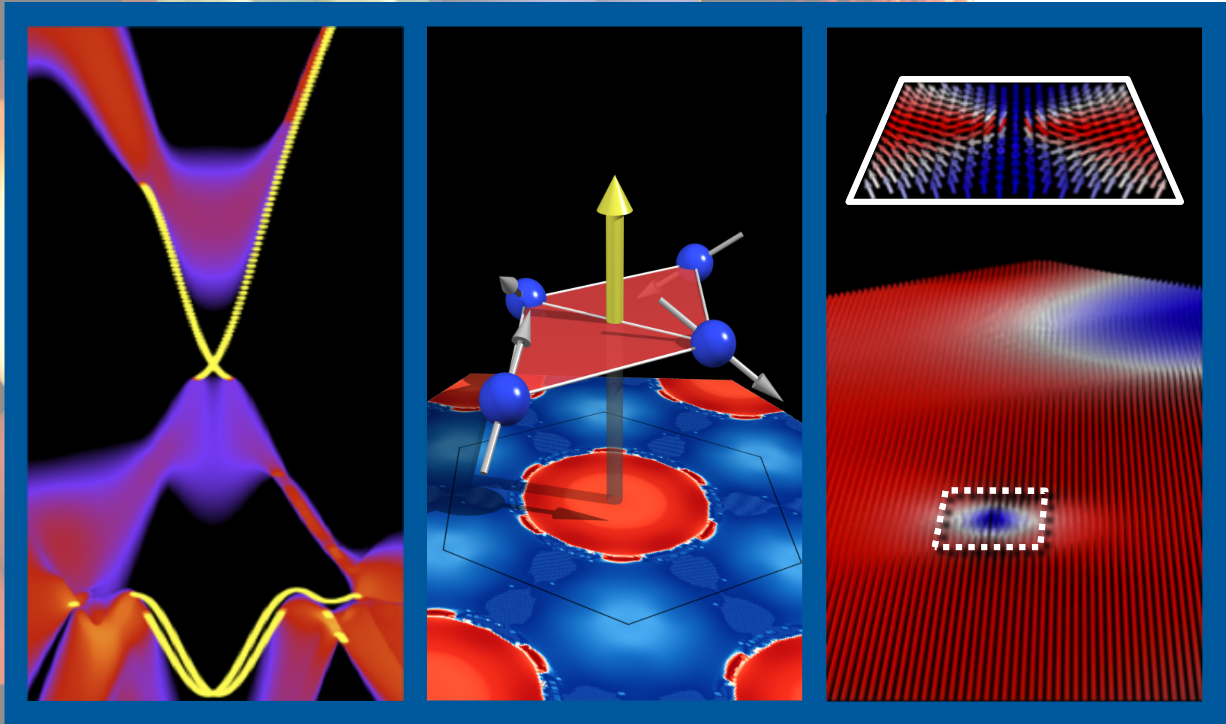
Spin-Orbit Interaction – A Path to Topological Matter in Real and Momentum Space

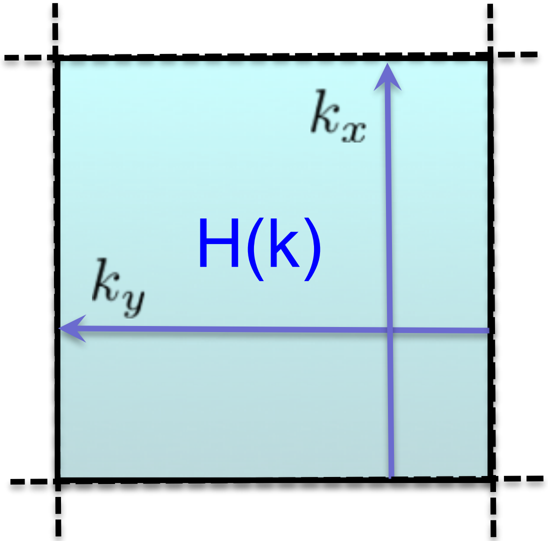


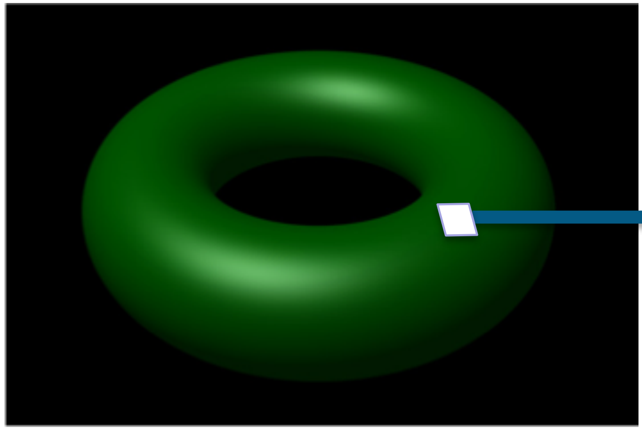
Peter Grünberg Institute and Institute for Advanced Simulation

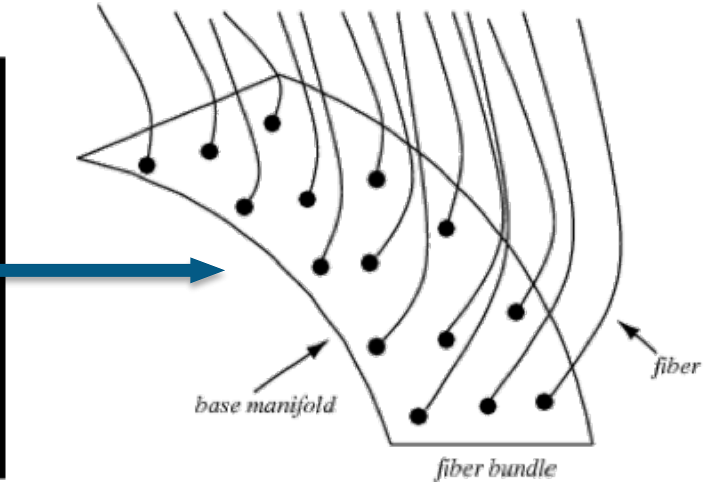
Stefan Blügel

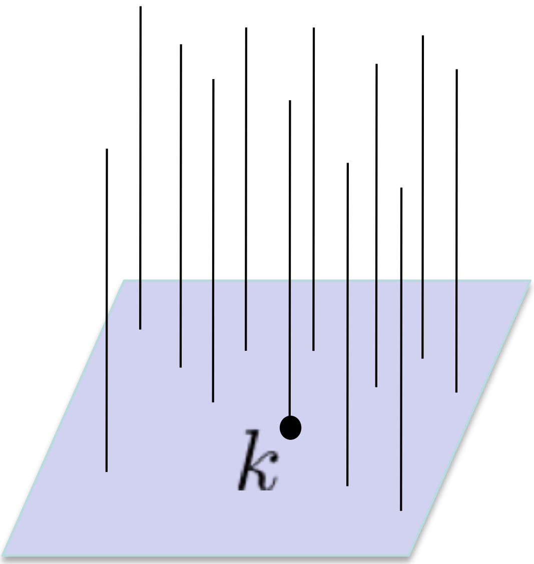
Trieste MaX Conference, 31. Jan. 2018

Topology of electrons in an insulator



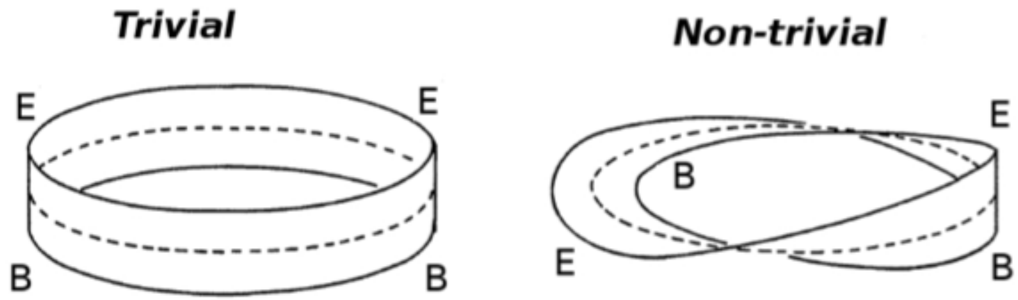






$$u_{n\mathbf{k}} \rightarrow e^{i\varphi} u_{n\mathbf{k}}$$

Fibre bundle theory

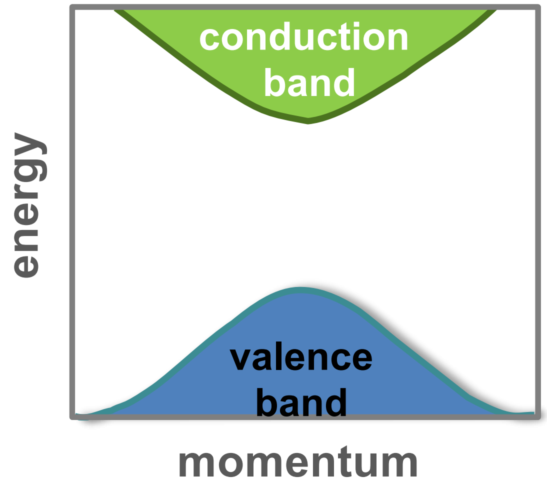


integer **Chern number** – topological invariant of fibre bundles

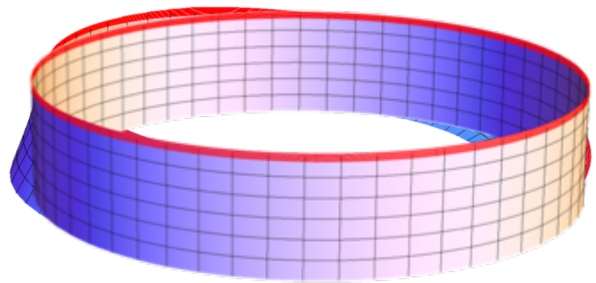
Nash and Sen, *Topology and Geometry for Physicists*

Topological insulators

- Topological matter



- Topology of Bloch wavefunction

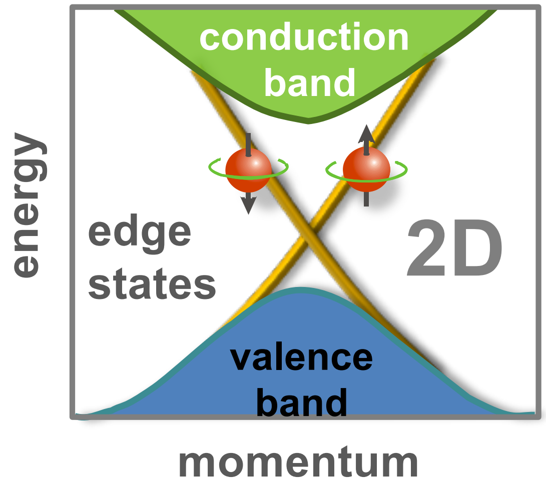


- Topological classification

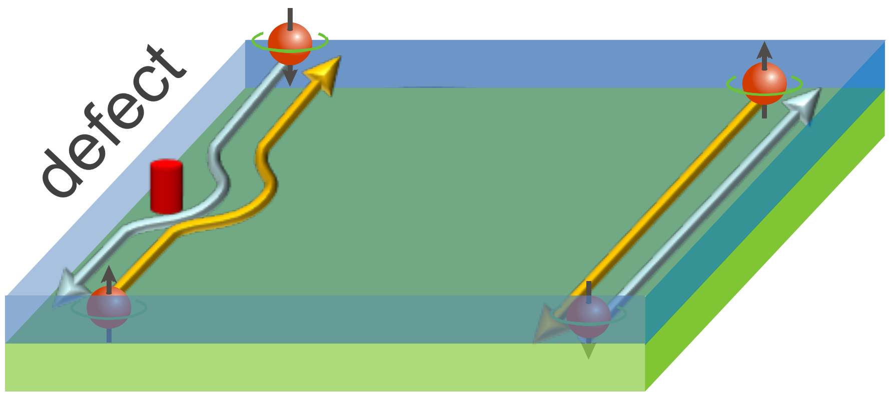
$\mathbb{Z}_2 = 0$

Topological insulators

- Topological matter



- Dissipationless edge states



Quantum Spin Hall Effect

Topological Characterization of Solids

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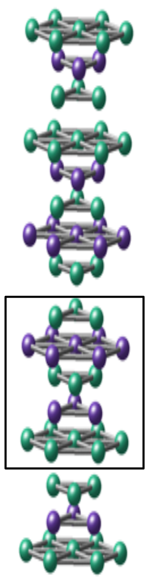
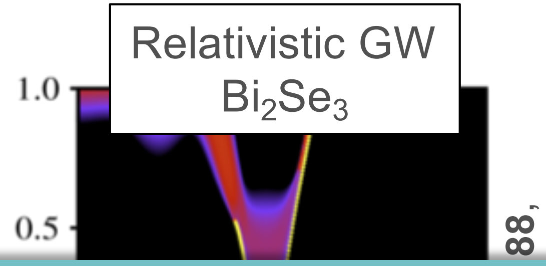
3D Topological Insulators

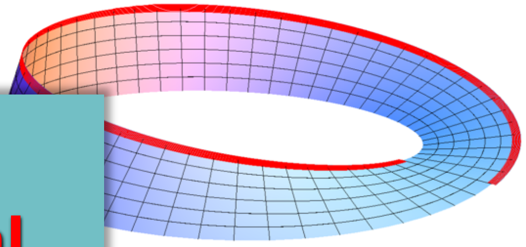


Bi_2Te_3
Bi_2Se_3
Sb_2Te_3



Response Properties

electronic structure causes non-trivial topological invariants



Berry curvature

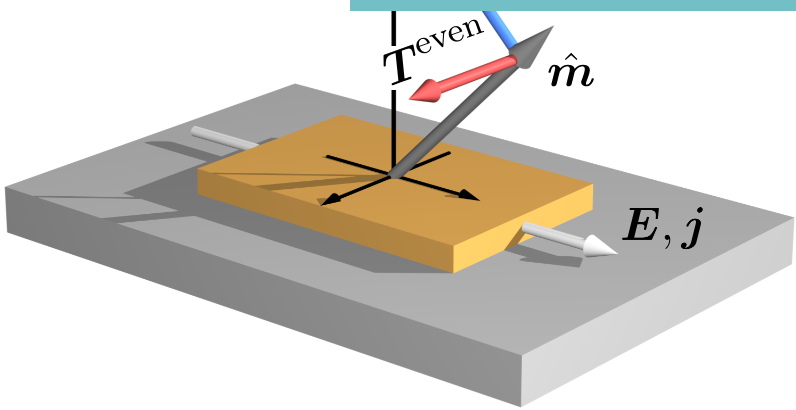
$$\iint \Omega^{\hat{m}k_x} dk_x d\hat{m}$$

Goal:

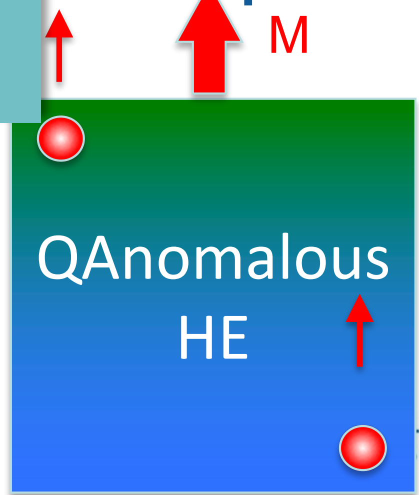
- **Exploration of topological phase space**

$$\{\mathbf{r}, \mathbf{p}, \mathbf{M}, t\}$$

Spin Orbit T…

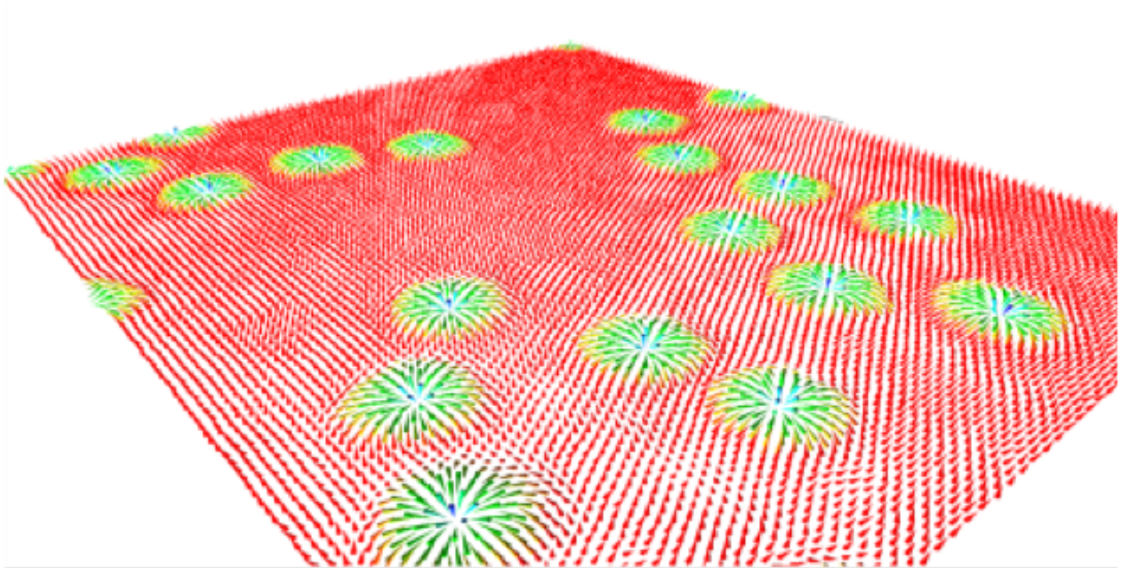


…ion of Spin-Currents



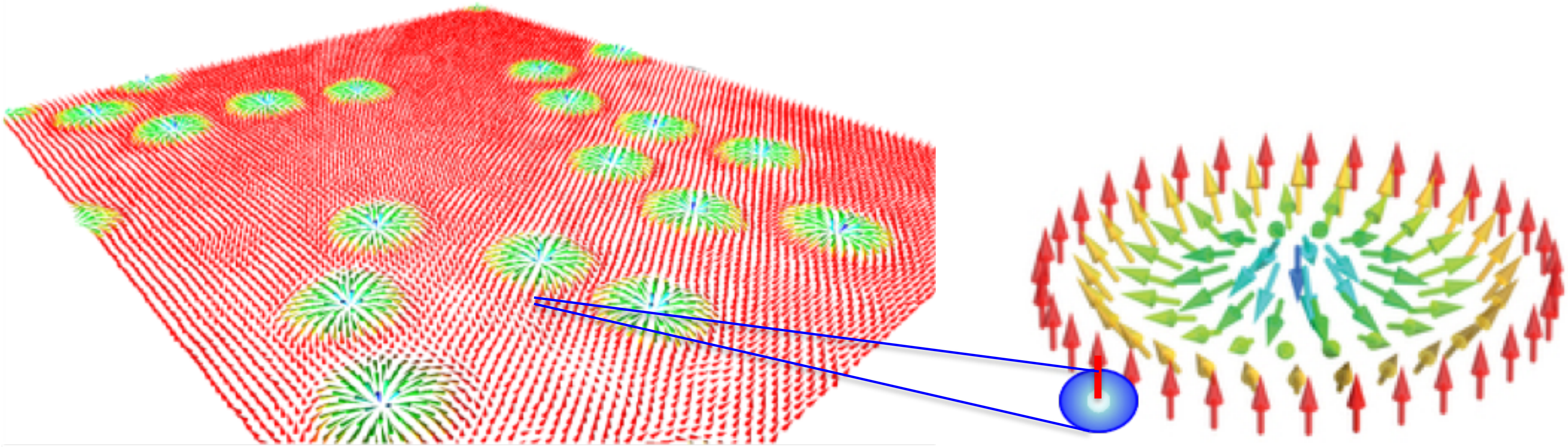
H. Zhang *et al.*, PRL (2012)

Chiral magnetic skyrmion



from Bertrand Dupé

Chiral magnetic skyrmion



from Bertrand Dupé

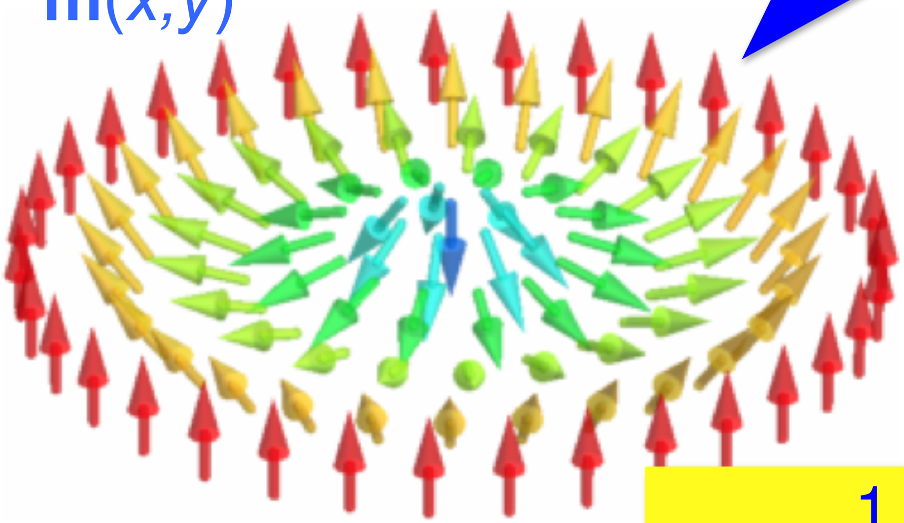
from Karin Everschor-Sitte

Chiral magnetic skyrmion

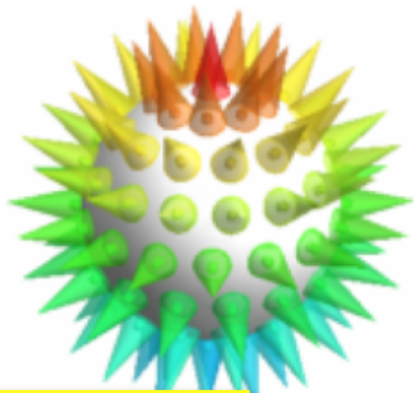
Skyrmion= non-trivial, smooth mapping from S_d to order parameter space ("trivial winding at infinity") magnetization direction

hedgehog vector field of magnetization direction $\mathbf{m}(x,y) = \mathbf{M}/M$

$\mathbf{m}(x,y)$



Smooth mapping
Here d=2, $S_2 \rightarrow S_2$



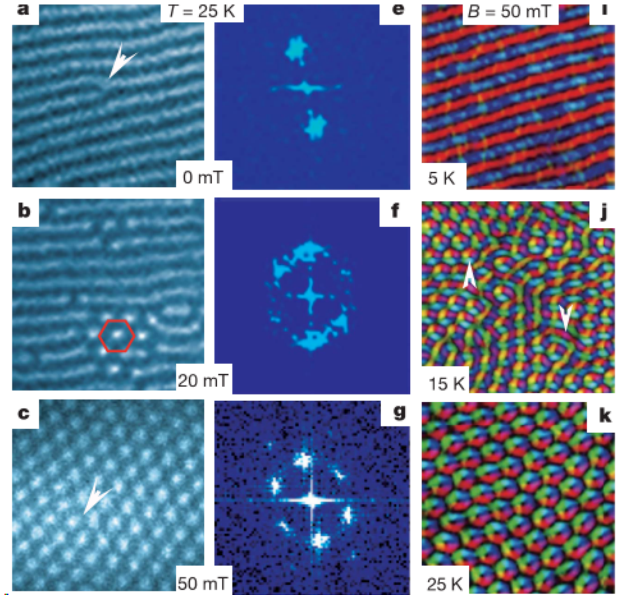
$$Q = \frac{1}{4\pi}\int_{\mathbb{R}^2} \mathbf{m}\cdot\left(\frac{\partial \mathbf{m}}{\partial x}\times\frac{\partial \mathbf{m}}{\partial y}\right) dxdy$$

Skyrmions: Experimental observations

Layers of materials with intrinsic chirality
(cubic helimagnets FeGe, MnSi, $Fe_{1-x}Co_xSi$)

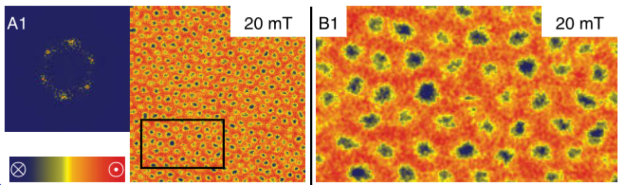
Lorentz Transmission Electron Microscopy

X.Z. Yu et al. *Nature* **465**, 90 (2010)



Magnetic Force Microscopy

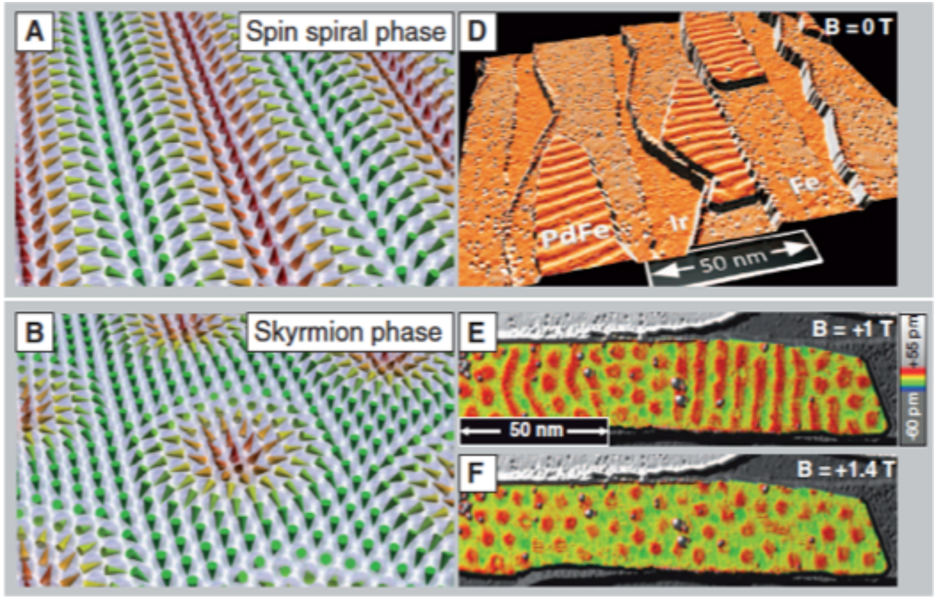
P. Milde et al., *Science* **340,** 1076 (2013)



Ultrathin films with induced chirality
(Fe/Ir, Mn/W, Pd/Fe/Ir)

Spin-Polarized Scanning Tunneling Microscopy

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



$B_{app} \neq 0$

Multiscale modeling

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❖ Micromagnetic-model:

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

❖ Spin-Lattice Model:

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

❖ DFT-model: $E_{\mathrm{tot}}^{\mathrm{DFT}}(\mathbf{q}, \hat{e}_{\mathrm{rot}}) = E_{\mathrm{noSOC}}^{\mathrm{DFT}}(\mathbf{q}) + \Delta E_{\mathrm{SOC}}^{\mathrm{DFT}}(\mathbf{q}, \hat{e}_{\mathrm{rot}})$

From total energy calculation to

- A, **D**, **K**
- J_{ij}, $\mathbf{D}_{ij}$

www.flapw.de

Fleur

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

ELMHOLTZ GEMEINSCHAFT

Multiscale modeling

- Micromagnetic-model:

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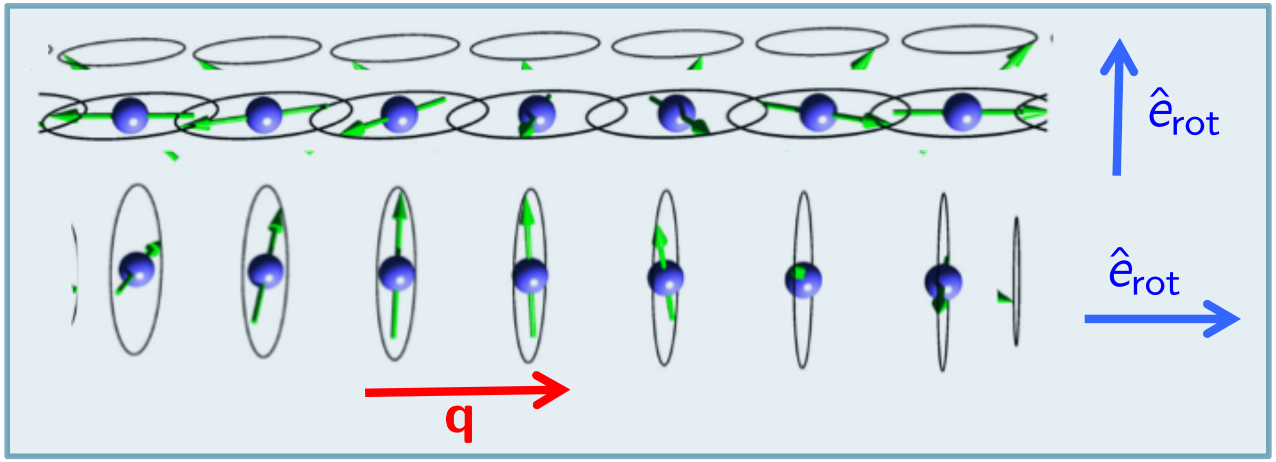
- Spin-Lattice Model:

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

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



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

Ab-initio A, D, K

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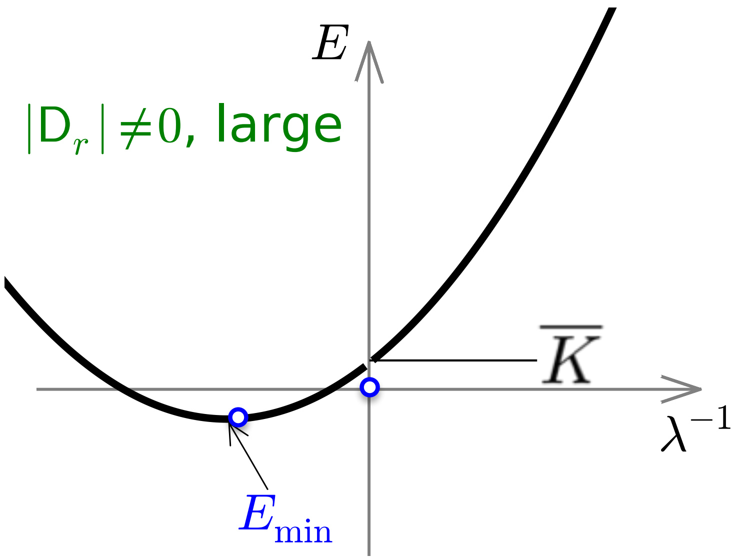
❖ Micromagnetic-model:

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

❖ Spin-Lattice Model:

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

❖ DFT-model: $E_{\text{tot}}^{\text{DFT}}(\mathbf{q}, \hat{e}_{\text{rot}}) = E_{\text{noSOC}}^{\text{DFT}}(\mathbf{q}) + \Delta E_{\text{SOC}}^{\text{DFT}}(\mathbf{q}, \hat{e}_{\text{rot}})$



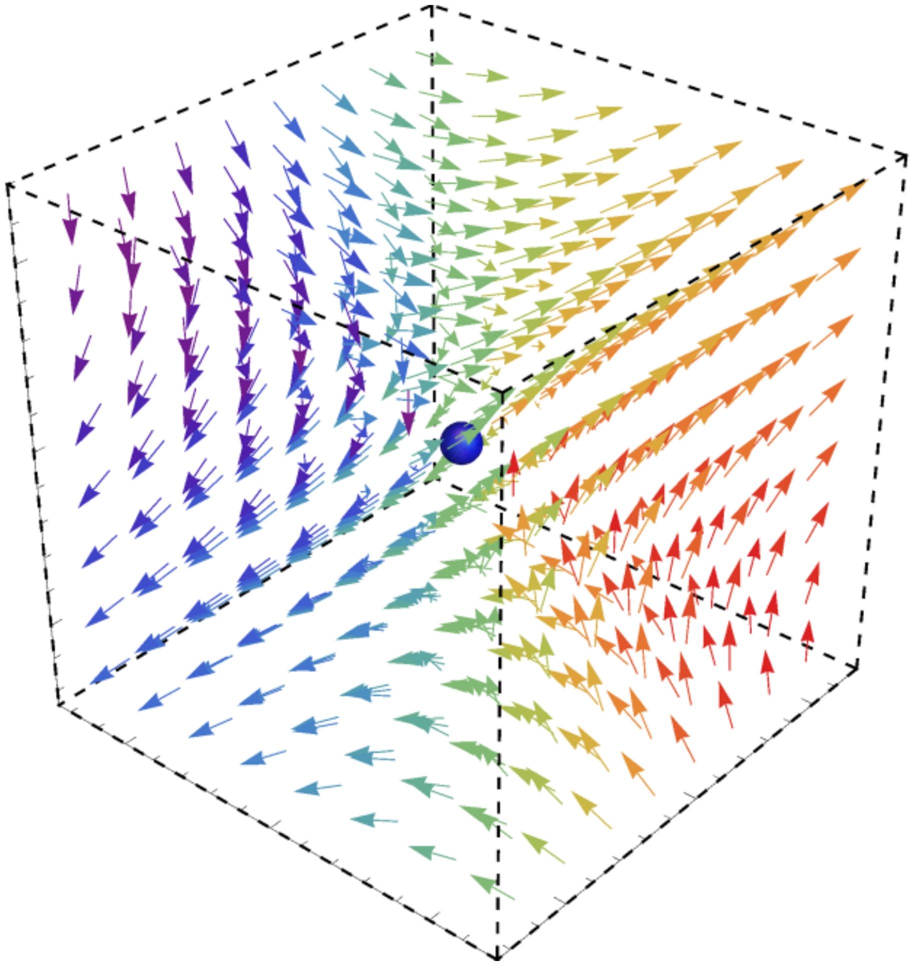
- Spin Stiffness:

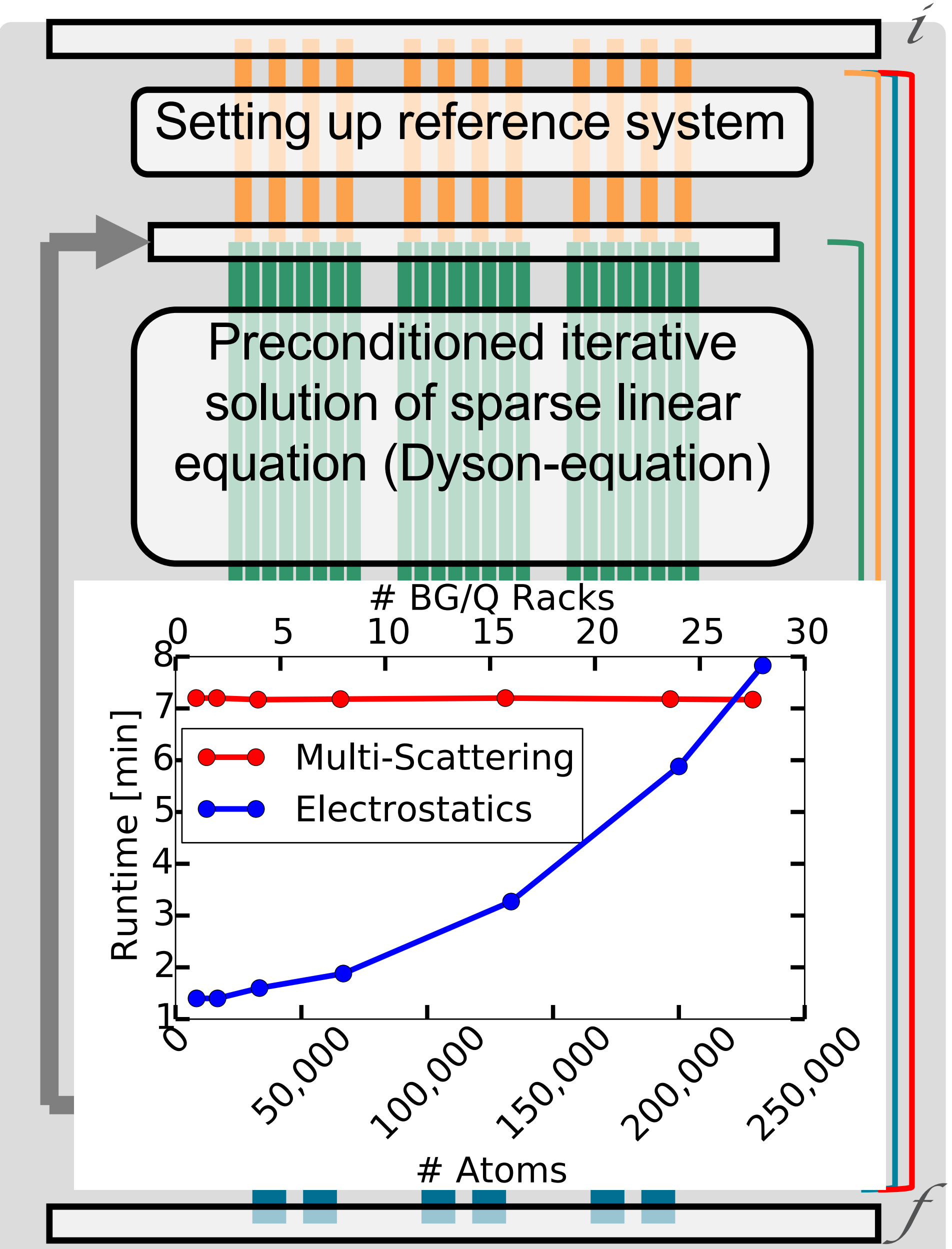
$$A = \frac{\partial^2}{\partial \mathbf{q}^2} E_{\text{tot}}^{\text{DFT}}(\mathbf{q}) \propto \sum_{j>0} J_{0j} R_{0j}^2$$

- Spiralization (micromagnetic D)

$$\underline{\mathbf{D}} = \frac{\partial}{\partial \mathbf{q}} E_{\text{tot}}^{\text{DFT}}(\mathbf{q}) \propto \sum_{j>0} \mathbf{D}_{0j} \otimes \mathbf{R}_{0j}$$

KKRnano: all-electron linear scaling for thousands of atoms

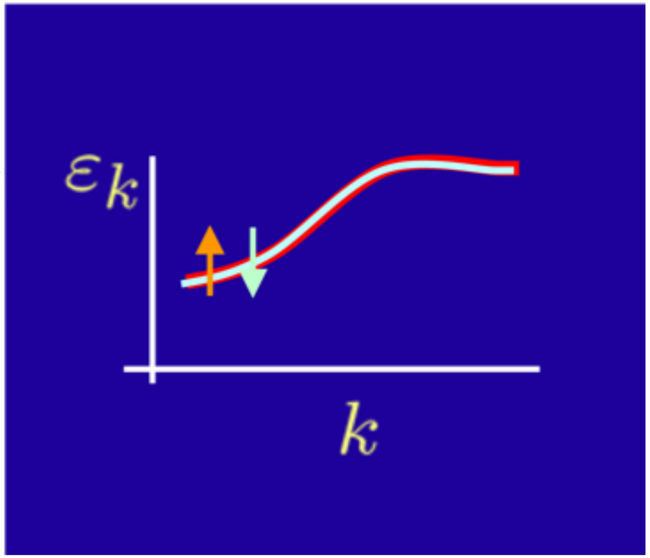




Schematic representation of workflow in KKRnano

What happens when space inversion symmetry broken

(GaAs, InSb, interfaces, surfaces, ...)



Time reversal + space inversion symmetry

$$\epsilon_{\mathbf{k}\uparrow} = \epsilon_{\mathbf{k}\downarrow}$$

Time reversal only

$$\epsilon_{\mathbf{k}\uparrow} = \epsilon_{-\mathbf{k}\downarrow} \quad , \quad \epsilon_{\mathbf{k}\uparrow} \neq \epsilon_{\mathbf{k}\downarrow}$$

Effective spin-orbit ("magnetic") field Ω:

$$H_1(\mathbf{k}) = \frac{\hbar}{2}\Omega(\mathbf{k}) \cdot \sigma$$

Time reversal symmetry:

$$\Omega(-\mathbf{k}) = -\Omega(\mathbf{k})$$

I. Žutić, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004).

Spin-Orbit Coupling

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- spin-orbit coupling has fascinating realizations and ramifications in solids

Examples:

- Orbital and topological orbital magnetic moment
- Magnetic Anisotropy
- Dzyaloshinskii-Moriya Interaction
- Rashba Effect , Dresselhaus Effect
- Topological Insulator, Weyl Semimetals
- Spin-Relaxation (Elliot-Yafet, Dyakonov-Perel)
- Anomalous Hall Effect, Spin Hall Effect
- Spin-Orbit torque
- Quantum Spin Hall Effect, Quantum Anomalous Hall Effect

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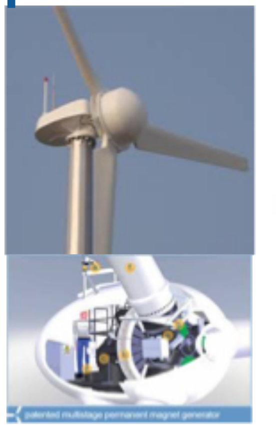
Magnetic materials & spintronics have a market

Energy

permanent magnets



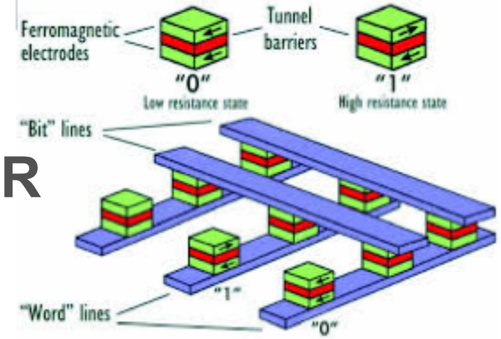
Storage

hard disk drive

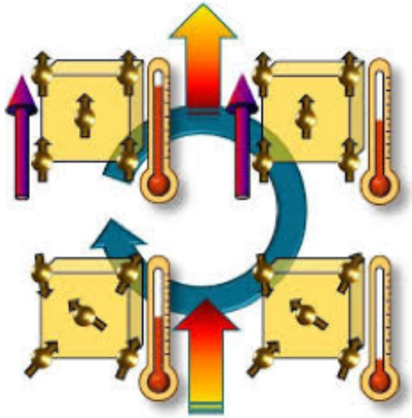
Memory

MRAM

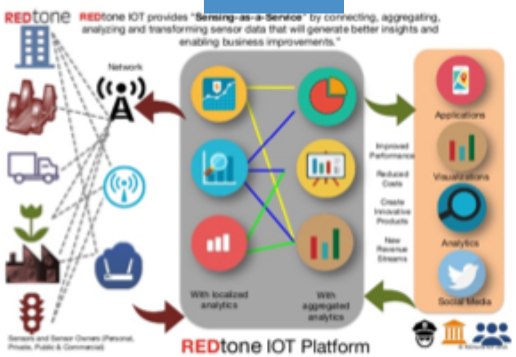
TMR



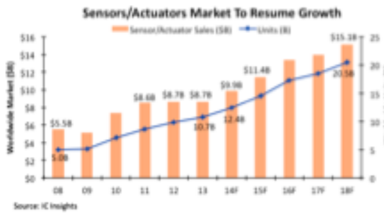
magneto-caloric materials



IoT



magnetic sensors



Example 1:
Bandstructure of topological insulator

GW with spin-orbit coupling (SOC)

MOST *GW* WORKS PUBLISHED → *a posteriori* SOC:

LDA (without SOC) **+** *GW* (without SOC) **+** SOC(LDA)

GW+SOC

GW with spin-orbit coupling (SOC)

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MOST *GW* WORKS PUBLISHED → *a posteriori* SOC:

LDA (without SOC) **+** *GW* (without SOC) **+** SOC(LDA)

GW+SOC

OUR WORK → full SOC:

Sakuma *et al.*, PRB **84** 085144 (2011)

LDA (with SOC) **+** *GW* (with SOC)

(more accurate but ~10 times more time-consuming)

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$G^{SOC}W^{SOC}$

HELMHOLTZ GEMEINSCHAFT

GW with spin-orbit coupling (SOC)

JÜLICH FORSCHUNGSZENTRUM

MOST *GW* WORKS PUBLISHED ***a posteriori* SOC:**

LDA (without SOC) **+** *GW* (without SOC) **+** SOC(LDA)

GW+SOC

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Sakuma *et al.*, PRB **84** 085144 (2011)

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(more accurate but ~10 times more time-consuming)

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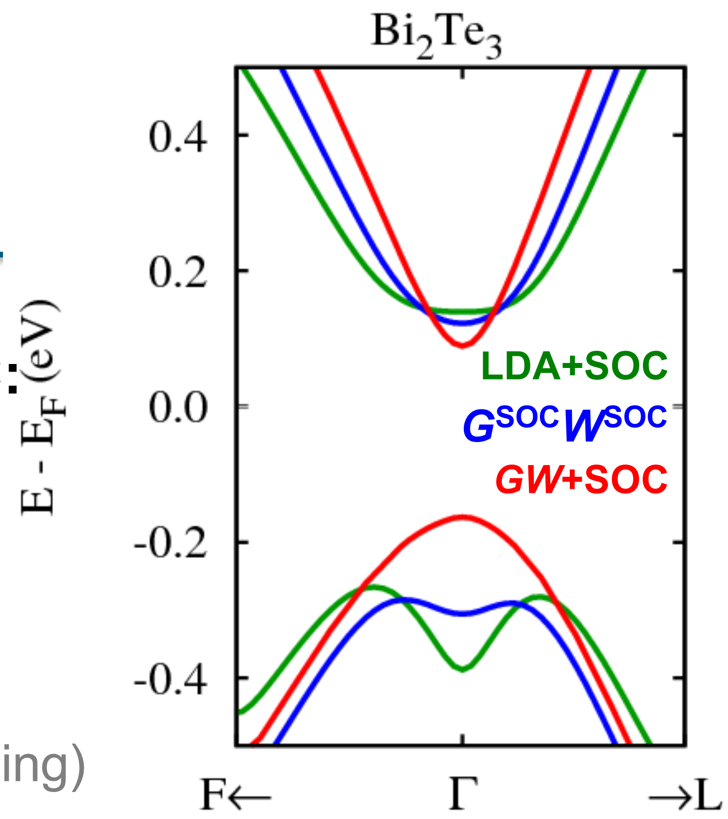
Fleur

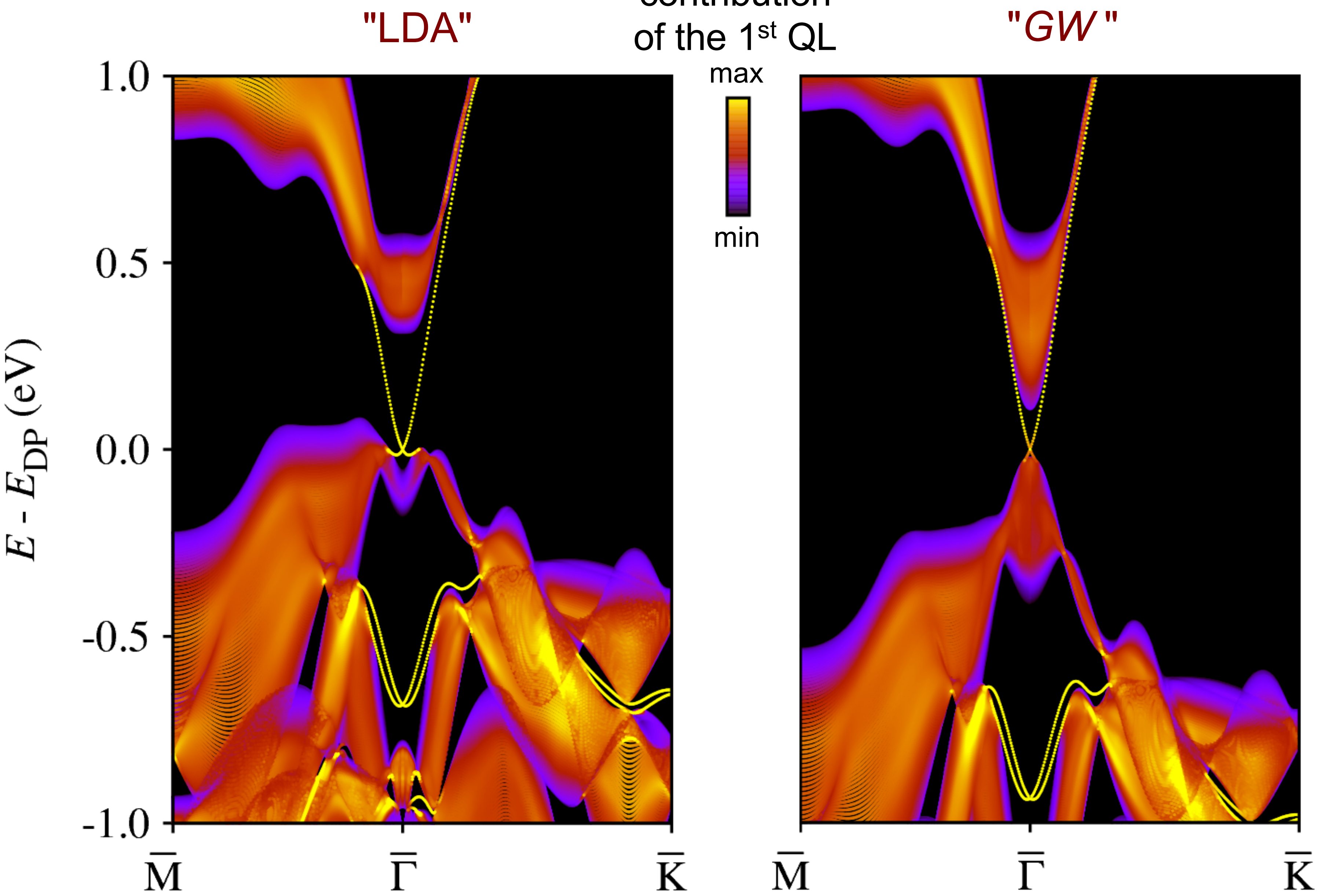
$G^{SOC}W^{SOC}$



Aguilera, Friedrich, Blügel, PRB **88**, 165136 (2013)

100 QL slab of Bi_2Se_3

(~100 nm)



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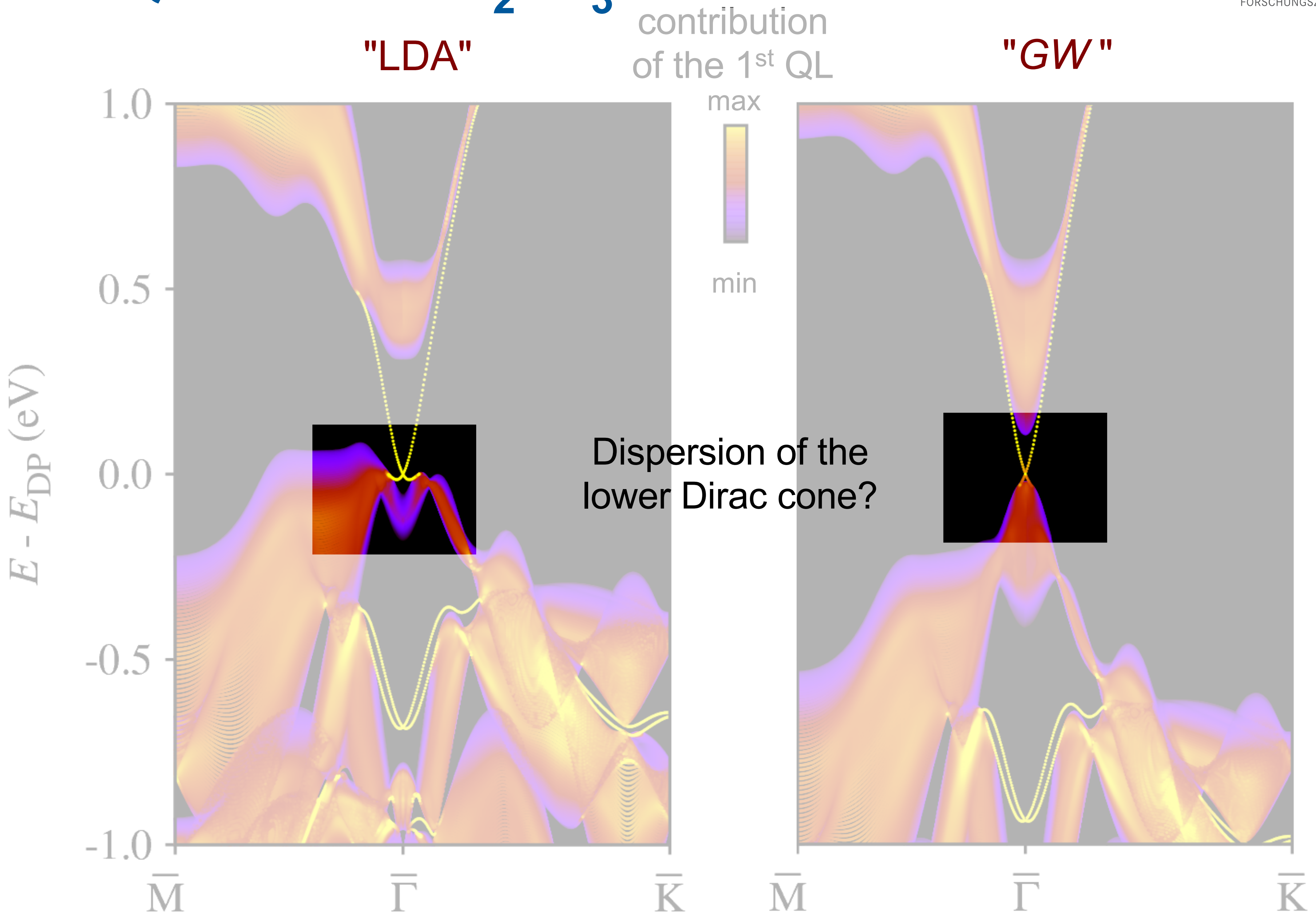
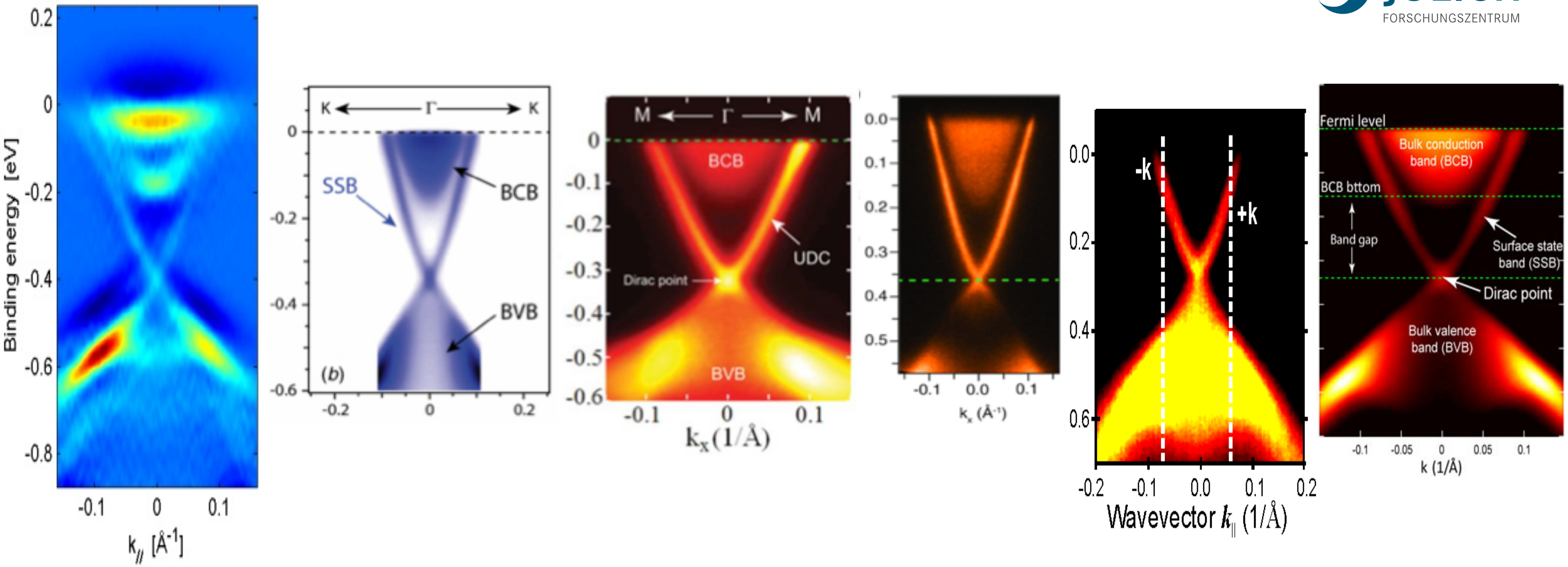
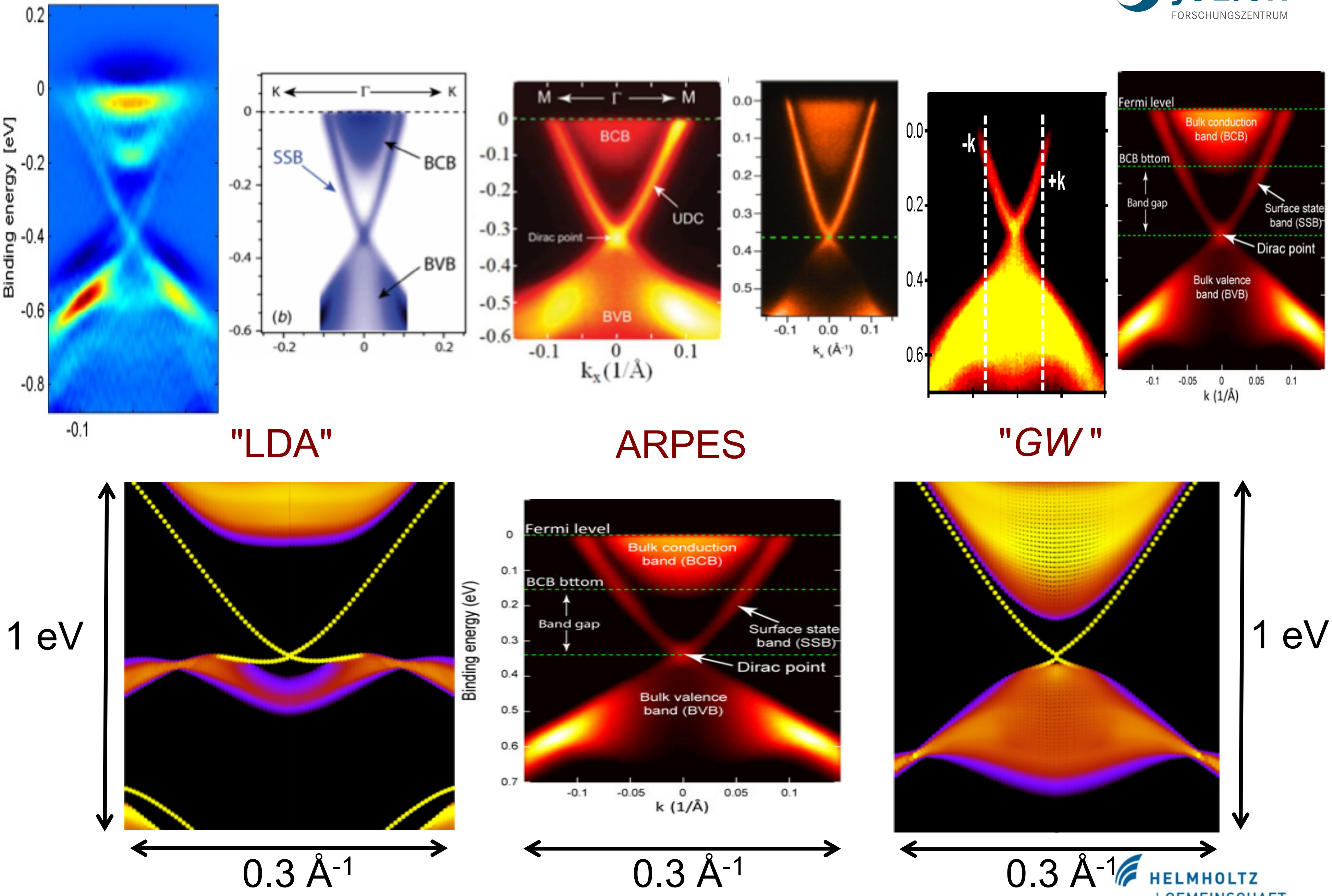


Comparison with ARPES: Bi_2Se_3



Comparison with ARPES: Bi_2Se_3



Example 2:
Skyrmion design

Skyrmions for Spintronics

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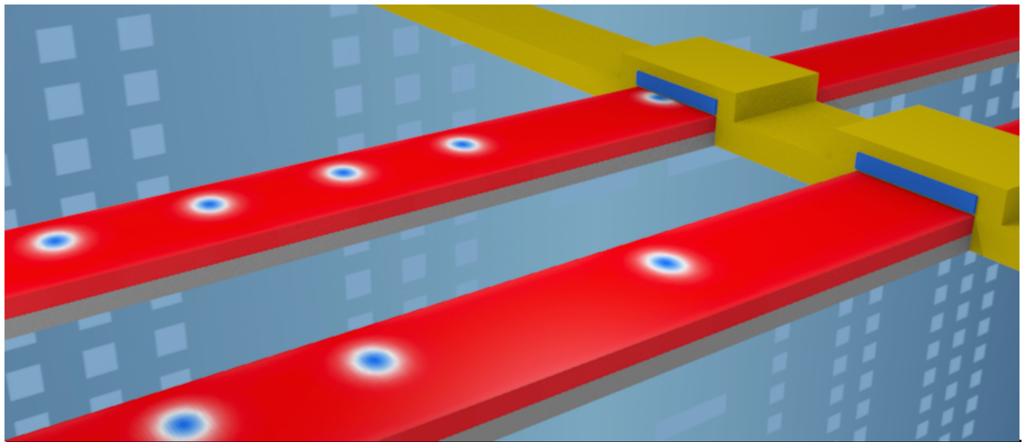
The Fert criteria

- Chiral magnetism in thin films, but not too thin (min 3 layers)
- Try find small but not too small skyrmions ≈ 5-10 nm
- Above room temperature and zero magnetic field
- Fit to the field of spintronics: *injection*, *transport*, *detection*, manipulation at reasonable fields and *currents*
- Fast & energy efficient
- Also for logic operation
- Metallic magnetism



Albert Fert, Vincent Cross and João Sampaio, Nature Nanotechnology **8**, 152 (2013)

Multiscale modeling

❖ Micromagnetic-model:

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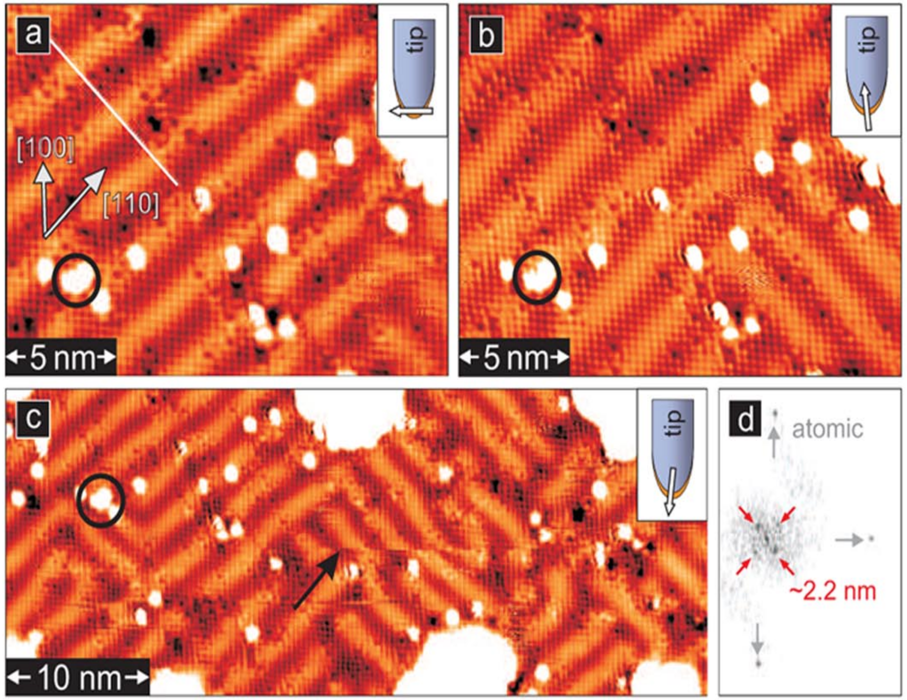
$$H = \frac{1}{2} \sum_{ij} J_{ij}\, \mathbf{m}_i \mathbf{m}_j + \sum_{ij} \mathbf{D}_{ij} \overbrace{\mathbf{m}_i \times \mathbf{m}_j}^{c} + \sum_i \mathbf{m}_i\, \underline{\mathbf{K}}\, \mathbf{m}_i + \sum_{ij} \frac{1}{r_{ij}^3} \left[\mathbf{m}_i \mathbf{m}_j - (\mathbf{m}_i \hat{\mathbf{e}}_i)(\mathbf{m}_j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

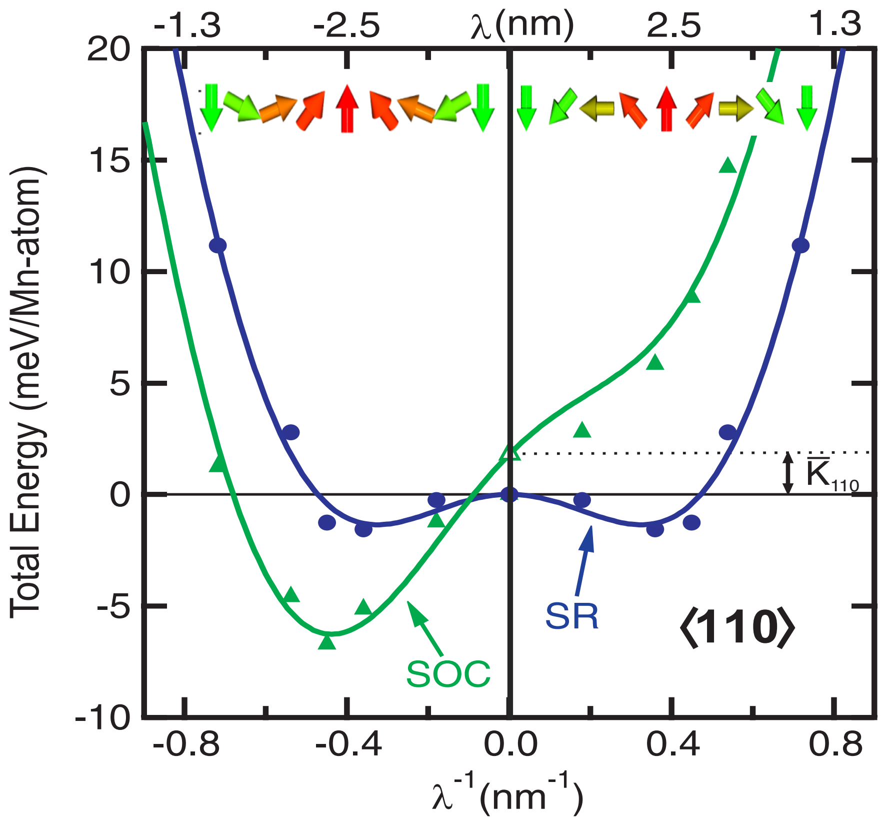
Exchange bias stabilized skyrmions

Mn/W(100)



Spin-polarized STM image

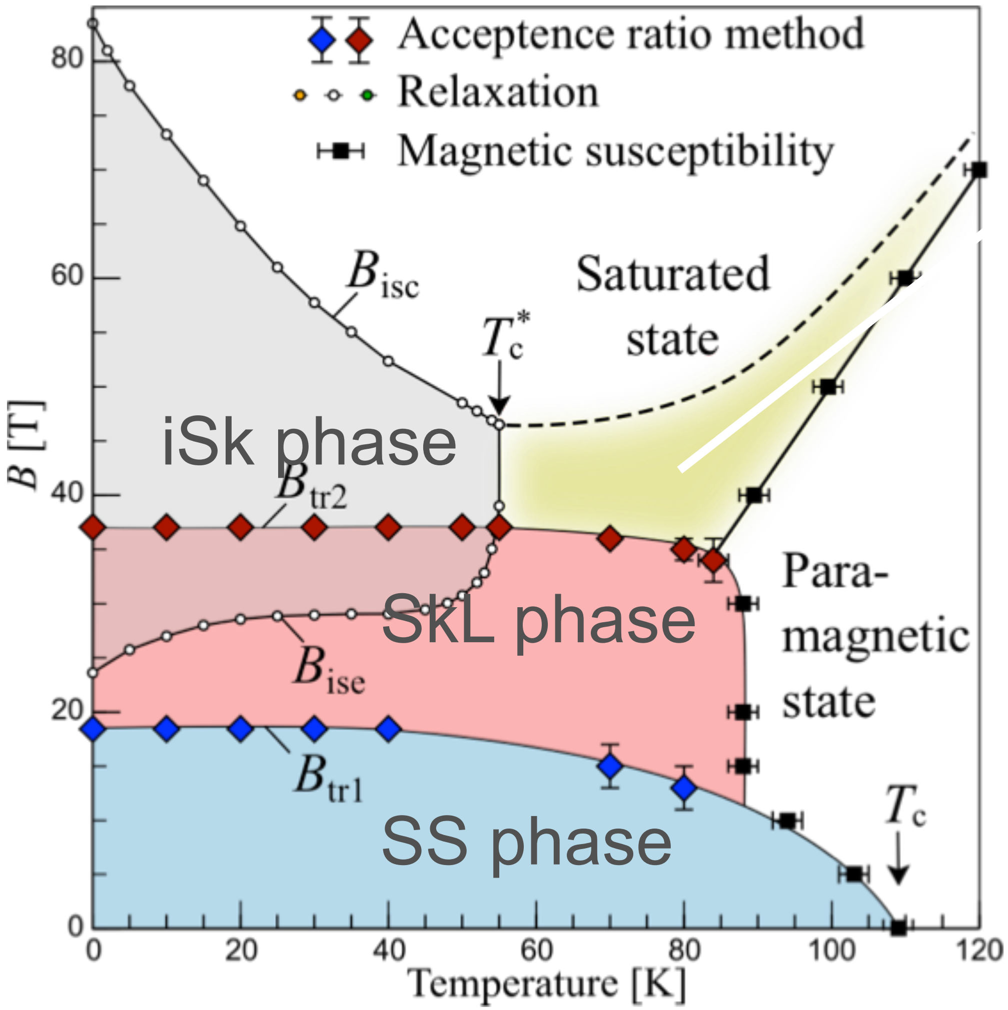
Ferriani *et al.*, PRL **101** 027201 (2008)



Theory result

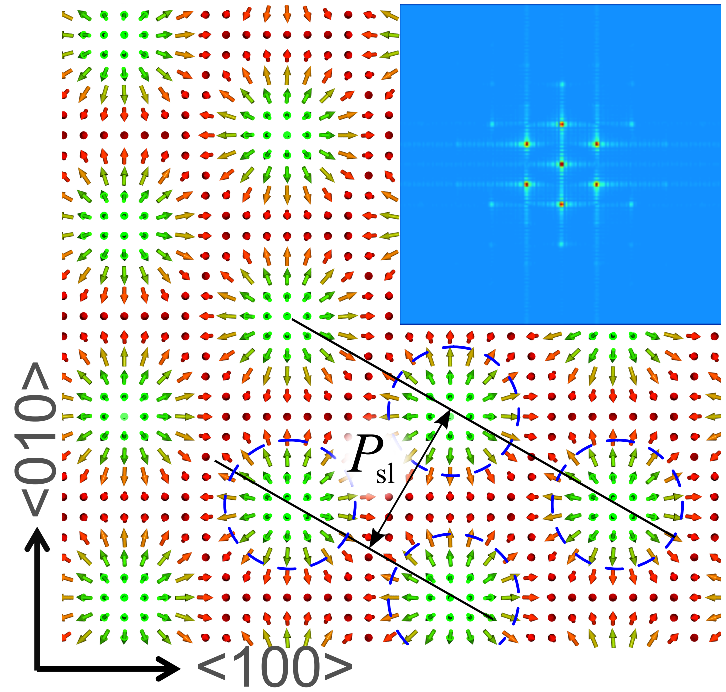
$$H = \frac{1}{2}\sum_{ij} J_{ij}\,\mathbf{m}_i\mathbf{m}_j + \sum_{ij} \mathbf{D}_{ij}\,\overbrace{\mathbf{m}_i \times \mathbf{m}_j}^{c} + \sum_i \mathbf{m}_i\,\underline{\mathbf{K}}\,\mathbf{m}_i + \sum_{ij}\frac{1}{r_{ij}^3}\left[\mathbf{m}_i\mathbf{m}_j - (\mathbf{m}_i\hat{\mathbf{e}}_i)(\mathbf{m}_j\hat{\mathbf{e}}_i)\right]$$

Interlayer Exchange Bias Skyrmions



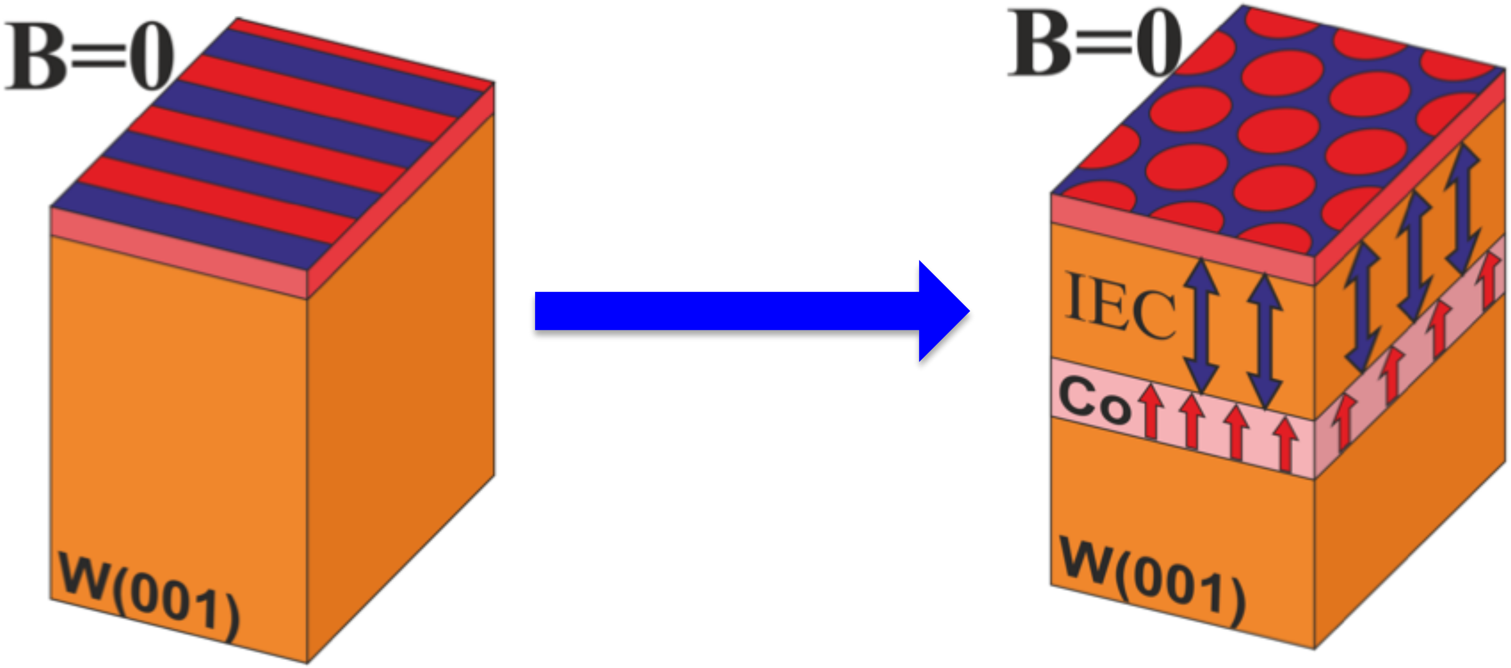
Spontaneous nucleation of individual skyrmion with finite life-time

Skyrmion lattice (SkL) phase



Nandy, Kiselev, Blügel, PRL.**116**, 177202 (2016)

Interlayer Exchange Bias Skyrmions



Nandy, Kiselev Blügel
PRL.**116**, 177202 (2016)

Interlayer exchange coupling (IEC) between reference and free magnetic layer may compensate the required magnetic field.

Skyrmions in zero applied field

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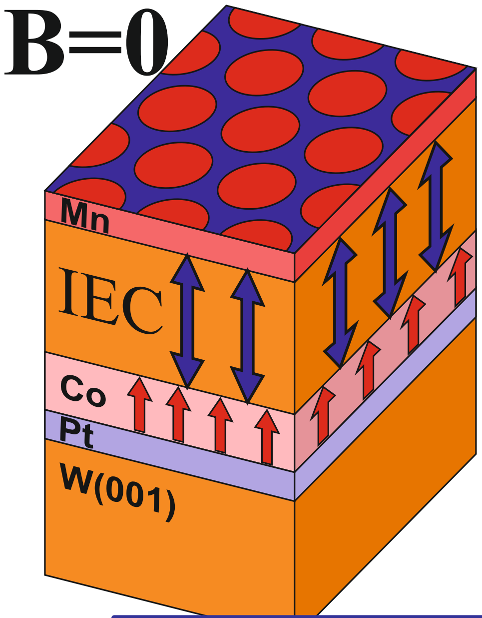
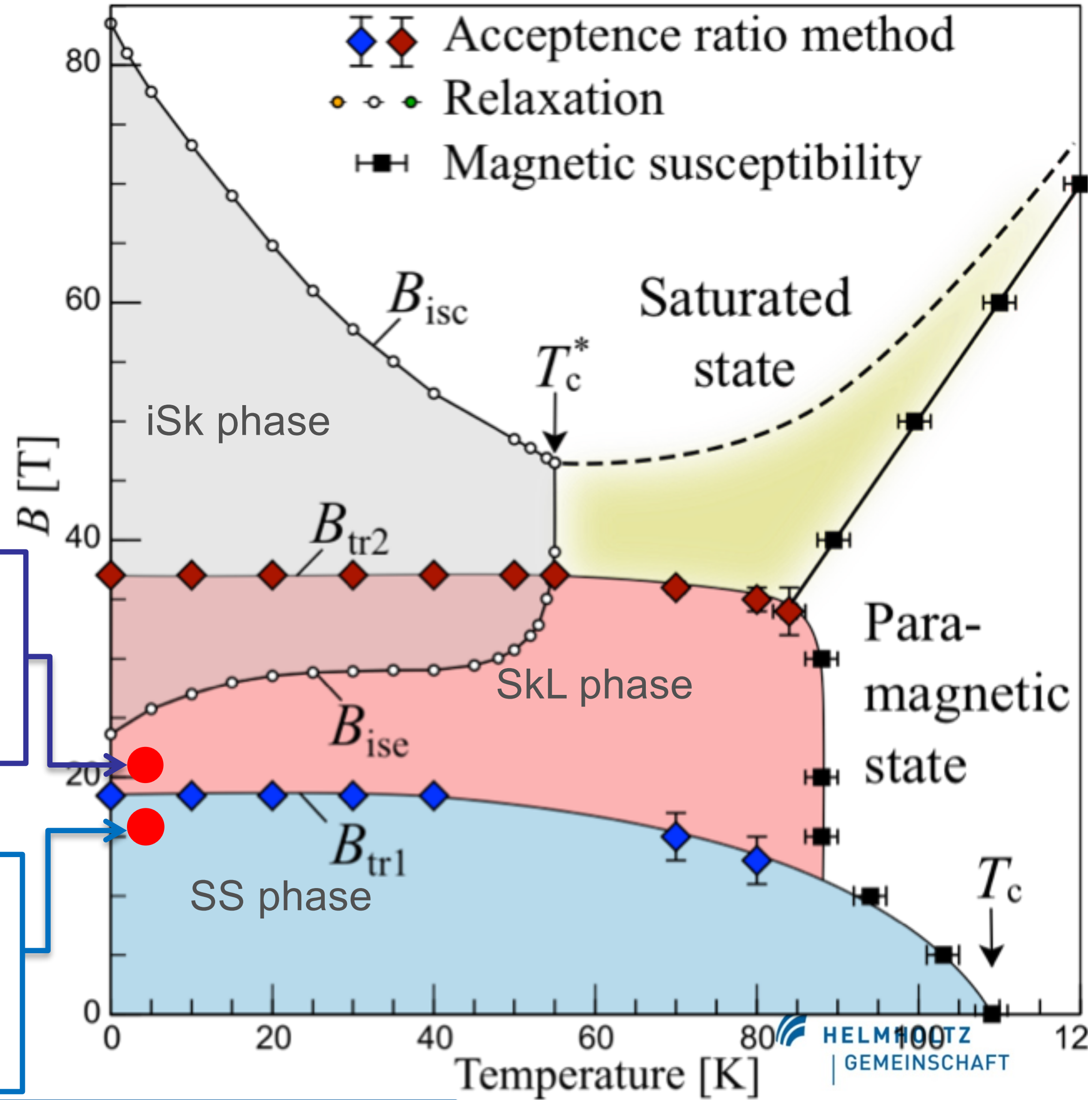


Mn/W$_6$/Co$_4$/Pt/W(001)
K_{Co} = 2.0 meV/Co,
B_{eff} = 20 T

Mn/W$_7$/Co$_4$/Pt/W(001)
K_{Co} = 2.7 meV/Co,
B_{eff} = 15 T



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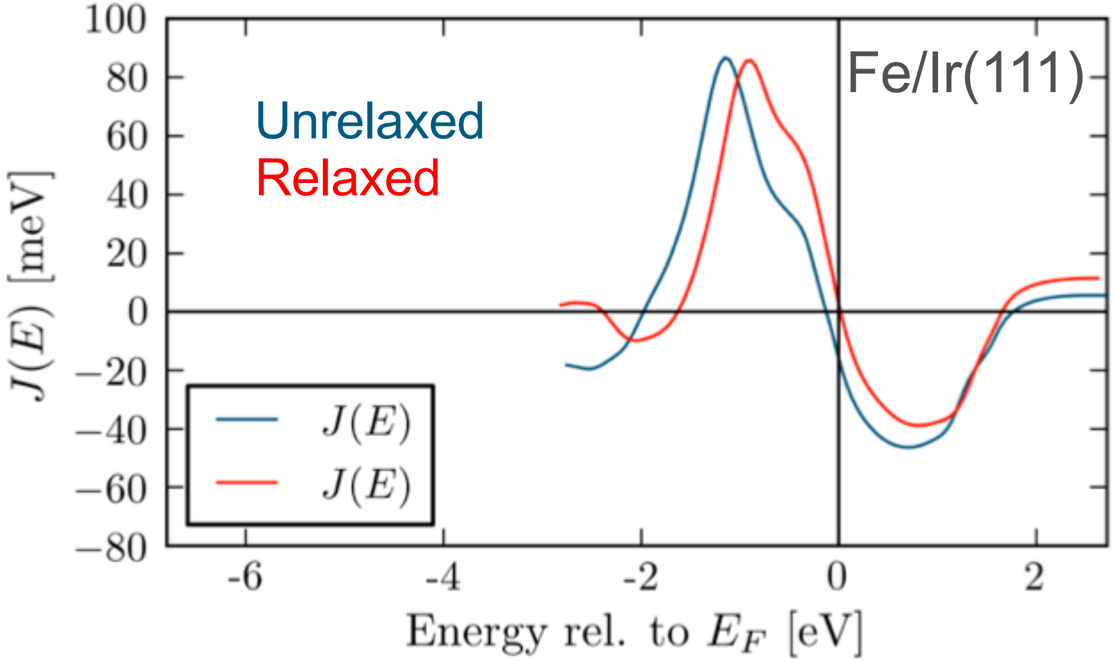
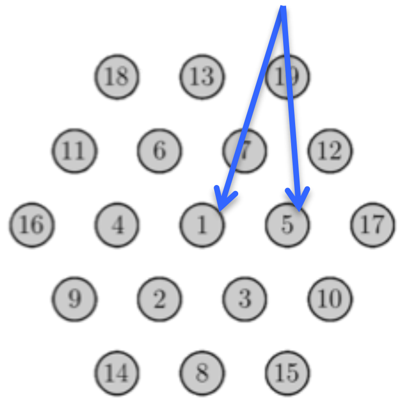
State resolved Heisenberg coupling

Steep slope at the Fermi energy
System is extremely sensitive on lattice relaxations
Energy shifts due to Hybridization effects

$$J_{1,5}(E) = -\frac{1}{3}\mathrm{Tr}_{\alpha,\beta}\,\frac{1}{\pi}\mathrm{Im}\int^{E_F} dE\,\mathrm{Tr}\left[\underline{\mathbf{G}}_{1,5}\,\underline{\mathbf{t}}_5^{\alpha}\,\underline{\mathbf{G}}_{5,1}\,\underline{\mathbf{t}}_1^{\beta}\right]$$

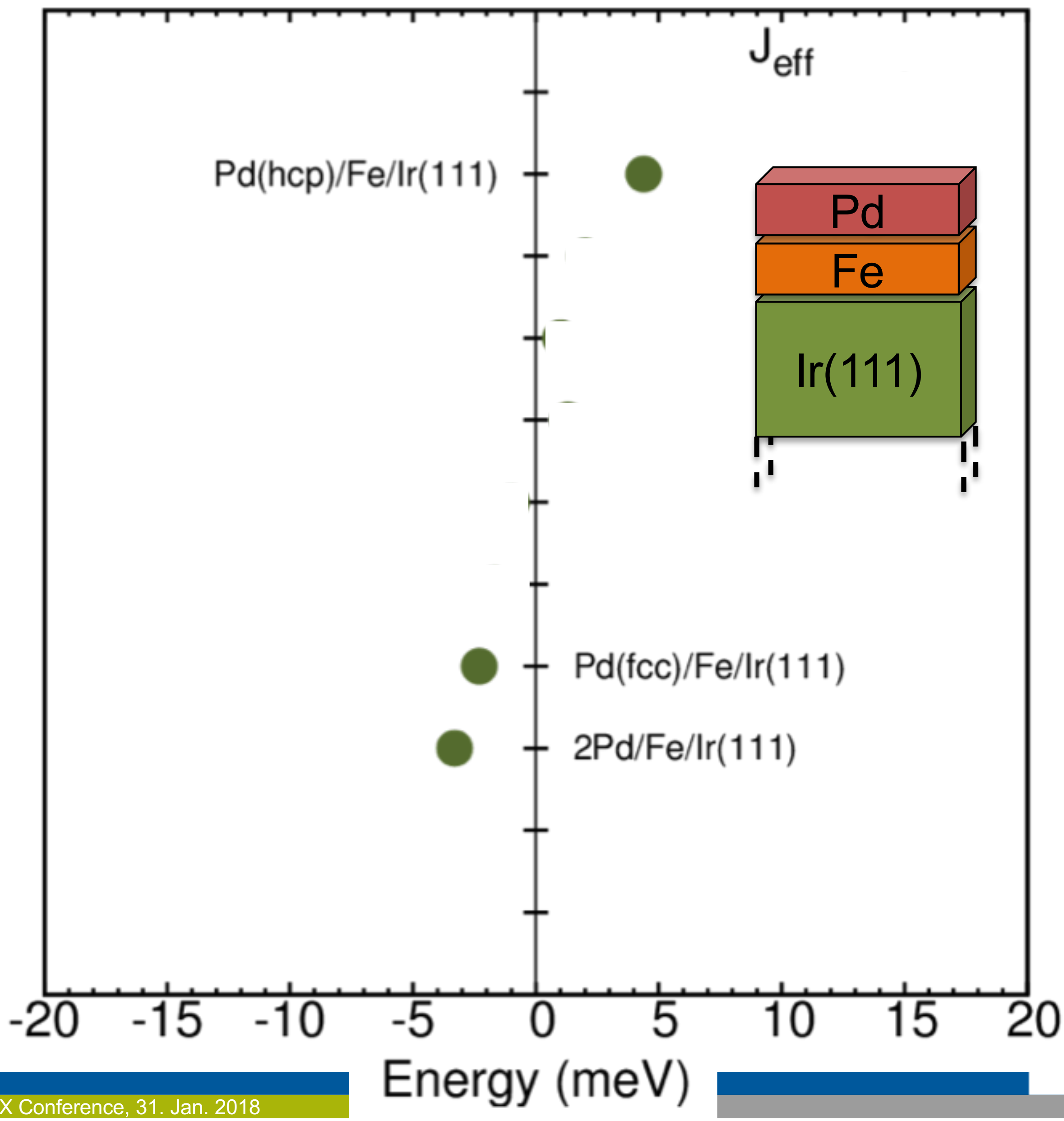
$$j(E) = \frac{dJ}{dE}$$





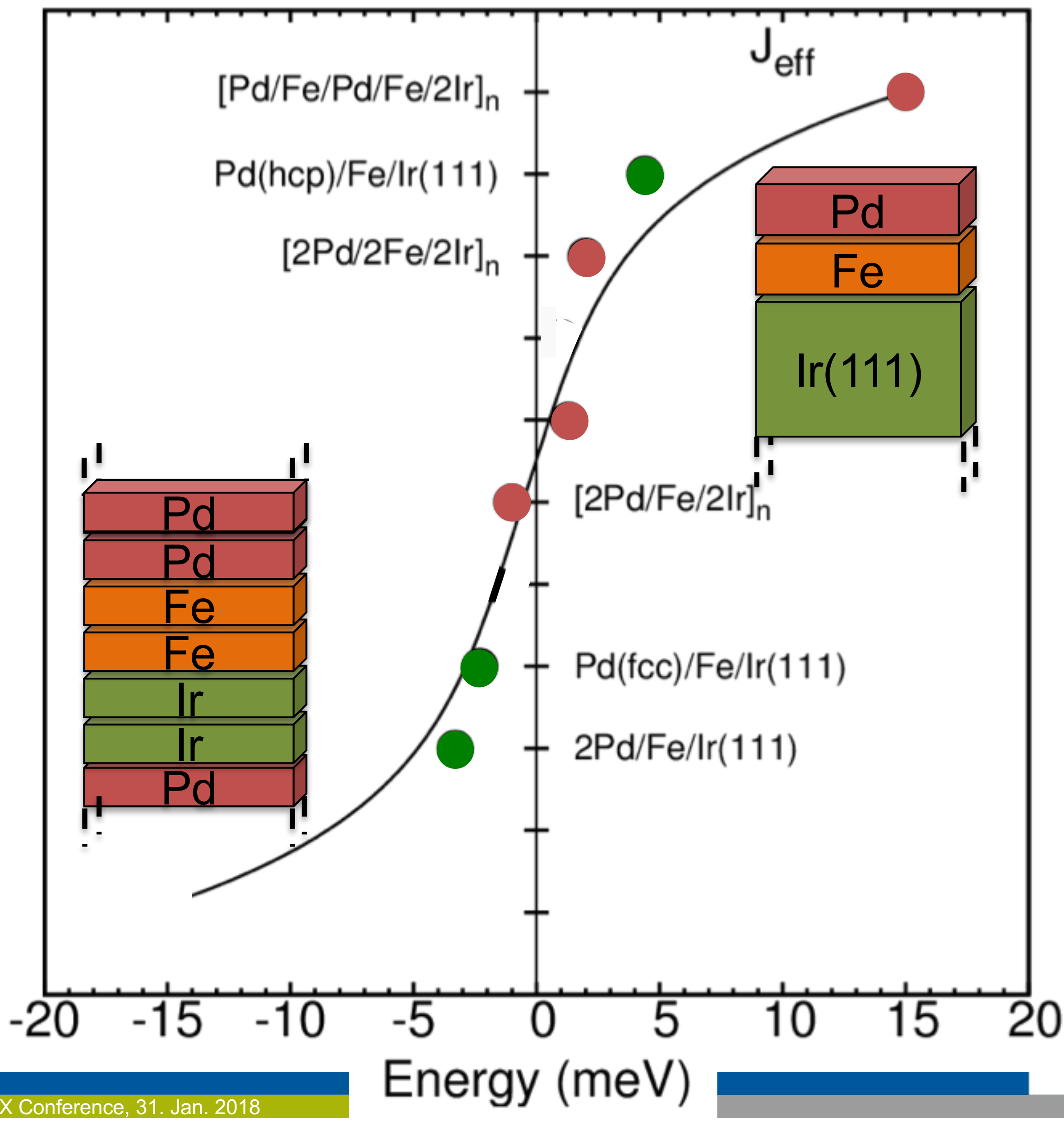
Bauer, Mavropoulos, Zeller, Blügel to be published

Skyrmion à la carte



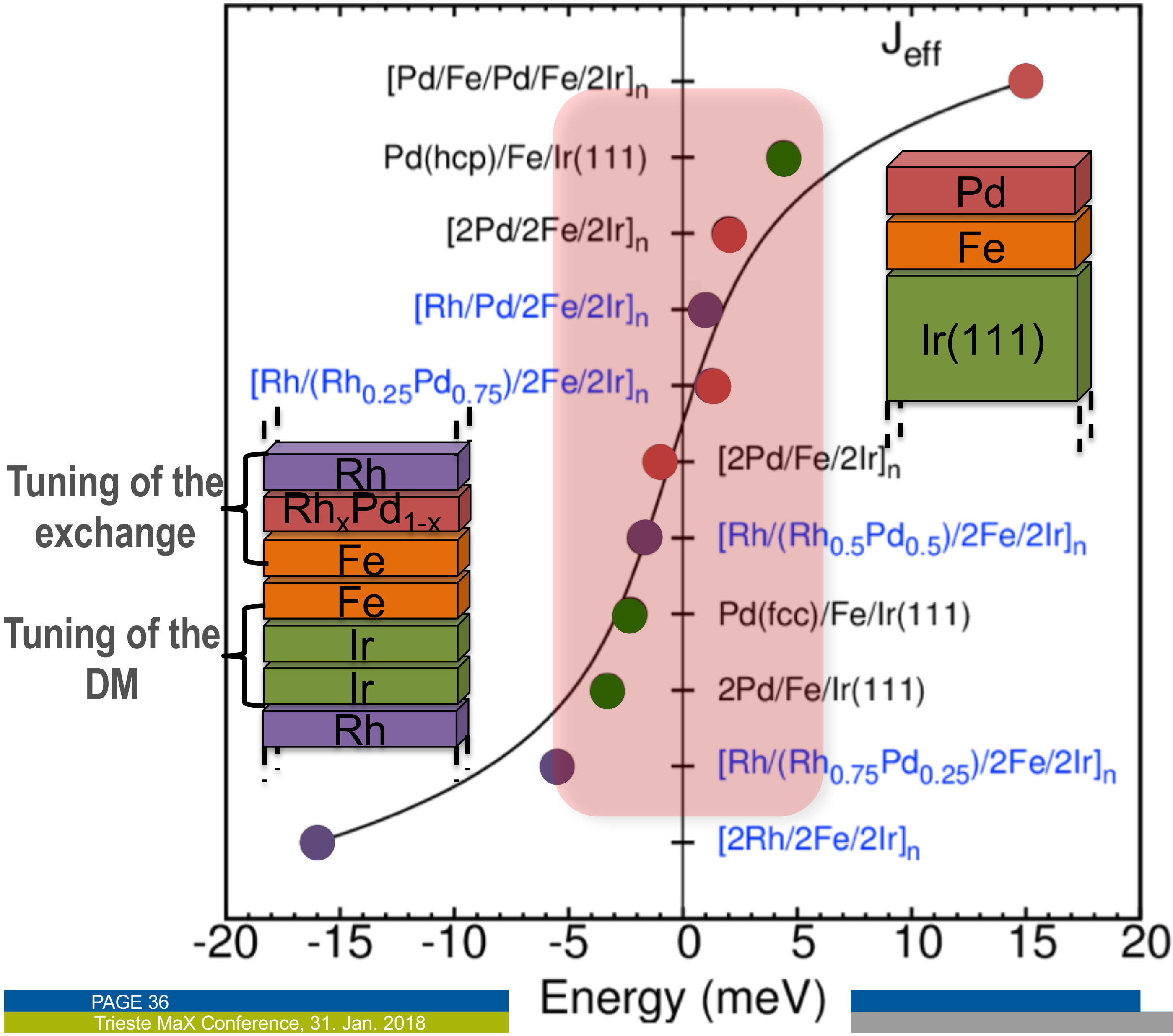
B. Dupé, G. Bihlmayer, S. Blügel, S. Heinze, Nature Comm. **7**, 11779 (2016)

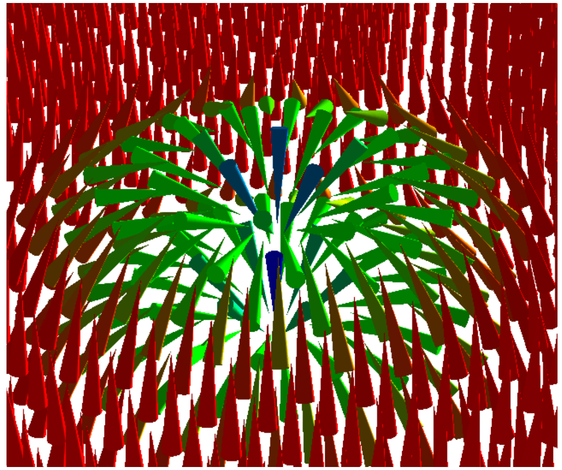
Skyrmion à la carte

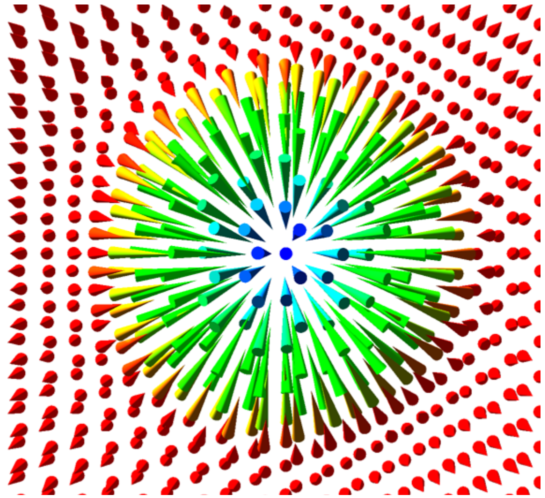


B. Dupé, G. Bihlmayer, S. Blügel, S. Heinze, Nature Comm. **7**, 11779 (2016)

Skyrmion à la carte

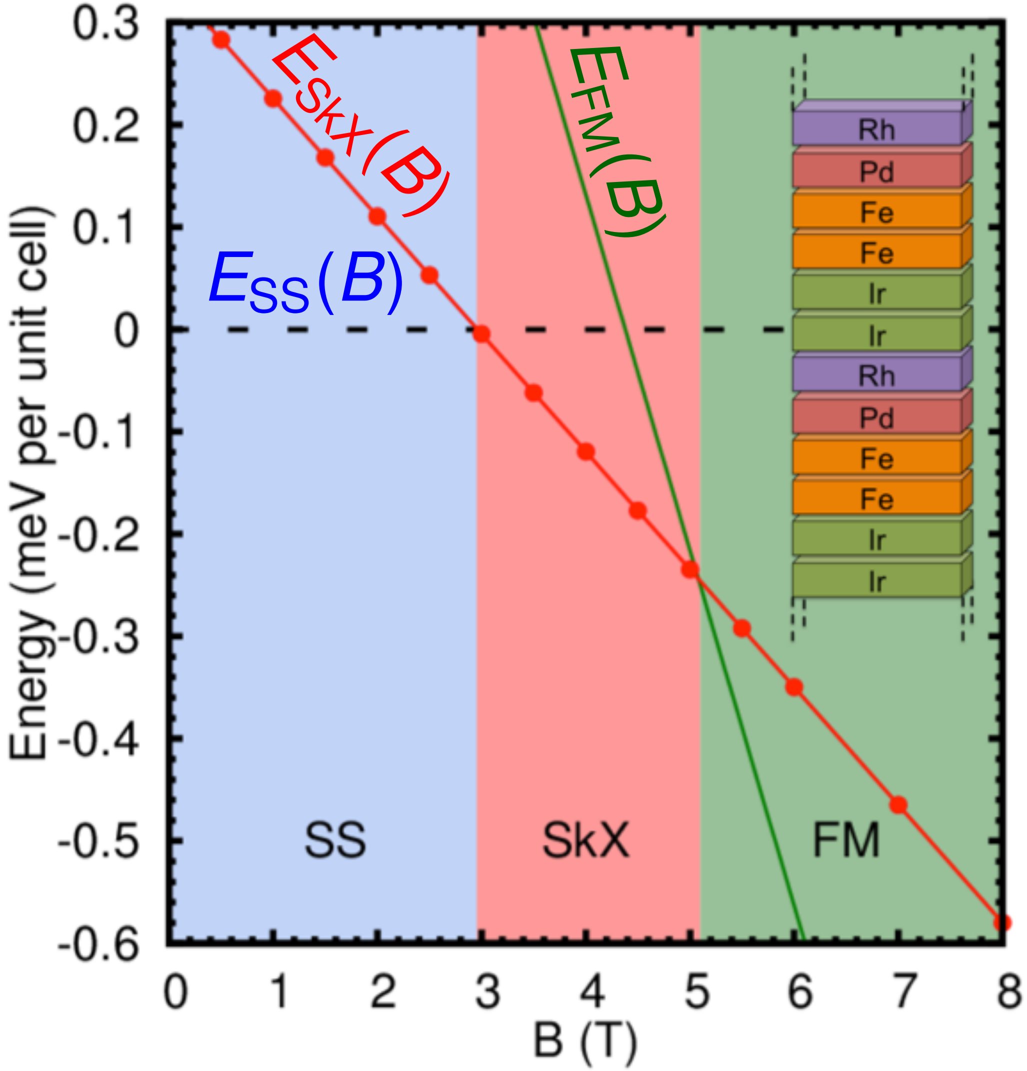






B. Dupé, G. Bihlmayer, S. Blügel, S. Heinze, Nature Comm. **7**, 11779 (2016)

Skyrmion à la carte



Dupe, Bihlmayer, Blügel, Heinze , Nature Comm. **7**, 11779 (2016)

Example 3:
Skyrmion detection

Small skyrmions from first-principles

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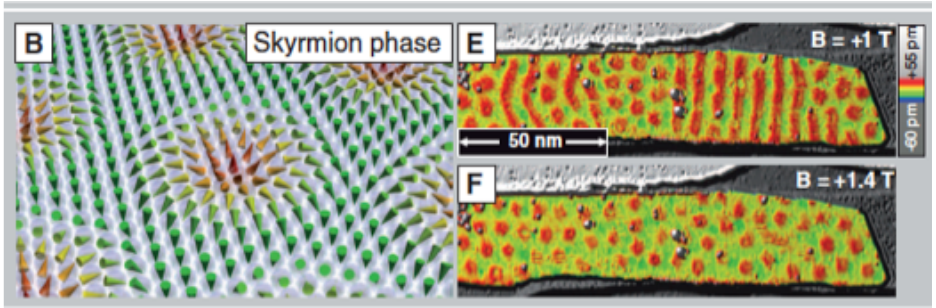
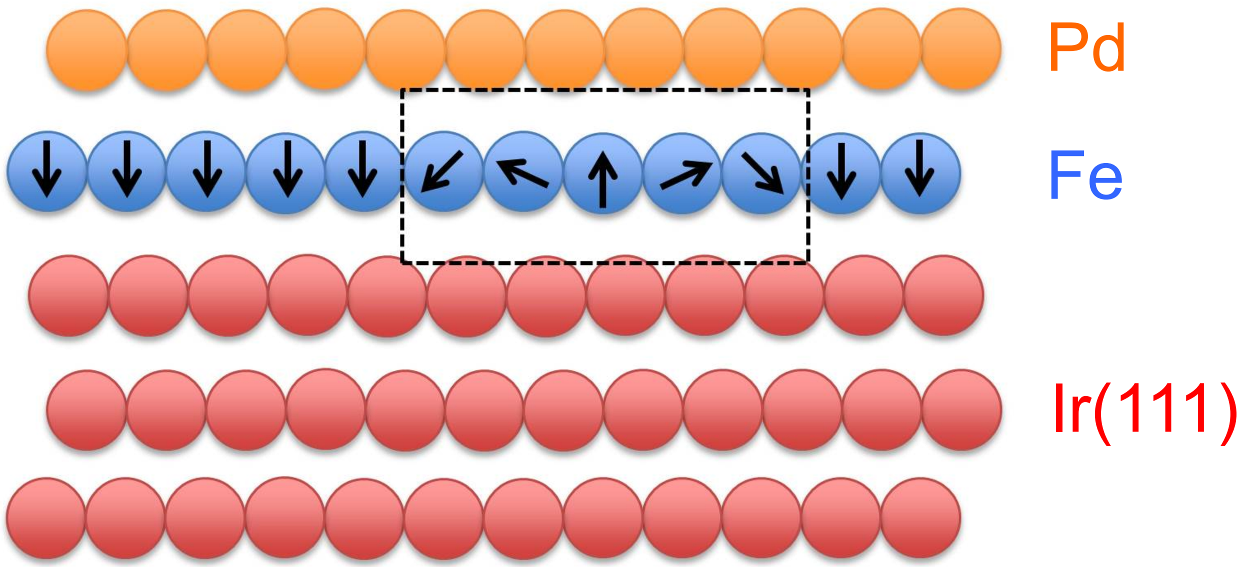
Spin-Polarized Scanning Tunneling Microscopy

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



Pd/Fe/Ir(111)



$$G_{Sky} = G_{FM} + G_{FM}\,\Delta V\,G_{Sky}$$

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Real-space spin relaxation of nano-skyrmions

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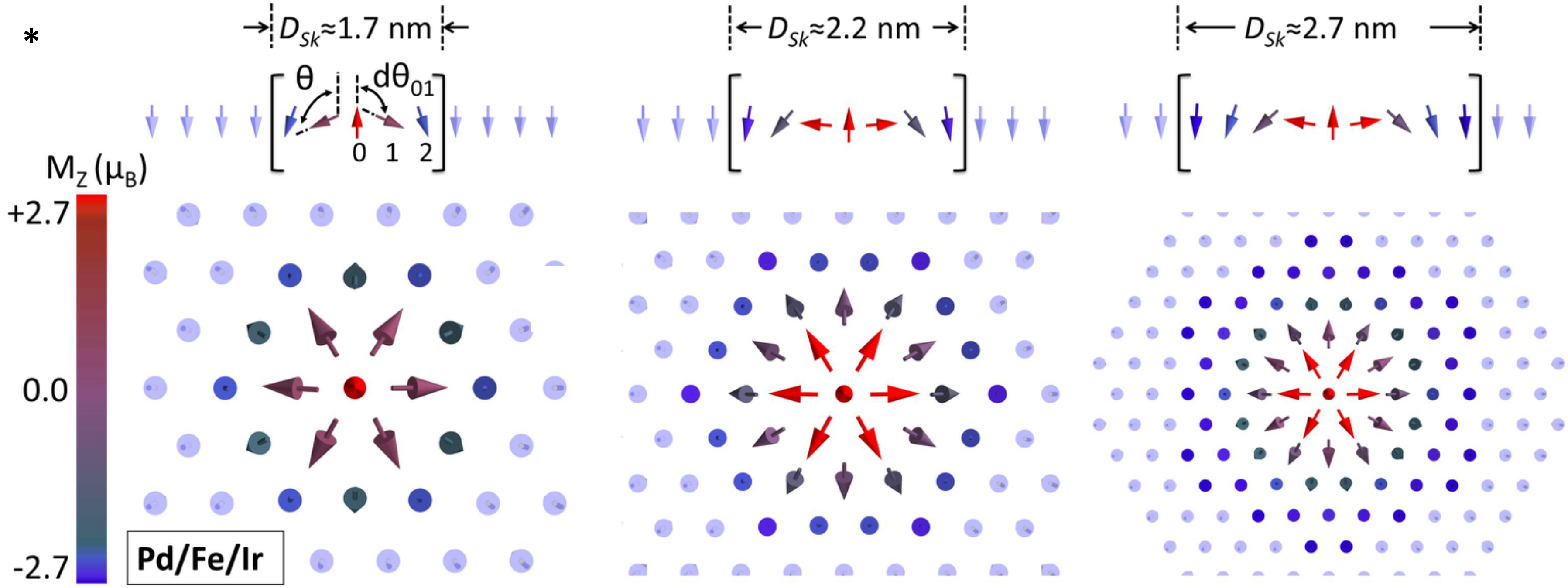
*



D. Crum, M. Bouhassoune, J. Bouaziz, B. Schwelinghaus, S. Blügel, S. Lounis , Nature Comm. **6**, 8541 (2015)

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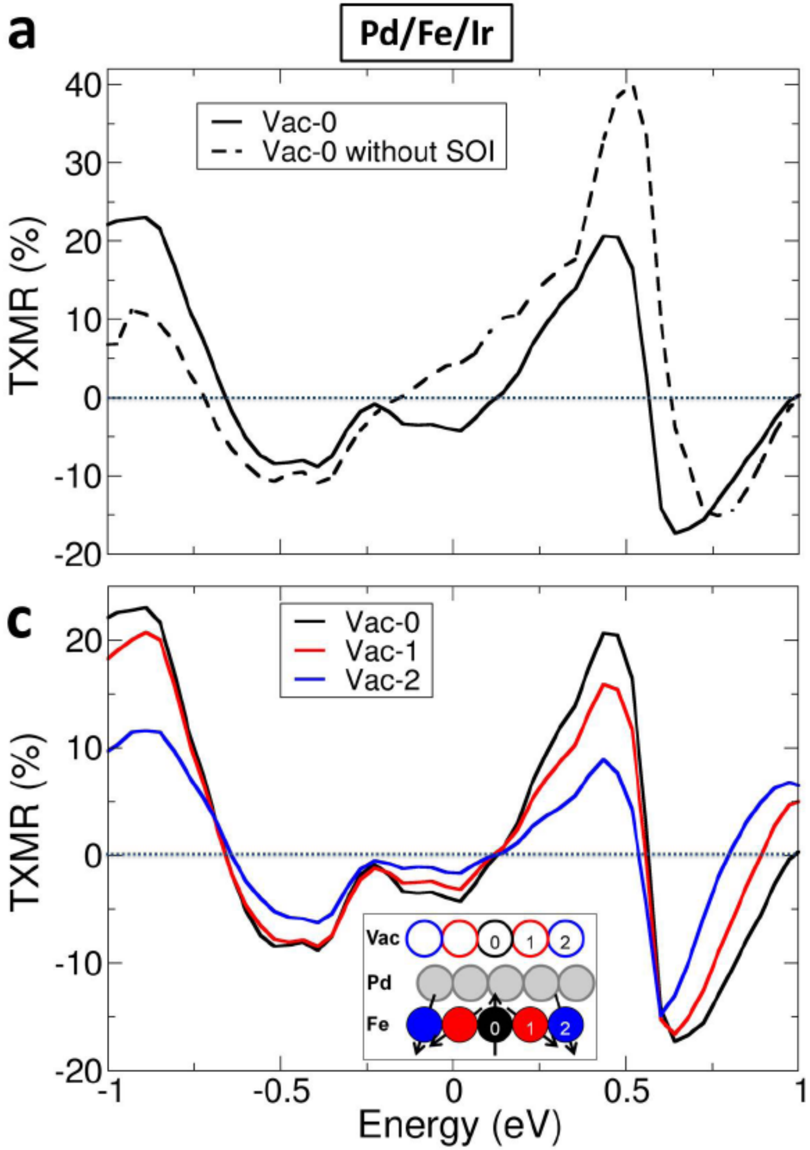
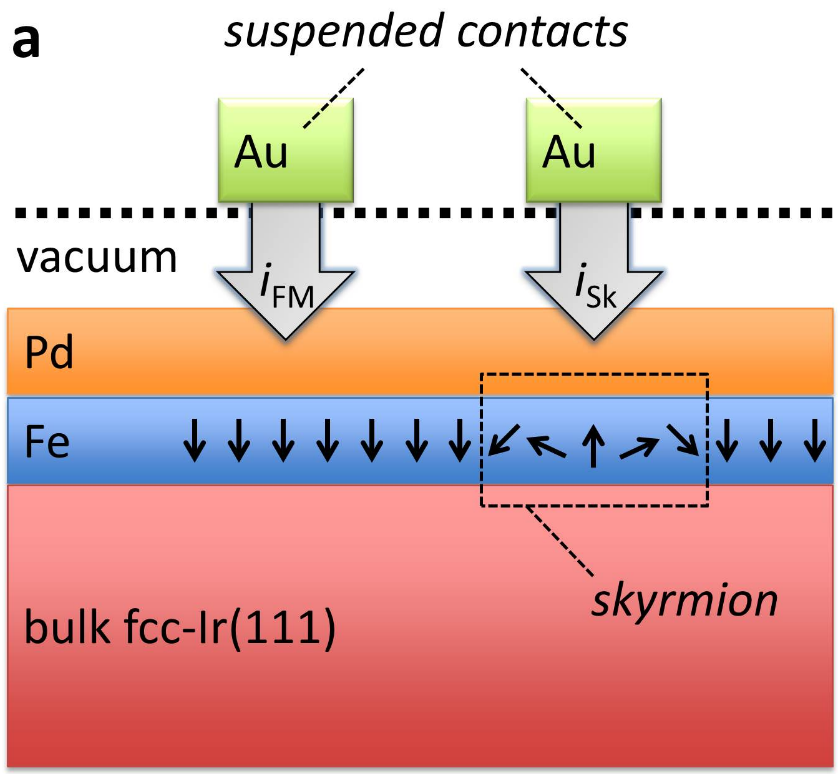
Spin-mixing magnetoresistance

*





$$\mathrm{TXMR}(\mathbf{r}) = \frac{\mathrm{LDOS}_{\mathrm{FM}}^{\mathrm{vac}} - \mathrm{LDOS}_{\{\mathbf{S}\}}^{\mathrm{vac}}}{\mathrm{LDOS}_{\mathrm{FM}}^{\mathrm{vac}}} \times 100\%$$

All-electric detection

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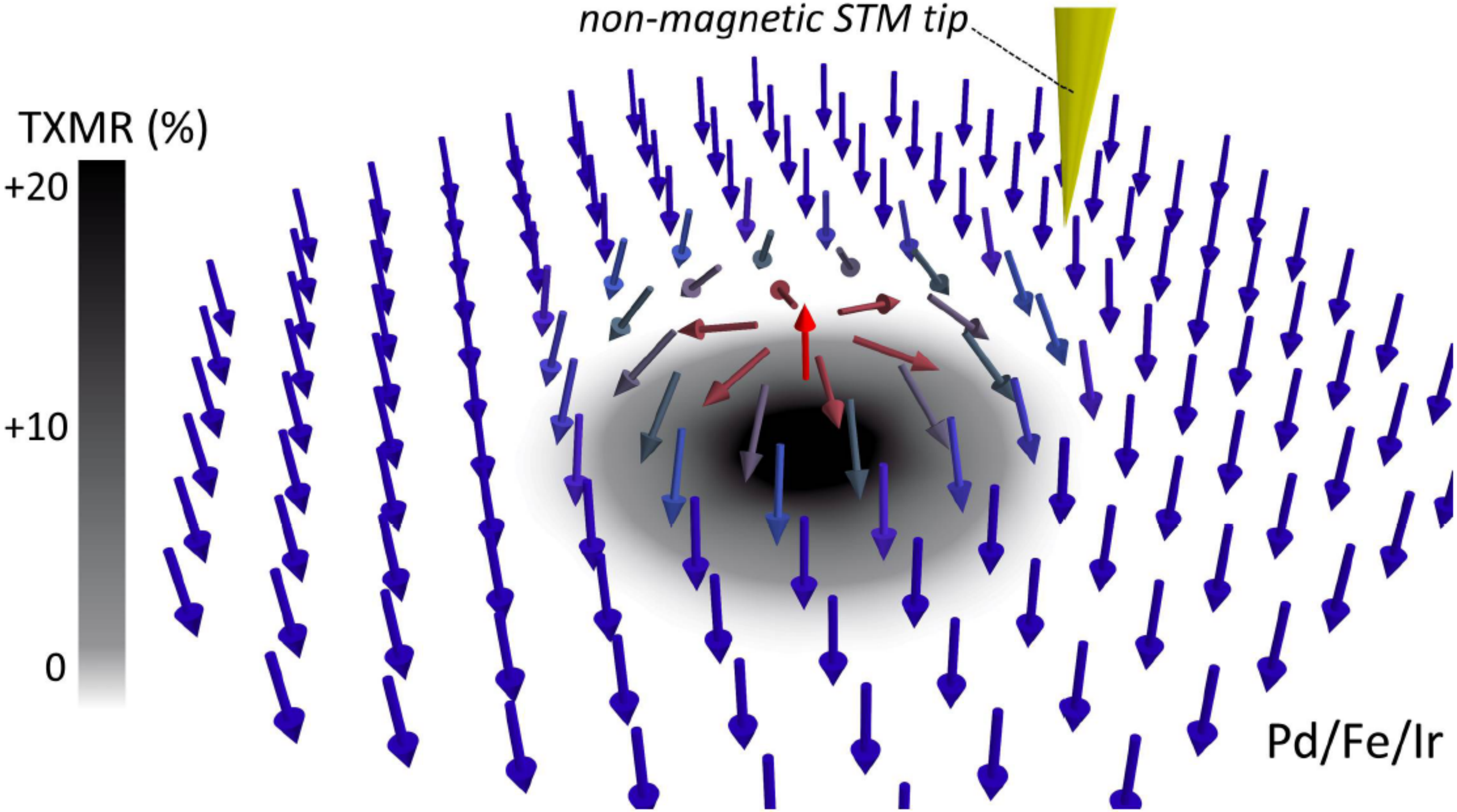

D. Crum, M. Bouhassoune, J. Bouaziz, B. Schwelinghaus, S. Blügel, S. Lounis , Nature Comm. **6**, 8541 (2015)

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Future Outlook

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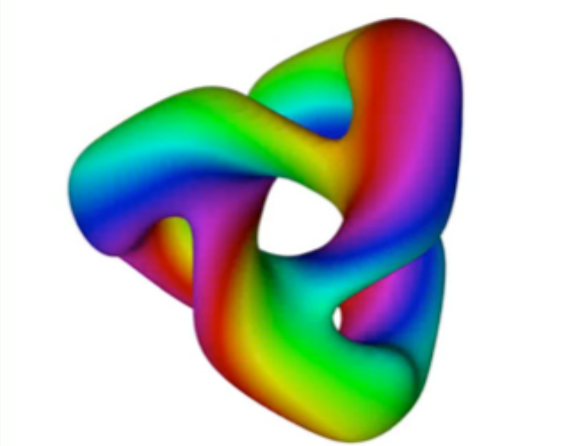

From Nicola Marzari

- **Spinorbitronics**
  - Spintextures for neuro-inspired computing
  - Ultrafast and antiferromagnetic spintronics
  - 3D nanoscale magnetic textures & dynamics
- **Quantum materials**
  - Emergent complex phase space topology
  - Topological superconductors for QC
- **Materials discovery lab – Computer**
  - Cognitive Materials and Functionality Discovery

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Quantum Phenomena for the New Information Age

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Thanks !

Fleur
www.flapw.de

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Paul Baumeister
Dirk Pleiter

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Jens Bröder
Daniel Wortmann

MAGic Sky

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