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UNIDADE DE PESQUISA DO MCTI

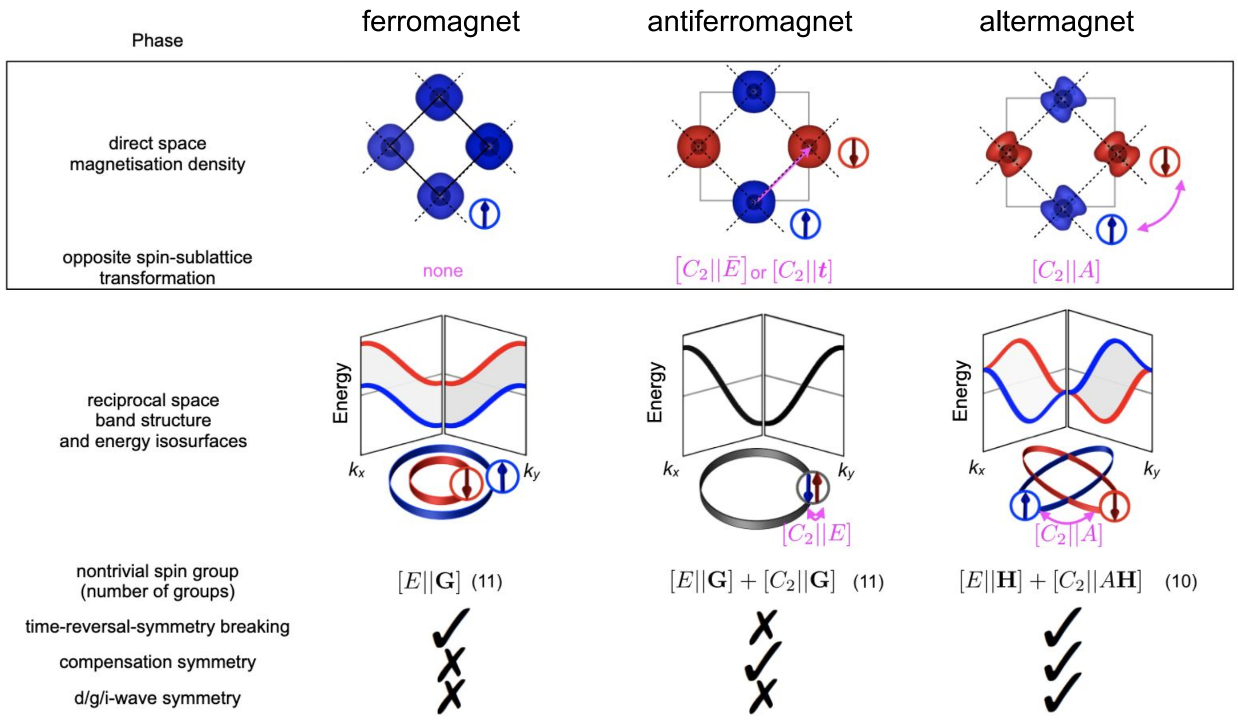
Construindo e explorando modelos de spin a partir de métodos de primeiros princípios

do magnetismo não colinear às ondas de spin topológicas

Prof. Flaviano José Marchiori dos Santos
Dr. rer. nat.

Magnetism: an old field but always new

New basic category: altermagnetism



L. Smejkal, J. Sinova, and T. Jungwirth, PRX 12, 031042 (2022)

Explain:

- Anomalous transport in some materials
- Degeneracy break in band structure of electrons and magnons
- Time-reversal symmetry breaking can coexist with zero net magnetization

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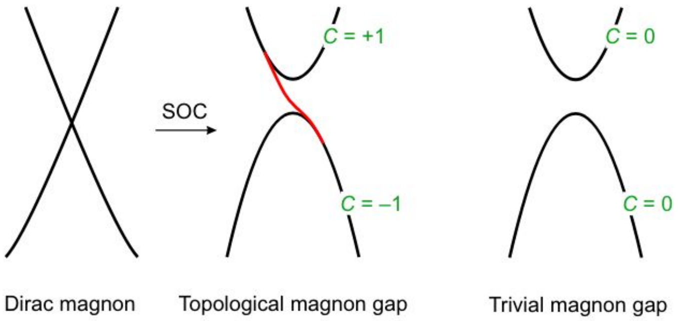
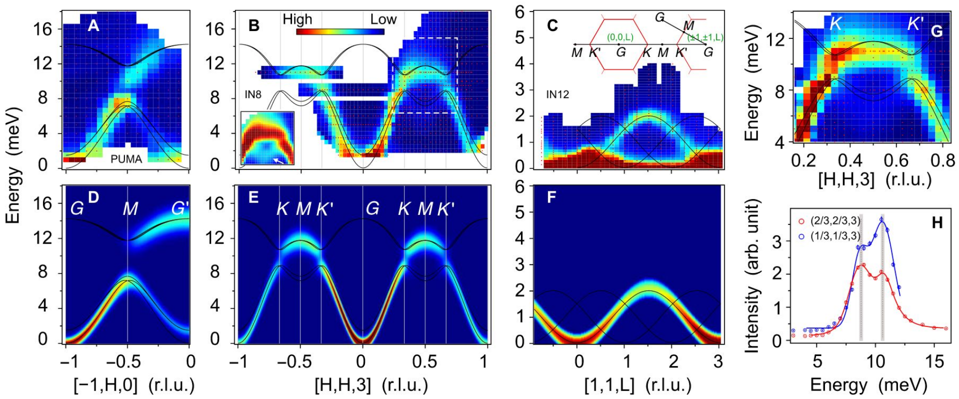
Topological magnons

Topological insulators



CrSiTe3, CrGeTe3, Mn5Ge3



F. Zhu, …**F.J. dos Santos**, et al., Sci. Adv. 7 (2021)

M. dos Santos Dias, N. Biniskos, **F. J. dos Santos** et al., Nat. Comm. 14, 7321 (2023)

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Zoo of noncollinear and topologically nontrivial magnetic textures

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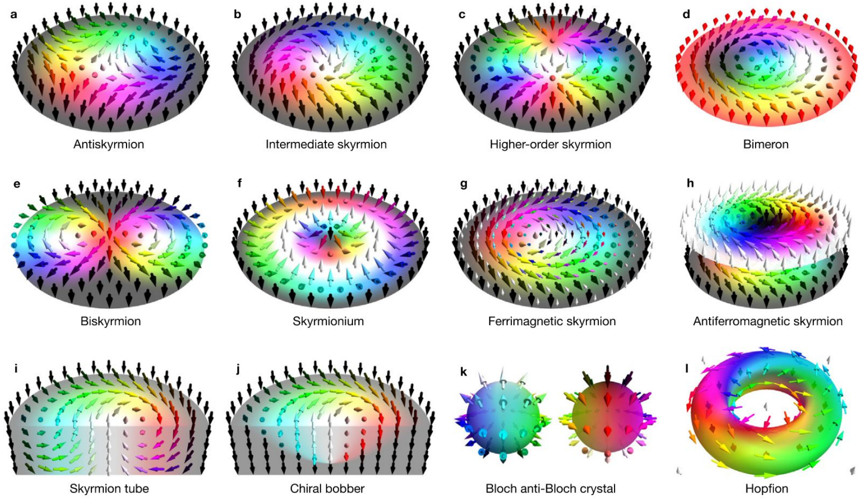
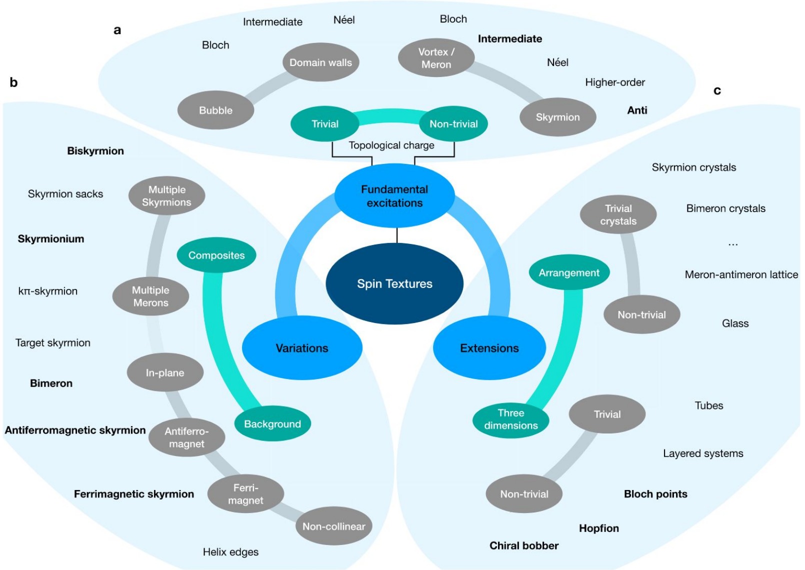
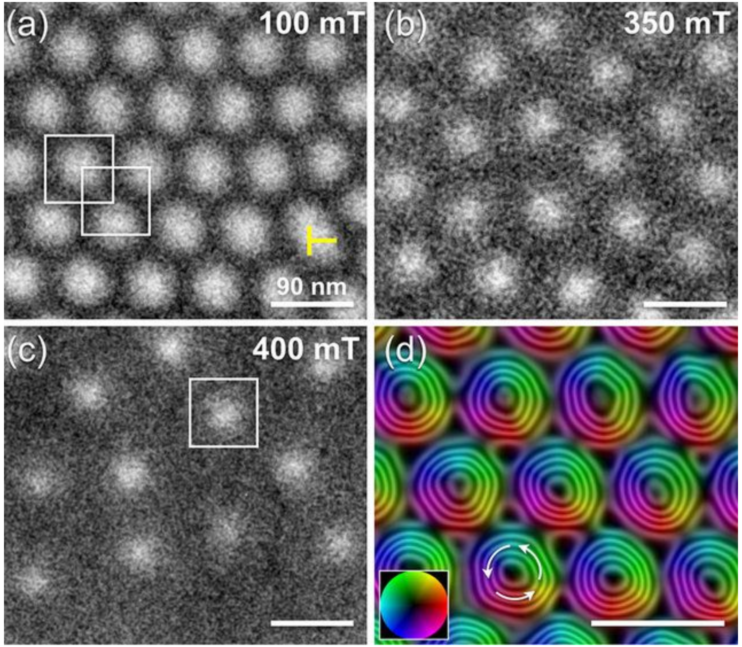


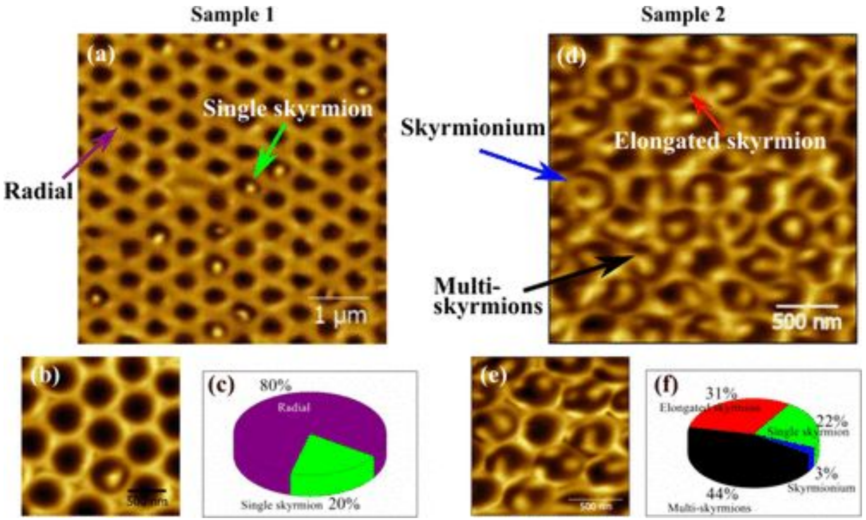


B. Göbel, I. Mertig and O.A. Tretiakov Physics Reports 895 (2021) 1–28

Zoo of noncollinear and topologically nontrivial magnetic textures



András Kovács et et al, Appl. Phys. Lett. 111(19):192410 (2017)



Damian Dugato et al, Nano Lett. 25, 22 (2025)

How to simulate these spin textures?

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Theoretical background

Heisenberg model Hamiltonian

- Systems with localized magnetic moments
- Slow motion of the moments with respect to the fast motion of the electrons
- Effective spin model describing the interaction between the localized magnetic moments in materials

Heisenberg model Hamiltonian

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

- It is useful to describe phase transitions, critical temperatures, exotic quasiparticles (skyrmions), spin excitations, topological magnons, etc.

How to compute the exchange parameters?

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Origin of the exchange interaction

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- Dominant magnetic interaction between discrete moments **does not** arise from their magnetic field: dipole-dipole, or spin-orbit coupling.
- The source is the *electrostatic* electron-electron interaction.
- Magnetic theories often disregard dipole-dipole and SOC.
- Spin correlation introduced by *Pauli's exclusion principle*: magnetic exchange interaction.
- *Spin-independent* Hamiltonian of a two-electron system

- General solution Ψ is a product of the purely orbital wavefunction ψ that satisfy the orbital Schrödinger equation:

$$-\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2)\psi + V(\mathbf{r}_1, \mathbf{r}_2)\psi = E\psi$$

with a linear combination of these four spin state: $|\uparrow\uparrow\rangle, \quad |\uparrow\downarrow\rangle, \quad |\downarrow\uparrow\rangle, \quad |\downarrow\downarrow\rangle$.

	S	S_z	
$\frac{1}{\sqrt{2}}(\|\uparrow\downarrow\rangle - \|\downarrow\uparrow\rangle)$	0	0	singlet
$\|\uparrow\uparrow\rangle$	1	1	triplet
$\frac{1}{\sqrt{2}}(\|\uparrow\downarrow\rangle + \|\downarrow\uparrow\rangle)$	1	0	
$\|\downarrow\downarrow\rangle$	1	-1	

- The strength of this correlation is given by the *exchange interaction*.

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Mapping DFT electronic structure calculation onto model Hamiltonian

How to obtain the parameters for the model Hamiltonian?

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

Two popular methods:

- Total energy differences
- Infinitesimal-rotations method

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Total energy differences

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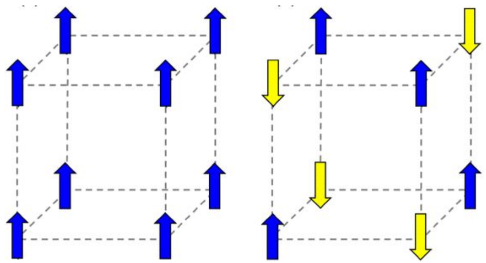
Ferromagnetic and antiferromagnetic configurations



E_{FM} E_{AFM}

DFT self-consistent total energie calculations

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

Assuming:

- A nearest-neighbour-only Hamiltonian
- Energy variation is only caused by the exchange interaction

$$J = (E_{\mathrm{AFM}} - E_{\mathrm{FM}}) \,/\, (2 \cdot N_{\mathrm{atom}} \cdot N_{\mathrm{neighbour}})$$

Convention:

- Both J_{ij} and J_{ji} are included
- S = 1

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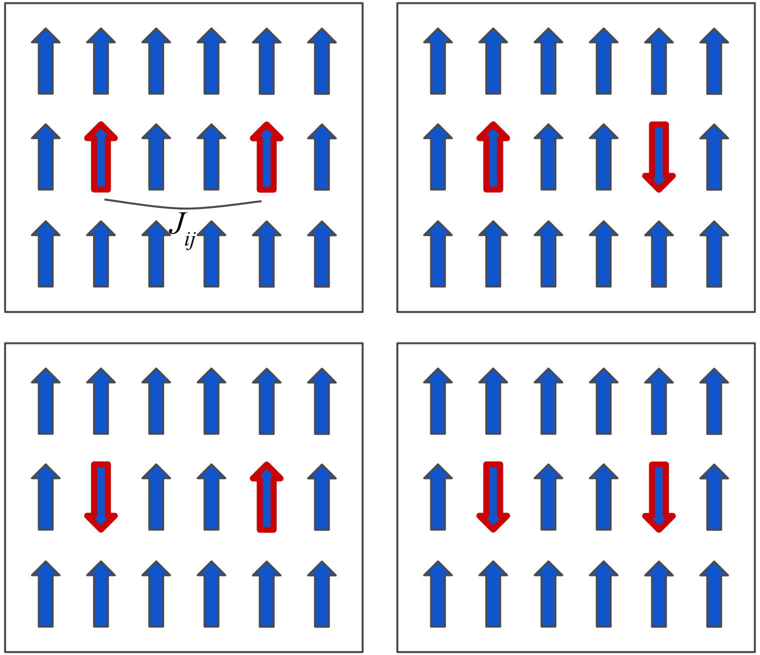
Total energy differences

Four-state method:



$$J_{ij} = (E_{\uparrow\uparrow} + E_{\downarrow\downarrow} - E_{\uparrow\downarrow} - E_{\downarrow\uparrow}) \,/\, (8\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j)$$

- Beyond nearest neighbours
- Energy variation is only caused by the exchange interaction
- It requires supercells

$$J_{ij} = (E_{\uparrow\uparrow} + E_{\downarrow\downarrow} - E_{\uparrow\downarrow} - E_{\downarrow\uparrow}) \,/\, (8\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j)$$

$$+ \quad \sum_R J_{ij}^{\,R} \boldsymbol{S}_i \cdot \boldsymbol{S}_j^{\,R}$$

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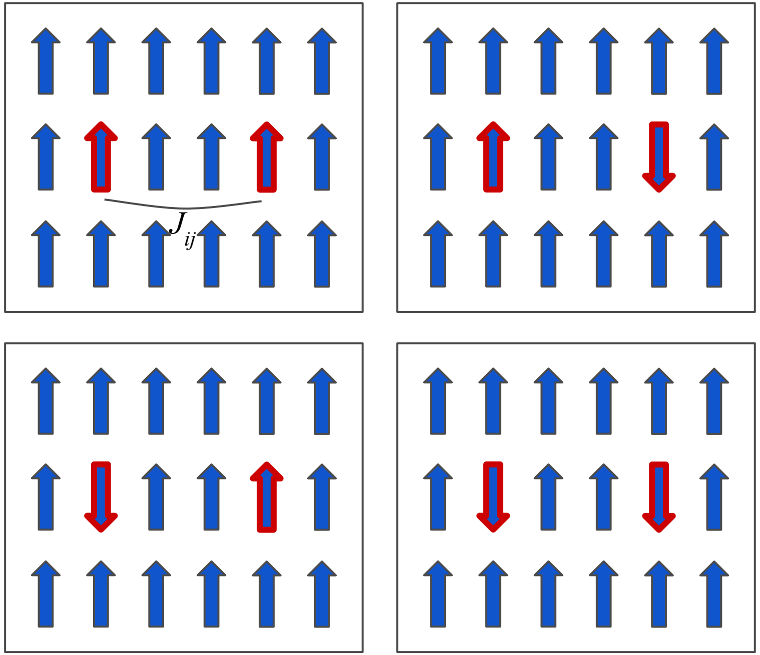
Xiang *et al.*, PRB 84, 224429 (2011)

Total energy differences

Four-state method:



$$J_{ij} = (E_{\uparrow\uparrow} + E_{\downarrow\downarrow} - E_{\uparrow\downarrow} - E_{\downarrow\uparrow}) / (8\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j)$$

Overview:

- Simple
- Assume the system is very Heisenberg-like
- Requires supercell and multiple DFT calculations
- Typically used for a few exchange coupling

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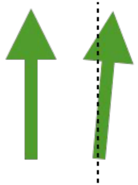
Xiang *et al.*, PRB 84, 224429 (2011)

Infinitesimal-rotations method



Hamiltonian: neglecting relativistic effects and longitudinal spin fluctuations

$$\mathcal{H} = -\sum_{i \neq j} J_{ij}\, \vec{e}_i \vec{e}_j .$$

Energy variation due to two spin rotations at sites *i* and *j*

$$\delta E(\vec{e}_i, \vec{e}_j) = \delta E(\vec{e}_i) + \delta E(\vec{e}_j) - (\vec{e}_i - \vec{e}_0)(\vec{e}_j - \vec{e}_0) J_{ij}$$

$$\begin{aligned} E_{ij}^{\mathrm{int}} &= \delta E(\vec{e}_i, \vec{e}_j) - \delta E(\vec{e}_i) - \delta E(\vec{e}_j) \\ &= -J_{ij}\, \delta\vec{e}_i \delta\vec{e}_j , \end{aligned}$$

László Oroslány *et al.*
Phys. Rev. B 99, 224412 (2019)

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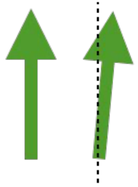
Infinitesimal-rotations method



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From Magnetic force theorem and Lloyd's formula:

$$\delta E_{\mathrm{KS}} = \frac{1}{\pi}\int_{-\infty}^{\varepsilon_{\mathrm{F}}} d\varepsilon \,\mathrm{Im}\mathrm{Tr}\ln(\hat{I} - \delta\hat{V}\hat{G}(\varepsilon))$$

Green's function

$$\hat{G}(z) = (z\hat{I} - \hat{H})^{-1}$$

Assuming now that $\delta\hat{V}_i$ and $\delta\hat{V}_j$ are operators that describe the local perturbations corresponding to spin rotations at sites i and j

$$\ln(\hat{I} - \delta\hat{V}_i\hat{G} - \delta\hat{V}_j\hat{G})$$
$$= \ln(\hat{I} - \delta\hat{V}_i\hat{G}) + \ln(\hat{I} - \delta\hat{V}_i\hat{G}) + \ln(\hat{I} - \hat{T}_i\hat{G}\hat{T}_i\hat{G}),$$

where the scattering operator $\hat{T}_i$ is defined as

$$\hat{T}_i = \delta\hat{V}_i(\hat{I} - \hat{G}\delta\hat{V}_i)^{-1}.$$

Since we are interested in small perturbations around the ground state, we can safely use the Born approximation $\hat{T}_i \approx \delta\hat{V}_i$, and we also expand the logarithm as $\ln(1-x) \approx -x$, thus

$$E_{ij}^{\mathrm{int}} = -\frac{1}{\pi}\int_{-\infty}^{\varepsilon_{\mathrm{F}}} d\varepsilon \,\mathrm{Im}\mathrm{Tr}[\delta\hat{V}_i\hat{G}(\varepsilon)\delta\hat{V}_j\hat{G}(\varepsilon)]$$

Hamiltonian in a tight-binding scheme:

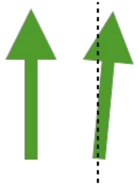
$$H_{nLs,n'L's'} = H^c_{nL,n'L'}\delta_{ss'} + H^s_{nL,nL'}\,\vec{e}_n.\vec{\sigma}_{ss'}$$

Which allow us to represent the perturbation:

$$\underline{\underline{\delta\hat{V}_i}}_{nn'} = \delta_{in}\delta_{in'}\underline{H^s_{ii}}\,\delta\vec{e}_i\vec{\sigma}$$

László Oroslány *et al.*
Phys. Rev. B 99, 224412 (2019)

Infinitesimal-rotations method



$$\mathrm{Tr}[\delta\hat{V}_i\hat{G}\delta\hat{V}_j\hat{G}]$$
$$= \mathrm{Tr}_{Ls}\{\underline{H}^s_{ii}(\delta\vec{e}_i\vec{\sigma})[\underline{G}^c_{ij}I + \underline{G}^s_{ij}(\vec{e}_0\vec{\sigma})]$$
$$\underline{H}^s_{jj}(\delta\vec{e}_j\vec{\sigma})[\underline{G}^c_{ji}I + \underline{G}^s_{ji}(\vec{e}_0\vec{\sigma})]\},$$

$$\mathrm{Tr}[\delta\hat{V}_i\hat{G}\delta\hat{V}_j\hat{G}]$$
$$= 2\mathrm{Tr}_L[\underline{H}^s_{ii}\underline{G}^c_{ij}\underline{H}^s_{jj}\underline{G}^c_{ji}$$
$$- \underline{H}^s_{ii}\underline{G}^s_{ij}\underline{H}^s_{jj}\underline{G}^s_{ji}]\delta\vec{e}_i\delta\vec{e}_j$$
$$\cancel{+ 4\mathrm{Tr}_L[\underline{H}^s_{ii}\underline{G}^s_{ij}\underline{H}^s_{jj}\underline{G}^s_{ji}](\delta\vec{e}_i\vec{e}_0)(\delta\vec{e}_j\vec{e}_0)}$$
$$\cancel{+ 2i\mathrm{Tr}_L[\underline{H}^s_{ii}\underline{G}^s_{ij}\underline{H}^s_{jj}\underline{G}^c_{ji}}$$
$$\cancel{- \underline{H}^s_{ii}\underline{G}^c_{ij}\underline{H}^s_{jj}\underline{G}^s_{ji}]\vec{e}_0(\delta\vec{e}_i \times \delta\vec{e}_j),}$$

$$E^{\mathrm{int}}_{ij} = -J_{ij}\,\delta\vec{e}_i\delta\vec{e}_j$$

infinitesimal
where $\delta\vec{e}_i \perp \vec{e}_0$

nonrelativistic collinear

For $\delta\vec{e}_i \perp \vec{e}_0$, nonrelativistic collinear magnetic case, time-reversal symmetry, and lots of algebra, we get the LKAG formula (Liechtenstein formula)

$$J_{ij} = \frac{2}{\pi}\int_{-\infty}^{\varepsilon_F} d\varepsilon\,\mathrm{Im}\mathrm{Tr}_L[\underline{H}^s_{ii}\underline{G}^{\uparrow}_{ij}\underline{H}^s_{jj}\underline{G}^{\downarrow}_{ji}]$$

$$\underline{H}^{c/s}_{nn} = \frac{1}{2}(\underline{H}^{\uparrow}_{nn} \pm \underline{H}^{\downarrow}_{nn})$$

$$\hat{G}(z) = (z\hat{I} - \hat{H})^{-1}$$

László Oroszlány *et al.*
Phys. Rev. B 99, 224412 (2019)

Liechtenstein, Katsnelson, Antropov, Gubanov
J. Magn. Magn. Mater. **67**, 65 (1987)

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Método multi-escala

Calculos de DFT

JuKKR

- Korrings-Kohn-Rostoker (KKR)
- Green function
- Full potential
- Spin-orbit coupling
- LDA, PBE

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- Plane-wave basis
- Very large use/development community
- Pseudopotential (fast)
- Spin-orbit coupling
- DFT+U+V and more new advancements

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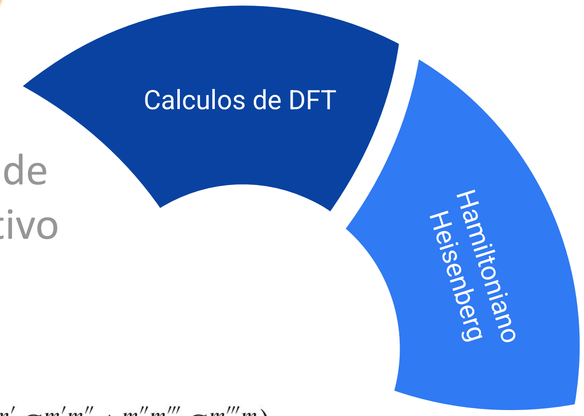
Método multi-escala



- Mapeamento da estrutura eletrônica de primeiros princípios num modelo efetivo
- Método das rotações infinitesimais

LKAG formula:

$$J_{ij} = -\frac{1}{2\pi} \int_{-\infty}^{E_F} d\varepsilon \sum_{\substack{mm' \\ m''m'''}} \mathrm{Im}\left(\Delta_i^{mm'} G_{ij,\downarrow}^{m'm''} \Delta_j^{m''m'''} G_{ji,\uparrow}^{m'''m}\right)$$

where

$$\Delta_i^{mm'} = \int_{\mathrm{BZ}} \left[H_{ii,\uparrow}^{mm'}(\mathbf{k}) - H_{ii,\downarrow}^{mm'}(\mathbf{k})\right] d\mathbf{k}$$

Liechtenstein, Katsnelson, Antropov, Gubanov
J. Magn. Magn. Mater. **67**, 65 (1987)

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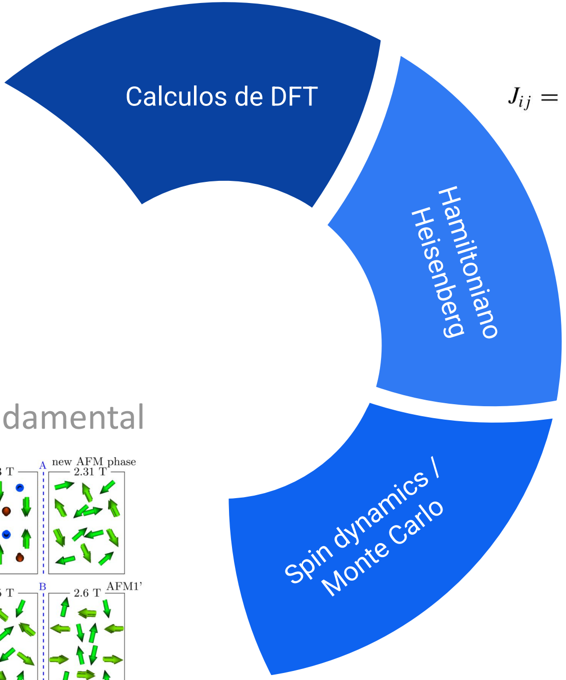
Método multi-escala



$$J_{ij} = -\frac{1}{2\pi}\int_{-\infty}^{E_F} d\varepsilon \sum_{\substack{mm'\\ m''m'''}} \mathrm{Im}\left(\Delta_i^{mm'} G_{ij,\downarrow}^{m'm''} \Delta_j^{m''m'''} G_{ji,\uparrow}^{m'''m}\right)$$

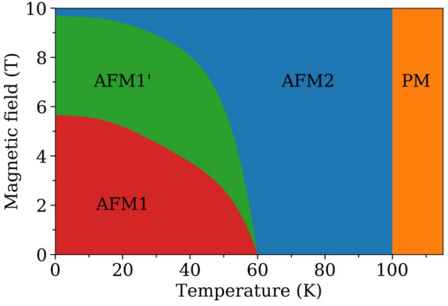
$$\Delta_i^{mm'} = \int_{\mathrm{BZ}} \left[H_{ii,\uparrow}^{mm'}(\mathbf{k}) - H_{ii,\downarrow}^{mm'}(\mathbf{k})\right] d\mathbf{k}$$

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{2}\sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$

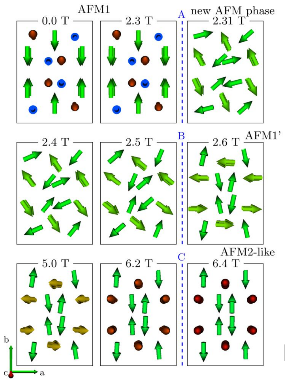
Landau-Lifshitz-Gilbert (LLG)

$$\frac{1}{\gamma}\frac{\mathrm{d}\,\mathbf{m}_i}{\mathrm{d}\,t} = -\underbrace{\left(\mathbf{m}_i \times \mathbf{B}_{\mathrm{eff}}^i\right)}_{\text{precessão}} - \underbrace{\lambda\left[\mathbf{m}_i \times \left(\mathbf{m}_i \times \mathbf{B}_{\mathrm{eff}}^i\right)\right]}_{\text{amortecimento}}$$

Diagrama de fase, Temperature critica



Estado fundamental



N. Biniskos, F. J. dos Santos et al., PRB 105, 104404 (2022)

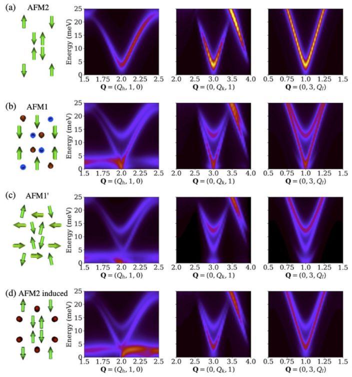
Método multi-escala

$$J_{ij} = -\frac{1}{2\pi}\int_{-\infty}^{E_F} d\varepsilon \sum_{\substack{mm'\\ m''m'''}} \mathrm{Im}\left(\Delta_i^{mm'} G_{ij,\downarrow}^{m'm''} \Delta_j^{m''m'''} G_{ji,\uparrow}^{m'''m}\right)$$

$$\Delta_i^{mm'} = \int_{\mathrm{BZ}} \left[H_{ii,\uparrow}^{mm'}(\mathbf{k}) - H_{ii,\downarrow}^{mm'}(\mathbf{k})\right] d\mathbf{k}$$

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\,\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{2}\sum_{ij}\mathbf{D}_{ij}\cdot(\mathbf{S}_i\times\mathbf{S}_j)$$

- Teoria linear de ondas de spin
- Teoria de espalhamento de nêutrons



N. Biniskos, F. J. dos Santos et al., APL Materials 11, 081103 (2023)

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Método multi-escala

$$J_{ij} = -\frac{1}{2\pi}\int_{-\infty}^{E_F} d\varepsilon \sum_{\substack{mm'\\ m''m'''}} \mathrm{Im}\left(\Delta_i^{mm'} G_{ij,\downarrow}^{m'm''} \Delta_j^{m''m'''} G_{ji,\uparrow}^{m'''m}\right)$$

$$\Delta_i^{mm'} = \int_{\mathrm{BZ}} \left[H_{ii,\uparrow}^{mm'}(\mathbf{k}) - H_{ii,\downarrow}^{mm'}(\mathbf{k})\right] d\mathbf{k}$$

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\,\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{2}\sum_{ij}\mathbf{D}_{ij}\cdot(\mathbf{S}_i\times\mathbf{S}_j)$$

- Python package desenvolvida no EPFL
- Automação, gerenciamento, e armazenamento de dados
- *High-throughput*
- Transferência de conhecimento

Método multi-escala

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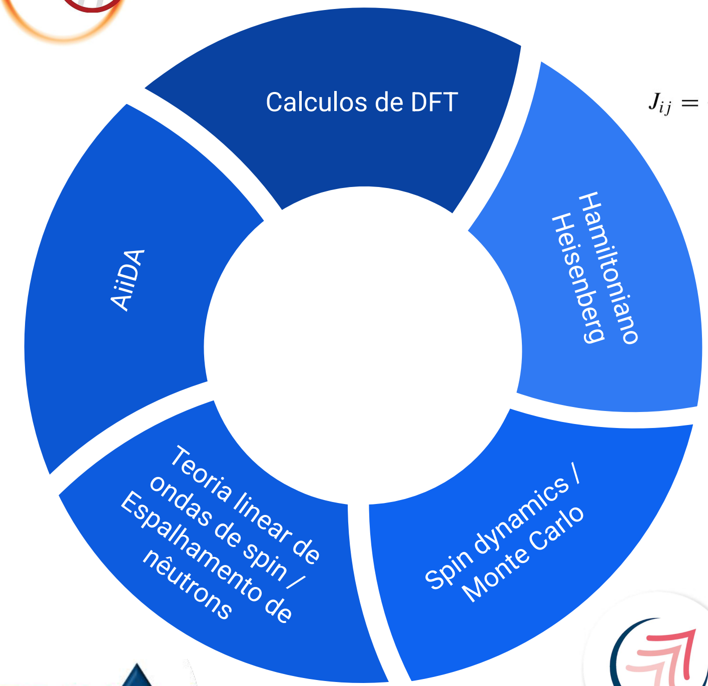
JuKKR

AiiDA



$$J_{ij} = -\frac{1}{2\pi}\int_{-\infty}^{E_F} d\varepsilon \sum_{\substack{mm' \\ m''m'''}} \mathrm{Im}\left(\Delta_i^{mm'} G_{ij,\downarrow}^{m'm''} \Delta_j^{m''m'''} G_{ji,\uparrow}^{m'''m}\right)$$

$$\Delta_i^{mm'} = \int_{\mathrm{BZ}} \left[H_{ii,\uparrow}^{mm'}(\mathbf{k}) - H_{ii,\downarrow}^{mm'}(\mathbf{k})\right] d\mathbf{k}$$

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{2}\sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$

spirit

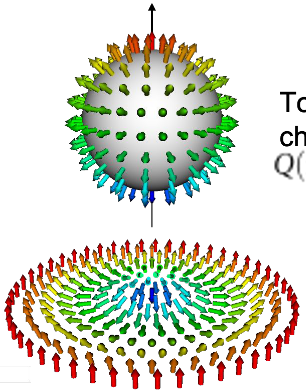
SWTS

Spin-resolved inelastic scattering by spin waves in noncollinear magnets

Flaviano José dos Santos et al., Phys. Rev. B 97, 024431 (2018)

Skyrmions magnéticos

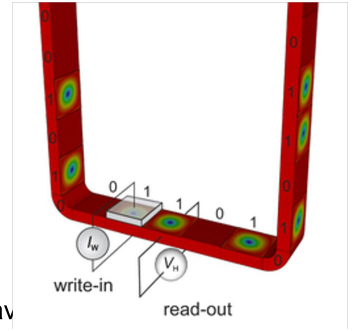
Skyrmion



Topological charge

$$Q(\mathbf{m}) = \frac{1}{4\pi}\int_{\mathbb{R}^2} \mathbf{m}\cdot(\partial_x \mathbf{m}\times \partial_y \mathbf{m})\,\mathrm{d}\mathbf{r}$$

Bogdanov *et al.*,
Zh. Eksp. Teor. Fiz. **95**, 178 (1989)



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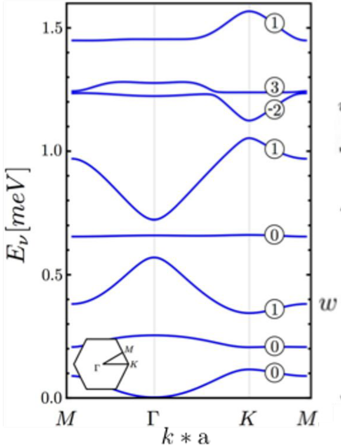
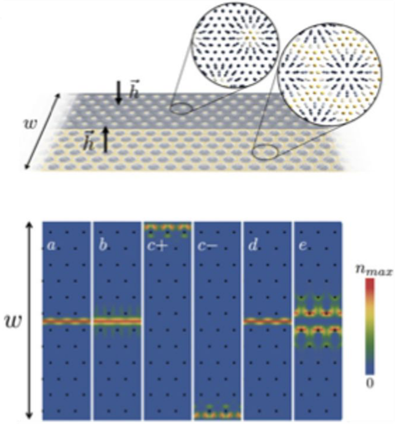
Fert *et al.*,
Nat. Nano. **8**, 152 (2013)

Zhang *et al.*,
Sci. Rep. **5**, 15773 (2015)

Topological spin waves





Roldán-Molina, *et al.*,
New J. Phys. **18**, 045015 (2016)

Díaz, *et al.*,
Phys. Rev. Lett. **122**, 187203 (2019)

Hamiltoniano de Heisenberg generalizado

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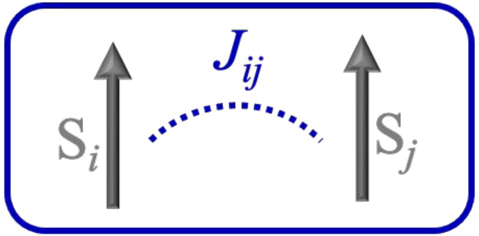
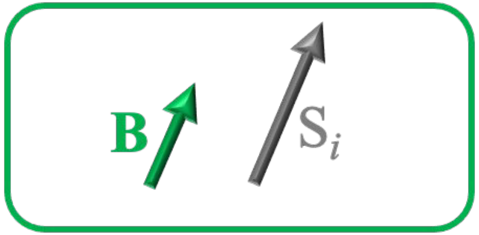




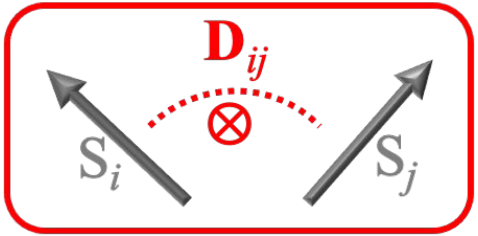
Mag. exchange interaction (MEI)

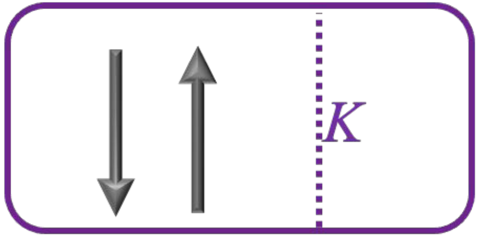
Dzyaloshinskii-Moriya Interaction (DMI)

Mag. field

Mag. anisotropy

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\,\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{2}\sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) - \sum_i \mathbf{B} \cdot \mathbf{S}_i - \sum_\alpha K^\alpha \sum_i (S_i^\alpha)^2$$





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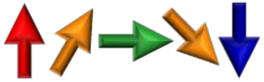
Teoria linear de spin wave para magnetos não-colineares

local ref. frame



HP transformation

$$\mathcal{H}_2 = \sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}^{\dagger} \tilde{\mathbf{J}}_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}$$

Holstein-Primakoff transformation $\mathbf{S}_i' = \mathbf{M}_i \mathbf{a}_i$

$$\mathbf{M}_i = \sqrt{\frac{S_i}{2}} \begin{pmatrix} 1 & 1 & 0 \\ -\mathrm{i} & \mathrm{i} & 0 \\ 0 & 0 & \sqrt{\frac{2}{S_i}} \end{pmatrix} \quad \text{and} \quad \mathbf{a}_i = \begin{pmatrix} a_i \\ a_i^{\dagger} \\ S_i - a_i^{\dagger} a_i \end{pmatrix}$$

Holstein and Primakoff,
Phys. Rev. 58, 1098 (1940)

Bogoliubov transformation

$$\mathcal{H}_2 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}$$

F.J. dos Santos,
Phys. Rev. B 97, 024431 (2018)

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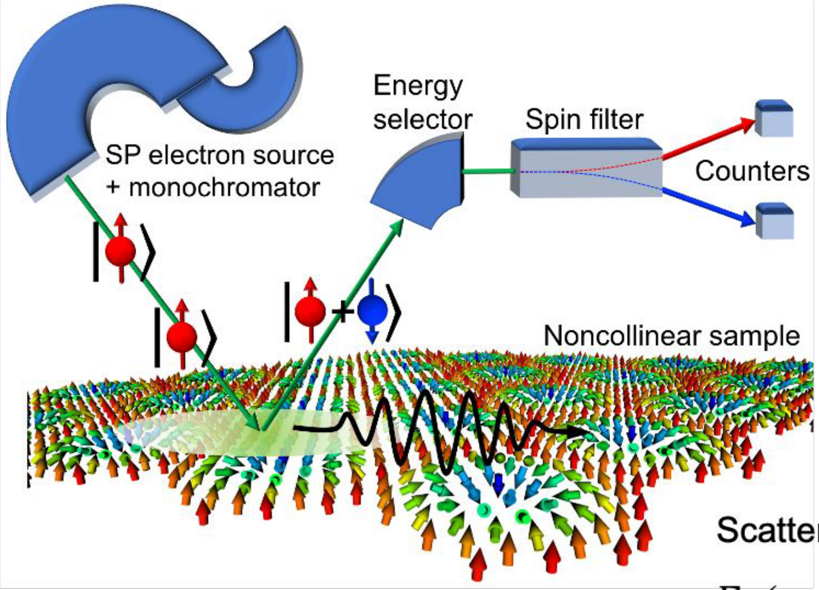
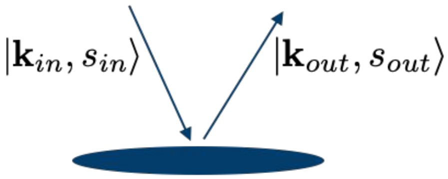
Spin-resolved electron-energy-loss spectroscopy (SREELS)





$$\omega = E_{\text{in}} - E_{\text{out}}$$
$$\mathbf{q} = \mathbf{k}_{\text{in}} - \mathbf{k}_{\text{out}}$$
$$s = s_{\text{in}} - s_{\text{out}}$$

s	$\uparrow$	$\downarrow$
$\uparrow$	0	-1
$\downarrow$	1	0

Scattering rate

$$\Gamma_m(\mathbf{q},\omega) \propto \sum_{\alpha\beta} \sigma^{\alpha}_{s_{\text{in}}s_{\text{out}}} \sigma^{\beta}_{s_{\text{out}}s_{\text{in}}} \sum_{\mu\nu} e^{\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\mu\nu}} \mathcal{N}^{\alpha\beta}_{\mu\nu}(\mathbf{q},\omega)$$

Spin-spin correlation functions

$$\mathcal{N}^{\alpha\beta}_{\mu\nu}(\mathbf{q},\omega) = 2\sqrt{S_\mu S_\nu} \sum_r \delta\big(E_0 + \omega - E_r(\mathbf{q})\big) \times \left[O^{\alpha+}_{\mu}(\mathcal{R}^{++}_{\mu r}(\mathbf{q}))^* + O^{\alpha-}_{\mu}(\mathcal{R}^{-+}_{\mu r}(\mathbf{q}))^*\right] \left[O^{\beta+}_{\nu}\mathcal{R}^{-+}_{\nu r}(\mathbf{q}) + O^{\beta-}_{\nu}\mathcal{R}^{++}_{\nu r}(\mathbf{q})\right]$$

dos Santos *et al.*,
Phys. Rev. B 97, 024431 (2018)

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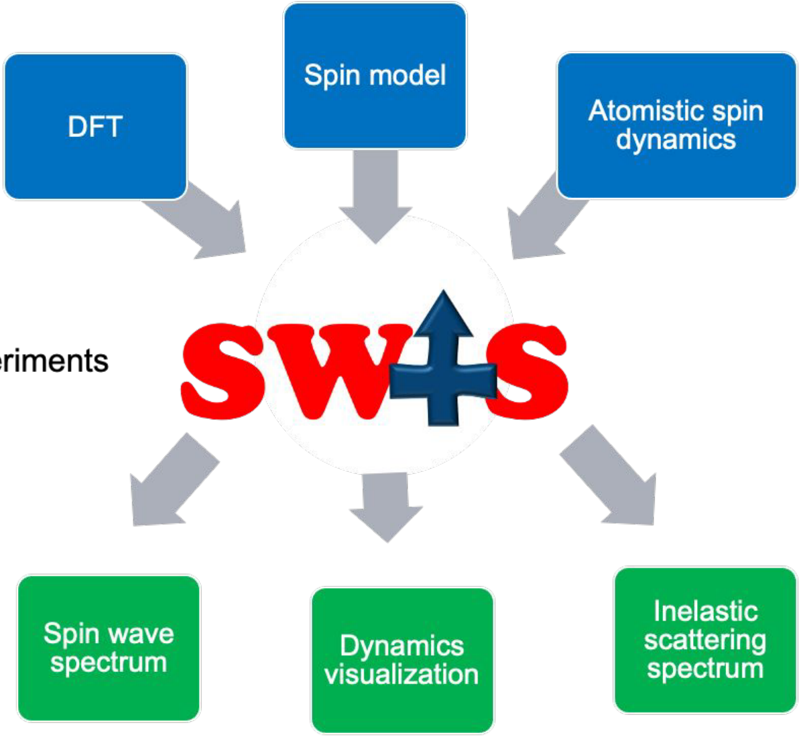
Spin Waves & Inelastic Scattering

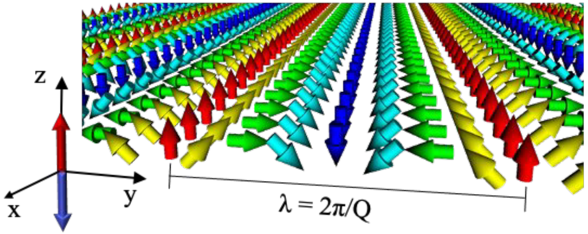
SWIS package



- ✓ Linear spin wave theory
- ✓ Arbitrary noncollinear spin texture
- ✓ Connection to inelastic scattering experiments
- ✓ Written in Fortran and Python
- ✓ Parallelized with OpenMP
- ✓ Easy-to-use
- ✓ Graphical user interface

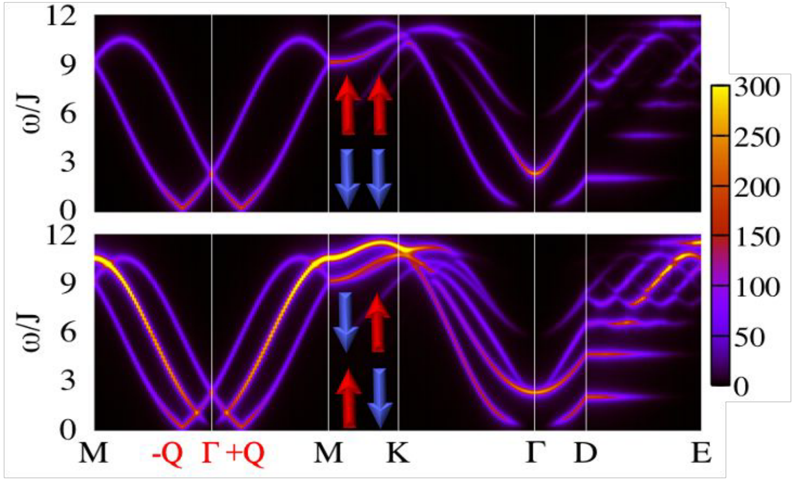
flaviano@cbpf.br

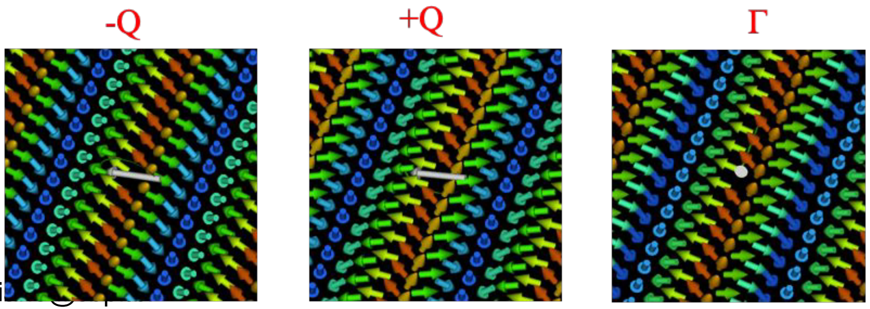
SREELS - Spiral de spin

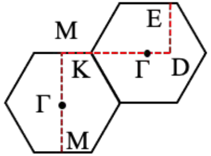


polarization along z

Spin-resolved inelastic spectra



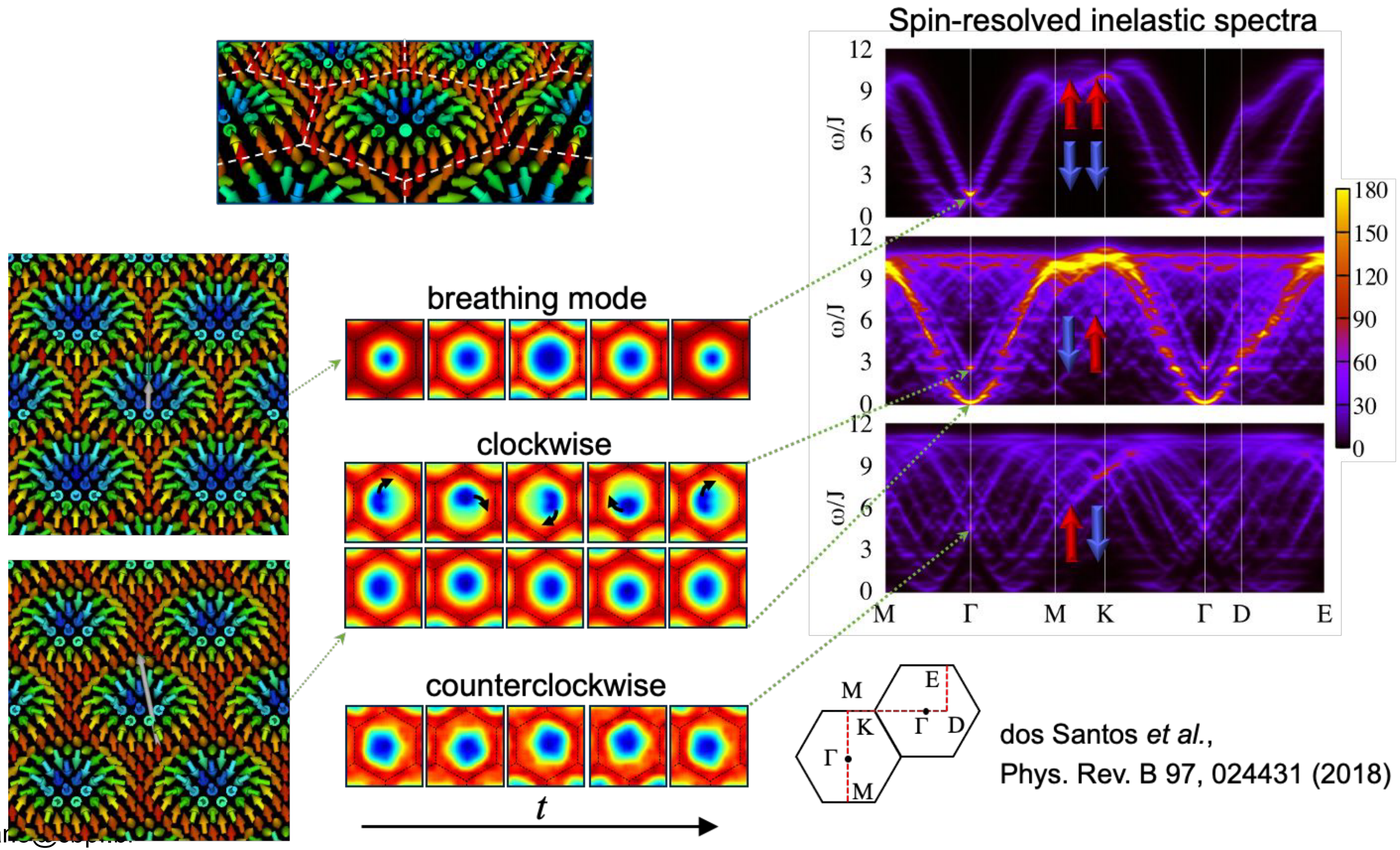




dos Santos *et al.*,
Phys. Rev. B 97, 024431 (2018)

flavi

SREELS - rede de Skyrmion



dos Santos *et al.*,
Phys. Rev. B 97, 024431 (2018)

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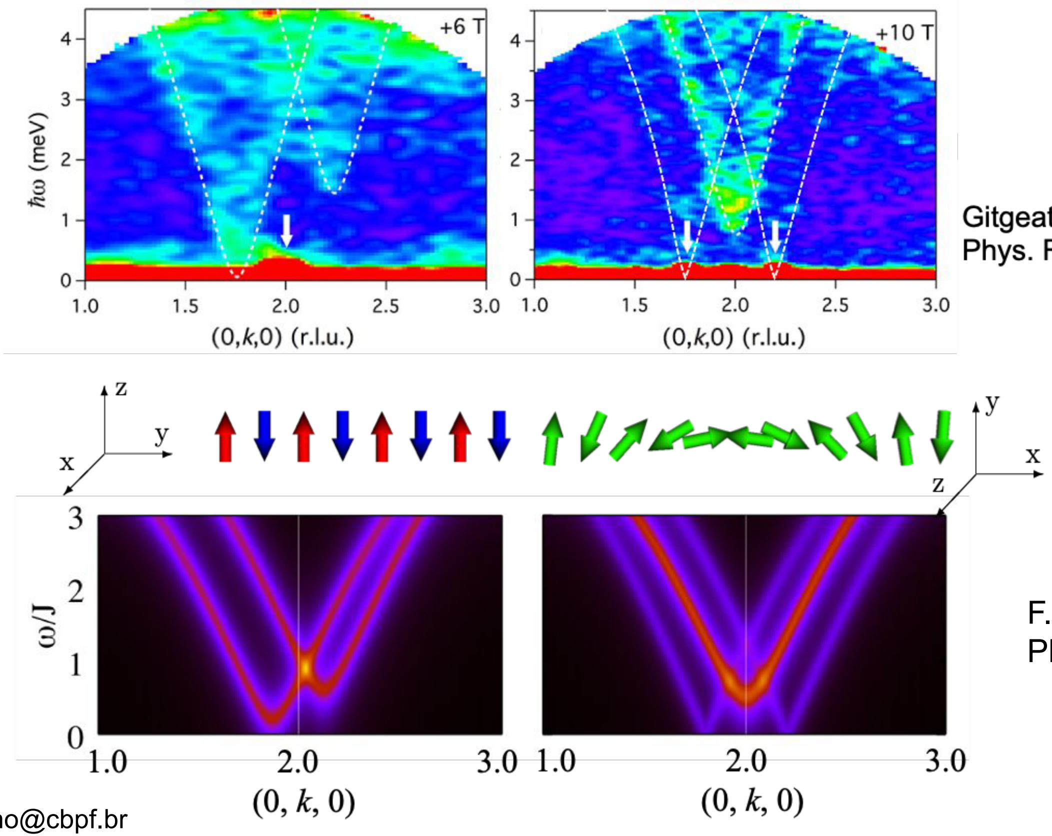
Comparison with experiment

Inelastic neutron scattering on bulk α-$Cu_2V_2O_7$



Gitgeatpong *et al.*,
Phys. Rev. Lett. **119**, 047201 (2017)

F.J. dos Santos,
Phys. Rev. B 102, 104436 (2020)

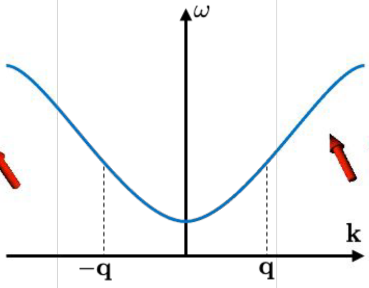
flaviano@cbpf.br

Nonreciprocity of spin waves in noncollinear magnets due to the Dzyaloshinskii-Moriya interaction

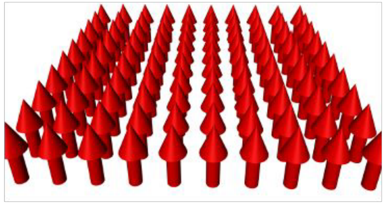
Flaviano José dos Santos et al., Phys. Rev. B 102, 104401 (2020)

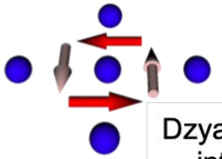
Nonreciprocity of spin waves

dispersion curve



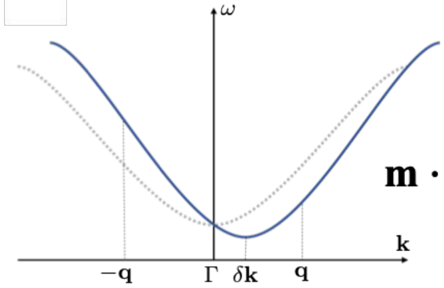
out-of-plane magnetization





Dzyaloshinskii-Moriya interaction (DMI)

nonreciprocal dispersion



$\mathbf{m} \cdot \mathbf{D}(\boldsymbol{k})$

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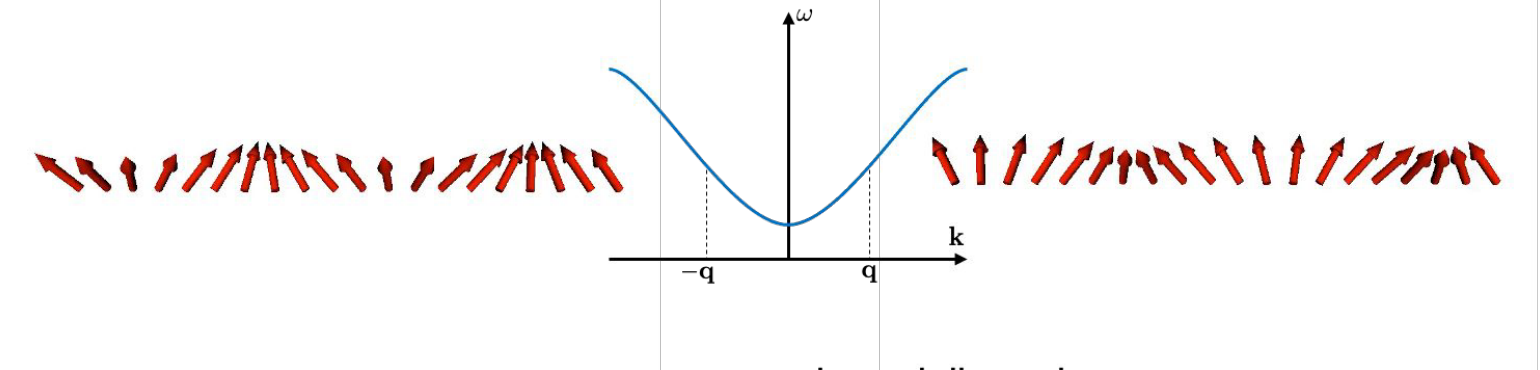
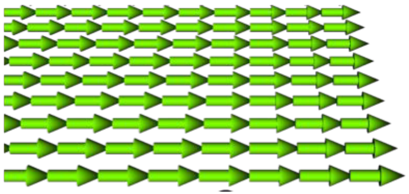
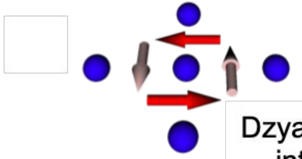
Nonreciprocity of spin waves

dispersion curve



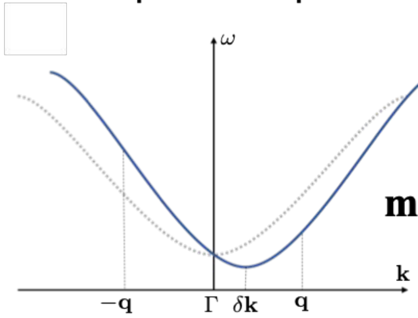
in-plane magnetization





Dzyaloshinskii-Moriya interaction (DMI)

nonreciprocal dispersion



$$\mathbf{m} \cdot \mathbf{D}(\boldsymbol{k})$$

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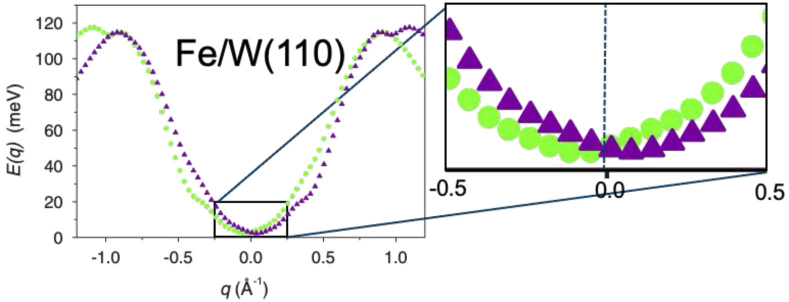
Application: measuring the DMI

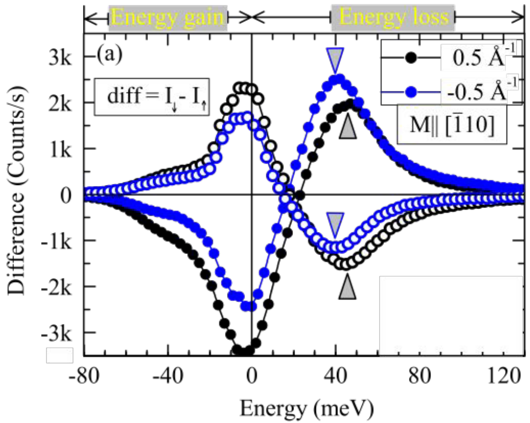
Theoretical prediction



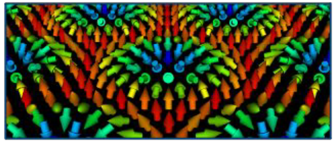
Udvardi, *et al.*, Phys. Rev. Lett. **102**, 207204 (2009)

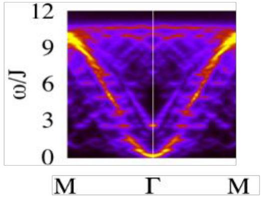
Costa, *et al.*, Phys. Rev. B **82**, 014428 (2010)

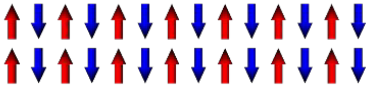
Experimental observation with EELS



Zakeri, *et al.*,
Phys. Rev. Lett. **104**, 137203 (2010)







$$\mathbf{m} \cdot \mathbf{D}(\boldsymbol{k}) = 0$$

?

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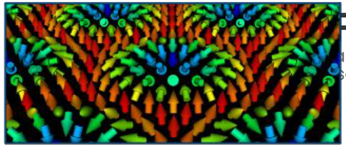
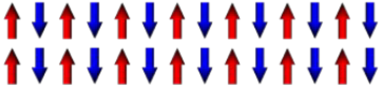
Sim, através do SREELS



sileiro
sas Físicas



Spin-wave angular mom.
is associated with
spin-wave chirality

Nonzero angular momentum

DMI parallel to spin-wave angular mom.: $s \parallel \mathbf{D}(\mathbf{k})$

Nonreciprocal inelastic spectrum

Spin-flip channel

Electron polarization parallel to spin-wave angular mom.: $s \parallel \mathbf{P}$

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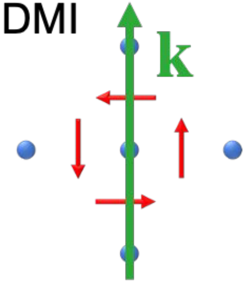
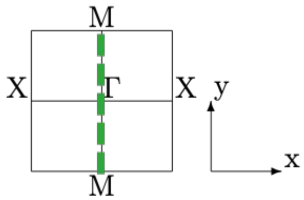
Sim, através do SREELS

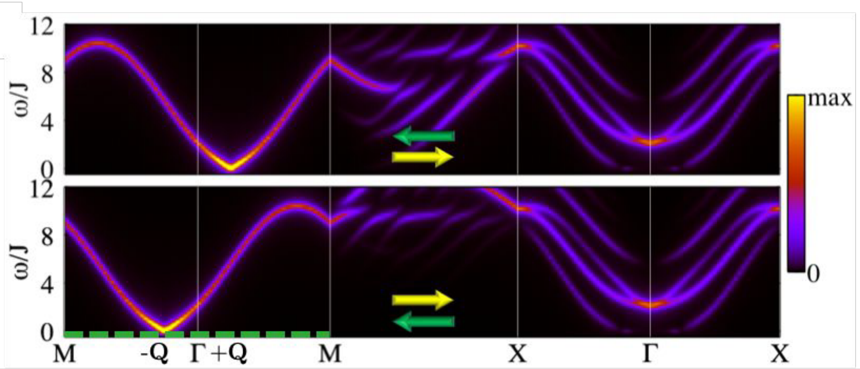
DMI



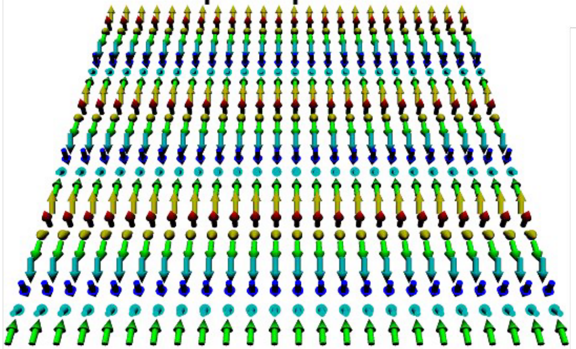
Brillouin zone



$\boldsymbol{s} \parallel \mathbf{D}(\mathbf{k}) \parallel \mathbf{P}$



Spin spiral



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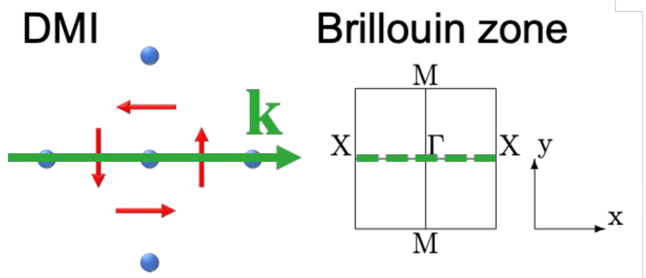
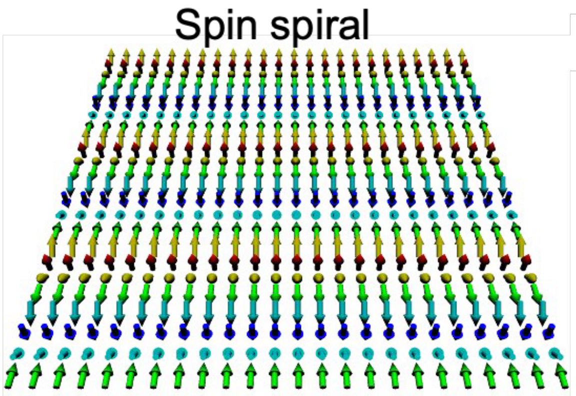
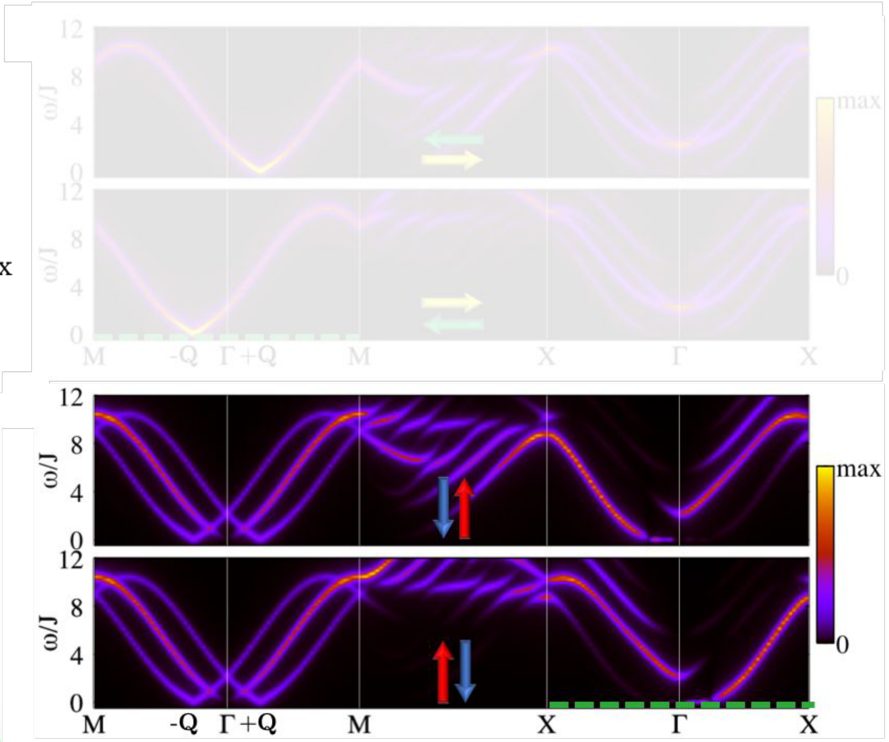
Sim, através do SREELS





$s \parallel \mathbf{D}(\mathbf{k}) \parallel \mathbf{P}$



Topological magnons in Mn_5Ge_3 and the impact of dimensionality

People involved

CBPF
Centro Brasileiro
de Pesquisas Físicas

Experiment

Nikolaos Biniskos
FZ Jülich & Charles U

Karin Schmalzl
FZ Jülich @ ILL

Jörg Persson
FZ Jülich

Frédéric Bourdarot
CEA & U Grenoble

Thomas Brückel
FZ Jülich

Theory

Manuel dos Santos Dias
Paul Scherrer Institut

Nicola Marzari
EPFL & PSI

Stefan Blügel
FZ Jülich

Samir Lounis
FZ Jülich & UDE

NEUTRONS
FOR SOCIETY

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

HORIZON 2020

CAPES

DFG
Deutsche
Forschungsgemeinschaft

Swiss National
Science Foundation

flaviano@cbpf.br

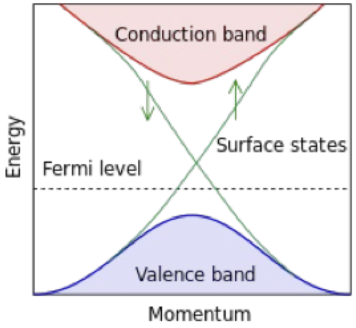
Topological insulator

CBPF
Centro Brasileiro
de Pesquisas Físicas

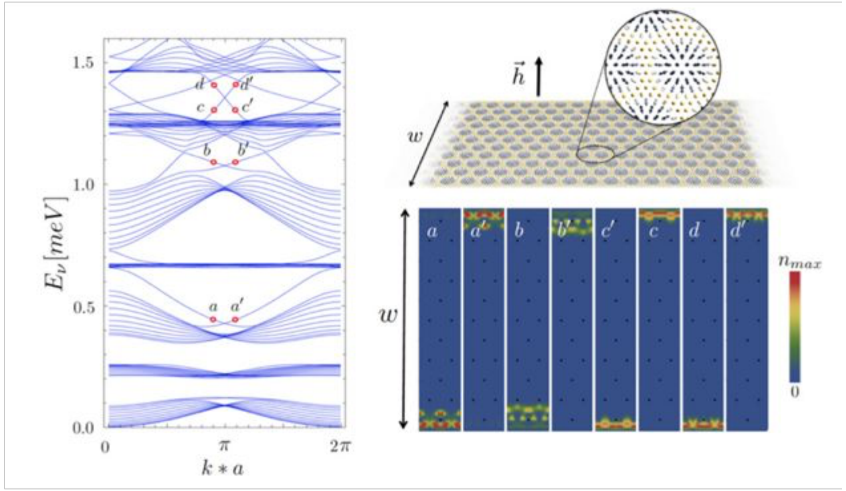
Electrons

Magnons

Topological insulator band structure



- Broken inversion symmetry
- Strong spin-orbit coupling



Roldán-Molina *et al.*,
New J. Phys. 18 (2016)
045015

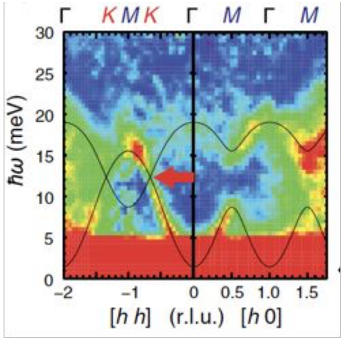
flaviano@cbpf.br

Topological magnons

Topological Spin Excitations in Honeycomb Ferromagnet CrI_3

Lebing Chen, Jae-Ho Chung, Bin Gao, Tong Chen, Matthew B. Stone, Alexander I. Kolesnikov, Qingzhen Huang, and Pengcheng Dai

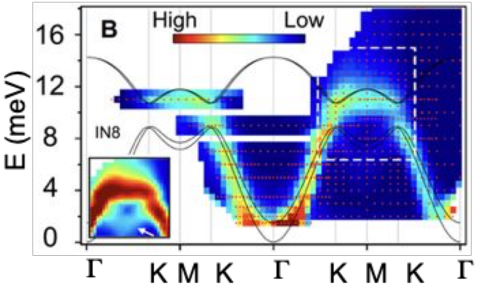
Phys. Rev. X **8**, 041028 – Published 14 November 2018

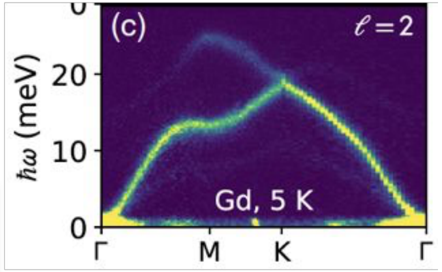


Topological magnon insulators in two-dimensional van der Waals ferromagnets $CrSiTe_3$ and $CrGeTe_3$: Toward intrinsic gap-tunability

FENGFENG ZHU, LICHUAN ZHANG, XIAO WANG, FLAVIANO JOSÉ DOS SANTOS, JUNDA SONG, THOMAS MUELLER, KARIN SCHMALZL, WOLFGANG F. SCHMIDT, ALEXANDRE IVANOV, JITAE T. PARK, JIANHUI XU, JIE MA, SAMIR LOUNIS, STEFAN BLÜGEL, YURIY MOKROUSOV, YIXI SU, AND THOMAS BRÜCKEL fewer Authors Info & Affiliations

SCIENCE ADVANCES • 10 Sep 2021 • Vol 7, Issue 37 • DOI: 10.1126/sciadv.abi7532





Dirac Magnons, Nodal Lines, and Nodal Plane in Elemental Gadolinium

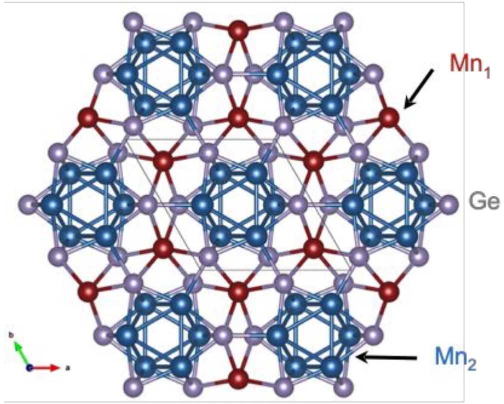
A. Scheie, Pontus Laurell, P. A. McClarty, G. E. Granroth, M. B. Stone, R. Moessner, and S. E. Nagler

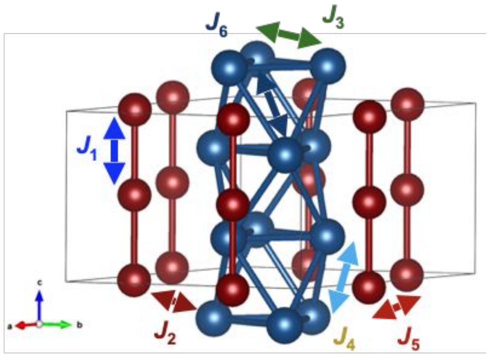
Phys. Rev. Lett. **128**, 097201 – Published 2 March 2022

 flaviano@cbpf.br

Mn_5Ge_3 metallic compound

CBPF Centro Brasileiro de Pesquisas Físicas





- $P6_3/mcm$
- **Centrosymmetric**
- Ferromagnetic

nature communications

Article https://doi.org/10.1038/s41467-023-43042-3

Topological magnons driven by the Dzyaloshinskii-Moriya interaction in the centrosymmetric ferromagnet Mn_5Ge_3

Received: 9 August 2023

Accepted: 31 October 2023

Published online: 11 November 2023

Check for updates

M. dos Santos Dias[1,2,3], N. Biniskos[4,10], F. J. dos Santos[5,6], K. Schmalzl[7], J. Persson[8], F. Bourdarot[9], N. Marzari[5,6], S. Blügel[1], T. Brückel[8] & S. Lounis[1,2]

The phase of the quantum-mechanical wave function can encode a topological structure with wide-ranging physical consequences, such as anomalous transport effects and the existence of edge states robust against perturbations.

First-principles Hamiltonian parametrization

- DFT calculations for structural properties
  - Optimize unit cell parameters and atomic positions
- DFT calculations for magnetic properties
  - Parameters for spin Hamiltonian

jukkr.fz-juelich.de

external field — on-site anisotropy — tensorial exchange

$$\mathcal{E} = \sum_i \sum_\alpha B_i^\alpha S_i^\alpha + \sum_i \sum_{\alpha,\beta} K_i^{\alpha\beta} S_i^\alpha S_i^\beta + \frac{1}{2} \sum_{i,j} \sum_{\alpha,\beta} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta$$

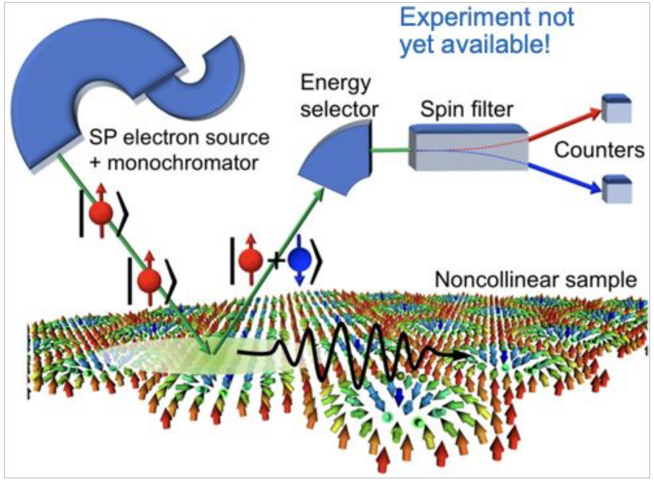
flaviano@cbpf.br

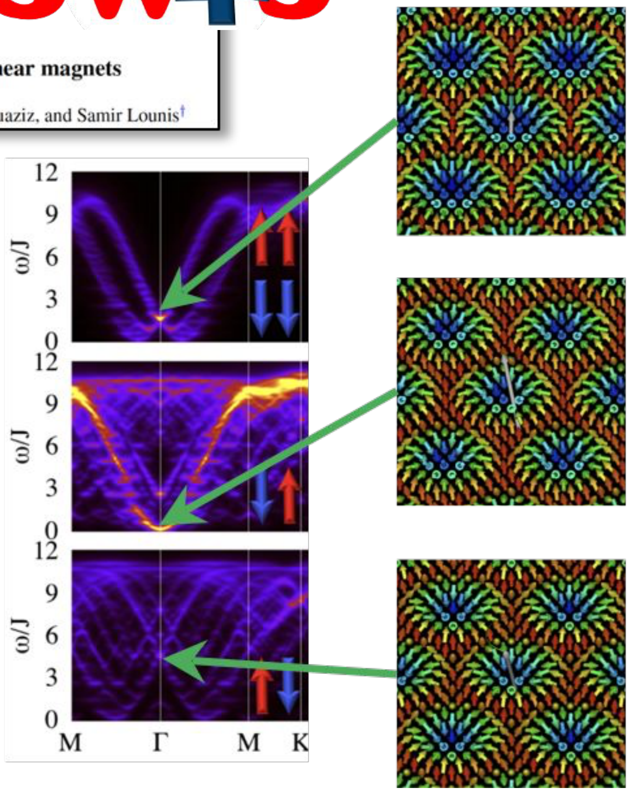
Linear spin-wave theory and inelastic scattering

PHYSICAL REVIEW B **97**, 024431 (2018)

Spin-resolved inelastic electron scattering by spin waves in noncollinear magnets

Flaviano José dos Santos,* Manuel dos Santos Dias, Filipe Souza Mendes Guimarães, Juba Bouaziz, and Samir Lounis†





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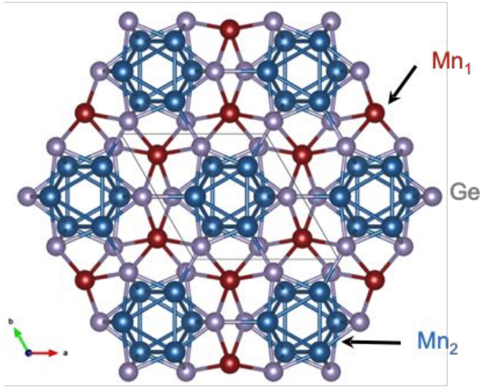
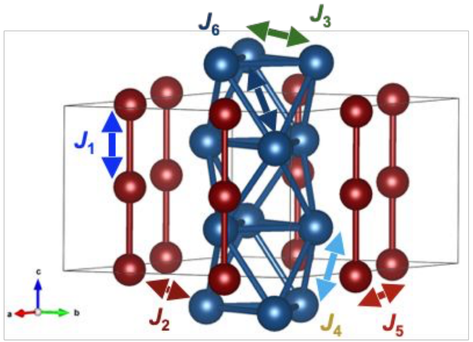
DFT calculations for Mn_5Ge_3

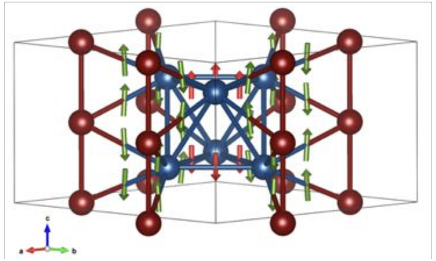


P6_3/mcm
(centrosymmetric)



meV

(meV)	type	APL 2009	This work
J_1	Mn_1-Mn_1	29.1	30.9
J_2	Mn_1-Mn_2	8.0	8.6
J_3	Mn_2-Mn_2	-2.0	-1.3
J_4	Mn_2-Mn_2	6.9	6.8
J_5	Mn_1-Mn_1	-1.4	-3.9
J_6	Mn_2-Mn_2	9.4	10.0
D_2	Mn_1-Mn_2	—	0.6
D_3	Mn_2-Mn_2	—	0.5



$$\mathcal{H} = K\sum_i (S_i^z)^2 - \sum_{i,j} J_{ij}\,\mathbf{S}_i\cdot\mathbf{S}_j - \sum_{i,j} \mathbf{D}_{ij}\cdot(\mathbf{S}_i\times\mathbf{S}_j)$$

K ~ 0.1 meV / Mn

dos Santos Dias et al.,
Nat. Commun. (2023)14:7321

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Theoretical spin-wave dispersion

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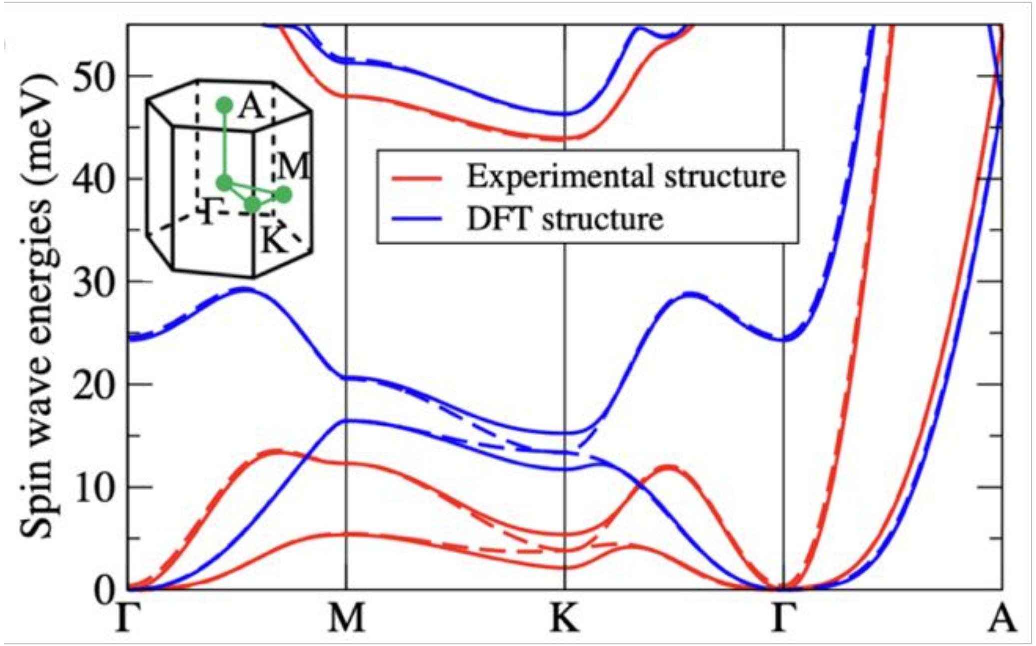

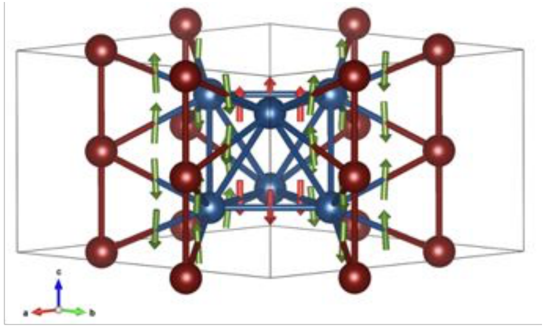

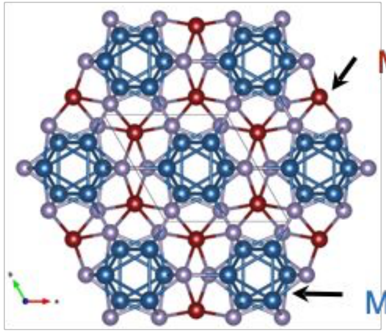

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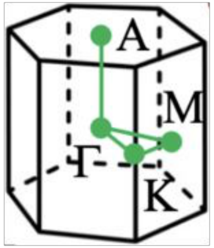
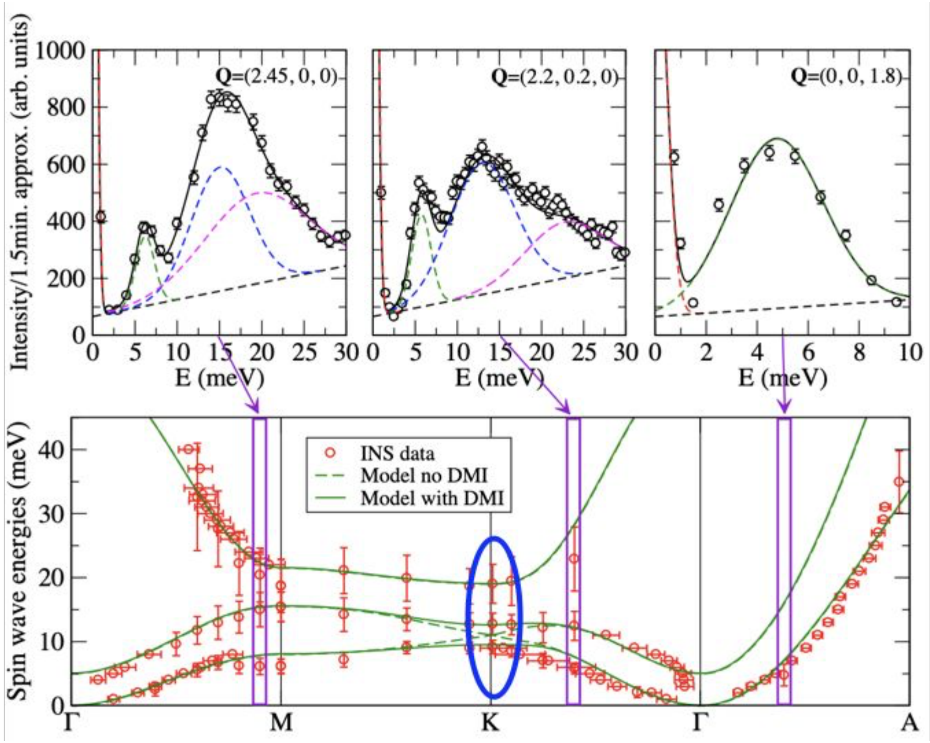
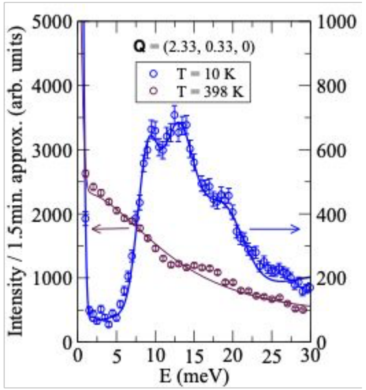
dos Santos Dias et al.,
Nat. Commun. (2023)14:7321

Inelastic-neutron-scattering measurements on Mn_5Ge_3

Institut Laue-Langevin (ILL)
CRG-Jülich and CRG-CEA
Grenoble







dos Santos Dias et al.,
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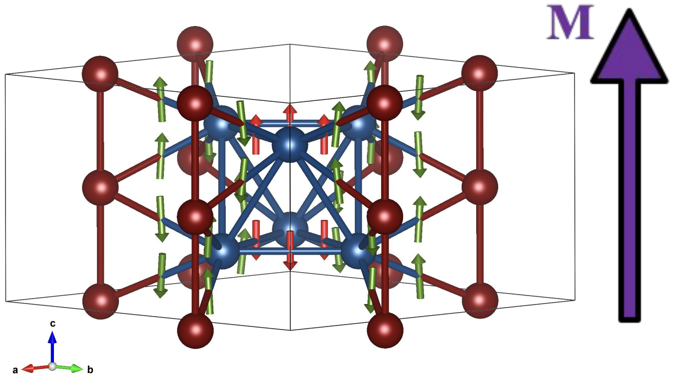

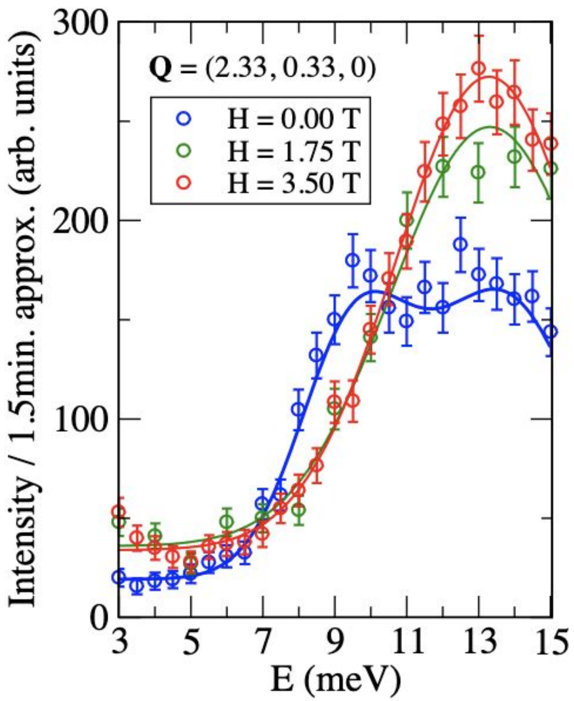

dos Santos Dias et al.,
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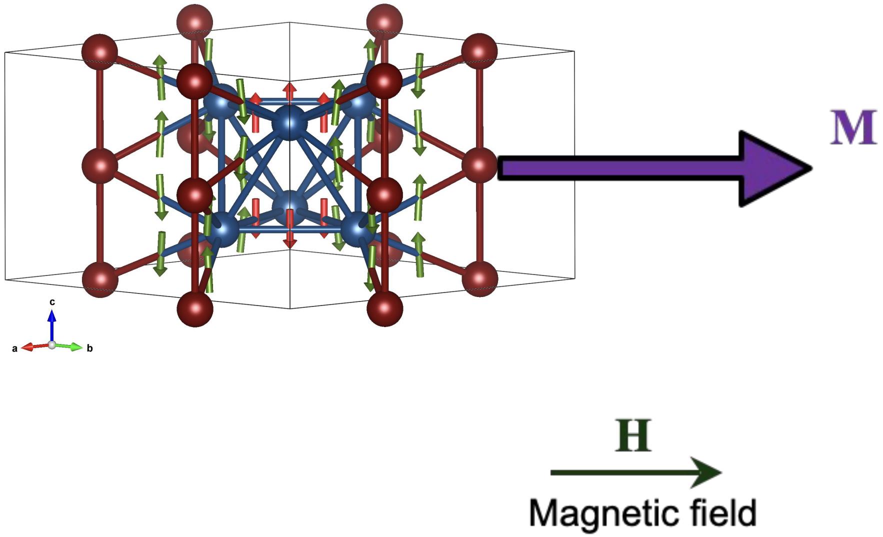
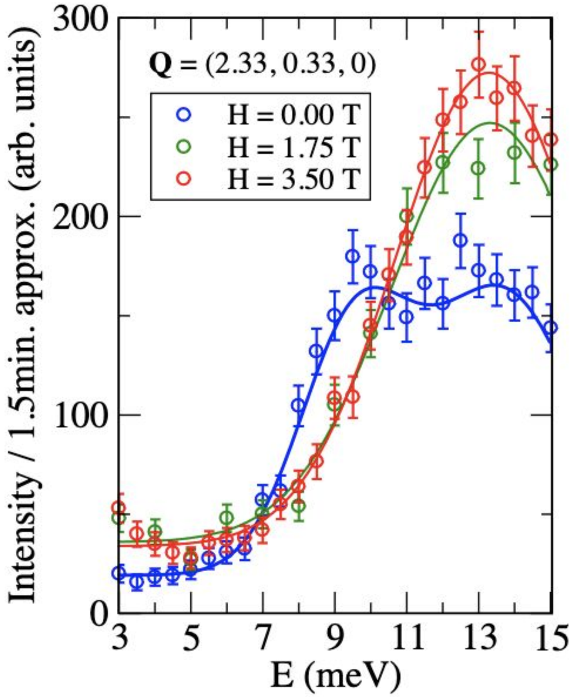
Inelastic-neutron-scattering measurements on Mn_5Ge_3





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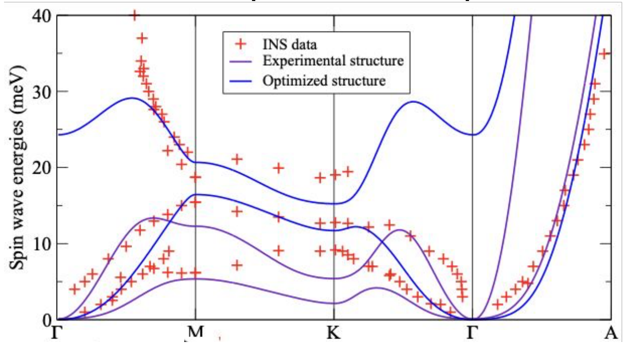
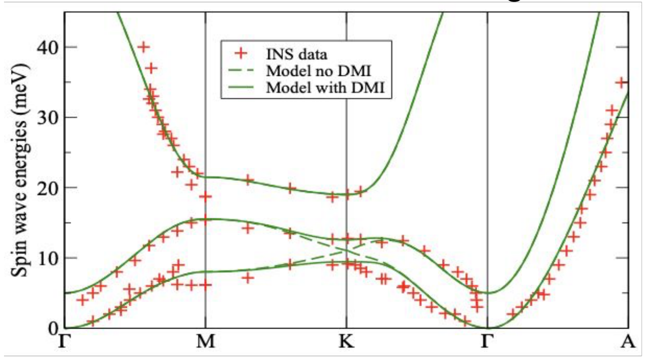
dos Santos Dias et al.,
Nat. Commun. (2023)14:7321

Minimal model: 3 spins

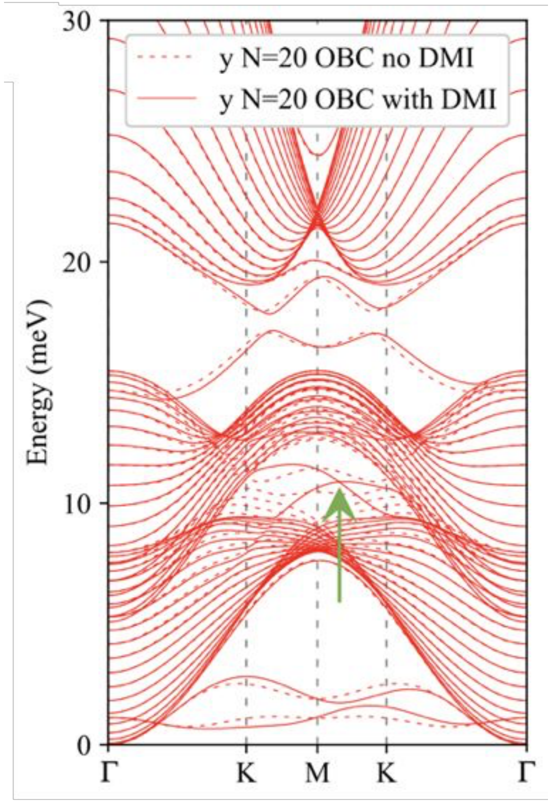
DFT vs exp. direct comparison



minimal model fitting



modelling a surface



Can we do better?

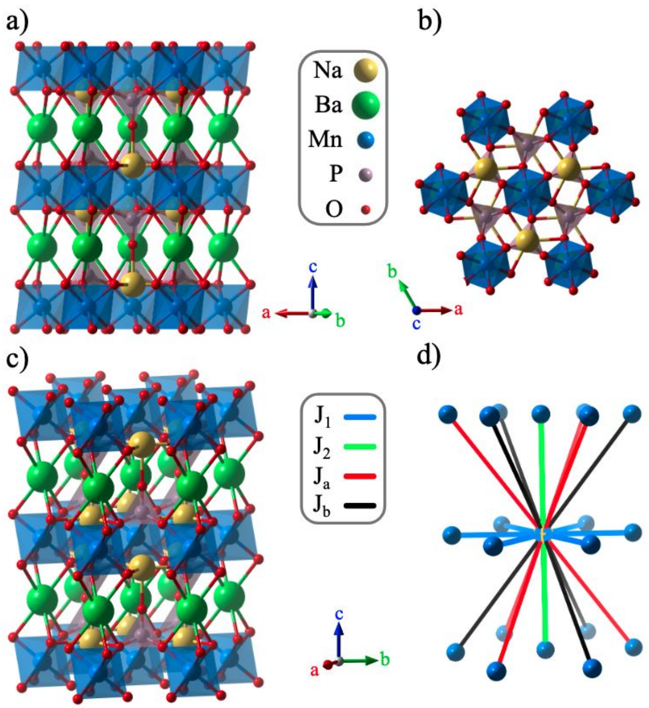
dos Santos Dias et al.,
Nat. Commun. (2023)14:7321

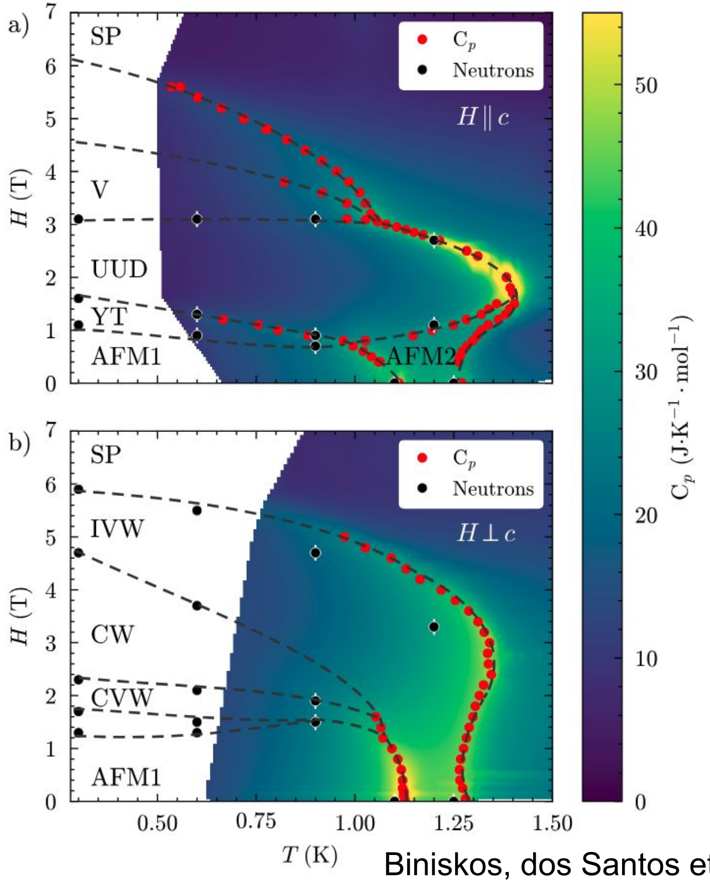
$Na_2BaMn(PO_4)_2$: a quantum spin liquid candidate

Nikolaos Biniskos, Flaviano José dos Santos, et al.

- Typical magnetic materials tend to develop ordered magnetic patterns, like ferromagnetic or antiferromagnetic order, as they cool.
- A quantum spin liquid (QSL) is an exotic phase of matter where the arrangement of magnetic spins does not freeze into a regular pattern even at very low temperatures. The spins remain in a constantly fluctuating, disordered state.

Spin-5/2 triangular-lattice antiferromagnet $Na_2BaMn(PO_4)_2$





Biniskos, dos Santos et al, in review

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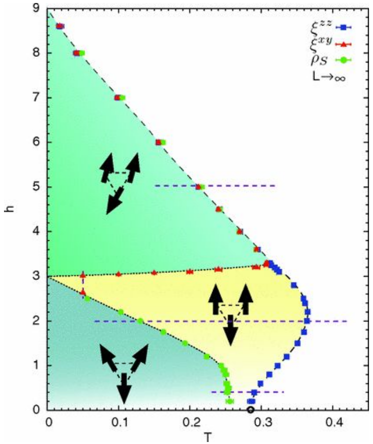
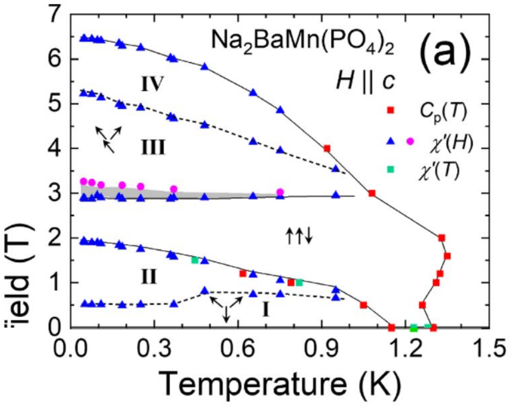
Results with a minimal model

frustrated triangular lattice



Luis Seabra et al,
Phys. Rev. B 84, 214418 (2011)

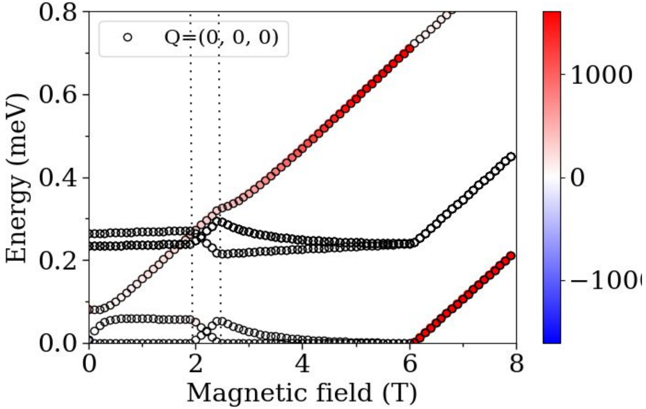
Experimental phase diagram



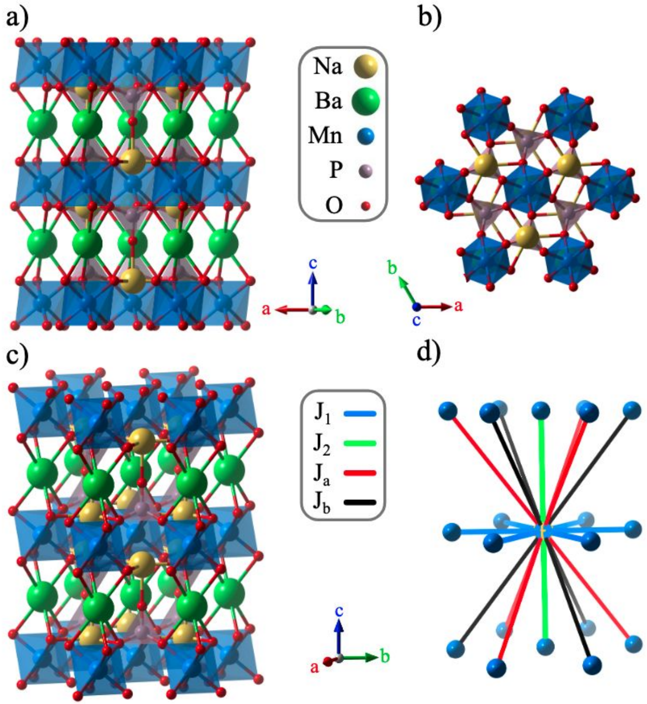
J Kim et al,
J. Phys.: Condens. Matter 34, 475803 (2022)

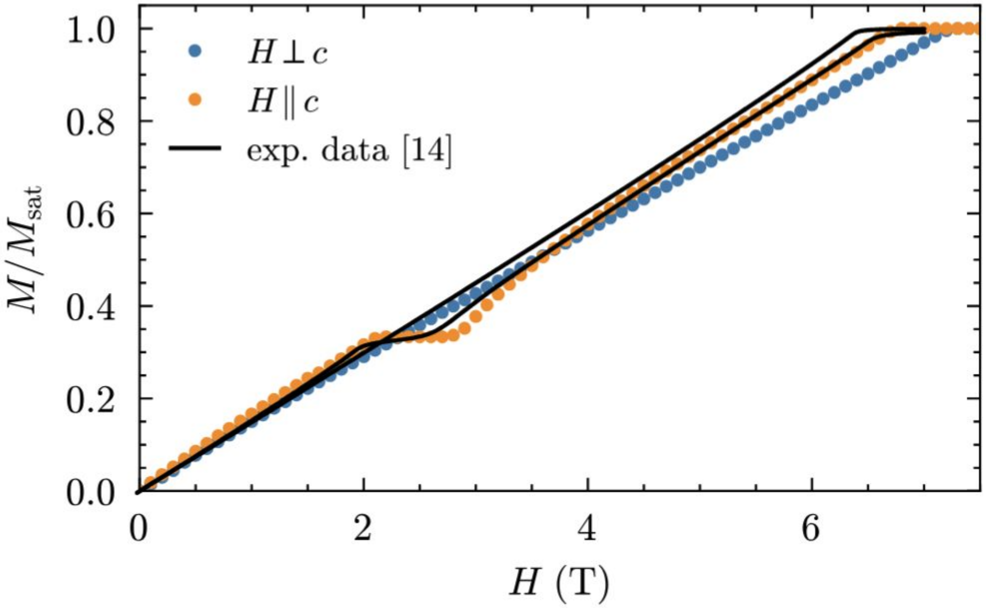
Our results

Spin-wave energies



Construction of minimal model: n.n. J and single-axis anisotropy





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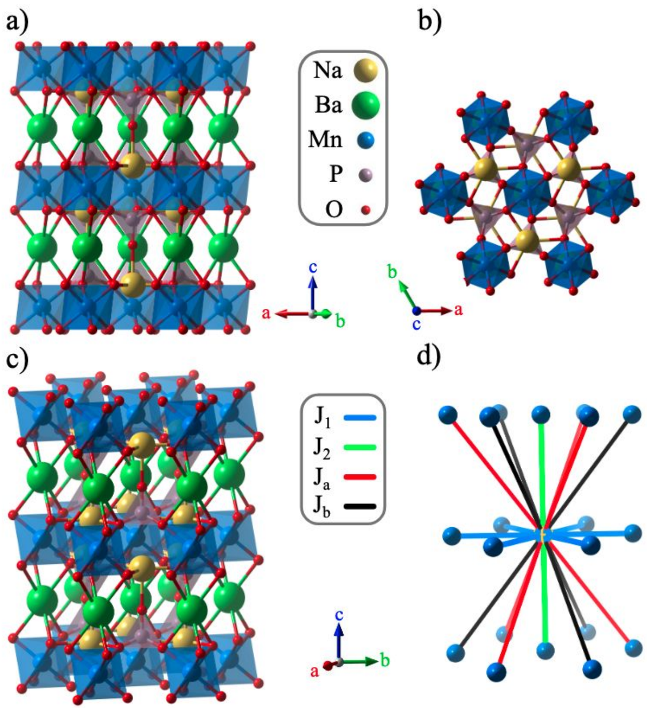
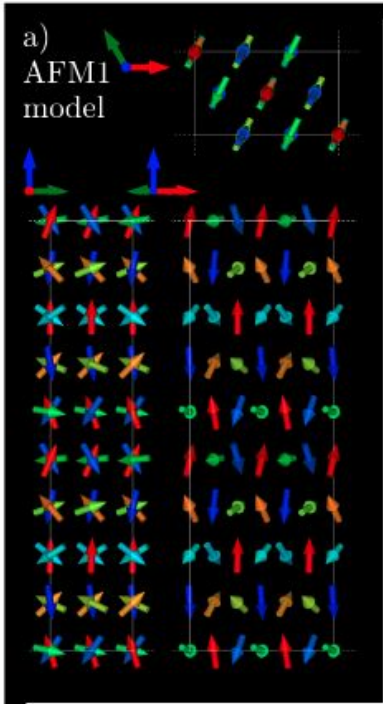
3D coupling and spin spirals

$$\tan(2\pi k_z) = \frac{3\sqrt{3}(J_b - J_a)}{3(J_b + J_a) - 2J_2}$$





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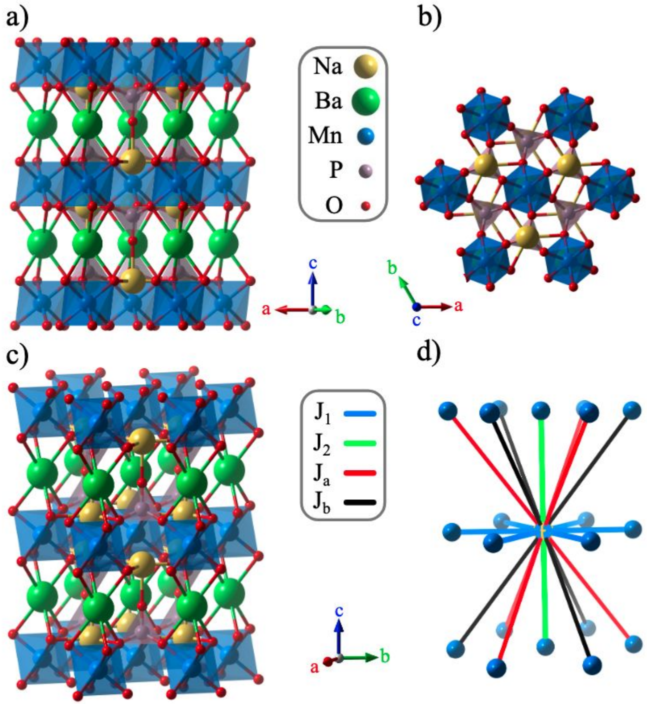

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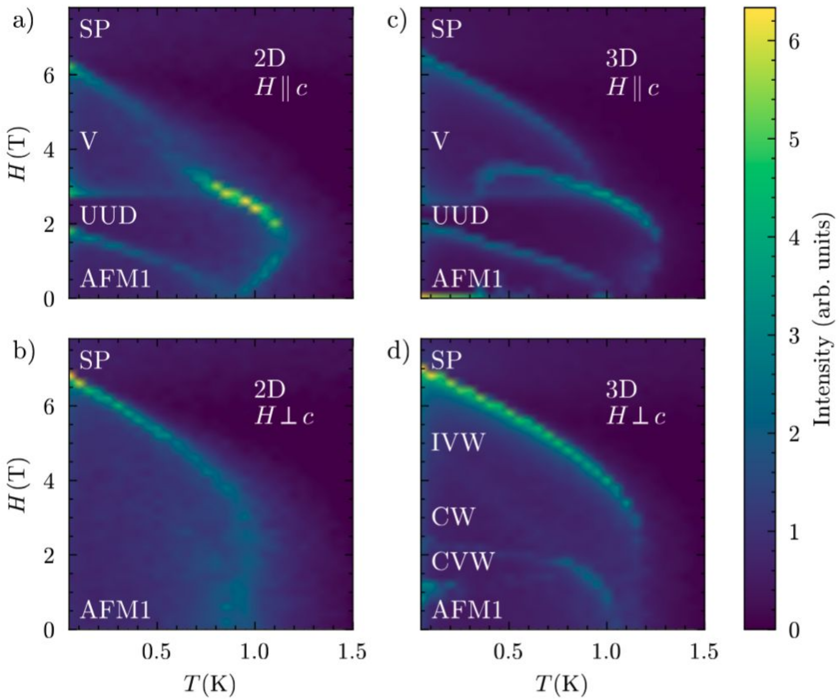

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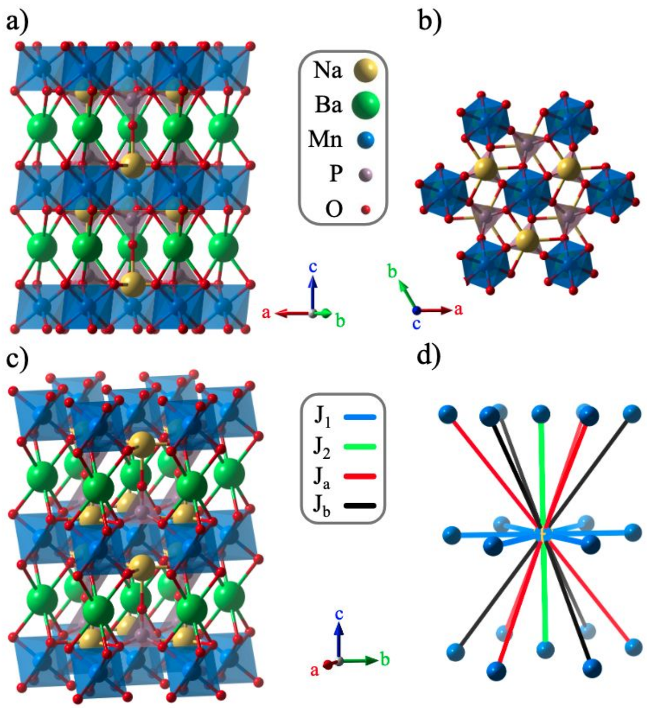

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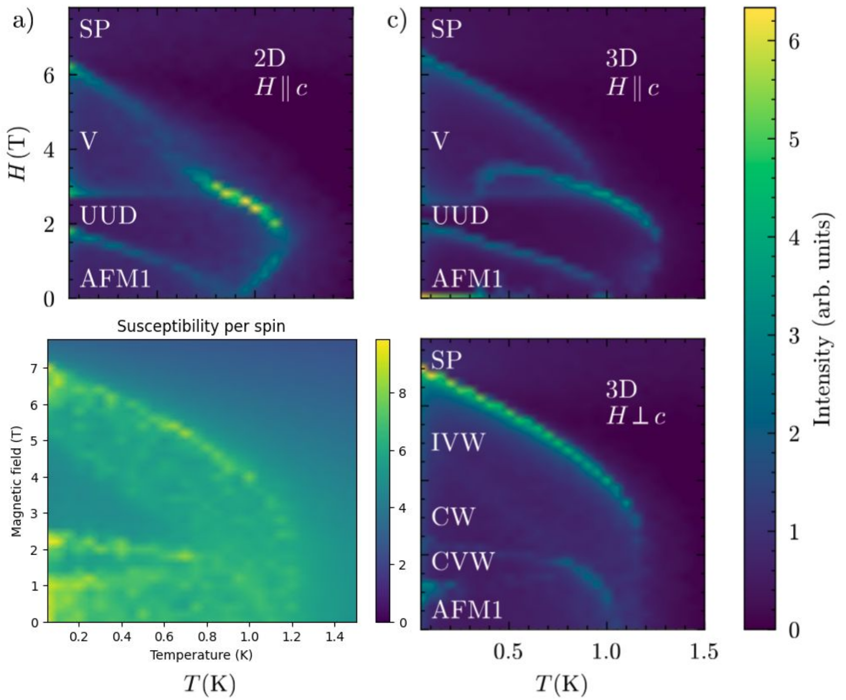

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Spin configurations: experiment vs simulation

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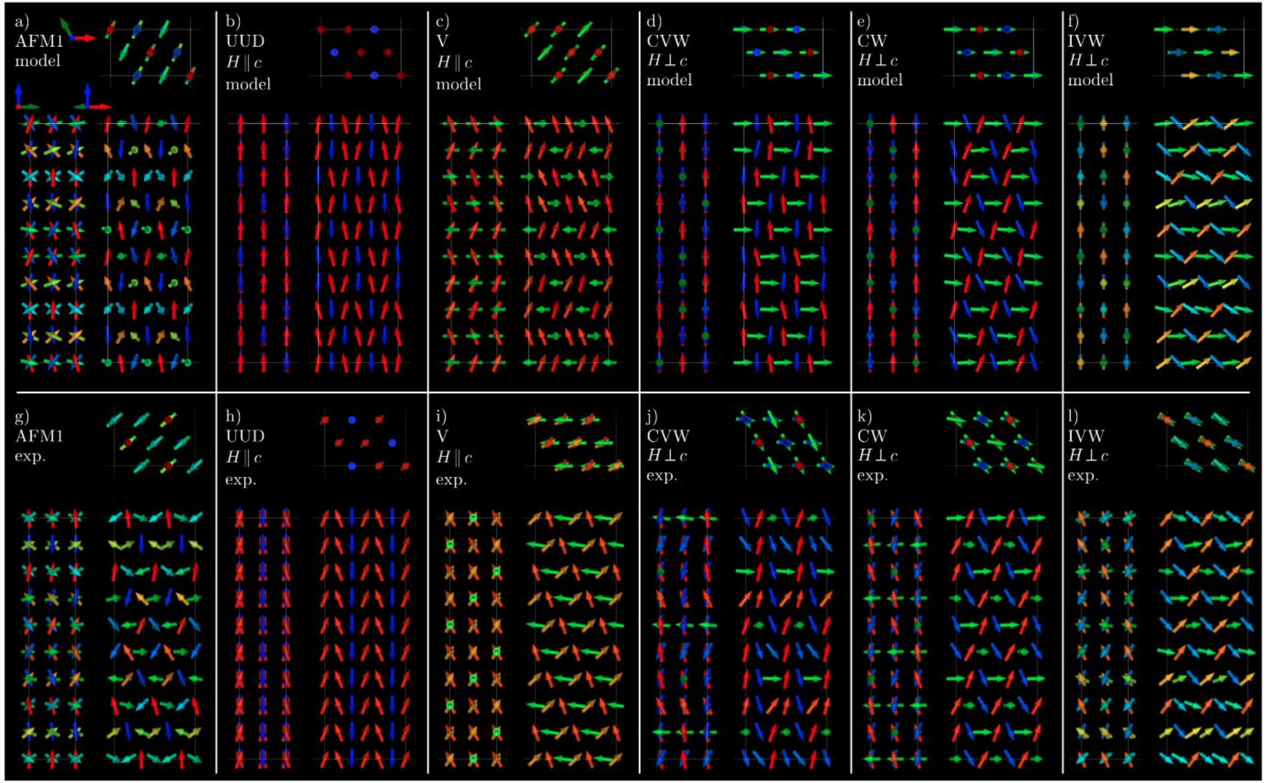
Centro Brasileiro de Pesquisas Físicas

Experimentally determined spin structure

Our simulations



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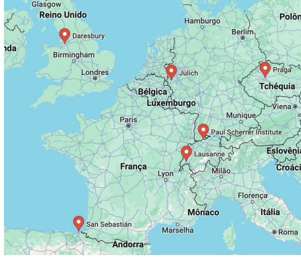
Colaboradores



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Petr Čermák

Paul Scherrer Institut, Suíça (Espalhamento de nêutrons)

Michel Kenzelmann

Jonathan White

David Tam

Outlook

- Magnetism is always new
- Exotic state of matter: topological spin textures and spin waves
- We can construct very useful models from first principles calculations
- There is a lot more to learn and discover

THANK YOU

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