Computational Topological Spintronics: from Hall effects to chiral skyrmions

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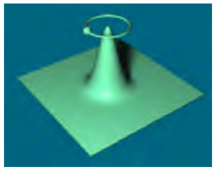
Jülich: Topological Nanoelectronics Group



Frank Freimuth
Jürgen Weischenberg
Timo Schena
Hongbin Zhang
Gustav Bihlmayer
Vikas Kashid
Phivos Mavropoulos
Bernd Zimmermann
Guillaume Geranton
Stefan Blügel

Köln: *Robert Bamler*
Achim Rosch

Berlin, Göttingen:
T. Kampfrath's group
M. Münzenberg's group

Nijmegen:
A. V. Kimel's group

Prague:
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Mainz: *Jacob Gayles*
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Hamburg:
R. Wiesendanger's group

Garching:
Ch. Pfleiderer's group

Leeds:
Ch. Marrows' group

Funding agencies:

Helmholtz Gemeinschaft

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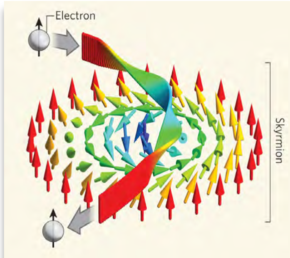
To name just a few...

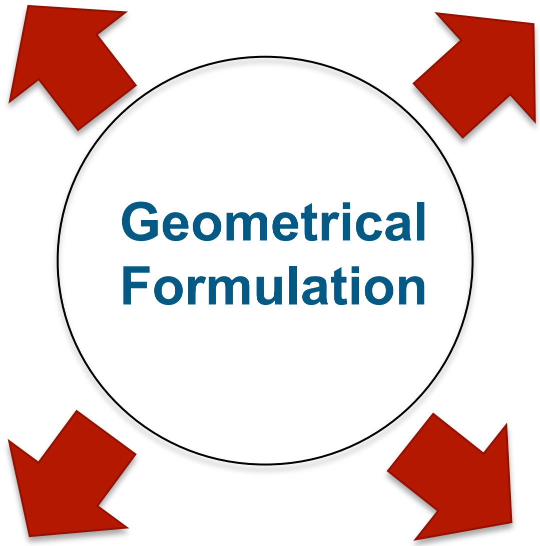


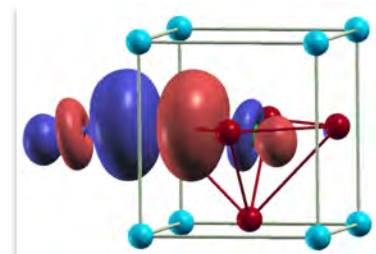
Topological Hall effect
Skyrmions

Pumping effects

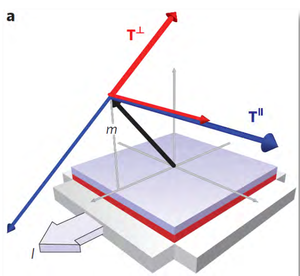
Electric Polarization

Dzyaloshinskii-Moriya interaction





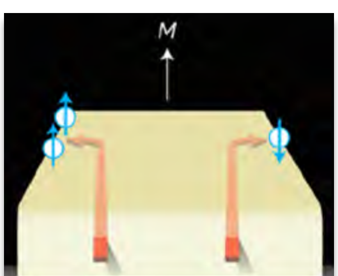
Spin-Orbit Torque



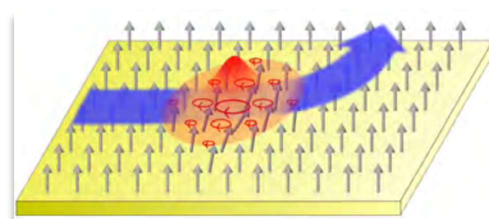
Thermal Hall effect

Gilbert damping

Magnon Hall effect
Exchange interactions



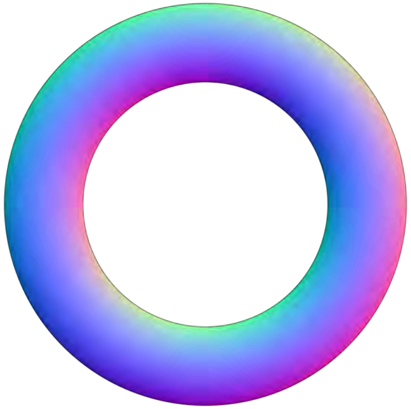
Anomalous Hall effect
Orbital Magnetization
Spin Hall effect
Quantized Hall effects
Topological Insulators

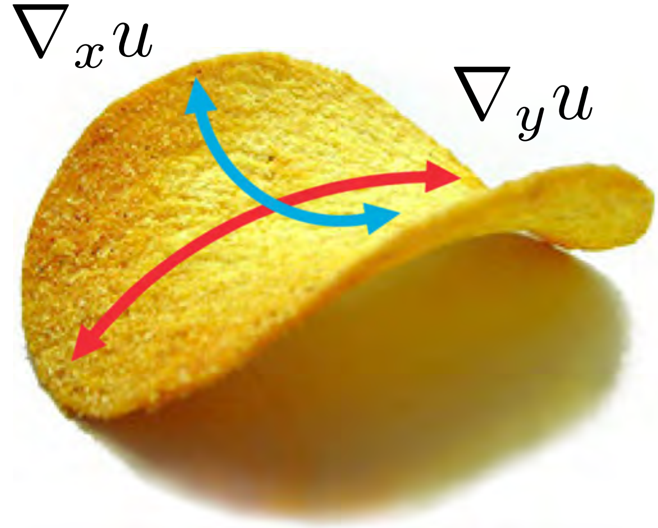


Outline

- Geometry and Solids
- Hall effects in metals
- Skyrmions
- Dzyaloshinskii-Moriya Interaction
- Spin-Orbit Torque

Geometry and Solids





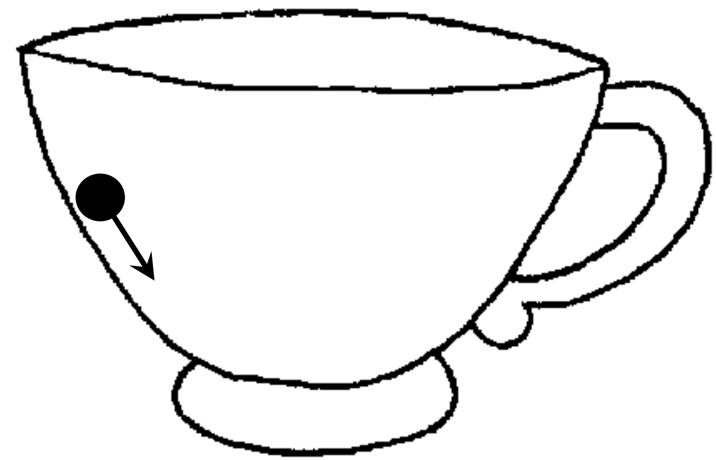
Berry Curvature characterizes how the electrons are glued together

Berry curvature = magnetic field

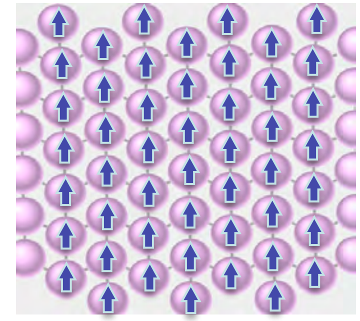
Picked phase = Berry phase

Aharonov-Bohm effect

Curvature determines electron dynamics!



Berry curvature in solids



Ferromagnet with spin-orbit interaction:

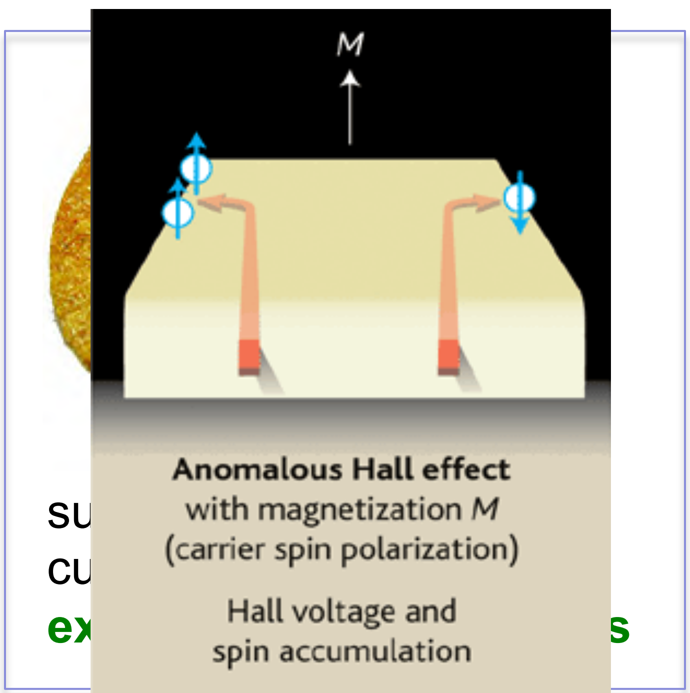
$$\mathbf{\Omega} = -2\mathrm{Im}\,\langle \nabla_x u | \nabla_y u \rangle$$

k_x k_y

push here (e.g. E-field)

Anomalous Hall effect

induce motion here!



Semiclassical picture (1950s – 2000s)

velocity $= \nabla_{\mathbf{k}}\varepsilon - \mathbf{E} \times \mathbf{\Omega}$

Hall conductance:

$$\sigma^H = \frac{1}{2\pi} \int_{\mathrm{k-space}} \mathbf{\Omega}\, d^2k$$

Metals

Berry curvature can be very complex in metals

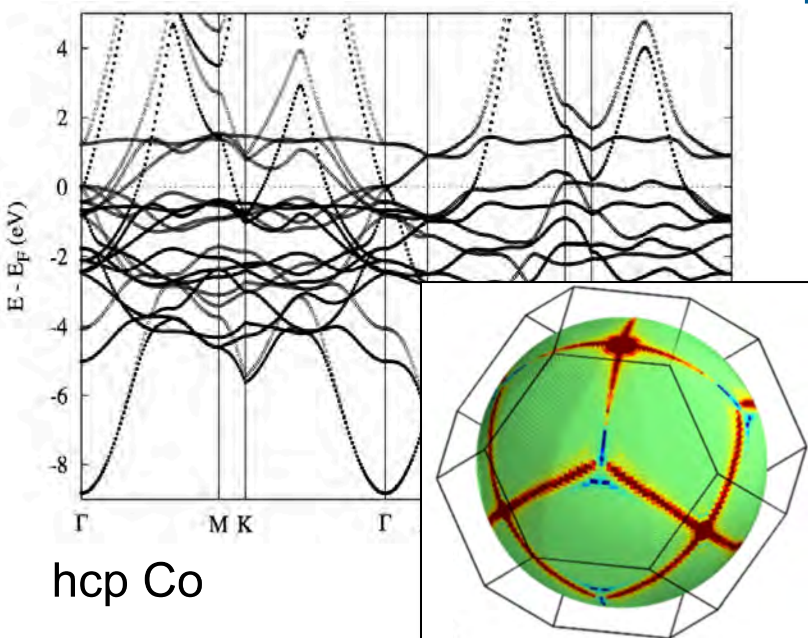
Motivates the use of complex computational techniques

➔ **density functional theory (DFT)**

Topological origin of spin and anomalous Hall effects

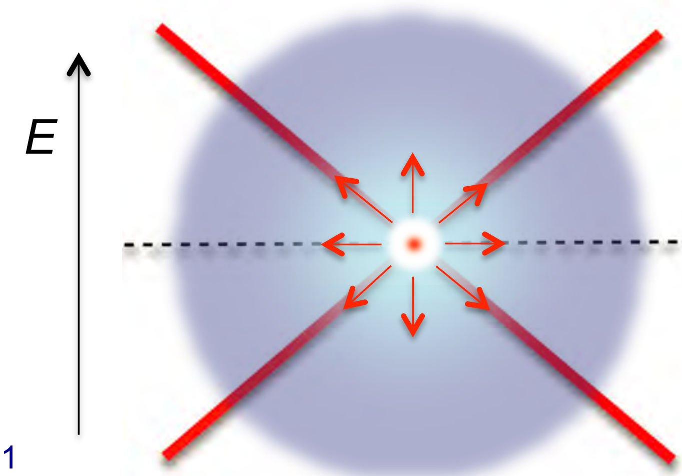
➔ **studied from DFT for one decade**

Dirac monopoles at band degeneracies



hcp Co

fcc Ni



Weischenberg, Freimuth, Sinova, Blügel, Mokrousov, PRL 2011

Beyond Berry curvature

Kubo linear response formalism

$$\sigma^{\mathrm{I}}_{\alpha\beta} = \frac{1}{4\pi V}\,\mathrm{Tr}\left[v^\alpha G^R(E_F) v^\beta G^A(E_F) - (\alpha \leftrightarrow \beta)\right]$$

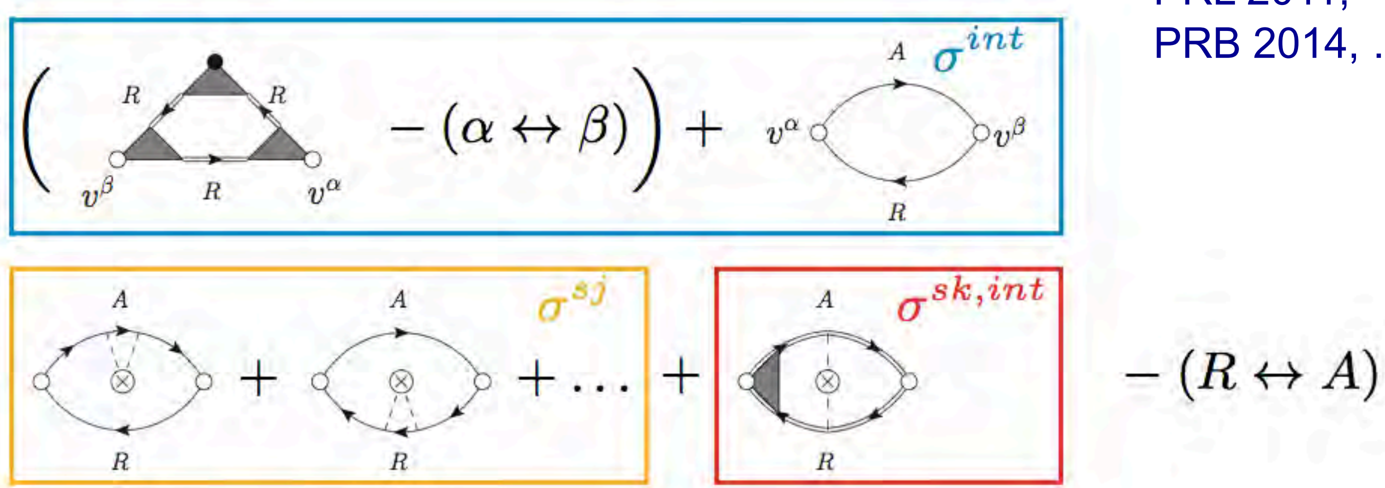
$$\sigma^{\mathrm{II}}_{\alpha\beta} = \frac{1}{2\pi V}\int_{-\infty}^{E_F} \mathrm{d}E\,\Re\left\{\mathrm{Tr}\left[v^\alpha G^R(E)^2 v^\beta G^R(E) - (\alpha \leftrightarrow \beta)\right]\right\}$$

Weischenberg, Czaja, Freimuth, Blügel, Sinova, Mokrousov, PRL 2011, PRB 2014, …

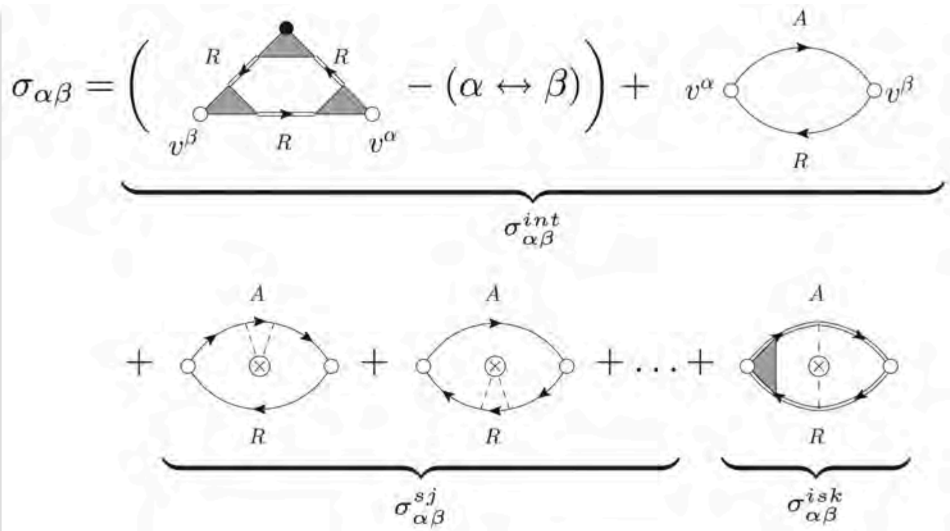
Disorder potential: $\hat{V} = U \sum_i \delta(\hat{\mathbf{r}} - \mathbf{R}_i)$

All scattering-independent contributions to the AHE:

→ $\sigma_{\alpha\beta} =$



Scattering-independent Hall effects

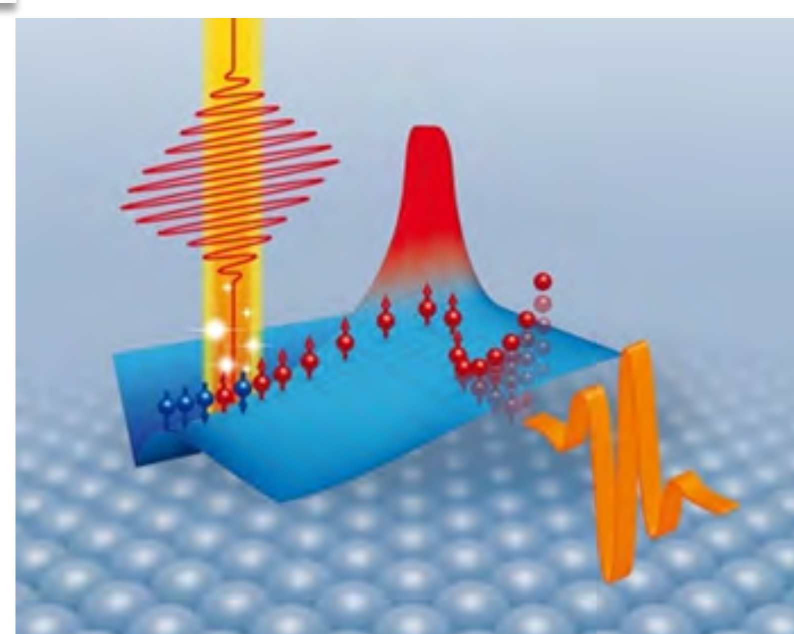


All scattering-independent contributions can be identified

Dominant for moderately dirty metals

Nature Nanotech. **8**, 256 ‘13

True not only for static, but also high-frequency electric fields



Weischenberg, Czaja, Freimuth, Sinova,
Kampfrath’s group, Münzenberg’s group,
Blügel, Zimmermann, Long, Mavropoulos,
Mokrousov,
PRLs, PRBs, Nature Nano.: 2009 and on...

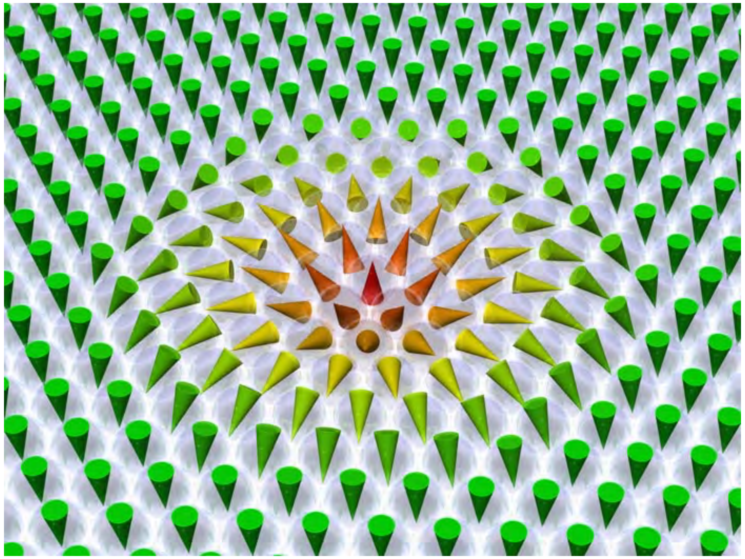
Chiral magnetic skyrmions

T. H. R. Skyrme, Nucl. Phys. 31, 556 (1962)

Skyrmions: soliton-like solutions for baryons in non-linear sigma model

Tony Skyrme

Chiral magnetic skyrmions



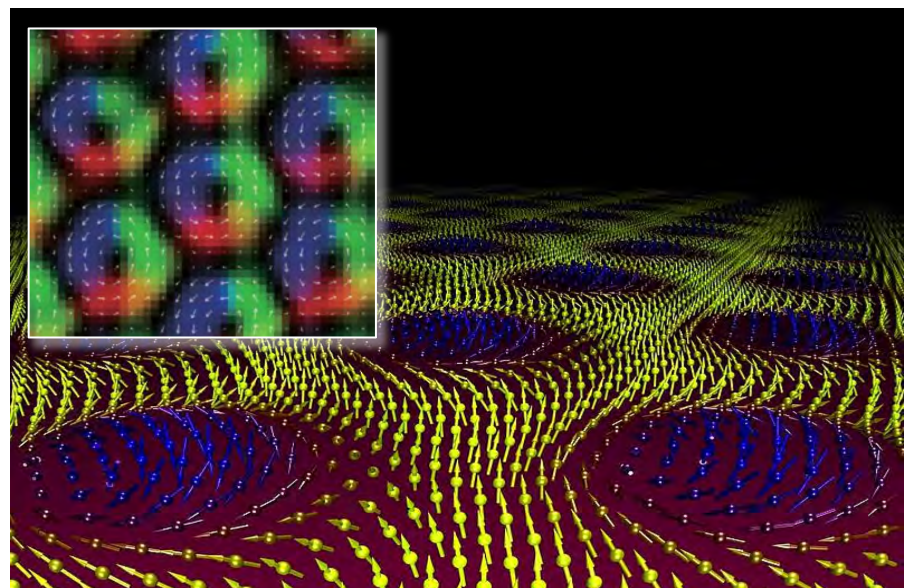
T. H. R. Skyrme, Nucl. Phys. 31, 556 (1962)

Observed in magnetic systems:

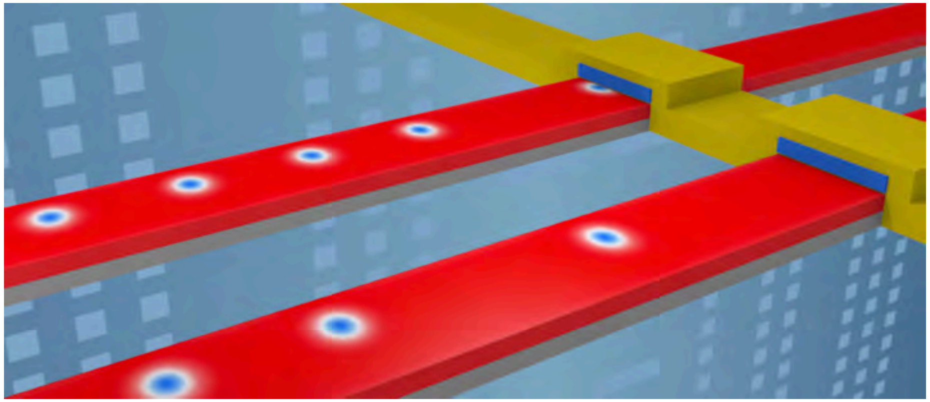
2D, 3D, metals, insulators

C. Pfleiderer, A. Rosch, Nature **465**, 880 (2010)
T. Schultz et al., Nature Physics **8**, 301 (2012)...
Tokura & Nagaosa Nat. Nano. **8**, 899 (2013)
Schulzet al. Nat. Phys. **8**, 301 (2012)
Fert et al. Nature Nano. **8**, 152 (2013)
Iwasaki et al., Nat. Comms., **4**, 1463 (2013)

Tony Skyrme



Chiral magnetic skyrmions



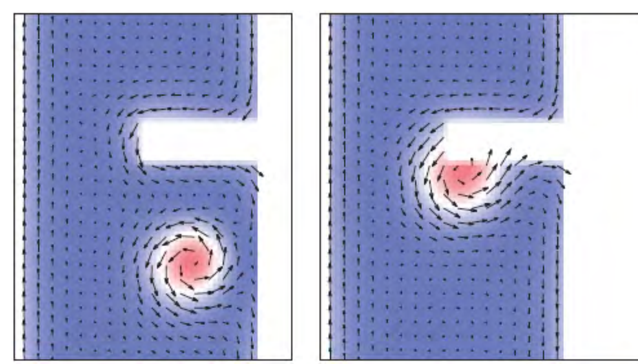
Albert Fert, Vincent Cross and João Sampaio, Nature Nanotechnology **8**, 152 (2013)

Many things are believed to do with:

non-trivial topology of skyrmions

Fascinating properties for spintronics:

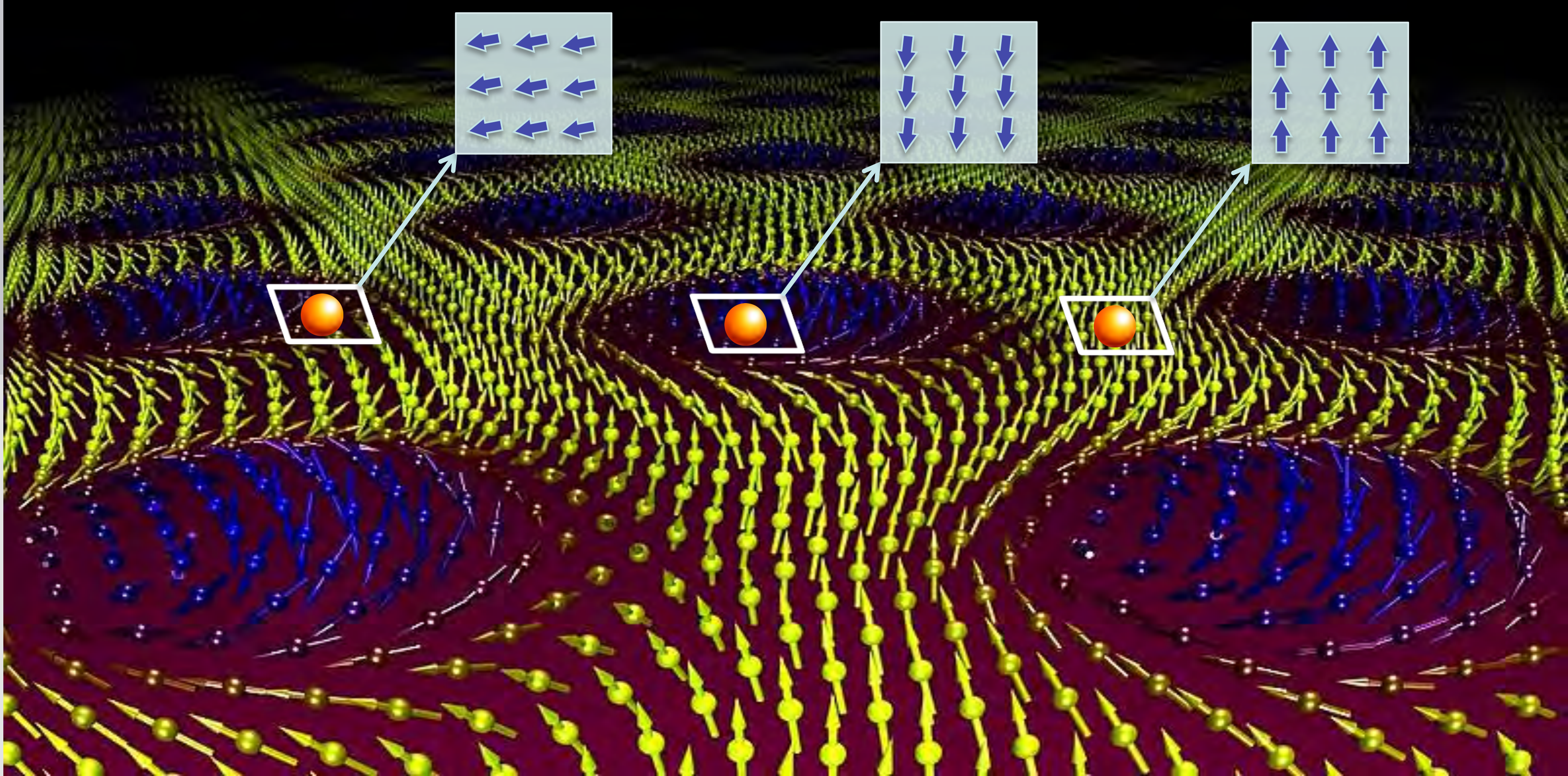
- low currents to move around
- suppressed scattering at defects
- various “skyrmion” transport effects



„Classical“ skyrmions: very large objects

MnSi
B_{20} compounds
etc….

Simplify the problem



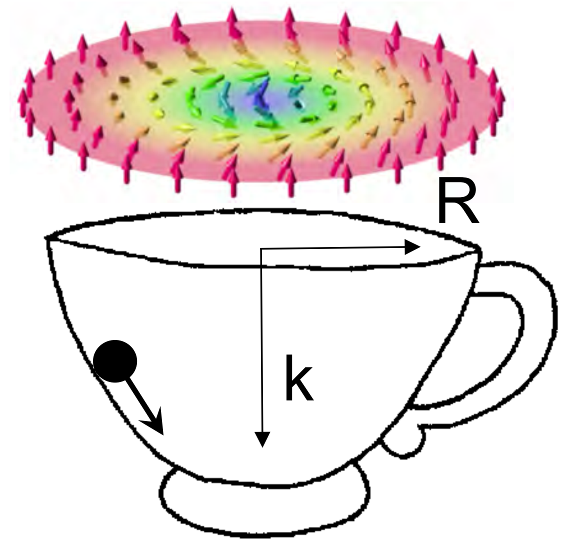
Electron dynamics in skyrmions

Equations of adiabatic electron dynamics:

Freimuth, Bamler, Mokrousov, Rosch, PRB 2013

$$H = H(\mathbf{k}, \mathbf{R})$$

$$(\mathbf{\Omega} - I)\dot{\mathbf{x}} = \frac{\partial \varepsilon}{\partial \mathbf{x}}, \quad \mathbf{x} = (\mathbf{R}, \mathbf{k})$$



"skyrmionic" cup

Berry curvature tensor:

k-space Berry curvature ← $\mathbf{\Omega_k}$ due to **k**-dependence of the states

real-space Berry curvature ← $\mathbf{\Omega_R}$ due to **R**-dependence of the states

mixed Berry curvature ← $\mathbf{\Omega_{kR}}$ due to states' **k**- and **R**-dependence

Electron dynamics in skyrmions

Equations of adiabatic electron dynamics:

Freimuth, Bamler, Mokrousov, Rosch, PRB 2013

$$H = H(\mathbf{k}, \mathbf{R})$$

How valid is this picture for skyrmions?

What can we extract from it?

"skyrmionic" cup

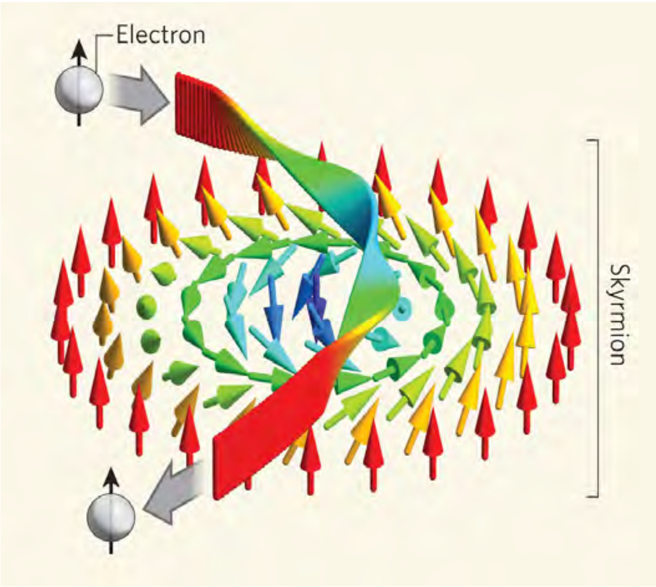
Berry curvature tensor:

k-space Berry curvature ← $\mathbf{\Omega_k}$ due to **k**-dependence of the states

real-space Berry curvature ← $\mathbf{\Omega_R}$ due to **R**-dependence of the states

mixed Berry curvature ← $\mathbf{\Omega_{kR}}$ due to states' **k**- and **R**-dependence

Real-space Berry curvature



Real space Berry curvature:

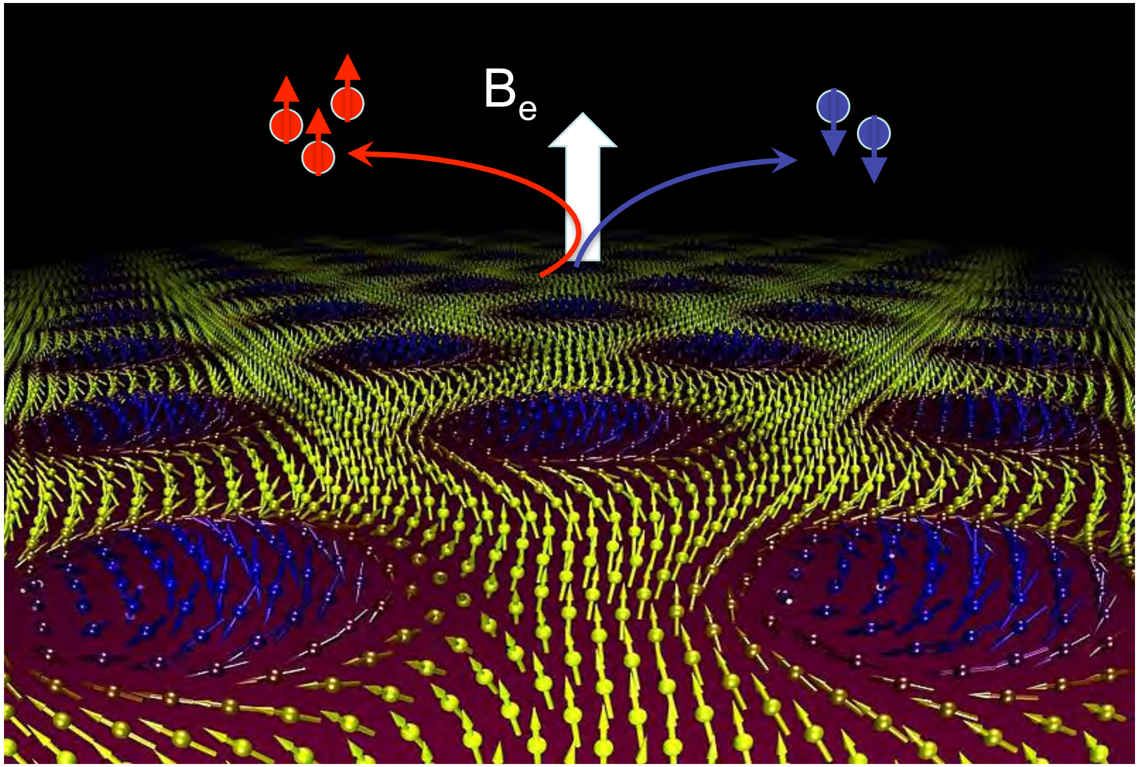
$$\Omega_{\mathbf{R}}^{ij,\sigma} = -2\mathrm{Im}\,\langle \partial_{\mathbf{R}_\mathrm{i}} \psi_\sigma(\mathbf{R}) | \partial_{\mathbf{R}_\mathrm{j}} \psi_\sigma(\mathbf{R}) \rangle$$

$$\Omega_{\mathbf{R}}^{ij,\sigma} = \sigma\, \mathbf{n} \cdot \left(\partial_{\mathbf{R}_i} \mathbf{n} \times \partial_{\mathbf{R}_j} \mathbf{n} \right) /2$$

emergent magnetic field

"topological charge"
"quantization"
"topological protection"

Emergent field and Hall effects



Neubauer *et al.* PRL 2009
Bruno *et al.* PRL 2004

MnSi:
emergent B-field ≈ 13 T

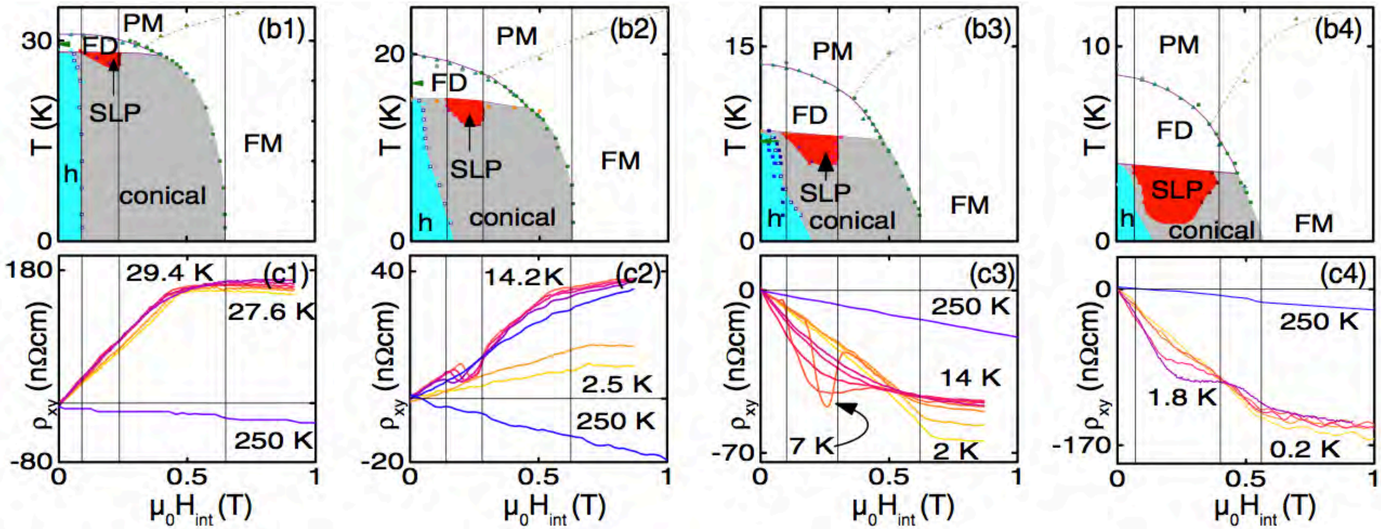
can reach
gigantic values

$\Omega^{\sigma}_{\mathbf{R}}$ produces Lorentz force opposite for opposite spin

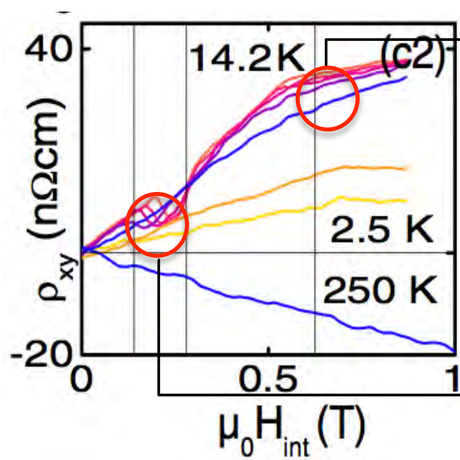
$$\downarrow$$

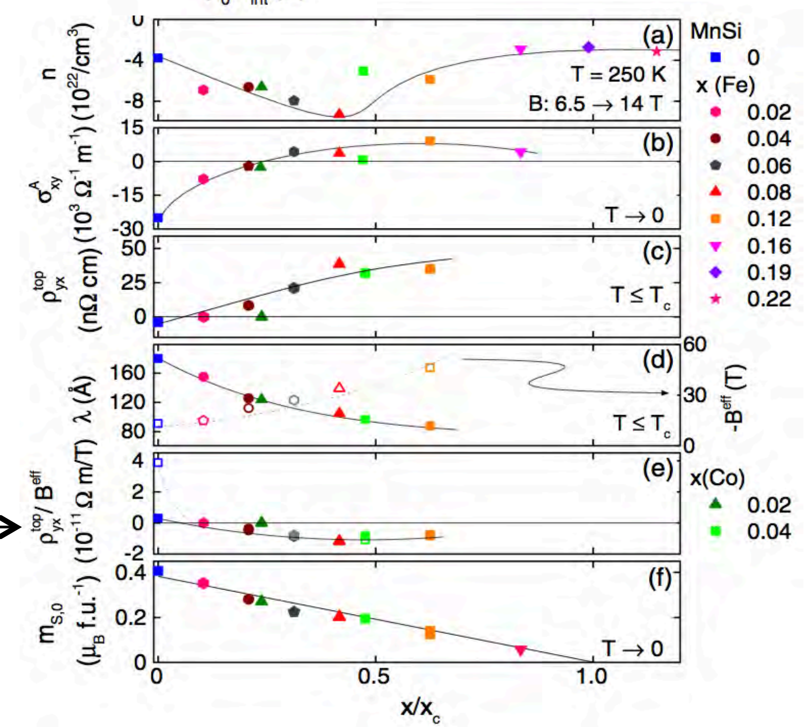
Topological Hall Effect (THE):
primary manifestation of skyrmionic topology

$Mn_{1-x}Fe_xSi$ alloys



Experiments: Chris Pfleiderer's group

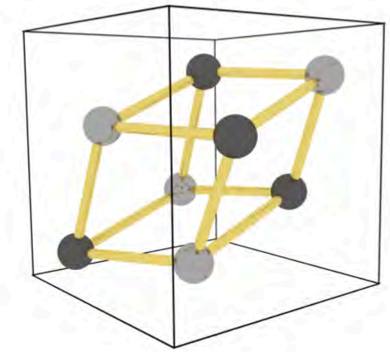


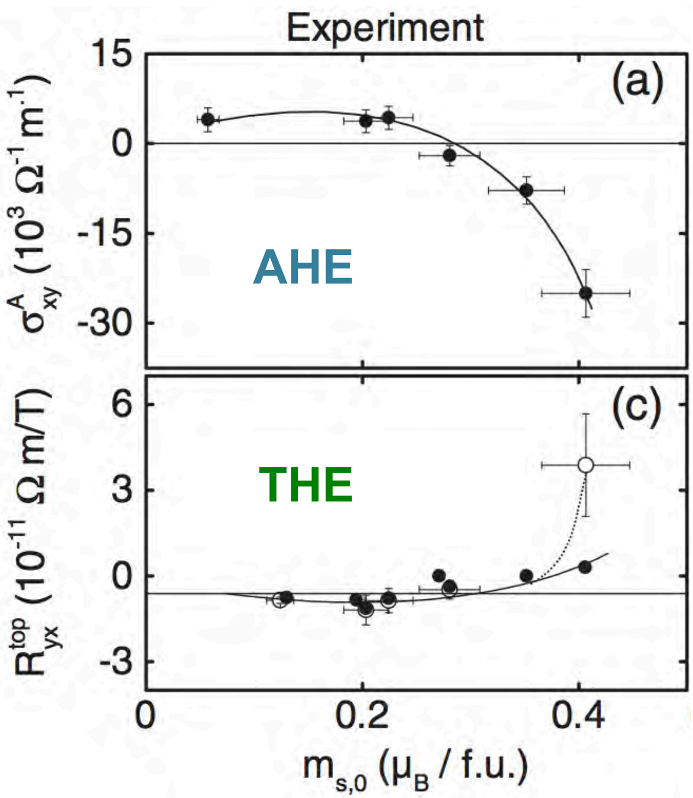


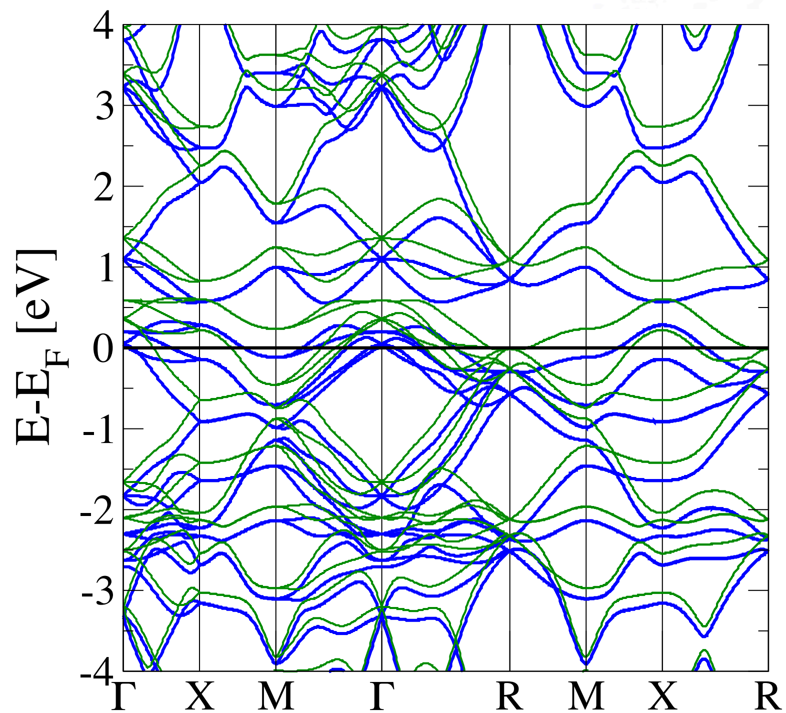
Franz, Freimuth, …, Blügel, Rosch, Mokrousov, Pfleiderer, PRL **112**, 186601 (2014)

AHE versus THE in $Mn_{1-x}Fe_xSi$ alloys

- Tuning Mn spin moment to fit experiment
- Alloying treated within virtual crystal approximation





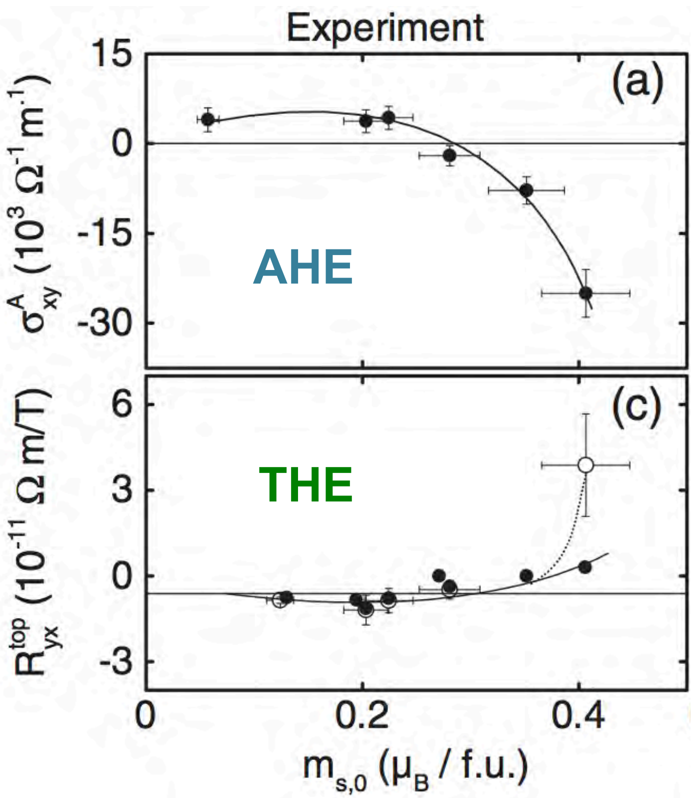


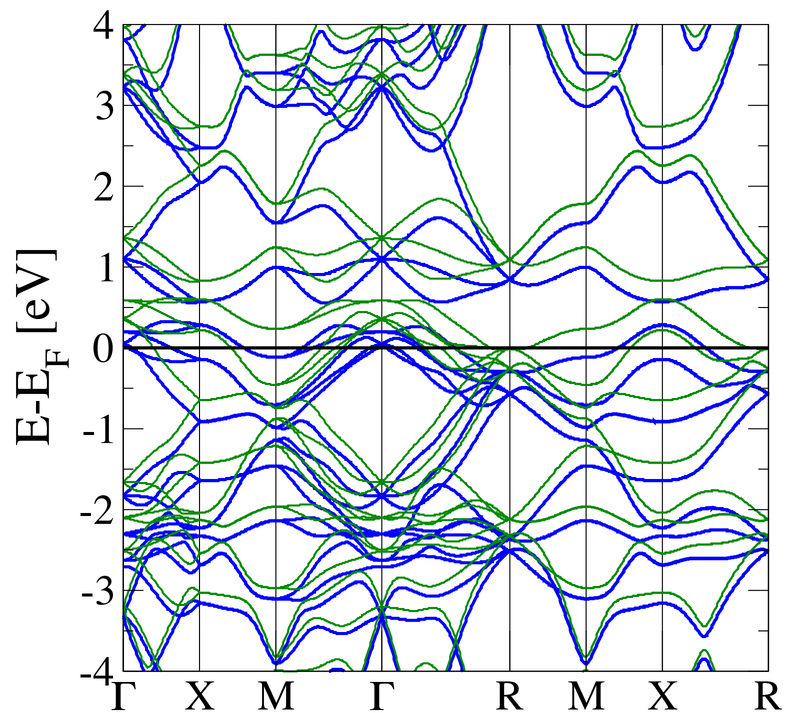
Franz, Freimuth, …, Blügel, Rosch, Mokrousov, Pfleiderer, PRL **112**, 186601 (2014)

AHE versus THE in $Mn_{1-x}Fe_xSi$ alloys

k-space Berry curvature AHE
Boltzmann theory for OHE

$$\rho_{yx}^{\mathrm{top}}(B^{\mathrm{eff}}) = \frac{\sigma_{xy}^{\mathrm{OHE},\uparrow}(B^{\mathrm{eff}}) - \sigma_{xy}^{\mathrm{OHE},\downarrow}(B^{\mathrm{eff}})}{(\sigma_{xx}^{\uparrow} + \sigma_{xx}^{\downarrow})^2} = R_{yx}^{\mathrm{top}} \cdot B_e$$





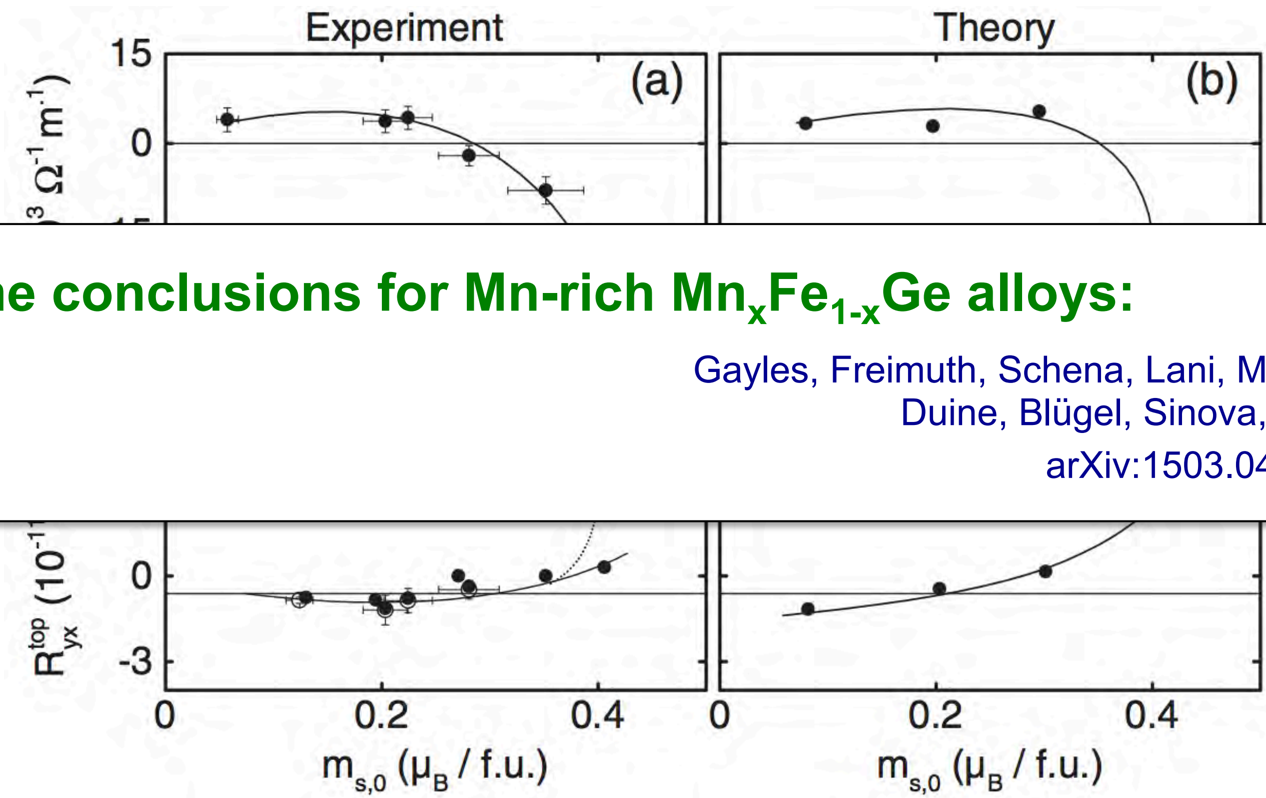
Franz, Freimuth, …, Blügel, Rosch, Mokrousov, Pfleiderer, PRL **112**, 186601 (2014)

AHE versus THE in $Mn_{1-x}Fe_xSi$ alloys

Excellent agreement between theory and experiment!

→ skyrmionic Berry phase picture is relevant

→ *ab initio* is precise enough to describe it



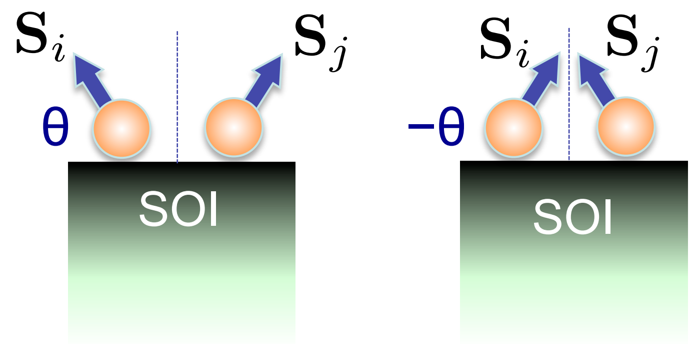
Same conclusions for Mn-rich $Mn_xFe_{1-x}Ge$ alloys:

Gayles, Freimuth, Schena, Lani, Mavropoulos, Duine, Blügel, Sinova, Mokrousov
arXiv:1503.04842 (2015)

Franz, Freimuth, …, Blügel, Rosch, Mokrousov, Pfleiderer, PRL **112**, 186601 (2014)

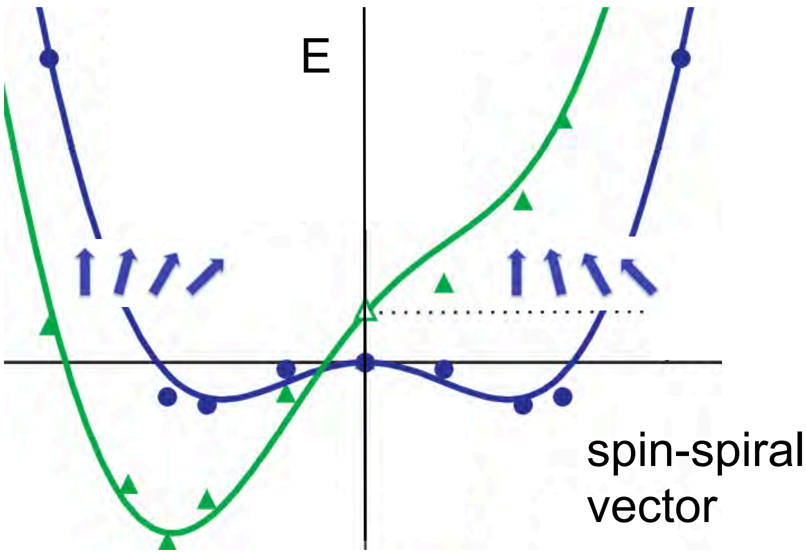
Dzyaloshinskii-Moriya interaction

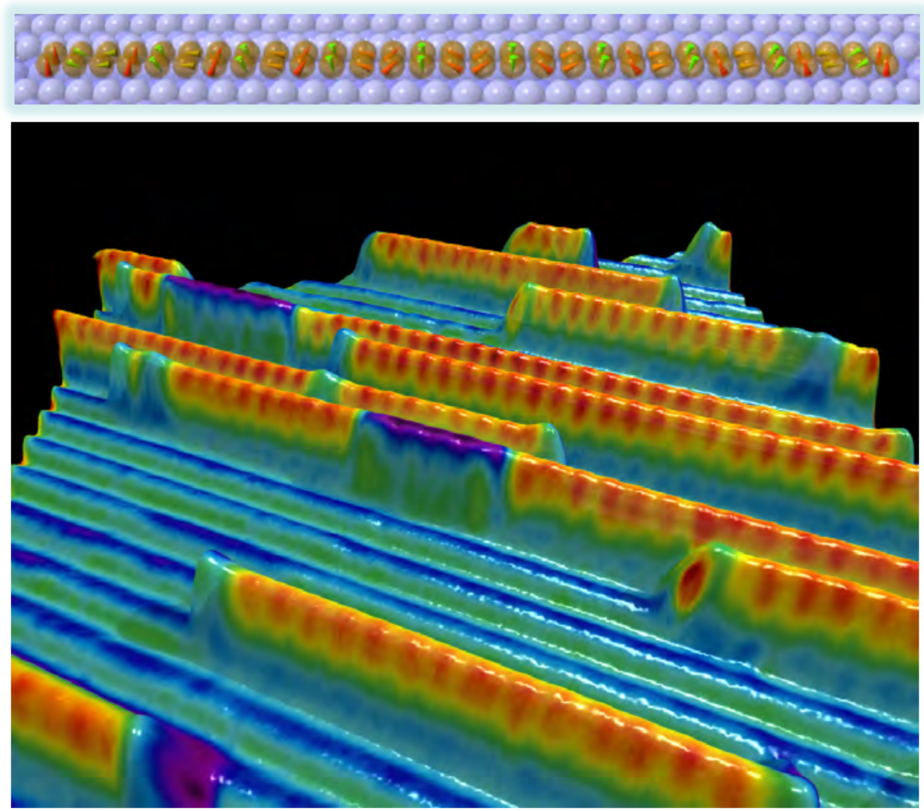
$$\Delta E \sim \mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$



Suggestion goes back to the 50s…

Menzel, Mokrousov, Wieser, Bickel, Vedmedenko, Blügel, Heinze, von Bergmann, Kubetzka, Wiesendanger, PRL **108**, 197204 (2012)

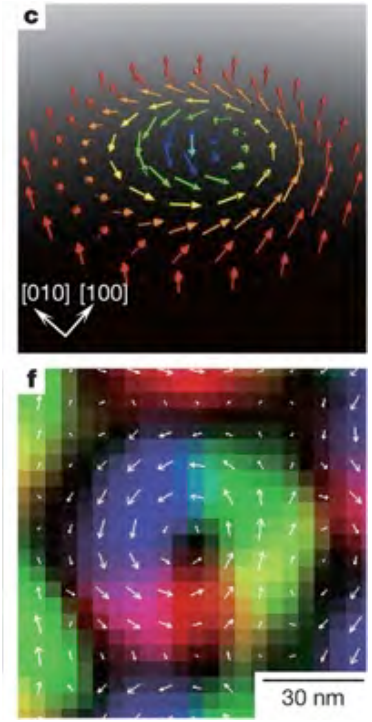




Fe bi-atomic chains on Ir(001) substrate

Dzyaloshinskii-Moriya interaction (DMI)

skyrmions



Nature **465**, 901 (2010)
Nat. Phys. **7**, 713 (2011)

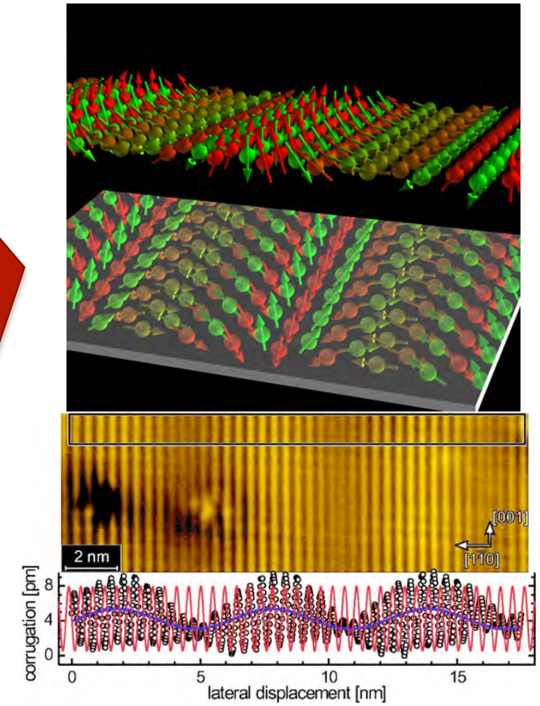
magnetism

spin-orbit coupling

inversion asymmetry

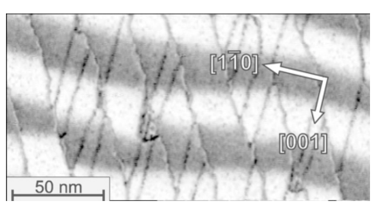
Dzyaloshinskii-Moriya interaction

chiral spin spirals



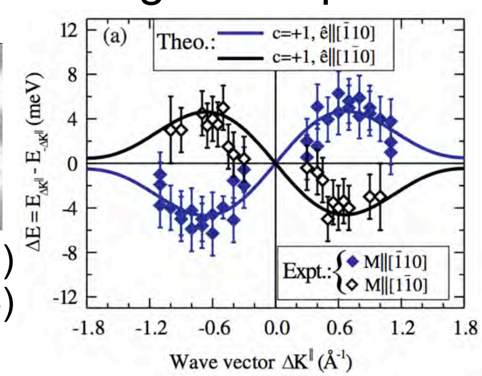
Nature **447**, 190 (2007)

chiral domain walls



PRL **88**, 057201 (2002)
PRB **78**, 140403 (2008)

magnon dispersion



PRL **102**, 207204 (2009)
PRL **104**, 137203 (2010)

DMI as a Berry phase theory

Response of free energy to a perturbation:

$$\delta F(\mathbf{R}) = D_{ij}(\mathbf{R})\,\hat{\mathbf{e}}_i \cdot \left(\hat{\mathbf{n}} \times \partial_{R_j} \hat{\mathbf{n}}\right)$$

Spiralization:

$$D_{ij}(\mathbf{R}) = \frac{1}{(2\pi)^d} \sum_n \int d\mathbf{k}\, f_{\mathbf{k}n} \left[A^{ij}_{n\mathbf{k}\mathbf{R}} - (\varepsilon_{n\mathbf{k}\mathbf{R}} - \mu) B^{ij}_{n\mathbf{k}\mathbf{R}}\right]$$

"localized" contribution

$\Omega_{\mathbf{kR}}$ Berry curvature in real and reciprocal (***k***,***R***)-space

		D_{yx} (meV Å/u.c.)
Co/Pt(111)	$\hat{\mathbf{n}} = \hat{\mathbf{e}}_z$	11.3
O/Co/Pt(111)	$\hat{\mathbf{n}} = \hat{\mathbf{e}}_z$	15.0
Al/Co/Pt(111)	$\hat{\mathbf{n}} = \hat{\mathbf{e}}_z$	20.7
	$\hat{\mathbf{n}} = \hat{\mathbf{e}}_x$	6.8

MnSi: $D = -4.1$ meV Å/u.c.

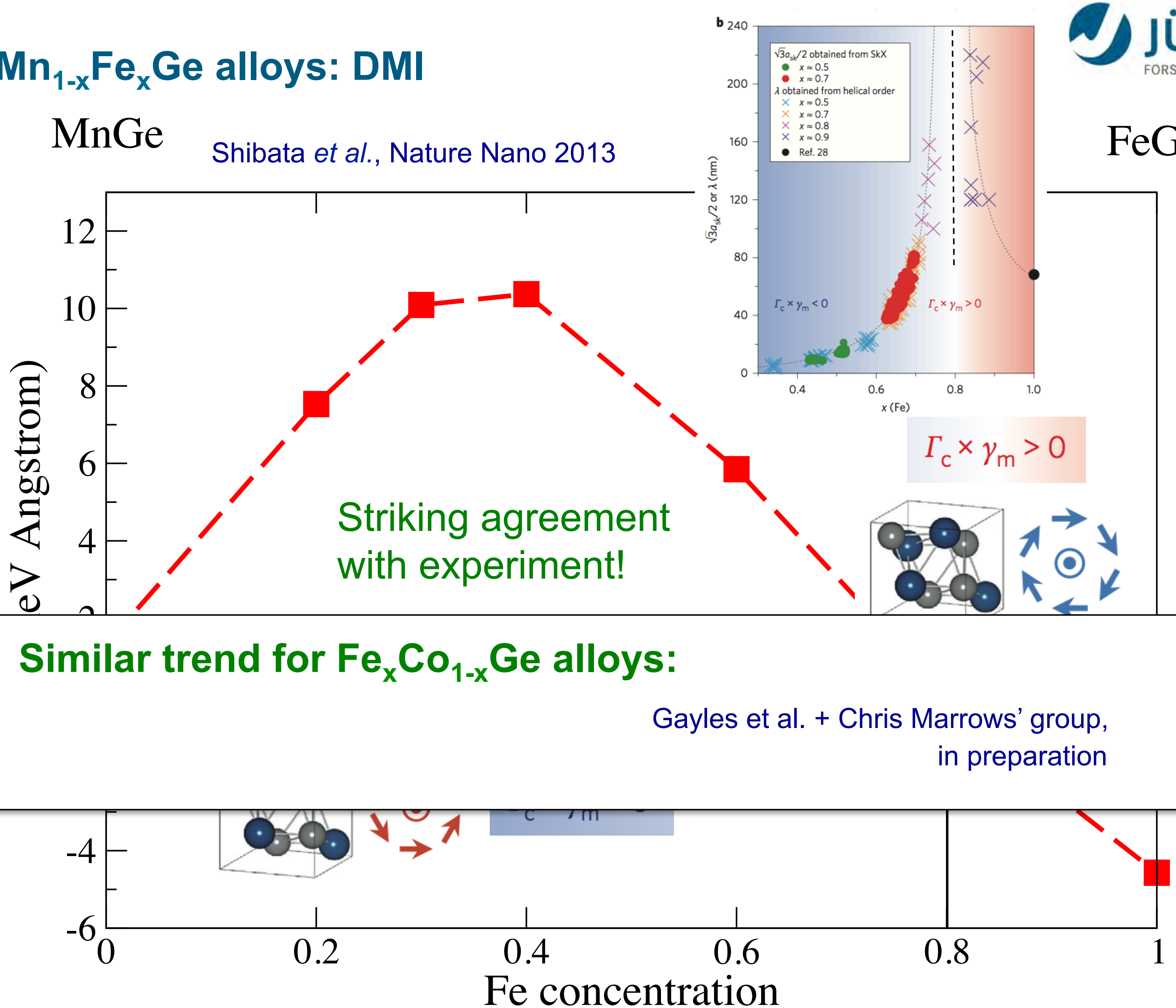
agrees quite well to experiment

Freimuth, Blügel, Mokrousov, JPCM **26**, 104202 (2014)

Freimuth, Blügel, Mokrousov, arxiv 2013 - 2014

Freimuth, Bamler, Mokrousov, Rosch PRB **88**, 214409 '13

$Mn_{1-x}Fe_xGe$ alloys: DMI



Similar trend for $Fe_xCo_{1-x}Ge$ alloys:

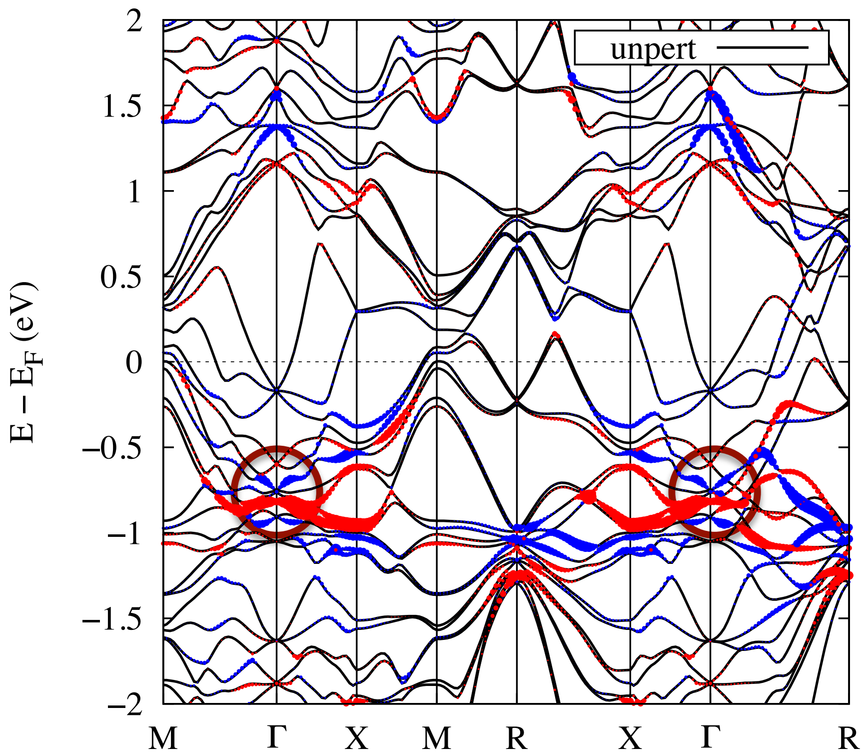
Gayles et al. + Chris Marrows' group, in preparation

Gayles, Freimuth, Schena, Lani, Mavropoulos, Duine, Blügel, Sinova, Mokrousov, arXiv:1503.04842 (2015)

Microscopics of the DMI

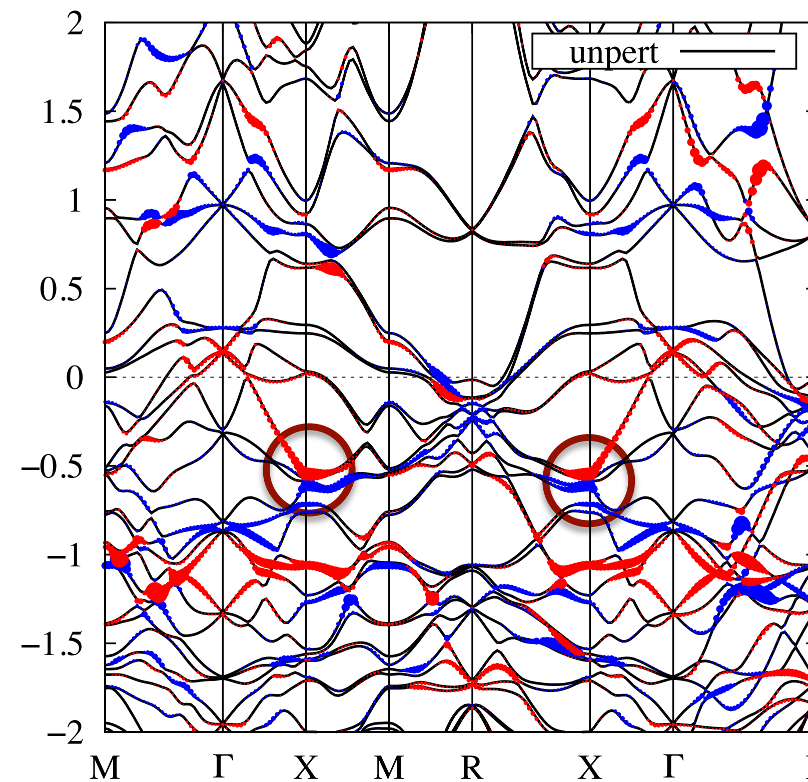
: SOC correction for a small spiral ***q***

➔ difficult to understand the trend



MnGe

FeGe

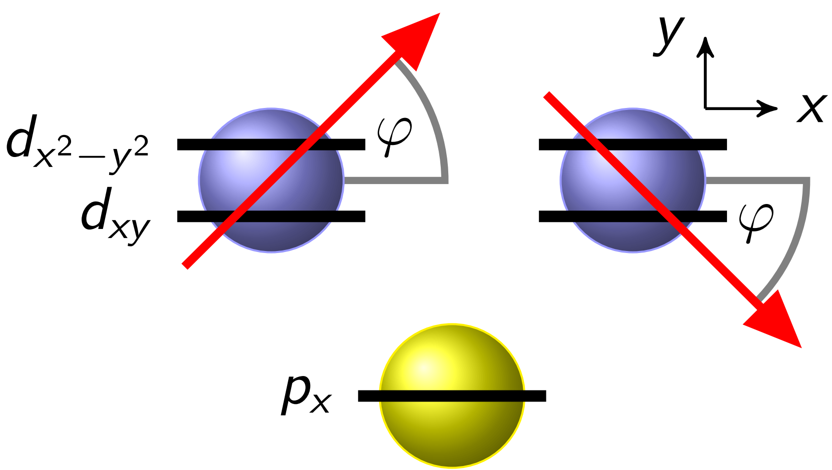


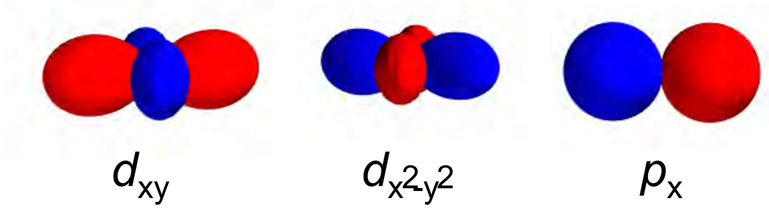
➔ driven by crossings of bands of different *spin* and *orbital* character

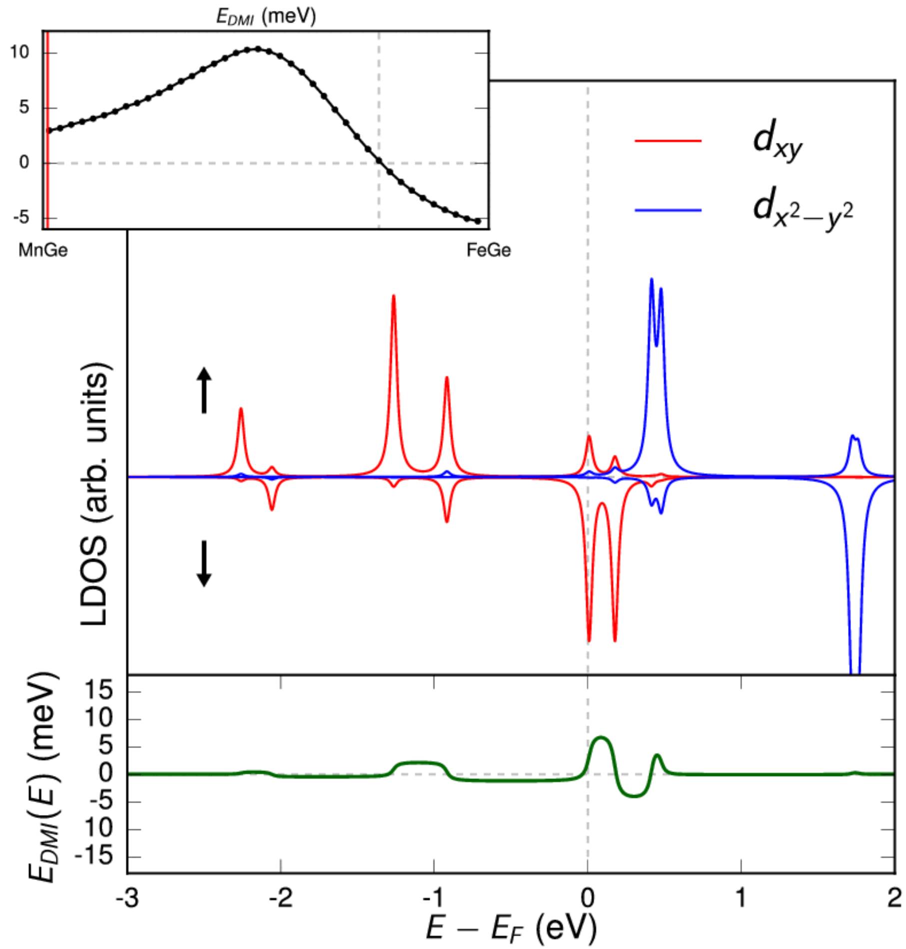
➔ spin-orbit on Ge not important

Gayles, Freimuth, Schena, Lani, Mavropoulos, Duine, Blügel, Sinova, Mokrousov, arXiv:1503.04842 (2015)

Simple model for DMI







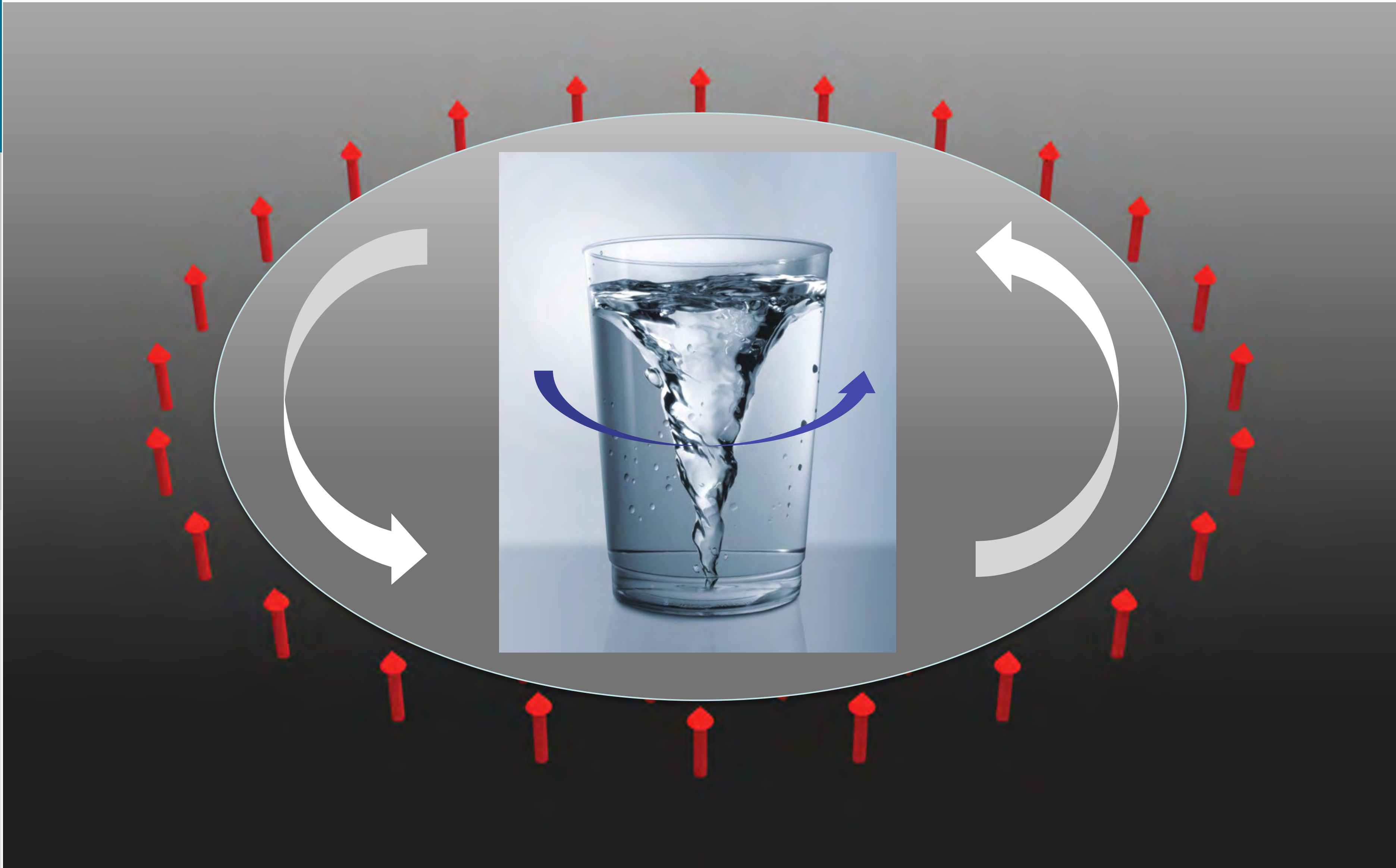
$$\delta\varepsilon_n = -\gamma \xi t_1 t_2 (-1)^i \sigma \sum_{\substack{n' (\neq n) \\ (i' \neq i)}} \frac{\tau\, \delta_{\sigma,-\sigma'} \tau'}{W_n^\sigma \left(\varepsilon_n^\sigma - \varepsilon_{n'}^{\sigma'}\right) W_{n'}^{\sigma'}}$$

Kashid, Schena, Zimmermann, Shah, Salunke, Mokrousov, Blügel, PRB **90**, 054412 (2014)

Gayles, Freimuth, Schena, Lani, Mavropoulos, Duine, Blügel, Sinova, Mokrousov, arXiv:1503.04842 (2015)

Berry curvature DMI

The electric field at the edge couples to the magnetization



Spin-Orbit Torque

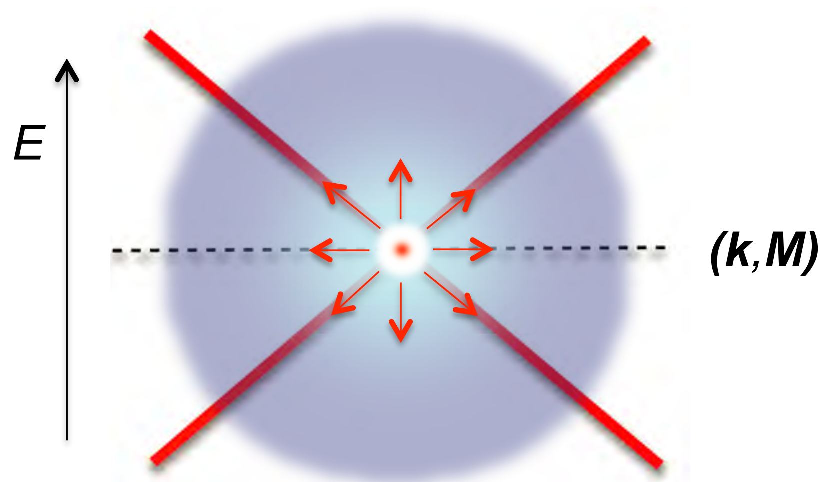
Spin-orbit torque = torque a current exerts on *collinear* magnetization

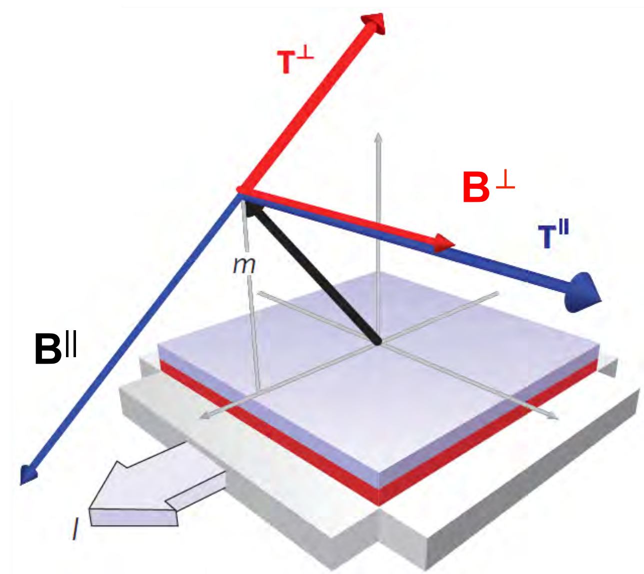
$$\mathbf{\Omega} = -2\mathrm{Im}\,\langle \nabla_x u | \nabla_y u \rangle$$

apply current (*k*)

change magnetization (*M*) !

Gambardella's group + Jülich, Nat. Nano. **8**, 587 '13
Freimuth, Geranton, Blügel, Mokrousov, PRBs, etc. '13 – '15
Kurebayashi, Sinova *et al.,* Nat. Nano. **9**, 211 '14





Beyond Berry curvature

Kubo linear response formalism for the **SOT**

$$t_{ij}^{\mathrm{I(a)}} = -\frac{e}{h}\int_{-\infty}^{\infty} d\mathcal{E}\frac{df(\mathcal{E})}{d\mathcal{E}} \quad \mathrm{Tr}\langle \mathcal{T}_i G^{\mathrm{R}}(\mathcal{E}) v_j G^{\mathrm{A}}(\mathcal{E})\rangle_{\mathrm{c}},$$

$$t_{ij}^{\mathrm{I(b)}} = \frac{e}{h}\int_{-\infty}^{\infty} d\mathcal{E}\frac{df(\mathcal{E})}{d\mathcal{E}} \mathrm{Re}\mathrm{Tr}\langle \mathcal{T}_i G^{\mathrm{R}}(\mathcal{E}) v_j G^{\mathrm{R}}(\mathcal{E})\rangle_{\mathrm{c}},$$

$$t_{ij}^{\mathrm{II}} = \frac{e}{h}\int_{-\infty}^{\infty} d\mathcal{E}\, f(\mathcal{E}) \quad \mathrm{Re}\mathrm{Tr}\langle \mathcal{T}_i G^{\mathrm{R}}(\mathcal{E}) v_j \frac{dG^{\mathrm{R}}(\mathcal{E})}{d\mathcal{E}} - \mathcal{T}_i \frac{dG^{\mathrm{R}}(\mathcal{E})}{d\mathcal{E}} v_j G^{\mathrm{R}}(\mathcal{E})\rangle_{\mathrm{c}},$$

Freimuth, Blügel, Mokrousov,
Phys. Rev. B 90, 174423 ‘14
JPCM **26**, 104202 ‘14

SOT and **DMI**:

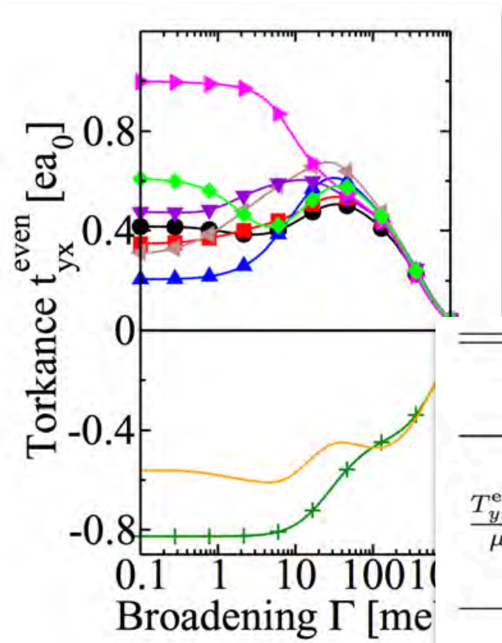
$$t_{ij} = \int \mathrm{d}\mathcal{E}\, \vartheta_{ij}(\mathcal{E})$$

$$D_{ij} = \frac{1}{eV}\int \mathrm{d}\mathcal{E}(\mathcal{E}-\mu)\vartheta_{ij}(\mathcal{E})$$

Disorder potential: $\hat{V} = U\sum_i \delta(\hat{\mathbf{r}} - \mathbf{R}_i)$ ....

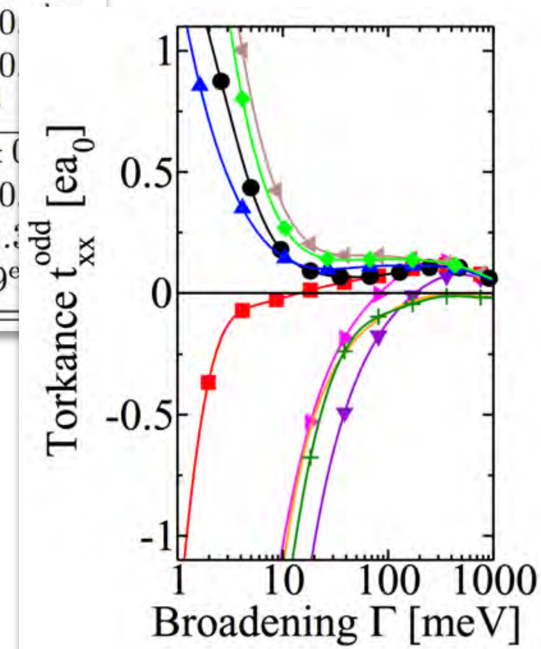
Spin-Orbit Torque

The formalism for the SOT can be worked out and confirmed by DFT



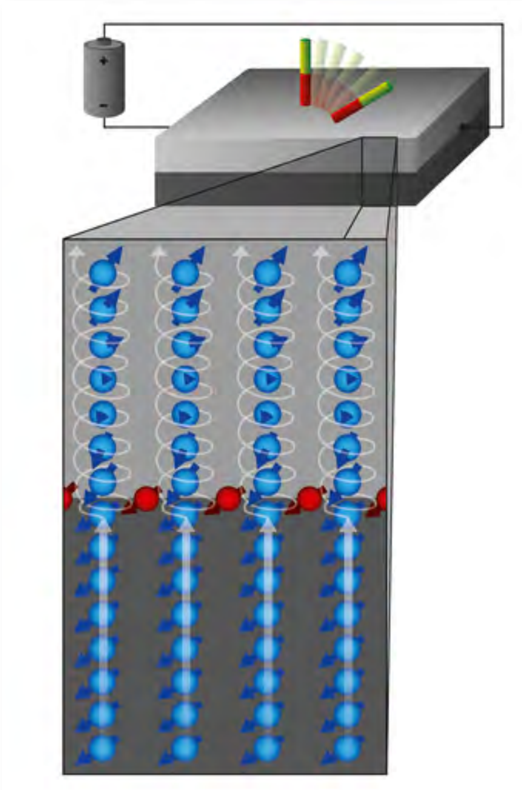
- ➔ "even" anti-damping part (AHE):
  Berry curature, *scattering-independent*
- ➔ "odd" field-like part ("diagonal" transport):
  diverges with vanishing disorder

	theor			expt
	Pt/Co	Pt/Co/O	Pt/Co/Al	Pt/Co/AlO$_x$
$\frac{T_{yx}^{\text{even}}}{\mu_S}$[mT]	3.2 (4.5)	5.1 (6.3)	3.9 (4.9)	5 ± 0.2^a 6.9 ± 0 1.7 ± 0 8^d
$\frac{T_{xx}^{\text{odd}}}{\mu_S}$[mT]	0.15 (0.73)	-3.0 (-3.0)	-5.6 (-3.6)	$-3.2 \pm ($ $-4 \pm 0.$ $0 \pm 1.$ -29^e



Gambardella's group + Jülich, Nat. Nano. **8**, 587 '13
Freimuth, Geranton, Blügel, Mokrousov, '14 – '15
Nottingham + Jülich + Prague, arXiv (2015)
Nijmegen + Porto + Braga + Jülich, arXiv (2015)

Spin-Orbit Torque

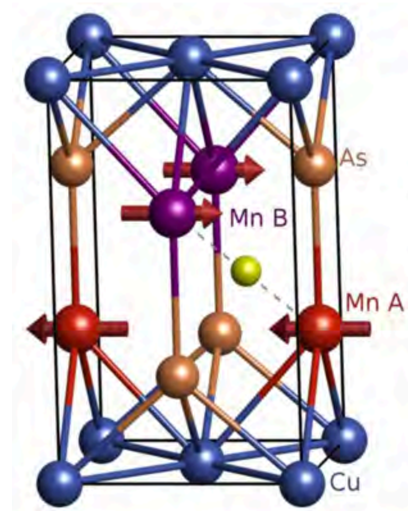


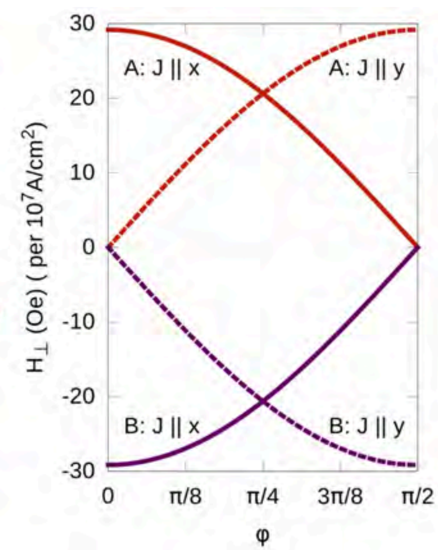
Switching magnetization with the current

- ➔ full electrical control of magnetization
- ➔ clear route towards miniaturization
- ➔ enhanced efficiency
- ➔ high-frequency dynamics
- ➔ switching in antiferromagnets!
- ➔ magnetic recording possible

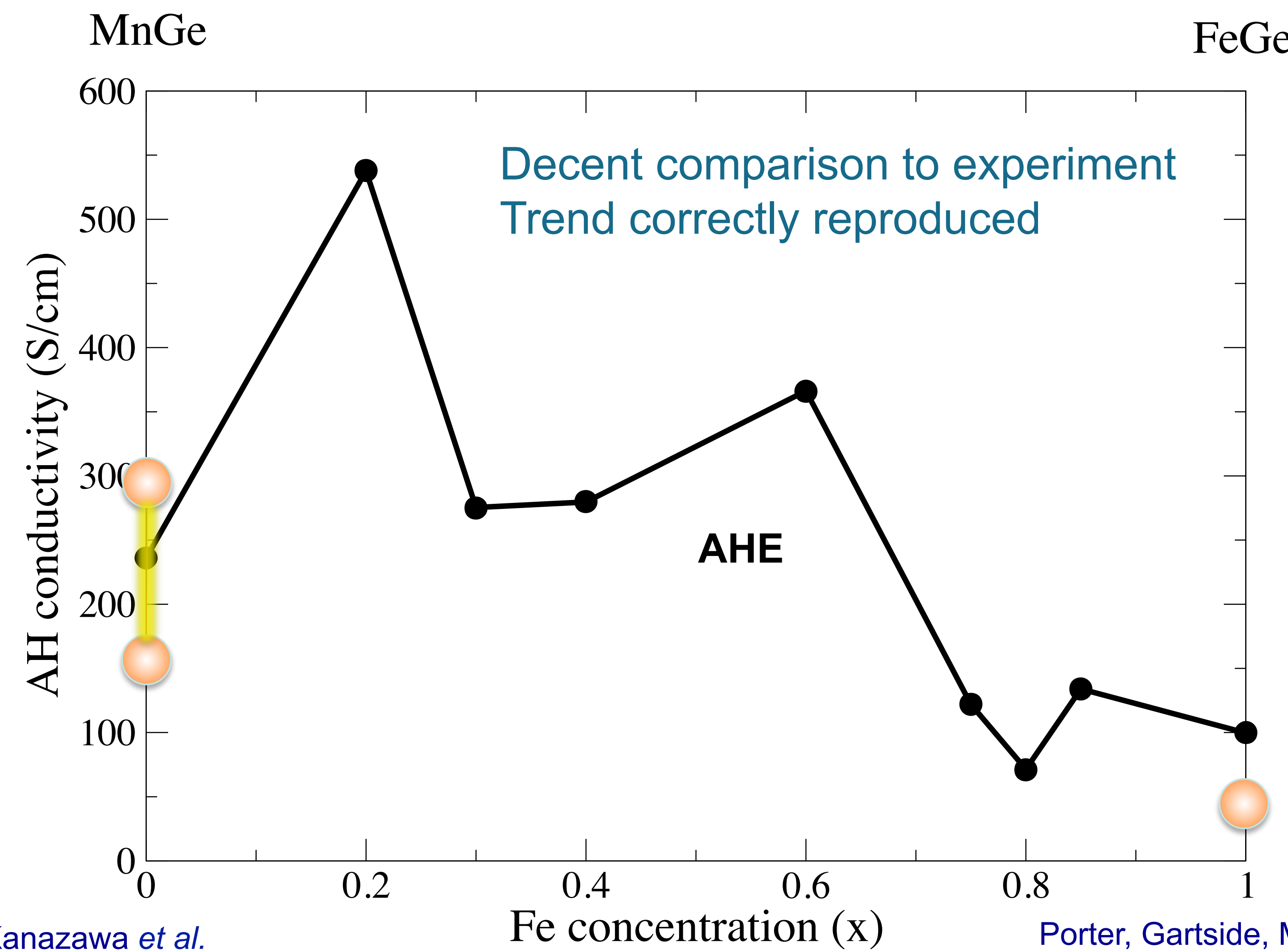
New vistas for ***antiferromagnetic* spintronics!**

Miron *et al.*, Nature **476**, 189 (2011)
Nijmegen + Porto + Braga + Jülich, arXiv (2015)
Nottingham + Jülich + Prague, arXiv (2015)
Gambardella's group + Jülich, Nat. Nano. **8**, 587 '13
Freimuth, Geranton, Blügel, Mokrousov, '14 – '15





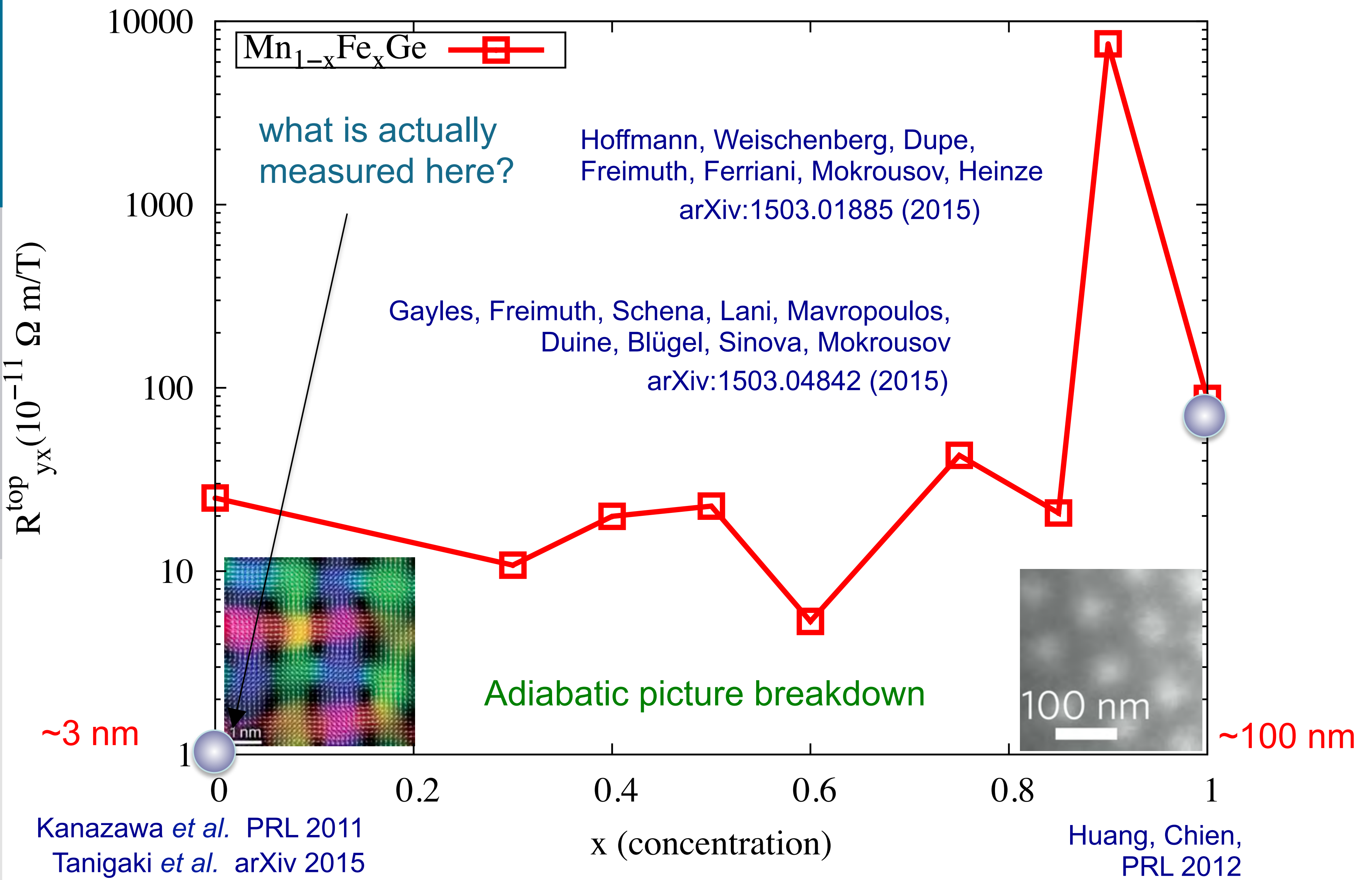
$Mn_{1-x}Fe_xGe$ alloys: scale the size by two orders



Kanazawa *et al.* PRL 2011

Porter, Gartside, Marrows, PRB 2014

$Mn_{1-x}Fe_xGe$ alloys: THE

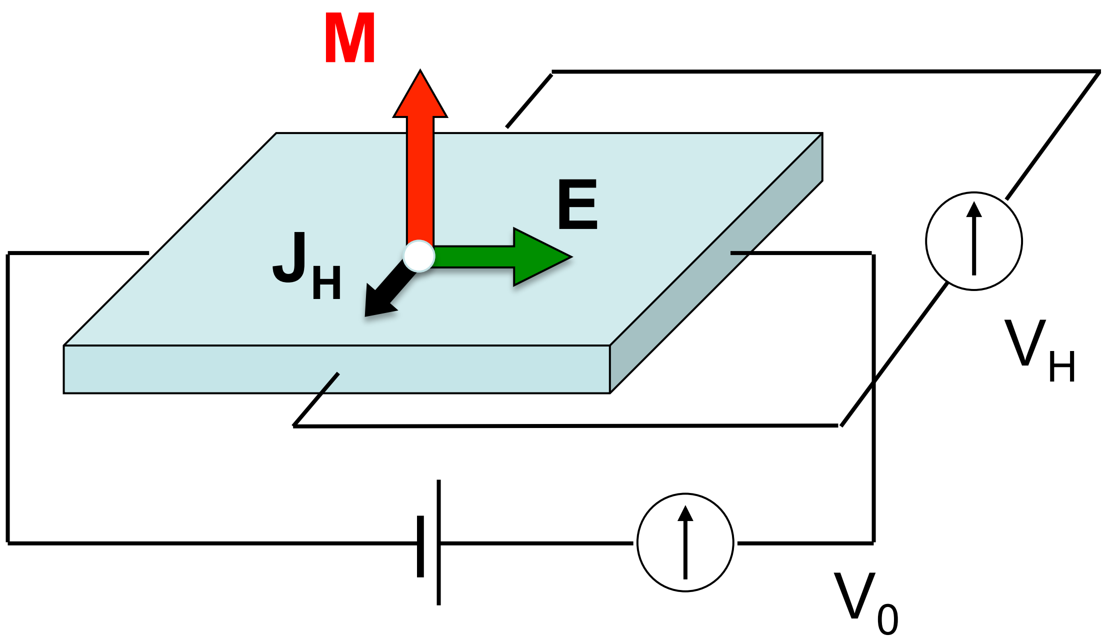


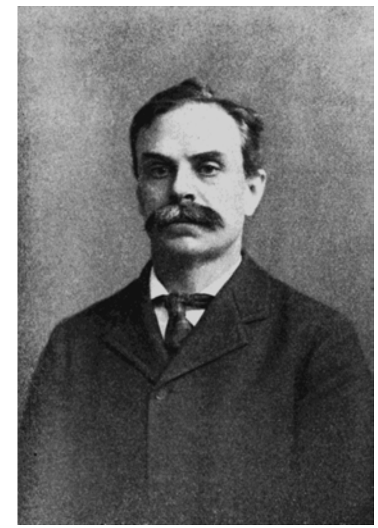
Anomalous Hall Effect
Ordinary Hall Effect (1879)

Anomalous Hall Effect (AHE) was discovered by Edwin Hall in 1880

Magnetic field exerts a *spin-insensitive* **Lorentz force** on conduction electrons

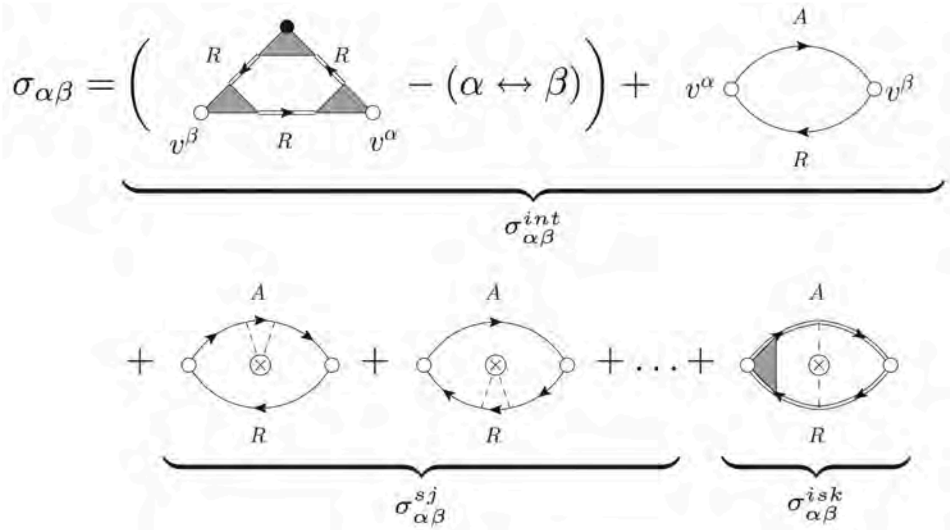
Anomalous Hall





AHE arises due to non-zero macroscopic **magnetization** and **spin-orbit interaction** in a magnetic sample

Scattering-independent Hall effects

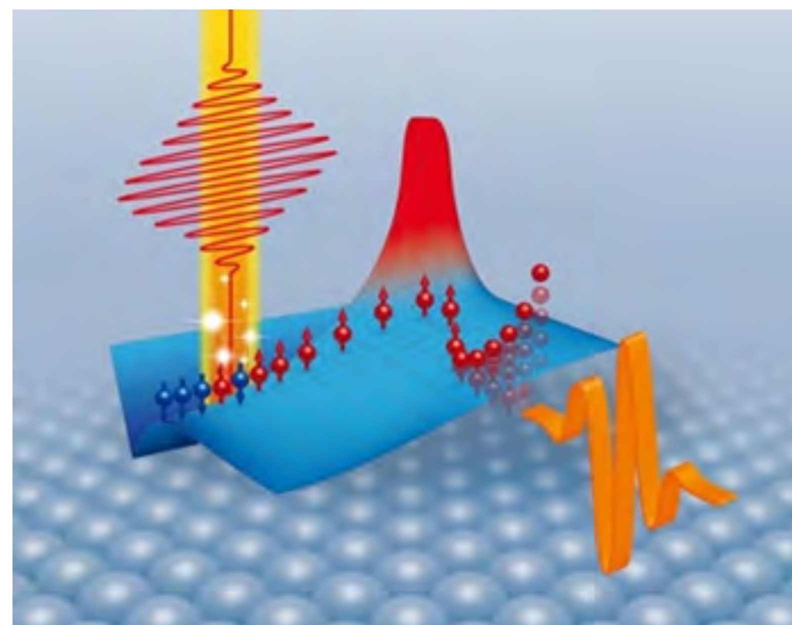


All scattering-independent contributions can be identified

Dominant for moderately dirty metals

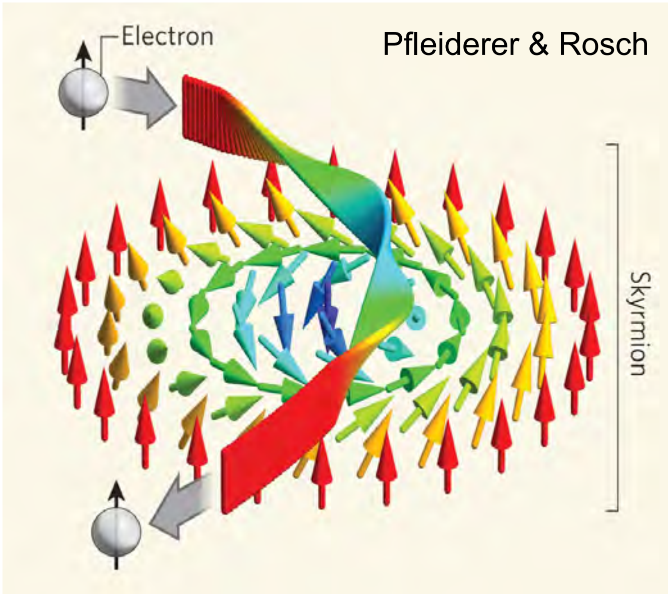
Nature Nanotech. **8**, 256 ‘13

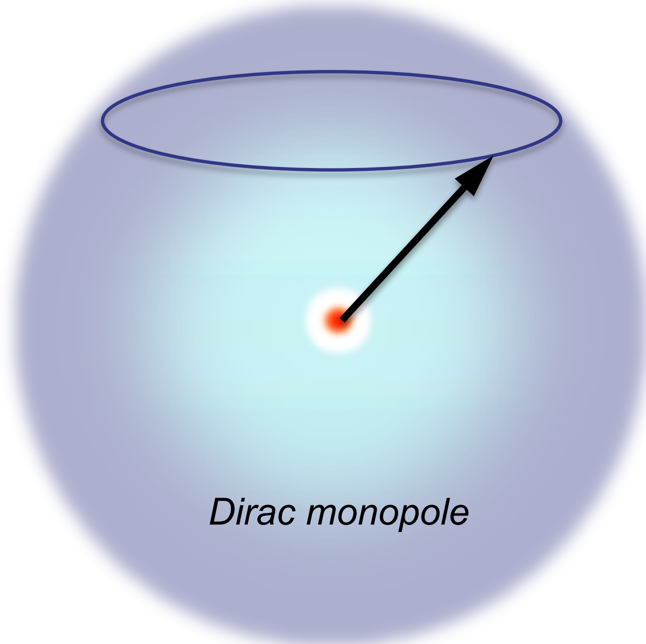
True not only for static, but also high-frequency electric fields



Weischenberg, Czaja, Freimuth, Sinova, Kampfrath’s group, Münzenberg’s group, Blügel, Zimmermann, Long, Mavropoulos, Mokrousov,
PRLs, PRBs, Nature Nano.: 2009 and on...

Real-space Berry curvature



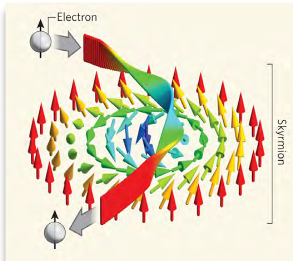


Flux of $\mathbf{\Omega}_\mathbf{R}$ = winding number ≈ flux of Dirac monopole field

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

➔ quantized topological charge
➔ topological protection
➔ key for spintronics applications

To name just a few...



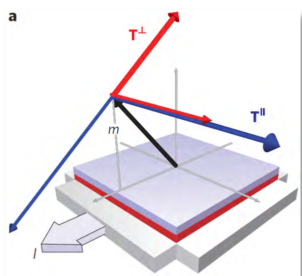
Topological Hall effect
Skyrmions (Ω_{RR})

Pumping effects (Ω_{kt})

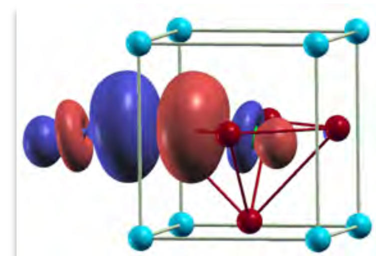
Electric Polarization ($\Omega_{k\lambda}$)

Dzyaloshinskii-Moriya interaction (Ω_{kR})

Spin-Orbit Torque (Ω_{kM})

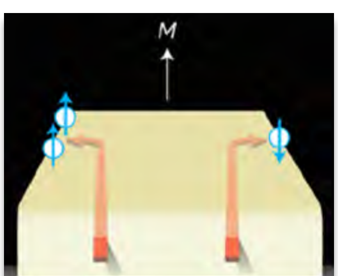


Geometrical Formulation



Thermal Hall effect (Ω_{kq})

Gilbert damping (Ω_{MM})



Ω_{kk}: Anomalous Hall effect
Orbital Magnetization
Spin Hall effect
Quantized Hall effects
Topological Insulators

Magnon Hall effect
Exchange interactions (Ω_{qq})