Skyrmion à la carte

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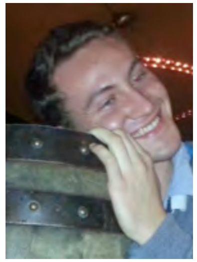
Acknowledgement

INSP/RE group
INTERDISCIPLINARY SPINTRONICS RESEARCH

C A U



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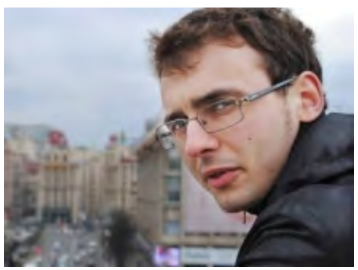

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Outline

I. Introduction

II. Methods
- ❑ Spin spiral calculations applied on Pd/Fe/Ir(111)
- ❑ DMI calculations applied on Pd/Fe/Ir(111)
- ❑ Effective extended Heisenberg Hamiltonian for MC and spin dynamics

III. Magnetic exchange frustration and its consequences
- ❑ Energy barriers for the collapse of skyrmion and antiskyrmion
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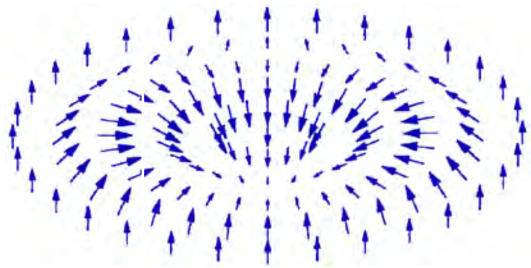
Micromagnetic model prediction

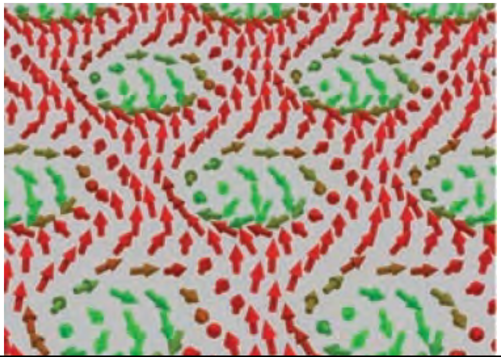
Existence of magnetic skyrmions

on a micrometer length scale



A. N. Bogdanov & D. A.Yablonskii, *Sov. Phys. JETP* **68**, 101 (1989).

Experimental discovery



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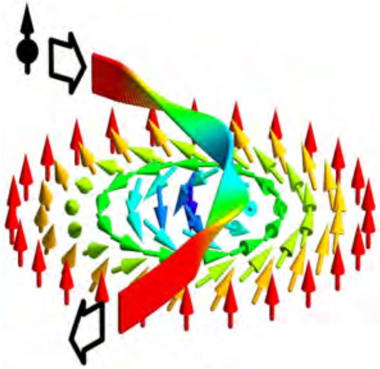
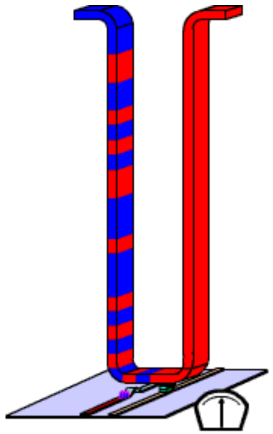
X. Z. Yu *et al* Nature **465**, 901 (2010).
A. Neubauer *et al* PRL **102**, 186602 (2009).
M. Lee *et al* PRL **102**, 186601 (2009).

Skyrmion race-track





S. Parkin *et al* Science **320,** 190 (2008).
F. Jonietz *et al* Science **330,** 1648 (2010).
A. Fert *et al* Nature Nanotech. **8**, 152 (2013).
C. Moreau-Luchaire *et al* Nature Nanotech. **11**, 444 (2016).
W. Jiang *et al* Science **349**, 283 (2015).

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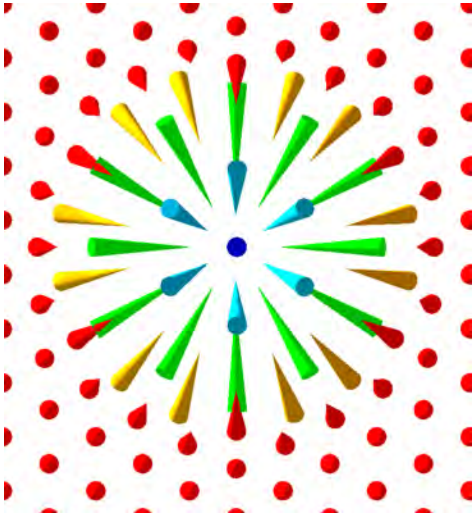
Skyrmions and topological charge

Skyrmion number (topological charge) of a vector field ***n****(x,y):*

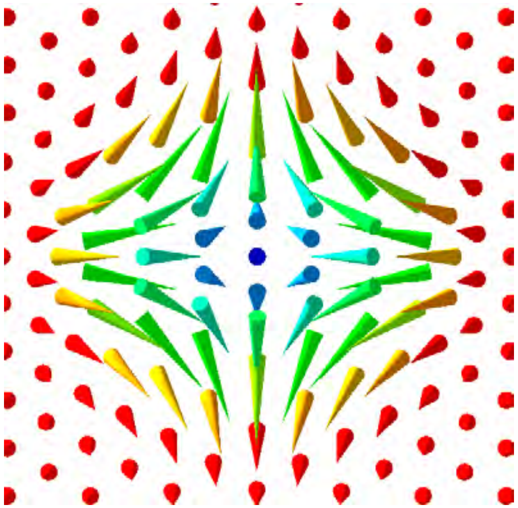
$$S = \frac{1}{4\pi} \int \mathbf{n} \cdot \left(\frac{\partial \mathbf{n}}{\partial x} \times \frac{\partial \mathbf{n}}{\partial y} \right) \, dx \, dy$$

Ferromagnet (*S*=0): topologically trivial state

Skyrmion (*S*=+1)



Antiskyrmion (*S*=–1)



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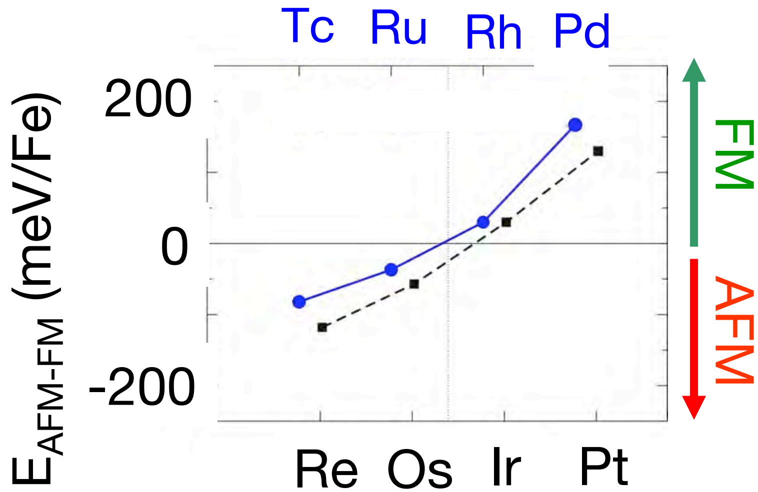
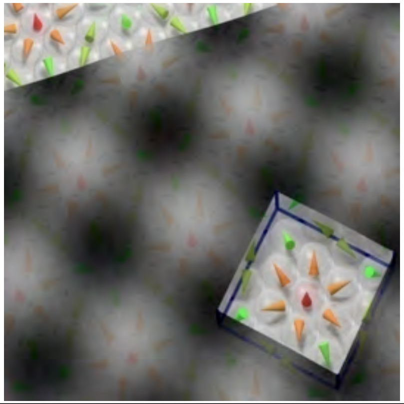
Versatility of magnetism in Fe ultra-thin films



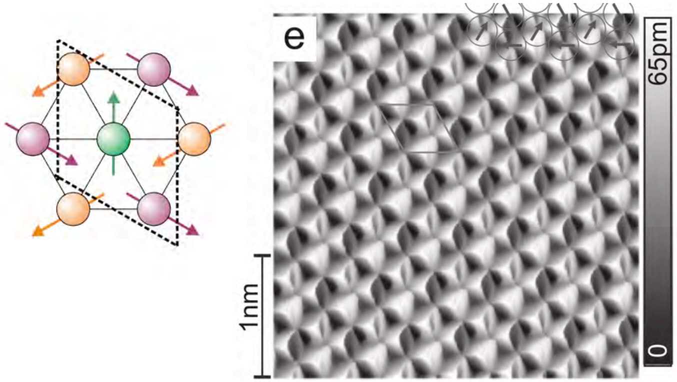
B. Hardrat *et al* PRB **79**, 094411 (2009).

Fe/Ir(111): nano-skyrmion lattice



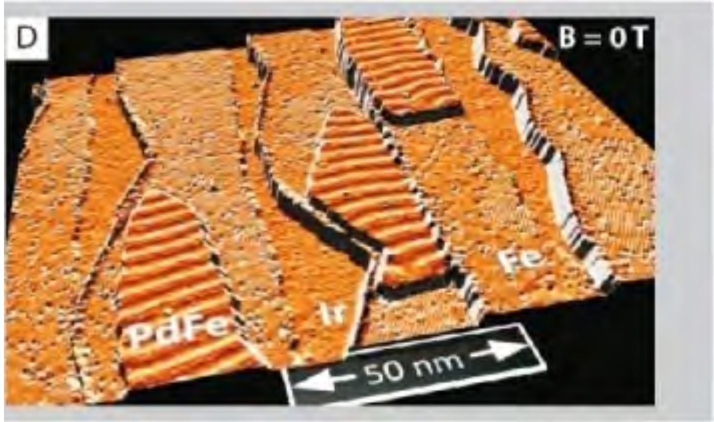
S. Heinze *et al* Nat. Phys. **7**, 713 (2011).

Fe/Re(0001) Néel state



S. Ouazi *et al* Sur. sci. **630**, 280 (2014).
S. Ouazi *et al* PRL **112**, 076102 (2014).

Pd/Fe/Ir(111) spin spiral ground state



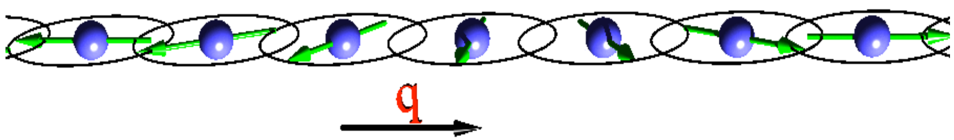
N. Romming *et al* Science **341**, 636 (2013).
B. Dupé *et al* Nature Comm. **5**, 4030 (2014).

First-principles based spin Hamiltonian

Density-functional theory (DFT) using the FLEUR code:

- energy of non-collinear magnetic structures
- energies of spiral spin-density waves

Spin spirals



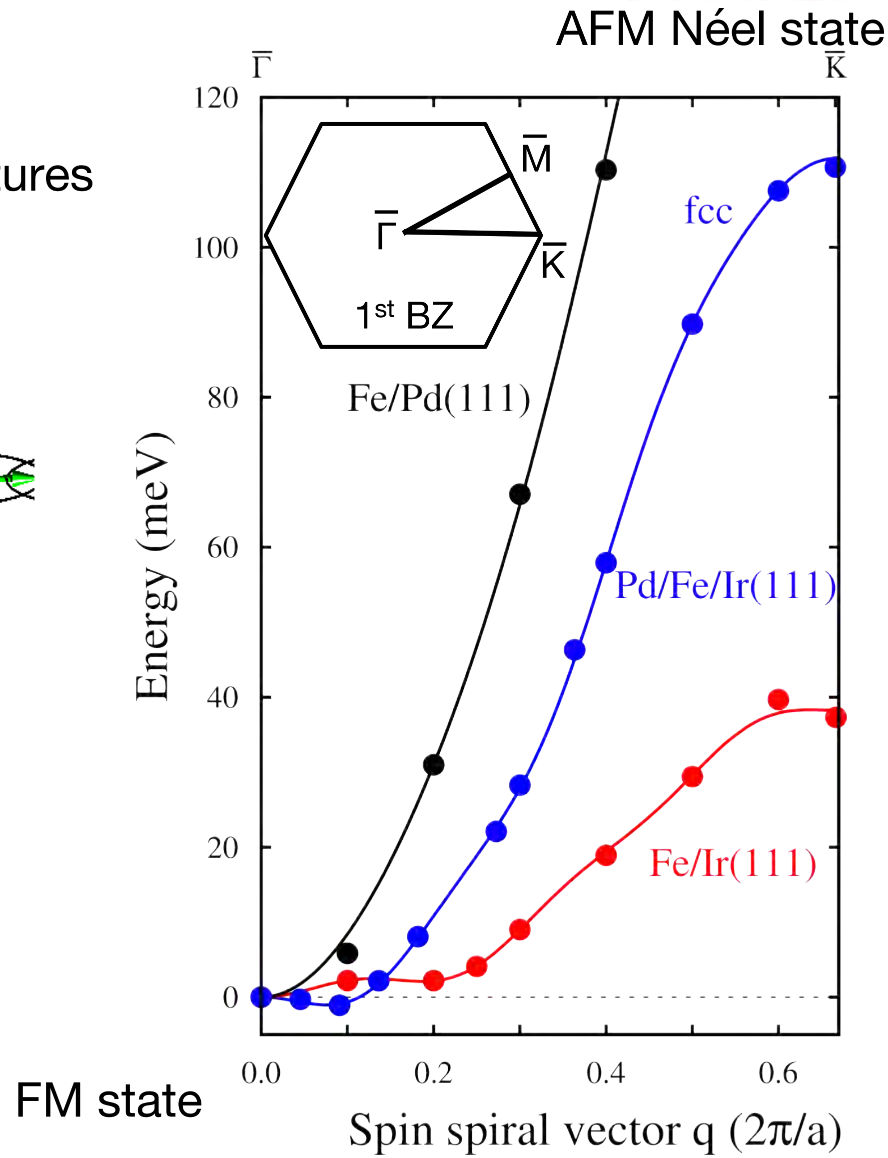
Energy dispersion

$$E(\boldsymbol{q}) = -N\sum_{\delta=1}^{NN} J_{0,\delta}\, e^{-i\boldsymbol{q}\boldsymbol{R}_{\delta}}$$

www.flapw.de

Fleur

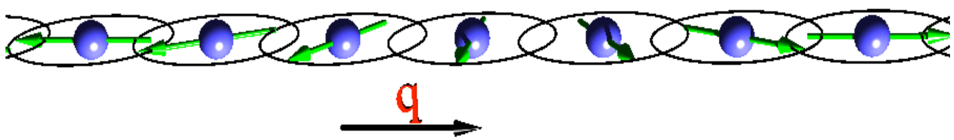
developed @ FZ Jülich



Density-functional theory (DFT) using the FLEUR code:

- energy of non-collinear magnetic structures
- energies of spiral spin-density waves
- with and without spin-orbit coupling

Spin spirals



DM interaction

$$E_{DM} = -\sum_{j \in NN_1} \boldsymbol{D}_{ij}.(\boldsymbol{M}_i \times \boldsymbol{M}_j)$$

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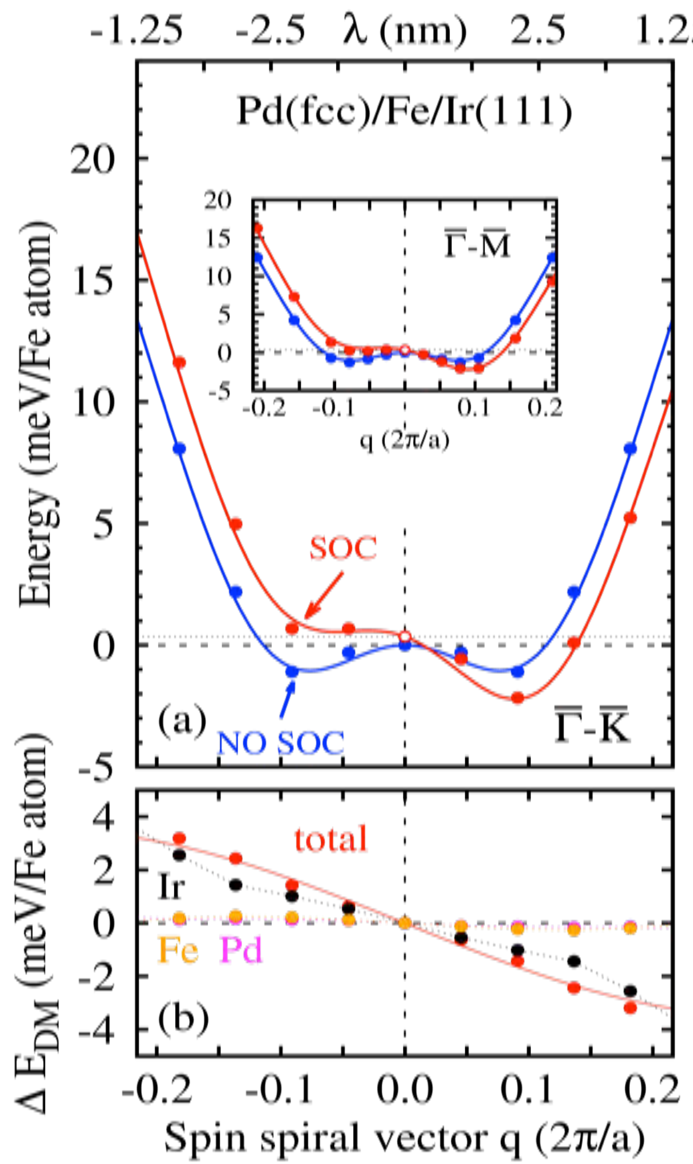
developed @ FZ Jülich



Spin Hamiltonian solved by Monte-Carlo & spin dynamics

$$H_i = -\sum_{j \in NN} J_{ij}.\boldsymbol{M}_i.\boldsymbol{M}_j$$ Magnetic exchange energy

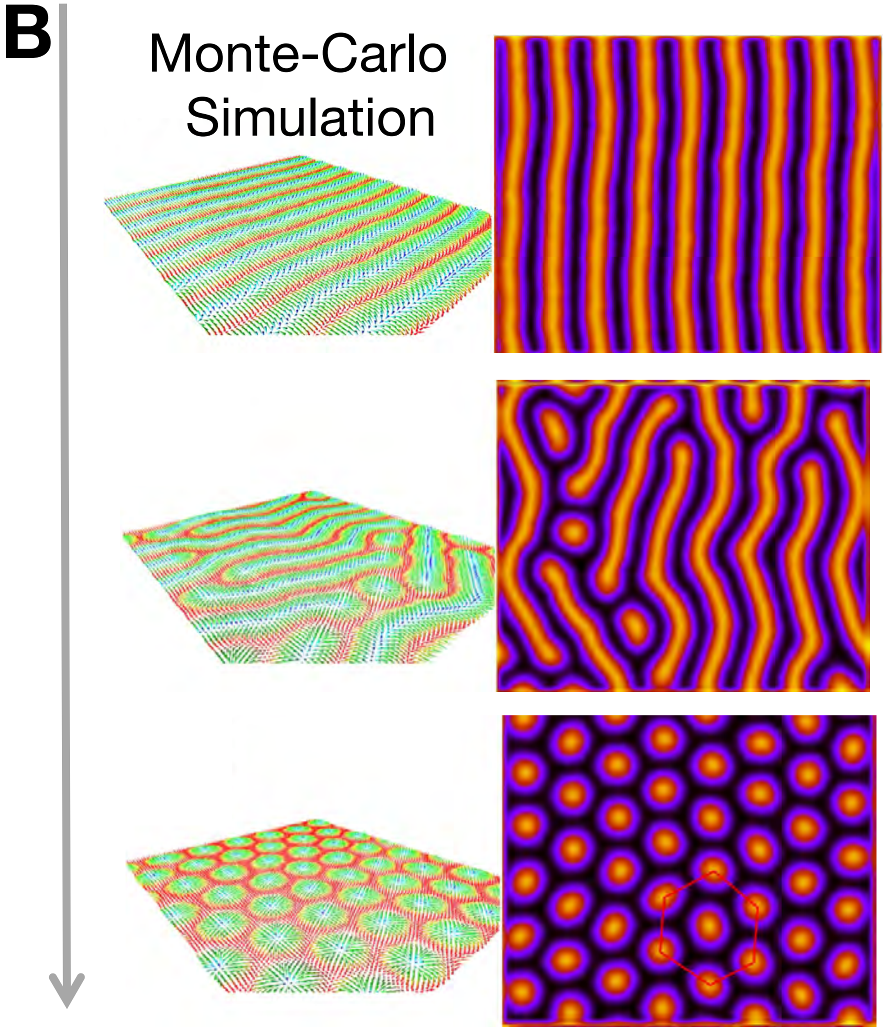
$$-\sum_{j \in NN} \boldsymbol{D}_{ij}.(\boldsymbol{M}_i \times \boldsymbol{M}_j)$$ Dzyaloshinskii-Moriya energy

$$-\boldsymbol{M}_i.\boldsymbol{B}$$ Zeeman energy

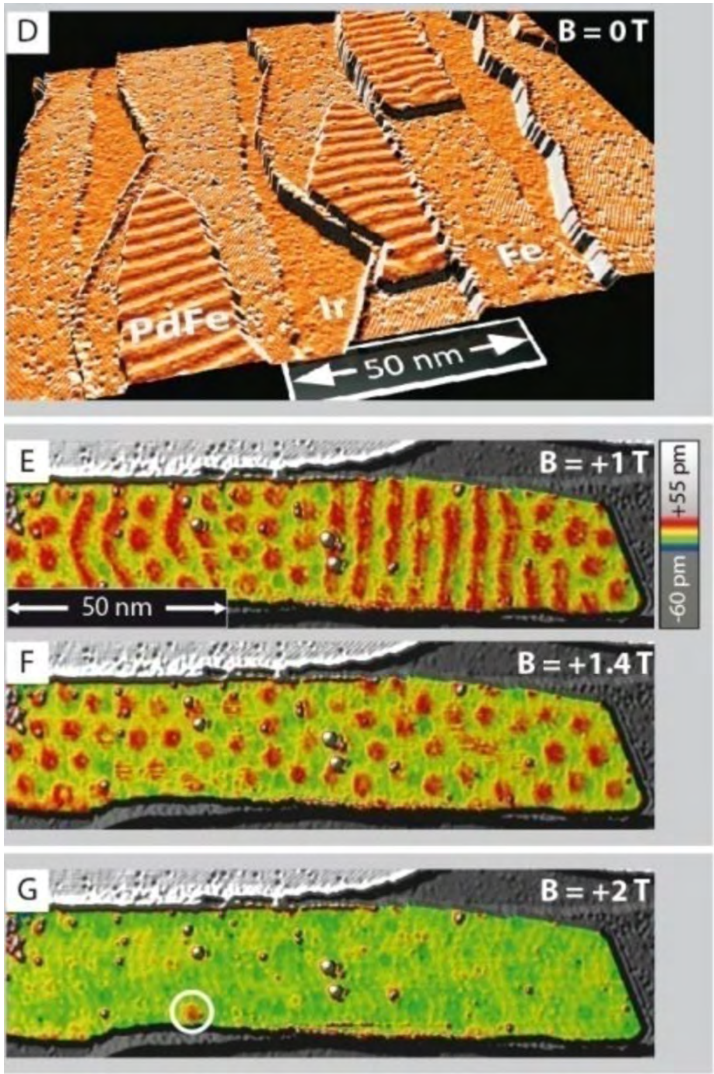
$$+K(\boldsymbol{\alpha}.\boldsymbol{M}_i)^2$$ Magnetocrystalline anisotropy energy

interaction constants calculated from DFT
No dipole-dipole interaction included

Stability diagram of Pd/Fe/Ir(111)



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



N. Romming *et al* Science (2013).

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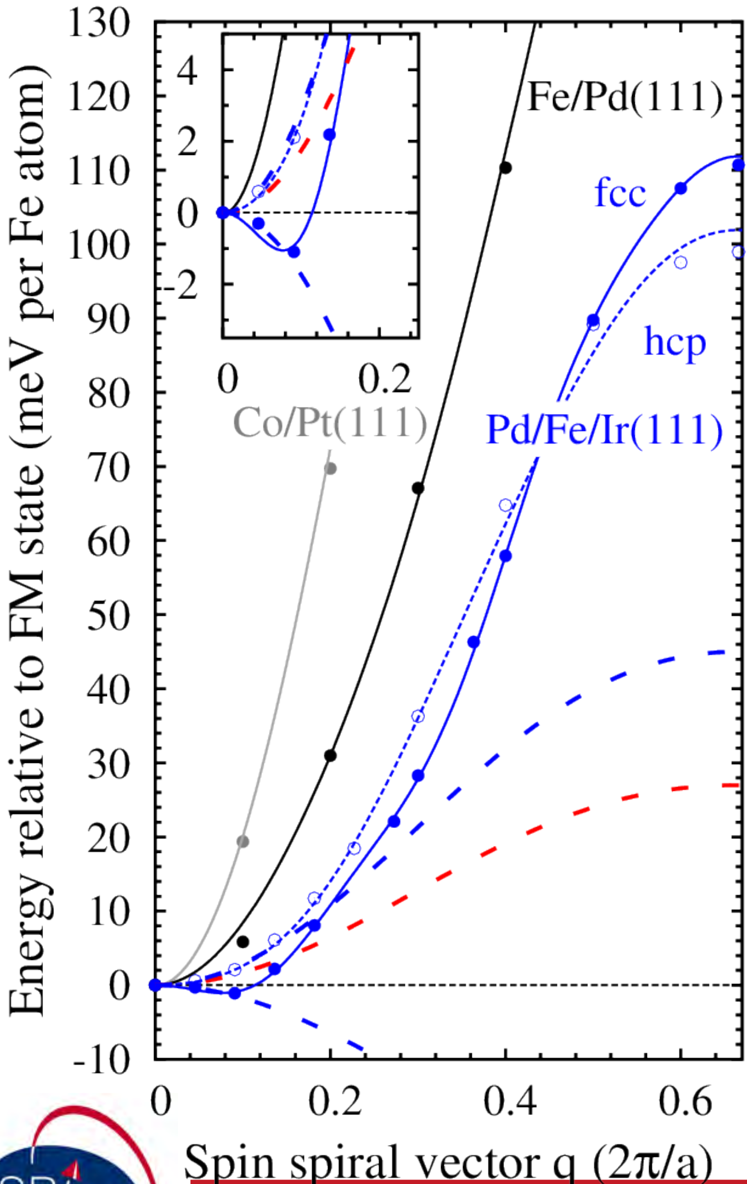
Frustration of exchange interaction: J_{eff}



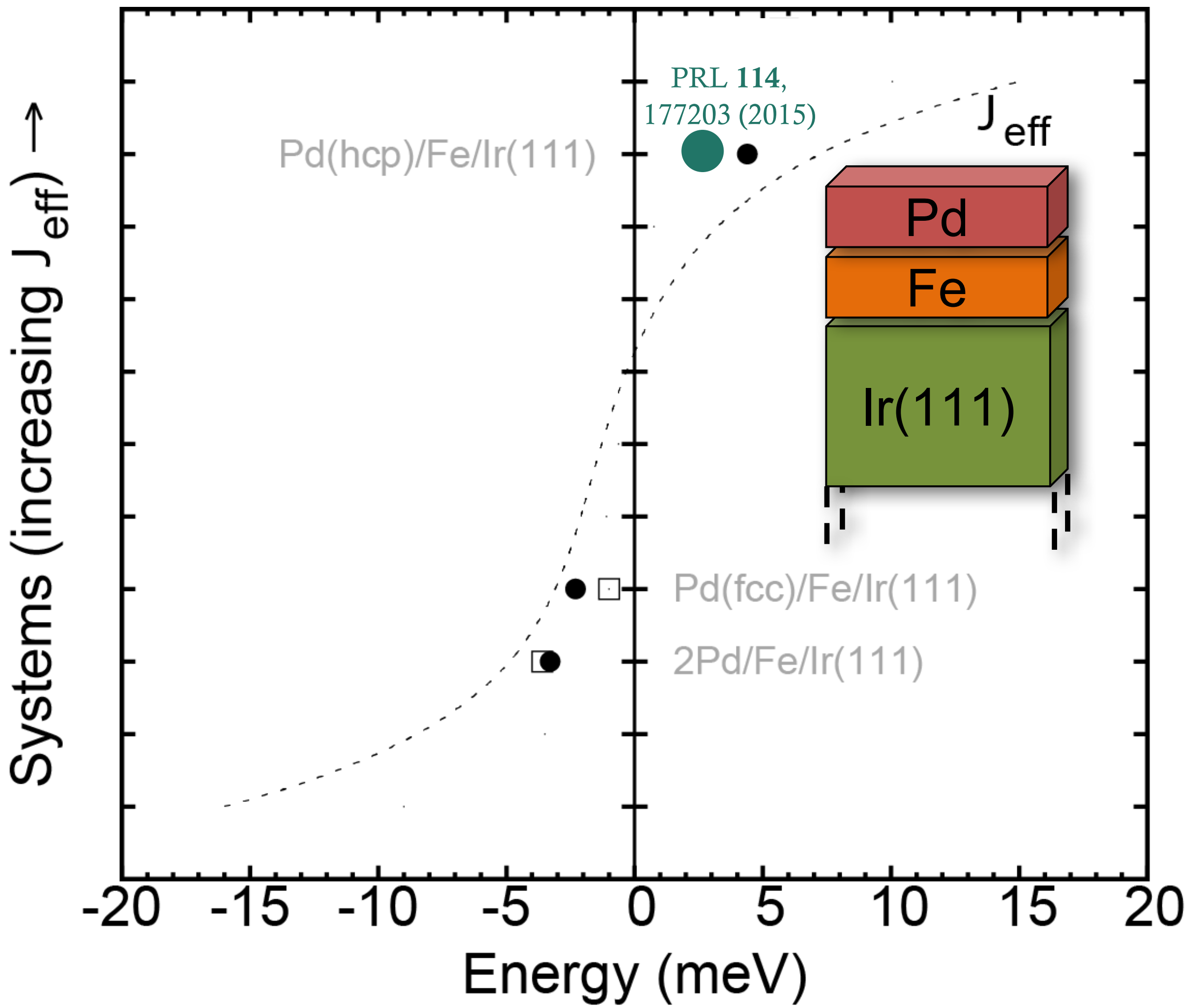
Spin spiral ground state

		hcp	fcc
J_1 (meV)		13.2	14.8
J_{eff}	(meV)	5.0	-3.0

→ A=2.0±0.4 pJ.m^{-1} from N. Romming et al. PRL **114**, 177203 (2015)

J_{eff}: approximation of spin stiffness only close to q=0

Frustration of exchange interaction: J_{eff}



B. Dupé *et al* Nature Comm. **7**, 11779 (2016).

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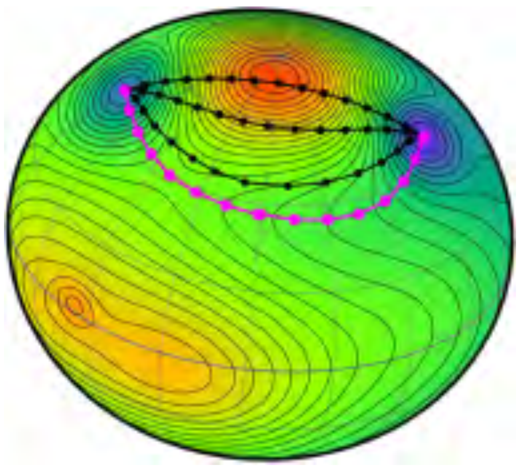
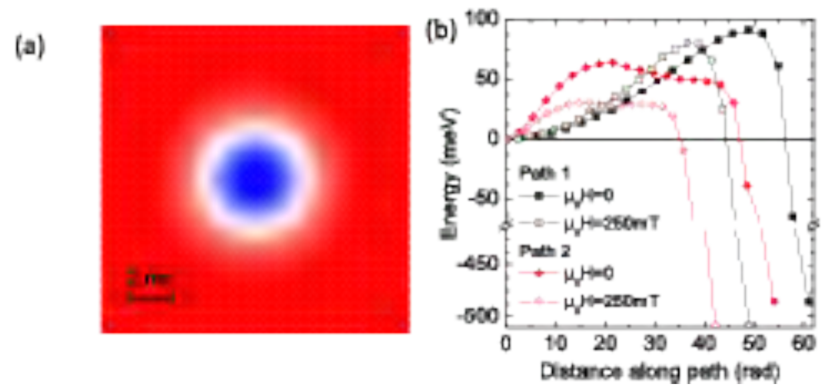
Calculation of the energy barrier: GNEB

Geodesic nudged elastic band: GNEB



P. Bessarab *et al* Computer Physics Communications **196**, 335 (2015).

Collapse of a skyrmion: first neighbor approximarion



S. Rohart *et al* Phys. Rev. B **93**, 214412 (2016).

Stability diagram of Pd/Fe/Ir(111)

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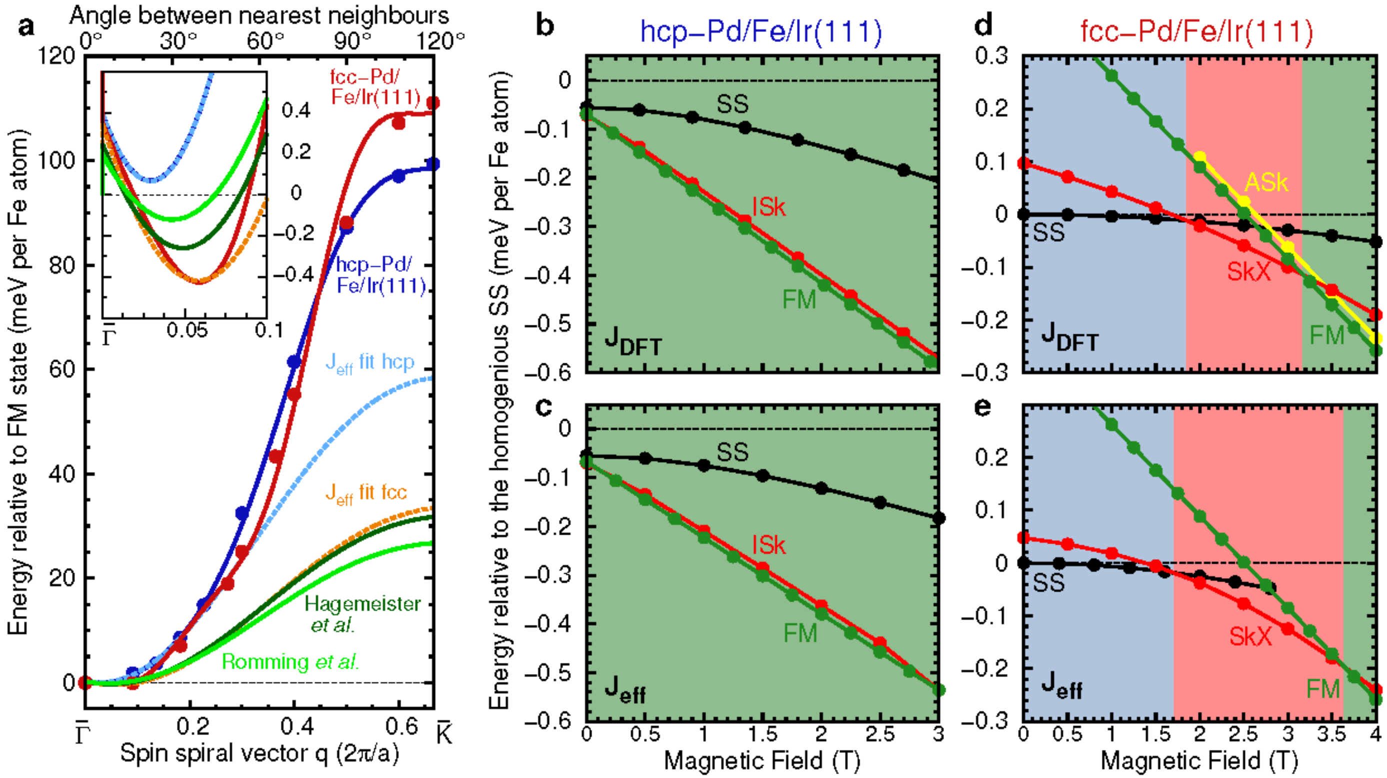
T= 0K



J_{eff} has very little effects on the stability diagram

S. von Malottki *et al* submitted Arxiv 1705.08122

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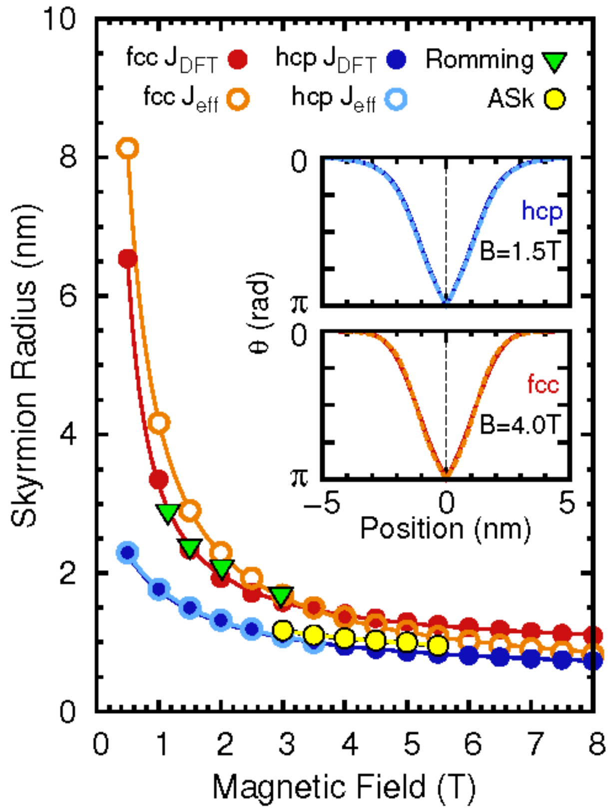
Radius depence with magnetic field



J_{eff} has very little effects on the stability diagram and very little effects on skyrmion properties with magnetic field at low temperature

S. von Malottki *et al* submitted Arxiv 1705.08122

Energy barrier with frustrated exchange

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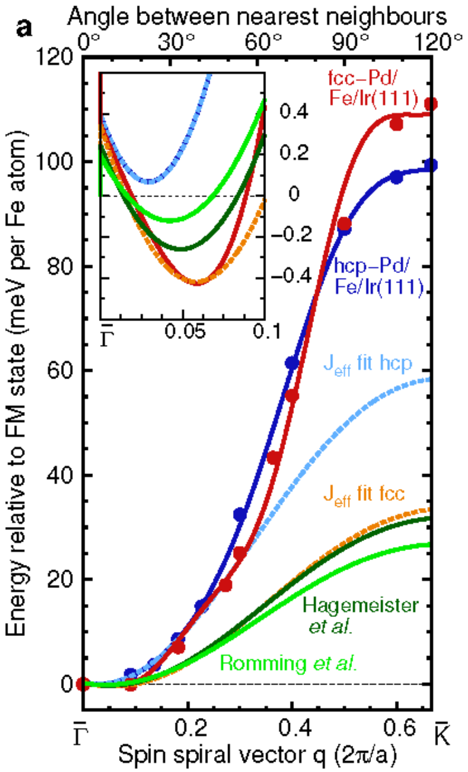
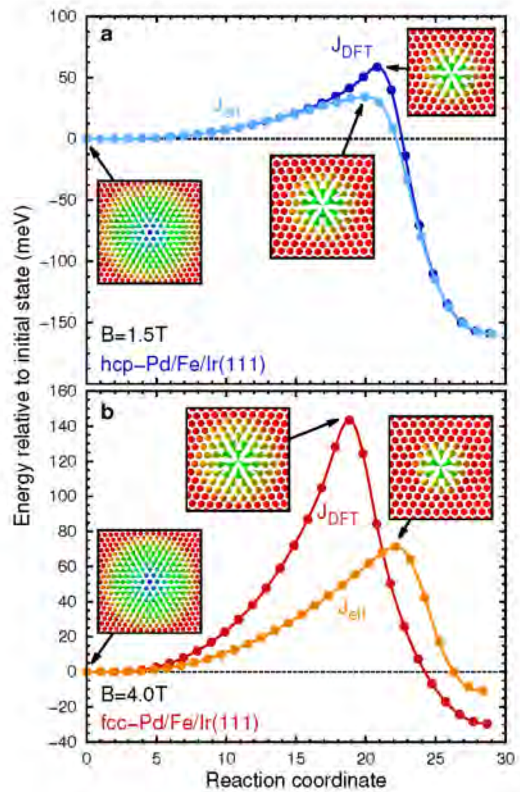
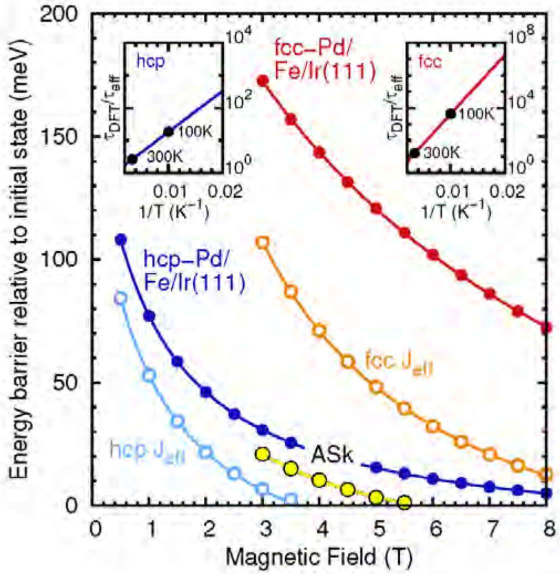


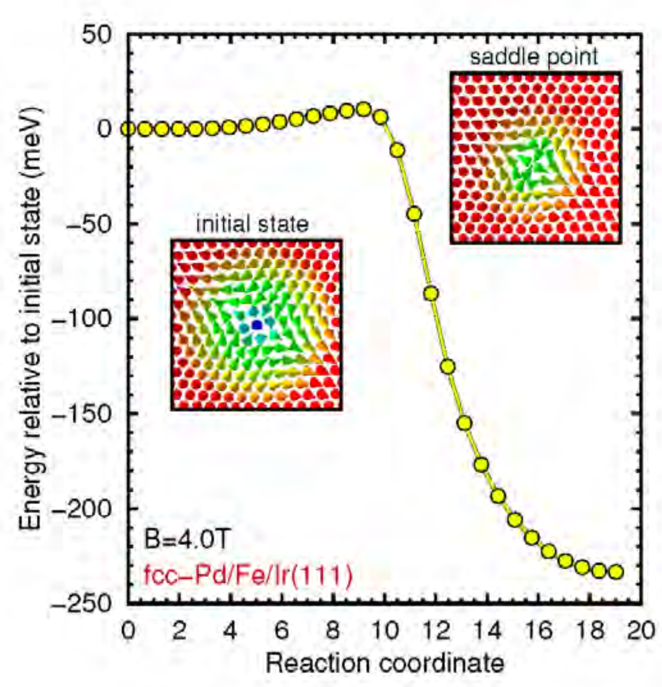




J_{eff} can not discribe excited states for a spin spiral ground state stabilized by magnetic exchange

S. von Malottki et al submitted Arxiv 1705.08122

Frustrated exchange stabilizes antiskyrmions



Frustration of exchange interaction can stabilize higher order topologically protected magnetic states

S. von Malottki et al submitted Arxiv 1705.08122

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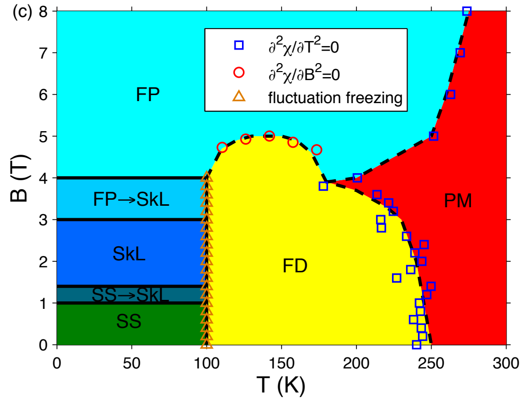
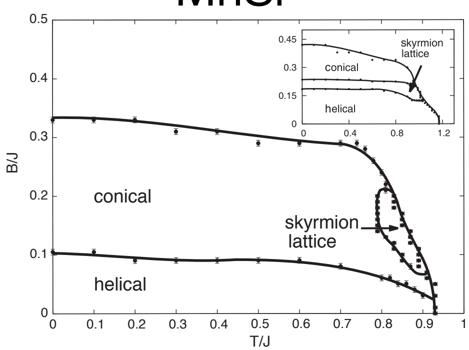
Previous works

Pd/Fe/Ir(111)



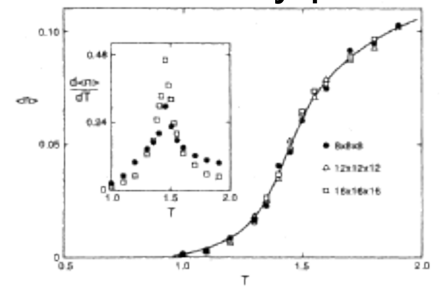
L. Rosza *et al* PRB **93**, 024417 (2016).

MnSi



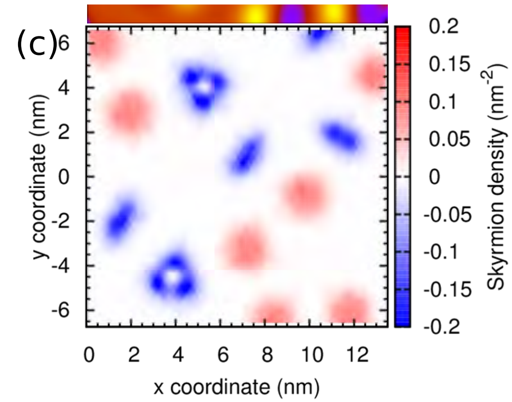
S. Bürhandt *et al* PRB **88**, 195137 (2013).

Creation of skyrmion/antiskyrmion density pairs



M. Lau *et al* PRB **39**, 7212 (1989).

Integrated skyrmion density is no order parameter



B. Dupé *et al* New Journ. Phys **18**, 055015 (2016).

Temperature dependence of order parameters

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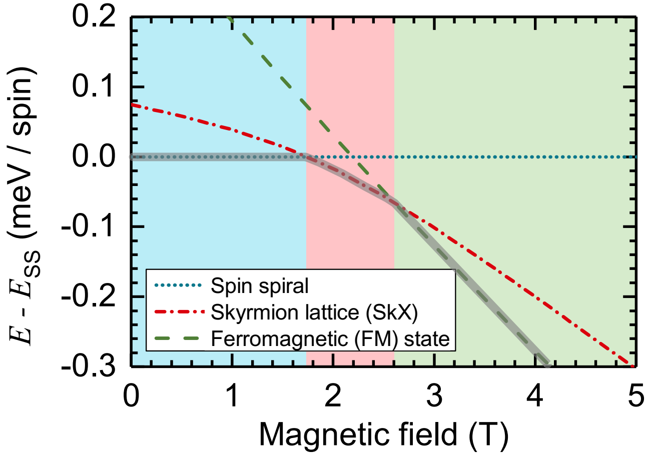
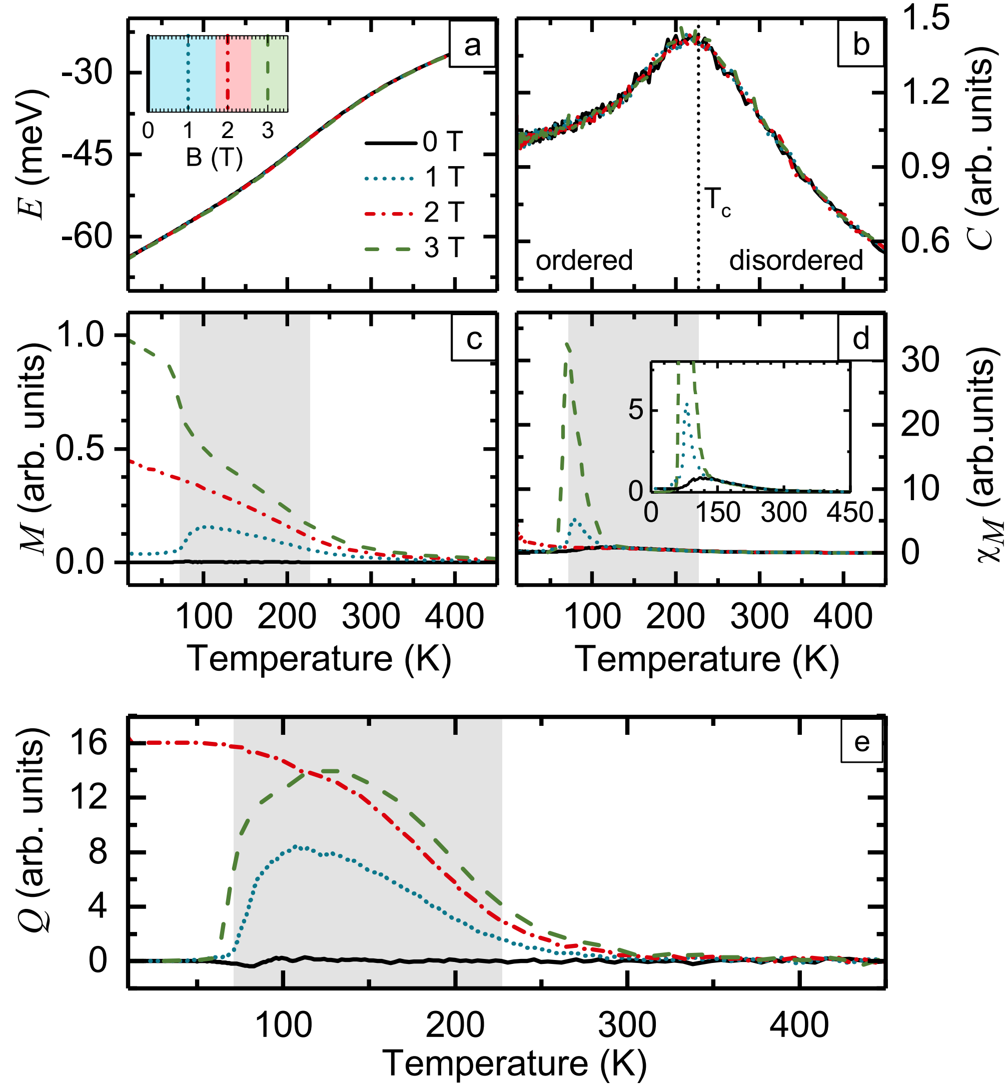
Stability diagram T=0K

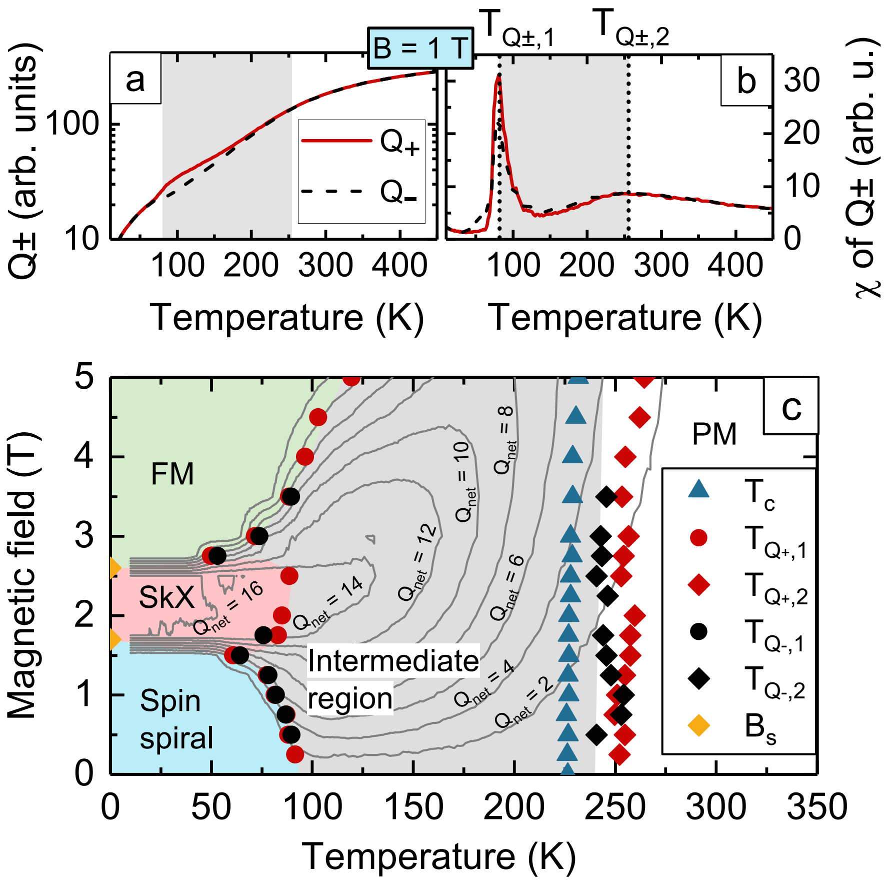


Finite temperature



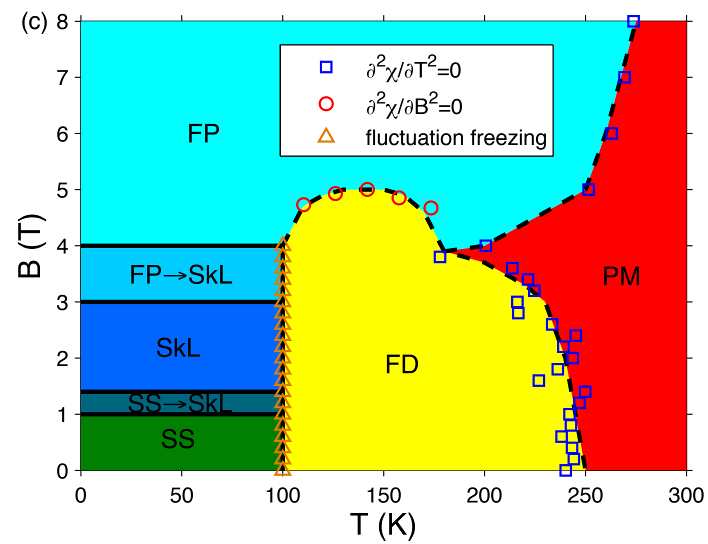
Phase diagram of Pd/Fe/Ir(111)

Parallel tempering



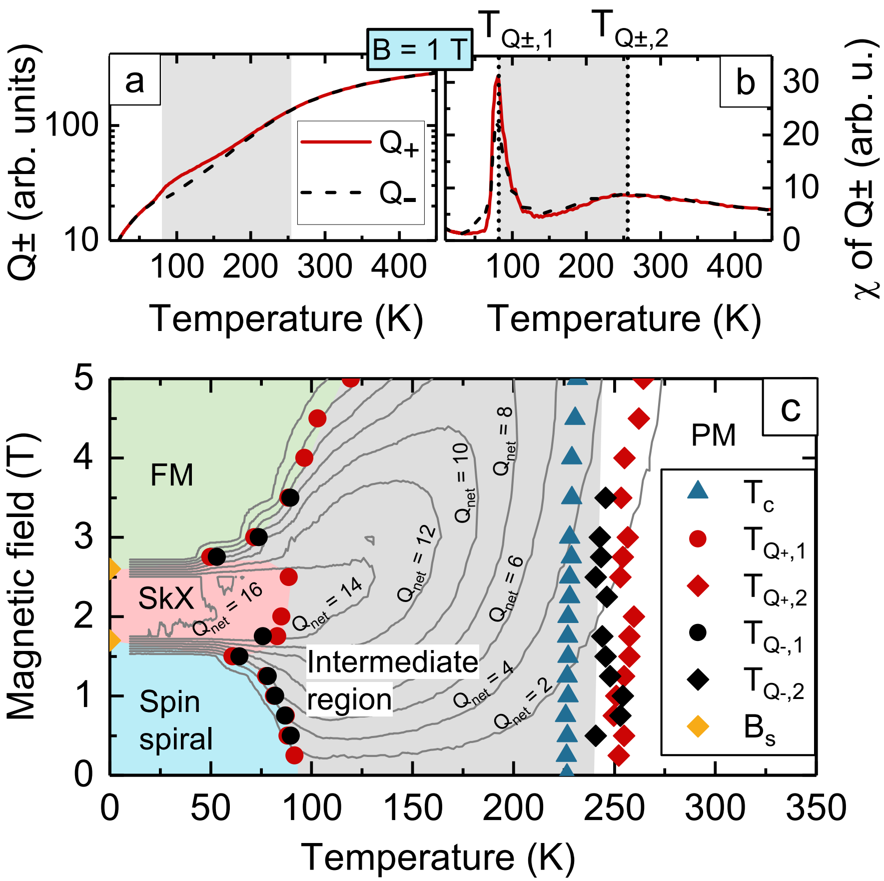
M. Böttcher *et al* submitted arXiv 1707.01708.

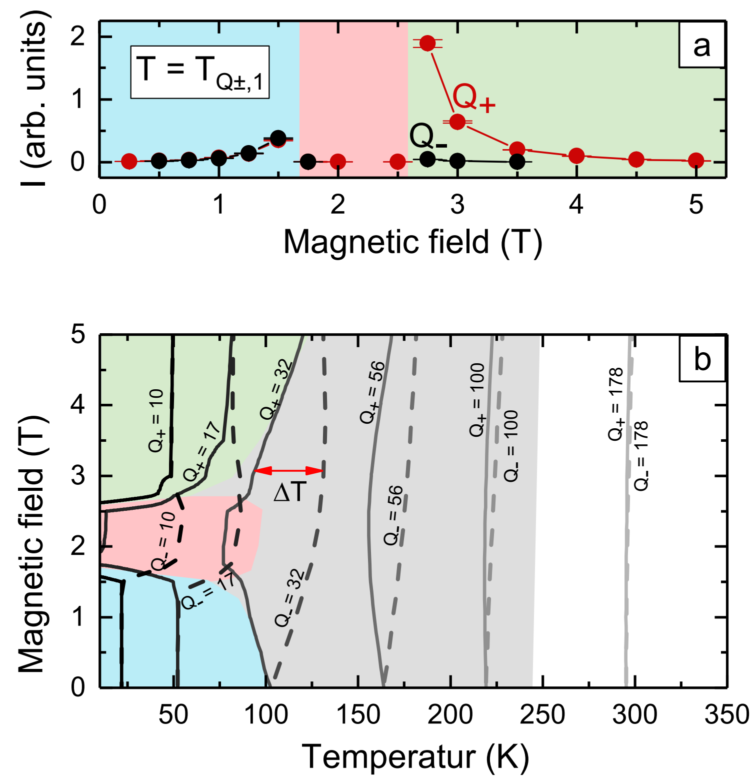
Metropolis



L. Rosza *et al* PRB **93**, 024417 (2016).

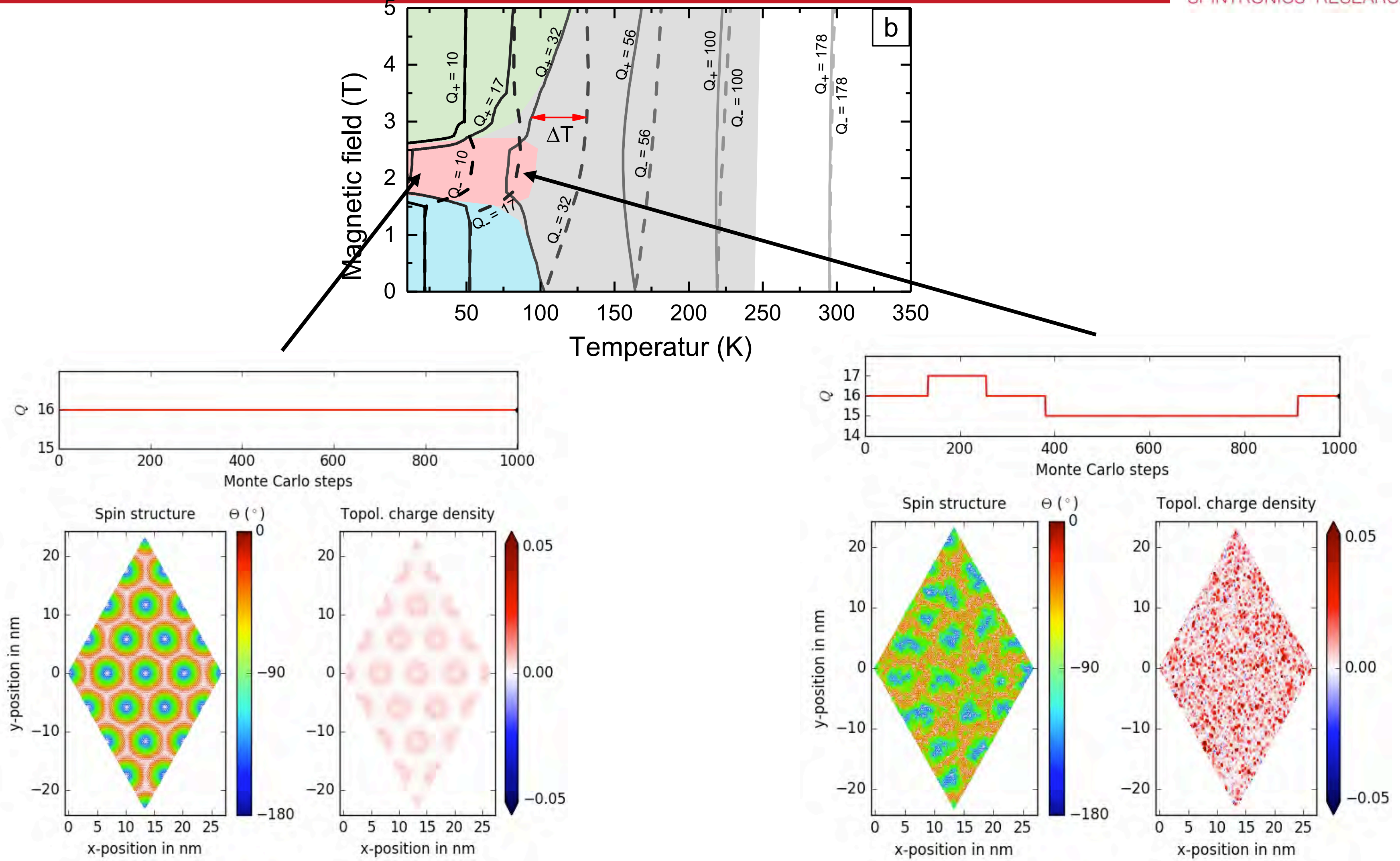
Skyrmion and anti-skyrmion density





Both skyrmion and antiskyrmion densities increase with temperature

M. Böttcher *et al* submitted arXiv 1707.01708.

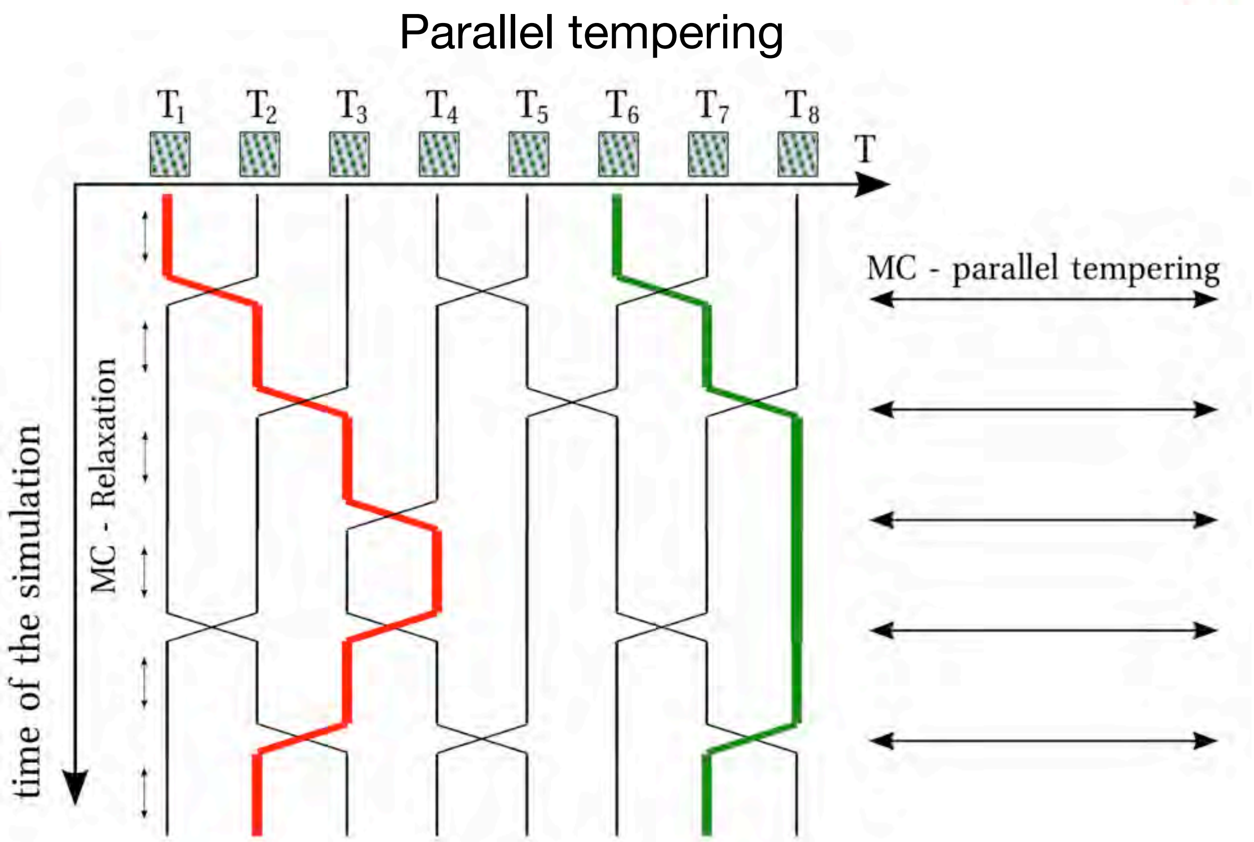


M. Böttcher *et al* submitted arXiv 1707.01708.

Conclusion

- Explain the occurrence of skyrmions based on ab initio calculations
- Tunability based on exchange and DMI
- Magnetic frustration can enhances stability
- Spin dynamics and MC simulations based of frustration of exchange and DMI in multilayer-like geometry

Parallel tempering Monte Carlo



$$p \propto e^{-\Delta E \beta}$$

Parallel tempering allows:

- To overcome local minima with temperature
- To calculate thermodynamical quantities over a large volume of the phase space