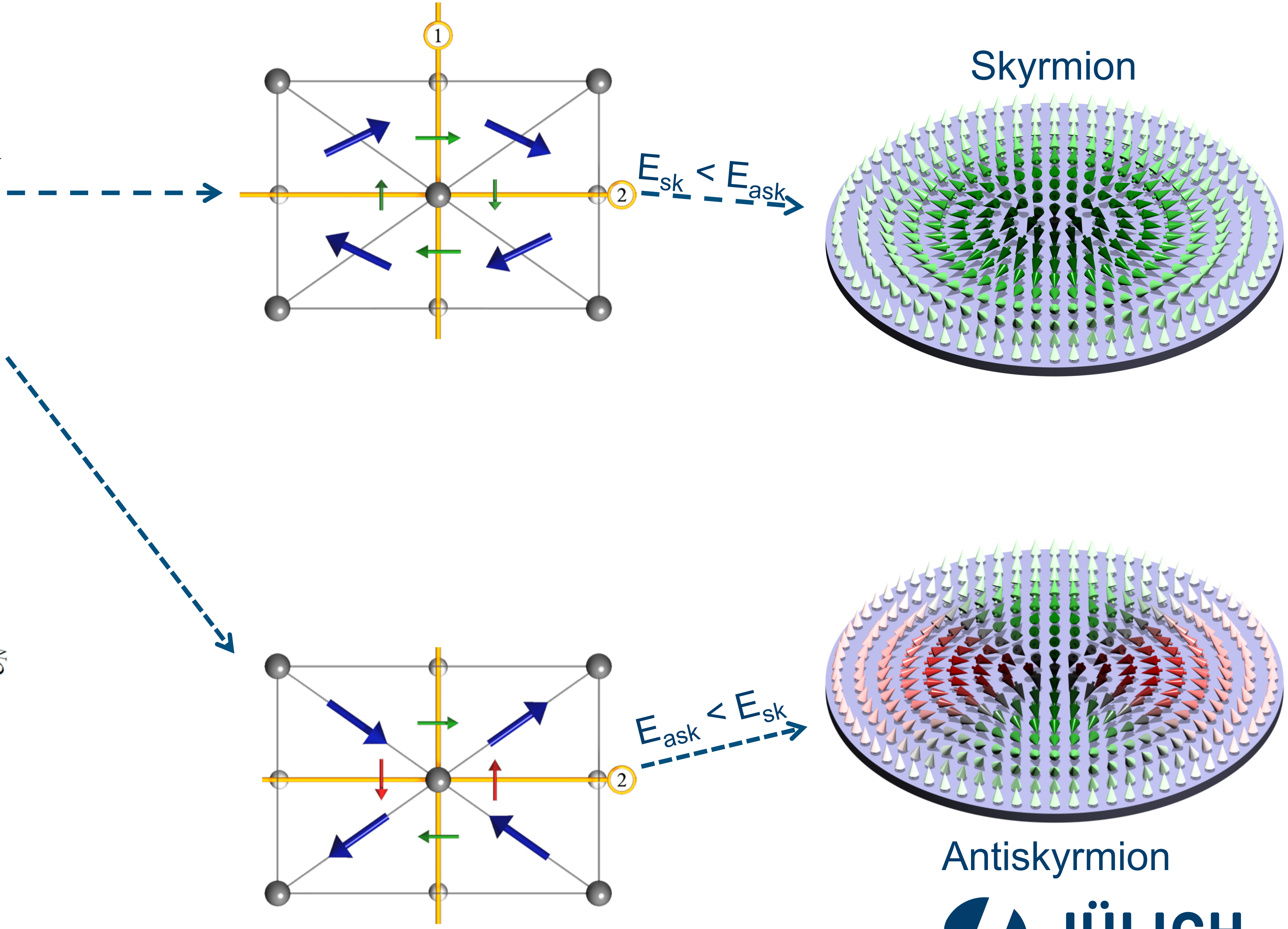
Magnetic structures in C_{2v} symmetry class



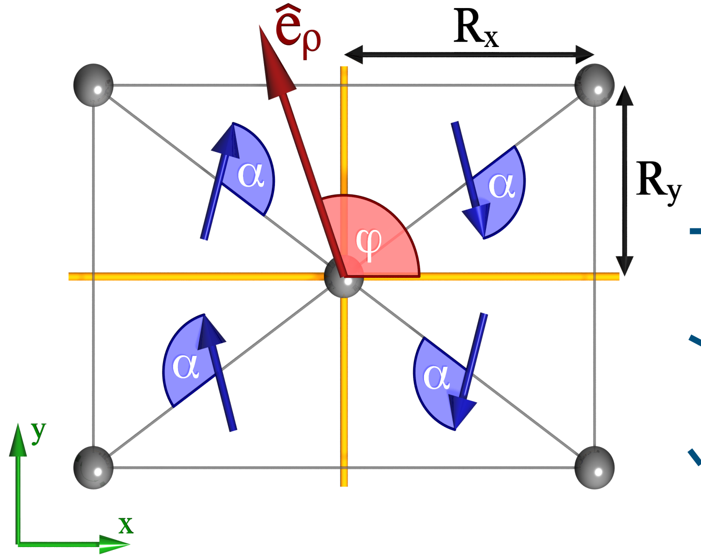


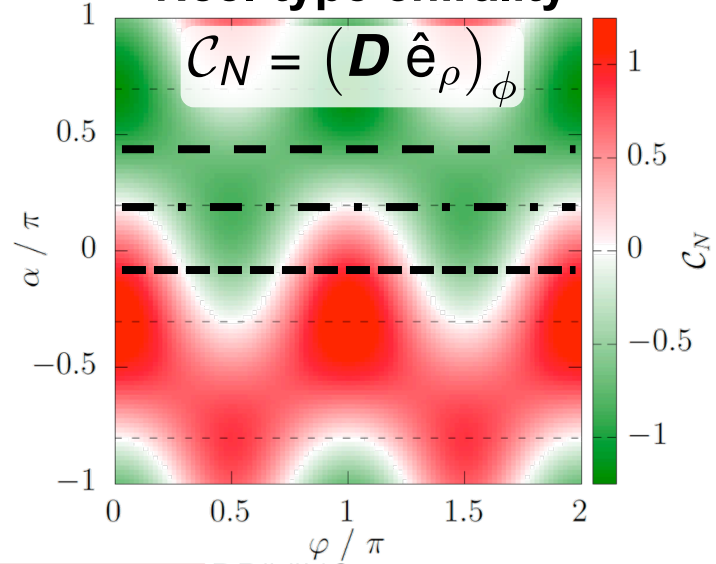
Magnetic structures in C_{2v} symmetry class

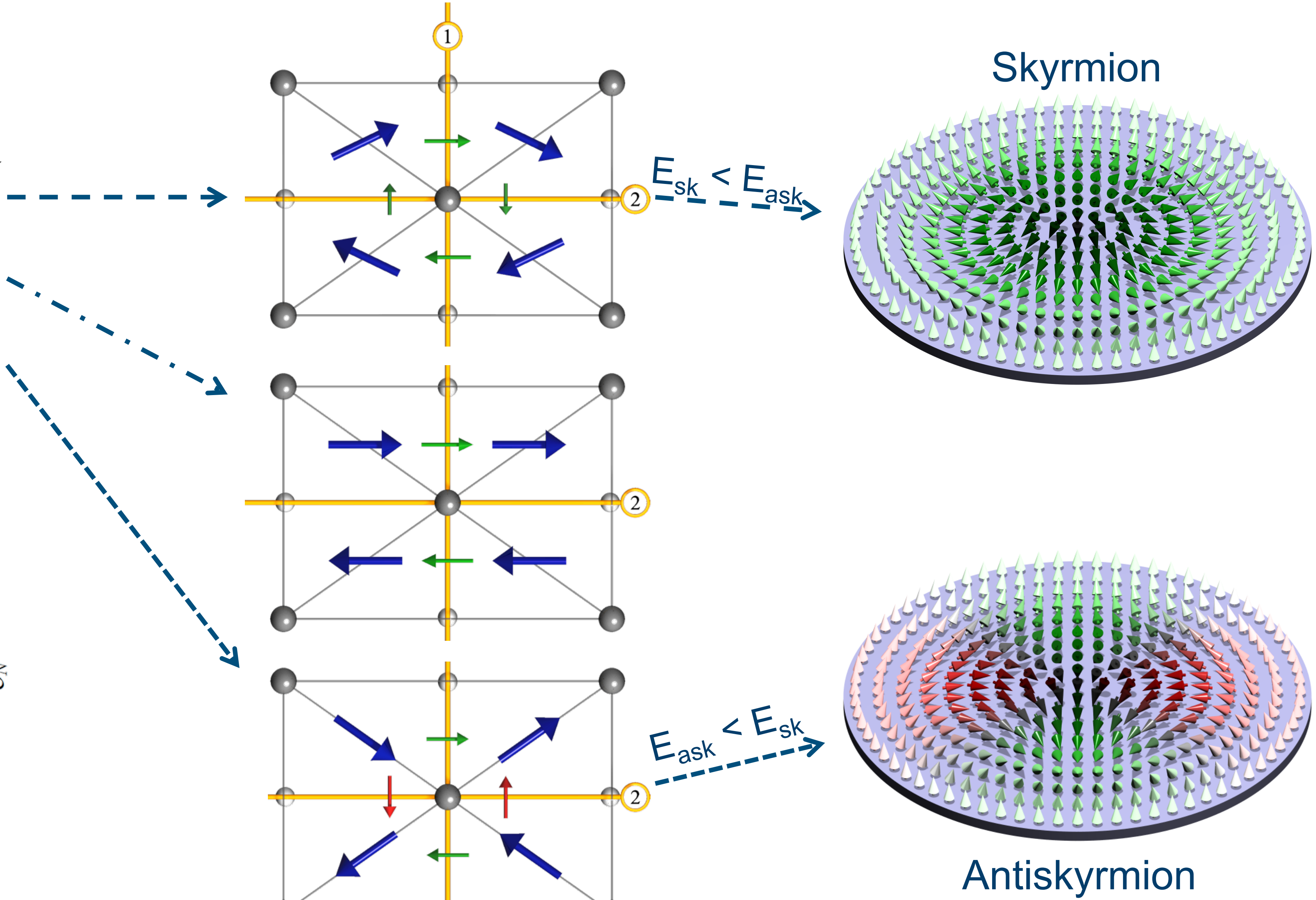




Magnetic structures in C_{2v} symmetry class







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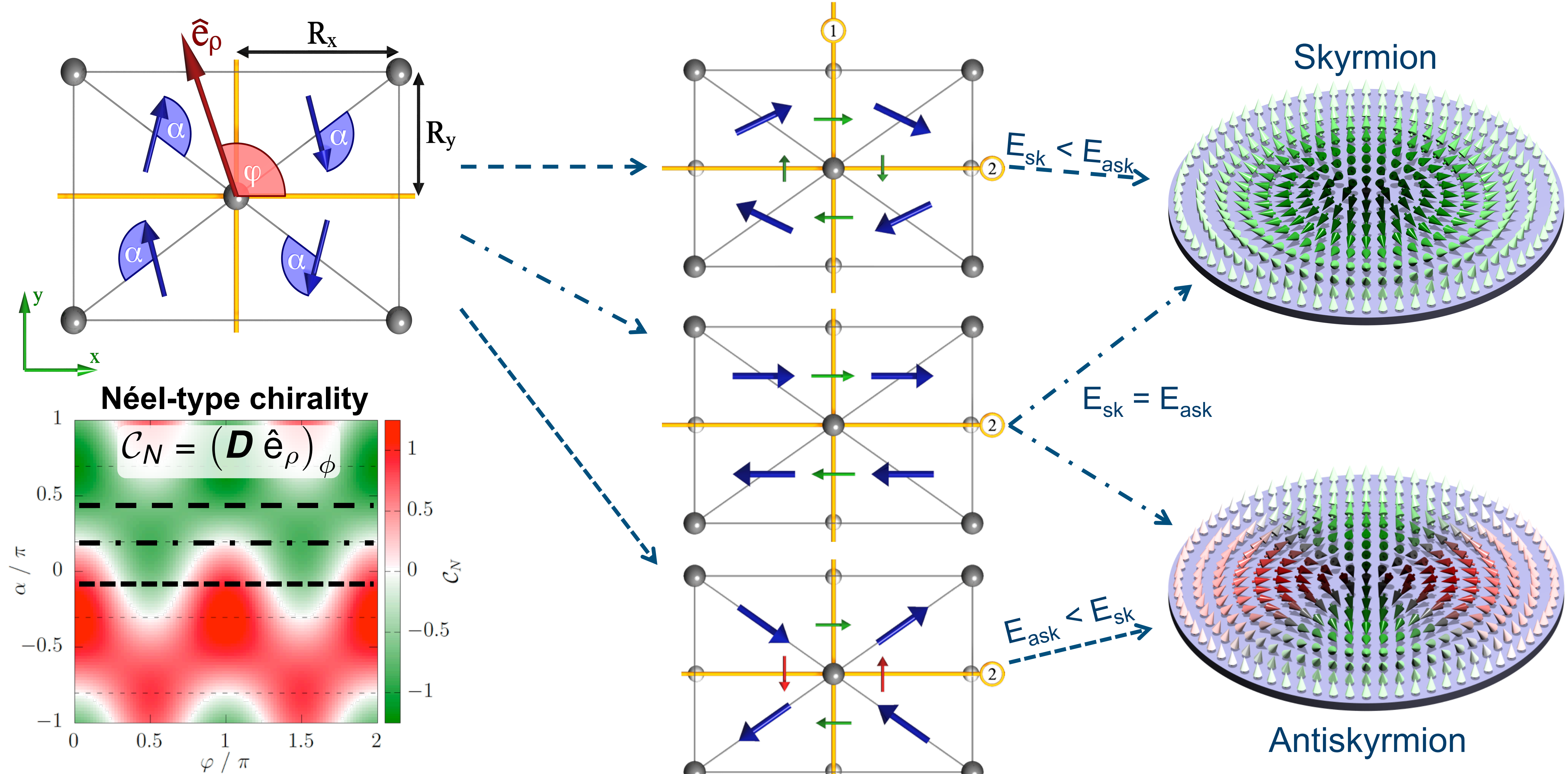

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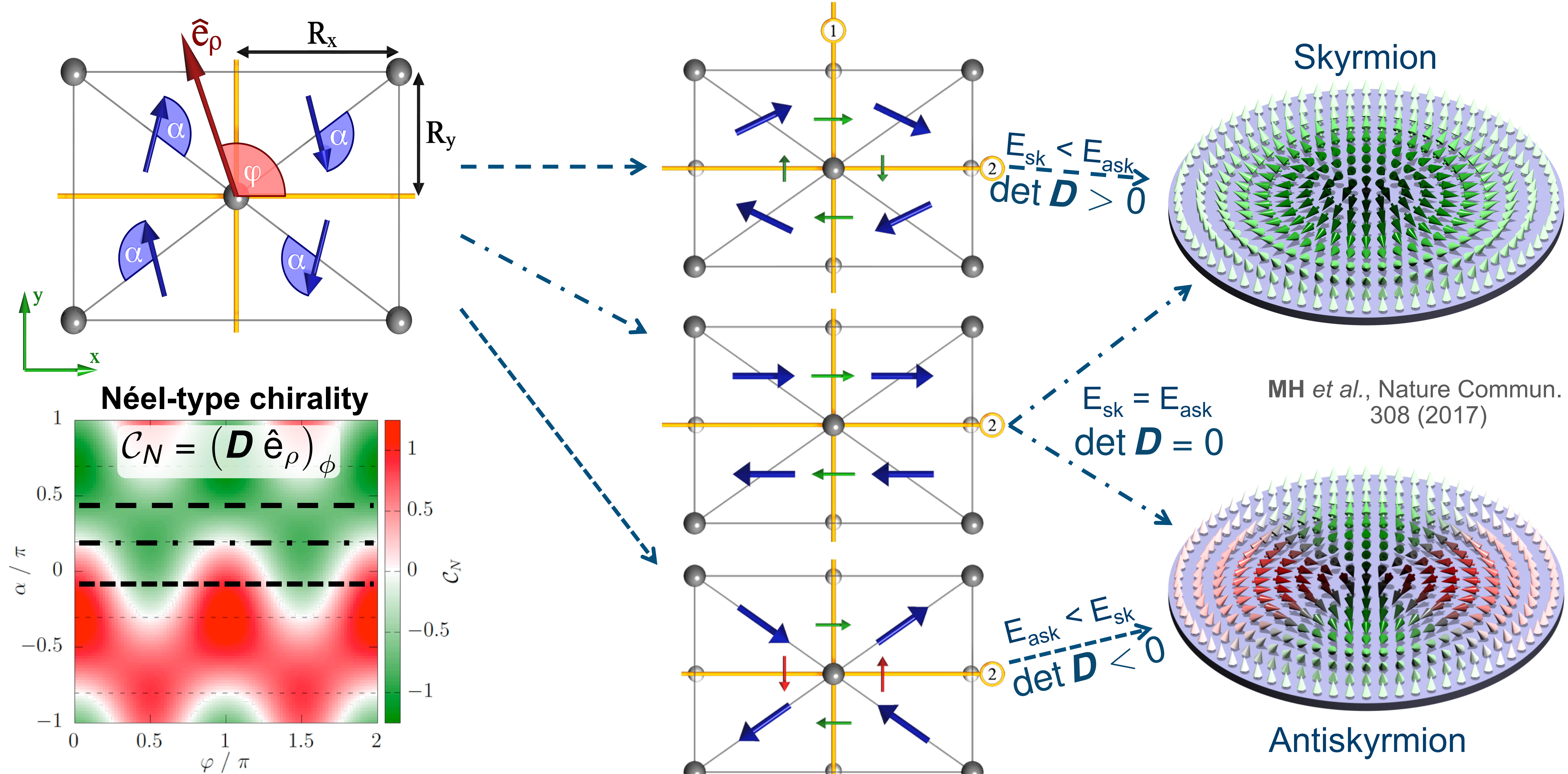
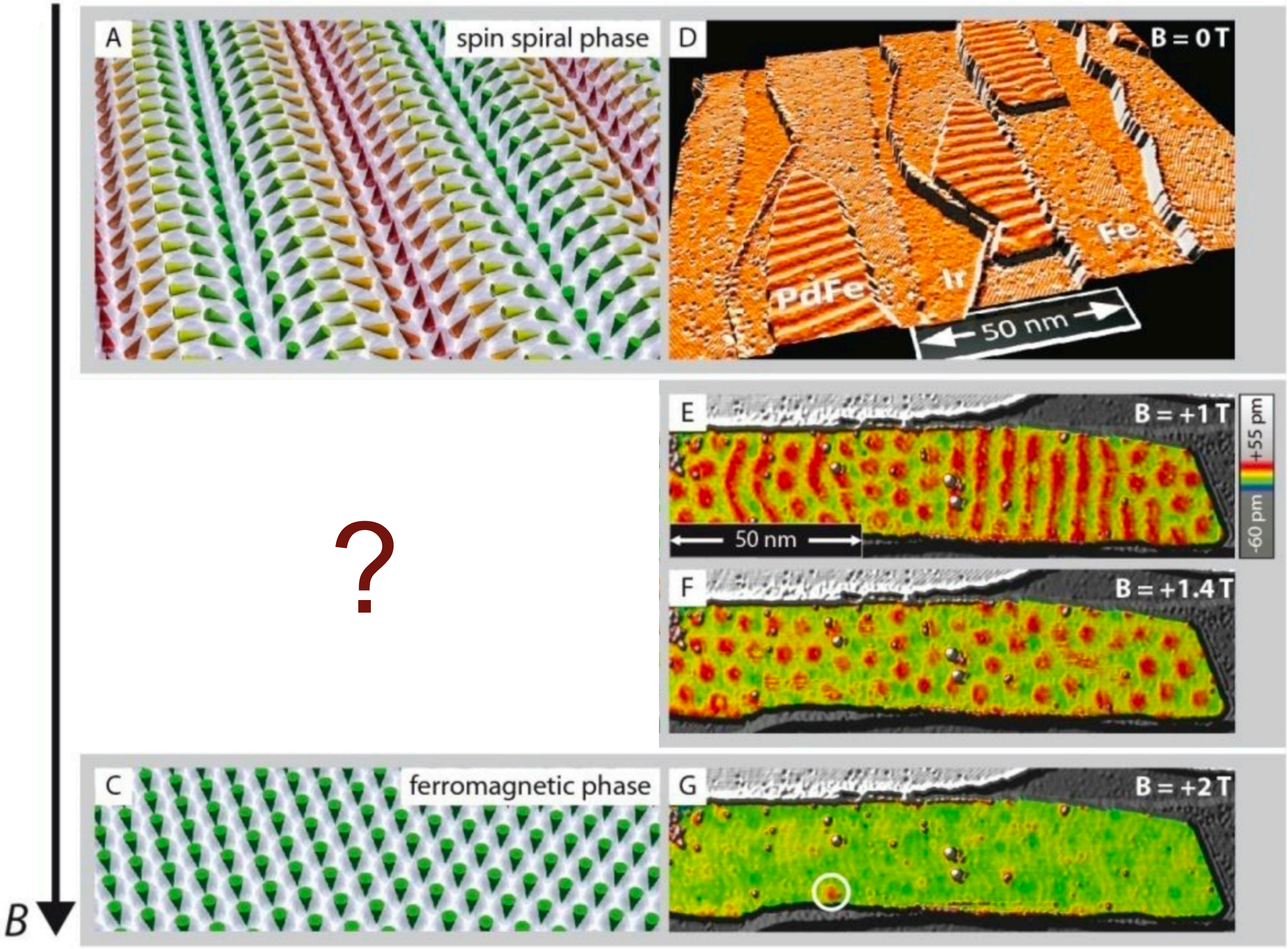


MH *et al.*, Nature Commun. **8**, 308 (2017)

Skyrmions in Pd/Fe/Ir(111)



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

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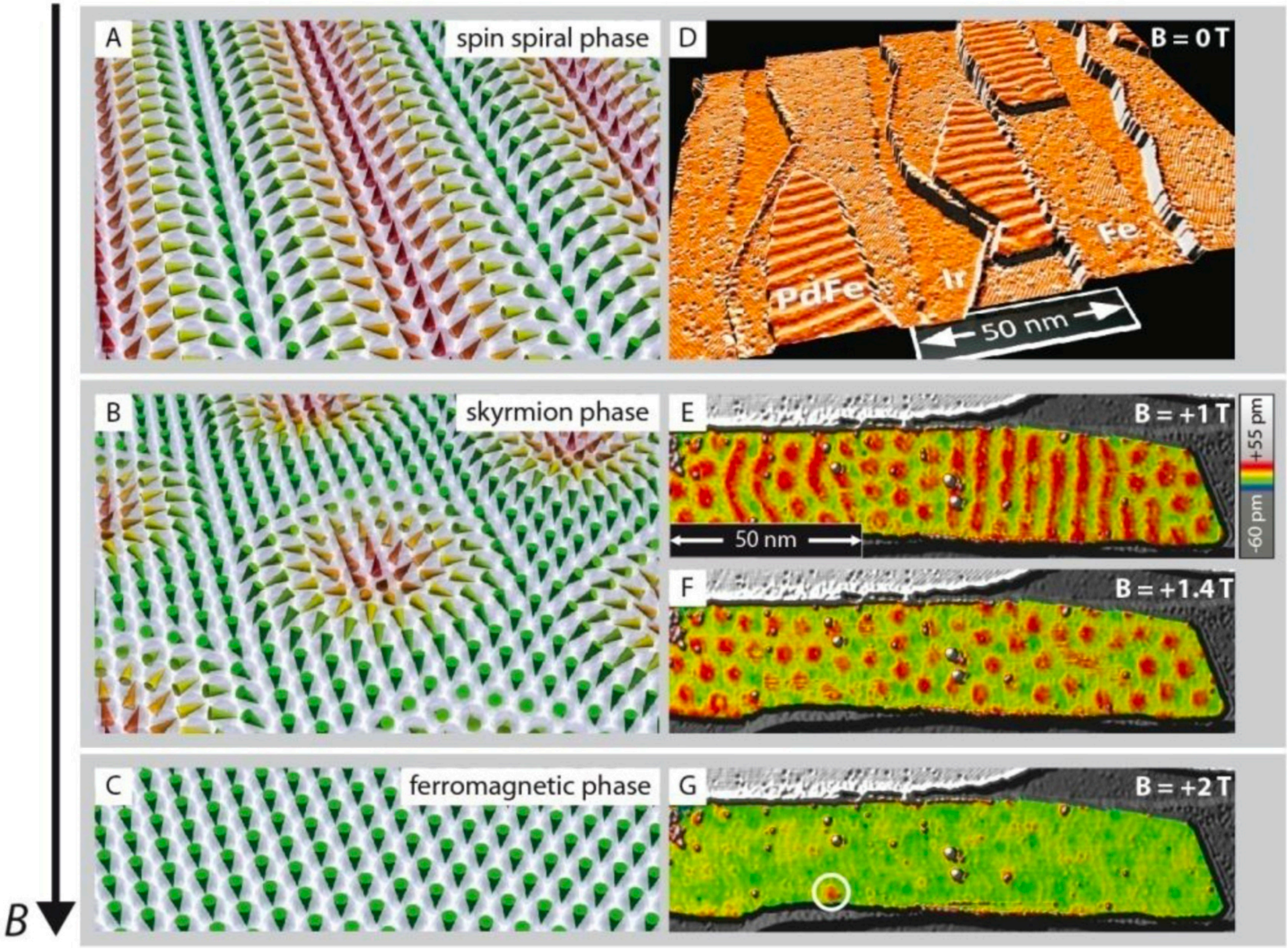

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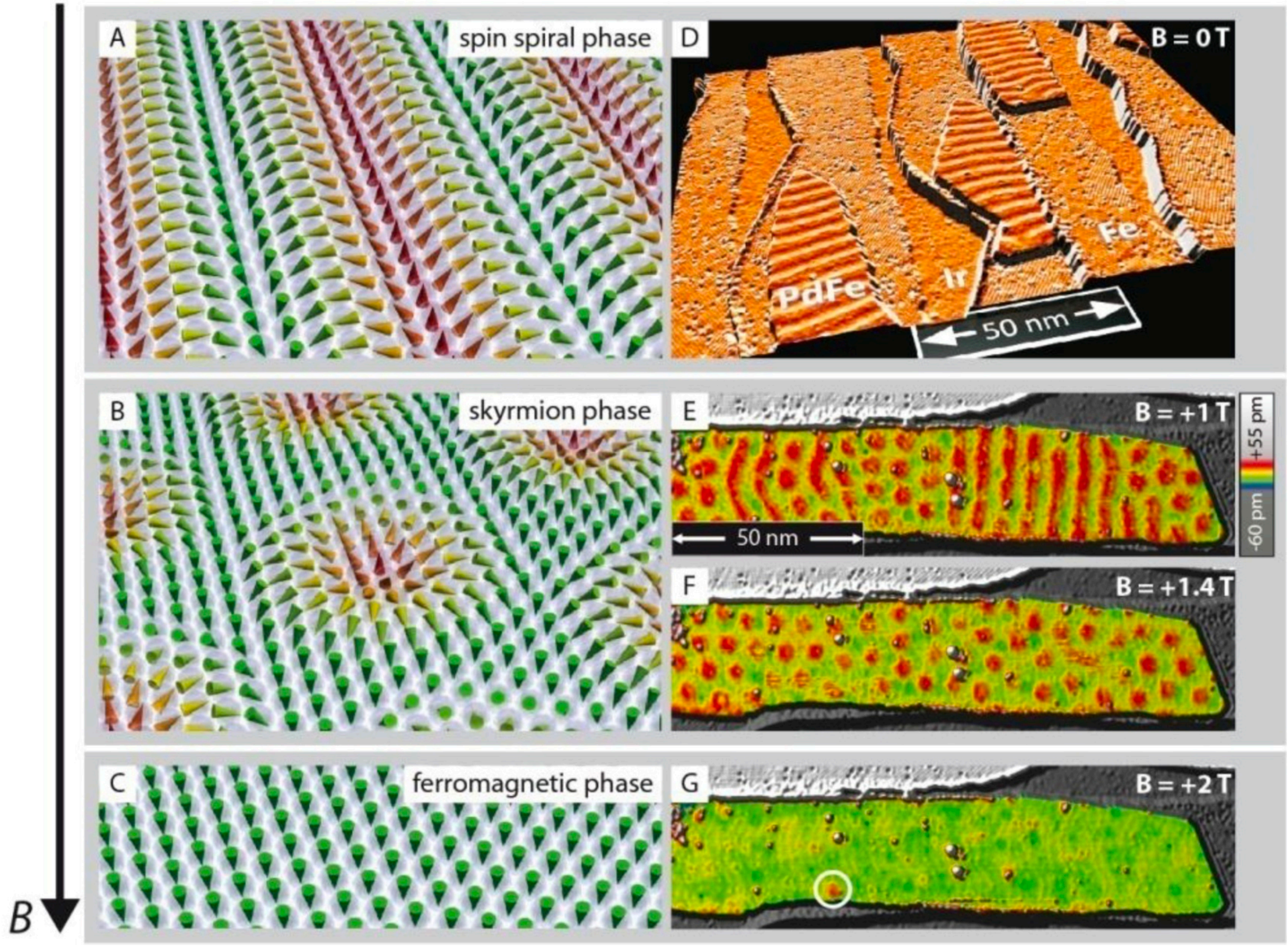

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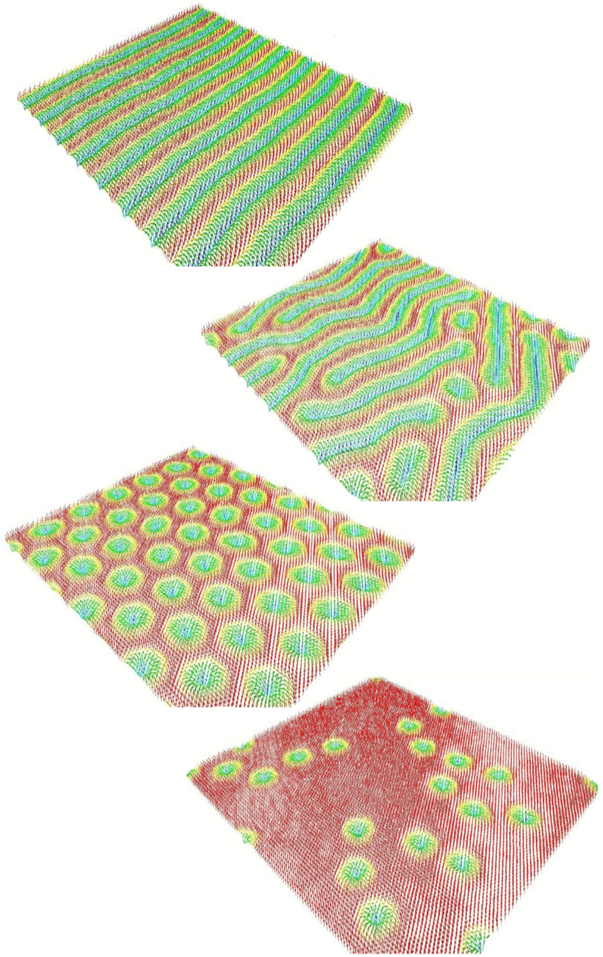

spin-spirals

↓

skyrmions in spiral-background

↓

skyrmion-**lattice**

↓

isolated skyrmions in ferromagnetic background

B

B. Dupé, **MH** *et al.*, Nature Commun. **5**, 4030 (2014)

Skyrmionic structures for technological applications

Nowadays data storage relies a lot on magnetic hard disk drive

https://en.wikipedia.org/wiki/Hard_disk_drive

- Data is stored in magnetic domains and is read by moving read-write-head
- Storage density as well as energy consumption are not optimal!

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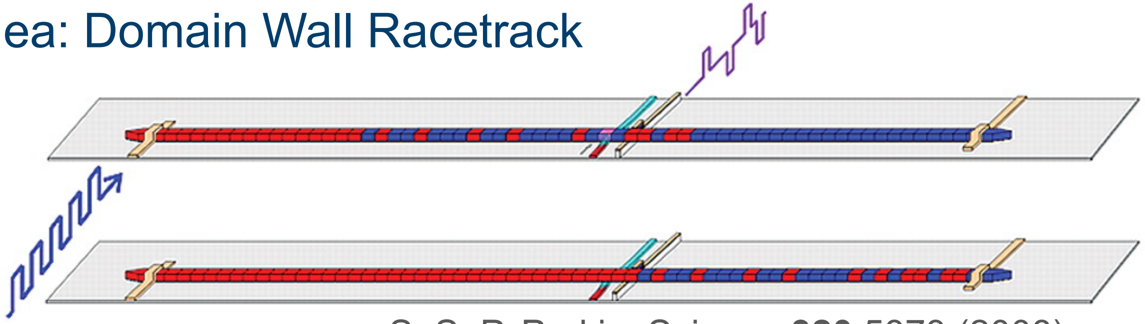
Idea: Domain Wall Racetrack



S. S. P. Parkin, Science **320** 5873 (2008)

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- faster, denser, less energy
- still not optimal: pinning (imperfections in material) can destroy information

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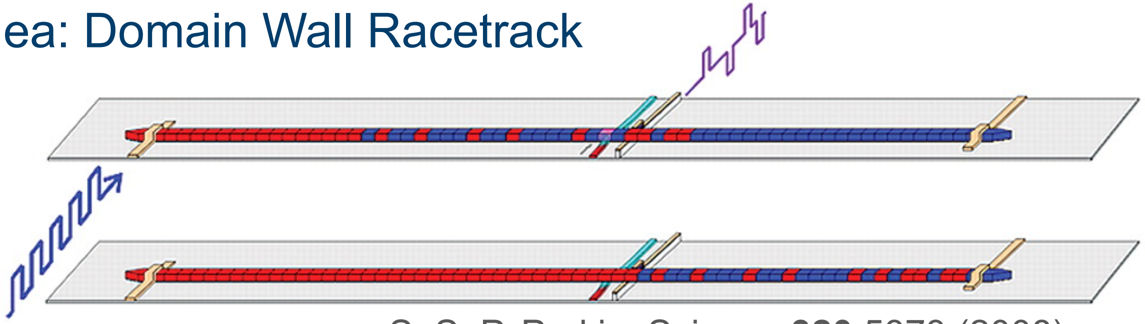

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Skyrmion racetrack memory

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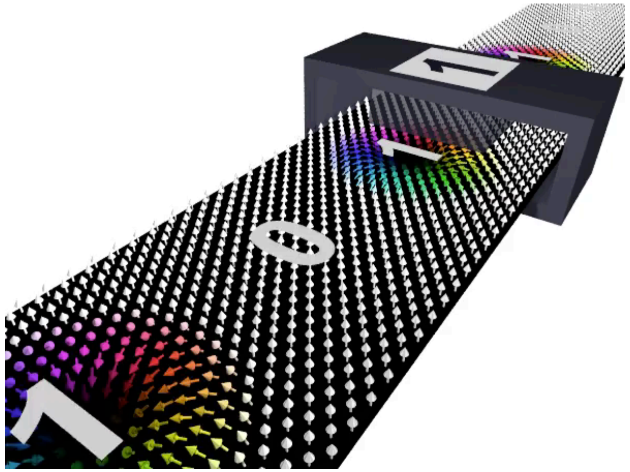
- less pinning



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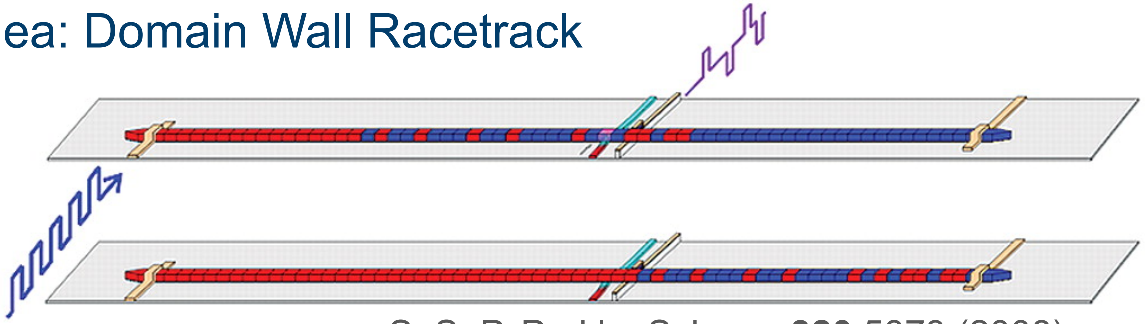

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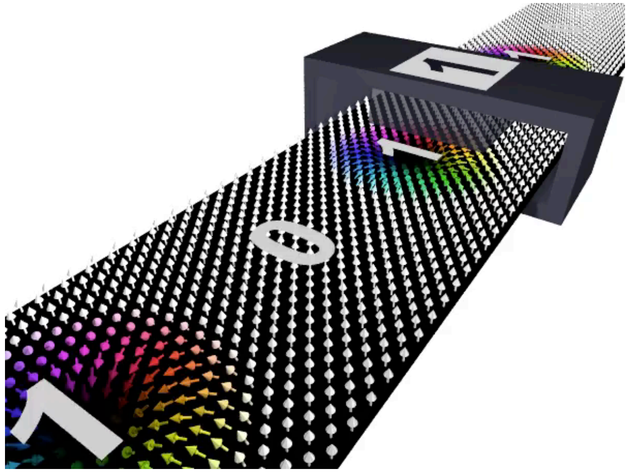

Spin-dynamics simulations

Spin-dynamics simulations

spirit
spirit-code.github.io

Atomistic Hamiltonian

$$H = -\sum_{ij} J_{ij} \left(\vec{S}_i \cdot \vec{S}_j\right) - \sum_{ij} \vec{D}_{ij} \cdot \left(\vec{S}_i \times \vec{S}_j\right) - \sum_i K_i \left(\vec{S}_i \cdot \hat{K}_i\right)^2 - \sum_i \vec{B} \cdot \vec{S}_i$$

Spin-dynamics simulations

spirit-code.github.io

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Landau-Lifshitz-Gilbert dynamics

$$\frac{\partial \vec{S}_i}{\partial t} = -\frac{\gamma}{(1+\alpha^2)\mu_i} \vec{S}_i \times \vec{B}_i^{\mathrm{eff}} - \frac{\gamma\alpha}{(1+\alpha^2)\mu_i} \vec{S}_i \times \left(\vec{S}_i \times \vec{B}_i^{\mathrm{eff}}\right)$$

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Spin-dynamics simulations

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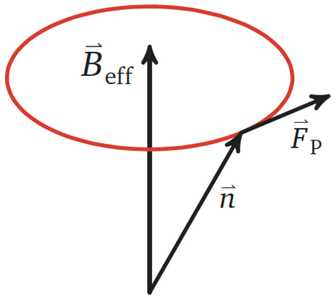

Precession

Spin-dynamics simulations

spirit-code.github.io

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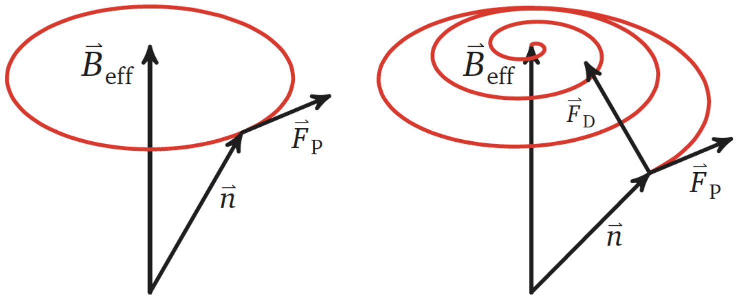

Spin-dynamics simulations

spirit

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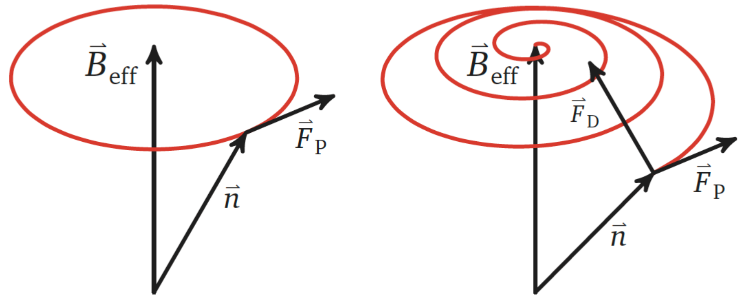

Precession Damping

Spin-dynamics simulations

spirit

spirit-code.github.io

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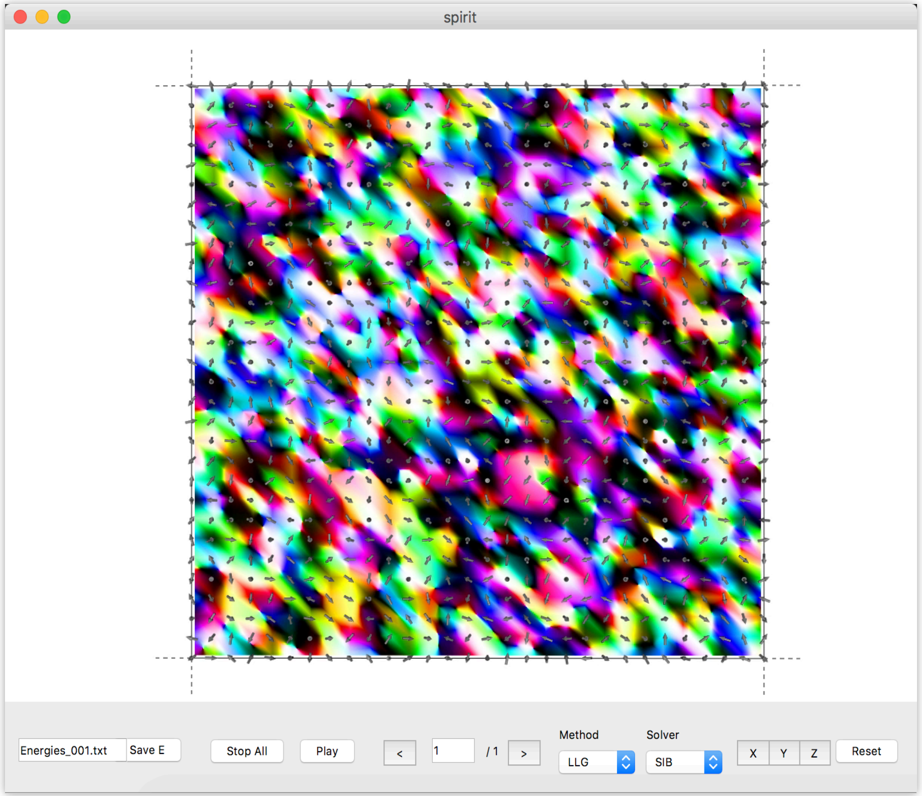
Precession

Damping

Spin Torque (electric current)
Precession-like

Non-adiabatic excitation
Damping-like



Spin-dynamics simulations

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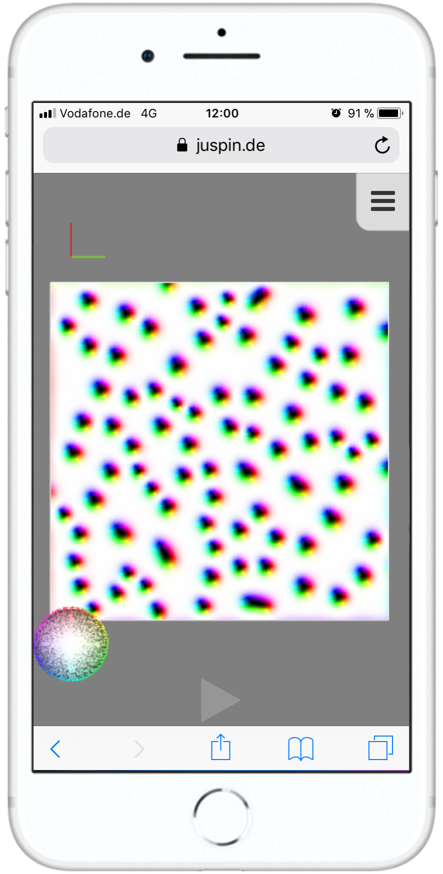
juspin.de



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Precession — Damping

Spin Torque (electric current)
Precession-like

Non-adiabatic excitation
Damping-like

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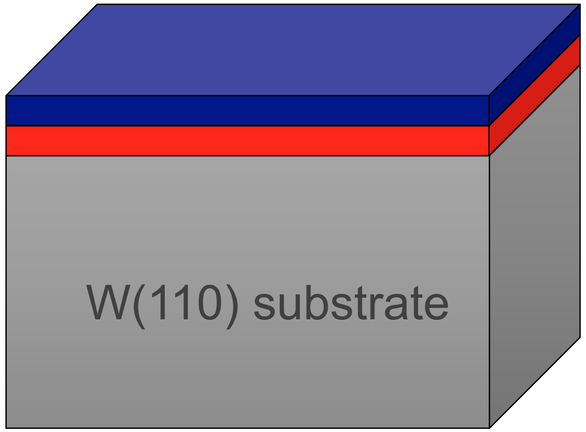
Recent example of research interest

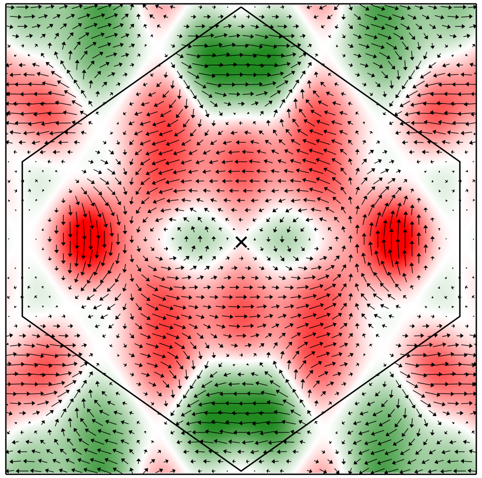
Antiskyrmions in 2Fe/W(110)

MH *et al.*, Nature Commun. **8**, 308 (2017)

2Fe/W(110): density functional theory calculations



D(q) in BZ



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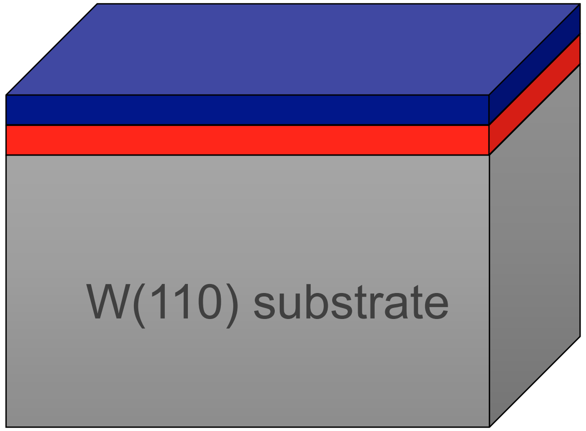
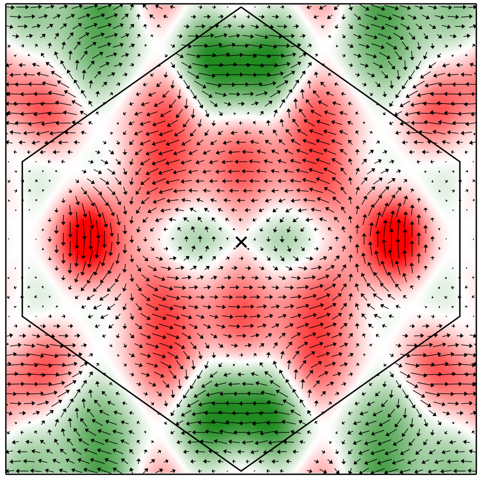


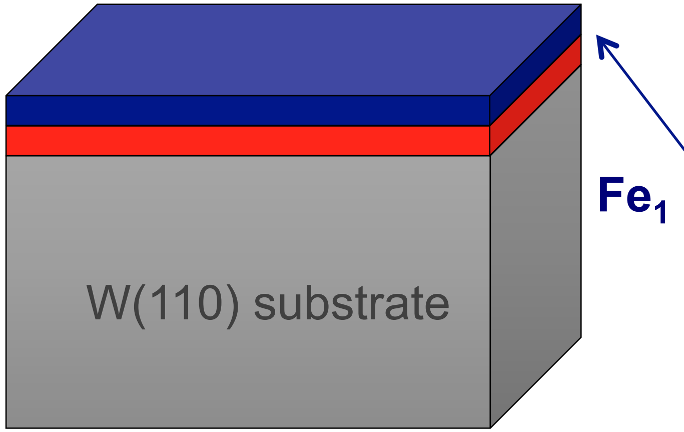
D(q) in BZ



FT

real-space: $\mathbf{D}_{0j}$

2Fe/W(110): density functional theory calculations



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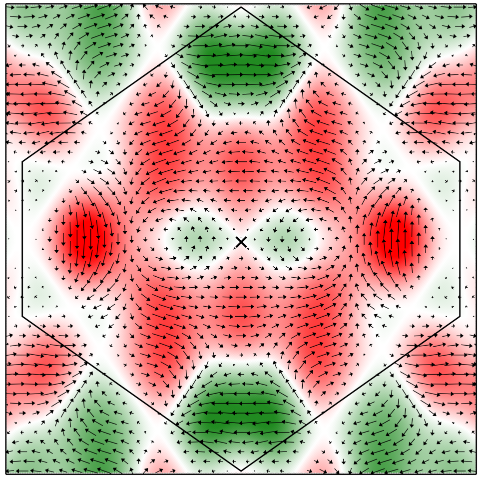

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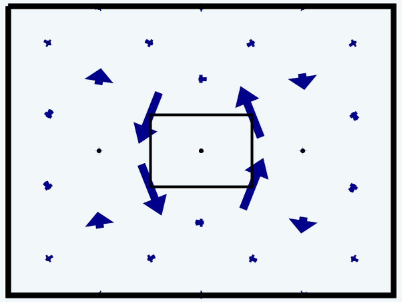

DRIVING THE EXASCALE TRANSITION

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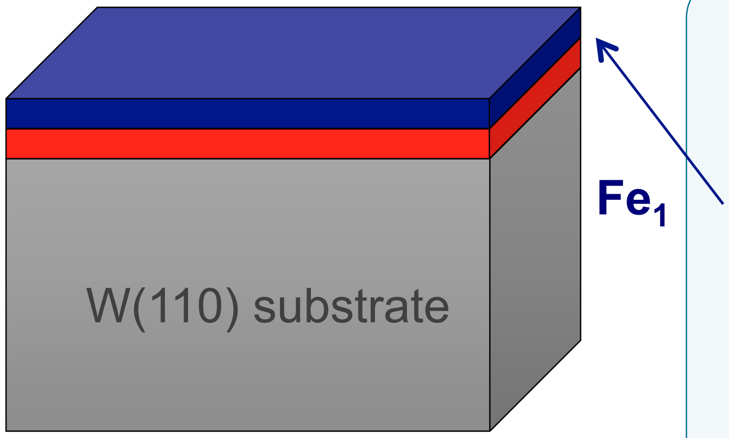

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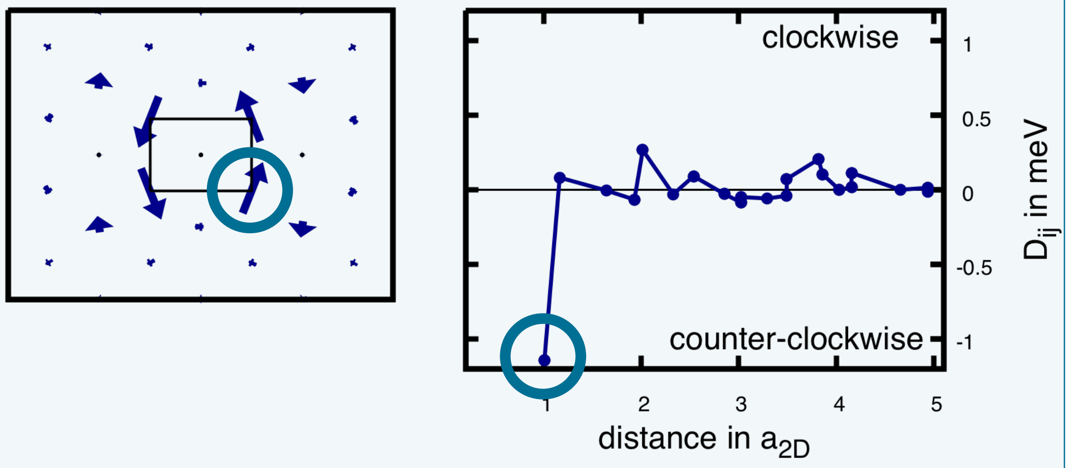
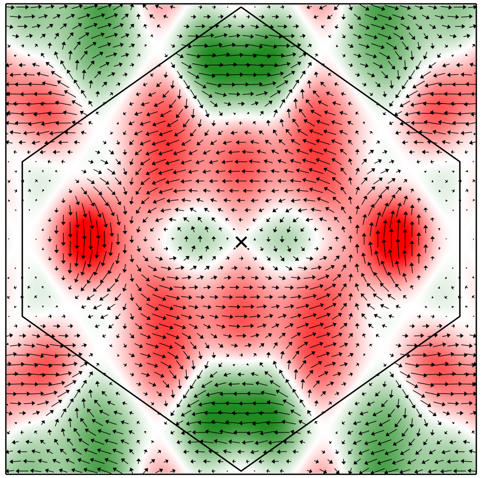


surface layer

- main contribution from 1st nearest neighbor

D(q) in BZ



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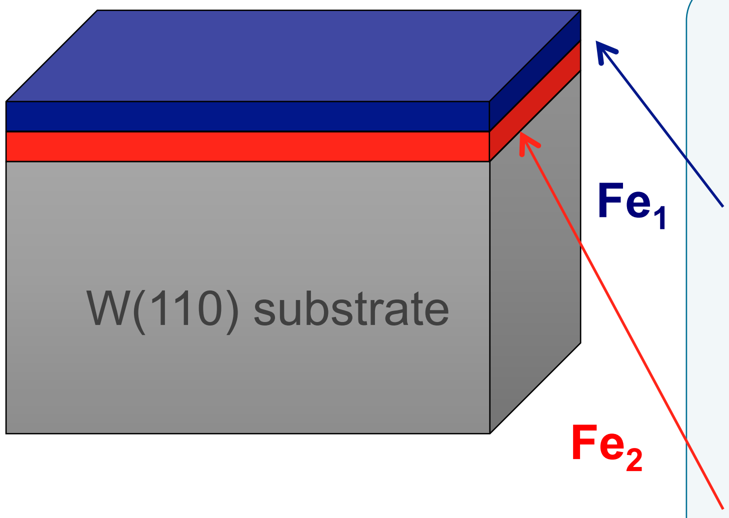

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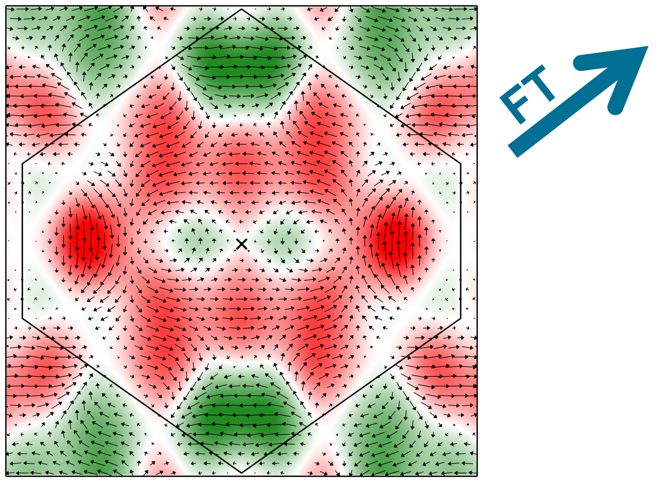

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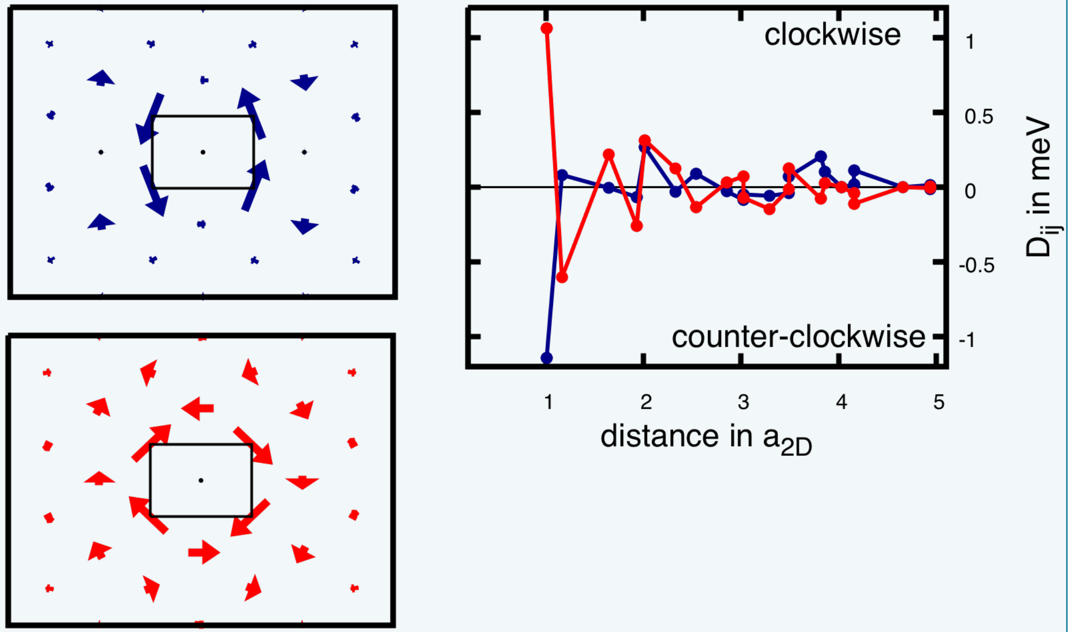

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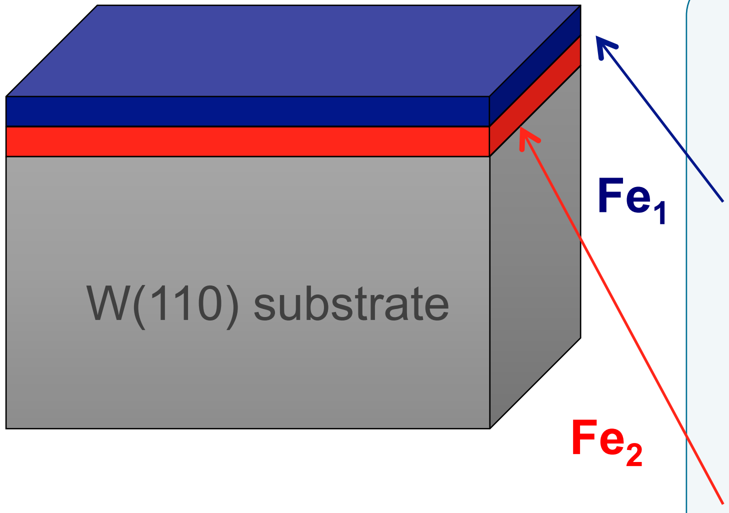

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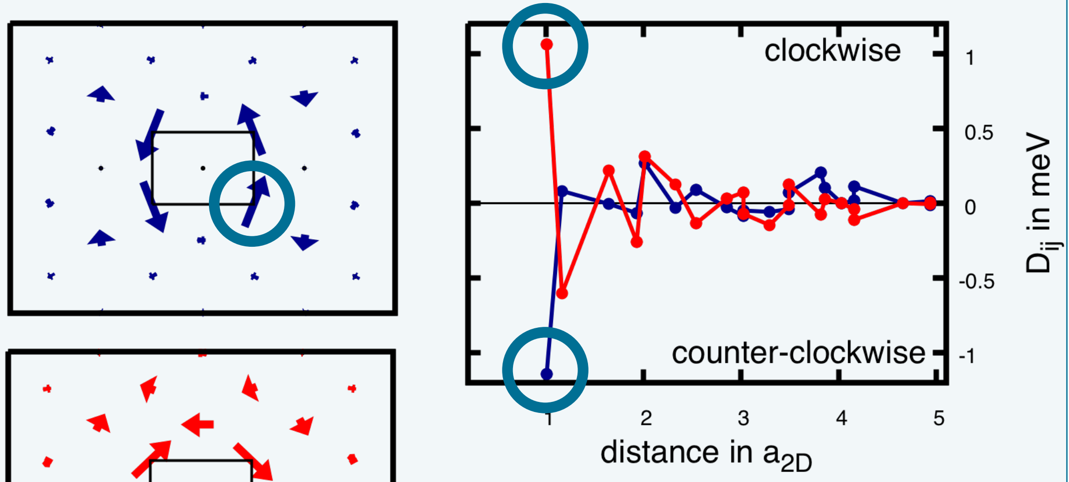

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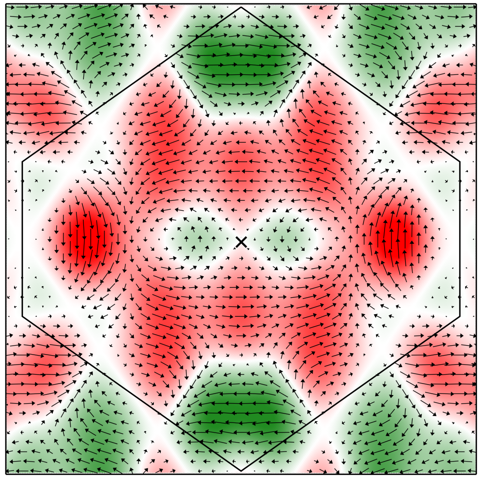
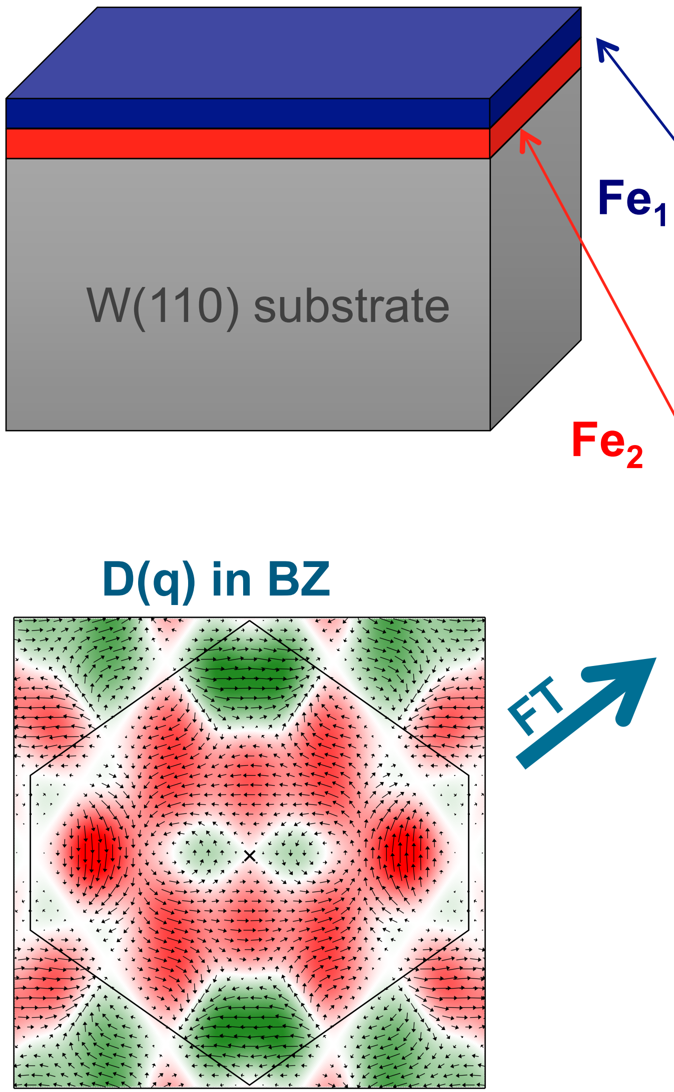


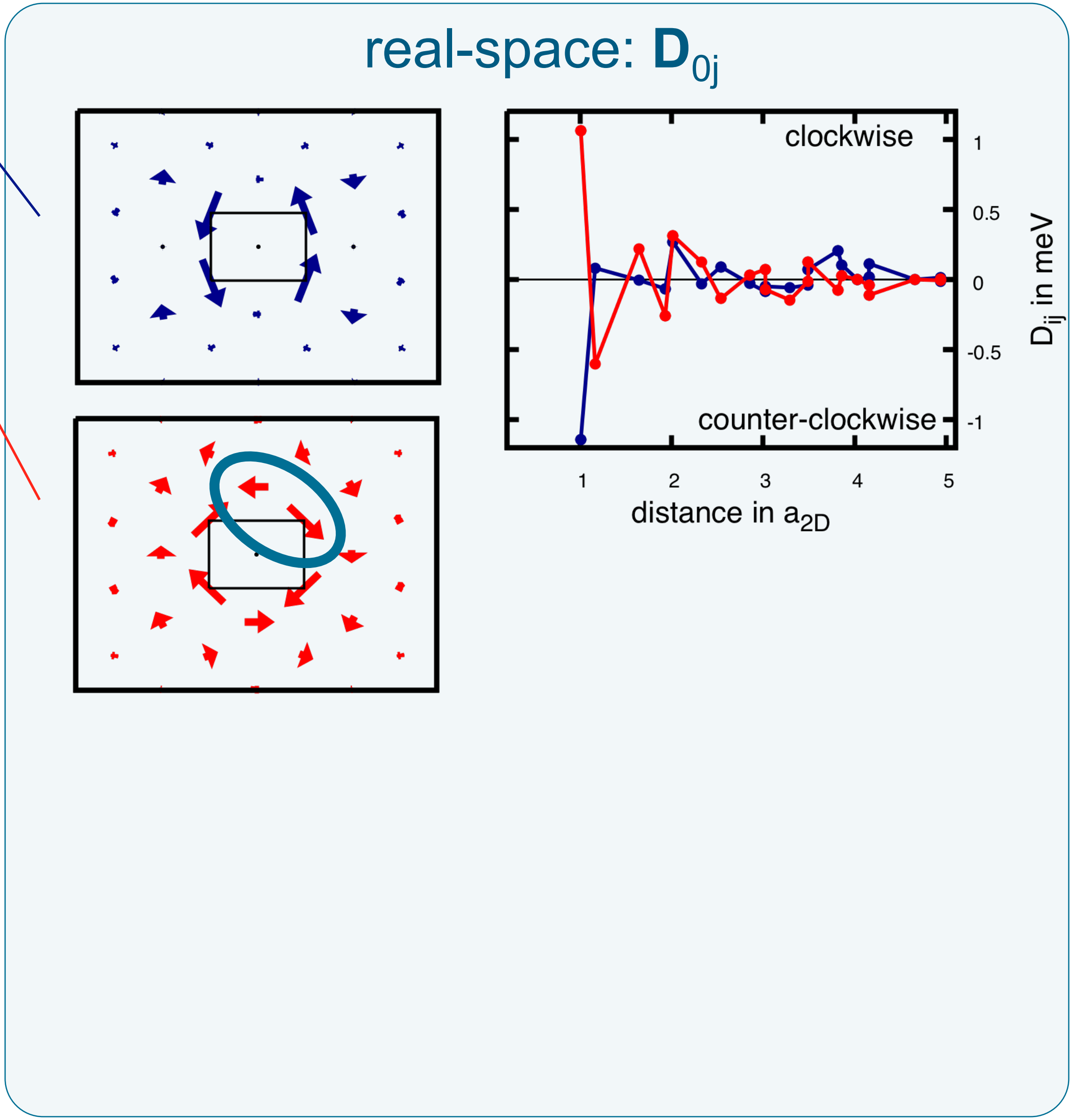
FT

surface layer
- main contribution from 1st nearest neighbor

n.n in both layers
- opposite rotational sense

2Fe/W(110): density functional theory calculations





surface layer

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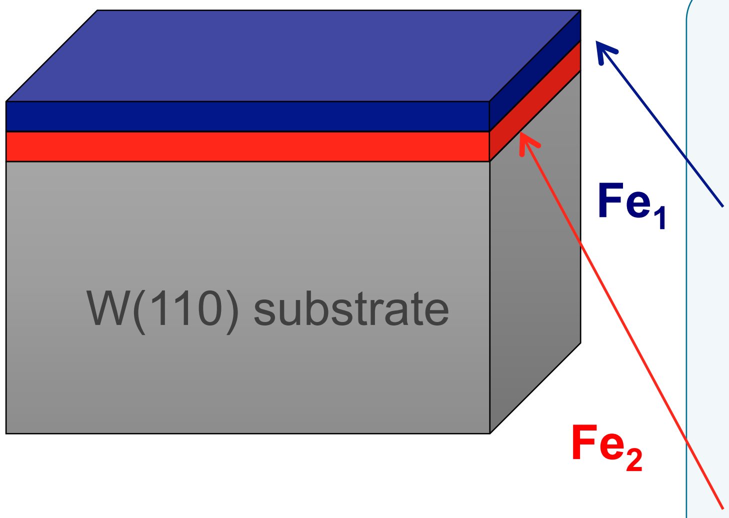
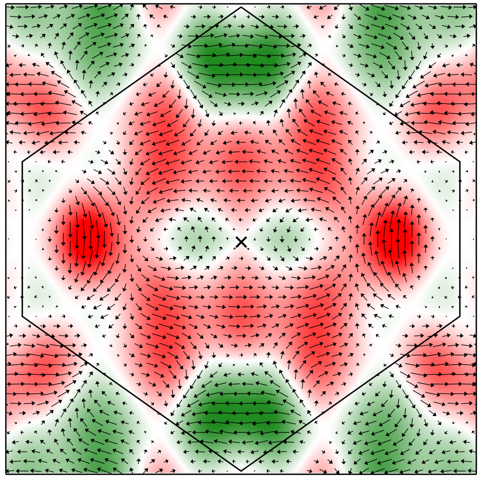
interface layer

- contribution from more neighbors
- different directions

2Fe/W(110): density functional theory calculations



D(q) in BZ



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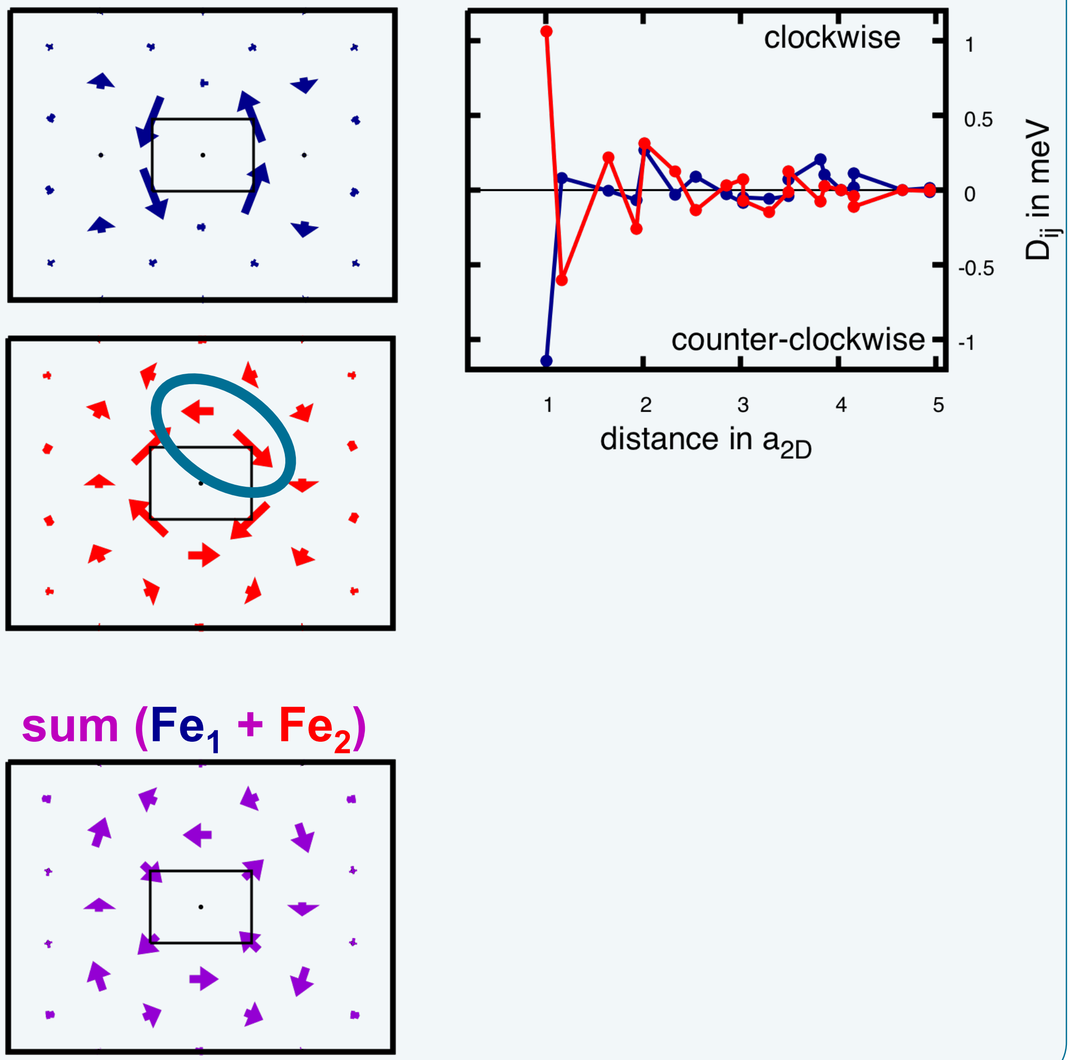

surface layer
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www.flapw.de Fleur

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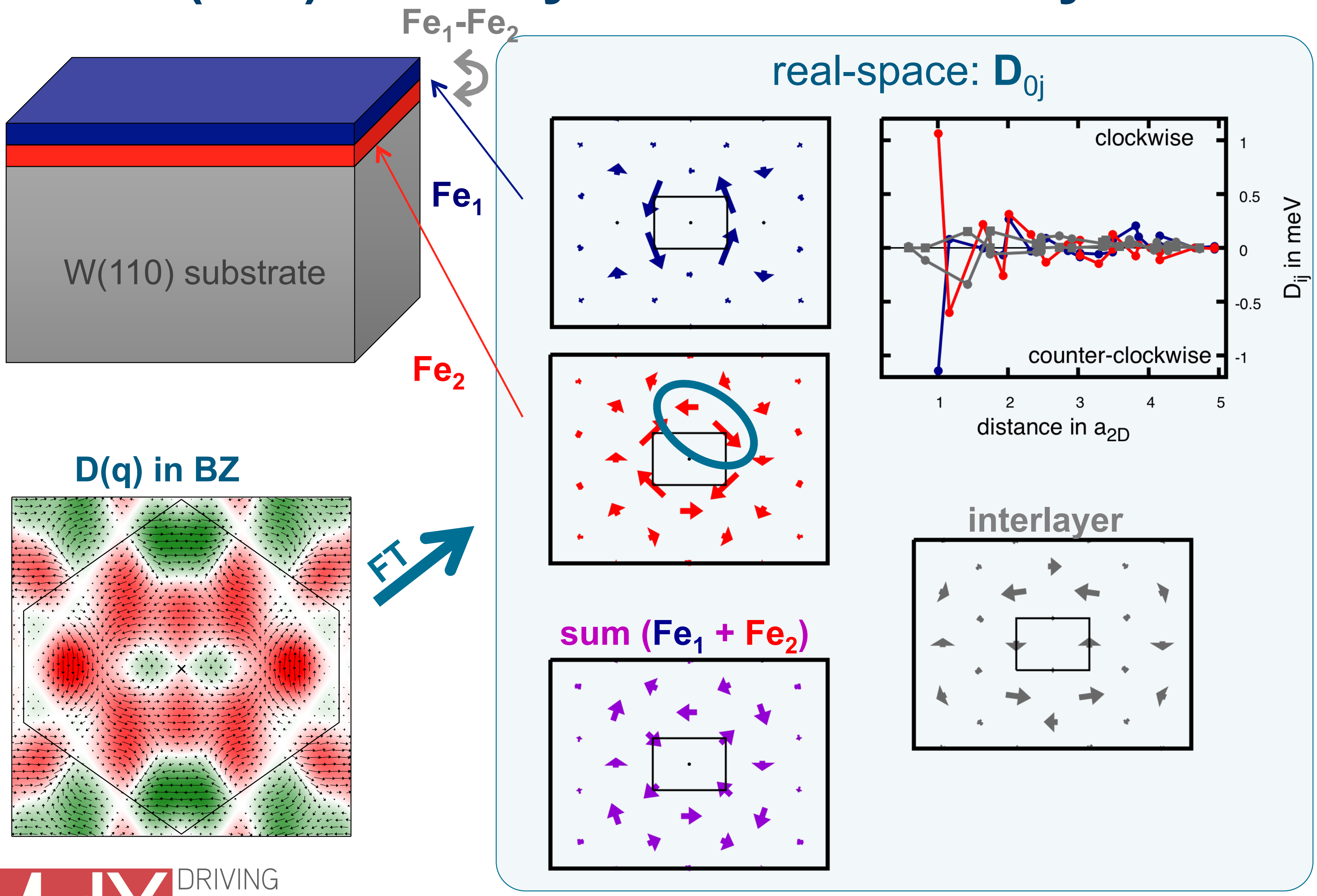
2Fe/W(110): density functional theory calculations



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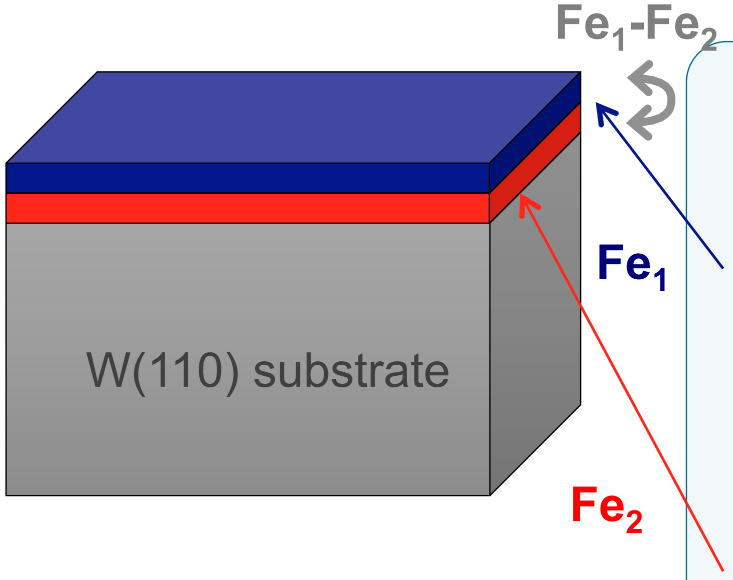

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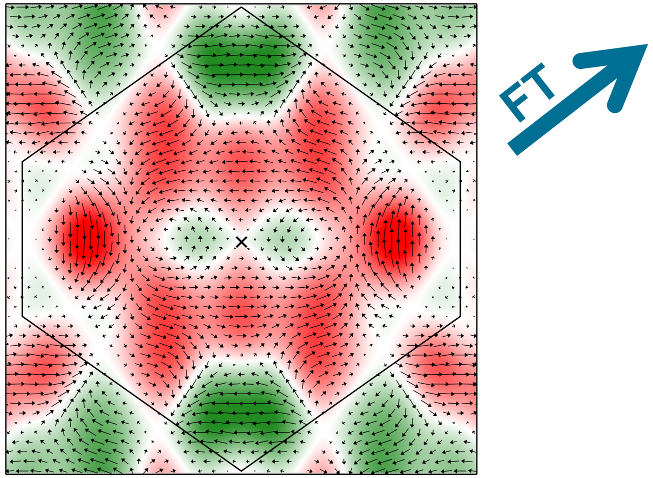

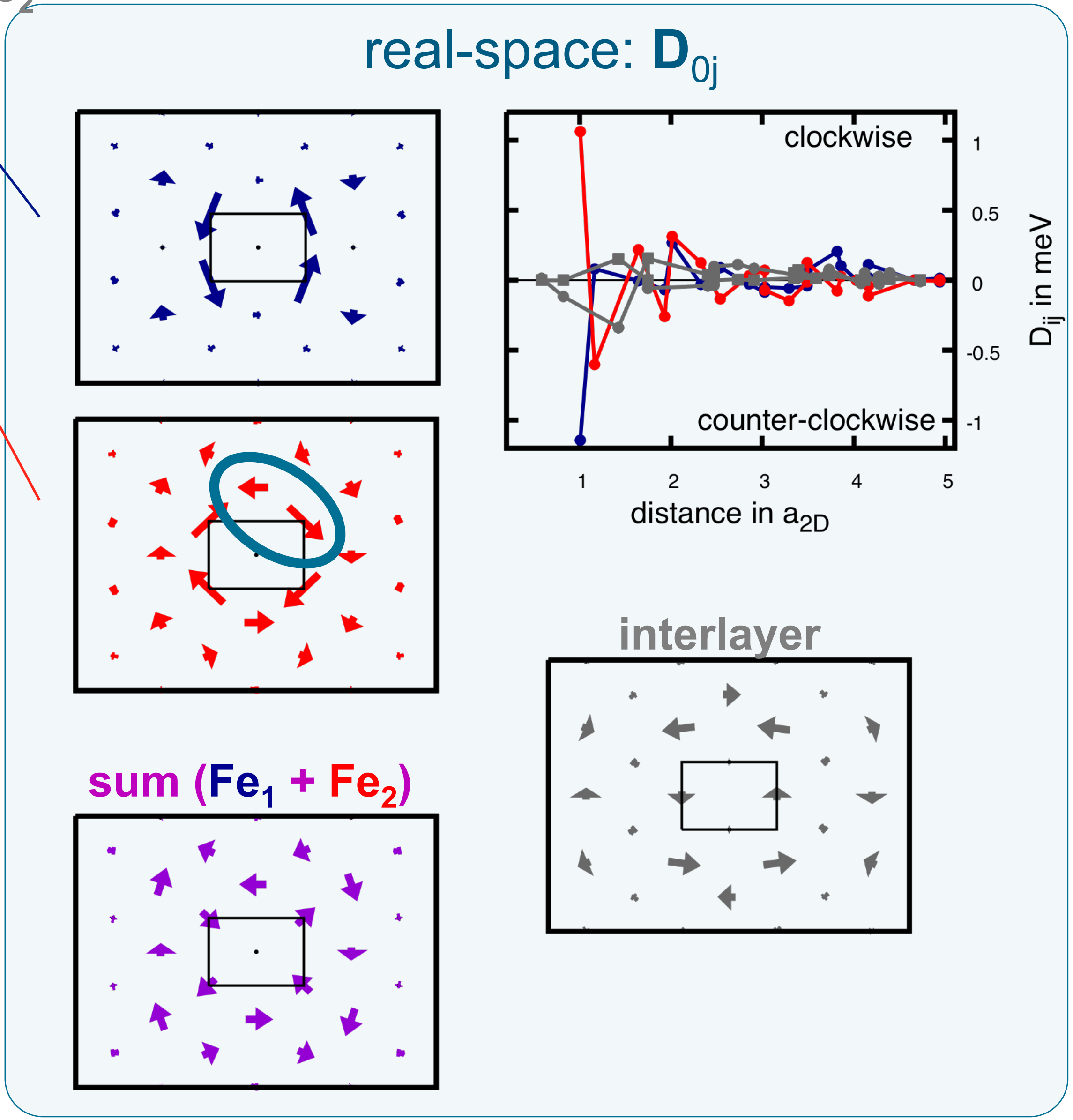

surface layer
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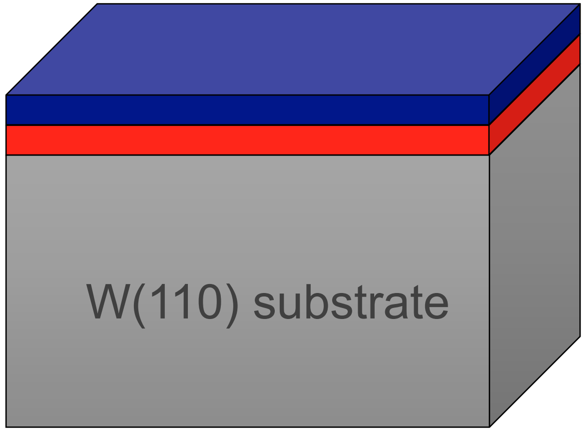
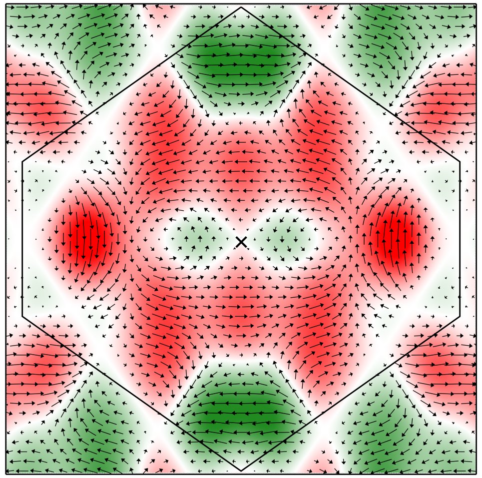
→ complex behavior

what kind of magnetic structures could be (meta-) stable in this system?

2Fe/W(110): density functional theory calculations



D(q) in BZ



reciprocal-space: **D(q)**

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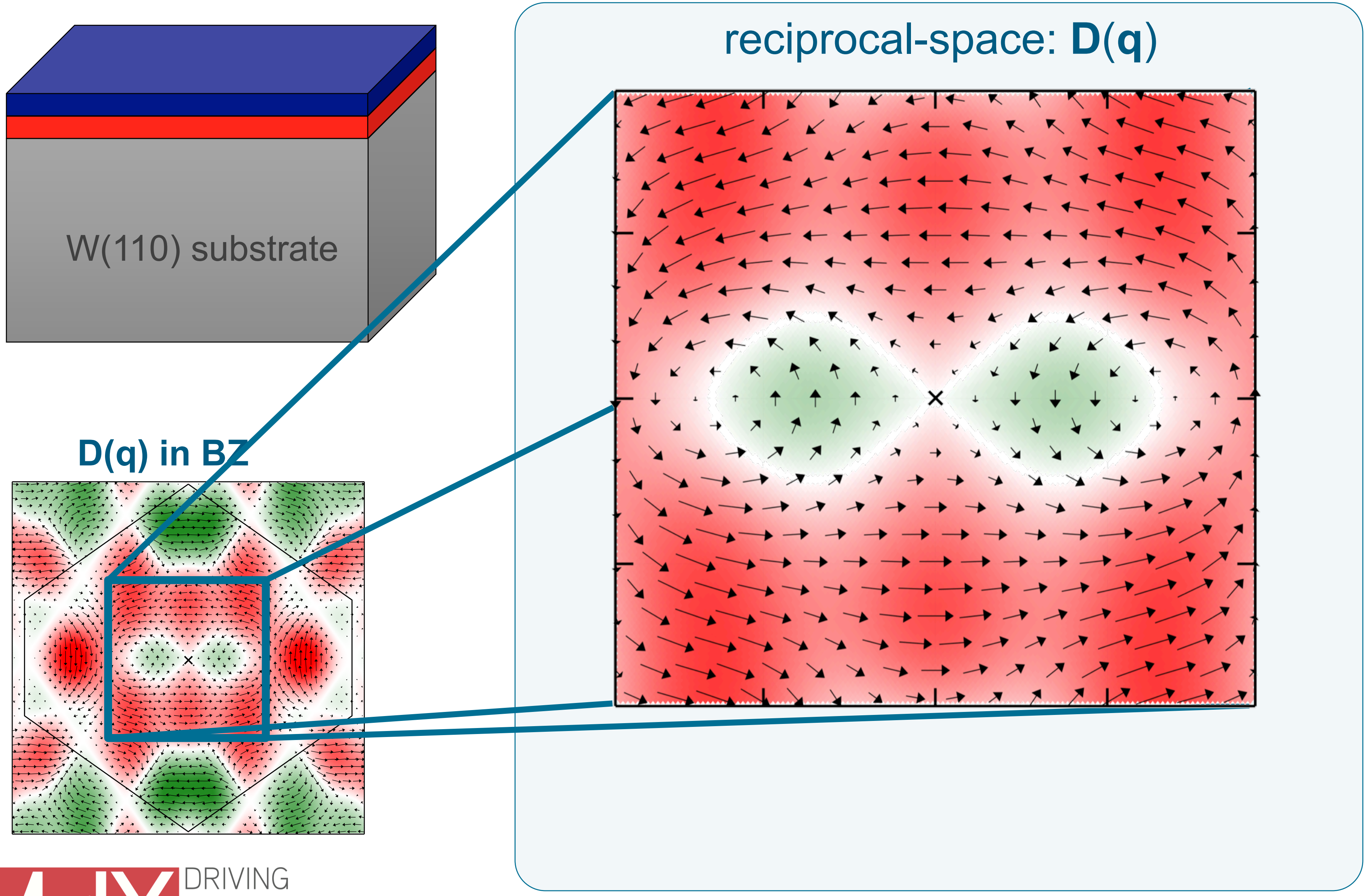

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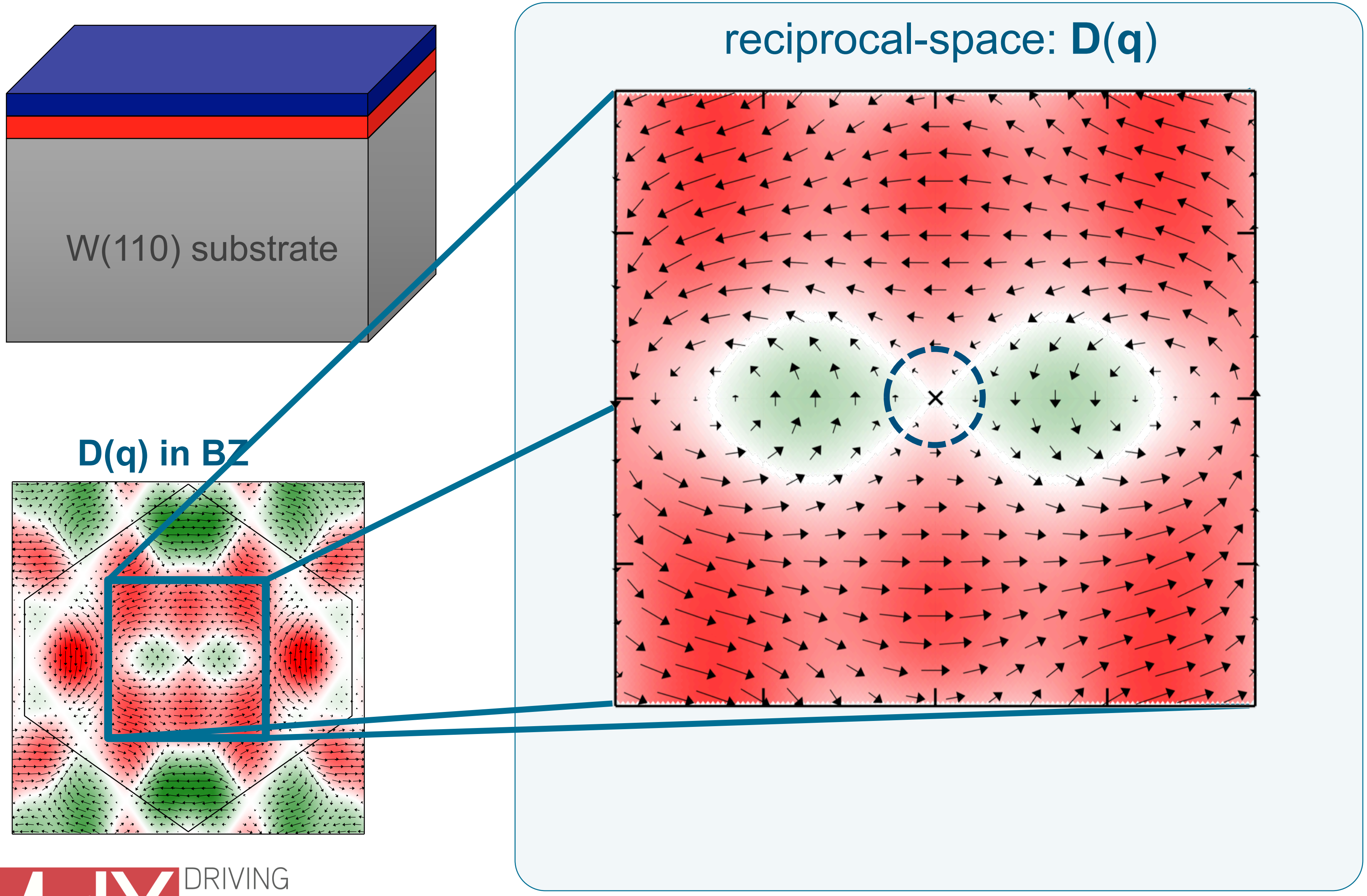
2Fe/W(110): density functional theory calculations

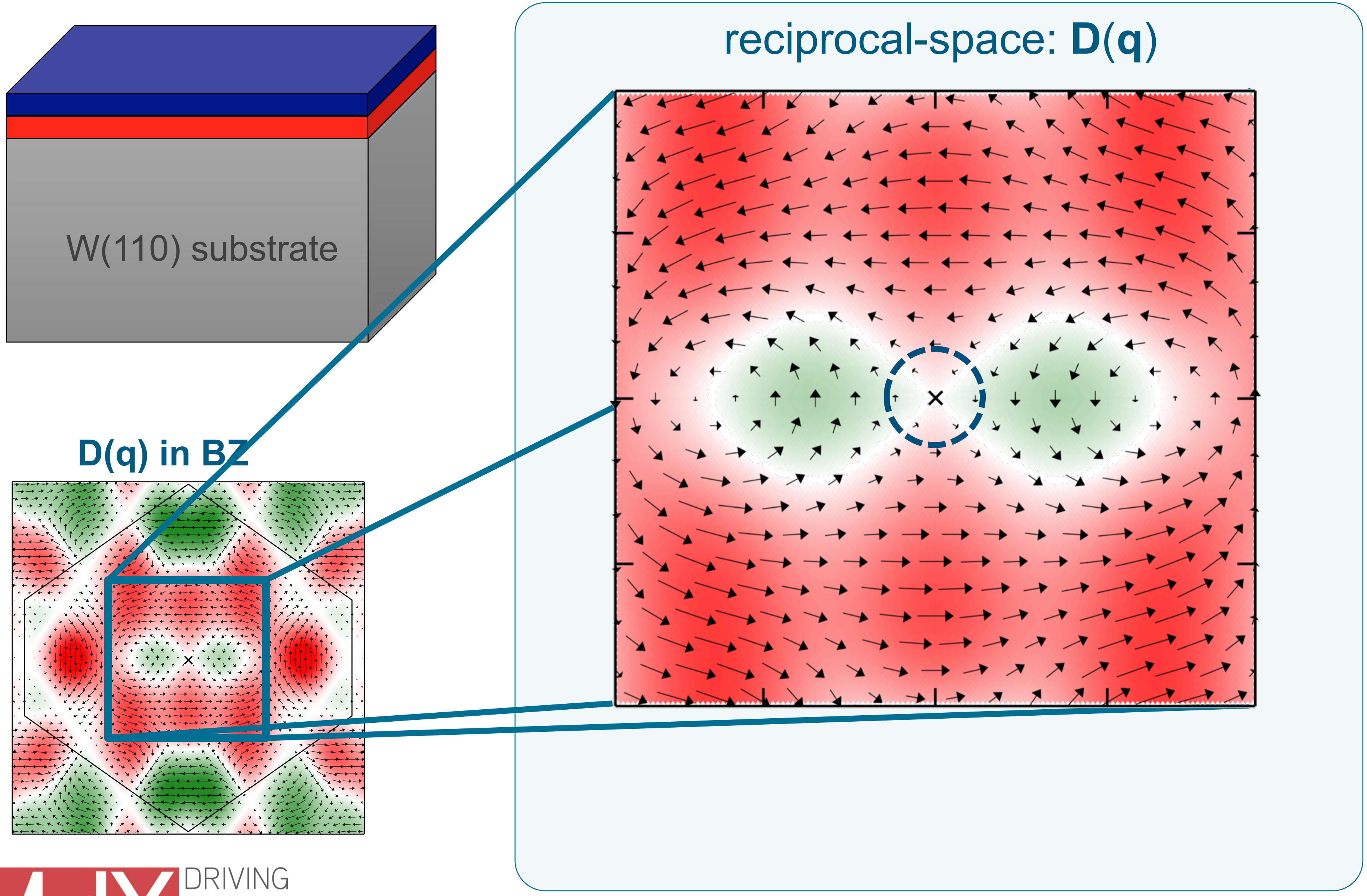


$$\hat{e}_{rot} \parallel \underline{\underline{\mathcal{D}}}\, \hat{e}_{\rho}$$

For small q-vectors, i.e. long periods:

opposite chirality (see color code) along different directions

2Fe/W(110): density functional theory calculations



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$\longrightarrow$ det $\boldsymbol{D} < 0$

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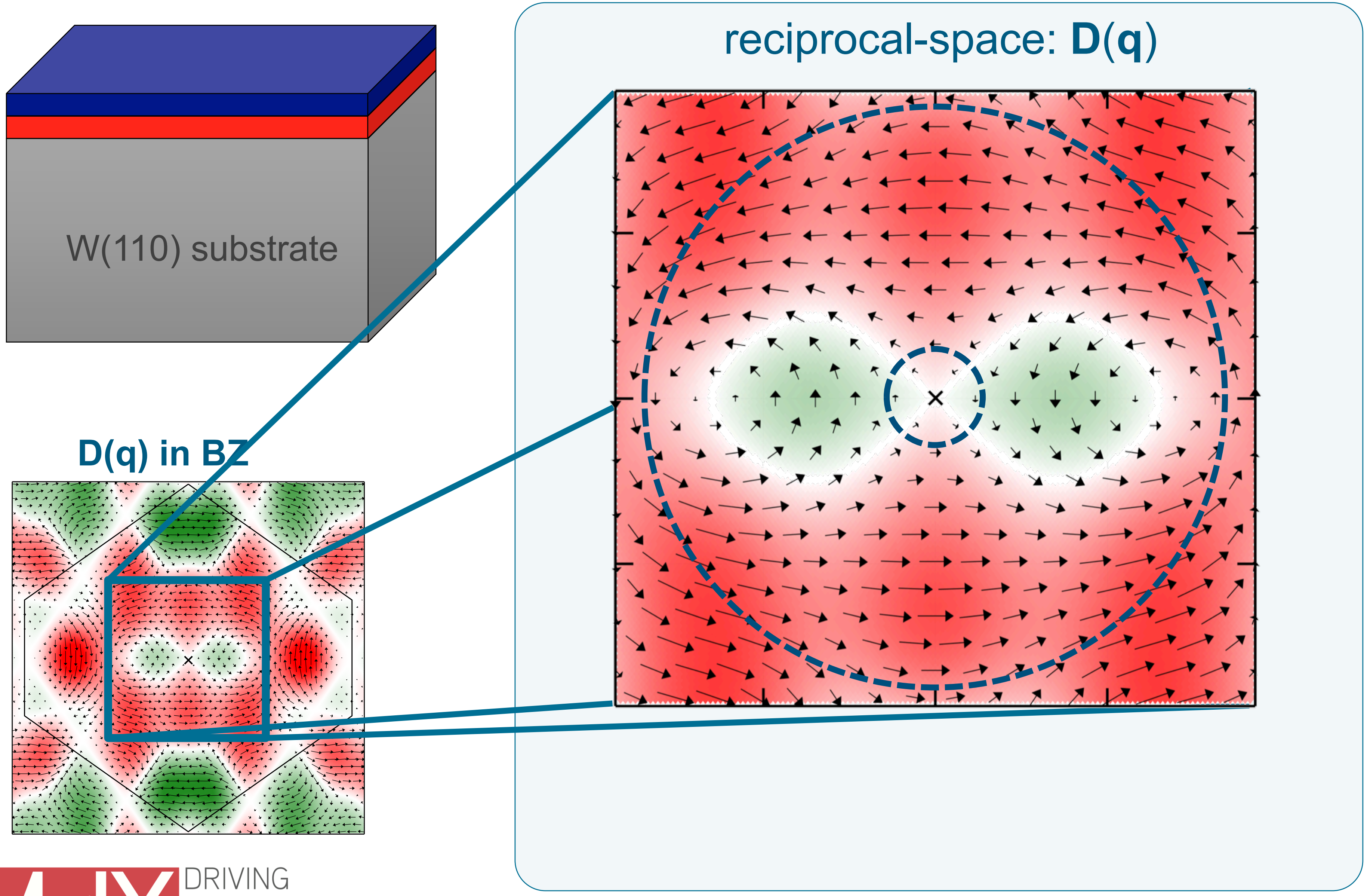

$\hat{e}_{rot} \parallel \underline{\underline{\mathcal{D}}}\, \hat{e}_\rho$

For small q-vectors, i.e. long periods:

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For larger q-vectors, i.e. short periods:

same chirality along different directions

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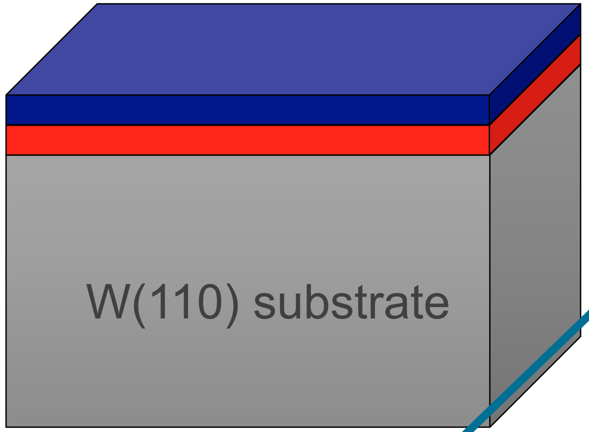
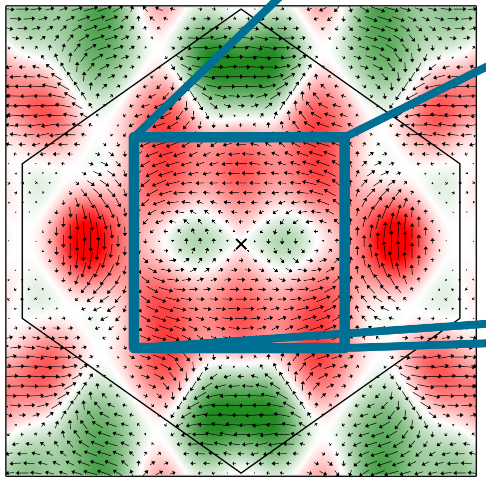
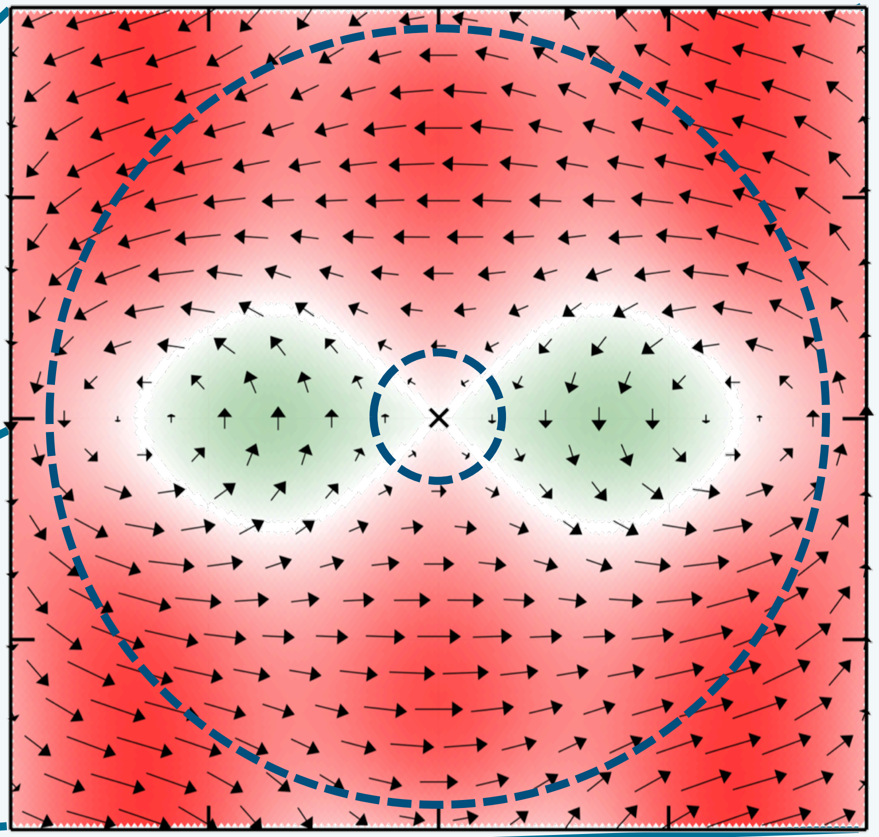
2Fe/W(110): density functional theory calculations



D(q) in BZ



reciprocal-space: **D(q)**



Are (anti-)skyrmions stable in 2Fe/W(110)?

$$\hat{e}_{rot} \parallel \underline{\underline{\mathcal{D}}}\, \hat{e}_\rho$$

For small q-vectors, i.e. long periods:

opposite chirality (see color code) along different directions

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$\longrightarrow$ det $\boldsymbol{D} > 0$

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2Fe/W(110): spin-dynamics simulations

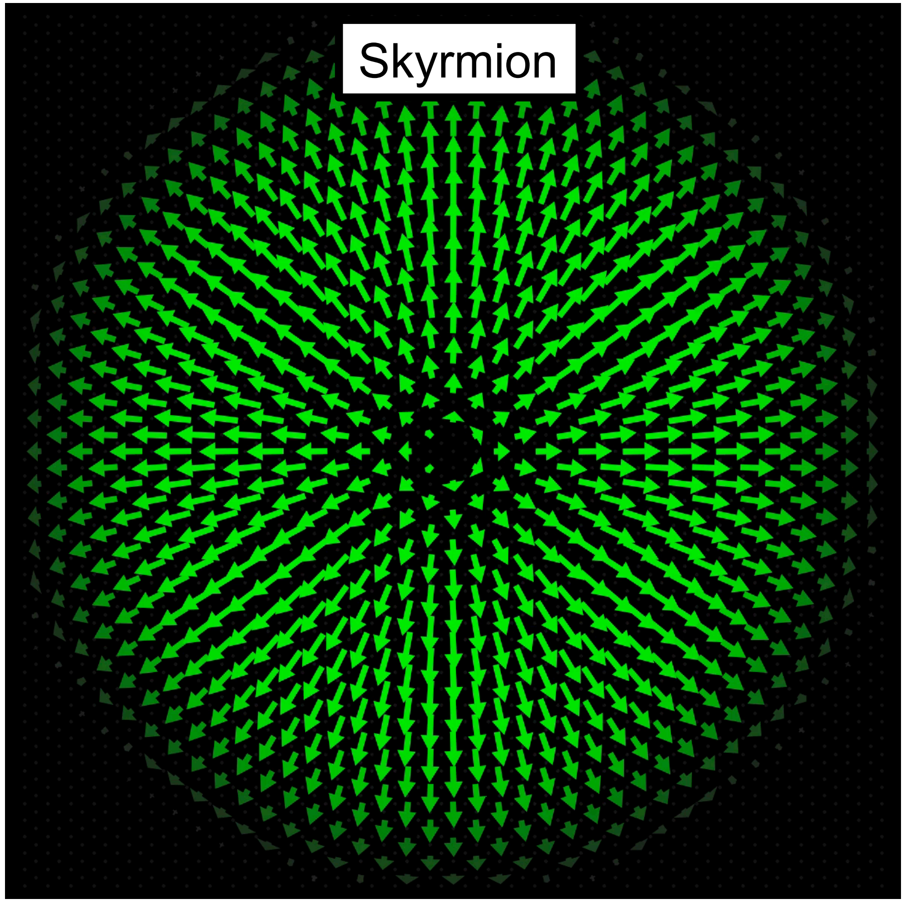
- start from **artificially created structure**

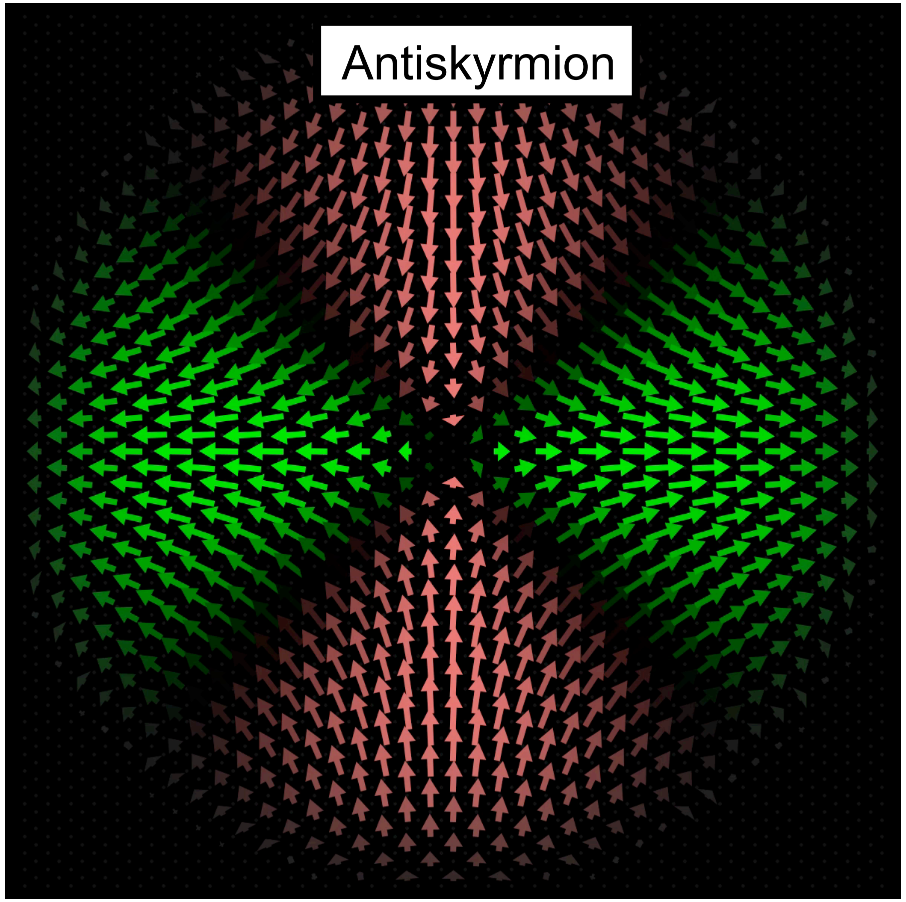
Skyrmion

Antiskyrmion

2Fe/W(110): spin-dynamics simulations

- start from **artificially created structure**





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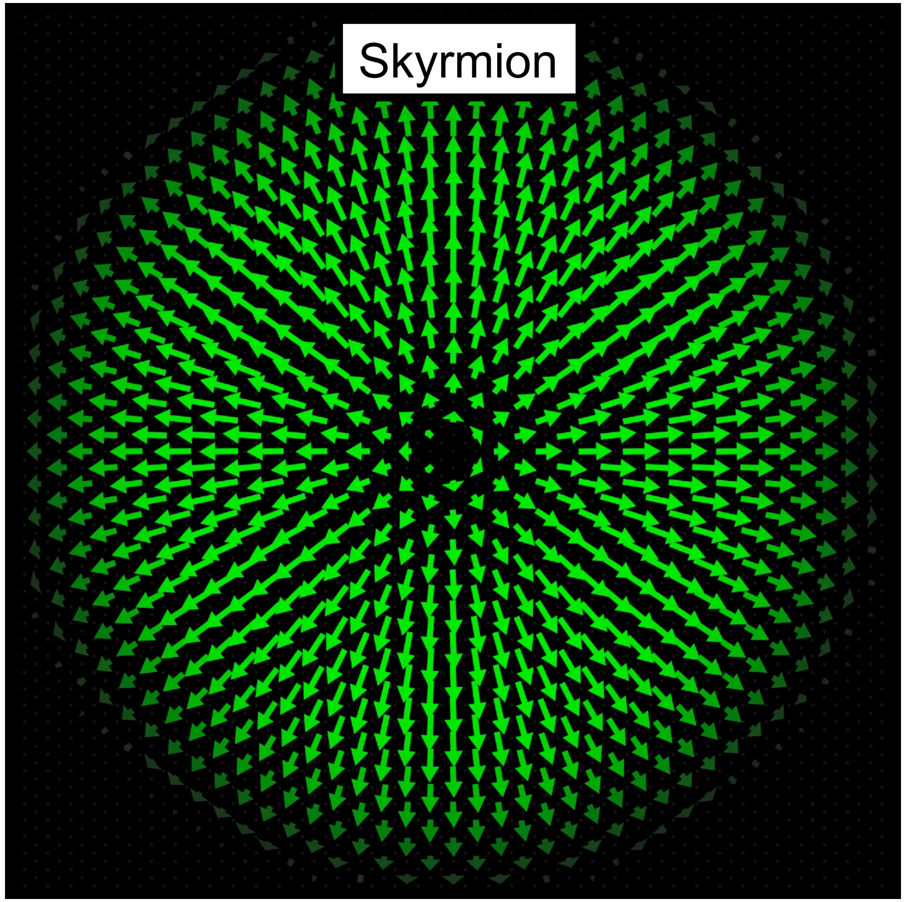

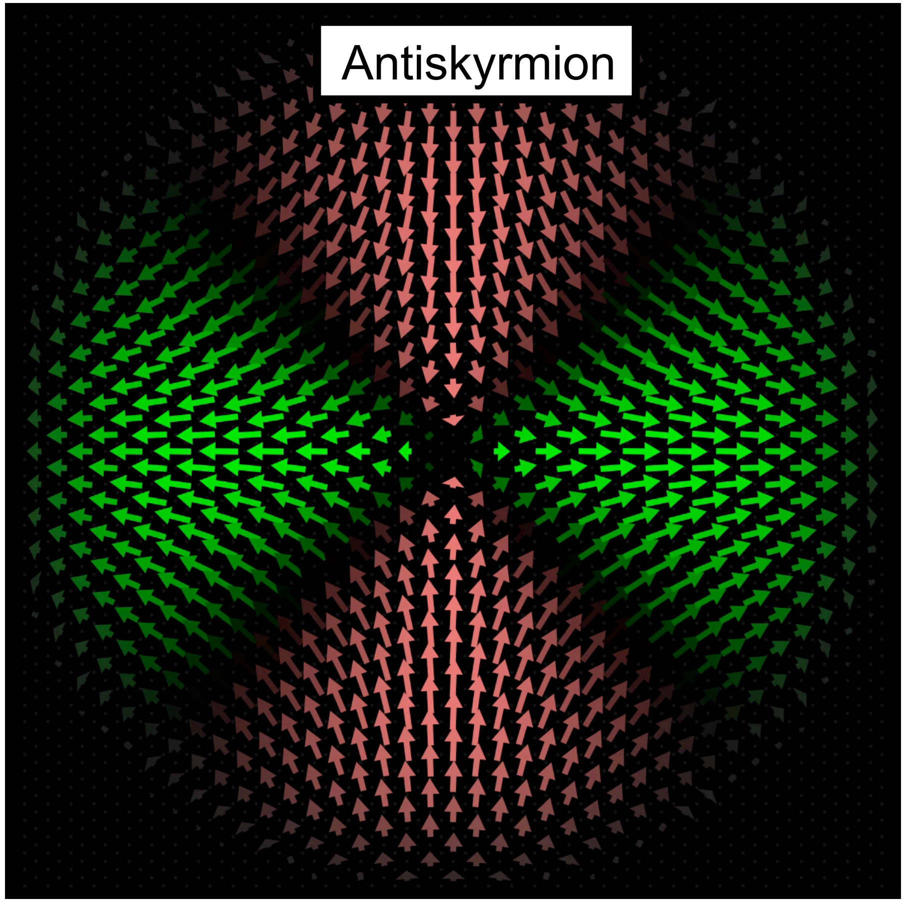

✗ Unstable

✔ Stable

2Fe/W(110): spin-dynamics simulations

- start from **random structure**

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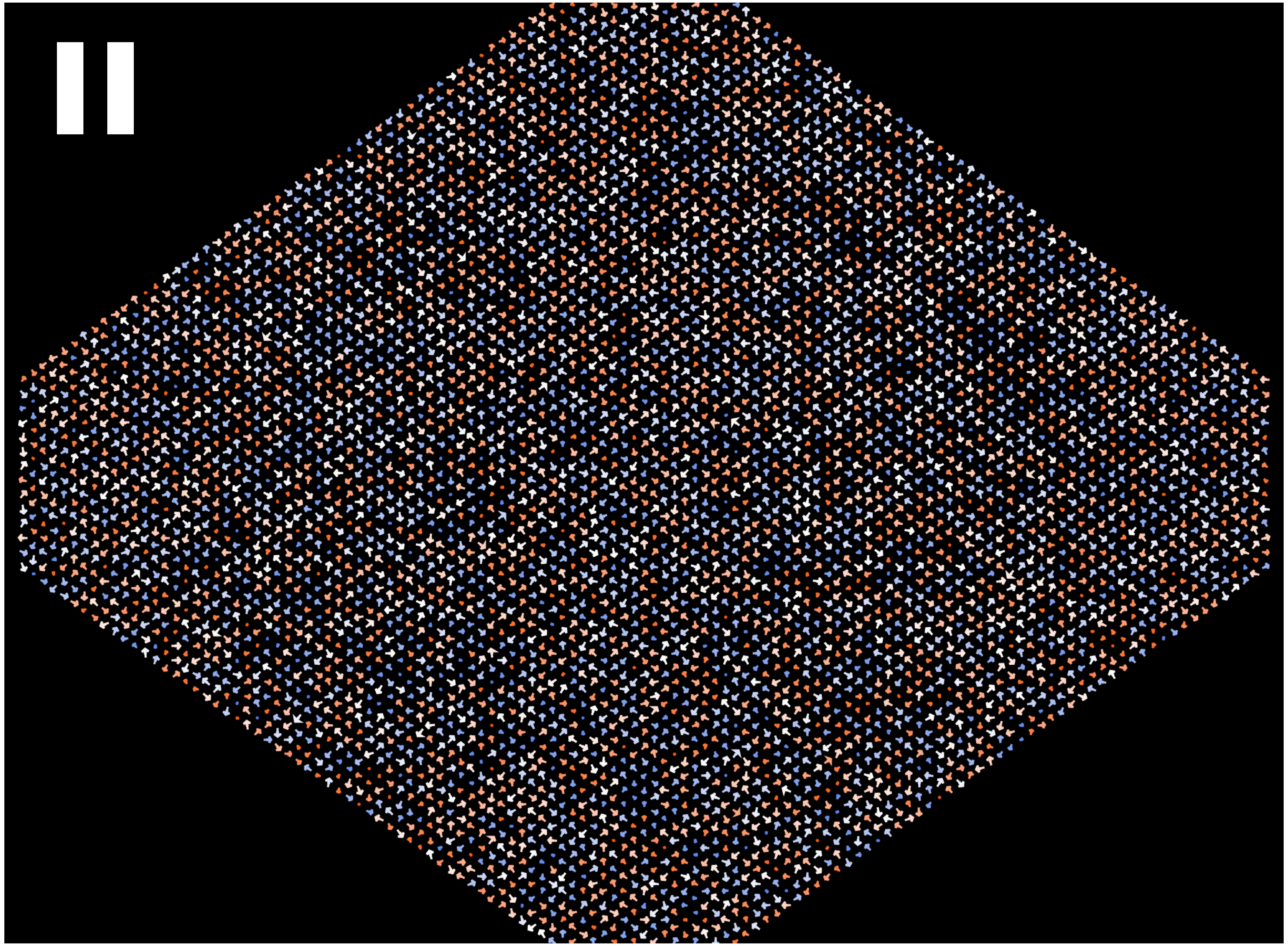

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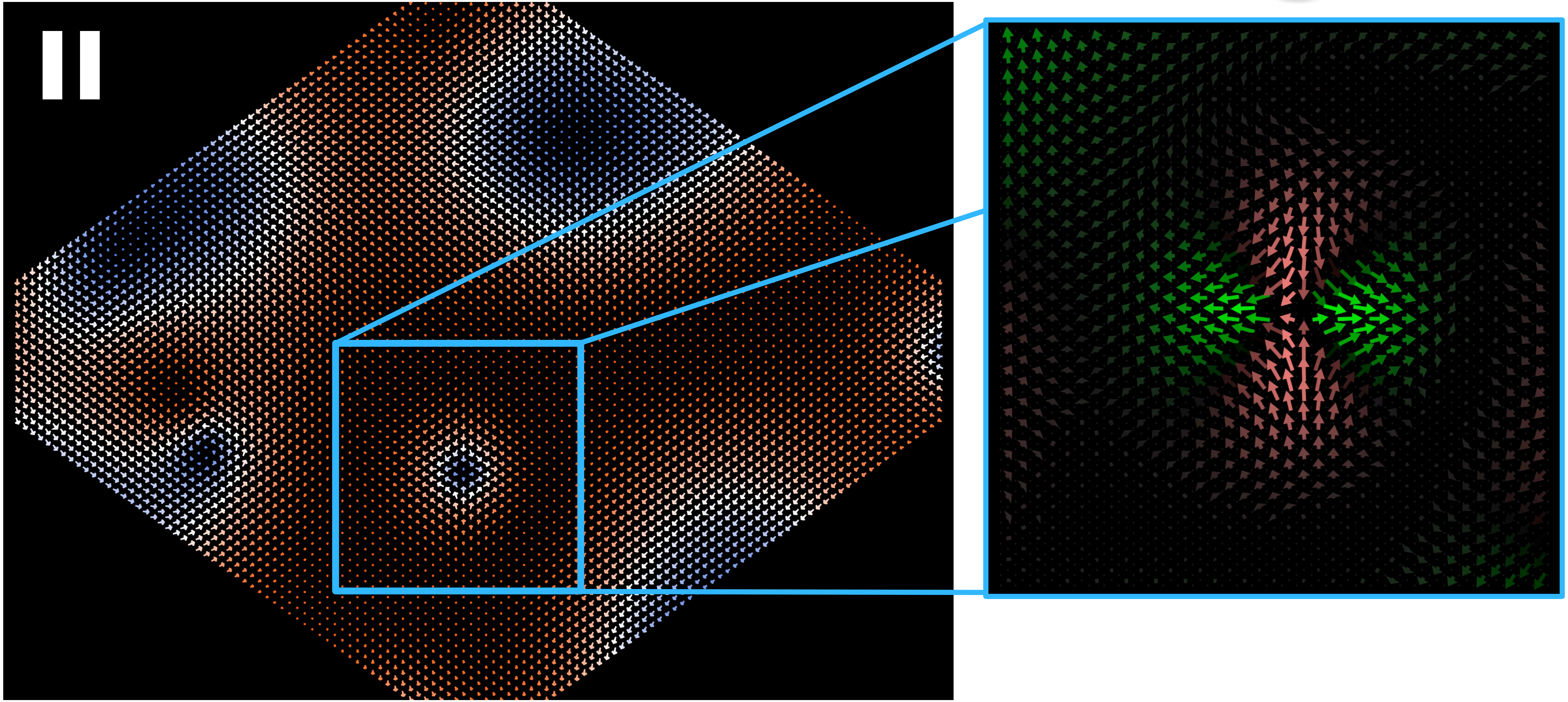

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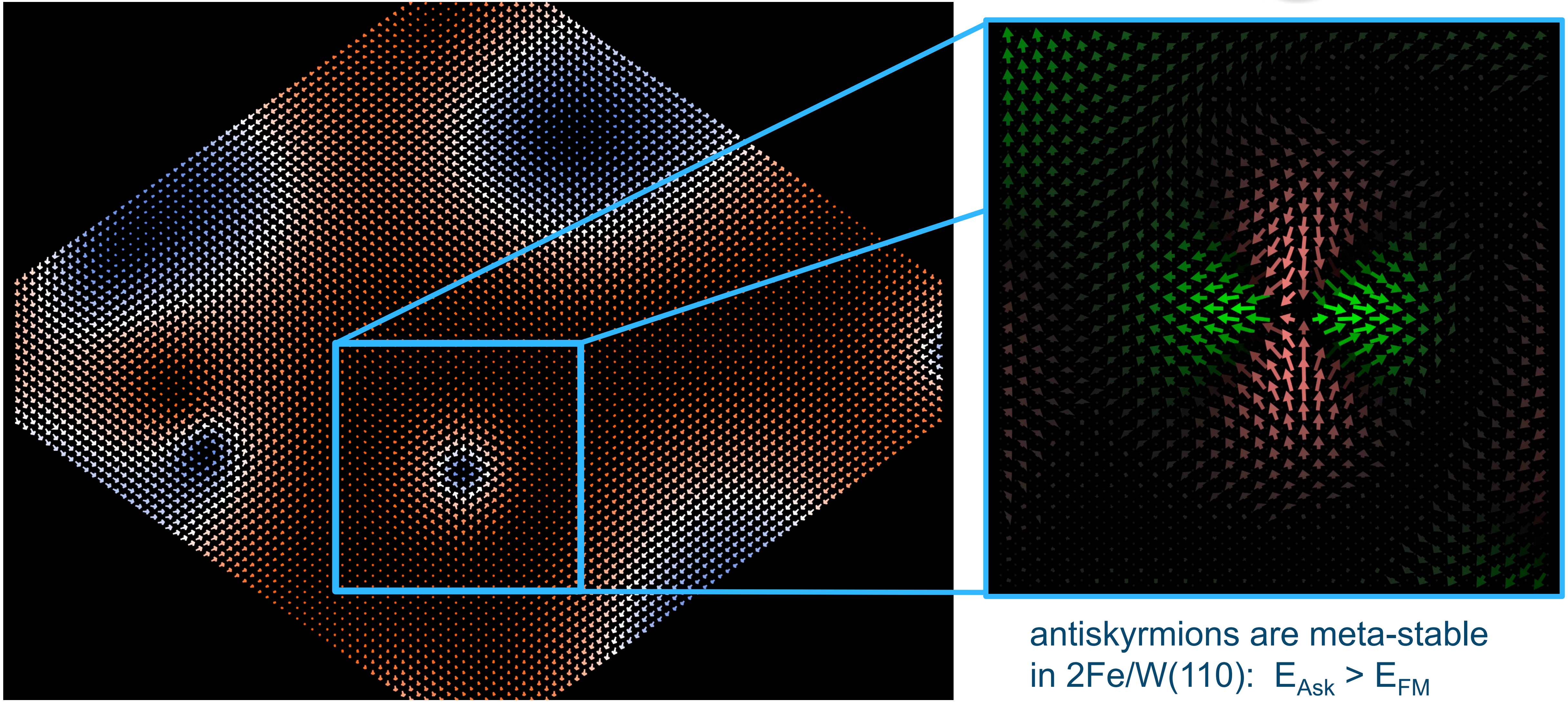


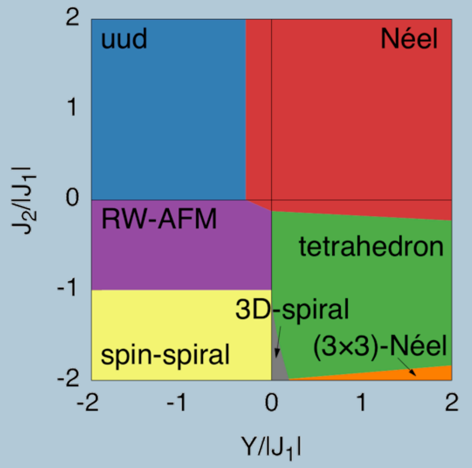
antiskyrmions are meta-stable in 2Fe/W(110): $E_{Ask} > E_{FM}$

Summary & Conclusion

Summary & Conclusion

- Higher-order exchange interactions can couple spin-spirals and result in many complex magnetic textures

  ⟶ plenty of opportunities for new discoveries!



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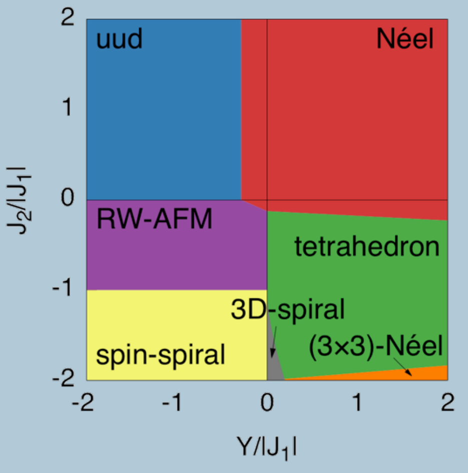
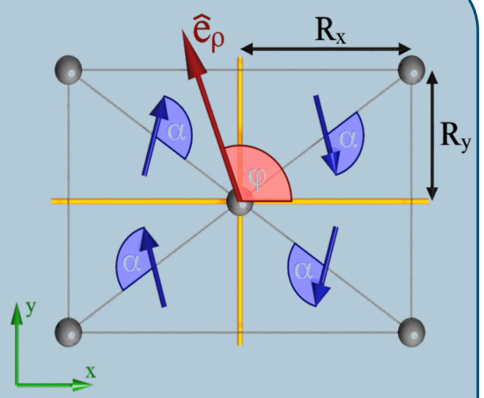


- Shape of DM interaction is defined by the underlying lattice symmetry
- C2v symmetry particularly interesting due to variety of possible preferred states



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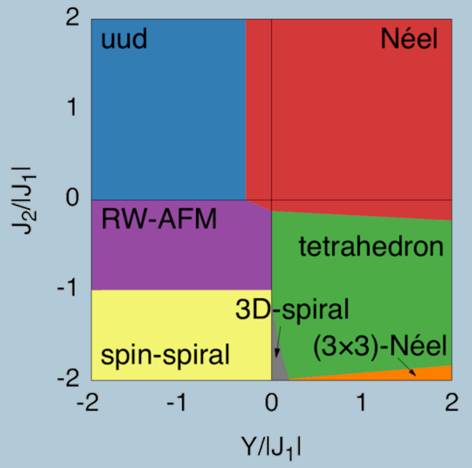

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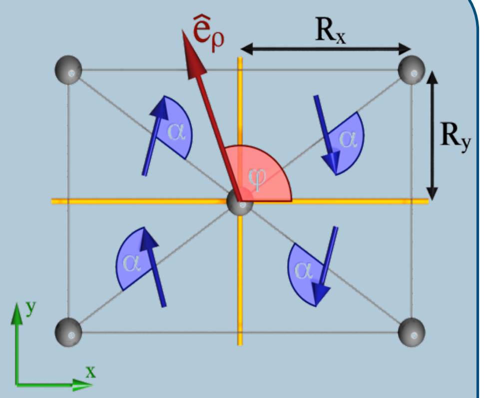

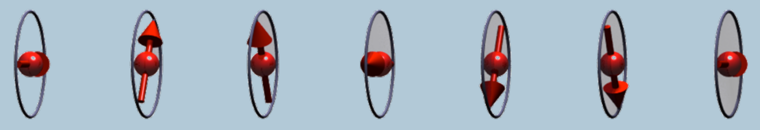

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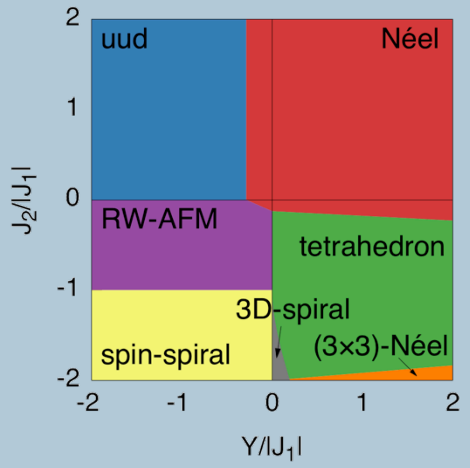

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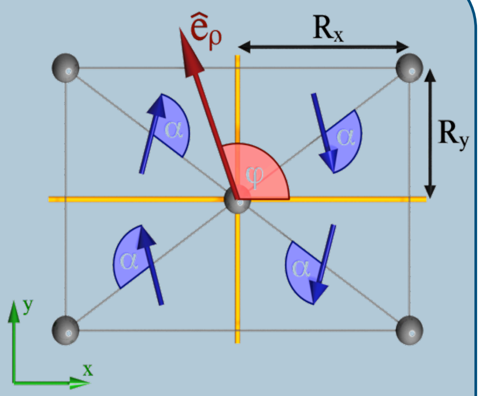

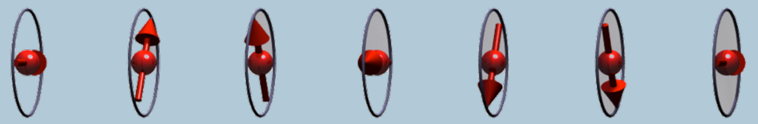

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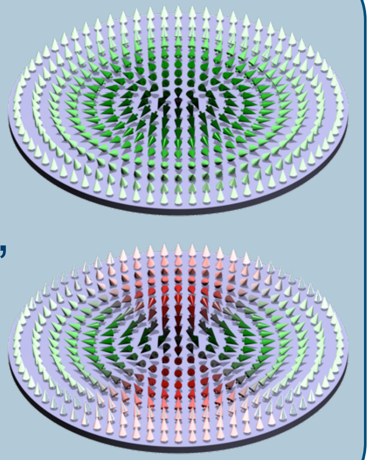
- ongoing search for such systems



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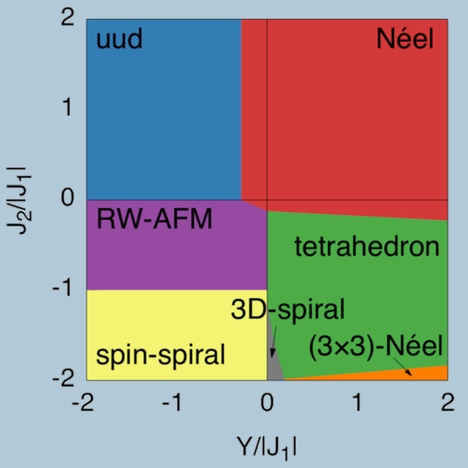

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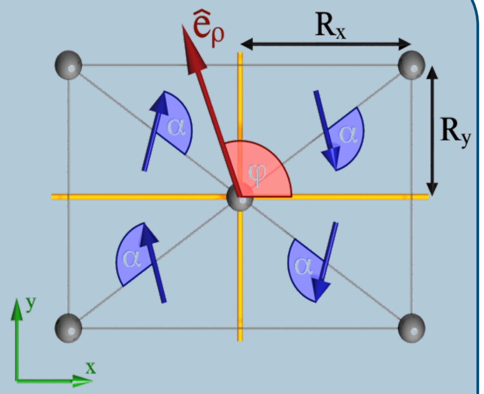
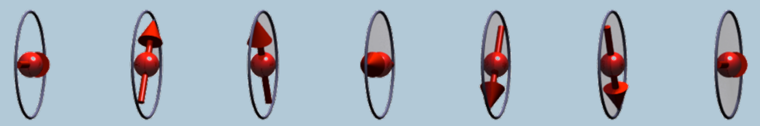


- rank-1 materials were not yet found! Find them!



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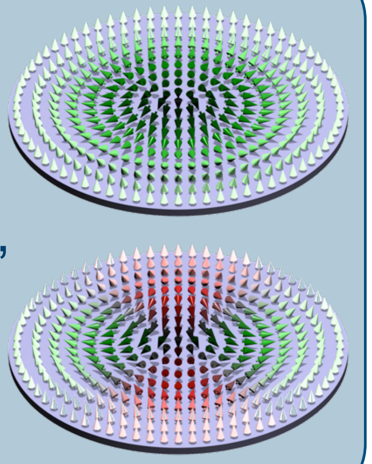

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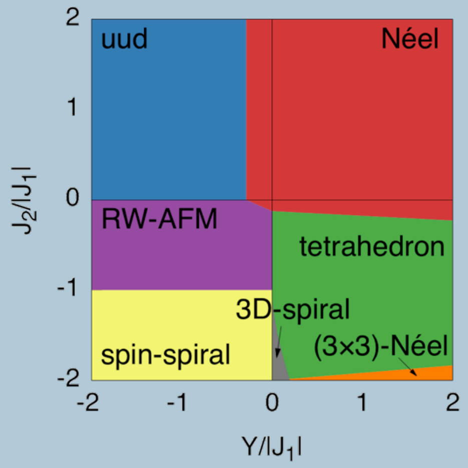

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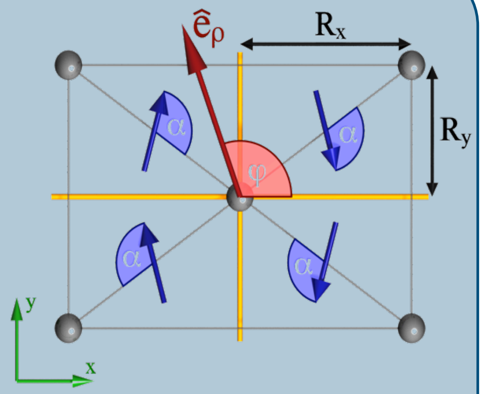

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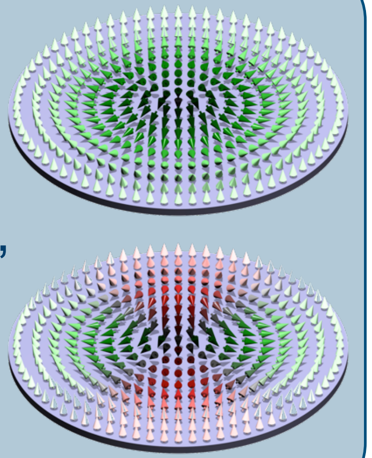

spirit

spirit-code.github.io

- Spin-dynamics simulations allow to determine (meta-) stable magnetic structures
- Spirit is useful tool for this.

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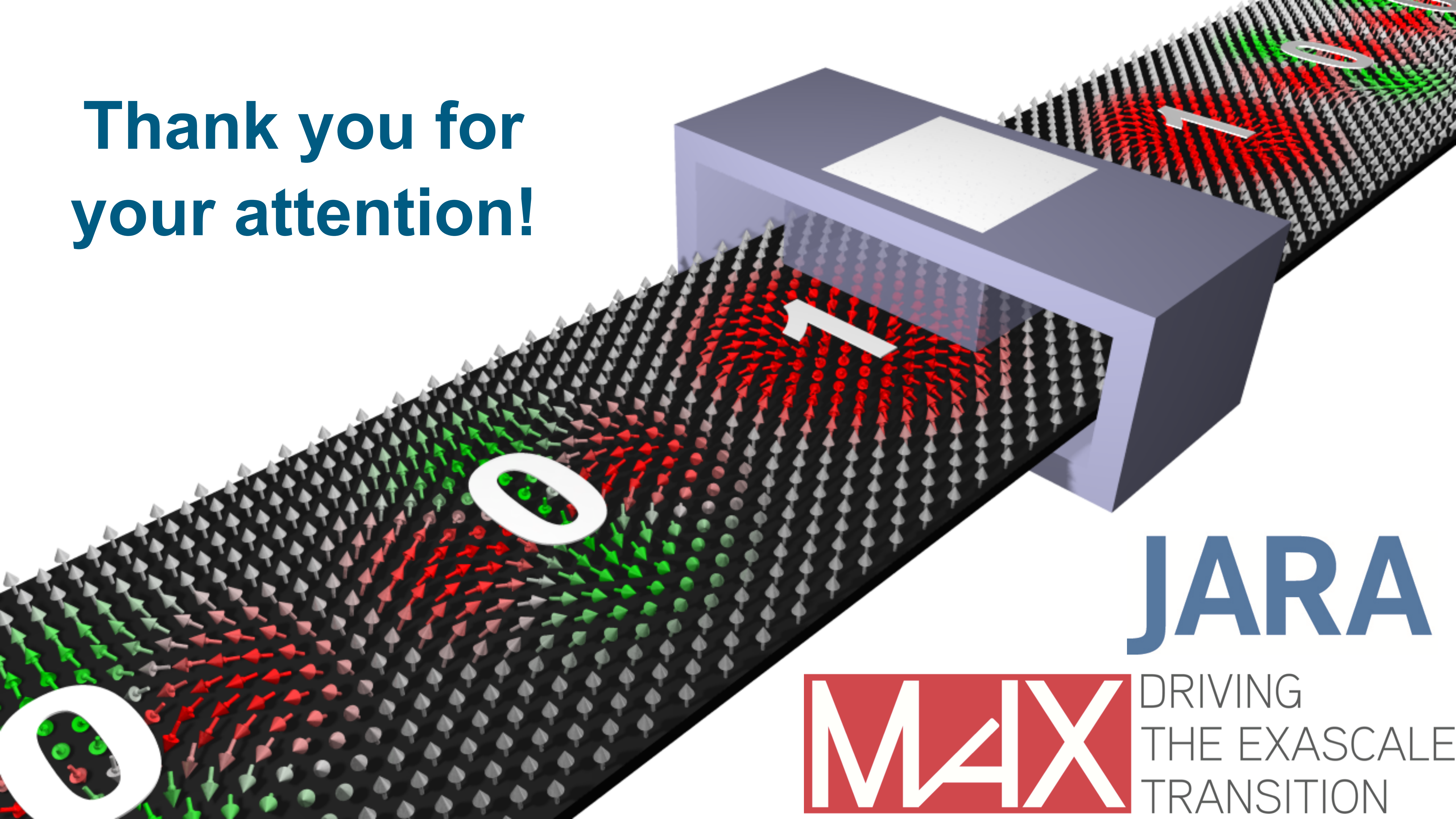
Thank you for your attention!



JARA

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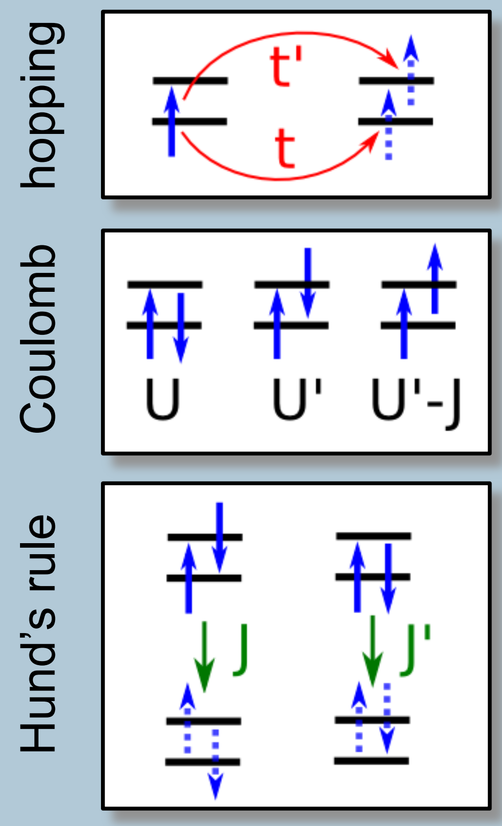
Higher-order exchange interactions: Hubbard model

Multi-band Hubbard model

electron-Hamiltonian



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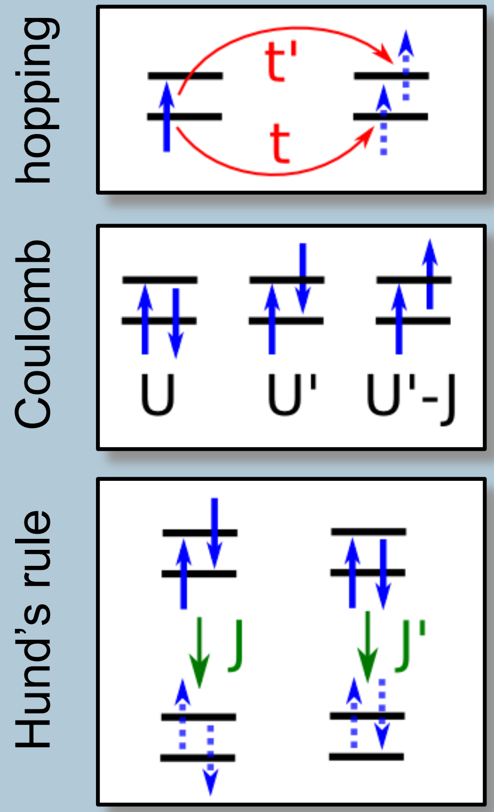
Multi-band Hubbard model

electron-Hamiltonian

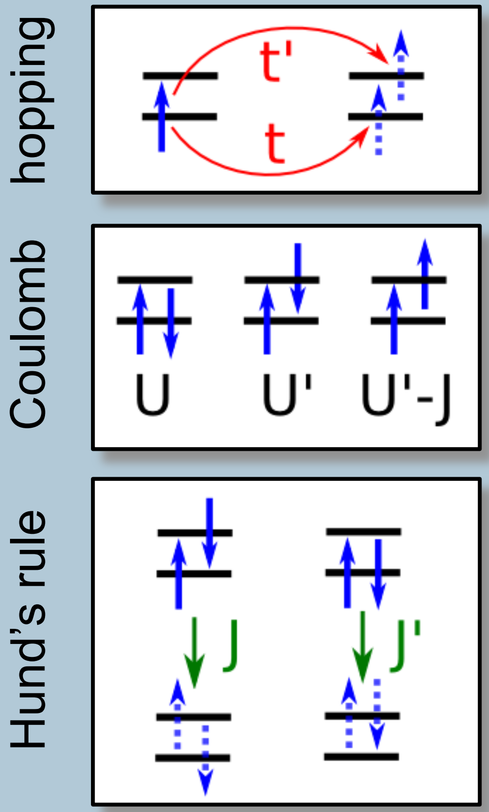


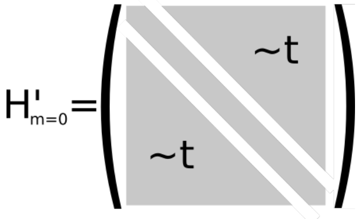
Effective *spin* Hamiltonian

Higher-order exchange interactions: Hubbard model

Multi-band Hubbard model

electron-Hamiltonian





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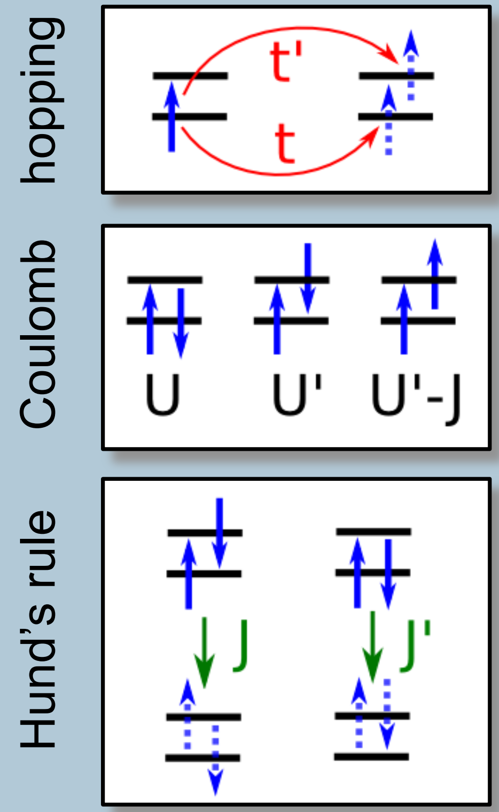

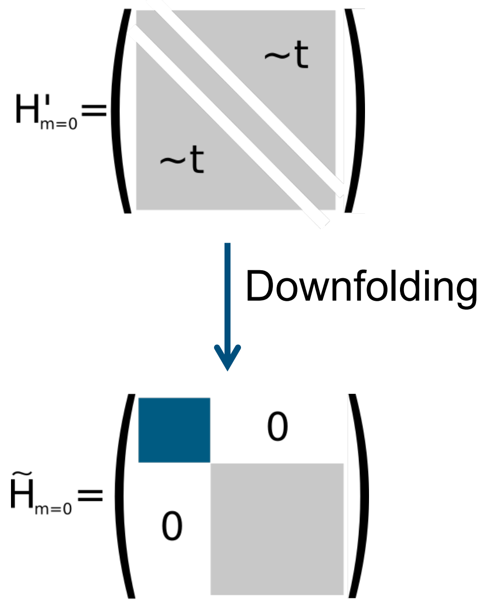

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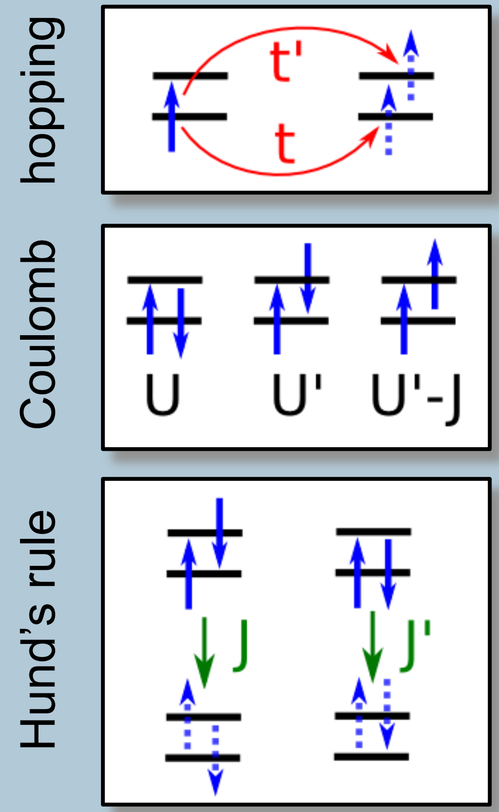

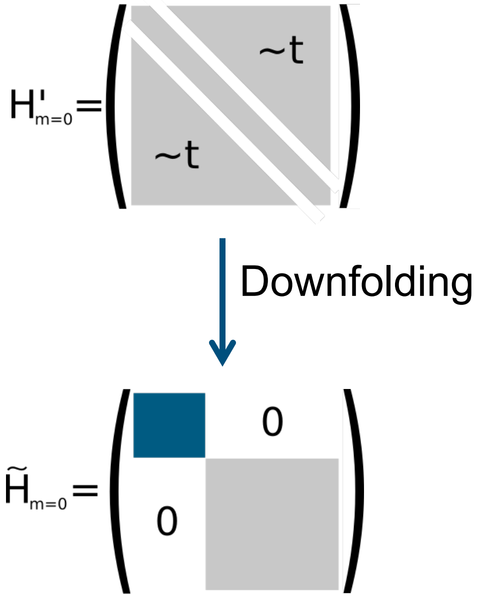

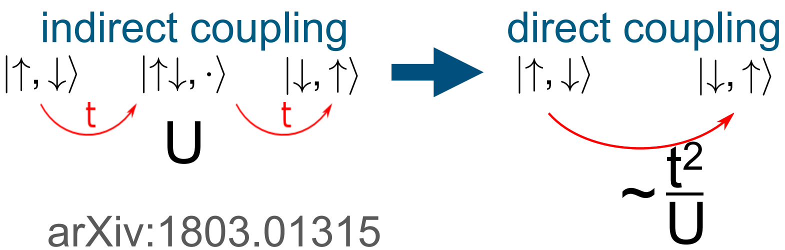

arXiv:1803.01315

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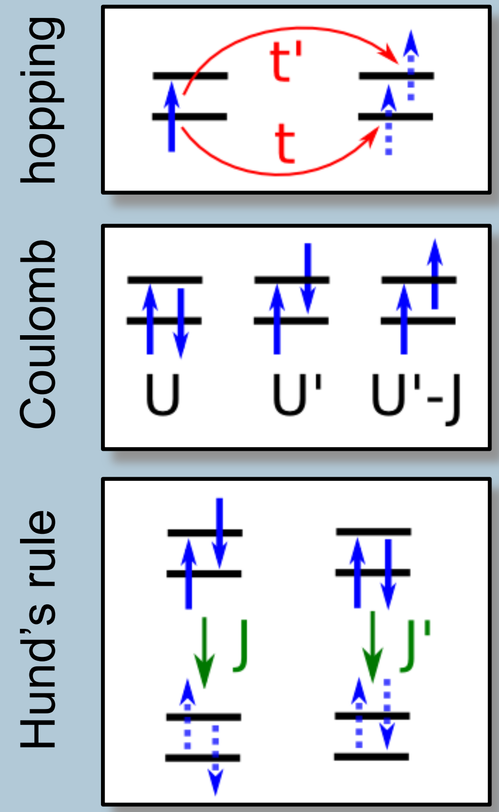
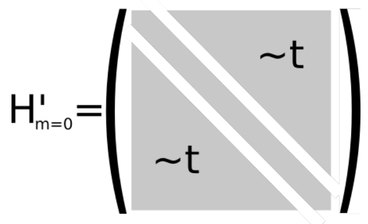
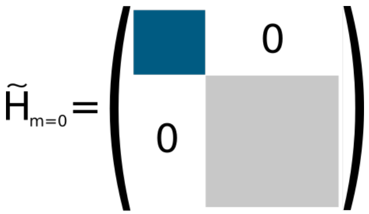


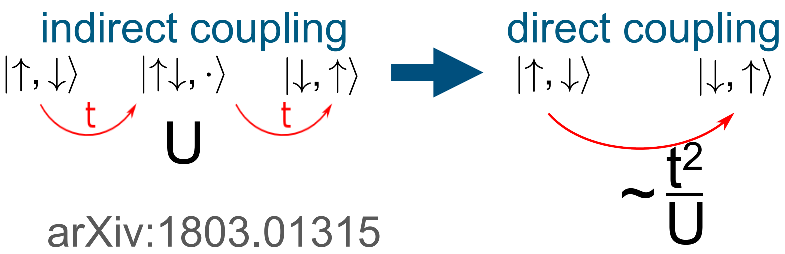


Downfolding



Mapping to spin Hamiltonian

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



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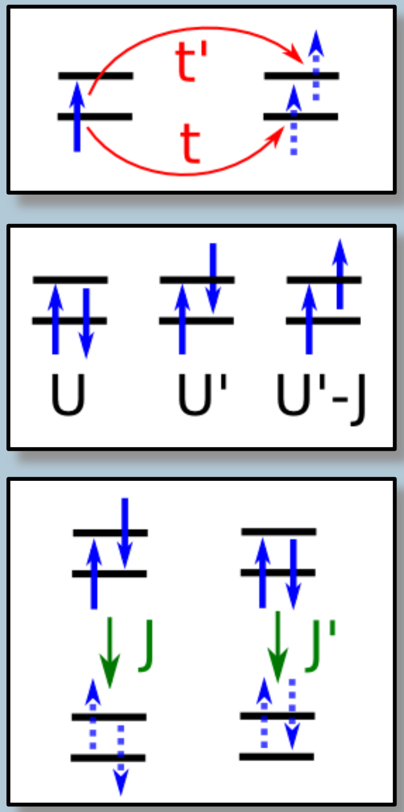
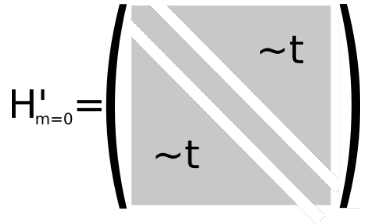
hopping

Coulomb

Hund's rule





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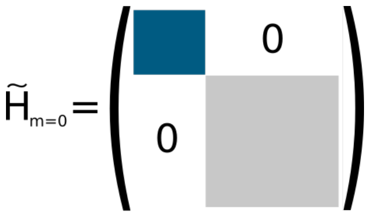

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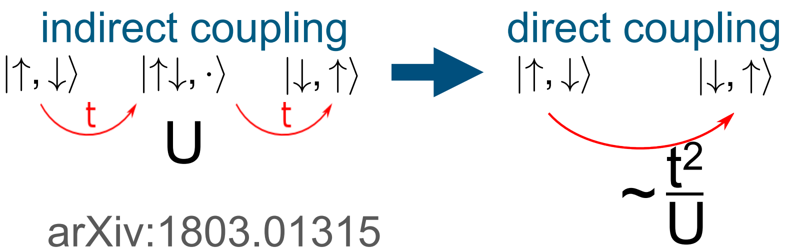

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Effective *spin* Hamiltonian

$$H = -\sum_{ij} J_{ij}\,(\mathbf{S}_i\cdot\mathbf{S}_j) - \sum_{ij} \mathbf{D}_{ij}\cdot(\mathbf{S}_i\times\mathbf{S}_j) - \sum_{ijkl} B_{ij}\,(\mathbf{S}_i\cdot\mathbf{S}_j)^2 - \sum_{ijk} Y_{ijk}\,(\mathbf{S}_i\cdot\mathbf{S}_j)(\mathbf{S}_i\cdot\mathbf{S}_k) - \sum_{ijkl} K_{ijkl}\,(\mathbf{S}_i\cdot\mathbf{S}_j)(\mathbf{S}_k\cdot\mathbf{S}_l)$$

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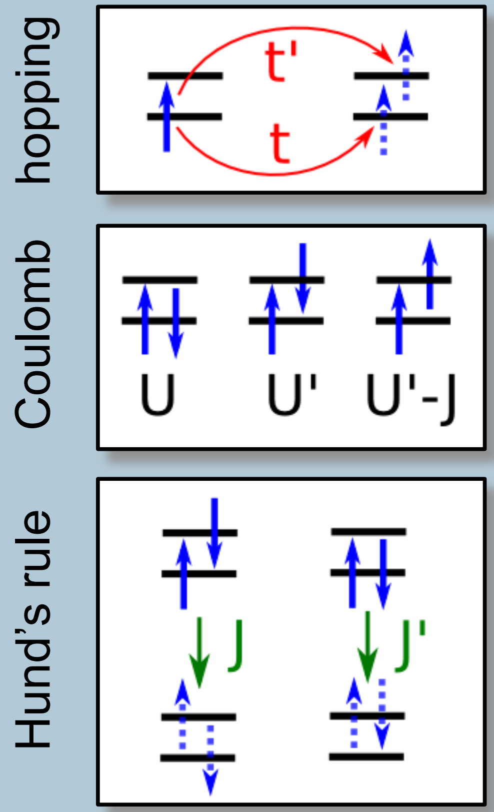

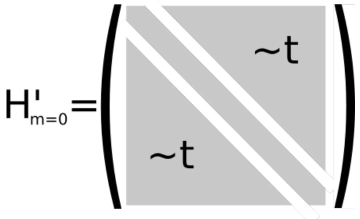

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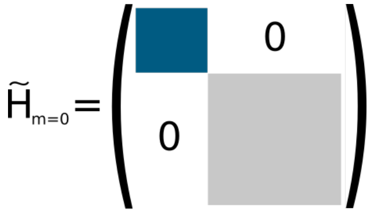

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indirect coupling → direct coupling

$|\uparrow,\downarrow\rangle \xrightarrow{t} |\uparrow\downarrow,\cdot\rangle \xrightarrow{t} |\downarrow,\uparrow\rangle$, U

$|\uparrow,\downarrow\rangle \rightarrow |\downarrow,\uparrow\rangle \sim \frac{t^2}{U}$

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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

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

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

DMI in the micromagnetic model

magnetization is described by a continuous magnetization density **m**(**r**)

DMI: $\sum_{\alpha\beta} D_{\alpha\beta}\,\mathcal{L}_{\alpha\beta}$ (general form)

α = spin coordinate
β = spatial coordinate

A. Bogdanov & A. Hubert, JMMM **138**, 255 (1994)

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Bulk systems

$$\underline{\underline{\mathcal{D}}} = \begin{pmatrix} D & 0 & 0 \\ 0 & D & 0 \\ 0 & 0 & D \end{pmatrix}$$

$$E_{\mathrm{DM}} = D\, \mathbf{m} \cdot (\nabla \times \mathbf{m})$$

Interfaces

$$\underline{\underline{\mathcal{D}}} = \begin{pmatrix} 0 & D & 0 \\ -D & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$E_{\mathrm{DM}} = D\left[(\mathbf{m} \cdot \nabla)\, m_z - m_z\, (\nabla \cdot \mathbf{m}) \right]$$

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Relation between micromagn. tensor ***D*** and atomistic $\mathbf{D}_{ij}$ vectors:

$$\boldsymbol{D} = \frac{1}{A_\Omega} \sum_j \mathbf{D}_{0j} \otimes \mathbf{R}_{0j}$$

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Calculation of skyrmion lifetimes

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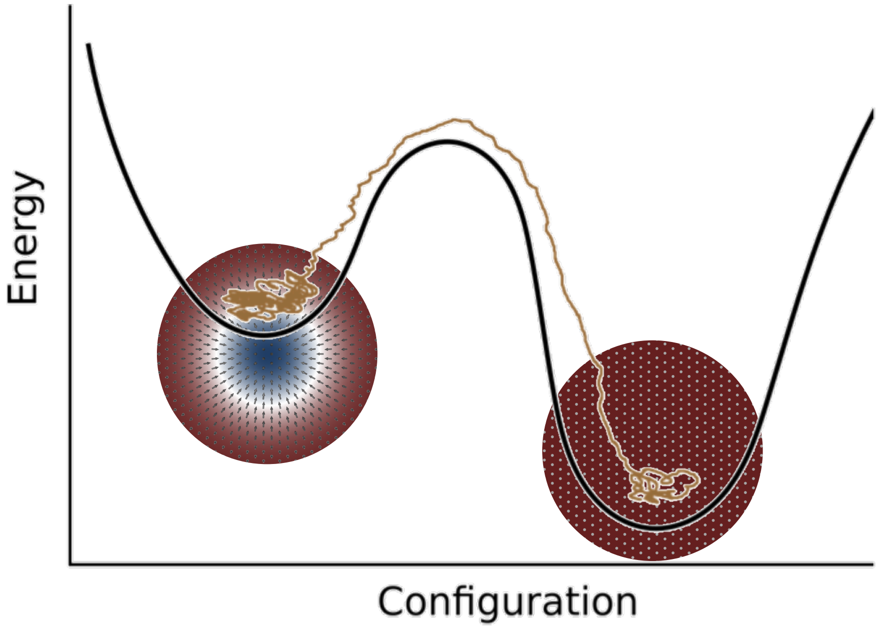
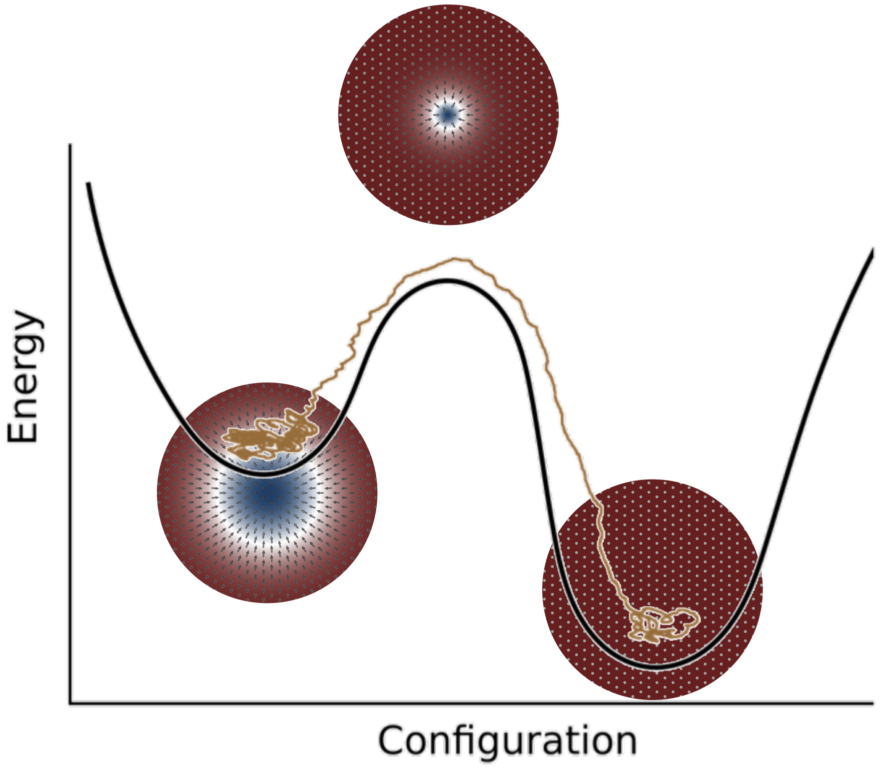


DRIVING
THE EXASCALE
TRANSITION

Calculation of skyrmion lifetimes



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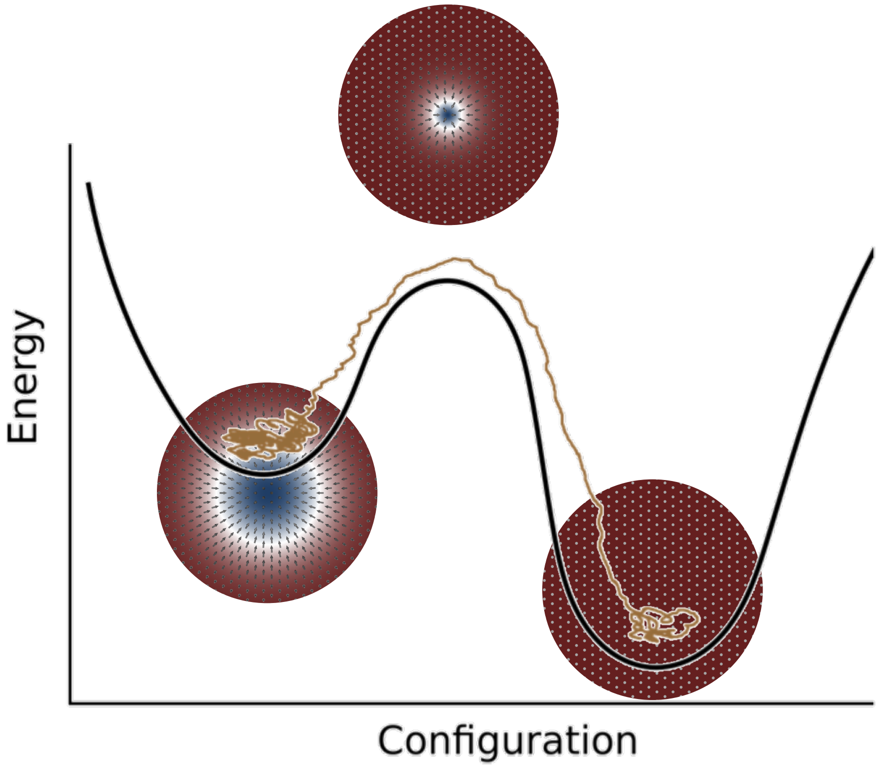
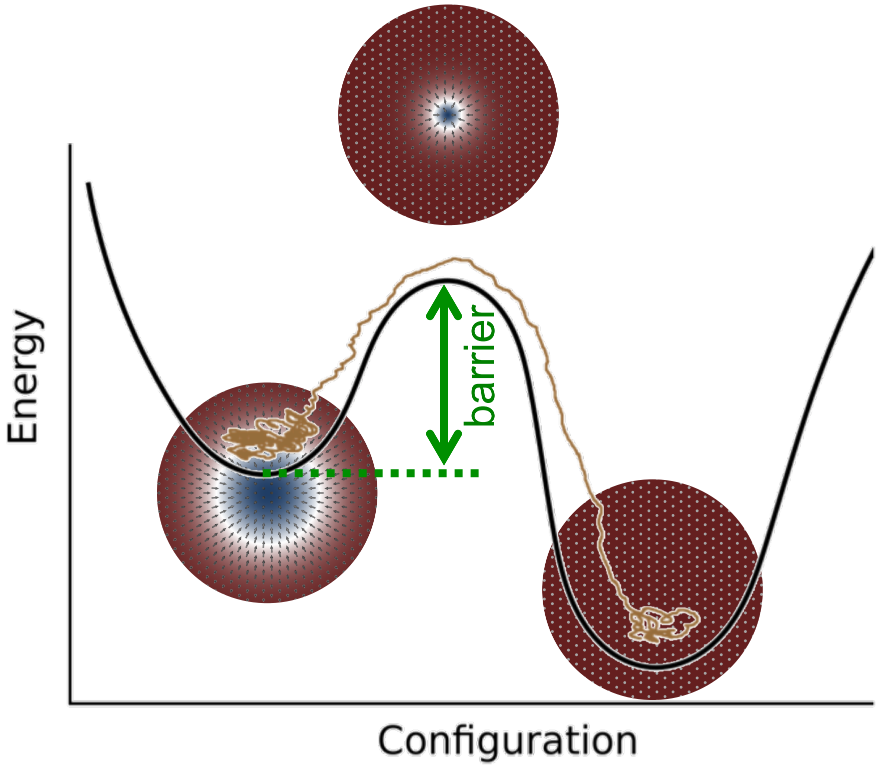


Lifetime

$$\tau = \nu \cdot e^{\Delta E / k_B T}$$

Calculation of skyrmion lifetimes



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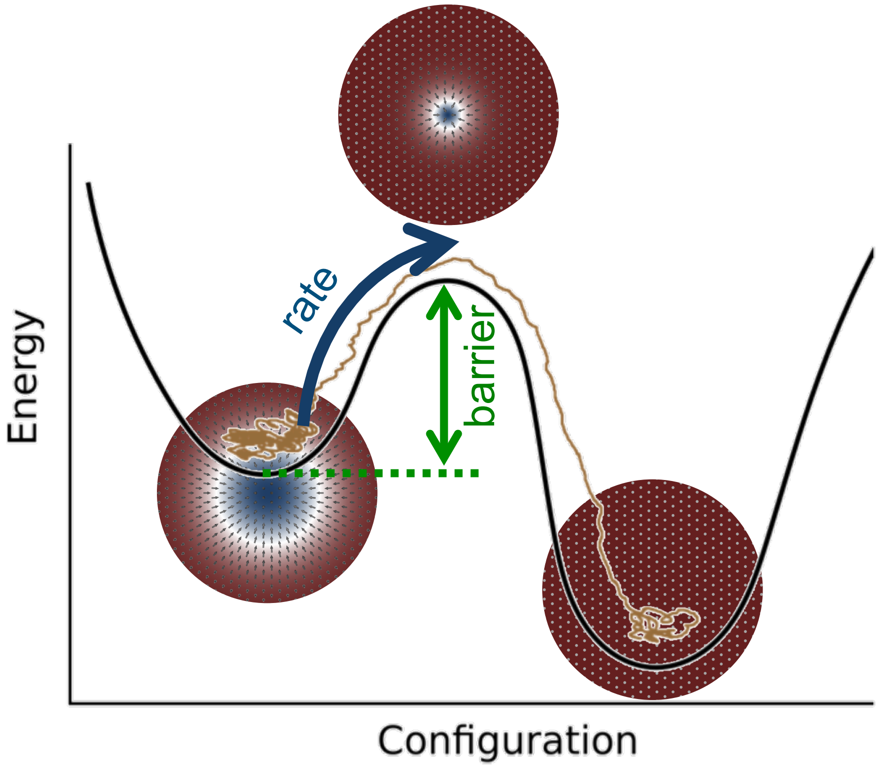
Calculation of skyrmion lifetimes

spirit



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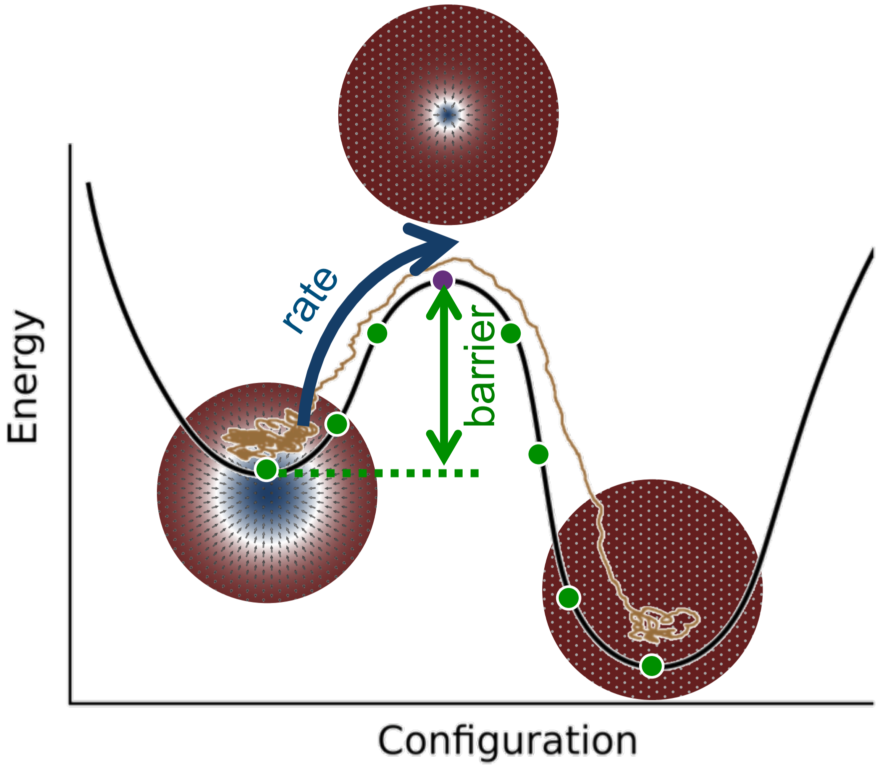
Calculation of skyrmion lifetimes

Geodesic nudged elastic band method (GNEB)

GNEB provides minimum energy path:

- saddle point structure
- energy barrier



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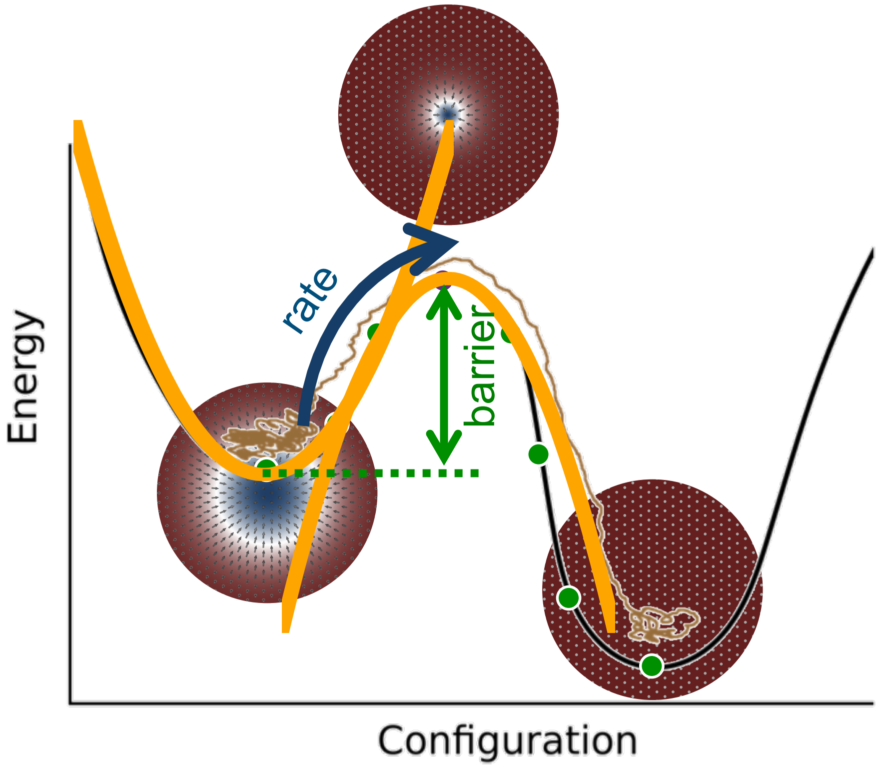

Harmonic transition state theory (HTST)

HTST provides attempt rate via harmonic approximation

Approximate energy landscape around initial state and saddle point:

$$E(x) = E_0 + G^k_\alpha n^k_\alpha + \frac{1}{2} n^k_\alpha H^{kl}_{\alpha\beta} n^l_\beta$$

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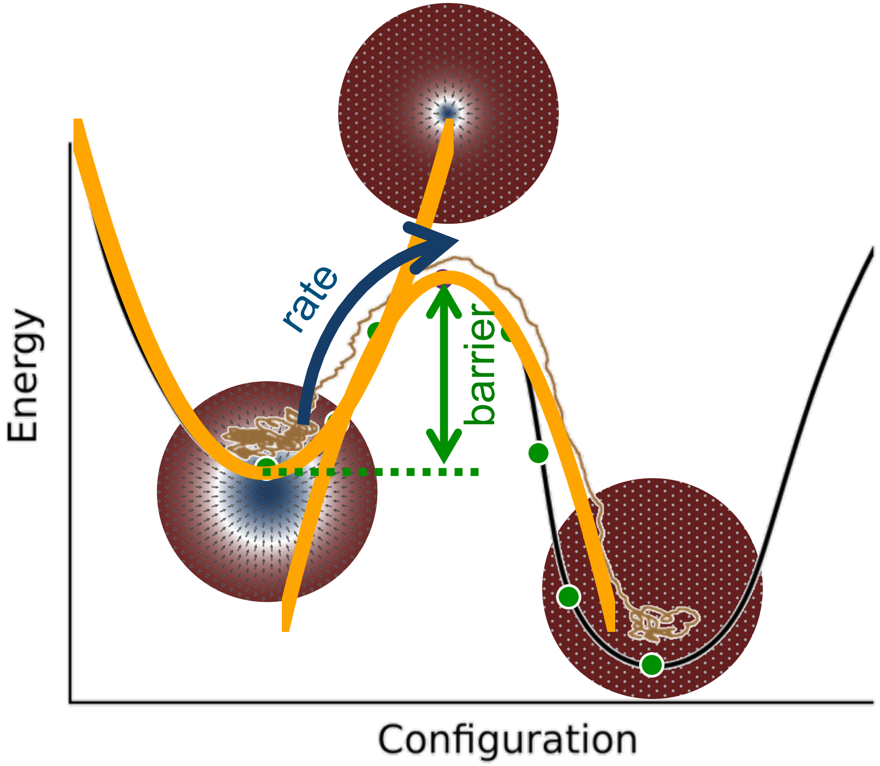

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$$\nu(T) \propto T^{-1} \left(\sum_j^N \frac{a_j^2}{\epsilon_{\mathrm{sp},j}} \right)^{-1/2} \frac{\prod_i \sqrt{\epsilon_{\mathrm{sp},i}}}{\prod_i \sqrt{\epsilon_{\mathrm{min},i}}}$$