

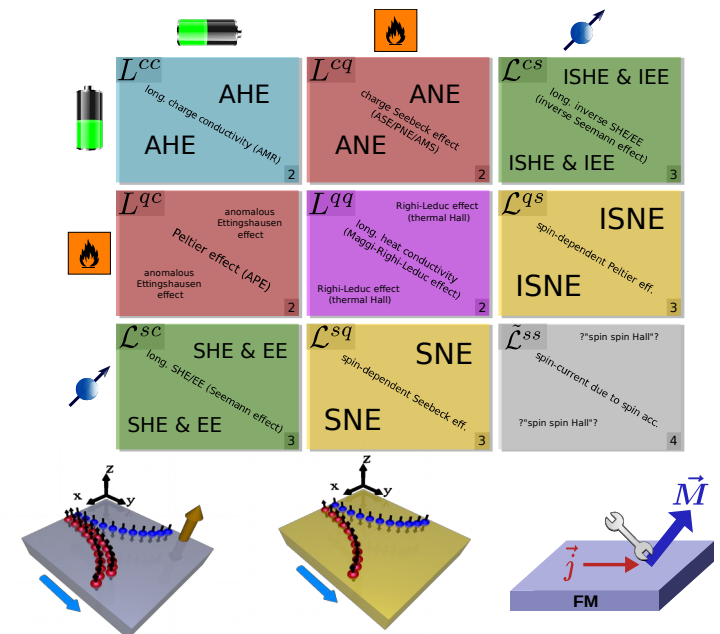
# New effects in spintronics derived from the symmetry of response functions

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## Outline

- Linear response formalism & group theory
- Application to electrical conductivity
- Application to spin-polarized conductivity
- Application to spin-orbit torques
- Summary and outlook



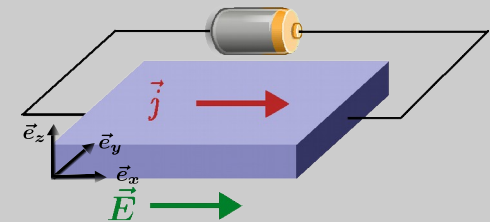


Response in  $\mathbf{B}$  caused by coupling to perturbation in  $\mathbf{A}$

$$\tau_{\hat{B}_i \hat{A}_j}(\omega, \vec{H}) = \int_0^\infty dt e^{-i\omega t} \int_0^\beta d\lambda \left\langle \rho(\vec{H}) \hat{A}_j \hat{B}_i(t + i\hbar\lambda; \vec{H}) \right\rangle$$

Example – electric current

$$\tau_{\hat{j} \hat{j}}(\omega) = \int_0^\infty dt e^{-i\omega t} \int_0^\beta d\lambda \text{Tr} \left( \rho_0 \hat{j} \hat{j}(t + i\hbar\lambda) \right)$$



$$\tau_{\hat{j} \hat{j}} = \sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

- symmetric part:  
longitudinal charge conductivity  
Anisotropic Magnetoresistance (AMR)
- antisymmetric part:  
transverse, anomalous Hall effect (AHE)



Response in **B** caused by coupling to perturbation in **A**

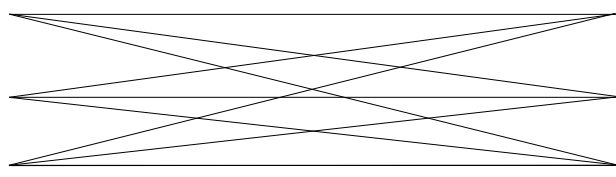
$$\tau_{\hat{B}_i \hat{A}_j}(\omega, \vec{H}) = \int_0^\infty dt e^{-i\omega t} \int_0^\beta d\lambda \left\langle \rho(\vec{H}) \hat{A}_j \hat{B}_i(t + i\hbar\lambda; \vec{H}) \right\rangle$$

observable

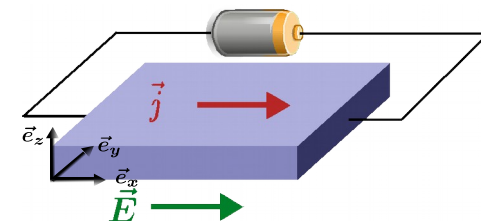
perturbation

Charge,  
heat or  
spin  
current

$\vec{j}^c$   
 $\vec{j}^q$   
 $J^s$



$\vec{j}^c$   
 $\vec{j}^q$   
 $J^s$

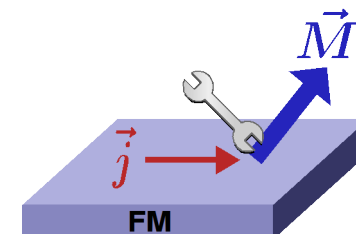


Torque

$\vec{T}$

spin-orbit torque

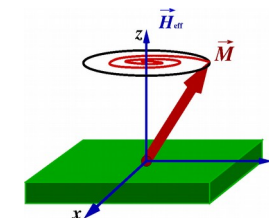
$\vec{j}^c$



$\vec{T}$

Gilbert damping

$\vec{T}$





- Make use of transformation properties of involved operators
- Account for symmetry operations in space as well as space and time

space

unitary operations

u

space + time

anti-unitary operations  
with time reversal  $T$  $a = T v$ 

	non-magnetic	magnetic
space groups	230	1651
point groups	32	122
Laue groups	12	37

symmetry determination: **FINDSYM**

ISOTROPY Software Suite, [iso.byu.edu](http://iso.byu.edu).

H. T. Stokes & D. M. Hatch, J. Appl. Cryst. 38, 237 (2005)



$$\sigma_{ij} = \tau_{\hat{j}_i \hat{j}_j}(\omega, \vec{H}) = \int_0^\infty dt e^{-i\omega t} \int_0^\beta d\lambda \left( \rho(\vec{H}) \hat{j}_j \hat{j}_i(t + i\hbar\lambda; \vec{H}) \right)$$

for **unitary** operators  $u$ :

$$\sigma_{ij} = \sum_{kl} \sigma_{kl} D(P_R)_{ki} D(P_R)_{lj}$$

for **anti-unitary** operators  $a$ :

$$\sigma_{ij} = \sum_{kl} \sigma_{lk} D(P_R)_{ki}^* D(P_R)_{lj}^*$$

#### Pseudoalgorithm

- determine symmetry of system
- loop over symmetry operations
  - set up system of linear eqs. in elements  $\{\sigma_{ij}\}$
- solution gives restrictions
  - element is linear combination of other elements
  - element is its negative
    - element is zero

**Only the magnetic Laue group has to be considered**

same transformation behavior for thermal transport  same tensor shapes

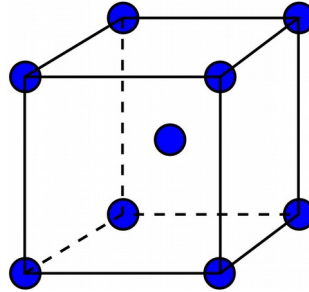
W. H. Kleiner, Phys. Rev. **142**, 318 (1966)



Only the magnetic Laue group has to be considered

paramagnetic

$m\bar{3}m1'$

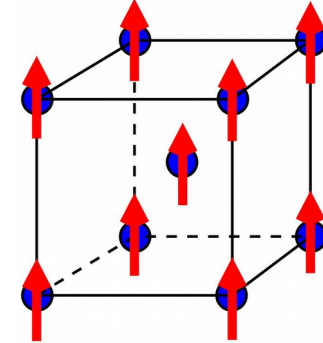


$$\sigma = \begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{xx} \end{pmatrix}$$

Isotropic conductivity

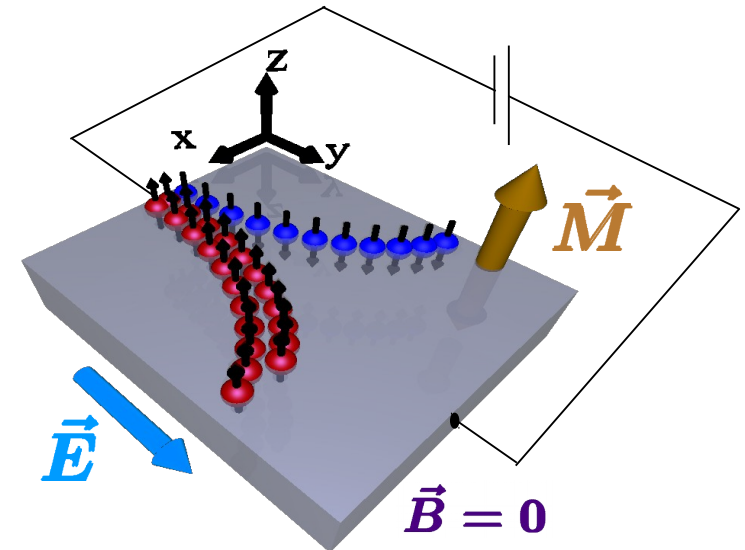
ferromagnetic

$4/mm'm'$



$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

Anomalous Hall effect



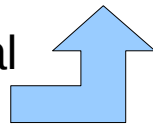
Results obtained by analytic computation using computer algebra system (CAS)

Non-magnetic materials

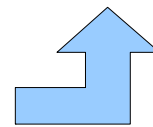
Magnetic materials

magnetic Laue group	$\underline{\tau}'$	$\underline{\sigma}$
$\bar{1}1'$	$\begin{pmatrix} \tau_{xx} & \tau_{yx} & \tau_{zx} \\ \tau_{xy} & \tau_{yy} & \tau_{zy} \\ \tau_{xz} & \tau_{yz} & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix}$
$2/m1'$	$\begin{pmatrix} \tau_{xx} & 0 & \tau_{zx} \\ 0 & \tau_{yy} & 0 \\ \tau_{xz} & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & \sigma_{xz} \\ 0 & \sigma_{yy} & 0 \\ \sigma_{xz} & 0 & \sigma_{zz} \end{pmatrix}$
$mmm1'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{yy} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$\bar{3}1', 4/m1', 6/m1'$	$\begin{pmatrix} \tau_{xx} & -\tau_{xy} & 0 \\ \tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$\bar{3}1m1', \bar{3}m11', 4/mmm1', 6/mmm1'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$m\bar{3}1', m\bar{3}m1'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{xx} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{xx} \end{pmatrix}$

Thermo-electrical  
response tensor



Electrical conductivity tensor



magnetic Laue group	$\underline{\tau}'$	$\underline{\sigma}$
$2'/m'$	$\begin{pmatrix} \tau_{xx} & -\tau_{yx} & \tau_{zx} \\ -\tau_{xy} & \tau_{yy} & -\tau_{zy} \\ \tau_{xz} & -\tau_{yz} & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ -\sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & -\sigma_{yz} & \sigma_{zz} \end{pmatrix}$
$m'm'm$	$\begin{pmatrix} \tau_{xx} & -\tau_{yx} & 0 \\ -\tau_{xy} & \tau_{yy} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$4'/m$	$\begin{pmatrix} \tau_{yy} & -\tau_{xy} & 0 \\ -\tau_{yx} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$4'/mm'm$	$\begin{pmatrix} \tau_{xx} & -\tau_{xy} & 0 \\ -\tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$4'/mmm'$	$\begin{pmatrix} \tau_{yy} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$\bar{3}1m', \bar{3}m'1, 4/mm'm', 6/mm'm'$	$\begin{pmatrix} \tau_{xx} & \tau_{xy} & 0 \\ -\tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$6'/m'$	$\begin{pmatrix} \tau_{xx} & -\tau_{xy} & 0 \\ \tau_{xy} & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$6'/m'm'm, 6'/m'mm'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$
$m\bar{3}m'$	$\begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{xx} & 0 \\ 0 & 0 & \tau_{xx} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{xx} \end{pmatrix}$

class a) contains time reversal  $T$

class c) contains combined operations  $a=v T$



$\text{Mn}_3\text{Ir}$  – a prototype non-collinear antiferromagnet

- $\text{Cu}_3\text{Au}$  structure
- moments in (111) plane (Kagome lattice)
- magnetic space group:  $R\bar{3}m'$

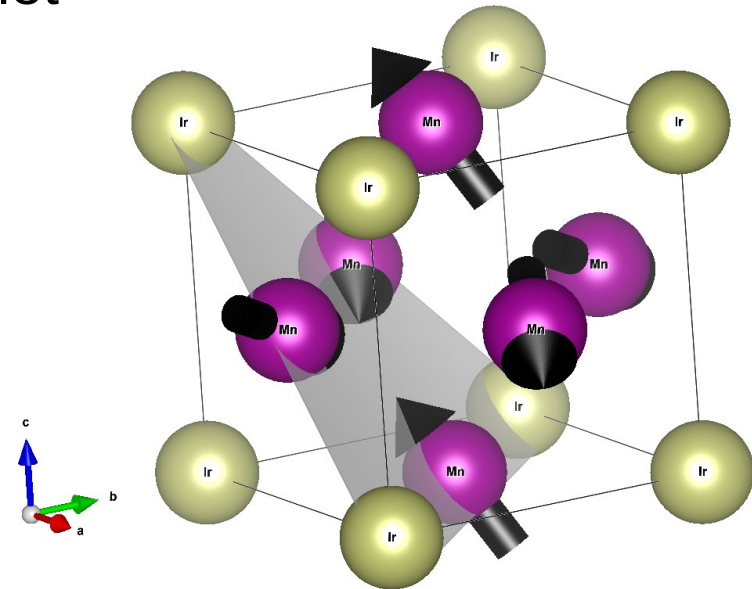
Prediction of **anomalous Hall effect (AHE)**  
and **magneto-optical Kerr effect (MOKE)**

- based on analysis of electronic structure

Chen, Niu, and MacDonald, PRL **112**, 017205 (2014)

- Natural consequence of Kleiner's tables  
for the shape of the conductivity tensor

Kleiner, PR **142**, 318 (1966)





Electrical conductivity tensor

$$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

numerical work based on Kubo-Středa equation

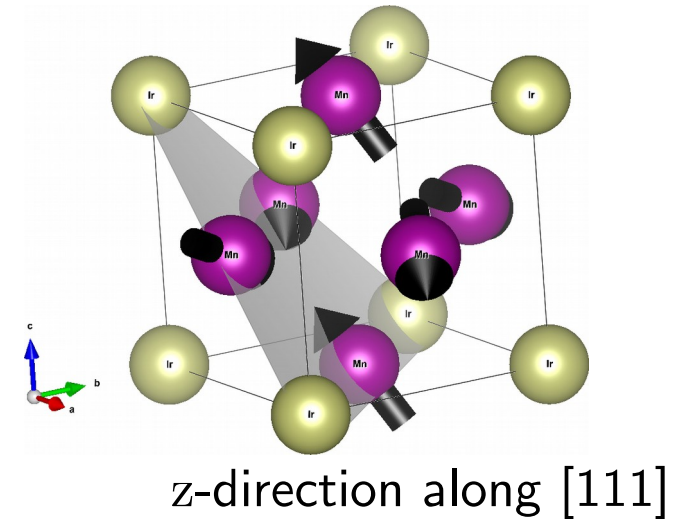
$$\sigma_{\mu\nu} = \frac{\hbar}{4\pi V} \text{Tr} \left\langle \hat{J}_\mu (G^+ - G^-) \hat{j}_\nu G^- - \hat{J}_\mu G^+ \hat{j}_\nu (G^+ - G^-) \right\rangle_c \\ + \frac{e}{4\pi i V} \text{Tr} \left\langle (G^+ - G^-) (\hat{r}_\mu \hat{J}_\nu - \hat{r}_\nu \hat{J}_\mu) \right\rangle_c$$

Smrčka and Středa, JPC 10, 2153 (1977)  
Lowitzer *et al.*, PRL **105**, 266604 (2010)

- confirms tensor shape
- Anomalous Hall conductivity

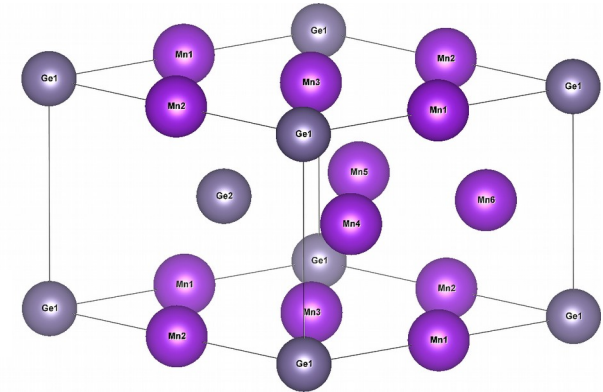
**275** (Ω cm)<sup>-1</sup> this work  
**218** (Ω cm)<sup>-1</sup> Chen *et al.* (2014)

comparable in size to Fe, Co, and Ni

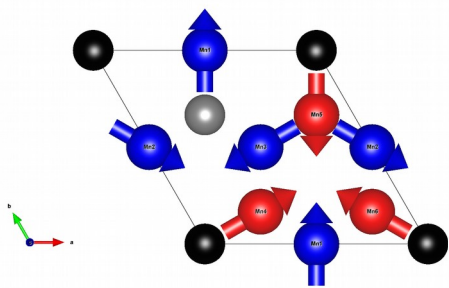




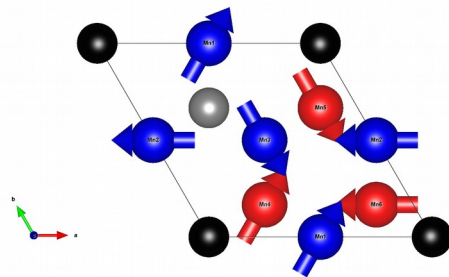
- Space group  $P6_3/mmc$  (194)
- Mn atoms couple antiferromagnetically on Kagome lattices (stacked along [0001])
- magnetic moments in {0001}
- various triangular configurations discussed



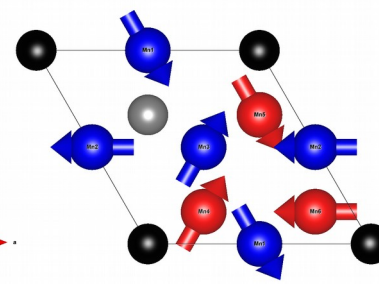
Zhang *et al.* JPCM **25**, 206006 (2013), Kübler and Felser, EPL **108**, 67001 (2014)



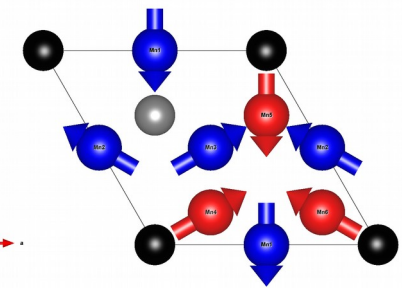
**AFM1**



**AFM2**



**AFM3**



**AFM4**

- AHC predicted by Kübler and Felser (for **AFM3** & **AFM4**)
- Excluded for **AFM1**



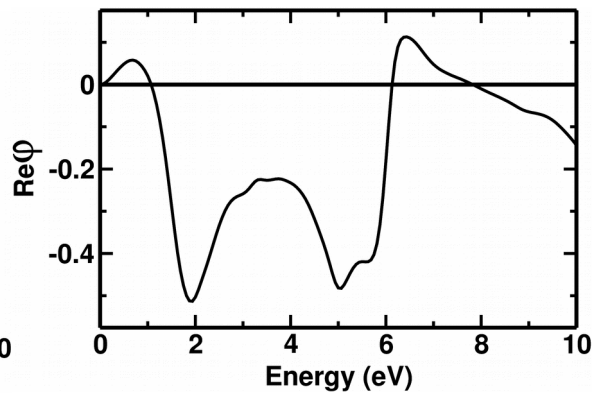
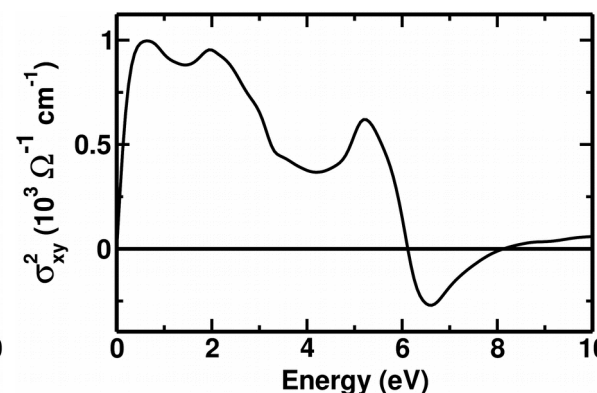
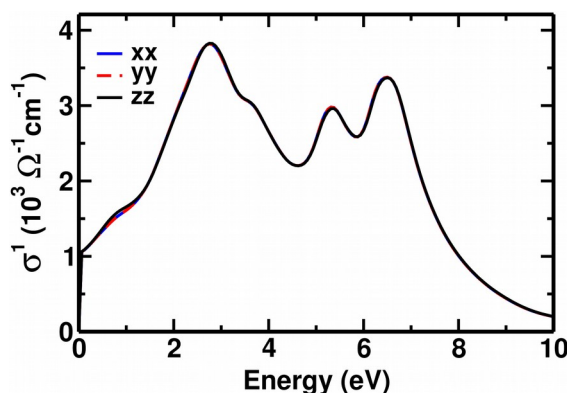
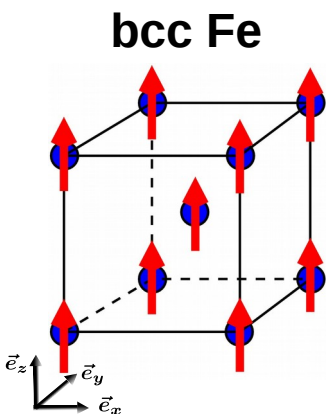
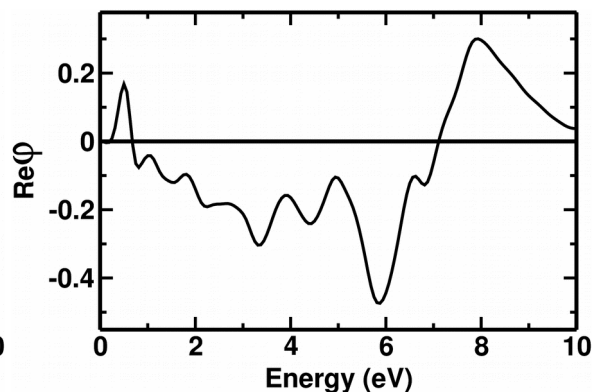
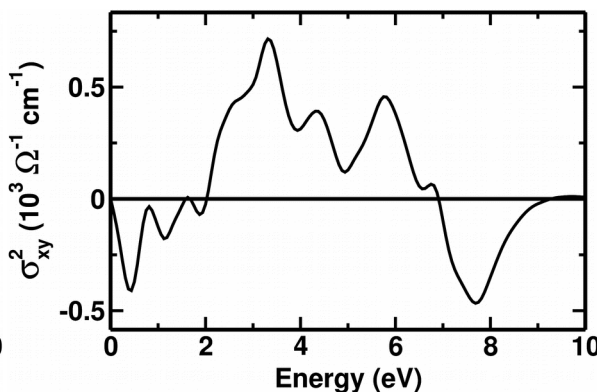
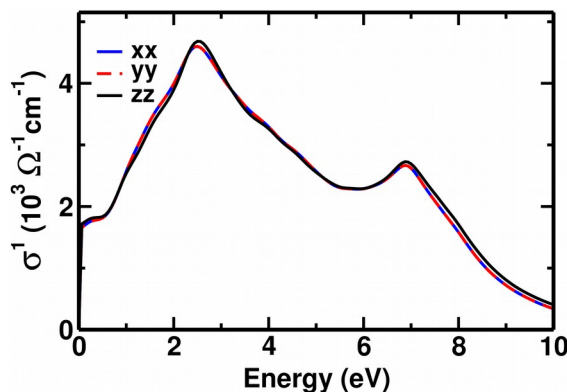
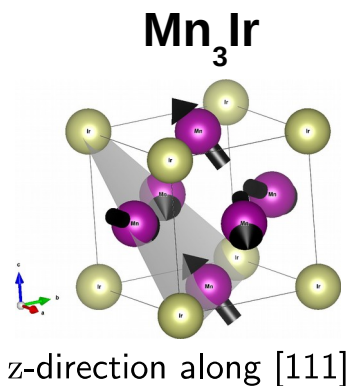
- Electrical conductivity
  - predicted tensor shapes (MSGs determined using **FINDSYM**)

$$\begin{pmatrix} \sigma_{xx} & 0 & \sigma_{xz} \\ 0 & \sigma_{yy} & 0 \\ -\sigma_{xz} & 0 & \sigma_{zz} \end{pmatrix} \begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix} \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ -\sigma_{xz} & -\sigma_{yz} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} \sigma_{xx} & 0 & \sigma_{xz} \\ 0 & \sigma_{yy} & 0 \\ -\sigma_{xz} & 0 & \sigma_{zz} \end{pmatrix}$$

	<b>AFM1</b>	<b>AFM2</b>	<b>AFM3</b>	<b>AFM4</b>
MSG	Am'm'2	P-6'2c'	Pm'	Am'm'2
<u>MLG</u>	<u>m'm'm</u>	<u>6'/m'mm'</u>	<u>2'/m'</u>	<u>m'm'm</u>

- numerical results confirm prediction **in all cases**
- Comparison to results obtained by Kübler & Felser [1]
  - Discrepancies for **AFM1** (no AHE) & **AFM4** (2 different AHCs)
  - **AFM2** not considered in [1]
  - Agreement for **AFM3**

[1] Kübler & Felser, EPL **108**, 67001 (2014)



- results in line with symmetry prediction

$$\sigma_{xx}^1(\omega) = \sigma_{yy}^1(\omega) \neq \sigma_{zz}^1(\omega) \quad \sigma_{xy}^2(\omega) = -\sigma_{yx}^2(\omega)$$

- same tensor shape as for bcc-Fe, comparable in magnitude

Wimmer, *et al.*, unpublished (2015)



- One-electron approximation to *Fermi's Golden Rule*

$$\mu_{q\lambda}^i(\omega) \propto \sum_f |\langle \Psi_f | X_{q\lambda} | \Psi_i \rangle|^2 \delta(E_f - E_i - \hbar\omega)$$

- Electron-photon interaction operator

$$X_{q\lambda}(\mathbf{r}) = -\frac{1}{c} \underbrace{\mathbf{j}_{el}} \cdot \mathbf{A}_{q\lambda}(\mathbf{r}) = e \alpha \cdot \hat{\mathbf{e}}_\lambda A e^{i\mathbf{q}\cdot\mathbf{r}}$$

**electric current density operator**

- Absorption coefficient in terms of Green function

$$\mu_{q\lambda}(\omega) \propto \sum_i \langle \Psi_i | X_{q\lambda}^\dagger \Im G^+(E_i + \hbar\omega) X_{q\lambda} | \Psi_i \rangle \theta(E_i + \hbar\omega - E_F)$$

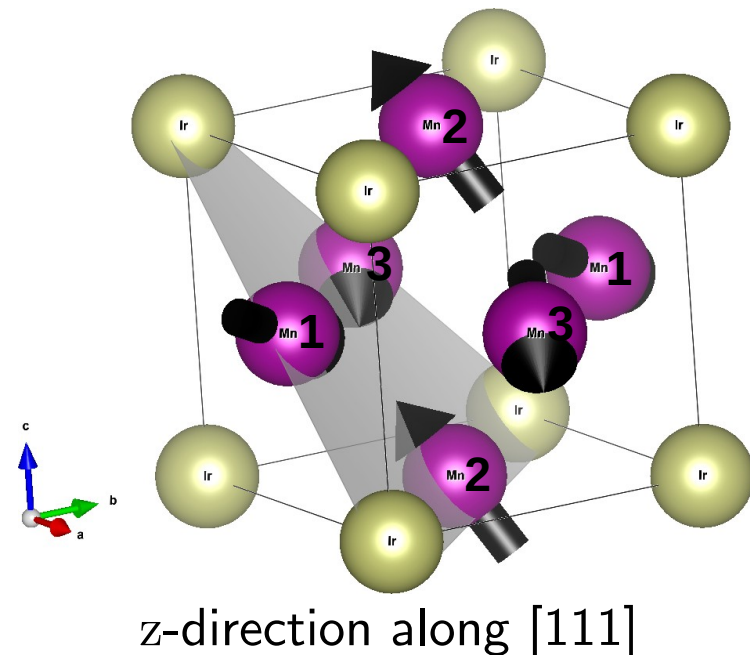
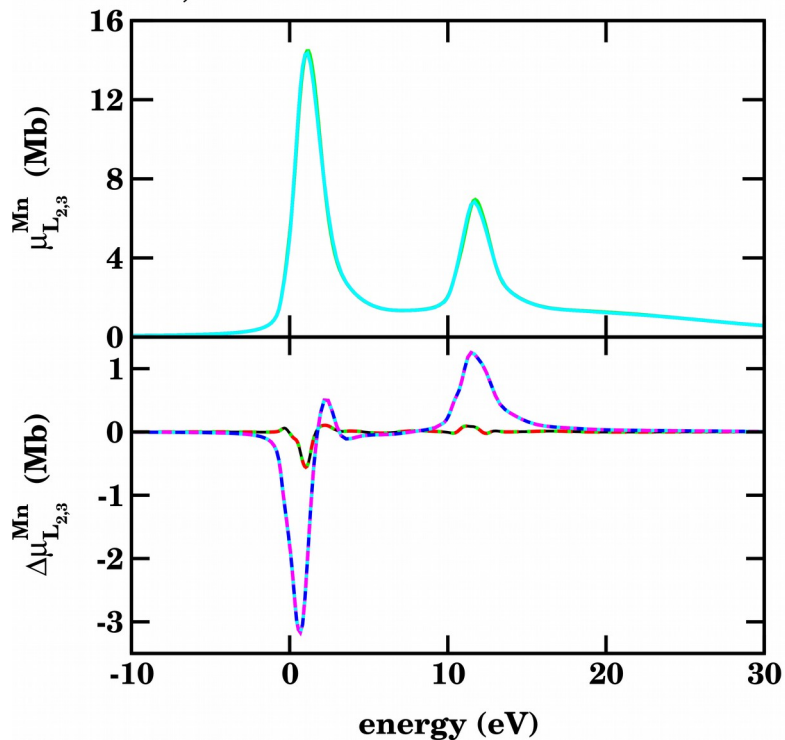
- Relation to transport effects

- XMCD ( $\mu_{q+} - \mu_{q-}$ )      **circular dichroism**  $\longleftrightarrow$  **AHE**

- XMLD ( $\mu_{q\bar{\lambda}} - \mu_{q'\bar{\lambda}}$ )      **linear dichroism**  $\longleftrightarrow$  **AMR**

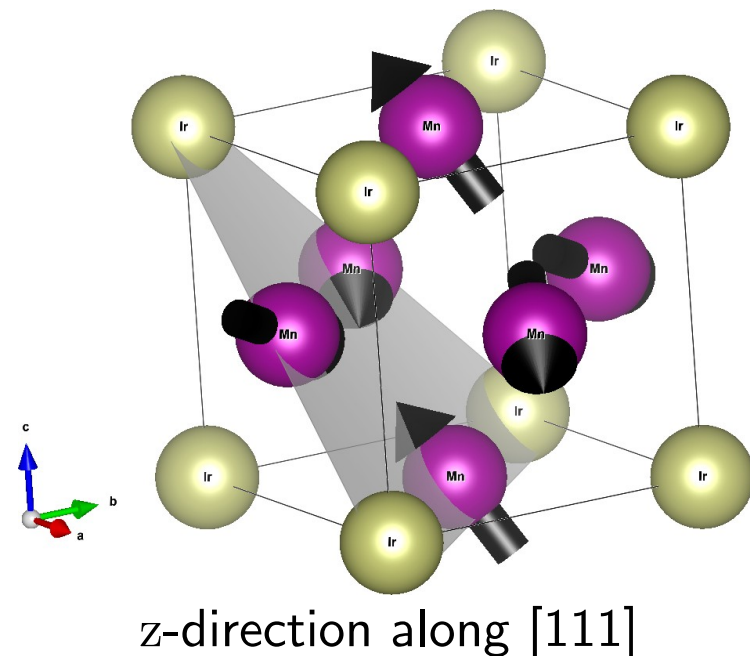
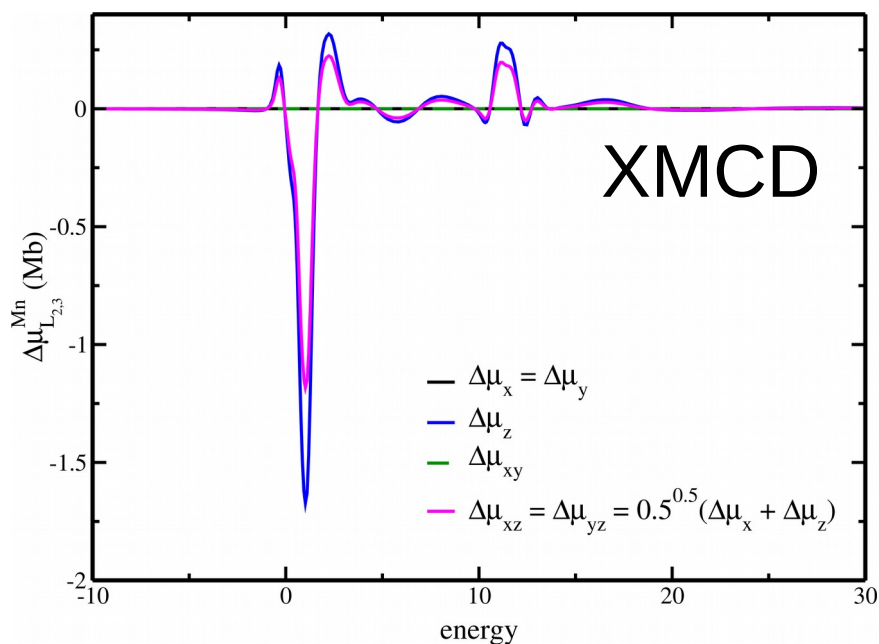
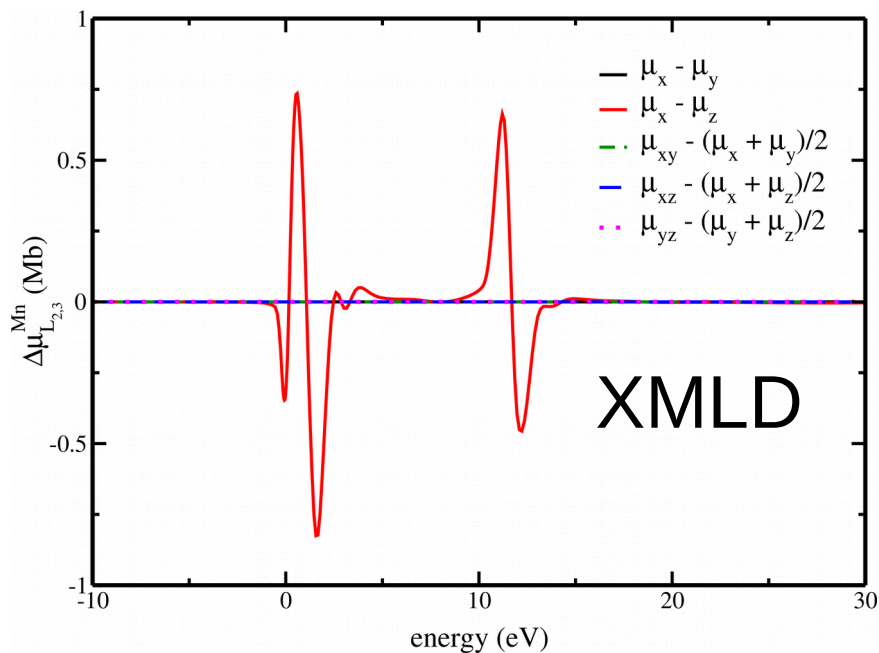
- Construction of spectra as sum of site-resolved absorption coefficients
- wavevectors  $\mathbf{q}$  along high symmetry directions  $\rightarrow$  connection to  $\underline{\sigma}$

### L<sub>2,3</sub>-XAS spectra of Mn in Mn<sub>3</sub>Ir



- spectra by superposition of site-resolved abs. coeffs.  $\mu_{\vec{q}\lambda}^n(\omega)$
- incidence  $\vec{q}$ : [111] vs. direction of  $\vec{m}_n$  (polar geometry)
  - same total absorption
  - in **both** cases XMCD (larger for polar geometry)

Wimmer, *et al.*, unpublished (2015)



$$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

Wimmer, *et al.*, unpublished (2015)



$$\tau_{(\mathcal{T}_k \hat{j}_i) \hat{j}_j}(\omega, \vec{H}) = \int_0^\infty dt e^{-i\omega t} \int_0^\beta d\lambda \left( \rho(\vec{H}) \hat{j}_j \mathcal{T}_k \hat{j}_i(t + i\hbar\lambda; \vec{H}) \right)$$

$$\hat{j}_j = -|e|c \alpha_j \leftarrow \text{Dirac matrix}$$

Using a relativistic spin polarization operator [1,2,3]:  $\mathcal{T}_k = \beta \Sigma_k - \frac{\gamma_5 \Pi_k}{mc}$

for **unitary** operators  $u$ :  $\sigma_{ij}^k = \sum_{lmn} D(P_R)_{li} D(P_R)_{mj} D(P_R)_{nk} \sigma_{lm}^n$

for **anti-unitary** operators  $a$ :  $\sigma_{ij}^k = - \sum_{lmn} D(P_R)_{li} D(P_R)_{mj} D(P_R)_{nk} \sigma_{lm}^{\prime n}$

**Only the magnetic Laue group has to be considered**

 Spin polarized conductivity tensor

[1] V. Bargmann, E. P. Wigner, Proc. Natl. Acad. Sci. U.S.A. **34**, 211 (1948)

[2] A. Vernes, B.L. Györfy, P. Weinberger, Phys. Rev. B **76**, 012408 (2007)

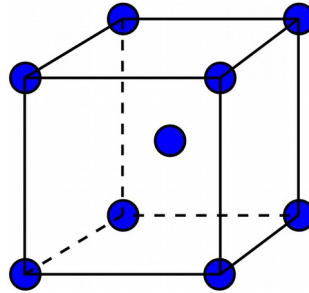
[3] S. Lowitzer, Ködderitzsch, H. Ebert, Phys. Rev. B **82**, 140402 (2010)



Only the magnetic Laue group has to be considered

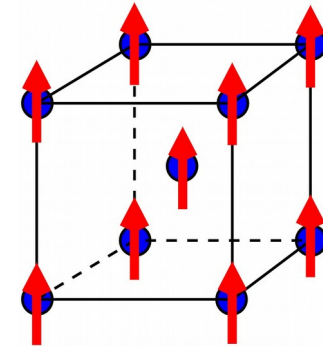
paramagnetic

$m\bar{3}m1'$



ferromagnetic

$4/mm'm'$

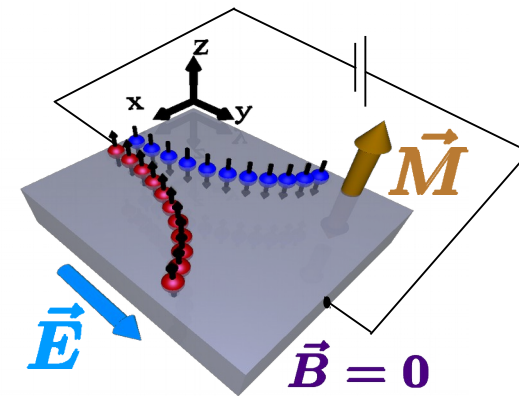
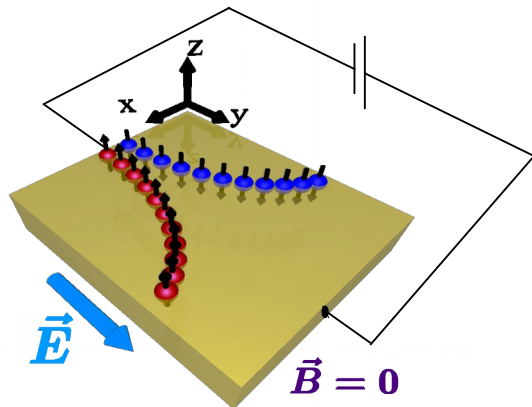


$$\begin{pmatrix} 0 & \sigma_{xy}^z & 0 \\ -\sigma_{xy}^z & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} \sigma_{xx}^z & \sigma_{xy}^z & 0 \\ -\sigma_{xy}^z & \sigma_{xx}^z & 0 \\ 0 & 0 & \sigma_{zz}^z \end{pmatrix}$$

Spin-Hall effect in paramagnet  
and  
ferromagnet

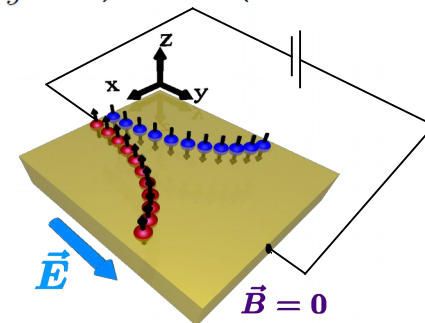
(no need for two-current-model)



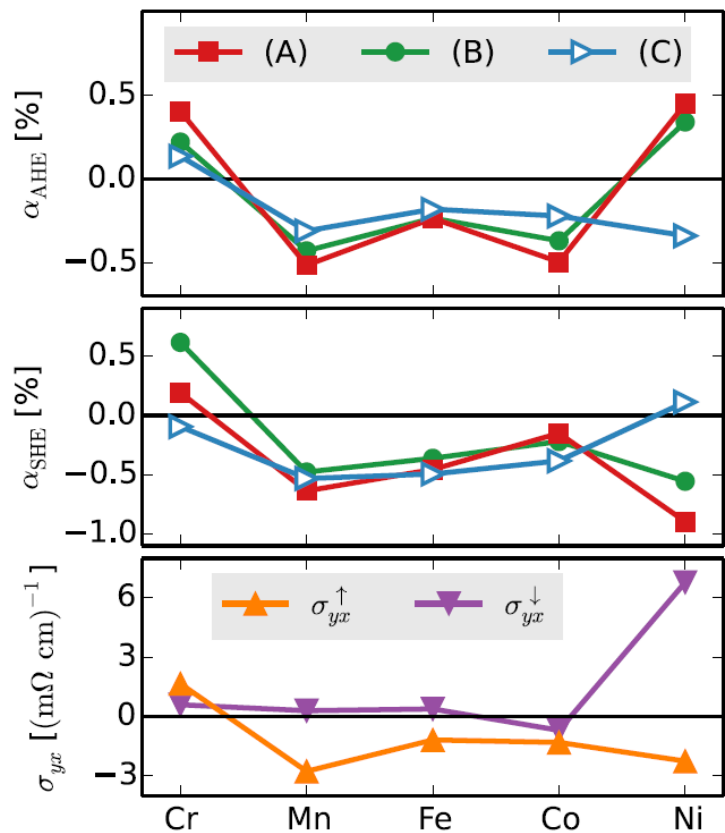




magnetic Laue group	$\underline{\sigma}$	$\underline{\sigma}^x$	$\underline{\sigma}^y$	$\underline{\sigma}^z$
$m\bar{3}m1'$ e.g.: Au	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{xx} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma_{yz}^x \\ 0 & -\sigma_{yz}^x & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -\sigma_{yz}^x \\ 0 & 0 & 0 \\ \sigma_{yz}^x & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \sigma_{yz}^x & 0 \\ -\sigma_{yz}^x & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$4/m\bar{m}'m'$ e.g.: FM bcc Fe	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \sigma_{xz}^x \\ 0 & 0 & \sigma_{yz}^x \\ \sigma_{zx}^x & \sigma_{zy}^x & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -\sigma_{yz}^x \\ 0 & 0 & \sigma_{xz}^x \\ -\sigma_{zy}^x & \sigma_{zx}^x & 0 \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx}^z & \sigma_{xy}^z & 0 \\ -\sigma_{xy}^z & \sigma_{xx}^z & 0 \\ 0 & 0 & \sigma_{zz}^z \end{pmatrix}$
$4/m1'$ e.g.: Au <sub>4</sub> Sc	$\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \sigma_{xz}^x \\ 0 & 0 & \sigma_{yz}^x \\ \sigma_{zx}^x & \sigma_{zy}^x & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -\sigma_{yz}^x \\ 0 & 0 & \sigma_{xz}^x \\ -\sigma_{zy}^x & \sigma_{zx}^x & 0 \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx}^z & \sigma_{xy}^z & 0 \\ -\sigma_{xy}^z & \sigma_{xx}^z & 0 \\ 0 & 0 & \sigma_{zz}^z \end{pmatrix}$
$2/m1'$ e.g.: Pt <sub>3</sub> Ge	$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \sigma_{xz}^x \\ 0 & 0 & \sigma_{yz}^x \\ \sigma_{zx}^x & \sigma_{zy}^x & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \sigma_{xz}^y \\ 0 & 0 & \sigma_{yz}^y \\ \sigma_{zx}^y & \sigma_{zy}^y & 0 \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx}^z & \sigma_{xy}^z & 0 \\ \sigma_{yx}^z & \sigma_{yy}^z & 0 \\ 0 & 0 & \sigma_{zz}^z \end{pmatrix}$

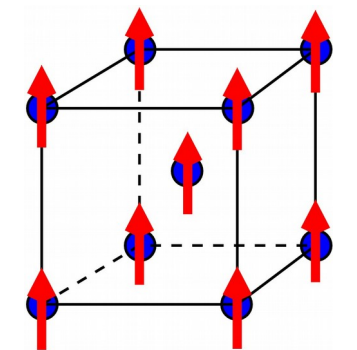


Wimmer, et al., arXiv:1502.04947 (2015)



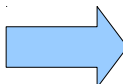
$$\text{AHE} \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

$$\text{SHE} \begin{pmatrix} \sigma_{xx}^z & \sigma_{xy}^z & 0 \\ -\sigma_{xy}^z & \sigma_{xx}^z & 0 \\ 0 & 0 & \sigma_{zz}^z \end{pmatrix}$$



ferromagnetic  
*4/mm'm'*

- complex electronic structure at  $E_F$
- skew scattering very sensitive to fine details



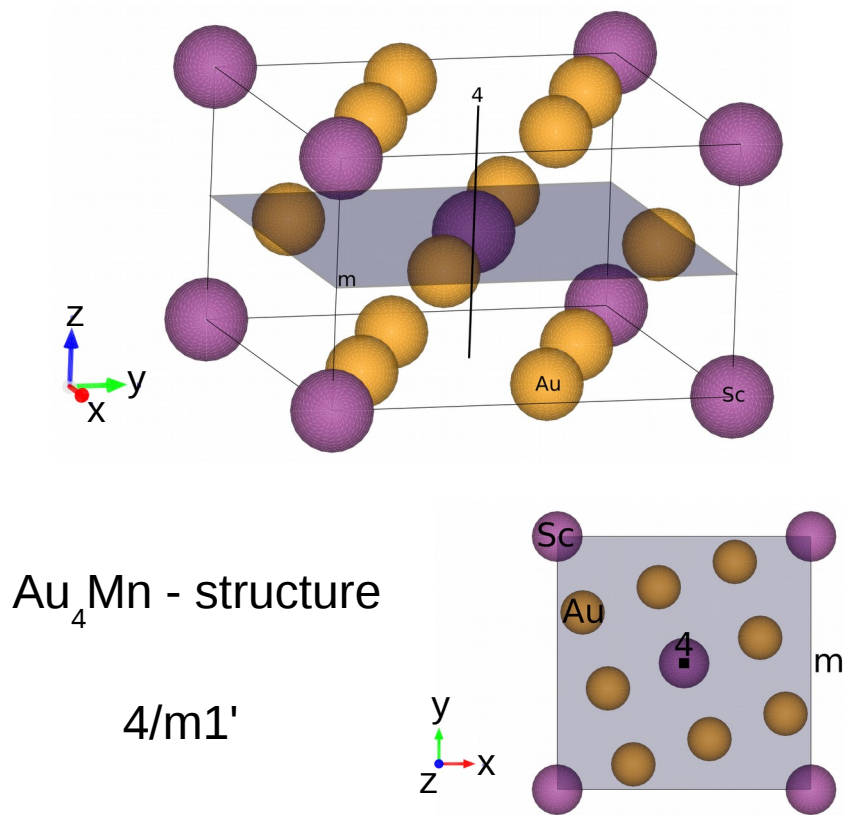
first-principles approach mandatory

skew scattering contributions to AHE, SHE  
1 % magnetic impurities in Pt host

Approach	Transport description	Electronic structure	Spin-orbit coupling
Method A	BE	FP	Pauli
Method B	BE	ASA	Dirac
Method C	KSF	ASA	Dirac

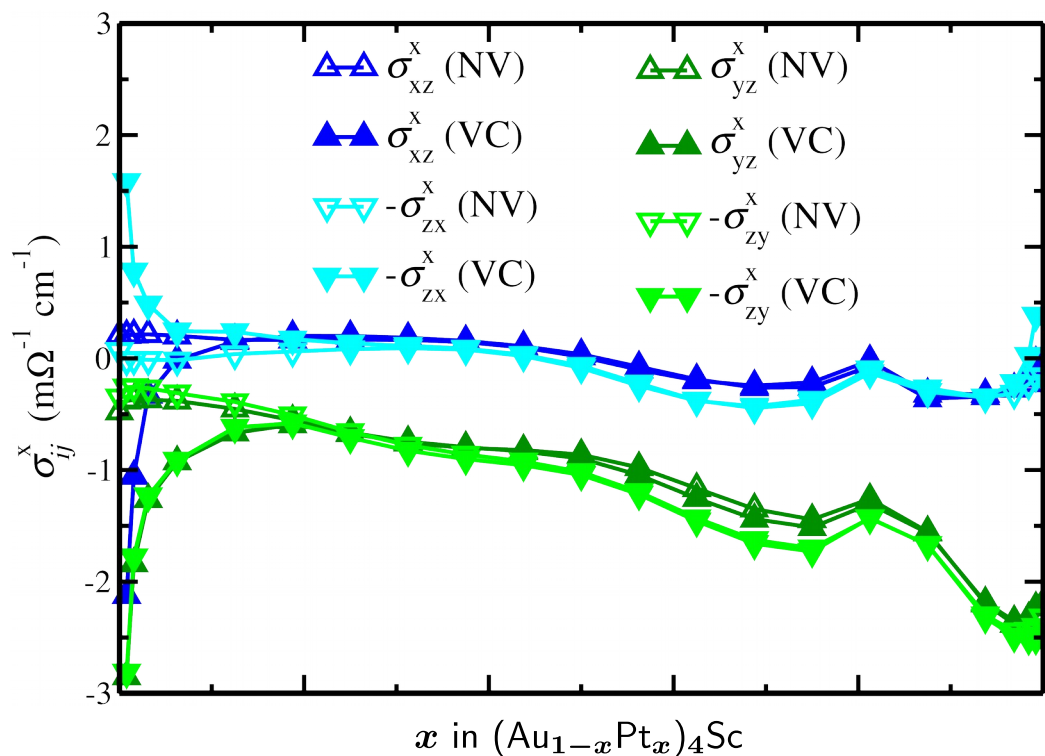
Zimmermann, *et al.* PRB **90**, 220403(R) (2014)



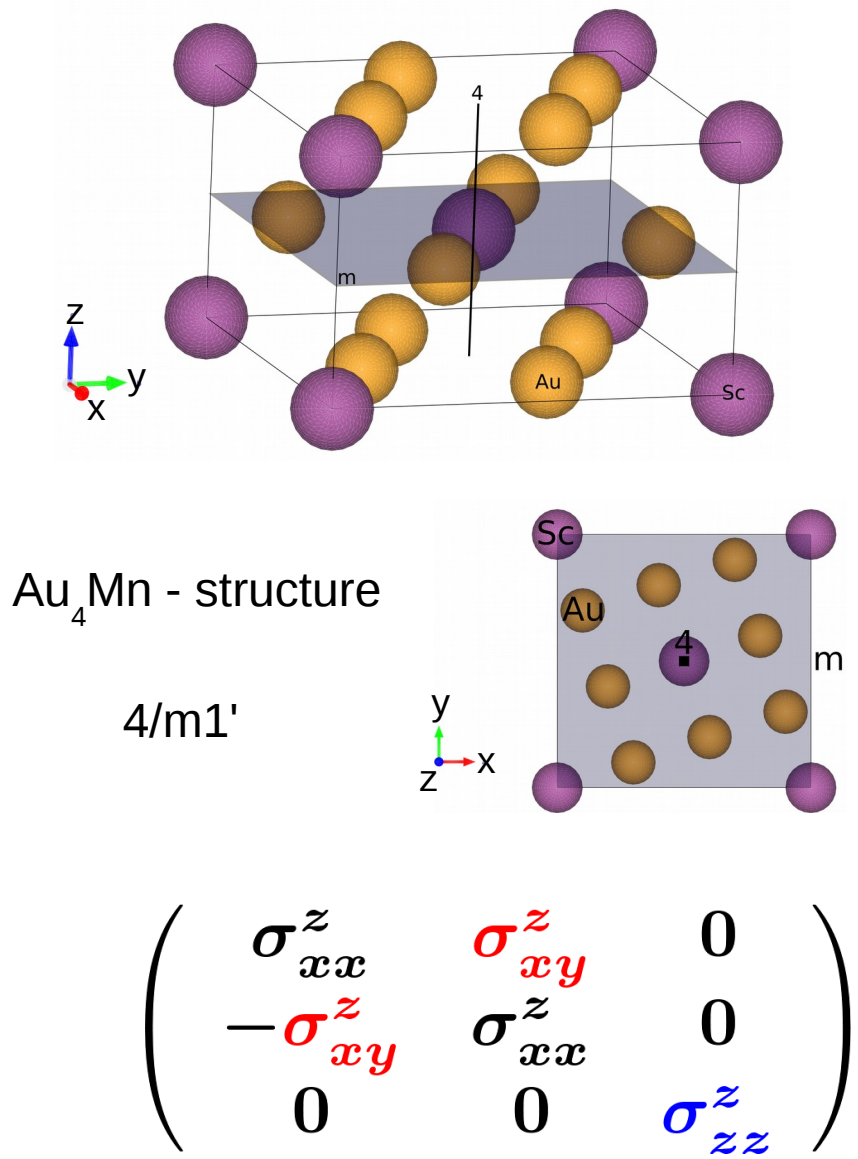


$$\begin{pmatrix} 0 & 0 & \sigma_{xz}^x \\ 0 & 0 & \sigma_{yz}^x \\ \sigma_{zx}^x & \sigma_{zy}^x & 0 \end{pmatrix}$$

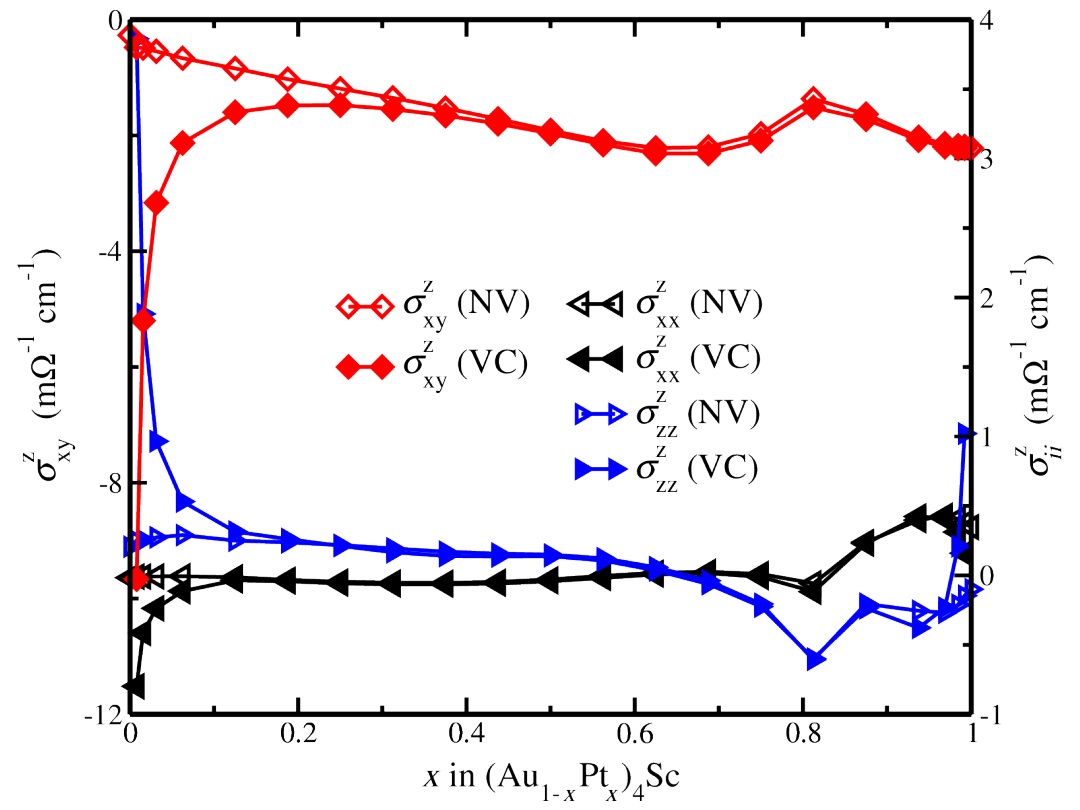
non-magnetic (Au<sub>1-x</sub>Pt<sub>x</sub>)<sub>4</sub>Sc - alloy



Wimmer, et al., arXiv:1502.04947 (2015)



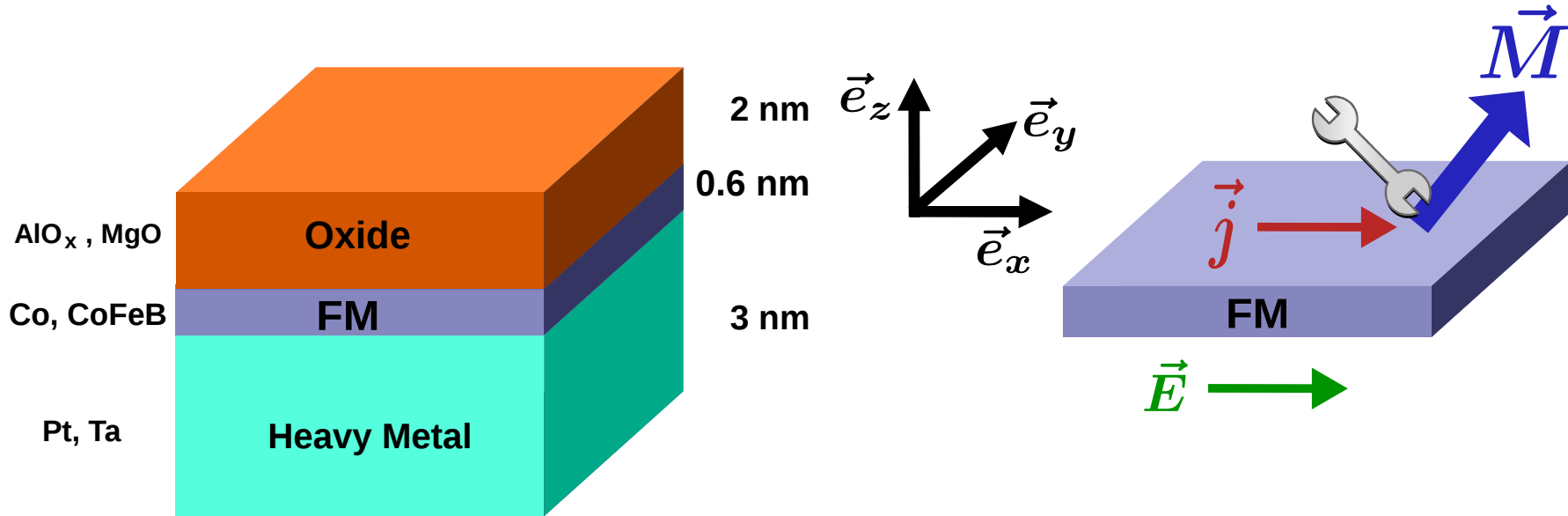
non-magnetic (Au<sub>1-x</sub>Pt<sub>x</sub>)<sub>4</sub>Sc - alloy



Wimmer, et al., arXiv:1502.04947 (2015)



## Systems lacking inversion symmetry



### Prediction:

Manchon & Zhang, PRB **79**, 094422 (2009)  
 Garate & MacDonald, PRB **80**, 134403 (2009)

### Experiments:

Miron *et al.*, Nat.Mat. **9**, 230 (2010)  
 Gambardella & Miron, Phil. Trans. R. Soc. A (2011) **369**, 3175  
 Garello *et al.*, Nat.Nanot. **8**, 587 (2013)

Torque

$$\vec{T} = t \vec{E}$$

Possible avenue to avoid large switching currents ( $10^7 \text{ A / cm}^2$ ) that currently hamper progress in STT-RAM technology.



$$\tau_{\hat{B}_i \hat{A}_j}(\omega, \vec{H}) = \int_0^\infty dt e^{-i\omega t} \int_0^\beta d\lambda \left\langle \rho(\vec{H}) \hat{A}_j \hat{B}_i(t + i\hbar\lambda; \vec{H}) \right\rangle$$

Freimuth, *et al*, arXiv: 1305.4873

For torkance

$$\hat{B}_i = \hat{T}_i \quad \hat{A}_j = \hat{j}_j$$

Torque operator

$$T_i = \frac{\partial}{\partial u_i} \hat{H}$$

Spin magnetisation

$$\vec{m} = m\vec{u}$$

Ebert & Mankovsky, PRB **79**, 045209 (2009)

Ebert, *et al*, PRL **107**, 066603 (2011)

Mankovsky, *et al*, PRB **87**, 014430 (2013)



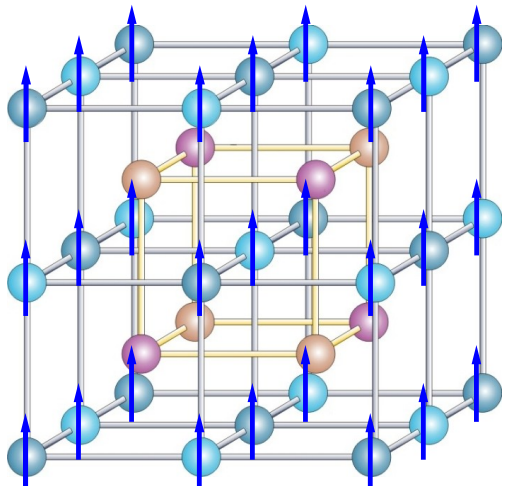
$$\vec{T} = t \vec{E}$$

Transformation of torkance under symmetry operations of magnetic space group

$$t_{ij} = \sum_{kl} t_{kl} D(R)_{ki} D(R)_{lj} \det(R) \quad \text{unitary operations} \quad \xrightarrow{\text{all } R} \quad \text{tensor shape}$$

$$t_{ij} = \sum_{kl} t'_{lk} D(R)_{ki}^* D(R)_{lj}^* \det(R) \quad \text{anti-unitary operations}$$

Example – inverse Heusler system



Cr<sub>2</sub>VSb

$$t = \begin{pmatrix} t_{xx} & t_{xy} & 0 \\ -t_{xy} & -t_{xx} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

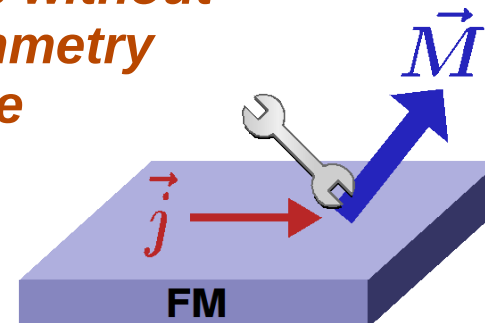


## Results obtained by analytic computation using computer algebra system (CAS)

magnetic point group	$\underline{t}$
$\bar{1}', 1, 2', m'$	$\begin{pmatrix} t_{xx} & t_{xy} & t_{xz} \\ t_{yx} & t_{yy} & t_{yz} \\ t_{zx} & t_{zy} & t_{zz} \end{pmatrix}$
$\bar{1}, \bar{3}, \bar{3}1m, \bar{3}1m', \bar{3}m'1, \bar{3}m1, \bar{4}3m, \bar{6}, \bar{6}2'm', \bar{6}2m, \bar{6}m'2', \bar{6}m2, 2'/m', 2/m, 4'/m, 4'/mm'm, 4'/mmm'm', 4/m, 4/mmm'm', 4/mmm, 6'/m, 6'/m', 6'/m'm'm, 6'/m'm'm', 6'/mm'm, 6'/mmm'm', 6/m, 6/mmm'm', 6/mmm, m\bar{3}, m\bar{3}m, m\bar{3}m', m'\bar{3}m, m'm'm, mmm$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$2, 2/m'$	$\begin{pmatrix} t_{xx} & 0 & t_{xz} \\ 0 & t_{yy} & 0 \\ t_{zx} & 0 & t_{zz} \end{pmatrix}$
$2'/m, m, m'm2'$	$\begin{pmatrix} 0 & t_{xy} & 0 \\ t_{yx} & 0 & t_{yz} \\ 0 & t_{zy} & 0 \end{pmatrix}$
$\bar{4}'2m', 222, 4'22', m'm'm'$	$\begin{pmatrix} t_{xx} & 0 & 0 \\ 0 & t_{yy} & 0 \\ 0 & 0 & t_{zz} \end{pmatrix}$
$\bar{4}', 2'2'2, 4', m'm'2$	$\begin{pmatrix} t_{xx} & t_{xy} & 0 \\ t_{yx} & t_{yy} & 0 \\ 0 & 0 & t_{zz} \end{pmatrix}$
$\bar{4}'m2', 4'mm', mm2$	$\begin{pmatrix} 0 & t_{xy} & 0 \\ t_{yx} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$m'mm$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & t_{yz} \\ 0 & t_{zy} & 0 \end{pmatrix}$
$\bar{3}', \bar{6}', 3, 312', 31m', 32'1, 3m'1, 4, 4/m', 42'2', 4m'm', 6, 6', 6/m', 62'2', 6m'm'$	$\begin{pmatrix} t_{xx} & t_{xy} & 0 \\ -t_{xy} & t_{xx} & 0 \\ 0 & 0 & t_{zz} \end{pmatrix}$
$\bar{4}, \bar{4}2'm', \bar{4}m'2', 4'/m'$	$\begin{pmatrix} t_{xx} & t_{xy} & 0 \\ t_{xy} & -t_{xx} & 0 \\ 0 & 0 & 0 \end{pmatrix}$

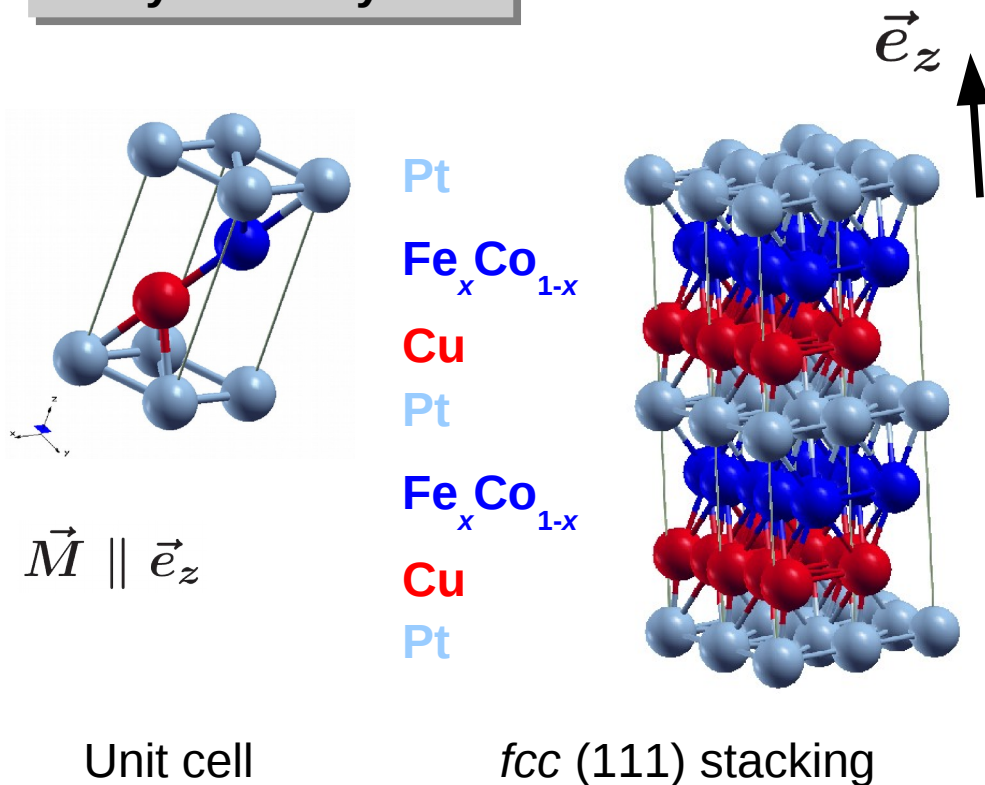
magnetic point group	$\underline{t}$
$\bar{4}2m, 4'/m'm'm$	$\begin{pmatrix} t_{xx} & 0 & 0 \\ 0 & -t_{xx} & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\bar{4}m2, 4'/m'mm'$	$\begin{pmatrix} 0 & t_{xy} & 0 \\ t_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\bar{4}'3m', 23, 4'32', 432, m'\bar{3}', m'\bar{3}'m'$	$\begin{pmatrix} t_{xx} & 0 & 0 \\ 0 & t_{xx} & 0 \\ 0 & 0 & t_{xx} \end{pmatrix}$
$\bar{3}'1m', \bar{3}'m'1, \bar{6}'2m', \bar{6}'m'2, 312, 321, 4/m'm'm', 422, 6'2'2, 6'22', 6/m'm'm', 622$	$\begin{pmatrix} t_{xx} & 0 & 0 \\ 0 & t_{xx} & 0 \\ 0 & 0 & t_{zz} \end{pmatrix}$
$\bar{4}'m'2, 4'2'2$	$\begin{pmatrix} t_{xx} & t_{xy} & 0 \\ t_{xy} & t_{xx} & 0 \\ 0 & 0 & t_{zz} \end{pmatrix}$
$\bar{3}'1m, \bar{3}'m1, \bar{6}'2'm, \bar{6}'m'2', 31m, 3m1, 4/m'mm, 4mm, 6'm'm, 6'mm', 6/m'mm, 6mm$	$\begin{pmatrix} 0 & t_{xy} & 0 \\ -t_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\bar{4}'2'm, 4'm'm$	$\begin{pmatrix} t_{xx} & t_{xy} & 0 \\ -t_{xy} & -t_{xx} & 0 \\ 0 & 0 & 0 \end{pmatrix}$

**only materials without inversion symmetry show torque**





## Trilayer test system

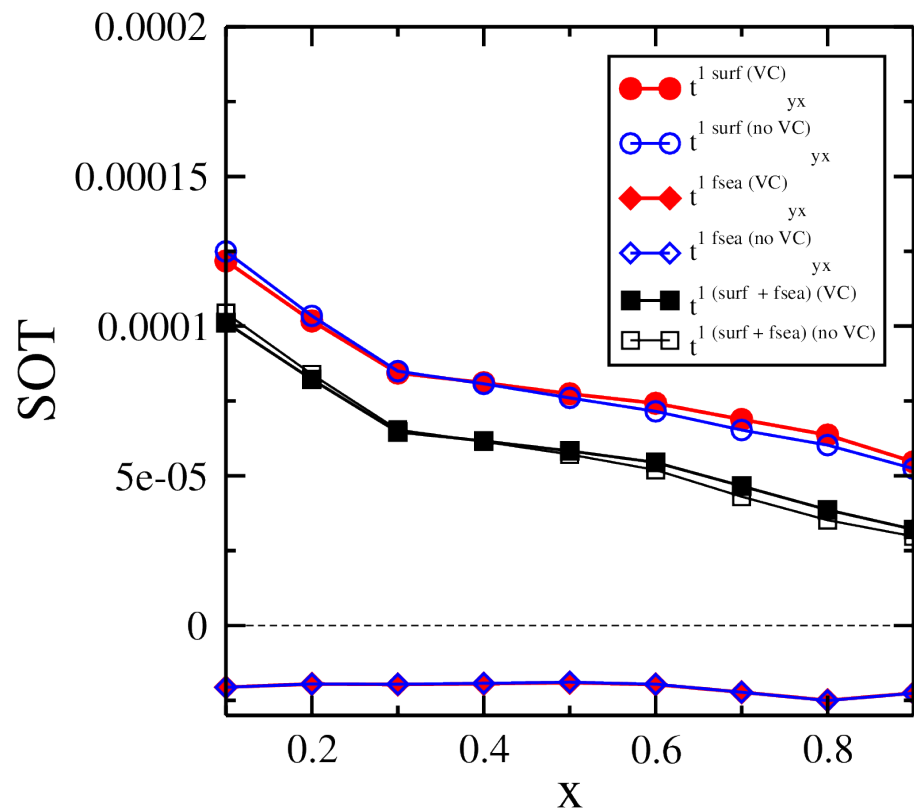


## Symmetry

$$t = \begin{pmatrix} t_{xx} & -t_{yx} & 0 \\ t_{yx} & t_{xx} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$t_{yx}$

even w.r.t.  $\vec{M} \rightarrow -\vec{M}$



- Fermi surface contribution dominant showing variation with concentration
- Fermi sea term almost constant



A universal scheme has been presented to

*predict the shape of any linear response tensor*

- **Electrical and spin conductivity**
  - Only magnetic Laue group relevant
  - AHE in non-collinear AFMs
  - Longitudinal Spin Conductivity
- **Torkance** (spin-orbit torque)
  - Only for systems without space inversion symmetry
- **Gilbert damping**
- **Edelstein effect**
- **Thermoelectric effects**
- **Layer-resolved conductivities**
- **Non-linear response**

*All results in full agreement with ab-initio calculations based on fully relativistic formalism*

*Further Applications not presented here*

Deutsche  
Forschungsgemeinschaft  
**DFG**

SFB 689



SPP 1538

Spin Caloric  
Transport

