Control of Dzyaloshinskii-Moriya interaction in $Mn_{1-x}Fe_xGe$: Toward skyrmion crystal engineering

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Collaborators

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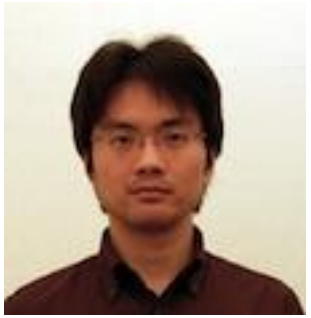


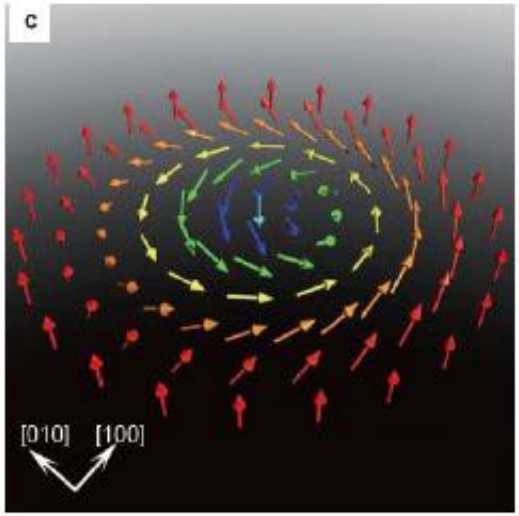
- Naoto Nagaosa
  (RINEN CEMS/Univ. Tokyo)

Scientific Reports, 5 13302 (2015)

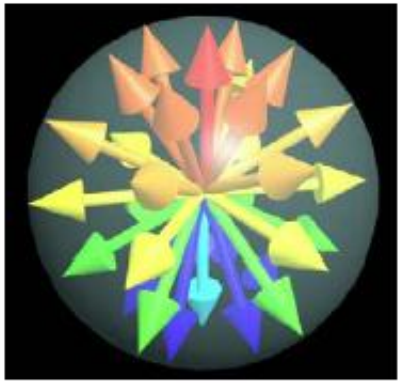
Outline

- Introduction
  - What is skyrmion ?
    A vortex spin structure which provides a playground of emergent electromagnetism
  - Possible application to magnetic memory
- Size & helicity control of skyrmion
  - Size & sign control of the DM interaction
- *Ab initio* calculation
  - How to estimate DMI from first principles?
  - How the band structure determines DMI ?
  - Materials design of DMI: toward skyrmion Xtal engineering
    - Sign, size, anisotropy …

What is skyrmion

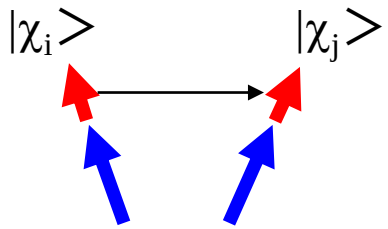


Mapping onto
the unit sphere



A vortex spin structure in which the spins point in all directions wrapping a sphere and can be characterized by a topological number

Emergent electromagnetism



Conduction electron

Localized spin
(or molecular field created by conduction electron themselves)

$$|\chi_i\rangle = \begin{pmatrix} \cos(\theta_i/2) \\ e^{i\phi_i}\sin(\theta_i/2) \end{pmatrix}$$

Two component spinor
spin wave function

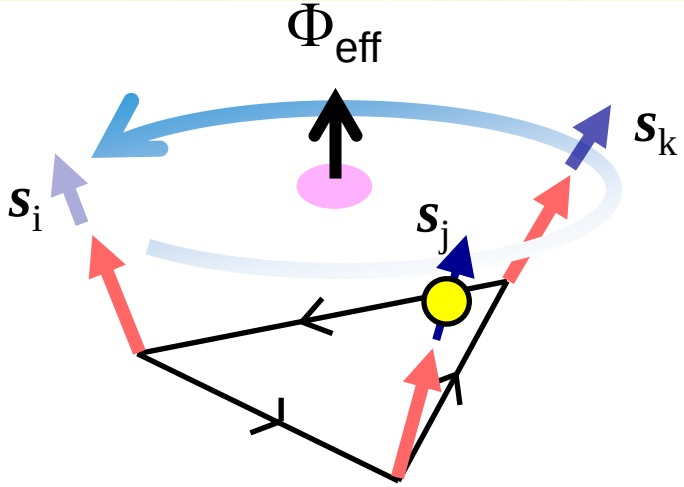
$$t_{ij}^{\text{eff}} = t_{ij}\langle\chi_i|\chi_j\rangle = t_{ij}e^{ia_{ij}}\cos\left(\frac{\theta_{ij}}{2}\right)$$

acquire a phase factor

acts like the Peierls phase and can be viewed as originating from a fictitious magnetic field which influences the orbital motion of the conduction electrons.

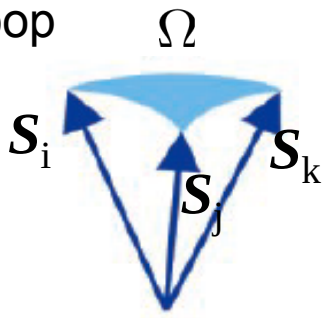
Emergent electromagnetism

The Peierls phase leads to a large gauge flux in the presence of noncoplanar spin configurations



Phase acquired by the electron's wave function around the loop

$$\langle \chi_i | \chi_k \rangle \langle \chi_k | \chi_j \rangle \langle \chi_j | \chi_i \rangle \propto \exp(i\Omega/2)$$



$$\Omega = \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$$

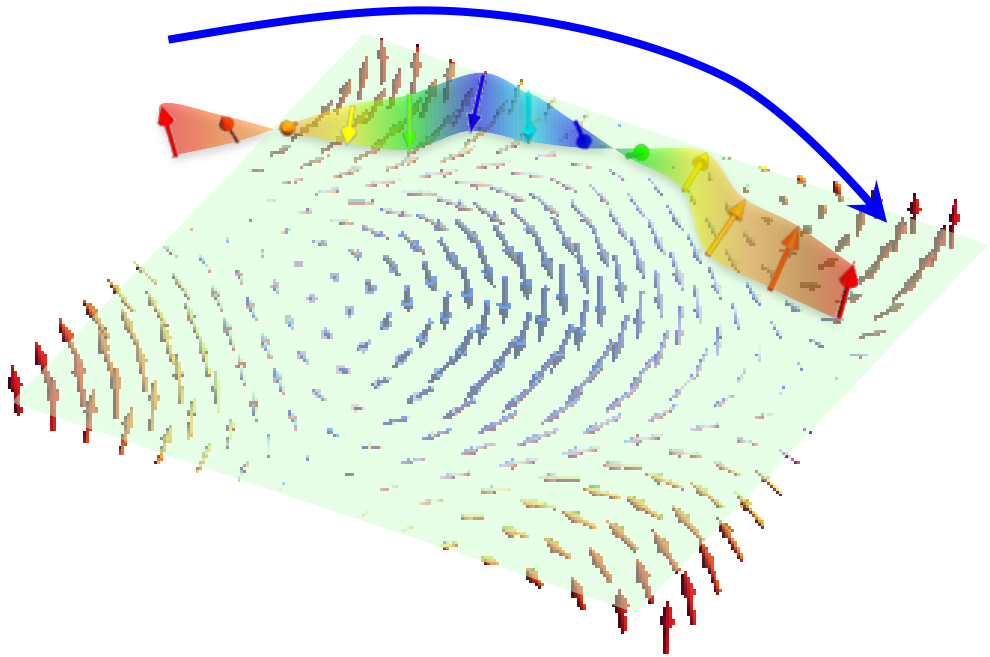
Solid angle subtended by the three spins on the unit sphere (Scalar spin chirality)

Equation of motion

$$\hbar\dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}} \times \mathbf{B} - \hbar\dot{\mathbf{r}} \times \mathbf{b}(\mathbf{r})$$

Large emergent magnetic field

Emergent electromagnetism



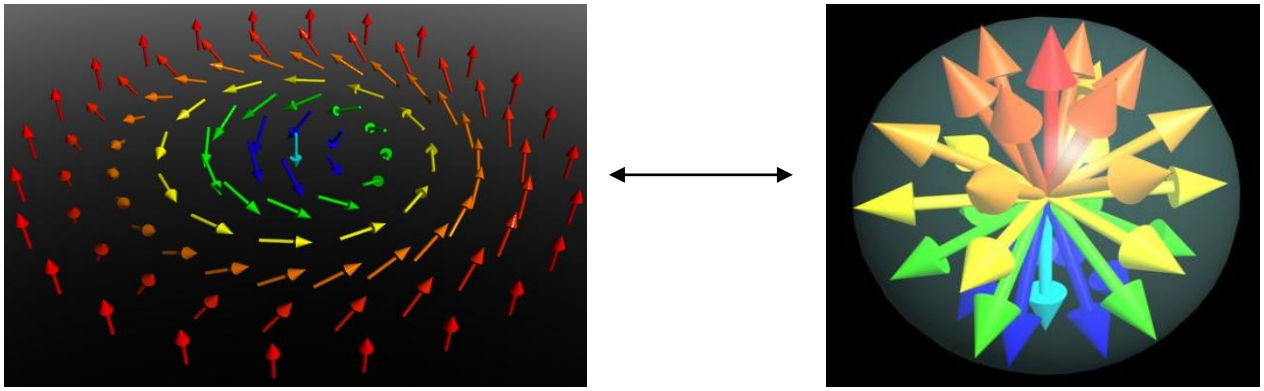
Emergent magnetic field due to Berry phase:

$$\Phi = \frac{1}{2}\int d\mathbf{r}\, \hat{\mathbf{n}} \cdot \left(\frac{\partial \hat{\mathbf{n}}}{\partial x} \times \frac{\partial \hat{\mathbf{n}}}{\partial y} \right)$$

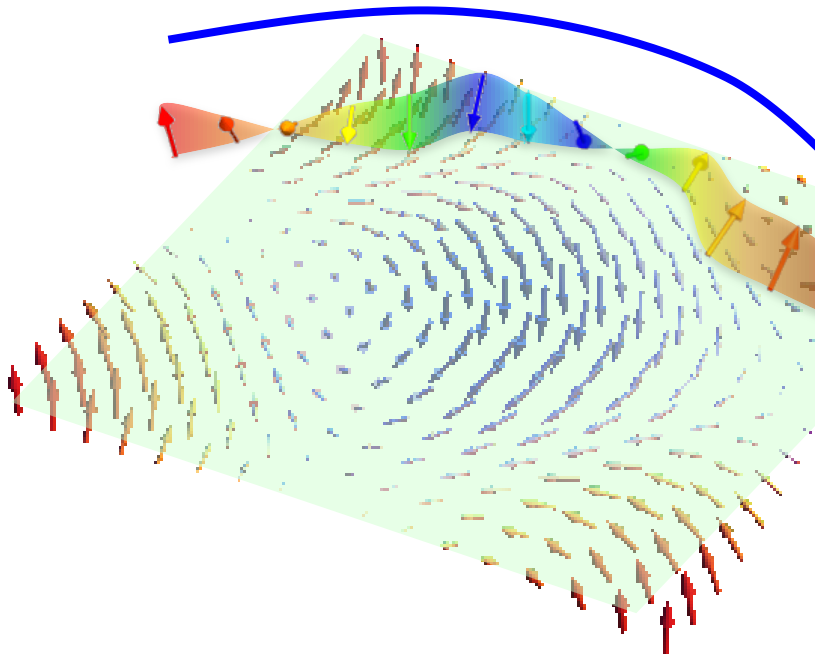
4π

One skyrmion (spins point in all directions wrapping a sphere)

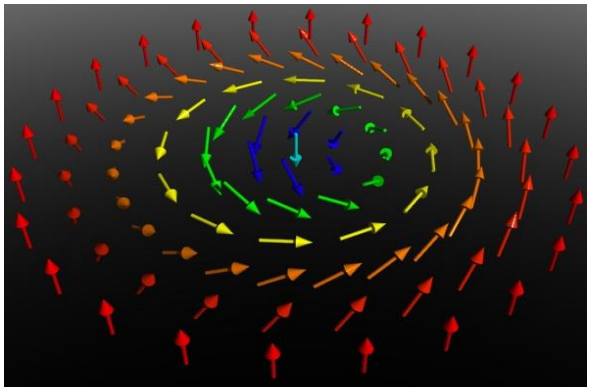
One magnetic flux $\phi_0 = h/e$



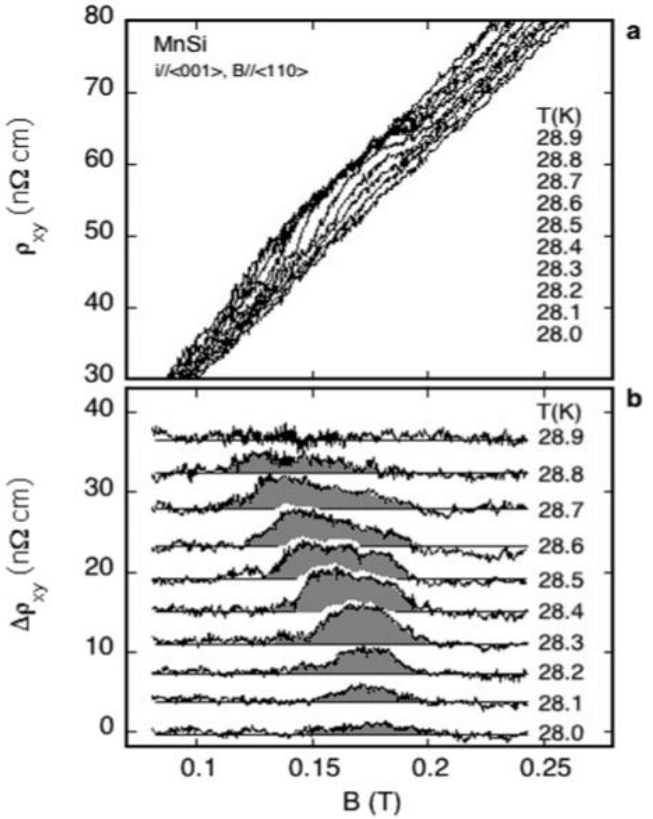
Emergent electromagnetism



One skyrmion (spins point in all directions wrapping a sphere)



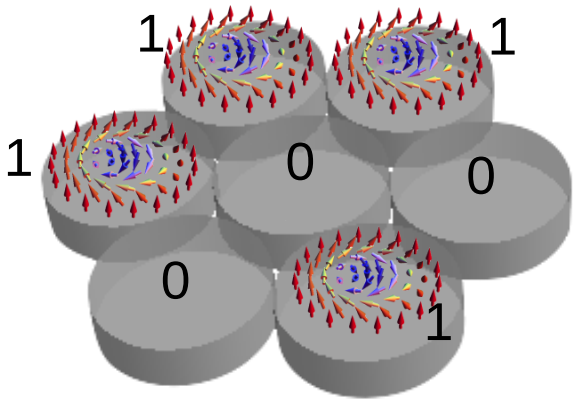
MnSi bulk

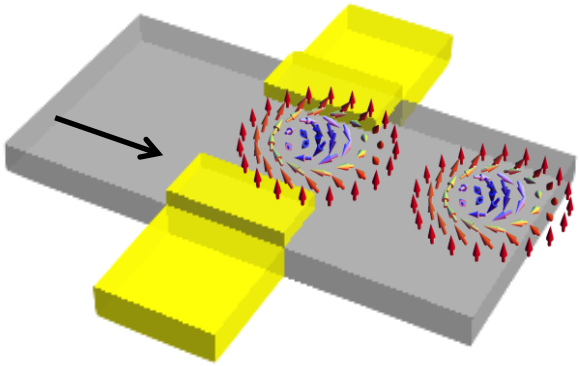


A. Neubauer *et al*, PRL **102,** 186602 (2009).

Possible application

Skyrmion-based magnetic memory

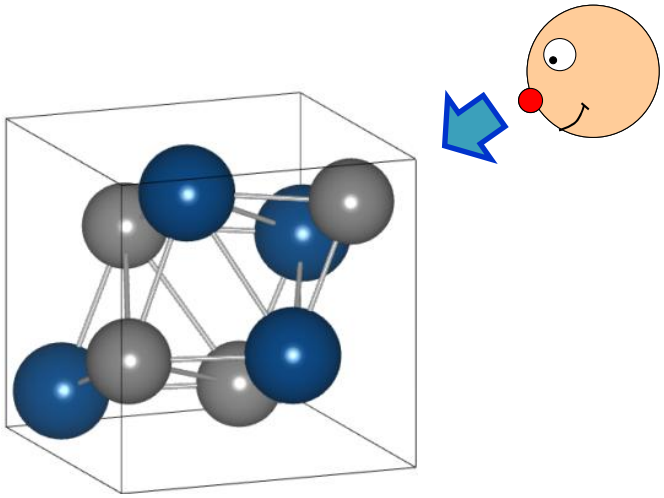


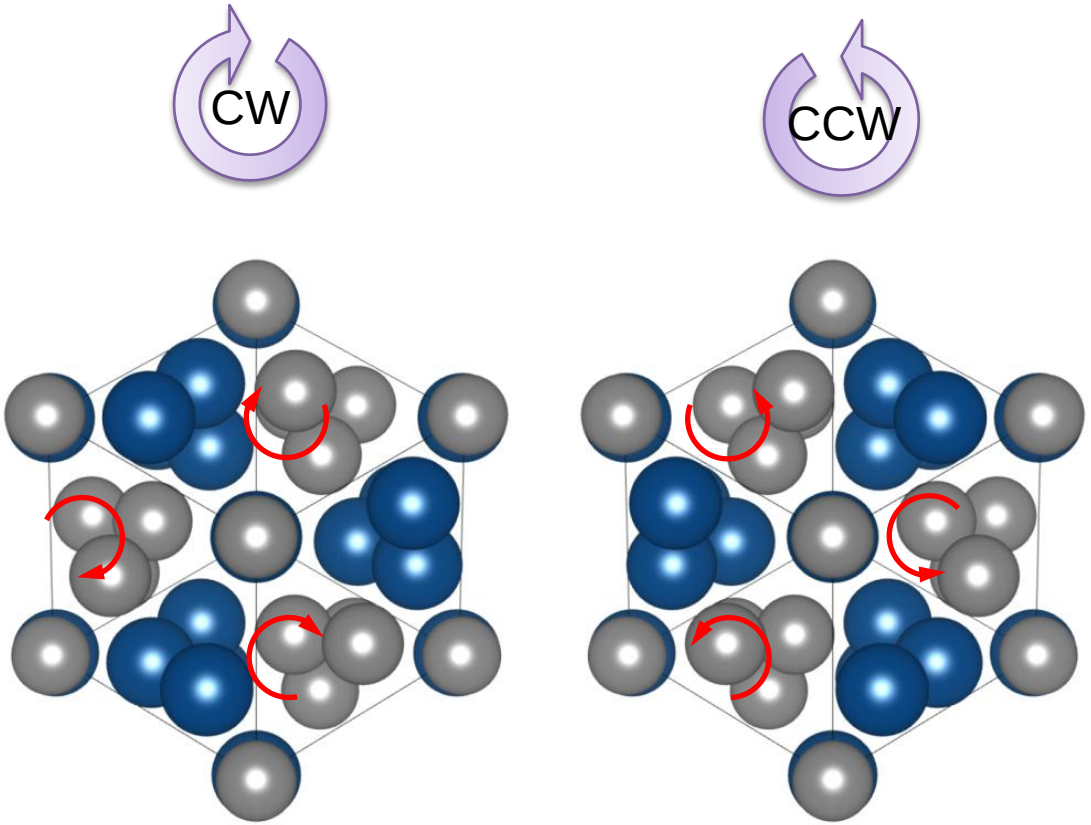


-Skyrmion = Topologically-protected particle
-High areal density (size ~ 3-200 nm)
-Very mobile under electric current

crystal engineering in terms of controlling the skyrmion crystal structure itself (including the lattice constant, lattice form and magnetic helicity) is not well established

Crystal structure of *B20* compound

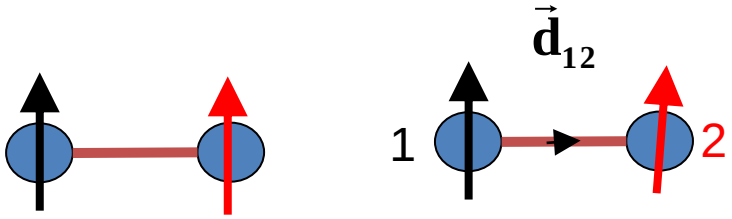




- : Transition-metal element
- : Si, Ge

  - Cubic ($P2_13$)
  - Noncentrosymmetric

Effective Hamiltonian



$$H = \sum [-J\mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_j)]$$ + weak anisotoropy

Ferromagnetic > Dzyaloshinsky-Moriya

Continuum magnetization $\mathbf{M}$ in a crystalline itinerant magnet

$$1 - \mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{2}(\mathbf{S}_i - \mathbf{S}_j)^2 \rightarrow \frac{1}{2}(\mathbf{M}(\mathbf{R}_i) - \mathbf{M}(\mathbf{R}_j))^2$$
$$-\mathbf{S}_i \times \mathbf{S}_j = \mathbf{S}_i \times (\mathbf{S}_i - \mathbf{S}_j) \rightarrow \mathbf{M}(\mathbf{R}_i) \times (\mathbf{M}(\mathbf{R}_i) - \mathbf{M}(\mathbf{R}_j))$$

$$\frac{J}{2}(\nabla \mathbf{M})^2 + \mathbf{D}_a \cdot \mathbf{M} \times (\partial_a \mathbf{M}) + \cdots$$

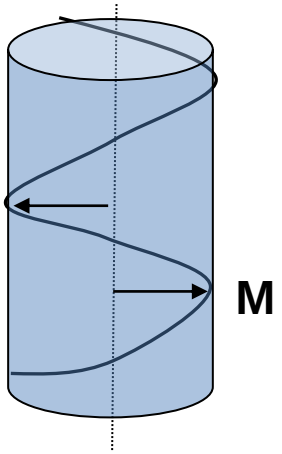
For the B20 structure

$$H = \int dr \left[\frac{J}{2}(\nabla M)^2 + DM \cdot (\nabla \times M)\right]$$

Effective Hamiltonian

$$H = \int dr \left[\frac{J}{2} (\nabla M)^2 + DM \cdot (\nabla \times M) \right]$$

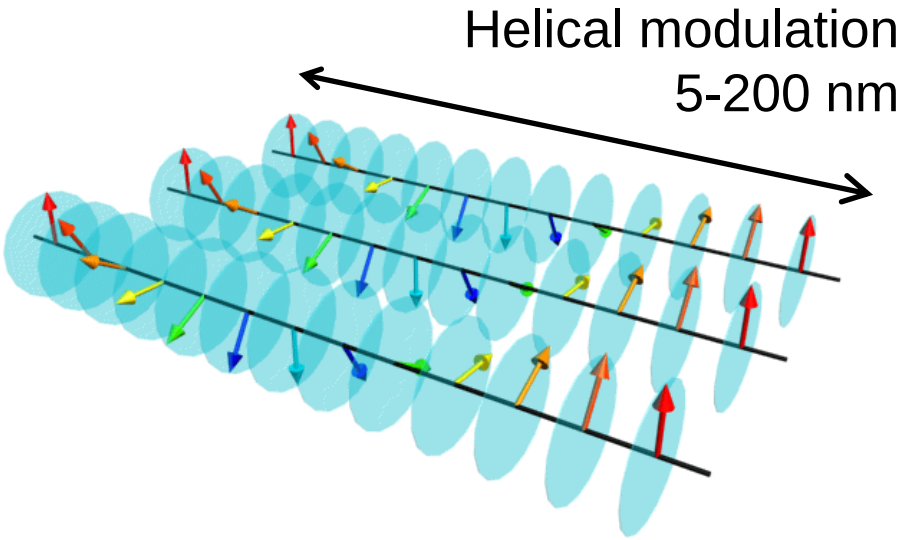
$$\mathbf{M}(z) = m(\mathbf{e}_x \cos(qz) + \mathbf{e}_y \sin(qz))$$

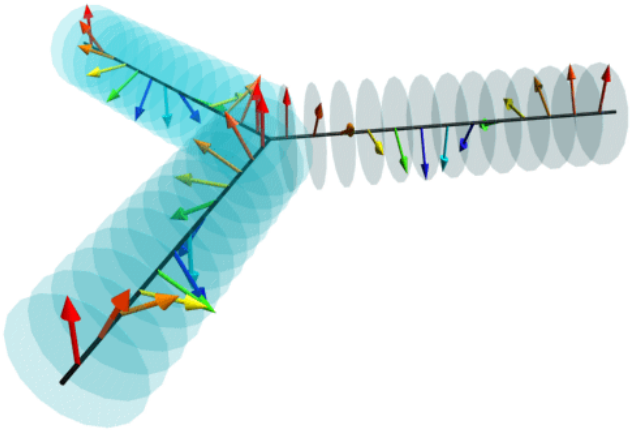


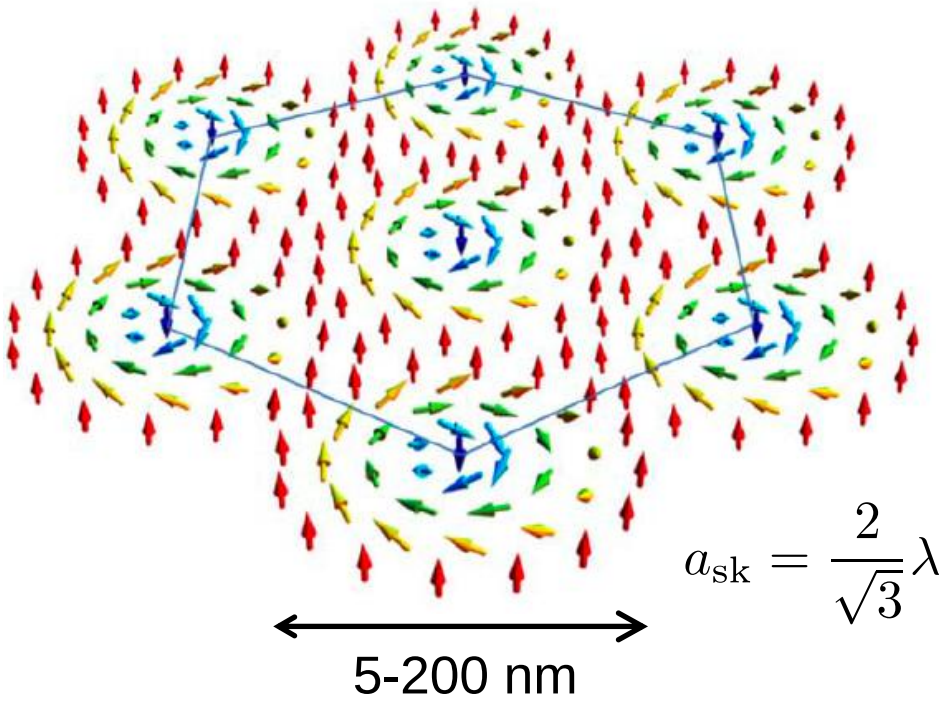
$$E(q) = Jq^2 + 2Dq$$

DMI prefers finite q=D/J ($\lambda = 2\pi J/D$)

Helical spin order in *B20*-type crystal

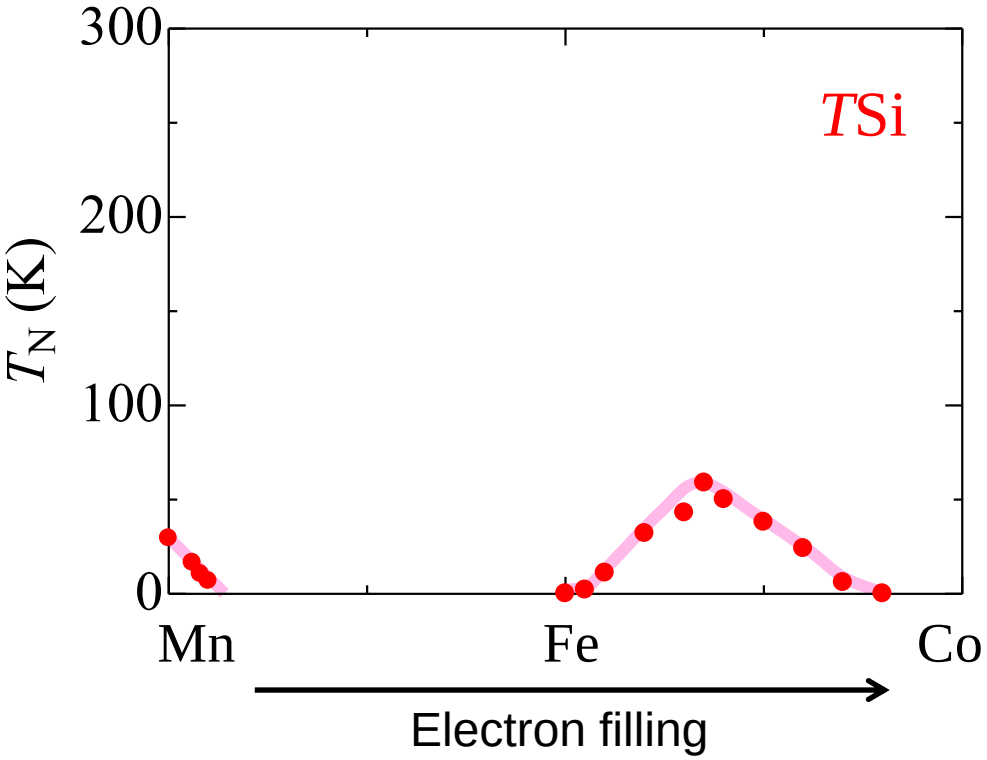


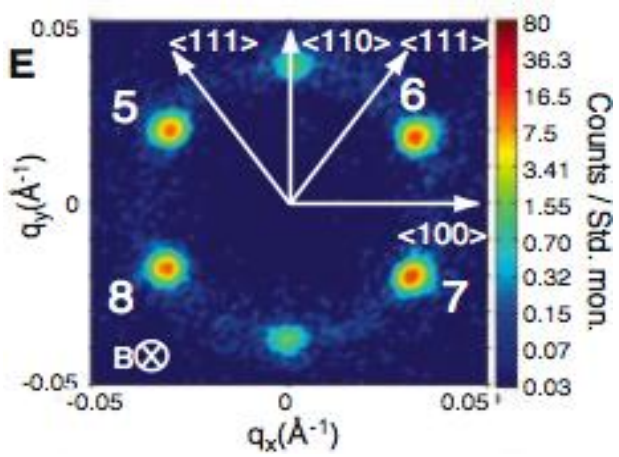




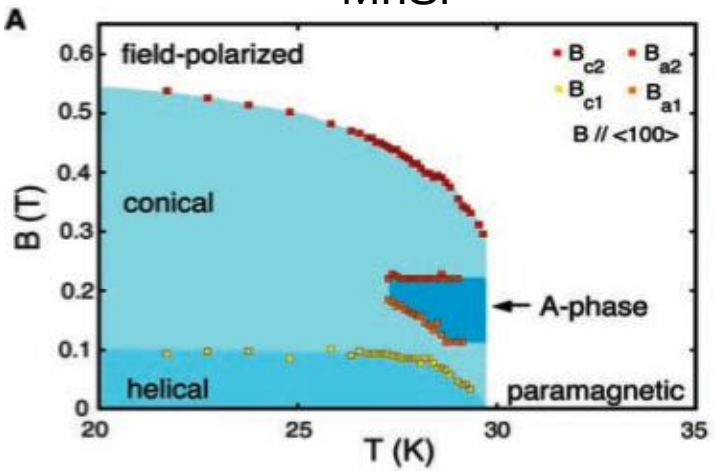
$$a_{\mathrm{sk}} = \frac{2}{\sqrt{3}}\lambda$$

Magnetic phase diagram in *T*Si





MnSi

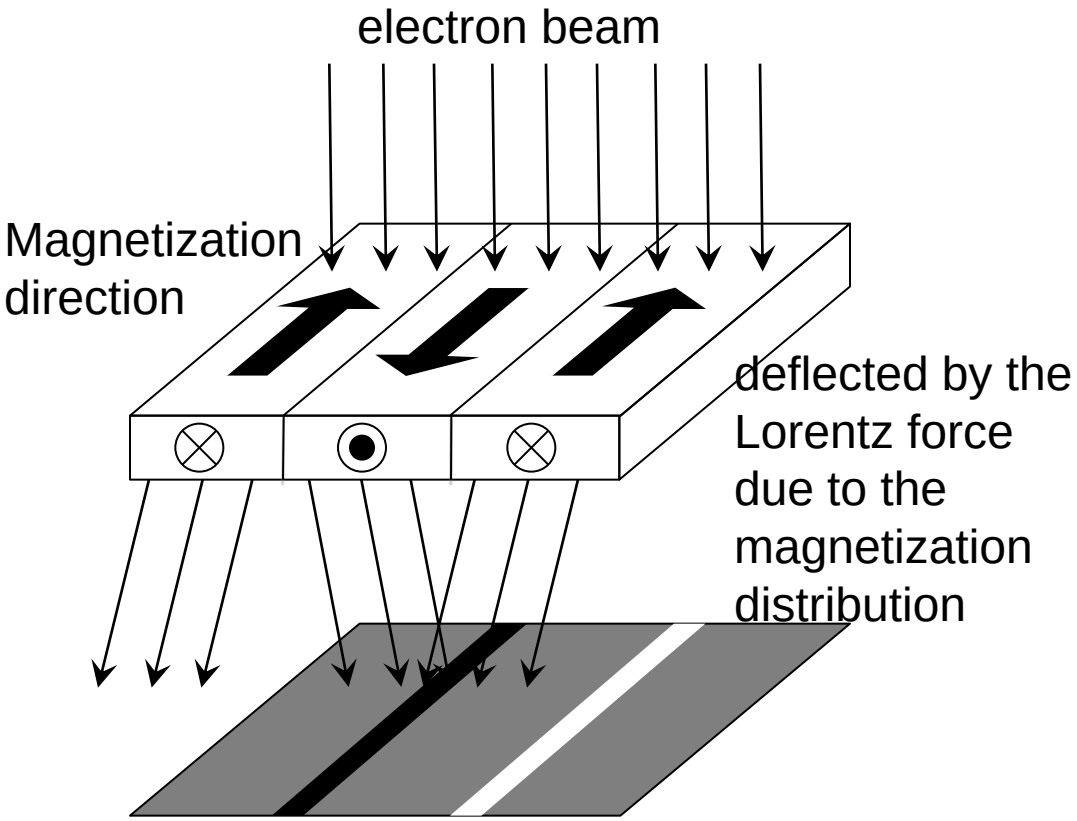


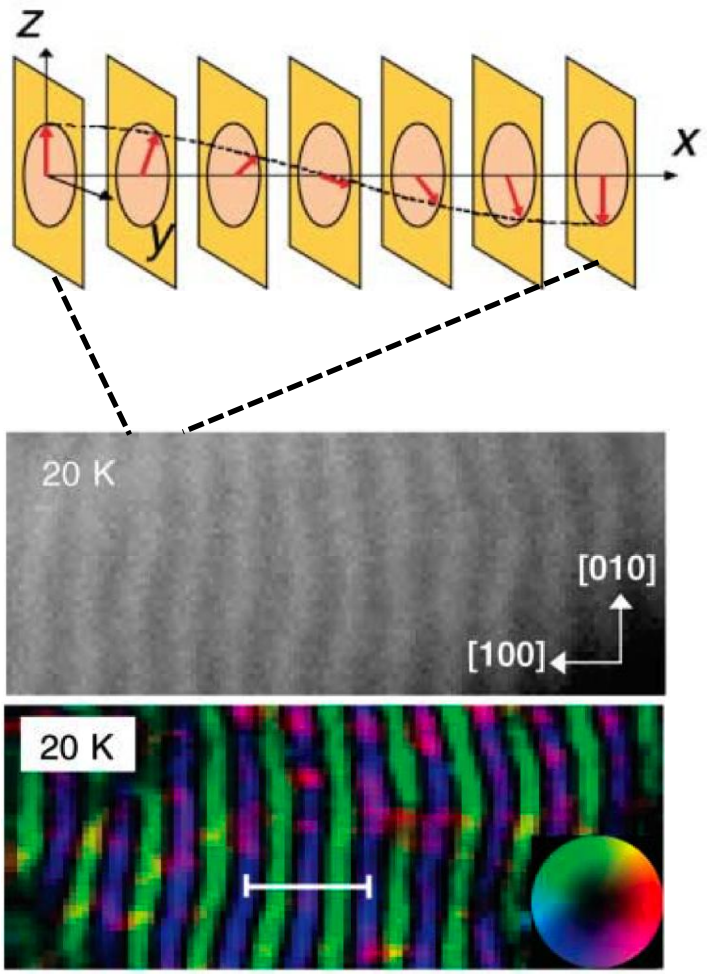
S. Mühlbauer *et al*, Science **323** 915 (2009)

S. V. Grigoriev et al., PRB 79, 144417 (2009).
Y. Onose et al., PRB 72, 224431 (2005).

Real-space observation by TEM

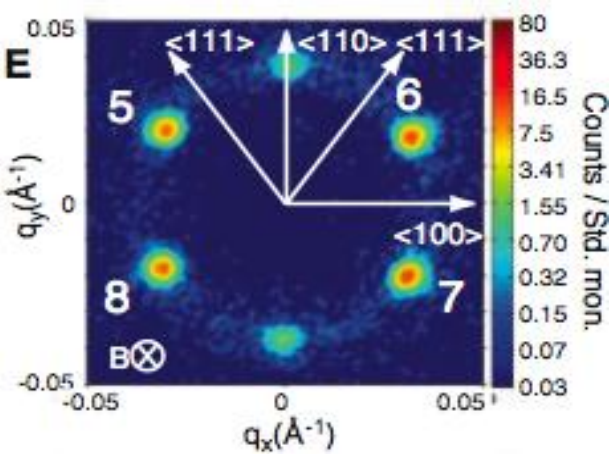
Mapping in-plane magnetization by transmission electron microscope



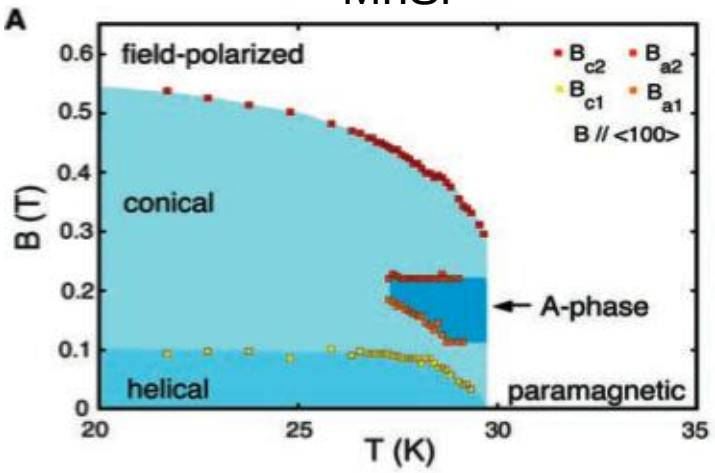


M. Uchida et al., Science **311**, 359 (2006)

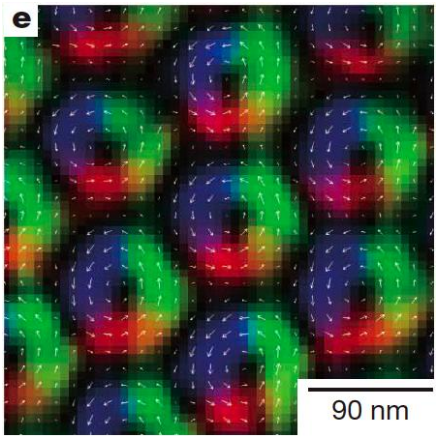
Real-space observation by TEM



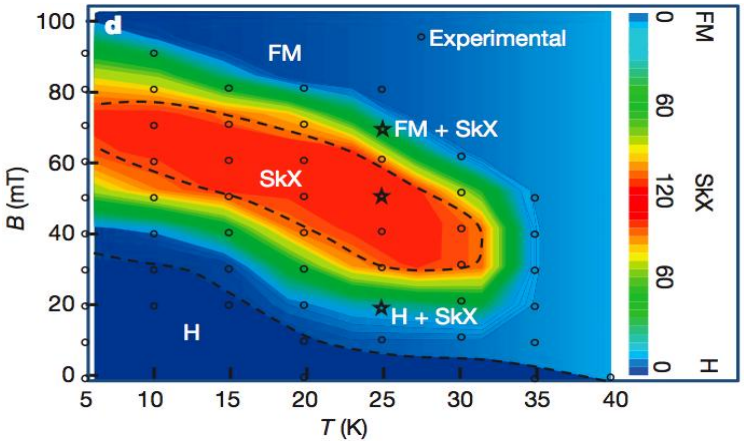
MnSi



S. Mühlbauer *et al*, Science **323** 915 (2009)



Stable skyrmions in thin film

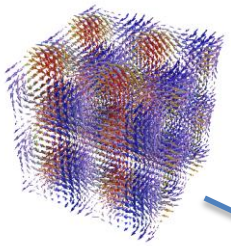


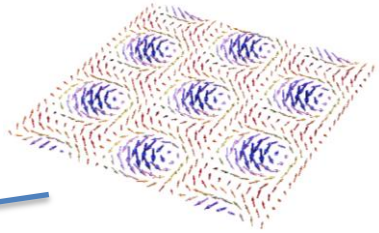
X. Z. Yu *et al*., Nature **465** 901 (2010)

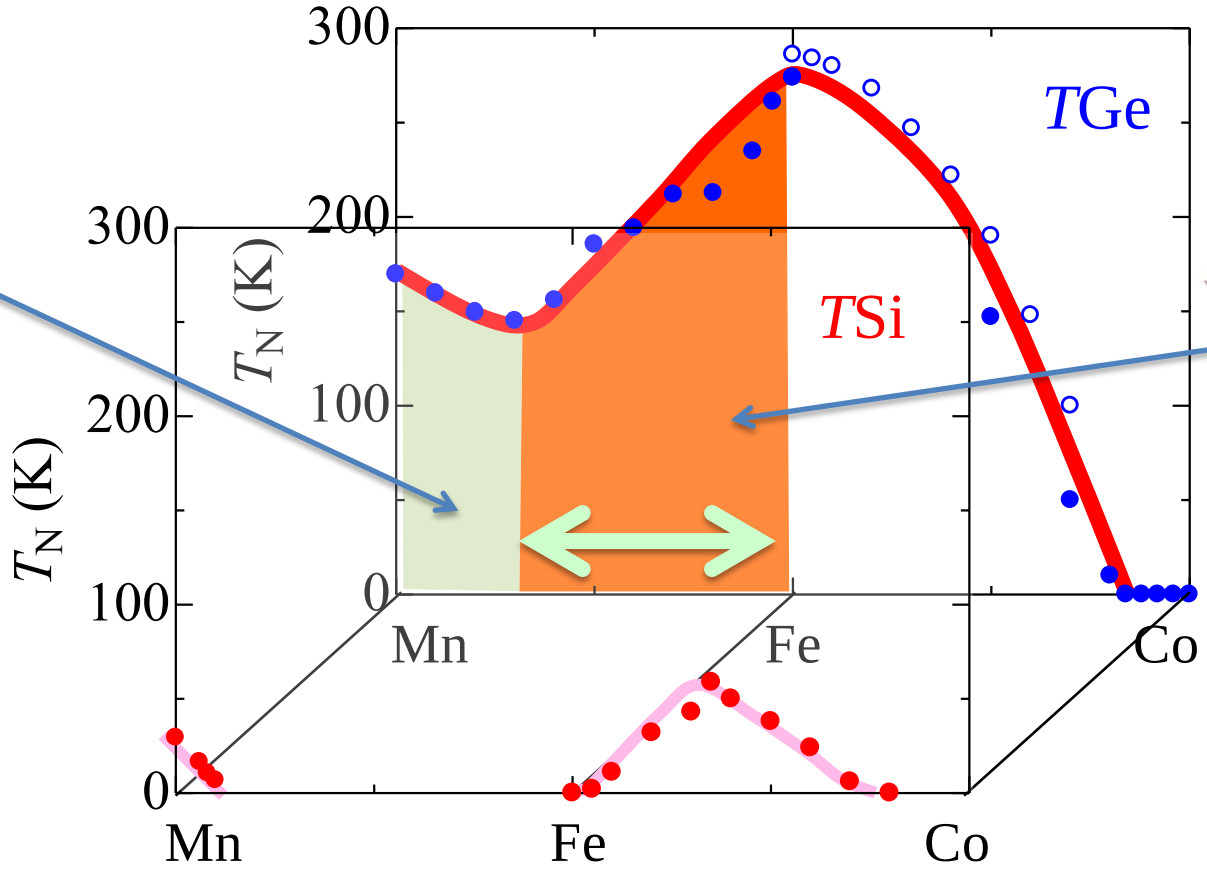
Magnetic phase diagram *T*Ge

K. Shibata *et al.*, Nat. Nanothech 8, 723 (2013)

Large variation of skyrmion size and reversal of helicity observed

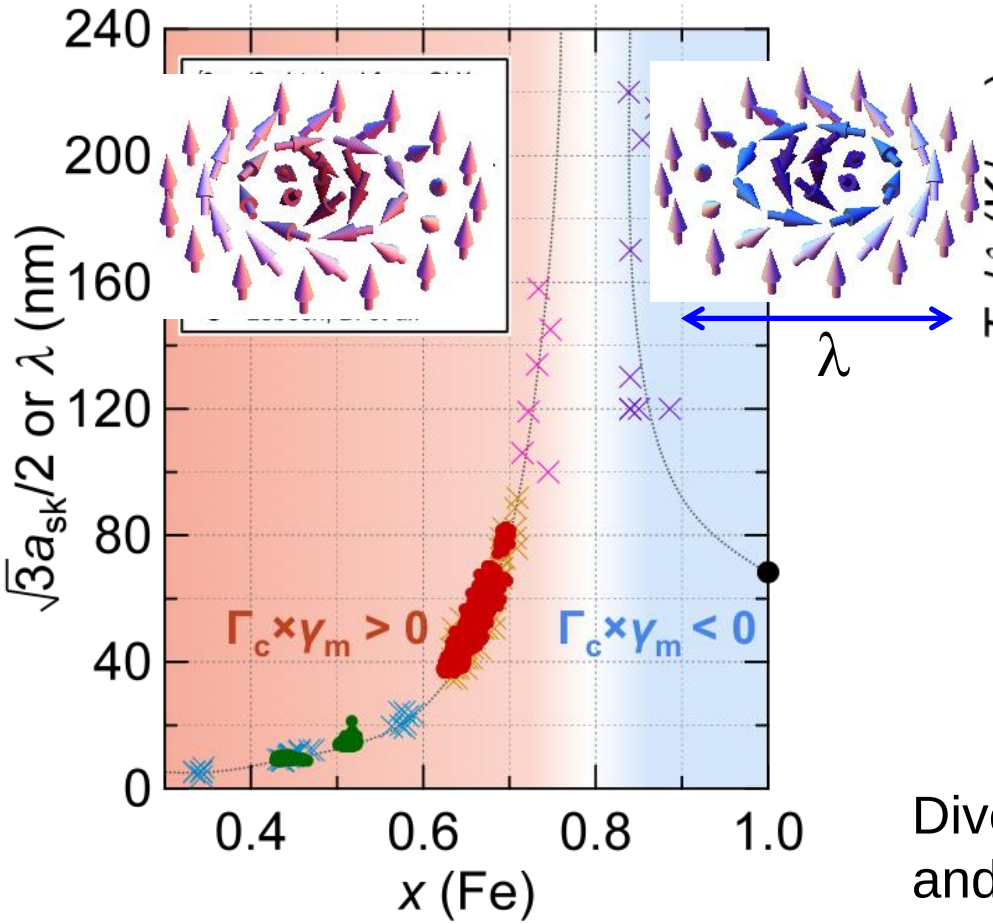


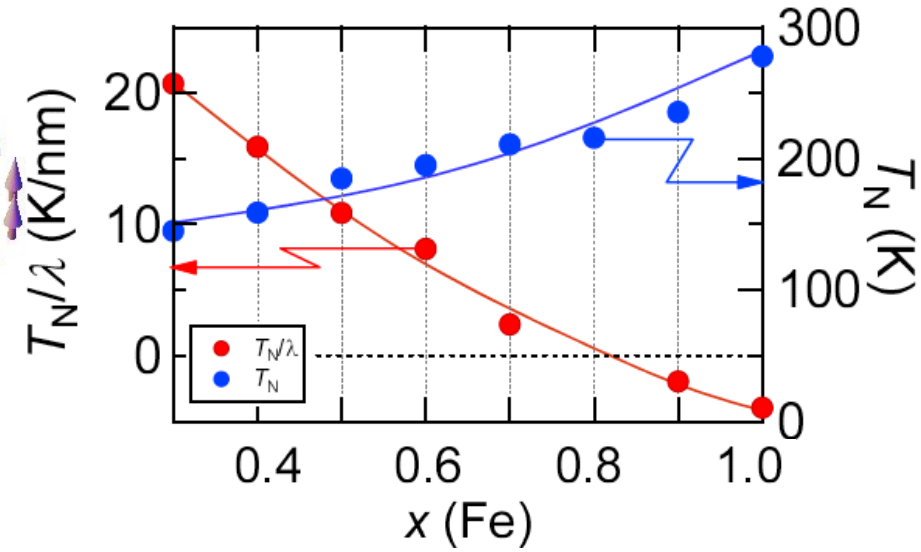




Skyrmion formation and helicity change in $Mn_{1-x}Fe_xGe$

K. Shibata *et al.*, Nat. Nanothech 8, 723 (2013)





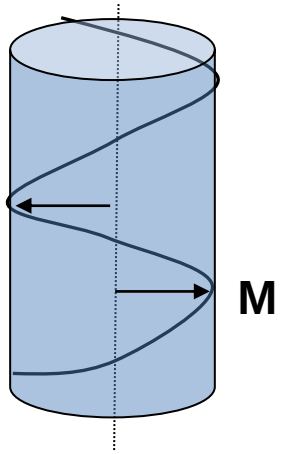
$$T_{\mathrm{N}} \propto J \qquad \lambda \propto J/D \longrightarrow D \propto T_{\mathrm{N}}/\lambda$$

Diverging skyrmion size
and reversal of helicity
→ DM int. changes its sign
Mechanism ???

How to estimate DMI from first principles

$$H = \int dr \left[\frac{J}{2} (\nabla M)^2 + DM \cdot (\nabla \times M) \right]$$

$$\mathbf{M}(z) = m(\mathbf{e}_x \cos(qz) + \mathbf{e}_y \sin(qz))$$



$$E(q) = Jq^2 + 2Dq$$

evaluate the linear slope of the dispersion energy of the spin-spiral solution
→ Large unit cell ?

Generalized Bloch's theorem

Heide et al., Physica B09

Generalized translation $\mathcal{T}_n$

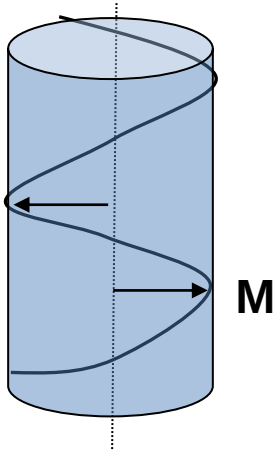
= translation + spin rotation

$$\mathbf{r} \rightarrow \mathbf{r} + \mathbf{R}_n \qquad \mathbf{U}(\mathbf{qR})$$

$$\mathcal{H}(\mathbf{r} + \mathbf{R}_n) = \mathbf{U}(\mathbf{qR}_n)\mathcal{H}(\mathbf{r})\mathbf{U}^{\dagger}(\mathbf{qR}_n)$$

$$U(\mathbf{qR}_n) = \begin{pmatrix} \exp(-i\varphi/2) & 0 \\ 0 & \exp(i\varphi/2) \end{pmatrix}$$

$$\varphi = \mathbf{q} \cdot \mathbf{R}_n$$



$\mathbf{R_n}$: lattice vector of the chemical lattice

$\mathbf{q}$: wave vector which determines the direction of spatial propagation of spiral spin density wave

Generalized Bloch's theorem

Heide et al., Physica B09

$$\begin{aligned}\mathcal{T}_n\mathcal{H}(\mathbf{r})\psi(\mathbf{r}) &= \mathbf{U}(-\mathbf{q}\mathbf{R}_n)\mathcal{H}(\mathbf{r}+\mathbf{R}_n)\psi(\mathbf{r}+\mathbf{R}_n)\\ &= \mathbf{U}(-\mathbf{q}\mathbf{R}_n)\mathcal{H}(\mathbf{r}+\mathbf{R}_n)\mathbf{U}^{\dagger}(-\mathbf{q}\mathbf{R}_n)\mathbf{U}(-\mathbf{q}\mathbf{R}_n)\psi(\mathbf{r}+\mathbf{R}_n)\\ &= \mathcal{H}(\mathbf{r})\mathbf{U}(-\mathbf{q}\mathbf{R}_n)\psi(\mathbf{r}+\mathbf{R}_n)\\ &= \mathcal{H}(\mathbf{r})\mathcal{T}_n\psi(\mathbf{r})\end{aligned}$$

$$\mathcal{H}(\mathbf{r})\mathcal{T}_n = \mathcal{T}_n\mathcal{H}(\mathbf{r})$$

$$\mathcal{T}_n\mathcal{T}_m = \mathcal{T}_m\mathcal{T}_n = \mathcal{T}_{n+m}$$

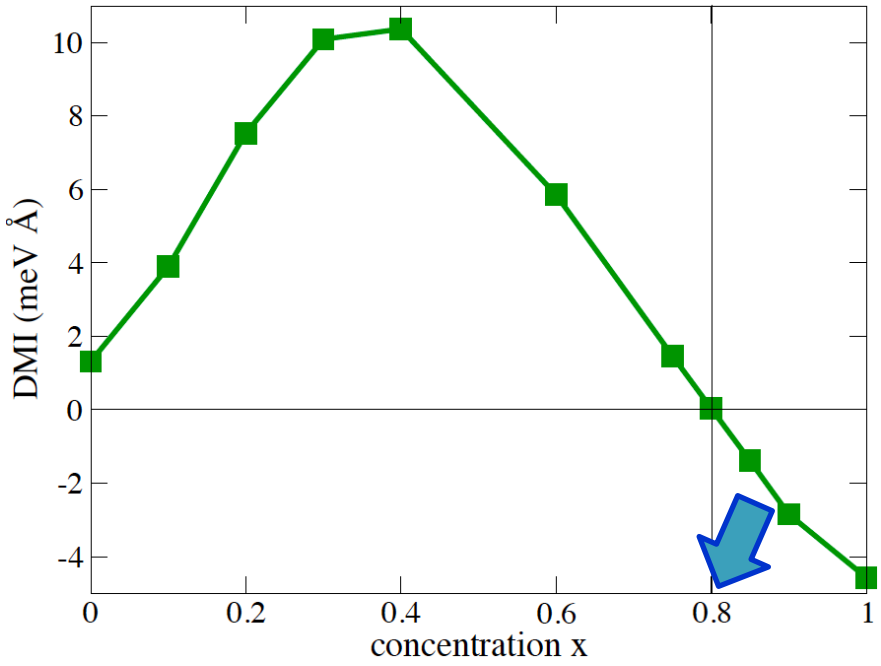
$$\mathcal{T}_n\psi(\mathbf{k},\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{R}_n)\psi(\mathbf{k},\mathbf{r})$$

$$\psi(\mathbf{k},\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})\begin{pmatrix}\exp(-i\mathbf{q}\cdot\mathbf{r})\alpha(\mathbf{k},\mathbf{r})\\ \exp(+i\mathbf{q}\cdot\mathbf{r})\beta(\mathbf{k},\mathbf{r})\end{pmatrix}$$

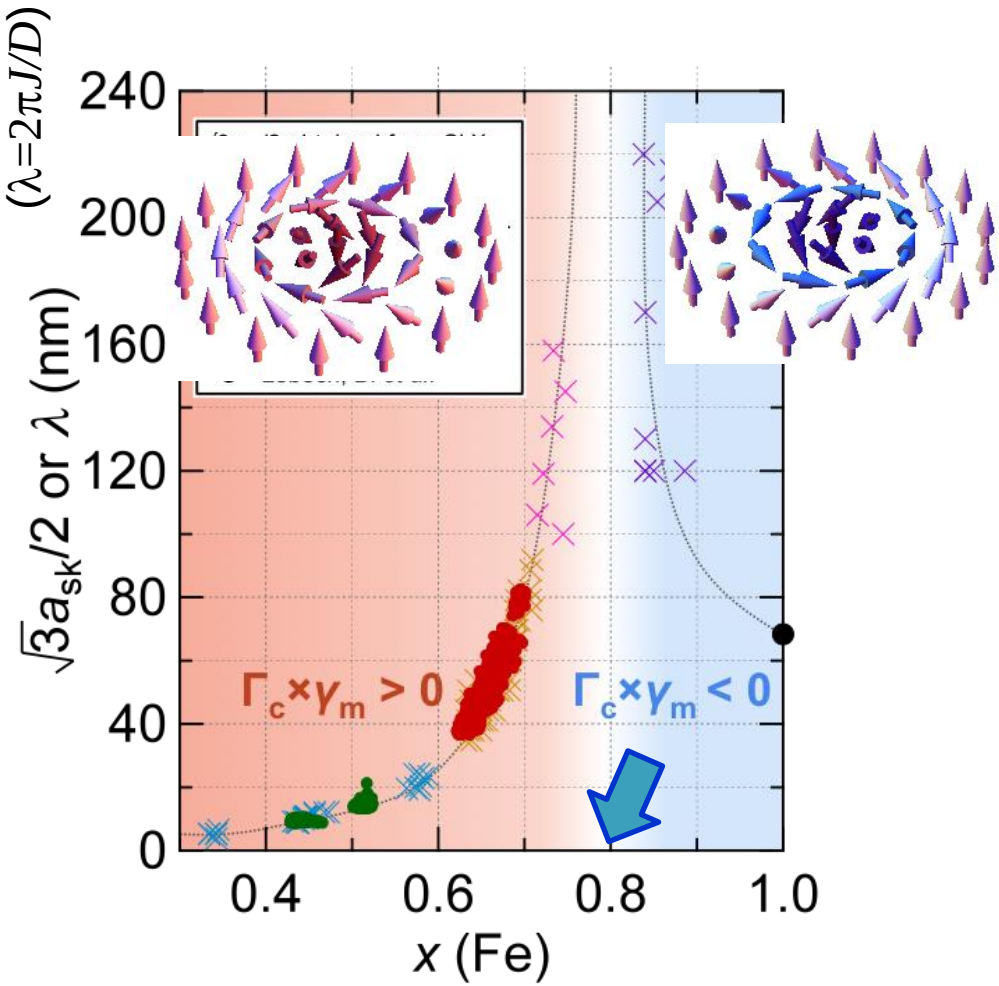
$$\alpha(\mathbf{k},\mathbf{r}) = \alpha(\mathbf{k},\mathbf{r}+\mathbf{R}_n) \quad \beta(\mathbf{k},\mathbf{r}) = \beta(\mathbf{k},\mathbf{r}+\mathbf{R}_n)$$

Calculation of DMI in $Mn_{1-x}Fe_xGe$

Gayles et al., PRL15



K. Shibata *et al.*, Nat. Nanothech13

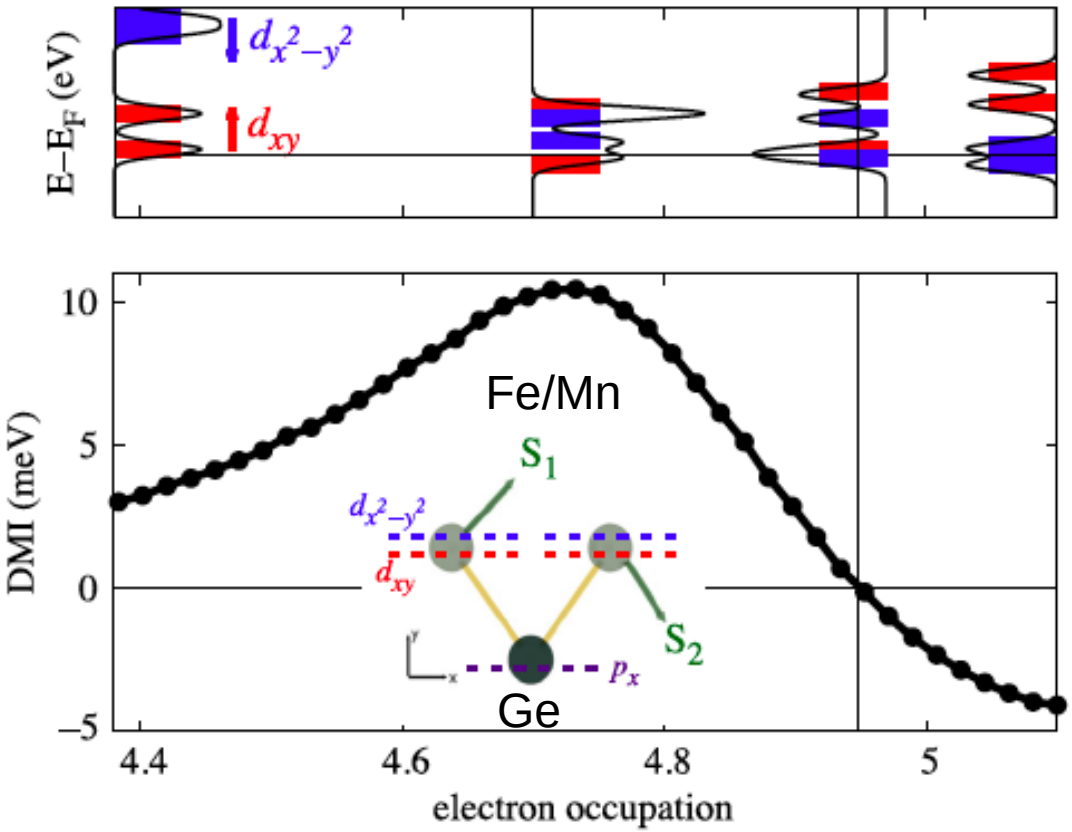


change of the sign of D at the critical concentration x~0.8, which results in the change of magnetic helicity of Skyrmions

→ in excellent agreement with the experimental observations

Mechanism of sign change in DMI

Gayles et al., PRL15



Construct a minimal tight-binding model for a finite trimer system

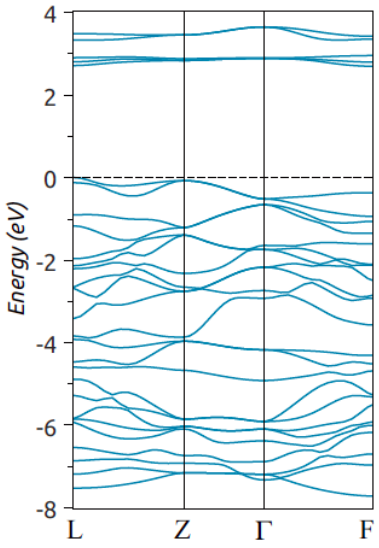
DMI is estimated from the difference in energy between two configurations of S_1 and S_2

Mimic the change of x by changing the electronic occupation of the orbitals, tuning the change in the spin moment and relative positions of the orbitals in accordance with first principles calculations

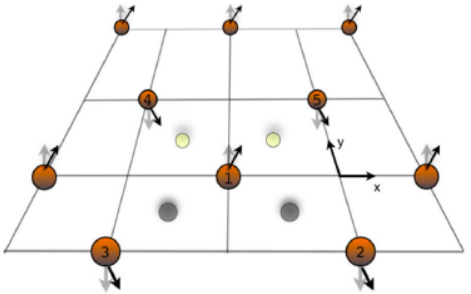
Guiding principles for controlling DMI ?

How to estimate DMI from first principles

DFT



Katsnelson et al., PRB10



Construct a tight-binding model

$$\hat{H} = \hat{H}_t + \hat{H}_u = \sum_{12} c_1^+ t_{12} c_2 + \frac{1}{2} \sum_{1234} c_1^+ c_2^+ U_{1234} c_3 c_4$$

Local rotation $\hat{R}_i = e^{i\delta\vec{\varphi}_i \hat{\vec{J}}_i}$ $\hat{\vec{J}}_i = \hat{\vec{L}}_i + \hat{\vec{S}}_i$

$$\delta\hat{H}_t = \sum_{ij} c_i^+ (\delta\hat{R}_i^+ \hat{t}_{ij} + \hat{t}_{ij}\delta\hat{R}_j) c_j$$

$$\frac{\delta E}{\delta\vec{\varphi}}$$

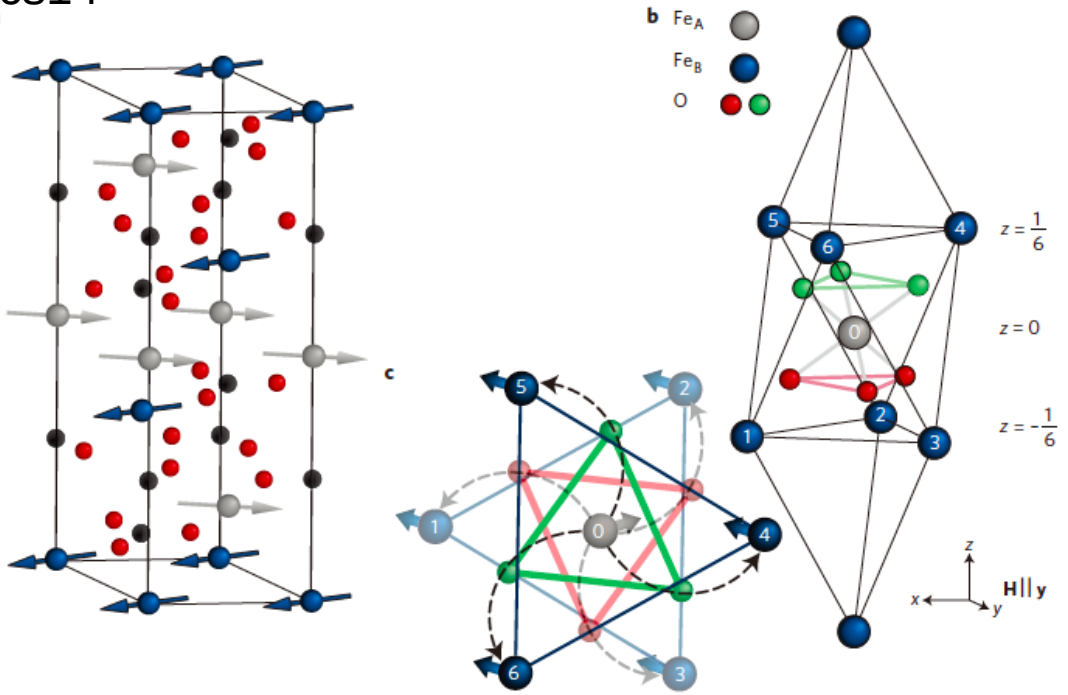
$$\vec{D}_{ij} = -\frac{i}{2}\mathrm{Tr}_{m,\sigma}\langle c_i^+ [\hat{\vec{J}}, \hat{t}_{ij}]_+ c_j \rangle = -\frac{i}{2}\mathrm{Tr}_{m,\sigma} N_{ji} [\hat{\vec{J}}, \hat{t}_{ij}]_+$$

Calculation of DMI in $FeBO_3$

Dmtrienko et al., Nature Physics14

DMI in iron borate (weak ferromagnet)

simple crystal structure, but nontrivial canted and locally twisted magnetic ordering pattern.

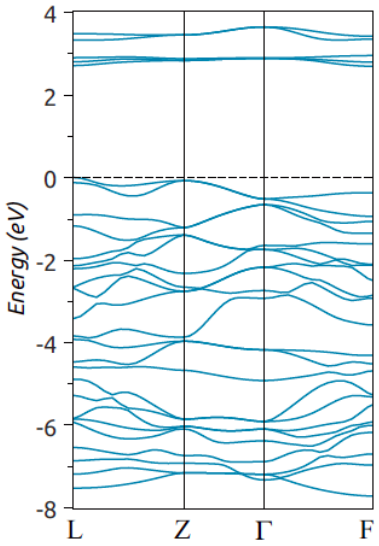


$$\mathbf{D}_{mn} = -\frac{i}{2}\mathrm{Tr}_{L,\sigma}\left\{N_{nm}[\hat{\mathbf{J}}, \hat{t}_{mn}]_+\right\}$$

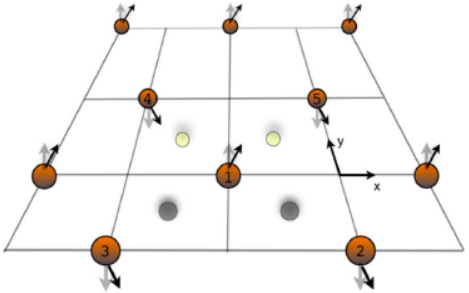
Bond $m-n$	$\mathbf{R}_{mn}$	$\mathbf{D}_{mn}$ (meV)
0-1	(1.0 ; 0.0 ; -0.904)	(-0.25; 0.0; -0.24)
0-2	(-0.5 ; $-\sqrt{3}/2$; -0.904)	(0.12 ; 0.22 ; -0.24)
0-3	(-0.5 ; $\sqrt{3}/2$; -0.904)	(0.12 ; -0.22 ; -0.24)
0-4	(-1.0 ; 0.0 ; 0.904)	(-0.25; 0.0 ; -0.24)
0-5	(0.5 ; $-\sqrt{3}/2$; 0.904)	(0.12 ; -0.22 ; -0.24)
0-6	(0.5 ; $\sqrt{3}/2$; 0.904)	(0.12 ; 0.22 ; -0.24)

How to estimate DMI from first principles

DFT



Katsnelson *et al*., PRB10



Construct a tight-binding model

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$$\vec{D}_{ij} = -\frac{i}{2}\mathrm{Tr}_{m,\sigma}\langle c_i^+ [\hat{\vec{J}}, \hat{t}_{ij}]_+ c_j \rangle = -\frac{i}{2}\mathrm{Tr}_{m,\sigma} N_{ji} [\hat{\vec{J}}, \hat{t}_{ij}]_+$$

Simple expression of D

Real space representation: not convenient to see the relation between the band structure and D

Berry phase formalism for DMI

Freimuth et al., J. Phys. Cond. Matt., 2014

Berry phase formalism for orbital magnetism

Shi *et al*, PRL07

Definition of orbital magnetization density:

$$\boldsymbol{M} = -\frac{1}{V}\left(\frac{\partial \Omega}{\partial \boldsymbol{B}}\right)_{T,\mu}$$

where $\Omega = E - TS - \mu N$ is the thermodynamic grand potential

$$\tilde{\boldsymbol{M}} \equiv -\frac{1}{V}\left(\frac{\partial K}{\partial \boldsymbol{B}}\right)_{T,\mu} \qquad K = E - \mu N \qquad \frac{\partial(\beta \boldsymbol{M})}{\partial \beta} = \tilde{\boldsymbol{M}},$$

$$\delta K(\boldsymbol{r}) = -\tilde{\boldsymbol{M}} \cdot \boldsymbol{B}(\boldsymbol{r}).$$

1st order perturbation

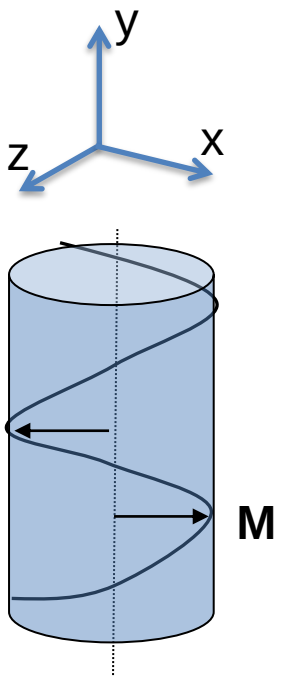
$$\delta K(\boldsymbol{r}) = \mathrm{Re}\sum_{nk}\{\delta f_{nk}\psi^*_{nk}\hat{K}_0\psi_{nk} + f_{nk}\psi^*_{nk}\hat{V}_{\boldsymbol{B}}\psi_{nk} + f_{nk}(\psi^*_{nk}\hat{K}_0\delta\psi_{nk} + \delta\psi^*_{nk}\hat{K}_0\psi_{nk})\}.$$

$$\boldsymbol{M} = \sum_{nk}\left\{\boldsymbol{m}_n(\boldsymbol{k})f_{nk} + \frac{e}{\hbar}\boldsymbol{\Omega}_n(\boldsymbol{k})\frac{1}{\beta}\ln(1 + e^{-\beta(\epsilon_{nk}-\mu)})\right\}$$

$$\boldsymbol{m}_n(\boldsymbol{k}) \equiv (e/2\hbar)i\langle\nabla_{\boldsymbol{k}}u_{nk}|[\epsilon_n(\boldsymbol{k}) - \hat{H}_0(\boldsymbol{k})]\times|\nabla_{\boldsymbol{k}}u_{nk}\rangle$$ Orbital moment

$$\boldsymbol{\Omega}_n(\boldsymbol{k}) = i\langle\nabla_{\boldsymbol{k}}u_n(\boldsymbol{k})|\times|\nabla_{\boldsymbol{k}}u_n(\boldsymbol{k})\rangle$$ Berry curvature

Berry phase formula for DMI



Freimuth et al., J. Phys. Cond. Matt., 14

$$\hat{\mathbf{n}} \sim (\eta \sin(\mathbf{q}\cdot\mathbf{r}), 0, 1)$$

$$\delta\Omega = \sum_j \mathbf{D}_j \cdot \left(\mathbf{n} \times \frac{\partial \hat{\mathbf{n}}}{\partial r_j}\right) = \eta \sum_j (\mathbf{D}_j \cdot \mathbf{e}_y) q_j \cos(\mathbf{q}\cdot\mathbf{r})$$

$$\delta K = \eta \sum_j \frac{\partial}{\partial \beta} \left(\beta (\mathbf{D}_j \cdot \mathbf{e}_y) q_j \cos(\mathbf{q}\cdot\mathbf{r})\right)$$

$$\Leftrightarrow \quad \delta K(\boldsymbol{r}) = -\tilde{\boldsymbol{M}} \cdot \boldsymbol{B}(\boldsymbol{r}).$$

$$D_{ij} = \frac{1}{\mathcal{N}V} \sum_{\mathbf{k}n} \left\{ f_{\mathbf{k}n} A_{\mathbf{k}nij} + \frac{1}{\beta} \ln[1 + \mathrm{e}^{-\beta(\varepsilon_{\mathbf{k}n} - \mu)}] B_{\mathbf{k}nij} \right\}$$

$$A_{\mathbf{k}nij} = \hbar \sum_{m \neq n} \mathrm{Im}\left[\frac{\langle u_{\mathbf{k}n}|\mathcal{T}_i|u_{\mathbf{k}m}\rangle \langle u_{\mathbf{k}m}|v_j(\mathbf{k})|u_{\mathbf{k}n}\rangle}{\varepsilon_{\mathbf{k}m} - \varepsilon_{\mathbf{k}n}}\right] \qquad B_{\mathbf{k}nij} = -2\hbar \sum_{m \neq n} \mathrm{Im}\left[\frac{\langle u_{\mathbf{k}n}|\mathcal{T}_i|u_{\mathbf{k}m}\rangle \langle u_{\mathbf{k}m}|v_j(\mathbf{k})|u_{\mathbf{k}n}\rangle}{(\varepsilon_{\mathbf{k}m} - \varepsilon_{\mathbf{k}n})^2}\right]$$

Torque operator $\quad \mathcal{T} = \frac{\partial H_0}{\partial \theta}\hat{\mathbf{e}}_\phi - \frac{1}{\sin\theta}\frac{\partial H_0}{\partial \phi}\hat{\mathbf{e}}_\theta$

Berry phase formula for orbital magnetization and DMI

Orbital magnetization

$$M(r) = \int \frac{dk}{(2\pi)^d} f(k) m(k) + \frac{1}{\beta} \int \frac{dk}{(2\pi)^d} \frac{e}{\hbar} \Omega(k) \ln(1 + e^{-\beta(\varepsilon - \mu)})$$

$$m(q) = -i \frac{e}{2\hbar} \langle \nabla_q u | \times [H(q) - \varepsilon(q)] | \nabla_q u \rangle$$

Berry curvature

$$\Omega_n(k) = i \langle \nabla_k u_n(k) | \times | \nabla_k u_n(k) \rangle$$

Shi *et al*, PRL07

DMI

$$D_{ij} = \frac{1}{\mathcal{N}V} \sum_{\mathbf{k}n} \left\{ f_{\mathbf{k}n} A_{\mathbf{k}nij} + \frac{1}{\beta} \ln[1 + e^{-\beta(\varepsilon_{\mathbf{k}n} - \mu)}] B_{\mathbf{k}nij} \right\}$$

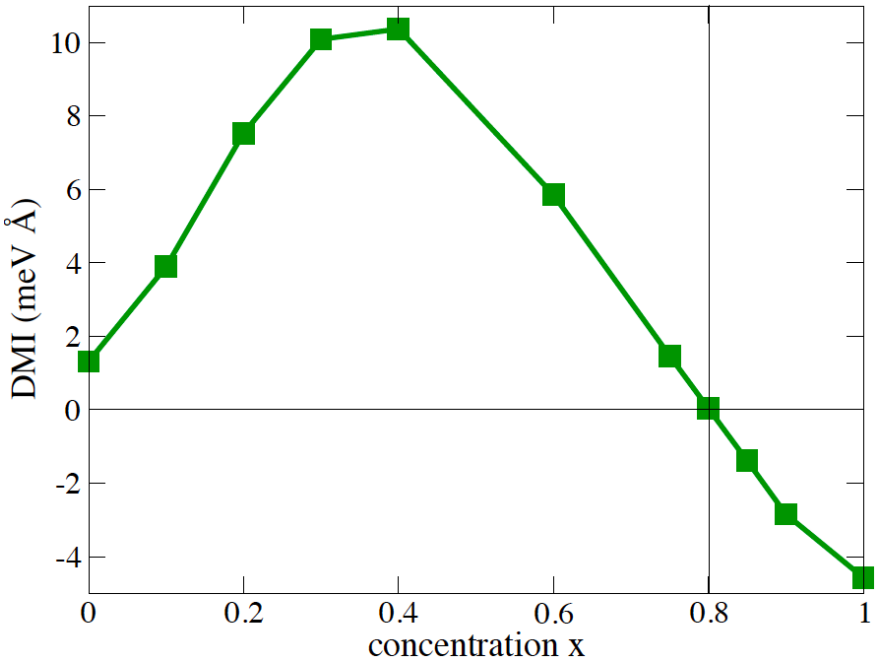
$$A_{\mathbf{k}nij} = -\hat{\mathbf{e}}_i \cdot \left[\hat{\mathbf{e}}_\phi \mathrm{Im} \left\langle \frac{\partial u_{\mathbf{k}n}}{\partial \theta} \middle| (\varepsilon_{\mathbf{k}n} - H_0(\mathbf{k})) \middle| \frac{\partial u_{\mathbf{k}n}}{\partial k_j} \right\rangle - \hat{\mathbf{e}}_\theta \frac{1}{\sin\theta} \mathrm{Im} \left\langle \frac{\partial u_{\mathbf{k}n}}{\partial \phi} \middle| (\varepsilon_{\mathbf{k}n} - H_0(\mathbf{k})) \middle| \frac{\partial u_{\mathbf{k}n}}{\partial k_j} \right\rangle \right],$$

$$B_{\mathbf{k}nij} = -2\hat{\mathbf{e}}_i \cdot \left[\hat{\mathbf{e}}_\phi \mathrm{Im} \left\langle \frac{\partial u_{\mathbf{k}n}}{\partial \theta} \middle| \frac{\partial u_{\mathbf{k}n}}{\partial k_j} \right\rangle - \hat{\mathbf{e}}_\theta \frac{1}{\sin\theta} \mathrm{Im} \left\langle \frac{\partial u_{\mathbf{k}n}}{\partial \phi} \middle| \frac{\partial u_{\mathbf{k}n}}{\partial k_j} \right\rangle \right]$$

Freimuth et al., J. Phys. Cond. Matt., 14

Berry phase formula for DMI

Gayles et al., PRL15

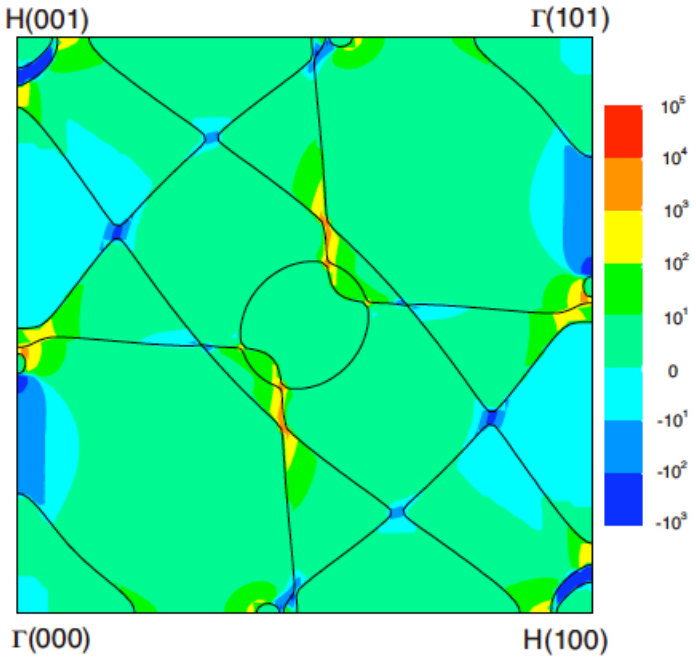


Berry phase formula vs evaluation of the linear term of E(q)

"The two methods coincide in the limit of weak SOI strength for cubic crystals. In the studied B20 compounds the exchange splitting of the order of 1 eV and the SOI of the order of 40~60 meV justifies the use of first order perturbation theory."

Berry phase formula for DMI

$$\boldsymbol{\Omega}_n(\boldsymbol{k}) = i\langle \nabla_{\boldsymbol{k}} u_n(\boldsymbol{k})| \times |\nabla_{\boldsymbol{k}} u_n(\boldsymbol{k})\rangle$$



fcc Fe Yao et al., PRL 2004

Easy to visualize
Convenient to discuss physical quantities such as σ_{xy}
in terms of the band structure

$$A_{\mathbf{k}nij} = -\hat{\mathbf{e}}_i \cdot \left[\hat{\mathbf{e}}_\phi \mathrm{Im} \left\langle \frac{\partial u_{\mathbf{k}n}}{\partial \theta} \middle| (\mathcal{E}_{\mathbf{k}n} - H_0(\mathbf{k})) \middle| \frac{\partial u_{\mathbf{k}n}}{\partial k_j} \right\rangle \right.$$
$$\left. - \hat{\mathbf{e}}_\theta \frac{1}{\sin\theta} \mathrm{Im} \left\langle \frac{\partial u_{\mathbf{k}n}}{\partial \phi} \middle| (\mathcal{E}_{\mathbf{k}n} - H_0(\mathbf{k})) \middle| \frac{\partial u_{\mathbf{k}n}}{\partial k_j} \right\rangle \right],$$

$$B_{\mathbf{k}nij} = -2\hat{\mathbf{e}}_i \cdot \left[\hat{\mathbf{e}}_\phi \mathrm{Im} \left\langle \frac{\partial u_{\mathbf{k}n}}{\partial \theta} \middle| \frac{\partial u_{\mathbf{k}n}}{\partial k_j} \right\rangle \right.$$
$$\left. - \hat{\mathbf{e}}_\theta \frac{1}{\sin\theta} \mathrm{Im} \left\langle \frac{\partial u_{\mathbf{k}n}}{\partial \phi} \middle| \frac{\partial u_{\mathbf{k}n}}{\partial k_j} \right\rangle \right]$$

Visualize ?

How to estimate DMI from first-principles

$$H_{\mathrm{DM}} = D\boldsymbol{S}\cdot(\boldsymbol{\nabla}\times\boldsymbol{S}) = iD\varepsilon^{\alpha\beta\gamma}S^{\alpha}q_{\beta}S^{\gamma}$$

$$\chi^{\alpha\gamma}(q_{\beta}) \propto iDq_{\beta} \quad (q_{\beta}\rightarrow 0)$$

$$\tilde{D}_{\beta} \equiv -\frac{\partial\chi^{\alpha\gamma}(q_{\beta})}{i\partial q_{\beta}}\bigg|_{q_{\beta}\rightarrow 0}$$

- Spin susceptibility at q~0 (long wavelength limit)
- Easy to calculate using DFT

How to estimate DMI from first-principles

- Possible to relate D with the band structure

$$\tilde{D}_\beta = \frac{1}{V}\sum_{\mathbf{k}} \tilde{D}_\beta(\mathbf{k})$$

$$\tilde{D}_\beta(\boldsymbol{k}) = \lim_{\boldsymbol{q}\to 0} \frac{\partial}{i\partial q_\beta} \sum_{n,n'} \frac{f(\varepsilon_{n'\boldsymbol{k}+\boldsymbol{q}}) - f(\varepsilon_{n\boldsymbol{k}})}{\varepsilon_{n'\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{n\boldsymbol{k}}} \times \langle n\boldsymbol{k}|\sigma^\alpha|n'\boldsymbol{k}+\boldsymbol{q}\rangle\langle n'\boldsymbol{k}+\boldsymbol{q}|\sigma^\gamma|n\boldsymbol{k}\rangle,$$

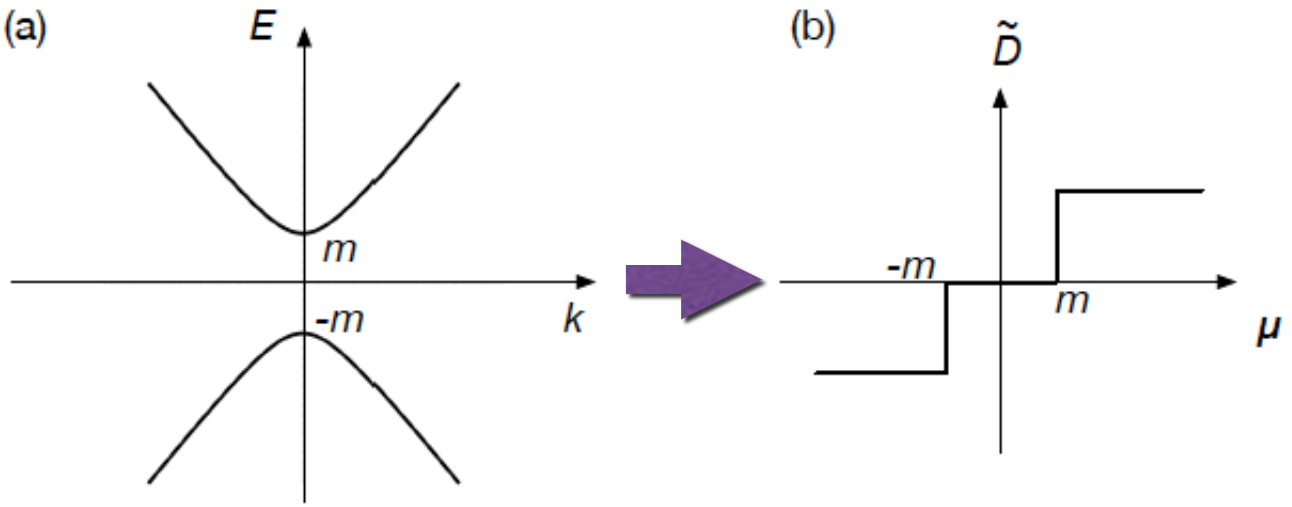
Convenient to see the momentum dependence

Convenient to see the relation between Đ and the band structure

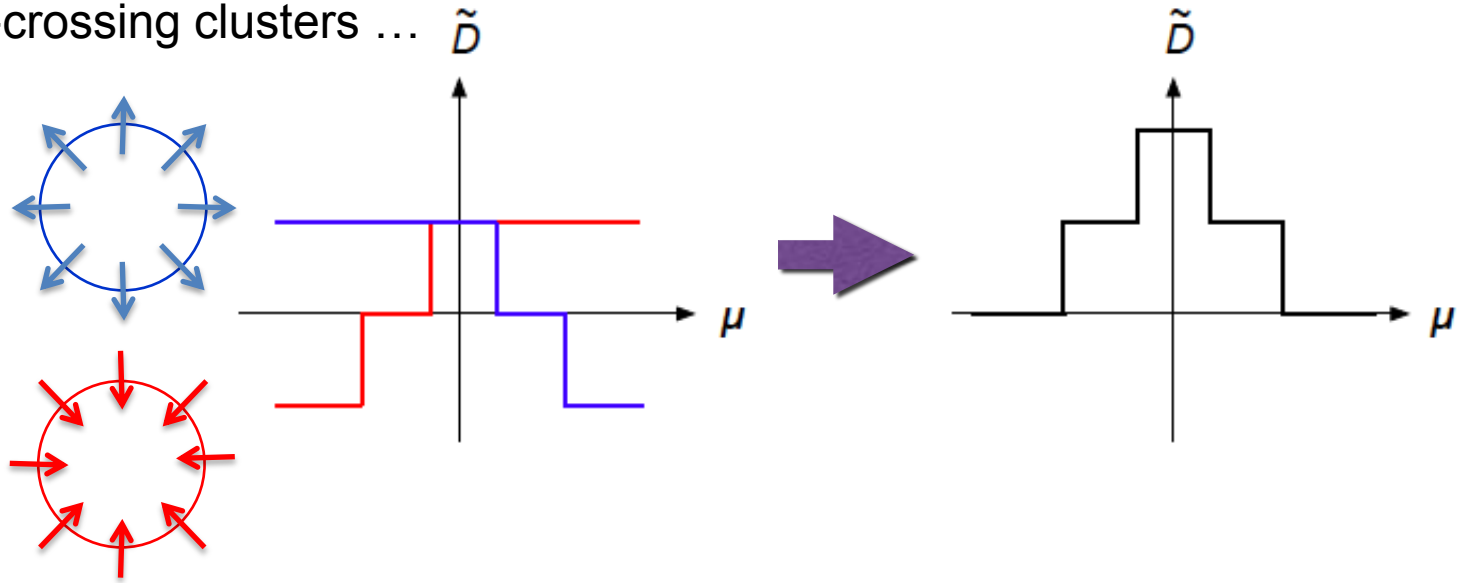
Contribution of band anti-crossing points

2 band model

$$\mathcal{H} = \boldsymbol{k} \cdot \boldsymbol{\sigma} + m\sigma_z$$

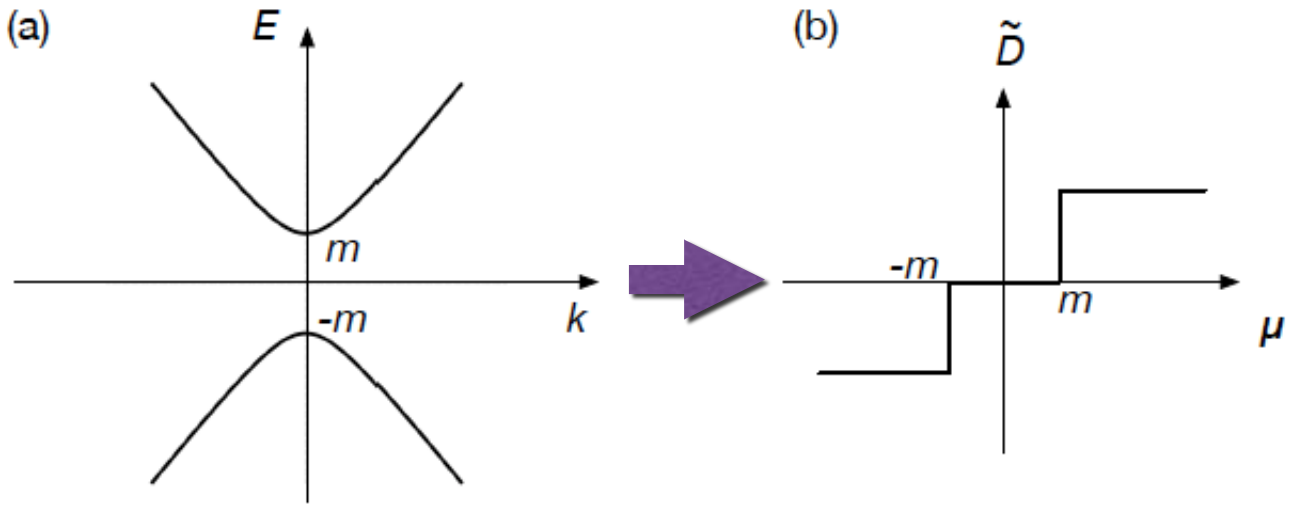


If anti-crossing clusters …

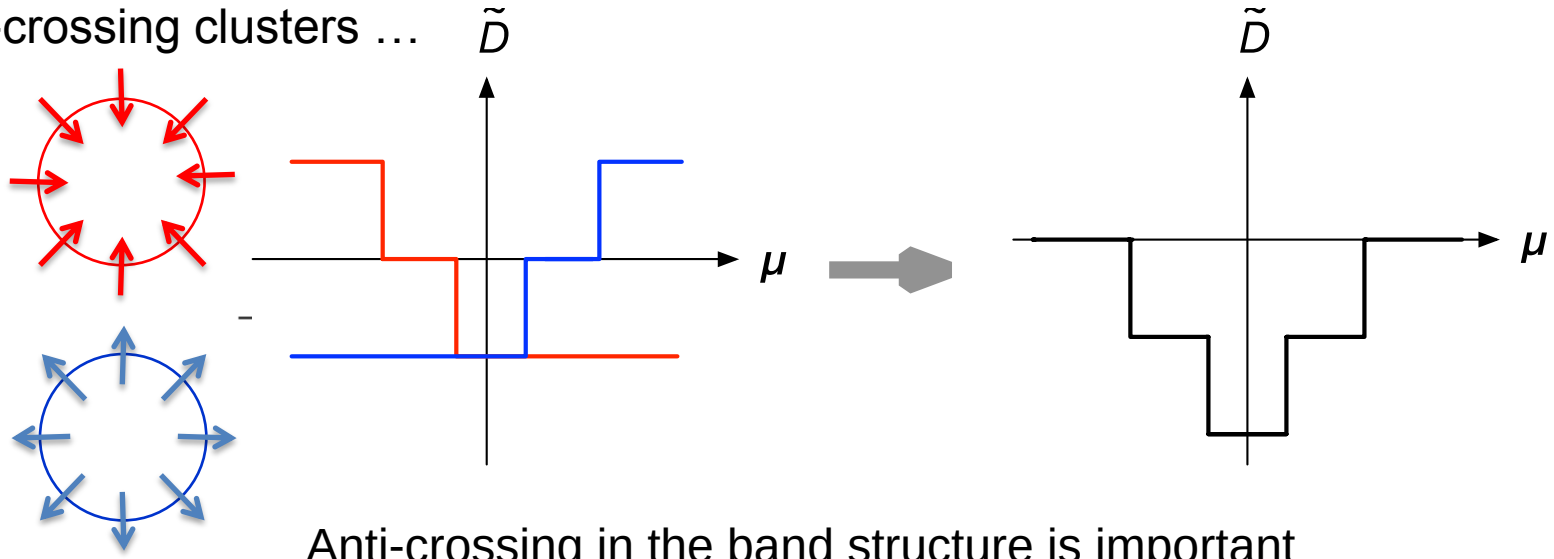


Contribution of band anti-crossing points

2band model (2D case) $\mathcal{H} = \boldsymbol{k} \cdot \boldsymbol{\sigma} + m\sigma_z$



If anti-crossing clusters …



Anti-crossing in the band structure is important

Anomalous Hall Effect

Onoda, Sugimoto, Nagaosa, PRL2006

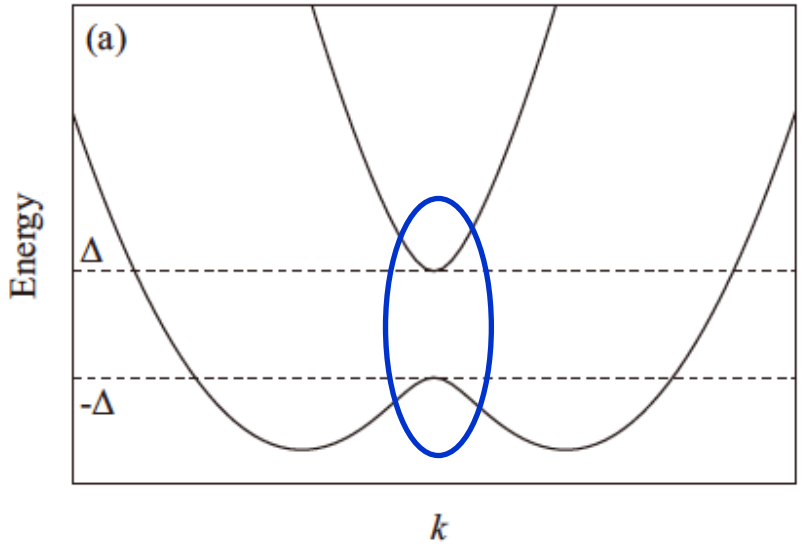
$$H = \frac{\hbar^2 k^2}{2m} + \lambda(\boldsymbol{k} \times \boldsymbol{\sigma}) \cdot \boldsymbol{e}_z - \Delta\sigma_z$$

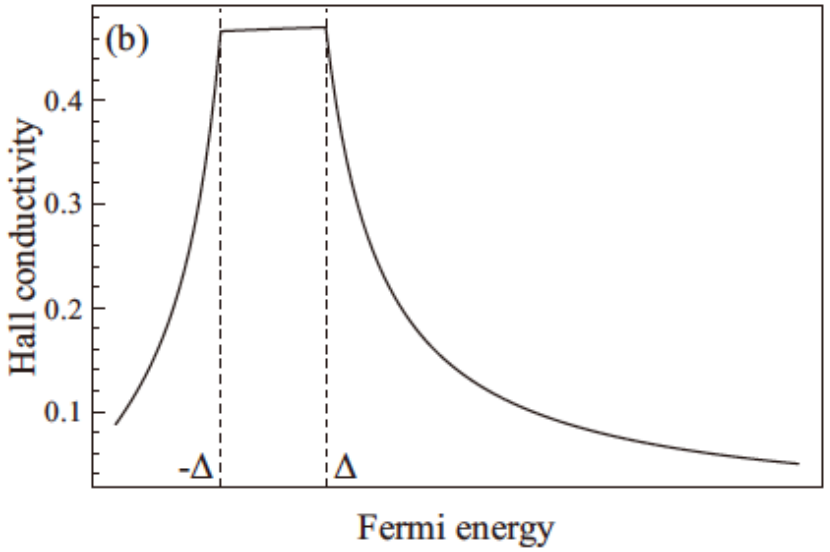
Berry curvature

$$\Omega_{\pm} = \mp \frac{\lambda^2 \Delta}{2(\lambda^2 k^2 + \Delta^2)^{3/2}}$$

Hall conductivity

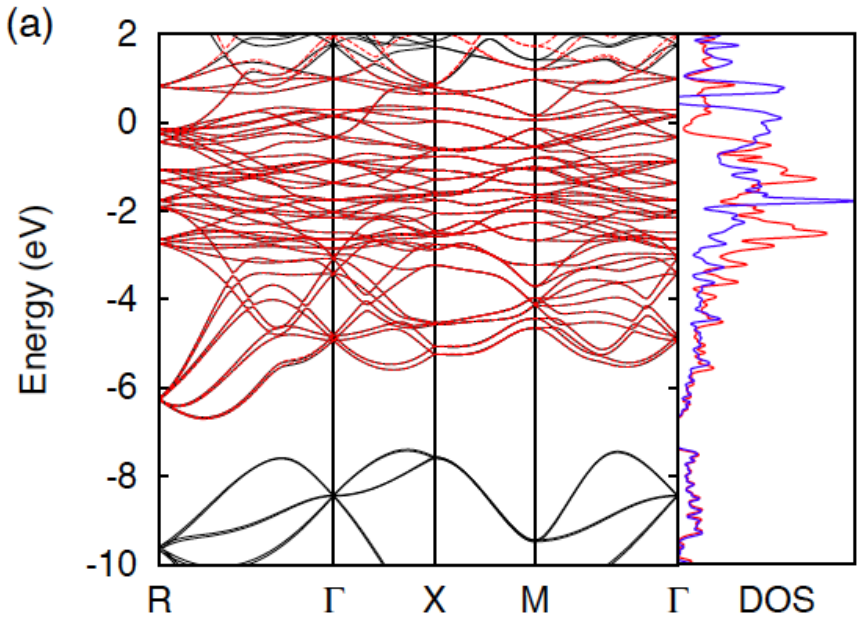
$$\sigma_{xy} = \frac{e^2}{\hbar} \int \frac{dk}{(2\pi)^d} f(\varepsilon_k) \Omega_{k_x k_y}$$

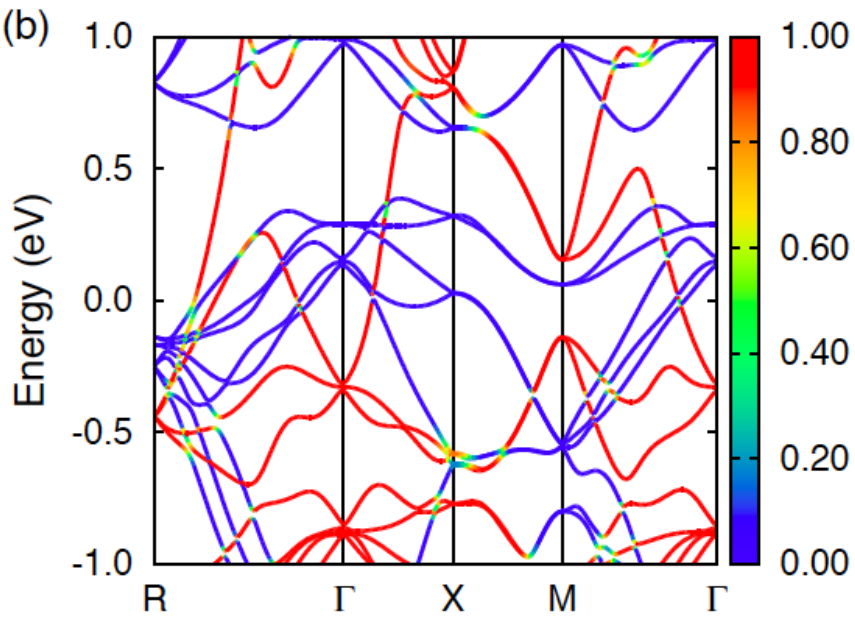




Anti-crossing in the band structure is important

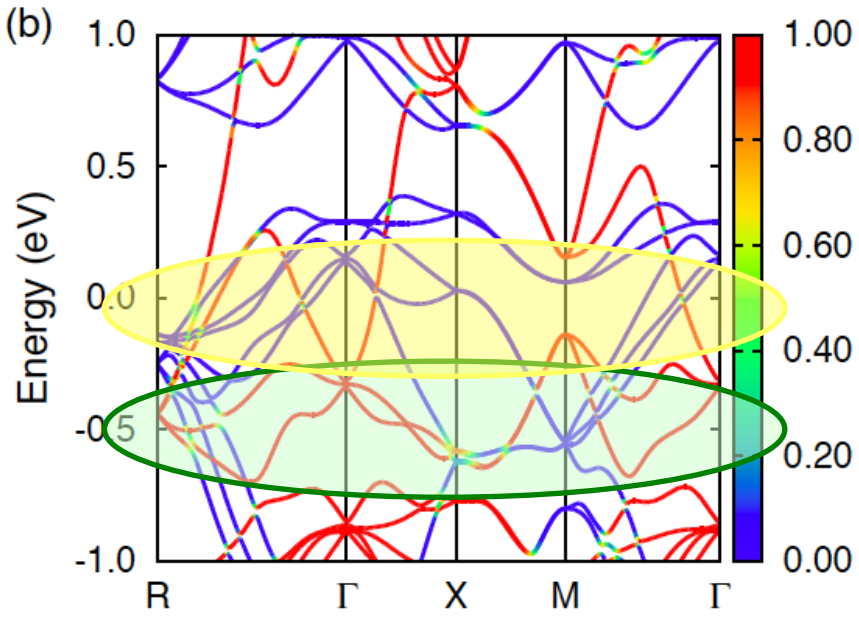
Band structure & DOS of FeGe

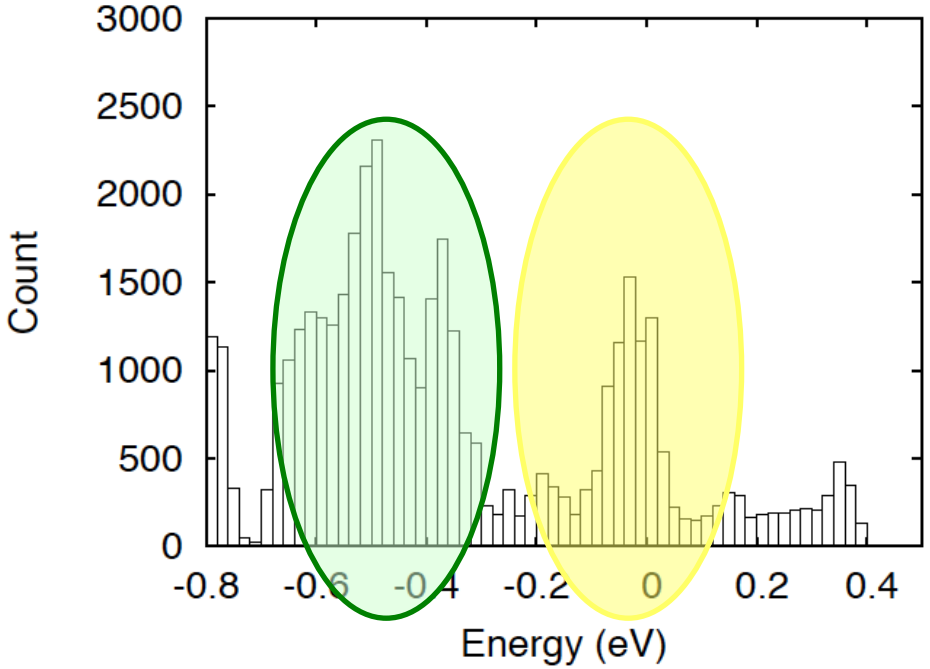




Detailed band structure around the Fermi level with colors representing the weight of up spin

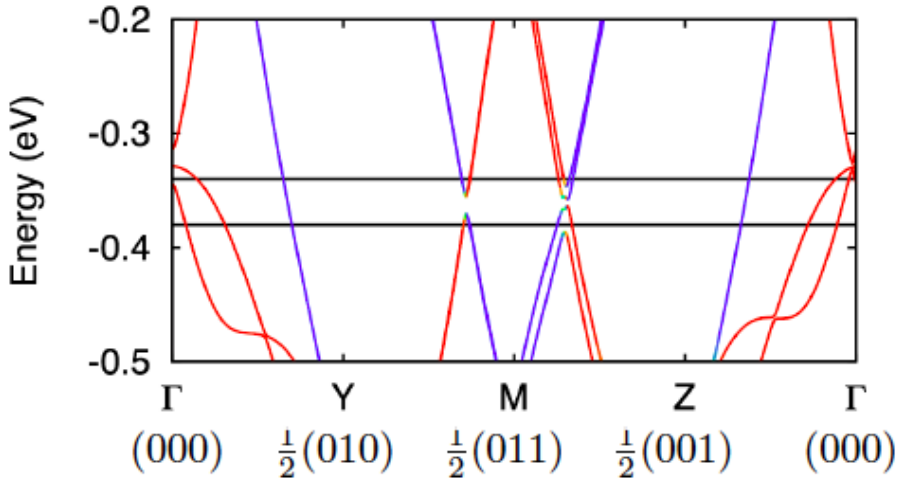
Distribution of band anti-crossing points





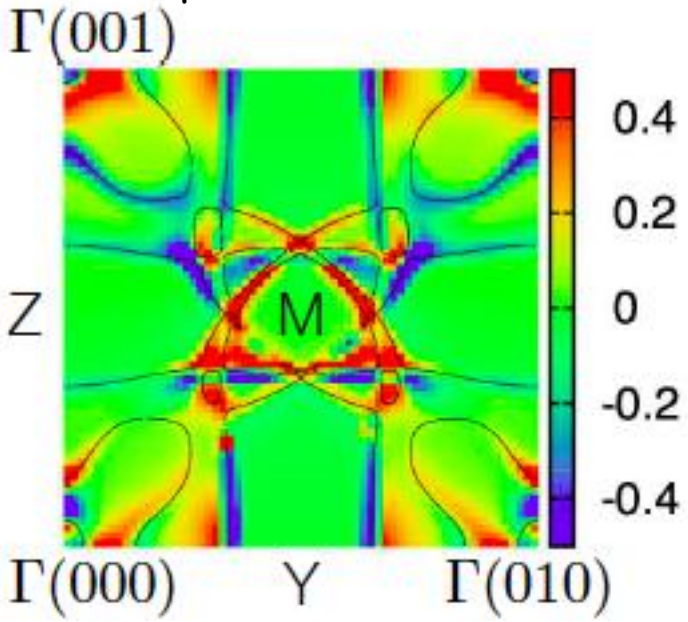
Number of k points in 64 × 64 × 64 mesh where the up-spin weight, **w↑**, satisfies **0.4 <w↑ < 0.6**.

Momentum dependence of $\tilde{D}(k)$

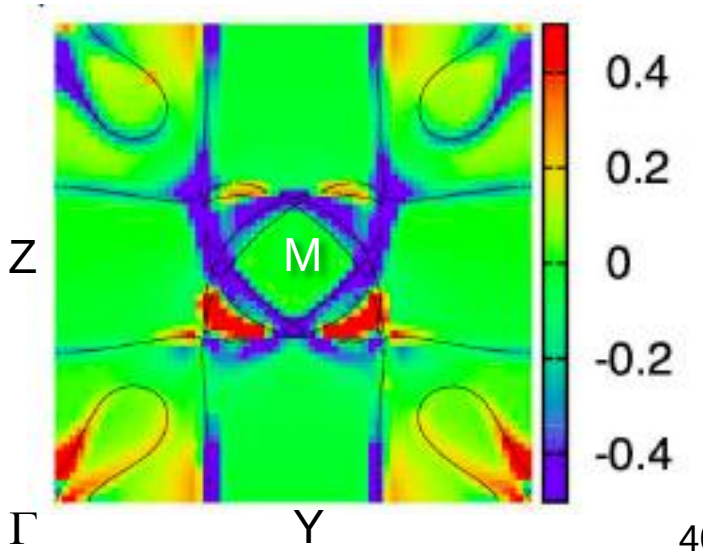


Band anti-crossing point is important

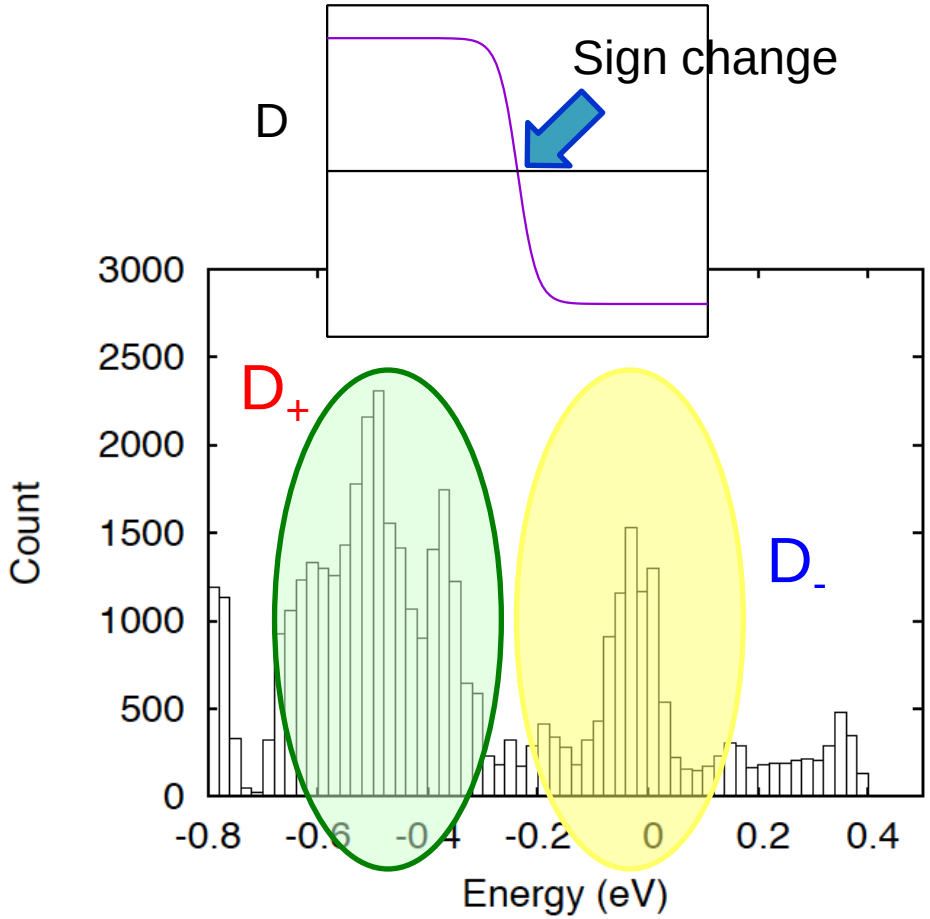
μ=-0.38 eV



μ=-0.34 eV

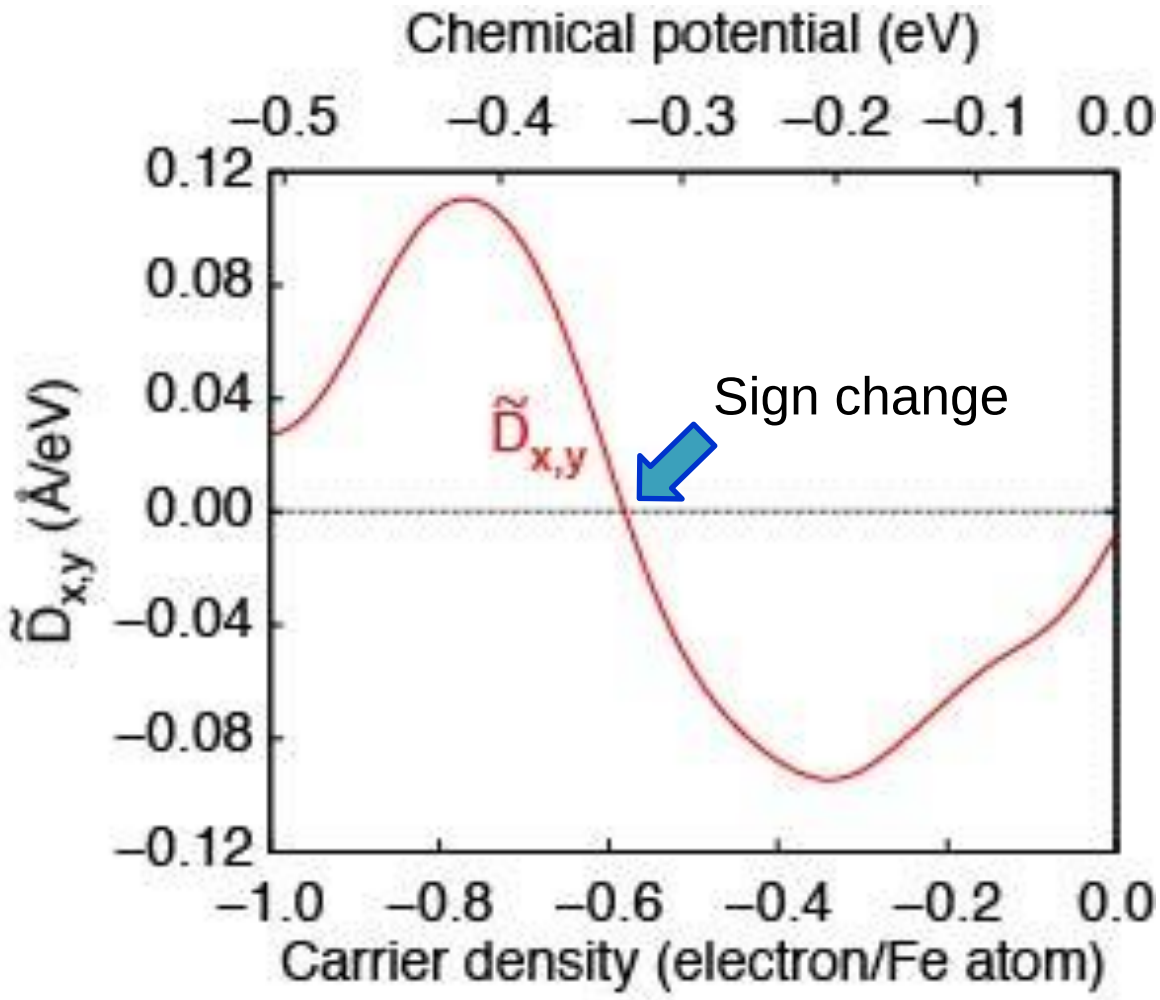


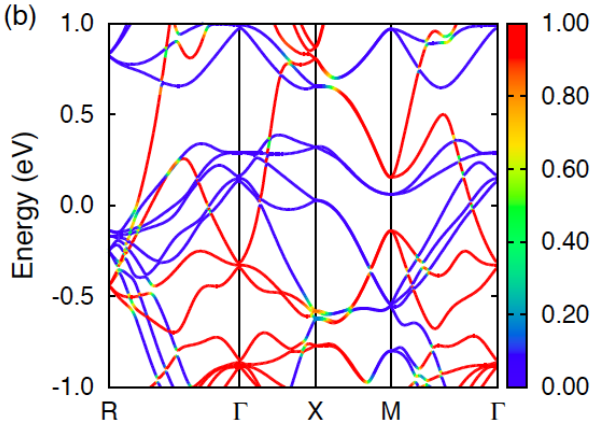
Distribution of band anti-crossing points



If $\tilde{D}_+$ and $\tilde{D}_-$ resides next to each other as a function of energy, then D should change its sign as a function of E_F

Cannier density dependence of $\tilde{D}$



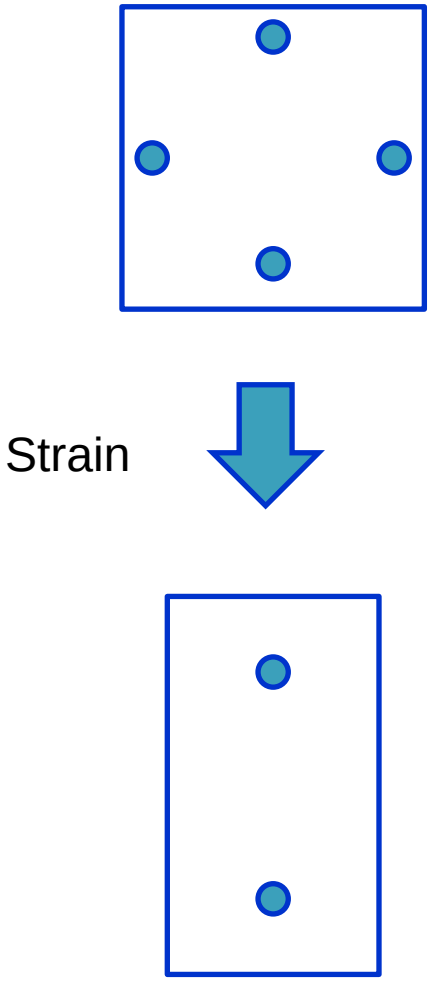


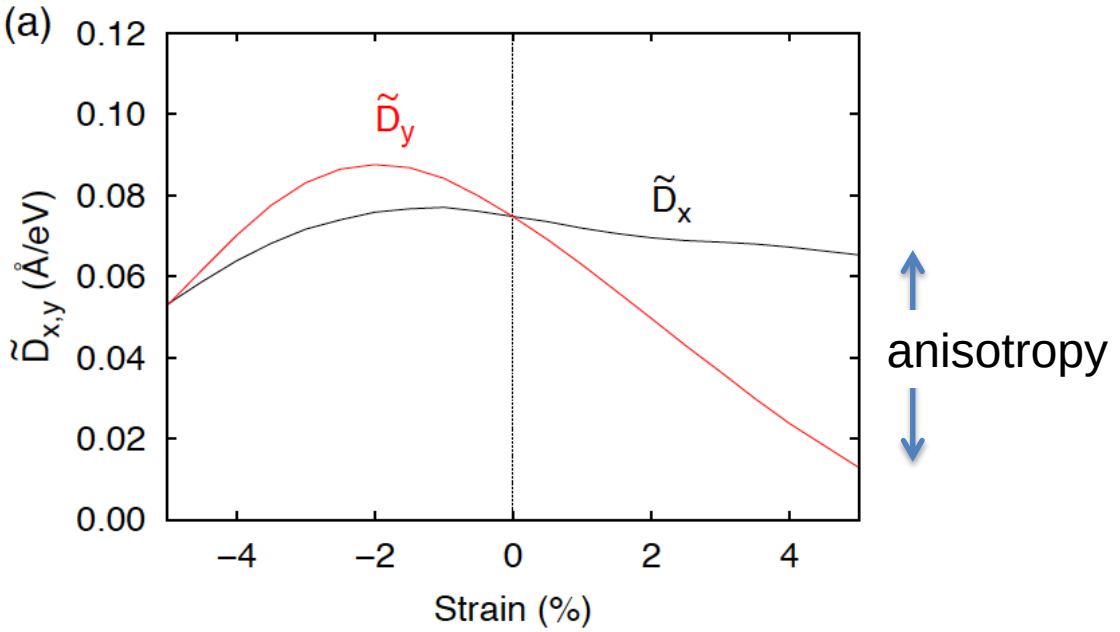
$\tilde{D}$ has opposite sign for MnGe and FeGe

Semi-quantitative description of sign change in D

Gigantic anisotropy induced by strain

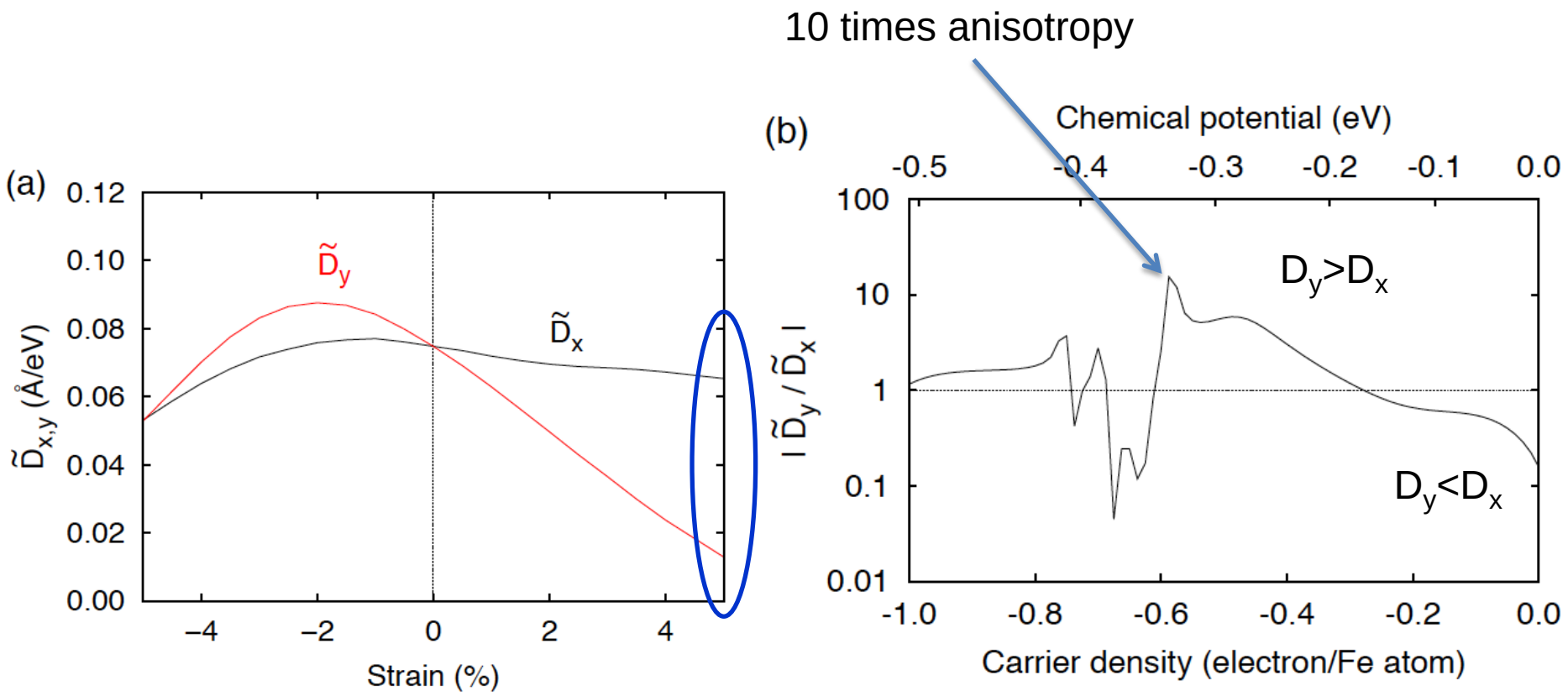
Distribution of anti-crossing points in BZ



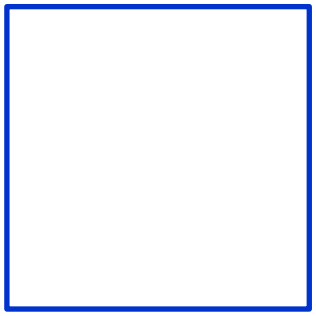


Gigantic anisotropy induced by strain

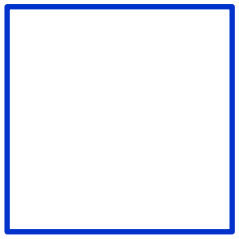
Doping dependence of anisotropy



Another possibility to control D̃

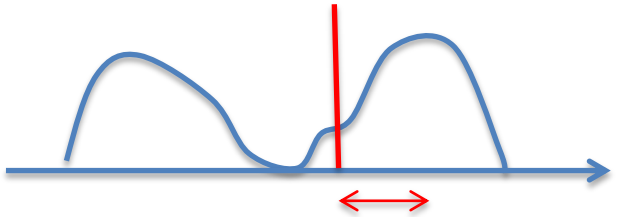


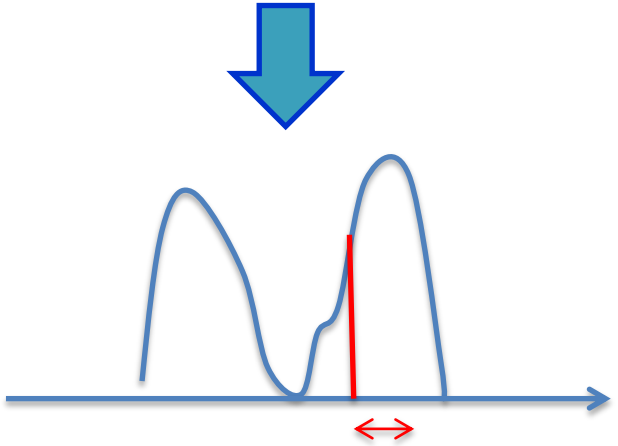
compress



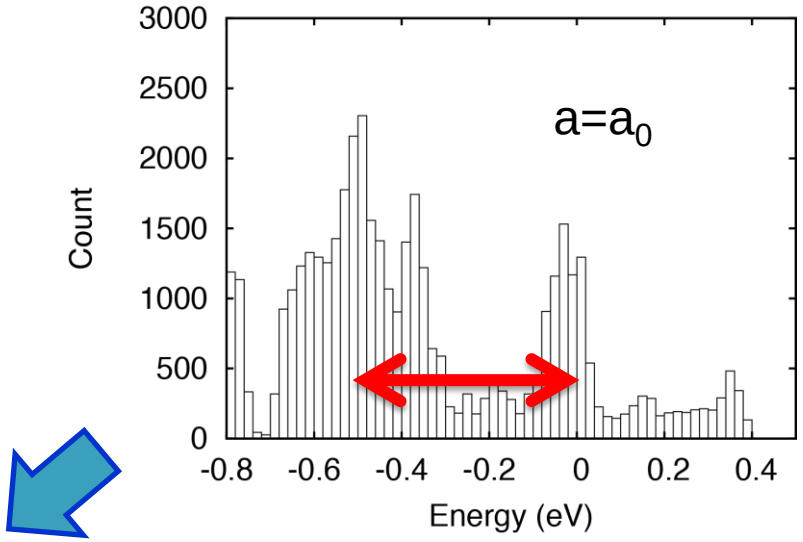
Transfer hopping
→ larger
Correlation
→ weaker
Exchange splitting
→ smaller

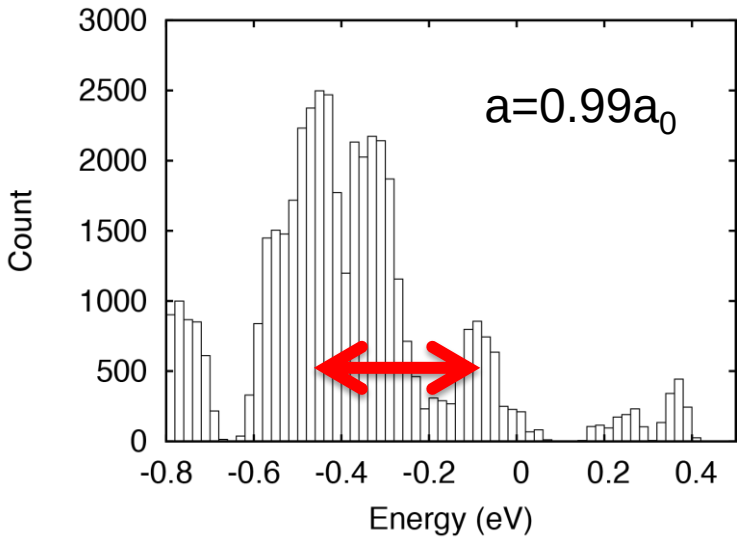
Distribution of band anti-crossing points



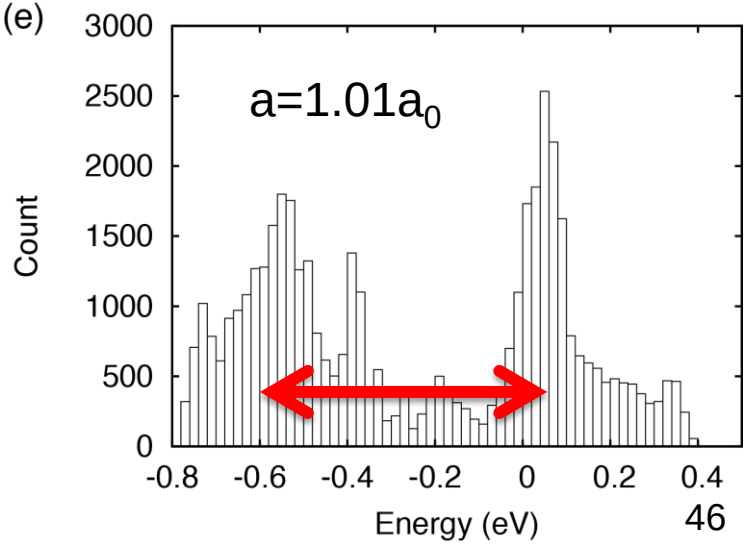


Distribution of band anti-crossing points

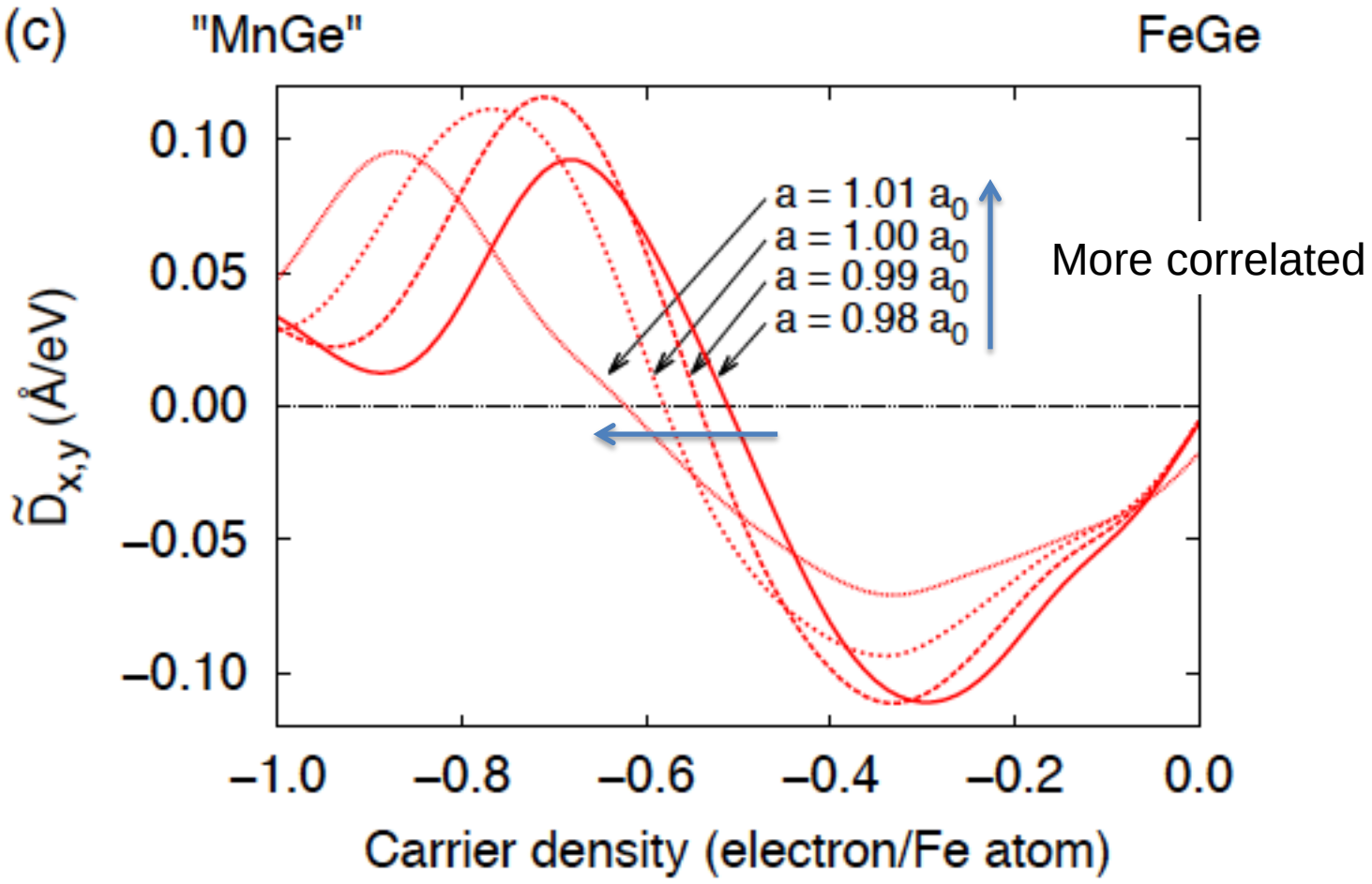




(e)



a_0 / carrier density dependence of $\tilde{D}$



Summary

- Size & helicity change of the DM interaction in $Mn_{1-x}Fe_xGe$ reproduced
- Distribution of the band anti-crossing points is important
- Huge anisotropy will be induced by applying strain to the system
- Control of D → Skyrmion crystal engineering