Cluster multipole theory for anomalous Hall effect in antiferromagnets

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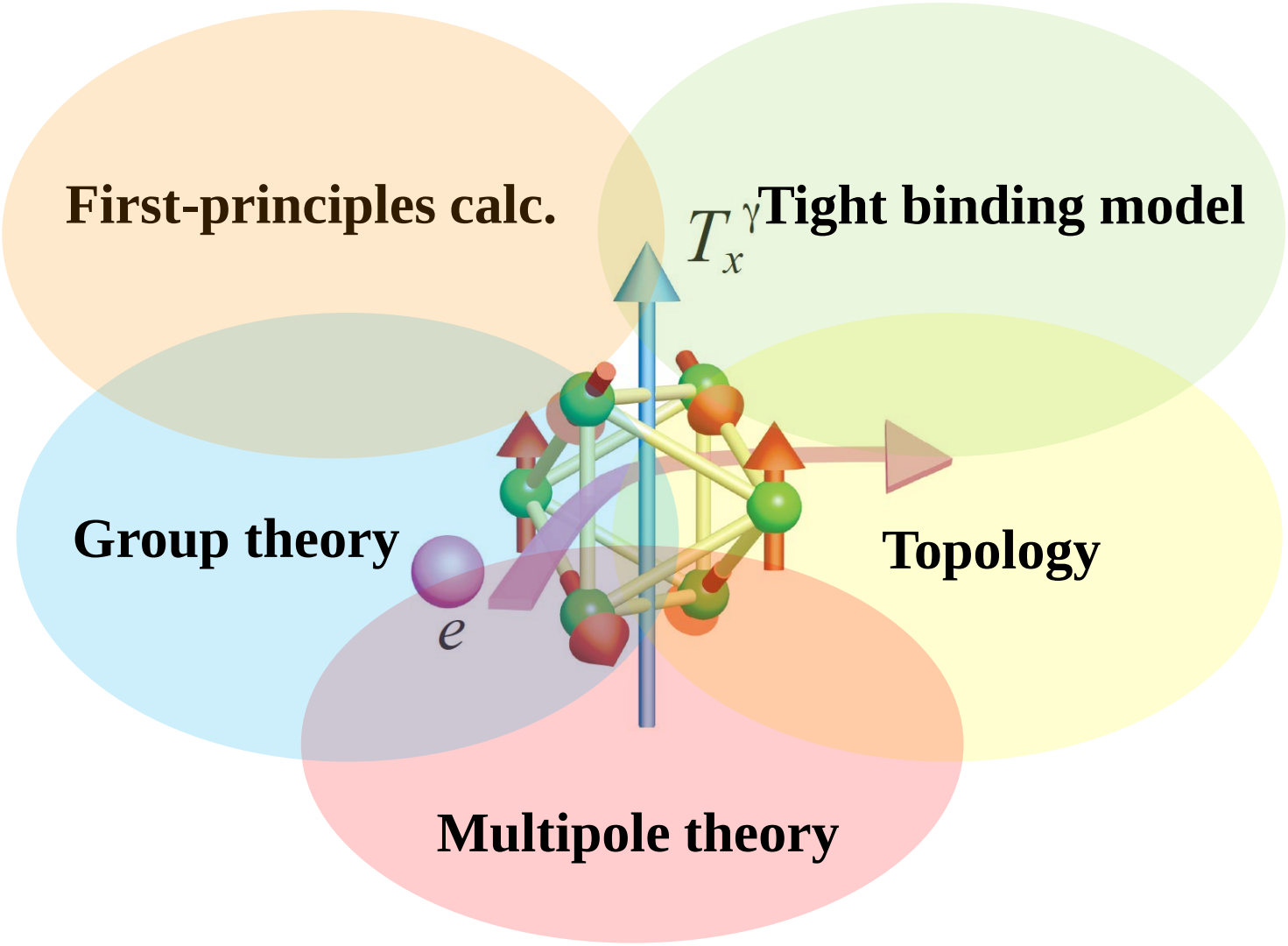
Osaka Univ.　Masayuki Ochi

MTS, T. Koretsune, M. Ochi, R. Arita, Phys. Rev. B **95**, 094406 (2017).

First-principles analysis



Anomalous Hall effect (AHE)

Hall effect induced without applied magnetic fields in magnetic compounds.

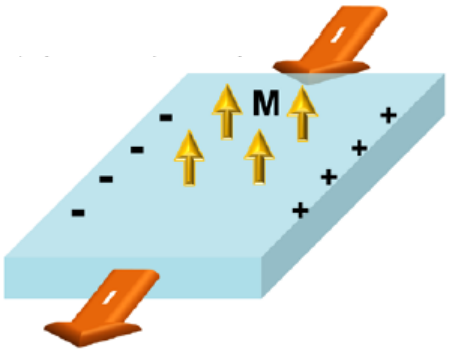


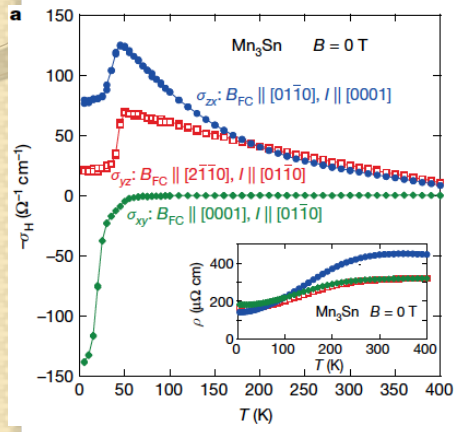
Figure from C.-Z. Chang and M. Li. (2016)

Anomalous Hall conductivity (AHC) had been believed to depend directly on the magnetization of materials.

AHE in antiferromagnets Mn_3Z (Z=Sn, Ge)

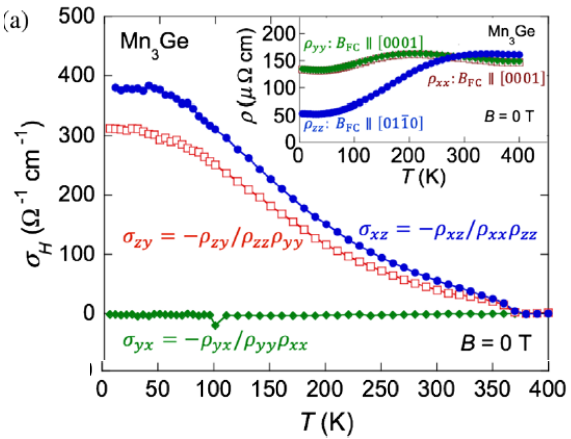
Large AHC was observed for the AFM states only with tiny magnetization !!

Mn_3Sn (M~0.002μ_B/Mn)



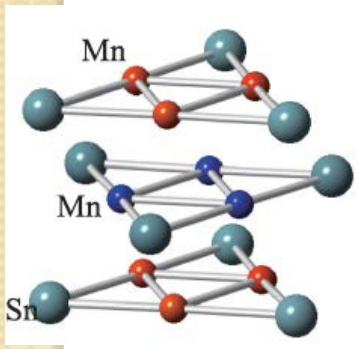
Nakatsuji, Kiyohara, Higo, Nature **527**, 212 (2015).

Mn_3Ge (M~0.007μ_B/Mn)



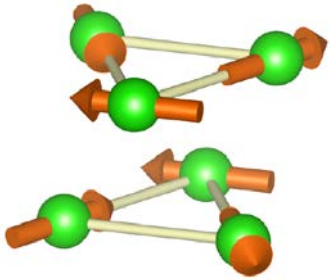
Kiyohara, Tomita, Nakatsuji, Phys. Rev. Appl. **5**, 064009 (2016).
A.K. Nayak et al, Science Advances **2**, e1501870 (2016).

Crystal structure



Hexagonal
S.G.: $P6_3mmc$ (No. 194)

Magnetic config. on Mn atoms



What is the mechanism of the AHE in antiferromagnets?

Anomalous Hall conductivity & Topology

Intrinsic anomalous hall conductivity (AHC)

$$\sigma_{\alpha\beta} = -\frac{e^2}{\hbar}\int \frac{d\mathbf{k}}{(2\pi)^3}\sum_n f(\varepsilon_n(\mathbf{k}))\boxed{\Omega_{n,\alpha\beta}(\mathbf{k})}$$

Berry curvature

n: Band index
α, β = x,y,z

Berry curvature

$$\Omega_{n,\alpha\beta}(\mathbf{k}) = -2\mathrm{Im}\sum_{m\neq n}\frac{v_{nm,\alpha}(\mathbf{k})v_{mn,\beta}(\mathbf{k})}{[\varepsilon_{m,\mathbf{k}}-\varepsilon_{n,\mathbf{k}}]^2}$$

$$v_{nm,\alpha}(\mathbf{k}) = \frac{1}{\hbar}\left\langle u_{n\mathbf{k}}\left|\frac{\partial\hat{H}(\mathbf{k})}{\partial k_\alpha}\right|u_{m\mathbf{k}}\right\rangle$$

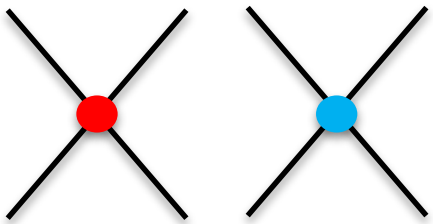
$$\hat{H}(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\hat{H}e^{i\mathbf{k}\cdot\mathbf{r}}$$

Wang. *et al*. Phys. Rev. B **74**, 195118 (2006)

Berry curvature characterizes *topology* of electronic structure.

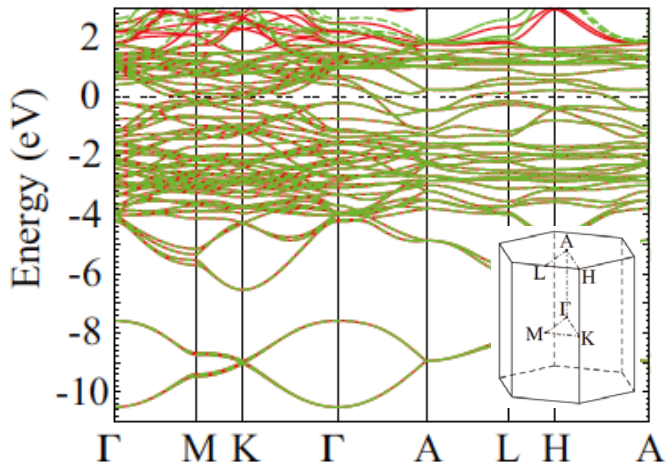
Chirality of Weyl node

$$\mathcal{C}_n(\mathcal{S}) = \frac{1}{2\pi}\oint_{\mathcal{S}} dS\hat{\mathbf{n}}\cdot\mathbf{\Omega}_n(\mathbf{k})$$



First-principles calculation (Quantum Espresso) → Tight binding model (Wannier90)

Band structure of AFM state in Mn_3Sn



Mn (s, d) & Sn (s, p)
88 orbital model

Red: Band calc.
Green: Tight binding

Berry curvature

$$\Omega_{n,\alpha\beta}(\mathbf{k}) = -2\mathrm{Im}\sum_{m\neq n}\frac{<u_{n,\mathbf{k}}|\partial_\alpha H(\mathbf{k})|u_{m,\mathbf{k}}><u_{m,\mathbf{k}}|\partial_\beta H(\mathbf{k})|u_{n,\mathbf{k}}>}{[\varepsilon_{m,\mathbf{k}}-\varepsilon_{n,\mathbf{k}}]^2}$$

Anomalous hall conductivity

$$\sigma_{\alpha\beta} = -\frac{e^2}{\hbar}\int\frac{d\mathbf{k}}{(2\pi)^3}\sum_n f(\varepsilon_n(\mathbf{k}))\Omega_{n,\alpha\beta}(\mathbf{k})$$

m, n: band index
k: wave number
α, β=x,y,z

Anomalous Hall conductivity of Mn_3Sn

	AHC	Mn Magnetic mom.
This work	129 (S/cm)	3.39 μ_B
Zhang *et al*. (2016)	133 (S/cm)	
Experiment	~100 (S/cm)	~ 3 μ_B

(Nakatsuji, Kiyohara, Higo, Nature (2015))

Agreement is good, but why can AHC be finite without net magnetization?

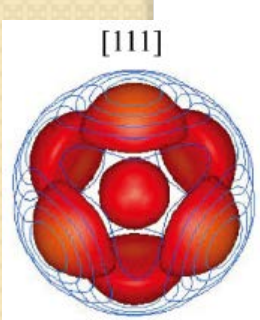
Cluster multipole theory

Magnetic multipole moment

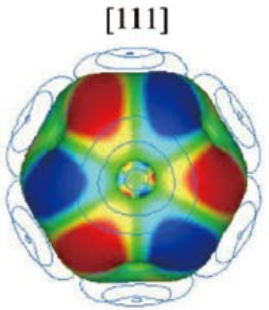
$$M_{\ell m} = \sqrt{\frac{4\pi}{2\ell+1}} \int d\boldsymbol{r} \nabla_i (r^\ell Y_{\ell m}(\hat{\boldsymbol{r}})^*) \cdot \boldsymbol{m}(\boldsymbol{r})$$

$\boldsymbol{m}(\boldsymbol{r})$: Magnetic density around an atom

Kusunose, J. Phys. Soc. Jpn. 77, 064710 (2008)



Magnetic dipole (ℓ=1)



Higher order multipole (ℓ >1)

MTS, Magnani, Oppeneer, Phys. Rev. B 88, 195146 (2013)

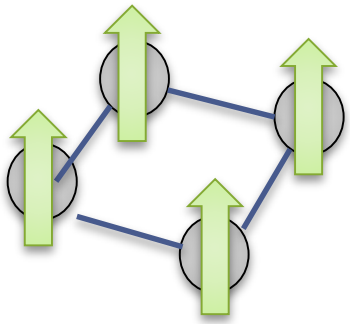
Characterize magnetic *distribution* around atom.

Cluster multipole (CMP) moment

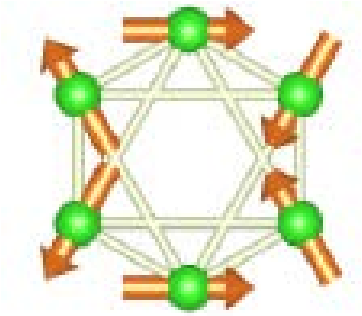
$$M_{\ell m} \equiv \sqrt{\frac{4\pi}{2\ell+1}} \sum_{i=1}^{N} \nabla_i (R_i^\ell Y_{\ell m}(\hat{\boldsymbol{R}}_i)^*) \cdot \boldsymbol{m}_i$$

$\boldsymbol{m}_i$: Magnetic moment on *i* th atom

MTS, T. Koretsune, M. Ochi, R. Arita, Phys. Rev. B (2017)



Dipole CMP (ℓ=1)



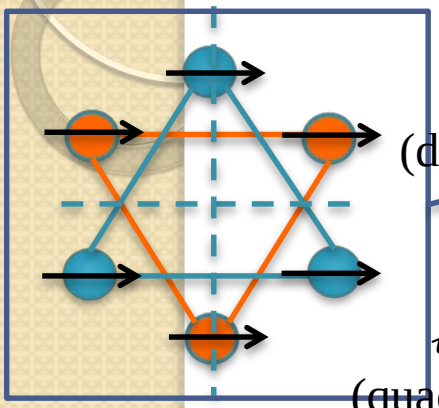
Higher order CMP (ℓ >1)

Characterize magnetic *configuration* in atom cluster.

Cluster multipole moments for Mn_3Sn

Multipole moments in Hexagonal axis (IREP. of D_{6h})

FM1

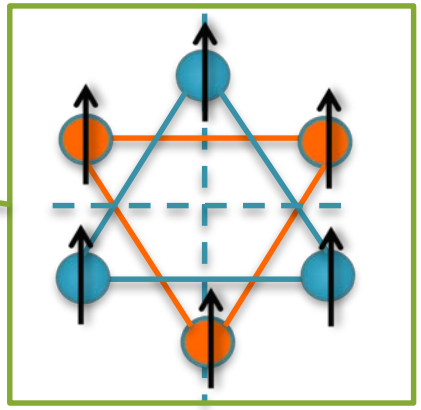


ℓ=1 (dipole)

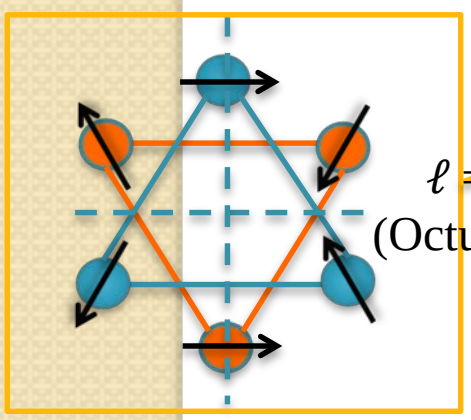
ℓ=2 (quadrupole)

IREP	CMP
A_{2g}	$J_z \equiv M_{10}$
E_{1g}	$J_x \equiv \frac{1}{\sqrt{2}}(-M_{11} + M_{1-1})$
	$J_y \equiv \frac{i}{\sqrt{2}}(M_{11} + M_{1-1})$
A_{1u}	$Q_{3z^2-r^2} \equiv M_{20}$
E_{2u}	$Q_{x^2-y^2} \equiv \frac{1}{\sqrt{2}}(M_{22} + M_{2-2})$
	$Q_{xy} \equiv \frac{i}{\sqrt{2}}(-M_{22} + M_{2-2})$
E_{1u}	$Q_{zx} \equiv \frac{1}{\sqrt{2}}(-M_{21} + M_{2-1})$
	$Q_{yz} \equiv \frac{i}{\sqrt{2}}(M_{21} + M_{2-1})$
A_{2g}	$T_z^{\alpha} \equiv M_{30}$
E_{1g}	$T_x^{\gamma} \equiv \frac{1}{\sqrt{2}}(-M_{31} + M_{3-1})$
	$T_y^{\gamma} \equiv \frac{i}{\sqrt{2}}(M_{31} + M_{3-1})$
E_{2g}	$T_{xyz} \equiv \frac{i}{\sqrt{2}}(-M_{32} + M_{3-2})$
	$T_z^{\beta} \equiv \frac{1}{\sqrt{2}}(M_{32} + M_{3-2})$
B_{2g}	$T_x^{\zeta} \equiv \frac{1}{\sqrt{2}}(-M_{33} + M_{3-3})$
B_{1g}	$T_y^{\zeta} \equiv -\frac{i}{\sqrt{2}}(M_{33} + M_{3-3})$

FM2

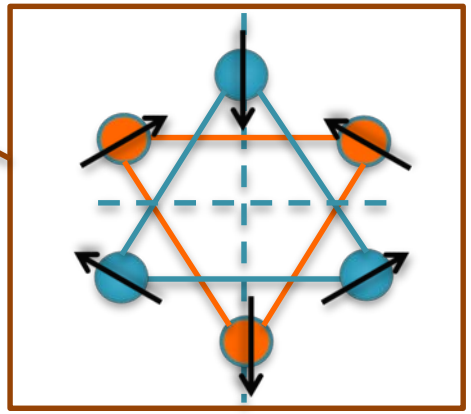


Mn_3Sn-AFM1



ℓ =3 (Octupole)

Mn_3Sn-AFM2



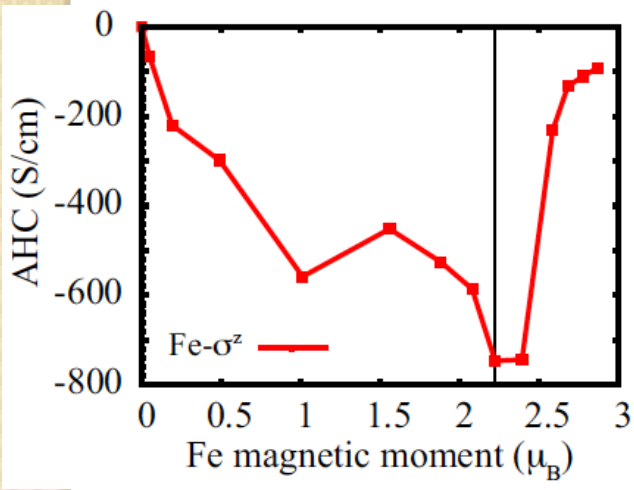
E_{1g}-octupole moments break the same symmetry as that of dipole moments.

Multipole moments dependence of AHC

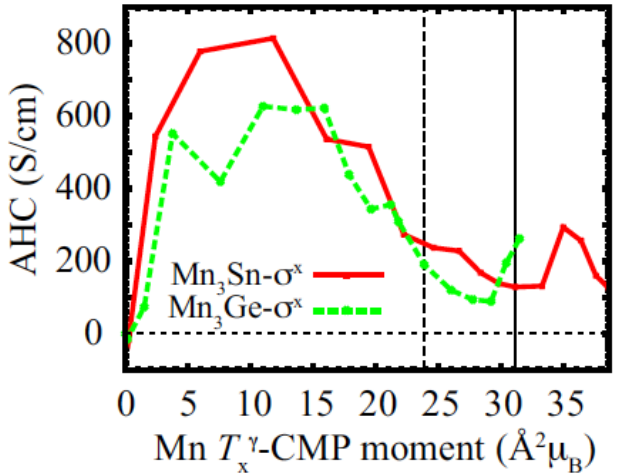
Interpolation of nonmagnetic and magnetic hopping Hamiltonians.

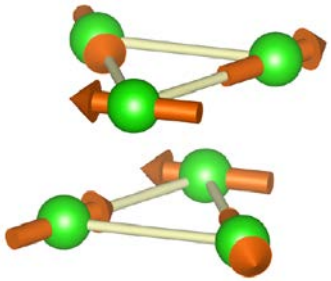
$$H_\lambda = H_{\mathrm{nonmag}} + \lambda(H_{\mathrm{mag}} - H_{\mathrm{nonmag}}) \ (\lambda \geq 0)$$

FM state of bcc-Fe



AFM state of Mn_3Sn

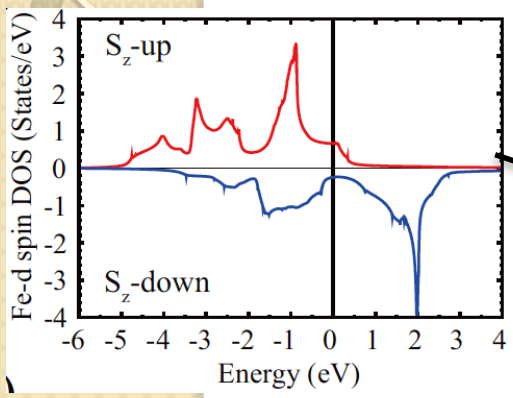


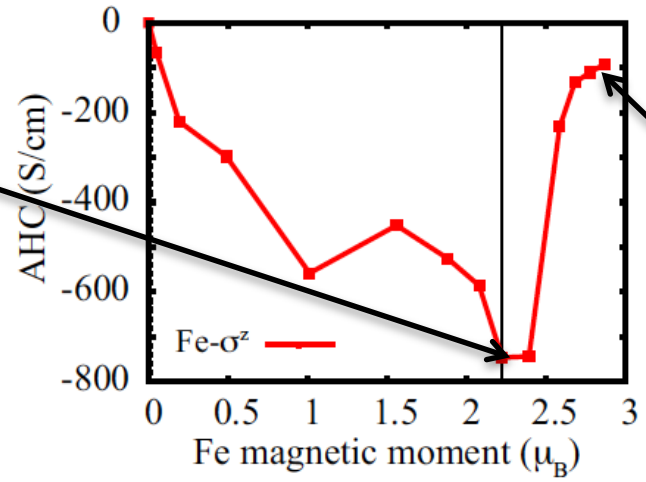


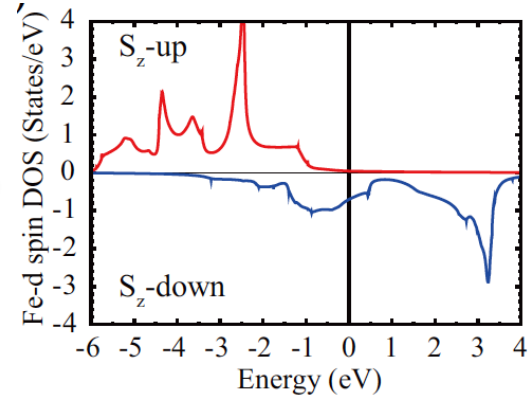
Similar multipole dependence of the AHC in ferromagnets and antiferromagnets.

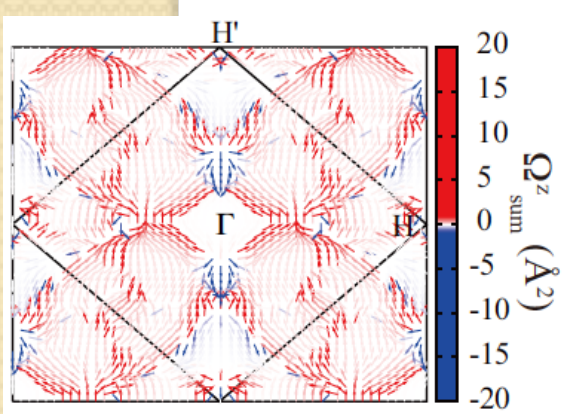
AHE and spin splitting of bcc-Fe

FM states of bcc-Fe



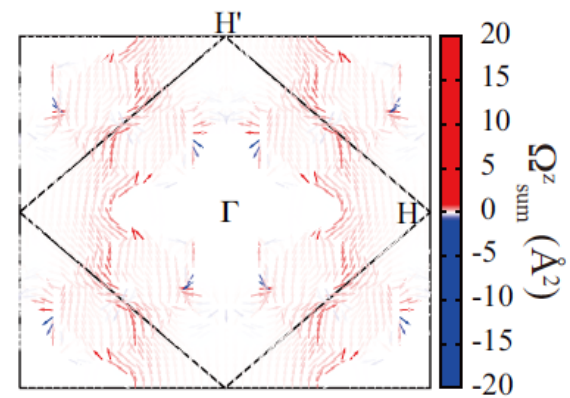






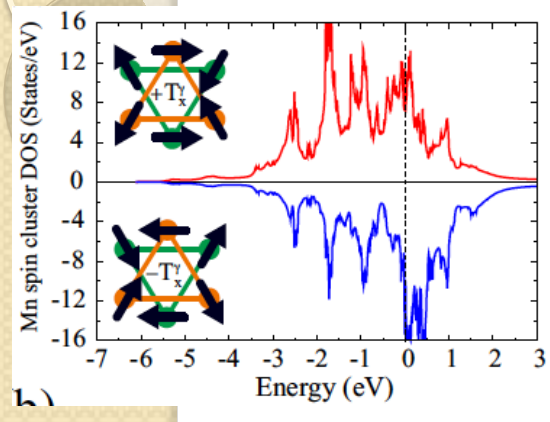
$$\sigma^z = -\frac{e^2}{\hbar}\int \frac{d\boldsymbol{k}}{(2\pi)^3}\boxed{\sum_n f(\varepsilon_n(\boldsymbol{k})-\mu)\Omega_n^z(\boldsymbol{k})}$$

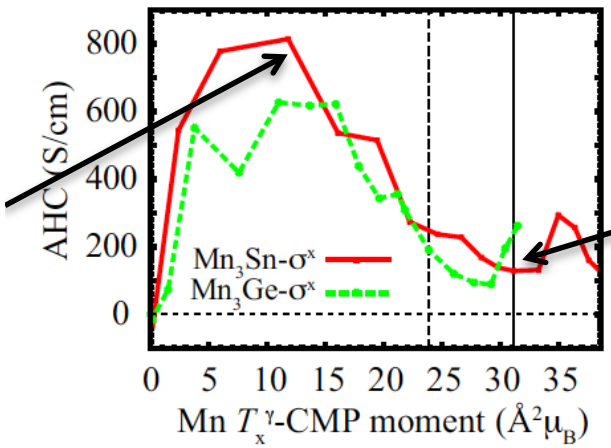
$$\Omega^z_{\mathrm{sum}}(\boldsymbol{k})$$

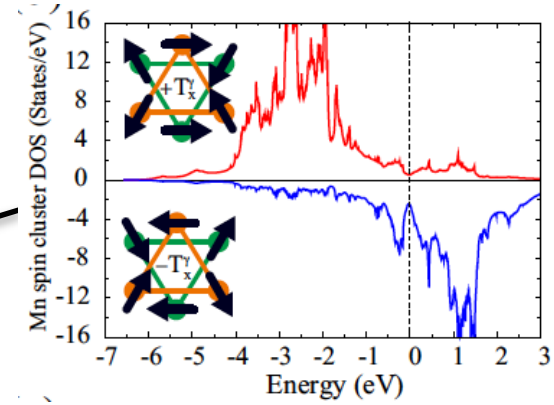


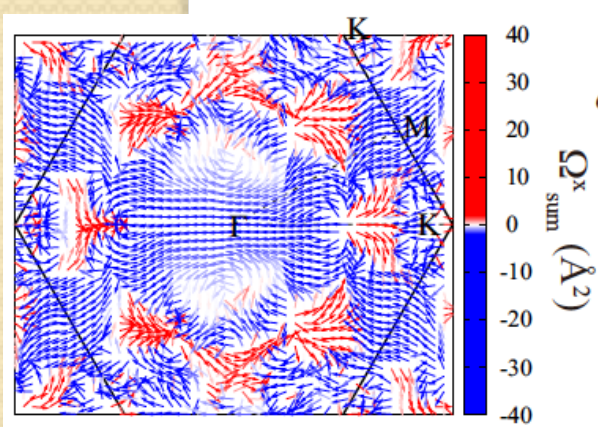
AHE and CMP orbital splitting of Mn_3Sn

AFM states of Mn_3Z (Z=Sn, Ge)



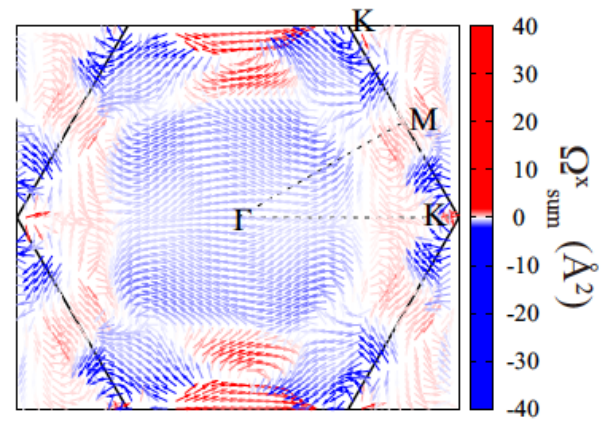






$$\sigma^x = -\frac{e^2}{\hbar}\int \frac{d\boldsymbol{k}}{(2\pi)^3}\boxed{\sum_n f(\varepsilon_n(\boldsymbol{k})-\mu)\Omega_n^x(\boldsymbol{k})}$$

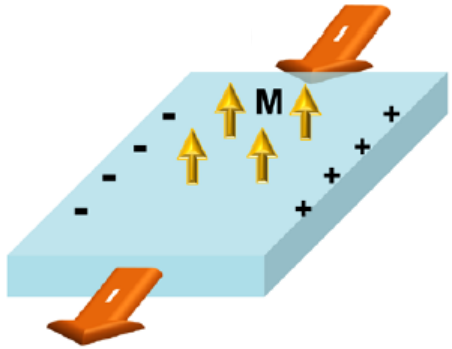
$$\Omega^x_{\mathrm{sum}}(\boldsymbol{k})$$



Conclusion

Cluster multipole theory provides unified view
for anomalous Hall effect in generic magnetic states.

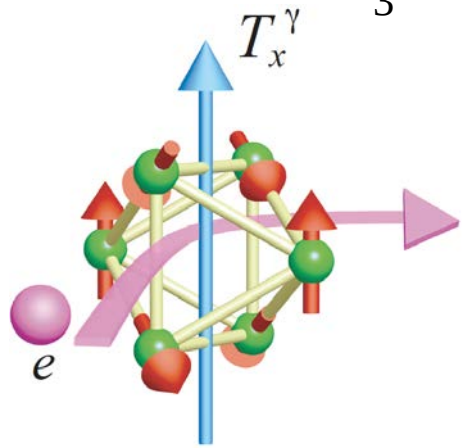
Ferromagnets



Cluster dipole moment (J_z)

AHE

AFM state of Mn_3Z



Cluster octupole moment (T_x^γ)

AHE

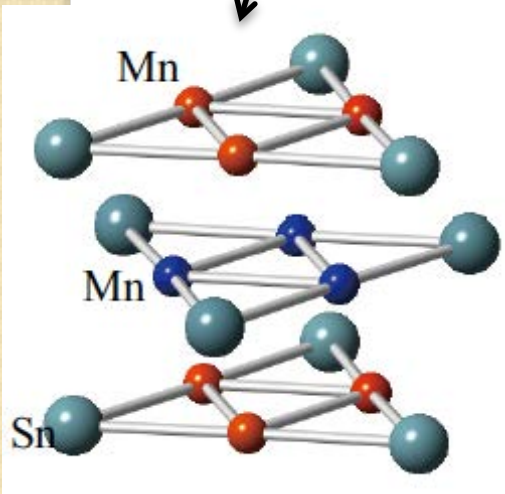
Analysis combining first-principles calc. with several theoretical tools fully demonstrate its power to reveal the transport mechanism.

Magnetization of CMP in Mn_3Z (Z=Sn, Ge)

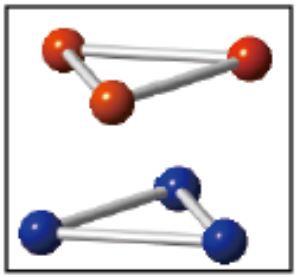
Space group of Mn_3Z

$$P6_3mmc = P\bar{3}m1 + \{C_{2z} \mid \tau\} P\bar{3}m1$$

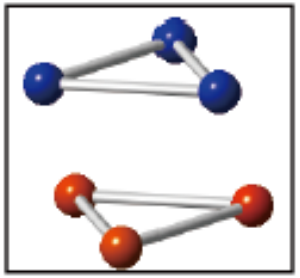
(Nonsymmorphic) (Symmorphic)

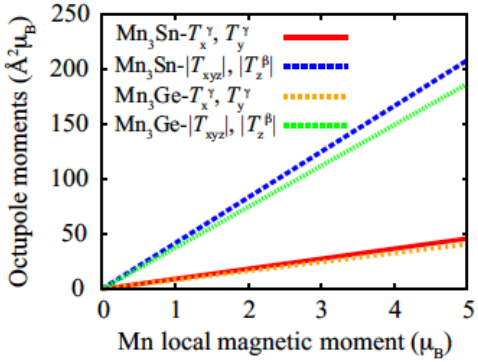


Mn-cluster 1



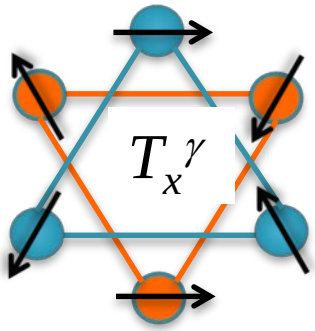
Mn-cluster 2





$+T_x^{\gamma}$ & $+T_{xyz}$

$+T_x^{\gamma}$ & $-T_{xyz}$



Macroscopic OP of AFM1: T_x^{γ}

MTS, Koretsune, Ochi, Arita, arXiv:1611.06042