A first-principles approach to orbital accumulation and orbital transport

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Outline

Aim: Develop electronic structure theory to compute and predict unusual spin and orbital effects

- Motivation: Spin-orbit torques
- Electronic structure methodology
- Results: Orbital Hall effect & orbital Nernst effect in 40 elements
- Magnetic spin Hall effect and magnetic orbital Hall effect in FMs & bilayers
- Detection of orbital accumulation in thin layers

Thanks to:

Leandro Salemi

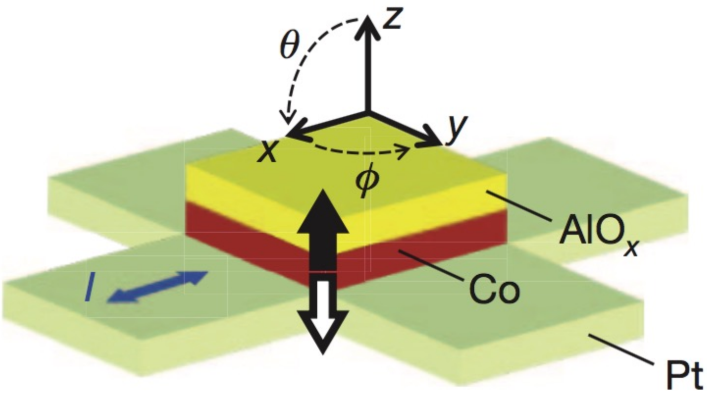
Marco Berritta

Sanaz Alikhah

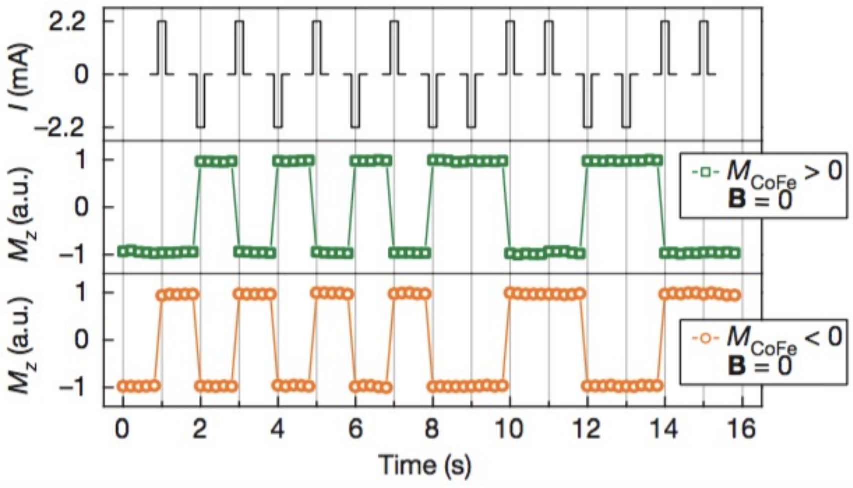
Knut och Alice Wallenbergs Stiftelse

Motivation - Spin-orbit torques

Magnetization switching with SOT



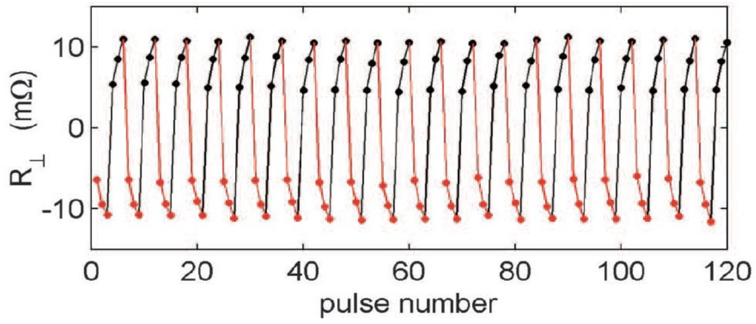
Spin Hall effect - small relativistic effect



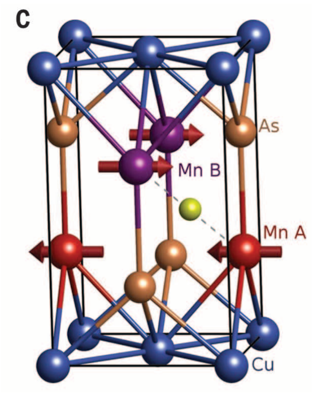
Miron et al, Nature **476**, 189 (2011)

Liu et al, Science **336**, 555 (2012)

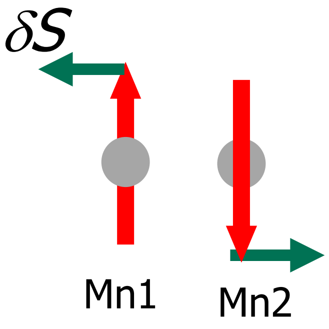
Staggered SOTs in special AFMs



CuMnAs



Rashba-Edelstein effect



Zelezny et al, PRL **113**, 157201 (2014)

Wadley et al, Science **351**, 587 (2016)

Zelezny et al, PRB **95**, 014403 (2017)

Review: Manchon et al, Rev.Mod.Phys. **91**, 035004 (2019)

From a device view point

Spin polarized currents
Spin transfer torque (STT)

→

Spin currents
Spin-orbit torque (SOT)

→

Orbital currents
??

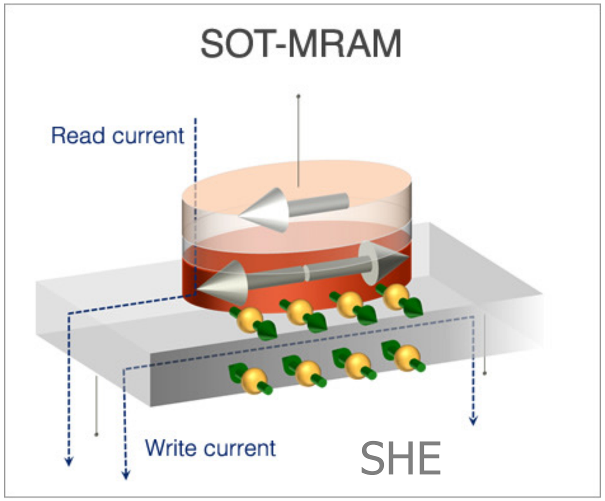
Slonczewski, 1996

STT-MRAM

Everspin, Samsung, IBM

market-ready product
after ~20 years

Hirsch 1999 (SHE)
Miron et al, 2011

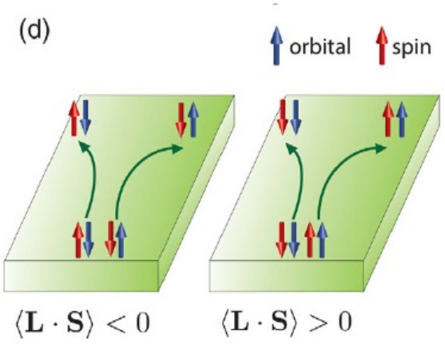


Technology being
developed for market

Observation SHE Pt:
Stamm et al, 2017

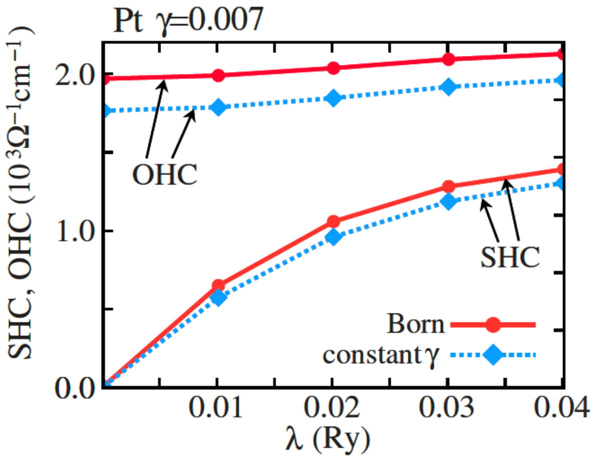
Go et al, ~2018 (OHE)

Orbital torque?



Current fundamental
research topic

Large orbital effects predicted



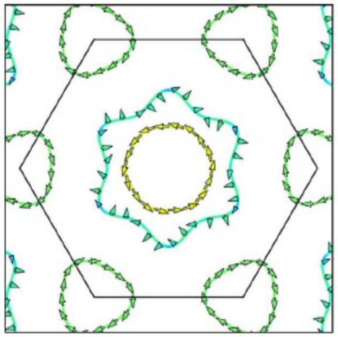
Orbital Hall effect predicted – without SOC

Tanaka et al, PRB **77**, 165117 (2008)

Orbital Rashba effect

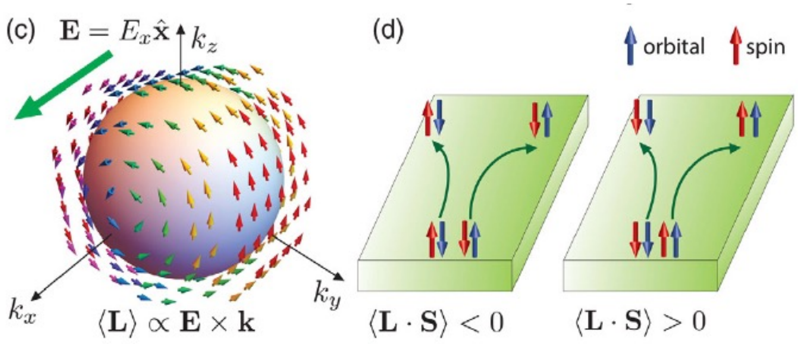
$$H_{\mathrm{OR}}(\mathbf{k}) = \frac{\alpha_{\mathrm{OR}}}{\hbar}\hat{\mathbf{L}}\cdot(\hat{\mathbf{z}}\times\mathbf{k})$$

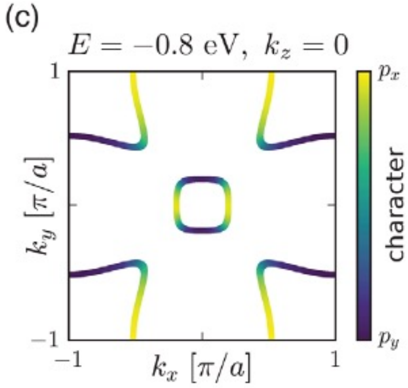
Orbital Rashba Hamiltonian



Go, Lee, Mokrousov, Blügel et al, Sci. Rep. **7**, 46742 (2017)

Explanation of OHE



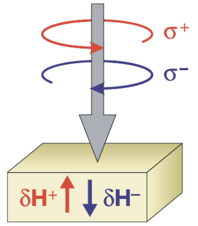


Orbital texture in k-space
Go, Jo, Kim & Lee, PRL **121**, 086602 (2018)

Electronic structure theory predictions

Orbital inverse Faraday effect –
not due to SOC

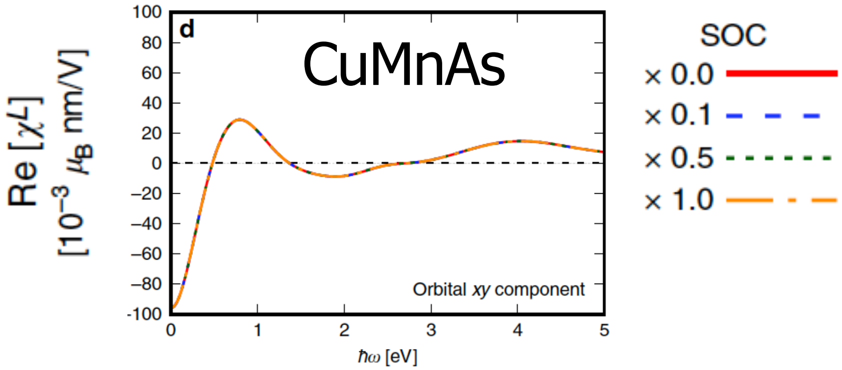
Berritta, Mondal, Carva, Oppeneer,
PRL **117**, 137203 (2016)



$$\overrightarrow{\delta M} \propto E^2 \vec{k}$$

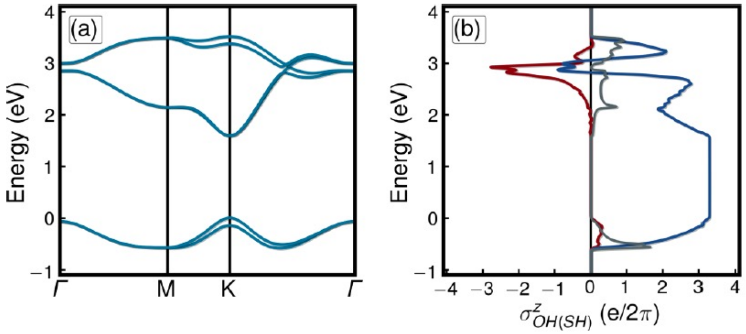
Orbital Rashba-Edelstein effect –
large, not due to SOC

Salemi, Beritta, Nandy, Oppeneer,
Nat. Commun. **10**, 5381 (2019)



Orbital Hall insul. phase in TMDCs

Canonico, Cysne, Molina, Muniz &
Rappoport, PRB **101**, 161409R (2020)

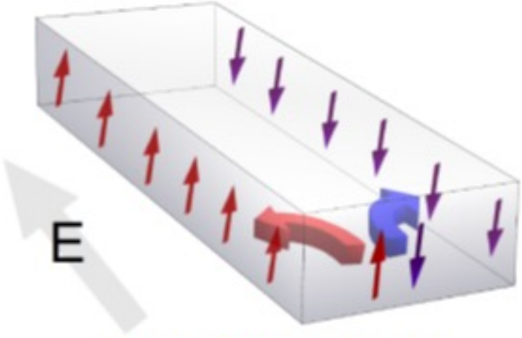


Many new papers in last years:

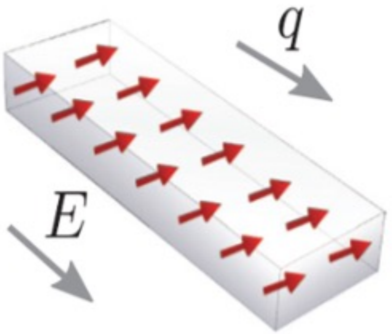
Go, Freimuth, Hanke, Xue et al, Phys.Rev.Res. **2**, 033401 (2020)
Go, Jo, Lee, Kläui & Mokrousov, EPL **135**, 37001 (2021)
Lee, Go, Park, Jeong et al, Nat. Commun. **12**, 6710 (2021)
Choi et al, arXiv 2109.14847

Phenomena: Charge-to-spin conversion – SHE & SREE

Spin Hall effect



Rashba-Edelstein effect,
inv. spin-galvanic effect



$\sigma_{yx}^{S_z}$ & χ_{yx}
time-reversal even

Transport

$$J_y^{S_z} = \sigma_{yx}^{S_z} \cdot E_x$$

Spin Conductivity Tensor

Local

$$\delta S_y = \chi_{yx} \cdot E_x$$

Spin Susceptibility Tensor

Dyakonov & Perel, JETP Lett. **13**, 467 (1971)

Hirsch, Phys.Rev.Lett. **83**, 1834 (1999)

Infinite bulk 3D crystal

http://zfmezo.home.amu.edu.pl/research.php

Edelstein, Solid State Comm. **73**, 233 (1990)

Originally: Rashba SOC + 2D symm.

Bychkov & Rashba, JETP Lett. **39**, 78 (1984)

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Methodology – Electronic structure calculations

Rashba-Edelstein effect

(requires inv. symmetry breaking)

$$\delta S_i = \chi^S_{ij} E_j$$

Spin magneto-electric susceptibility

$$\delta L_i = \chi^L_{ij} E_j$$

Orbital magneto-electric susceptibility

DFT + linear response theory

$A = \hat{L}$ or $\hat{S}$ (atomic sphere !)

$$\chi^A_{ij} = -\frac{ie}{m_e}\int_\Omega \frac{dk}{\Omega}\sum_{n\neq m}\frac{f_{nk}-f_{mk}}{\hbar\omega_{nmk}}\frac{A^i_{mnk}\,p^j_{nmk}}{-\omega_{nmk}+i\tau^{-1}_{\text{inter}}}$$

Interband (Fermi sea)

$$-\frac{ie}{m_e}\int_\Omega \frac{dk}{\Omega}\sum_{n}\frac{\partial f_{nk}}{\partial \epsilon}\frac{A^i_{nnk}\,p^j_{nnk}}{i\tau^{-1}_{\text{intra}}}$$

Intraband (Fermi Surface)

$$\hbar\omega_{nmk} = \epsilon_{nk} - \epsilon_{mk}$$

Relativistic WIEN2k

(own implementation)

$$\delta \boldsymbol{M} = \mu_B \delta(\boldsymbol{L} + 2\boldsymbol{S})$$

Salemi, Berritta, Nandy, Oppeneer, Nat. Commun. **10**, 5381 (2019)

Ab initio calculations

Spin Hall effect $$\boldsymbol{J}^{S_k} = \boldsymbol{\sigma}^{S_k} \boldsymbol{E}$$

Orbital Hall effect $$\boldsymbol{J}^{L_k} = \boldsymbol{\sigma}^{L_k} \boldsymbol{E}$$

$$A = \hat{\boldsymbol{j}}^{S_k} = \frac{\{\hat{S}_k, \hat{\boldsymbol{p}}\}}{2m_e V}$$

Spin/orbital current operator

Include scattering effects in an average through lifetimes $\tau_{intra}, \tau_{inter}$

(no explicit extrinsic effects such as side step or skew scattering)

SHE: Guo et al, PRL **100**, 096401 (2008)
OHE: Tanaka et al, PRB **77**, 165117 (2008)
Jo, Go, and Lee, PRB **98**, 214405 (2018)

Spin and orbital Nernst effects

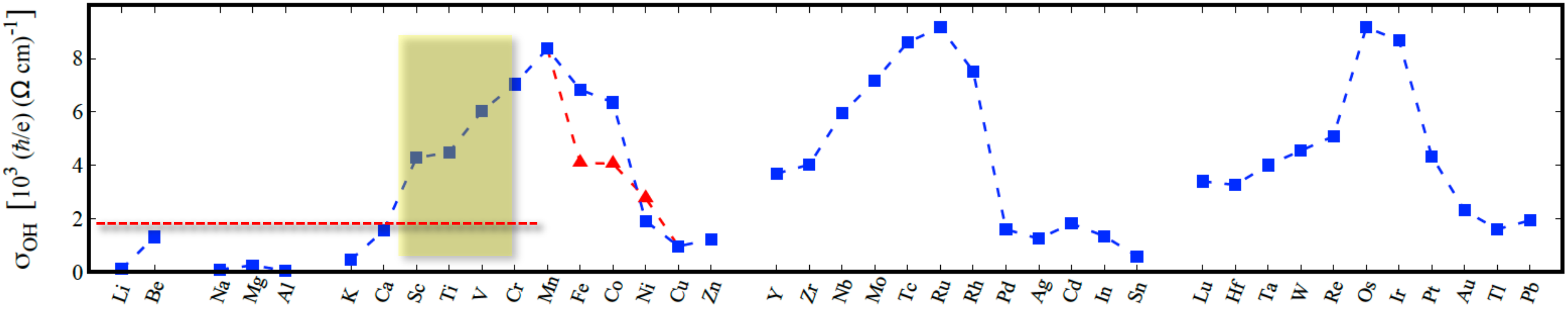
$$J_i^{S_k} = \sigma_{ij}^{S_k} E_j - \Lambda_{ij}^{S_k} \frac{dT}{dr_j}$$

Thermal gradient

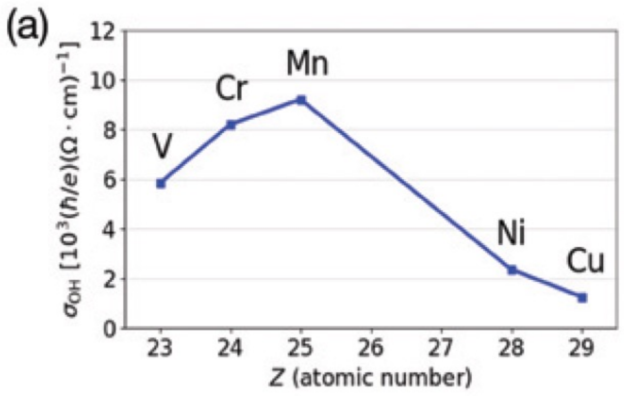
$$\Lambda_{ij}^{S_k(L_k)} = \frac{\pi^2 k_B^2 T}{-3e} \left(\frac{d}{dE} \sigma_{ij}^{S_k(L_k)}(E) \right)_{E=E_F}$$

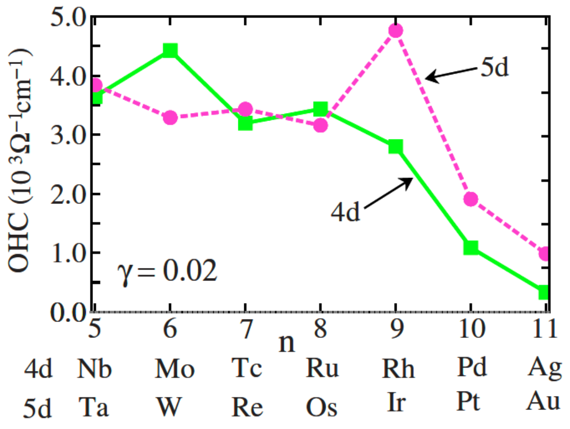
Spin Nernst effect: Meyer et al, Nat. Phys. **16**, 977 (2017)

Size of OHE for 40 elements



Jo et al, PRB **98**, 214405 (2018)





Tanaka et al, PRB **77**, 165117 (2008)

- Large effects for light 3d metals
- Good agreement with Jo et al (2018)
- Factor 2 & different trend from Tanaka et al (2008)
- Cheap, light metals for future orbitronics?

Salemi and Oppeneer, Phys.Rev.Mat. **6**, 095001 (2022)

Recently predicted new effects

Hall

SHE OHE

MSHE MOHE

Rashba-Edelstein

SREE OREE

MSREE MOREE

Nernst

SNE ONE

MSNE MONE

	SHE	MSHE	OHE	MOHE
Require SOC	*YES*	*YES*	*NO*	*YES*
Require magnetism (*T*-odd)	*NO*	*YES*	*NO*	*YES*
Intraband (Fermi surf.)	*NO*	*YES*	*NO*	*YES*

$\sigma_{yx}^{S_z}$, χ_{yx}^{S} & $\Lambda_{yx}^{S_z}$
time-reversal even

Tanaka et al, PRB **77**, 165117 (2008)
Sinova et al, Rev. Mod. Phys. **87**, 1213 (2015)
Kimata et al, Nature **565**, 627 (2019)
Salemi et al, Nat. Commun. **10**, 5381 (2019)

Edelstein, Solid State Comm. **73**, 233 (1990)
Meyer et al, Nat. Phys. **16**, 977 (2017)
Salemi and Oppeneer, PRB **106**, 024410 (2022)

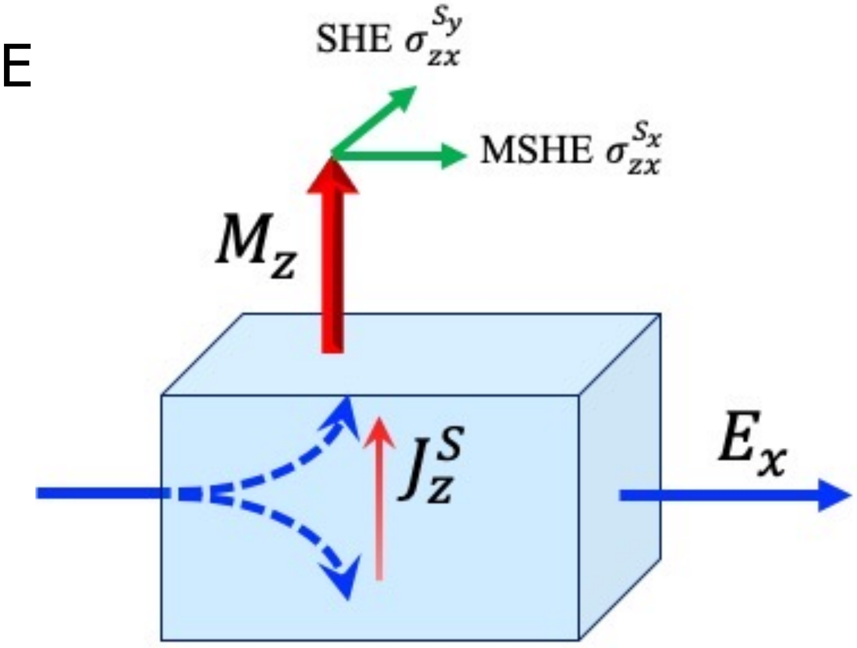
Unusual spin and orbital currents

Conventional SHE

$\vec{J}^S \perp \vec{E} \perp \vec{S}$

Time-reversal and *M* even

Fermi sea or interband



Anomalous component

$\vec{J}^S \perp \vec{E} \,||\, \vec{S}$

Time-reversal and *M* odd

Fermi surface or intraband $n = m$

Spin Berry curvature

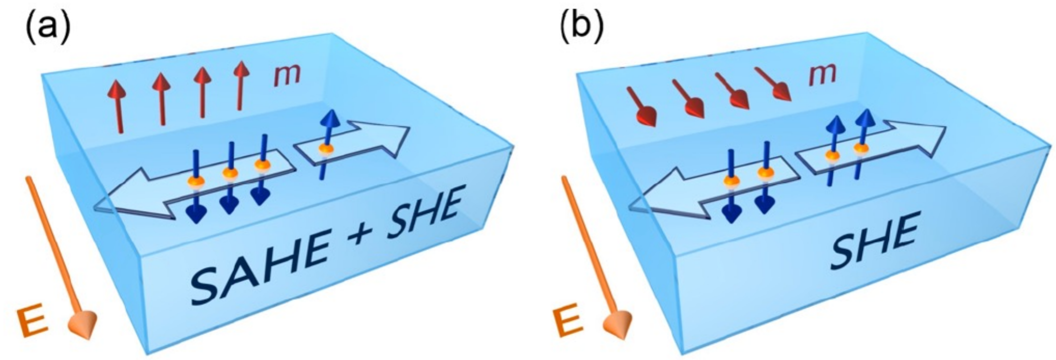
$$\sigma_{\mathrm{OH(SH)}} = \frac{e}{\hbar} \underline{\sum_{n \neq m}} \int \frac{d^3 k}{(2\pi)^3} (f_{m\mathbf{k}} - f_{n\mathbf{k}}) \Omega^{X_z}_{nm\mathbf{k}},$$

$$\Omega^{X_z}_{nm\mathbf{k}} = \hbar^2 \mathrm{Im} \left(\frac{\langle u_{n\mathbf{k}} | j_y^{X_z} | u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | v_x | u_{n\mathbf{k}} \rangle}{(E_{n\mathbf{k}} - E_{m\mathbf{k}} \underline{+ i\eta})^2} \right)$$

Calculations show: Always present for *magnetic* materials (MSHE and MOHE)

Salemi, Berritta, Oppeneer, PRMat. **5**, 074407 (2021)

Spin anomalous Hall effect (SAHE) in ferromagnets

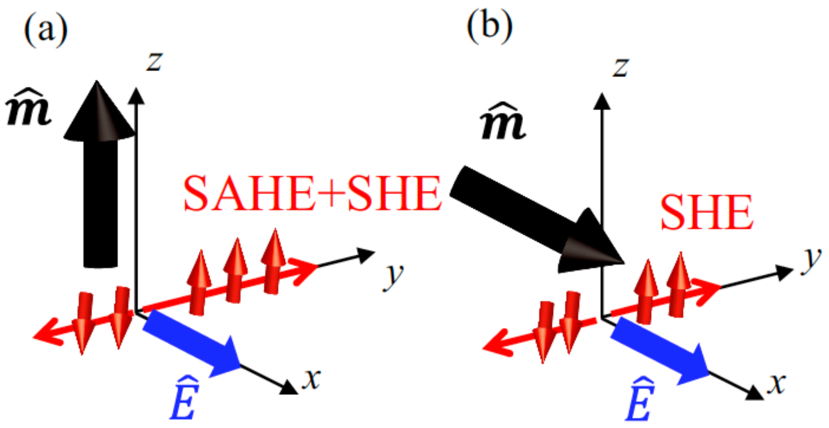


$$\vec{J}^S \perp \vec{E} \perp \vec{S}$$

$$\sigma_{\alpha\gamma}^{\beta} = -\frac{2e^2}{\hbar}\mathrm{Im}\int \frac{d\mathbf{k}}{(2\pi)^3} \sum_{\substack{n \in \text{occ.} \\ m \in \text{unocc.}}} \frac{\langle\psi_m|\hat{Q}_\alpha^\beta|\psi_n\rangle\langle\psi_n|\hat{v}_\gamma|\psi_m\rangle}{(E_n - E_m)^2}$$

Amin, Li, Stiles, Haney, PRB **99**, 220405R (2019)

(Fermi sea or interband term)



$\sigma_{yx}^{S_z}$ SHE-like, *T*-even

Miura & Masuda, PRMat. **5**, L101402 (2021)

Dependence on M direction

Symmetry analysis

Nonmagnetic metal

$$J_i^{S_k} = \underbrace{\sigma_{ij}^{S_k}}_{\epsilon_{ijk}\,\sigma_{\mathrm{SH}}} E_j$$

$$\sigma_{xy}^{S_z} = \sigma_{yz}^{S_x} = \sigma_{zx}^{S_y}$$

(Pt)

Ferromagnet

$$\sigma_{xy}^{S_z} \neq \sigma_{yz}^{S_x} \sim \sigma_{zx}^{S_y}$$

(Fe, Ni)

$$\sigma_{xy}^{S_z} \neq \sigma_{yz}^{S_x} \neq \sigma_{zx}^{S_y}$$

(Co)

$$\text{"}\sigma_{xy}^{SAHE}(\vec{m})\text{"}$$

Amin, Li, Stiles, Haney, PRB **99**, 220405R (2019)
Miura & Masuda, PRMat. **5**, L101402 (2021)

$$\mathbf{M} \parallel \mathbf{u}_z$$

$$\boldsymbol{\sigma}^{S_x} = \begin{pmatrix} 0 & 0 & \textcolor{red}{\sigma_{xz}^{S_x}} \\ 0 & 0 & \textcolor{blue}{\sigma_{yz}^{S_x}} \\ \textcolor{red}{\sigma_{zx}^{S_x}} & \textcolor{blue}{\sigma_{zy}^{S_x}} & 0 \end{pmatrix} \qquad \boldsymbol{\sigma}^{S_y} = \begin{pmatrix} 0 & 0 & \textcolor{blue}{\sigma_{xz}^{S_y}} \\ 0 & 0 & \textcolor{red}{\sigma_{yz}^{S_y}} \\ \textcolor{blue}{\sigma_{zx}^{S_y}} & \textcolor{red}{\sigma_{zy}^{S_y}} & 0 \end{pmatrix}$$

(and $\boldsymbol{\sigma}^{S_z}$)

SHE-like, *T*-even

ε_{ijk}

MSHE-like, *T*-odd

Repeated indices

Seemann, Ködderitzsch, Wimmer & Ebert, PRB **92**, 155138 (2015) Wang, Commun.Phys. **4**, 55 (2021)

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Calculated results Fe, Co, Ni

	T-even						*T*-odd			
	SHE			OHE			MSHE		MOHE	
	$\sigma_{yz}^{S_x}$	$\sigma_{zx}^{S_y}$	$\sigma_{xy}^{S_z}$	$\sigma_{yz}^{L_x}$	$\sigma_{zx}^{L_y}$	$\sigma_{xy}^{L_z}$	$\sigma_{xz}^{S_x}$	$\sigma_{zx}^{S_x}$	$\sigma_{xz}^{L_x}$	$\sigma_{zx}^{L_x}$
Fe	441	456	92	4697	4698	4707	-593	739	1343	848
Co	839	8	-44	5103	4718	4737	614	1074	-358	1356
Ni	1606	1543	824	3306	3297	3149	394	-290	-66	1033

$\frac{\hbar}{e}(\Omega\,\mathrm{cm})^{-1}$

$\hbar\tau^{-1} = 40$ meV

SAHE

OHE >> SHE

SHE components strongly *M*-anisotropic (SAHE)

MSHE ~ SHE => must be taken into account

MOHE (new) exists, but smaller than OHE

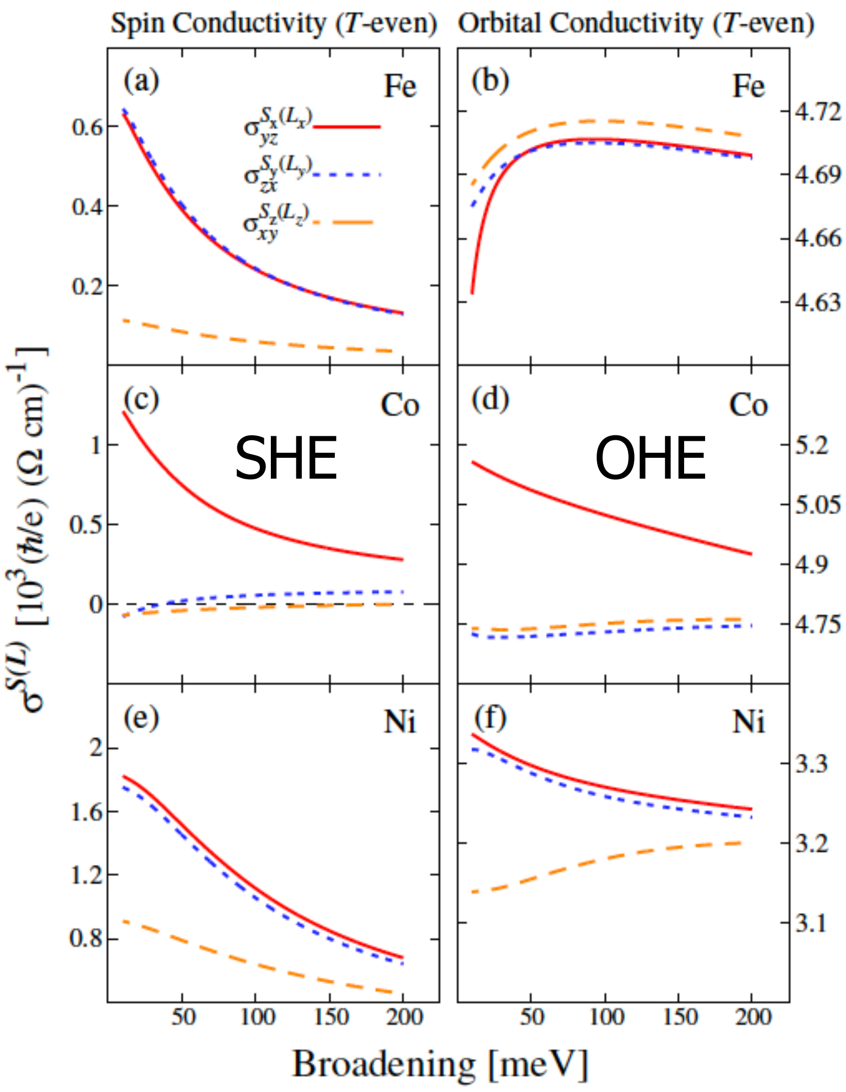
OHE present without SOC, all others require SOC

MSHE and MOHE (*intraband*) larger for pure samples

Salemi and Oppeneer, PRB 106, 024410 (2022)

Lifetime dependence

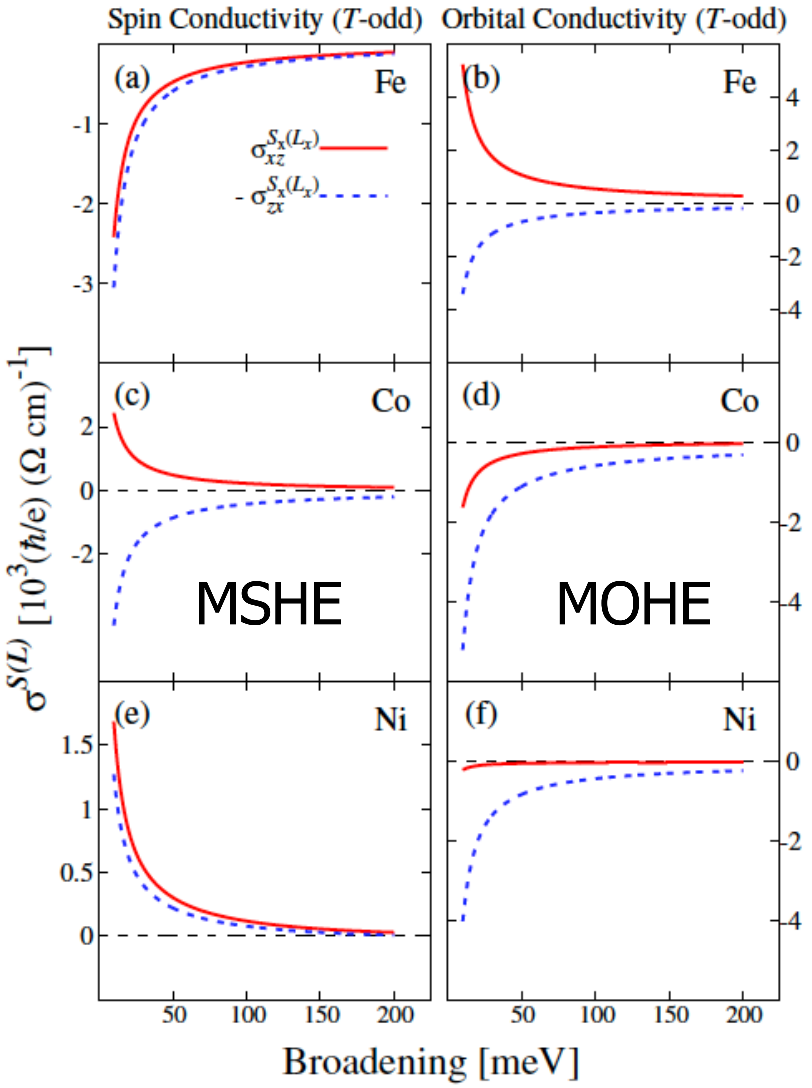
T-even



SHE

OHE

T-odd

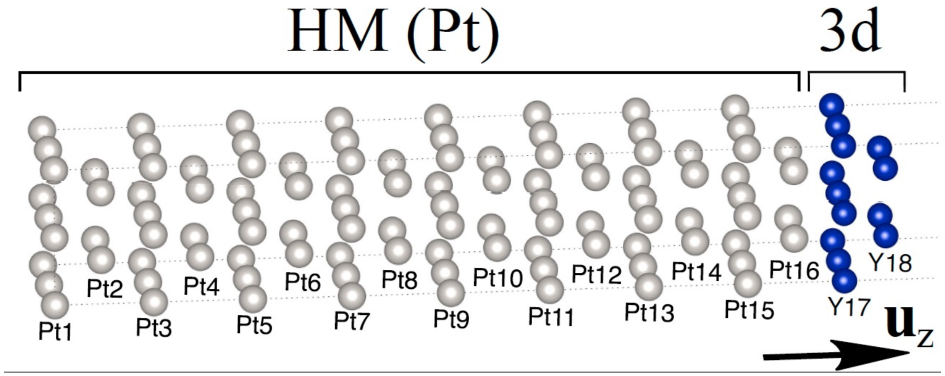


MSHE

MOHE

MSHE and MOHE (*intraband*) much larger for pure samples

SOTs at symmetry-broken interface Pt/3d FM



n Pt / 2 Y

Y = Ni, Co, Cu or Pt

n = 2 to 16

$$\delta \boldsymbol{S} = \boldsymbol{\chi}^S \ \boldsymbol{E}$$

$$\boldsymbol{J}^{S^\kappa} = \underline{\boldsymbol{\sigma}^{S_k}} \ \boldsymbol{E}$$

E along x

Ind. polarization

$$\begin{cases} \delta S_y = \chi^S_{yx} E_x & \textit{T}\text{-even} \\ \delta S_x = \chi^S_{xx} E_x & \textit{T}\text{-odd} \end{cases}$$

$$\boldsymbol{\mathcal{M}} = \boldsymbol{S}/|\boldsymbol{S}|$$

Effective torques

$$\boldsymbol{\mathcal{T}} = \boldsymbol{M} \times \delta \boldsymbol{B} \qquad \delta \boldsymbol{B} \approx |\boldsymbol{B}_{\mathrm{XC}}| \frac{\delta \boldsymbol{S}}{|\boldsymbol{S}|}$$

$$\boldsymbol{\mathcal{T}} = -2\mu_B |\boldsymbol{B}_{\mathrm{XC}}| \left[\boldsymbol{\mathcal{M}} \times \left(\boldsymbol{\chi}^S \boldsymbol{E} \right) \right]$$

$$\boldsymbol{\mathcal{T}}_{\mathrm{FL}} \propto \boldsymbol{M} \times (\boldsymbol{E} \times \boldsymbol{u}_z)$$

Time-rev. odd – field like

$$\boldsymbol{\mathcal{T}}_{\mathrm{DL}} \propto \boldsymbol{M} \times [\boldsymbol{M} \times (\boldsymbol{E} \times \boldsymbol{u}_z)]$$

Time-rev. even – damping like

Early work:

Haney, Lee, Lee, Manchon, Stiles, PRB **88**, 214417 (2013)

Freimuth, Blügel, Mokrousov, PRB **90**, 174423 (2014)

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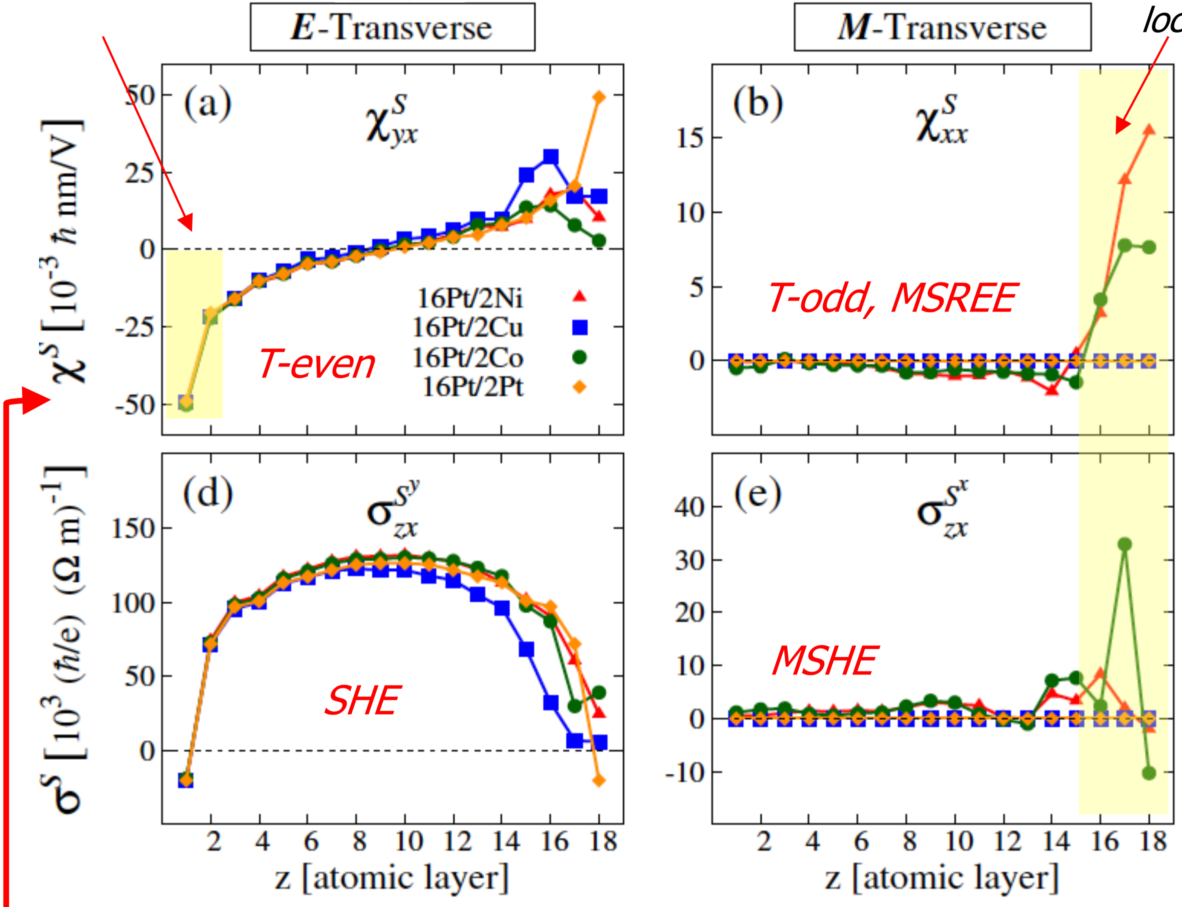
Layer-resolved induced spin polarization

δS_y SPIN δS_x $\boldsymbol{M} \parallel \boldsymbol{u}_z$

Spin accum.



local

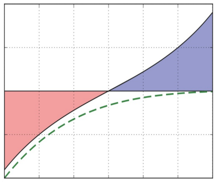
FL DL

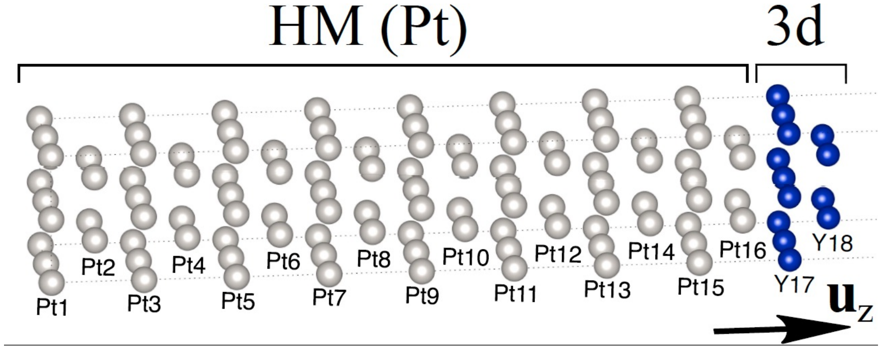
δS_y

- Typical transverse spin accumulation Pt
- Modified at the interface
- *M* and *T*-even effect

δS_x

- Very local response at interface, along E_x
- Only exists for *magn.* material (*M* and *T*-odd)
- Same size as δS_y





Salemi, Berritta, Oppeneer, PRMat. **5**, 074407 (2021)

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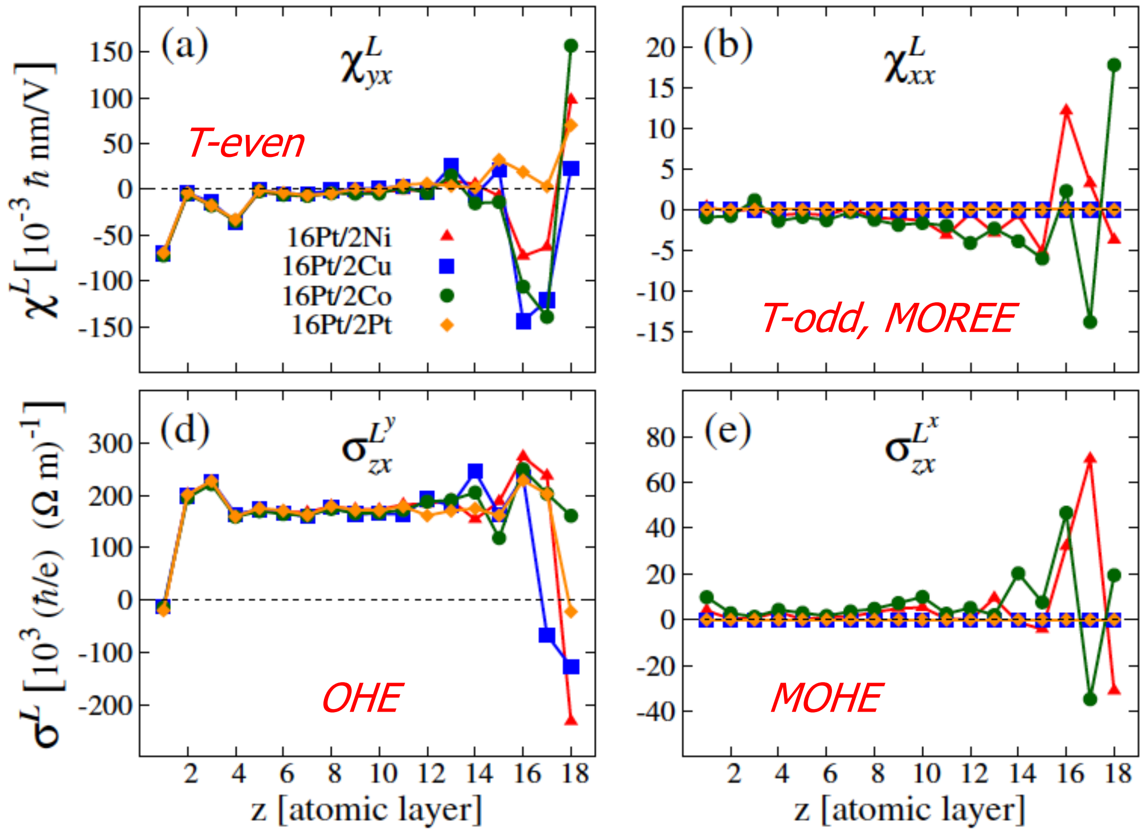
Results Pt/3d-bilayers –*orbital* polarization & current

δL_y ORBITAL δL_x $\boldsymbol{M} \parallel \boldsymbol{u}_z$

***E*-Transverse** ***M*-Transverse**



δL_y

- Huge OHE
- Orb. accumulation profile different from spin
- Enlarged at the interface
- *M*, *T*-even effect

δL_x

- Local response at interface, along E_x
- Only exists for magn. material (*M*, *T*-odd)
- Smaller than *E*-transv.

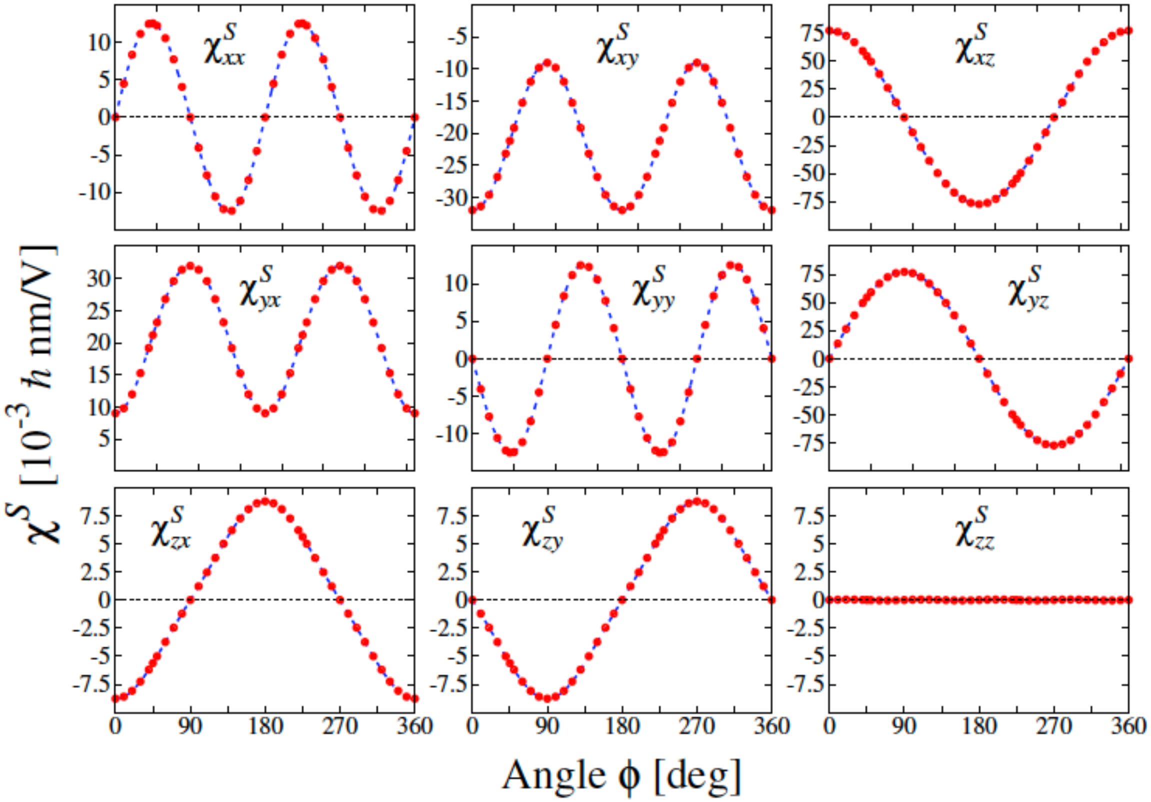
OHE and *E* -transv. orbital polarization not due to SOC

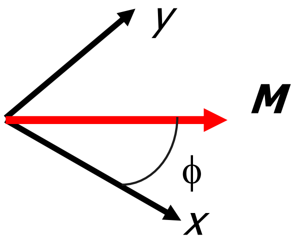
Salemi, Berritta, Oppeneer, PRMat. **5**, 074407 (2021)

Magnetization direction dependence

Dependence of χ^S on *M* direction

12Pt/2Co, 1st Co





In basal plane

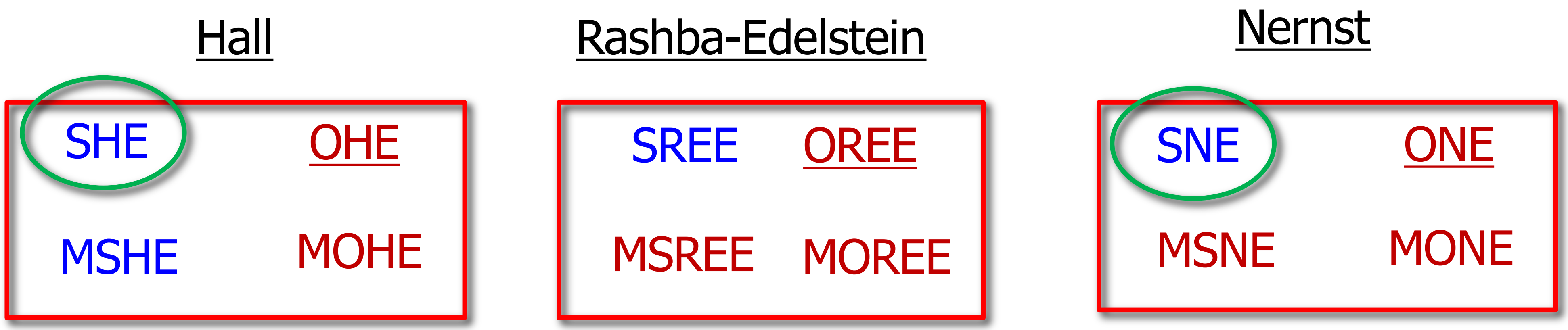
$$\mathcal{T} = -2\mu_B|\mathbf{B}_{\mathrm{XC}}|\left[\mathcal{M}\times\left(\underbrace{\chi^S\mathbf{E}}\right)\right]$$

Induced spin polarization, depends on direction of M

Even in M – 2ϕ – FL torque
Odd in M – ϕ – DL torque

- Accurate angle dependence from *ab initio* calculations
- Identify even in *M* and odd in *M* components => analytical expressions
- Next step: full switching dynamics in the time domain

Many predicted effects – direct observations?



Hall

SHE OHE

MSHE MOHE

Rashba-Edelstein

SREE OREE

MSREE MOREE

Nernst

SNE ONE

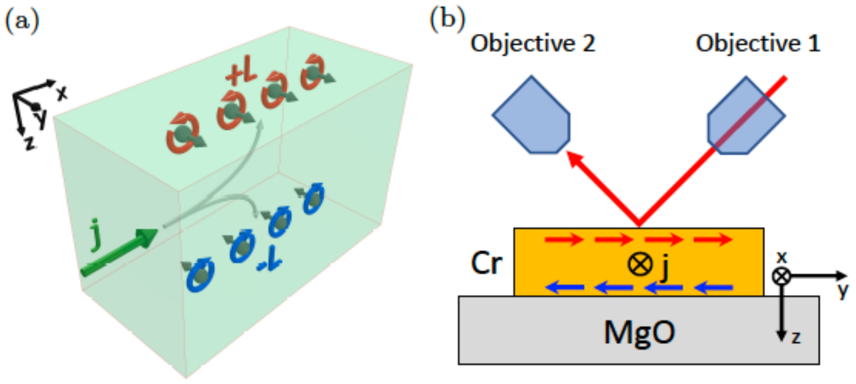
MSNE MONE

Tanaka et al, PRB **77**, 165117 (2008)
Sinova et al, Rev. Mod. Phys. **87**, 1213 (2015)
Kimata et al, Nature **565**, 627 (2019)
Salemi et al, Nat. Commun. **10**, 5381 (2019)

Stamm et al., PRL 119, 087203 (2017)
Meyer et al, Nat. Phys. **16**, 977 (2017)
Salemi and Oppeneer, PRB **106**, 024410 (2022)

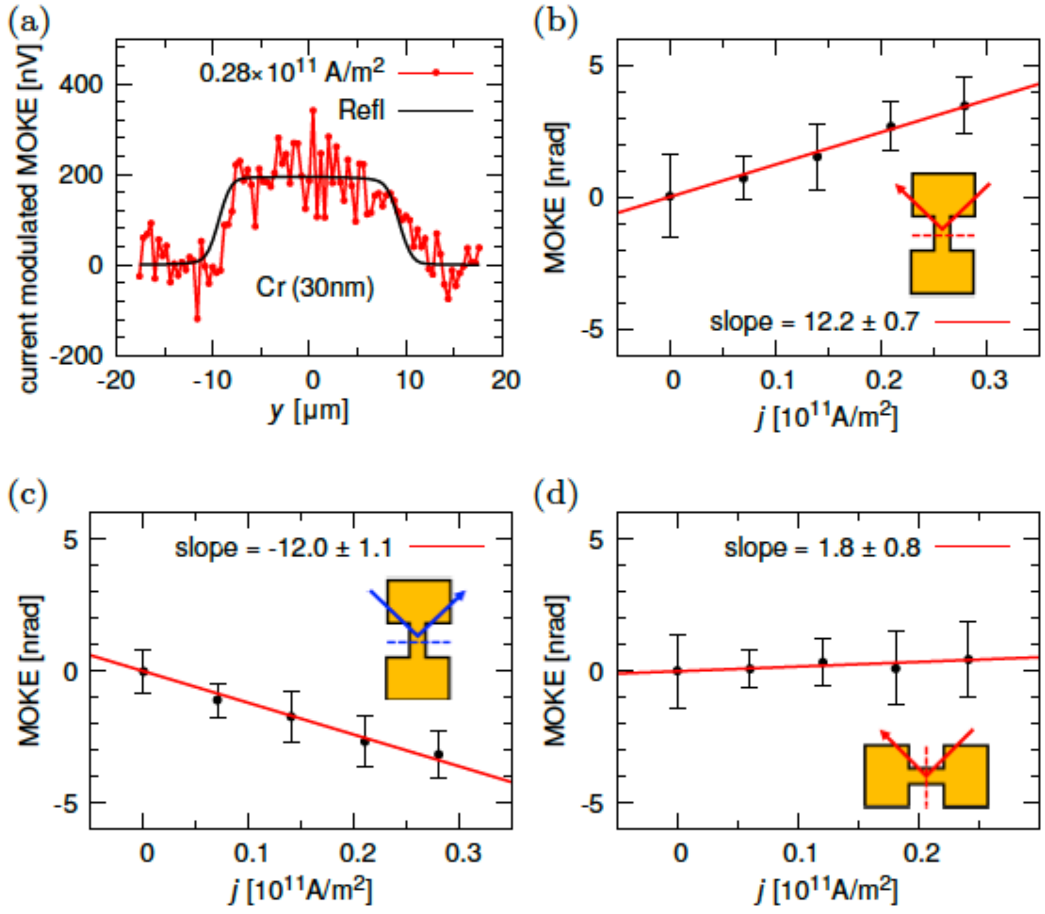
Experimental detection of orbital accumulation

L-MOKE on top surface



Cr film, t = 30 nm, w = 20 μm

Igor Lyalin, Roland Kawakami
(Columbus, Ohio)



nanorads!

See also: Choi, Jo et al., Nature, in press (2023)

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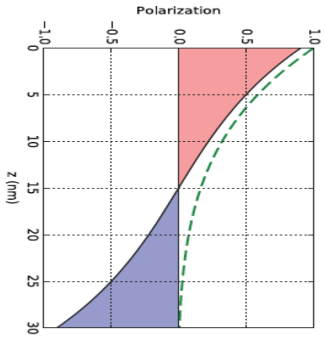
Electronic structure theory



OHE

Bulk complex MOKE

$$\theta_{\mathrm{K}}^{o} = \frac{l_o \sigma_{zx}^{\mathrm{OH}}\, \rho(t)^2 j D(E_{\mathrm{F}})\, \mathrm{e}^{\frac{t}{2l_o}}}{\cosh(\frac{t}{2l_o})} \mathrm{Re}\left\{ \Phi_{\mathrm{K}}^{bulk,o} \kappa \left(\frac{(\mathrm{e}^{-\kappa^- t} - 1)\mathrm{e}^{-\frac{t}{l_o}}}{\kappa^-} - \frac{\mathrm{e}^{-\kappa^+ t} - 1}{\kappa^+} \right) \right\}$$

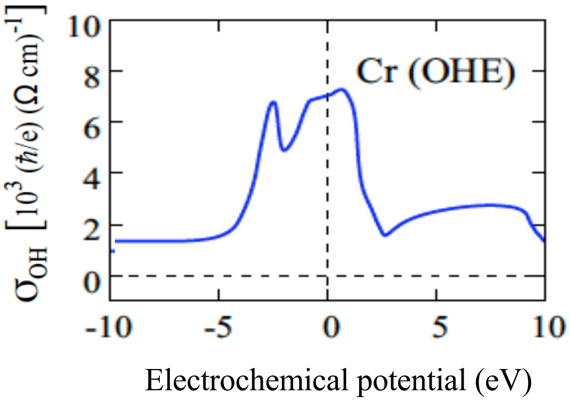
$$\kappa = (4\pi i \bar{n} \cos\psi)/\lambda$$

Orbital diffusion length (parameter)

$$\kappa^{\pm} = \kappa \pm 1/l_o$$

Refractive index

$$\cos\psi = (1 - \sin^2\phi_i/\bar{n}^2)^{1/2}$$



$$\sigma_{zx}^{OH} = 7000 \left(\frac{\hbar}{e}\right)[\Omega cm]^{-1}$$

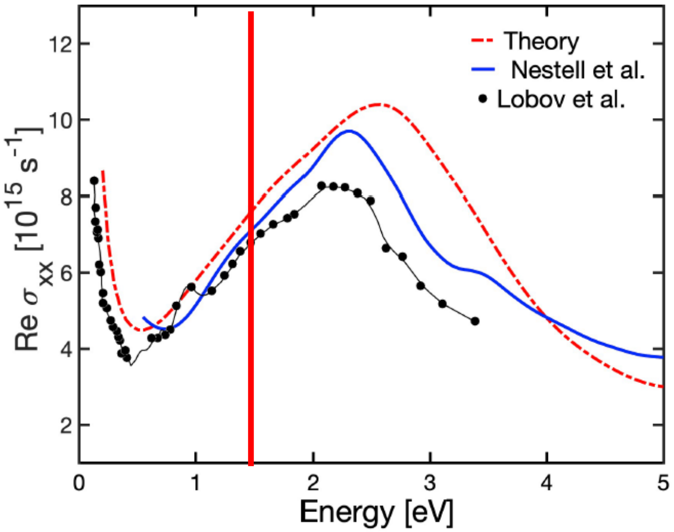
$$\sigma_{zx}^{SH} \approx -70 \left(\frac{\hbar}{e}\right)[\Omega cm]^{-1}$$

bcc Cr

Stamm et al., PRL **119**, 087203 (2017)

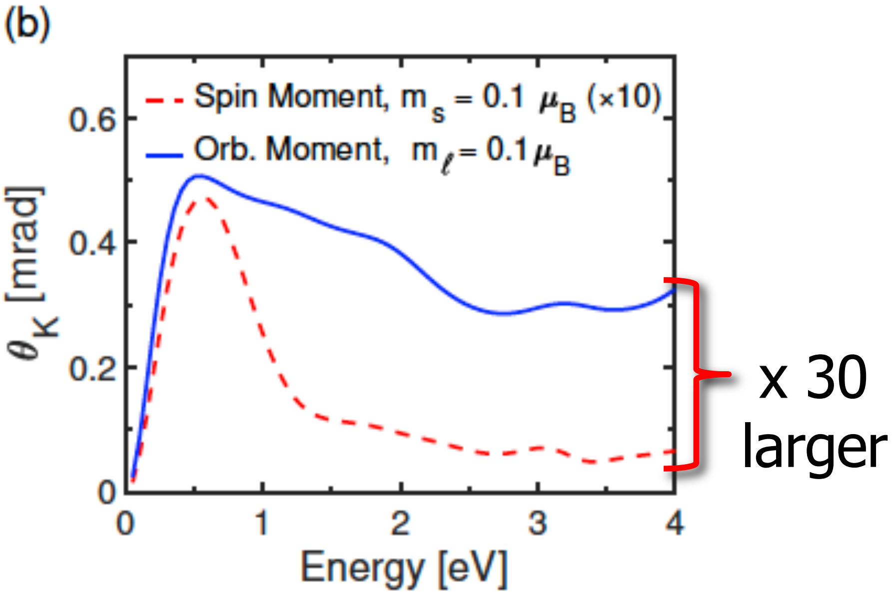
Ab initio based theory

Refractive index *n* from optical conductivity



Bulk complex MOKE, using rel. DFT plus Zeeman field

$$\mathcal{H} = \mu_{\mathrm{B}} \boldsymbol{B}_{ext} \cdot (\boldsymbol{\ell} + 2\boldsymbol{s})$$



$$\theta_{\mathrm{K}}^{L} + i\varepsilon_{\mathrm{K}}^{L} = \frac{iQ\bar{n}n_0}{\bar{n}^2 - n_0^2} \frac{\cos\phi_i \tan\phi_t}{\cos(\phi_i - \phi_t)}$$

WIEN2k FLAPW

$$\sigma_{\alpha\beta}(\omega) = -\frac{i\hbar}{V} \sum_{\boldsymbol{k}} \sum_{n \neq n'} \frac{f(\epsilon_{n\boldsymbol{k}}) - f(\epsilon_{n'\boldsymbol{k}})}{\epsilon_{n\boldsymbol{k}} - \epsilon_{n'\boldsymbol{k}}} \frac{\langle n'\boldsymbol{k}|j^{\alpha}|n\boldsymbol{k}\rangle\langle n\boldsymbol{k}|j^{\beta}|n'\boldsymbol{k}\rangle}{\hbar\omega - \epsilon_{n\boldsymbol{k}} + \epsilon_{n'\boldsymbol{k}} + i\hbar/\tau} + \sigma_{\mathrm{D}}(\omega)\delta_{\alpha\beta}$$

Determination of orbital diffusion length in Cr

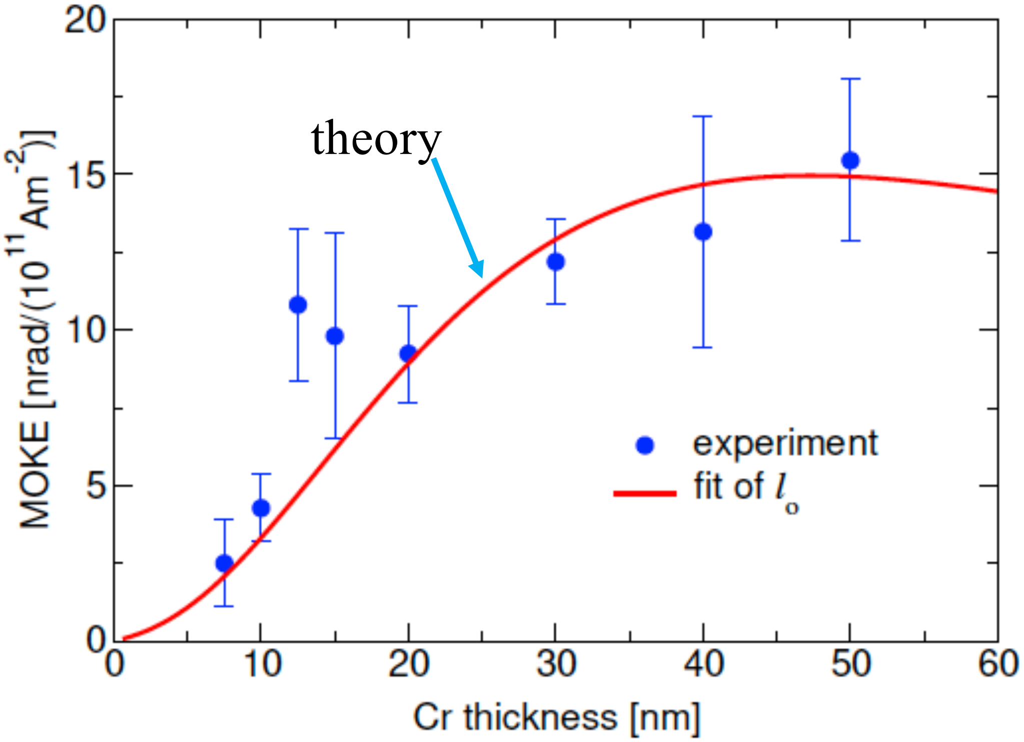
Fit MOKE or MOKE/ρ^2 to obtain l_o

$$l_0 = 6.6 \pm 0.6\, nm$$

$$\sigma_{zx}^{OH} = 7000 \left(\frac{\hbar}{e}\right)[\Omega cm]^{-1}$$

$$\theta_{\mathrm{K}}^{o} = \frac{l_o \sigma_{zx}^{\mathrm{OH}}\, \rho(t)^2 j D(E_{\mathrm{F}})\, \mathrm{e}^{\frac{t}{2l_o}}}{\cosh(\frac{t}{2l_o})} \times$$

$$\mathrm{Re}\left\{\Phi_{\mathrm{K}}^{bulk,o} \kappa \left(\frac{(\mathrm{e}^{-\kappa^{-}t} - 1)\mathrm{e}^{-\frac{t}{l_o}}}{\kappa^{-}} - \frac{\mathrm{e}^{-\kappa^{+}t} - 1}{\kappa^{+}} \right)\right\}$$



Igor Lyalin, Roland Kawakami
(Columbus, Ohio)

Choi, Jo et al., Nature, in press (2023): Orbital diffusion length l_o ~ 60 – 70 nm Ti

But had to scale σ^{OH} by a factor of 1/100

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Summary

Electronic structure calculations very powerful, predictive tool for development of spin-orbitronics and orbitronics

Ferromagnetic Fe, Co, Ni:

- Large magnetic spin Hall effect and MOHE coefficients (*T*-odd) predicted
- Expected to be present in other magnetic materials
- Leads to (novel) magnetic SNE and magnetic ONE (MSNE and MONE)

Pt/3d bilayers

- Presence of *T*-even and *T*-odd spin and orbital accumulations => diff. torques

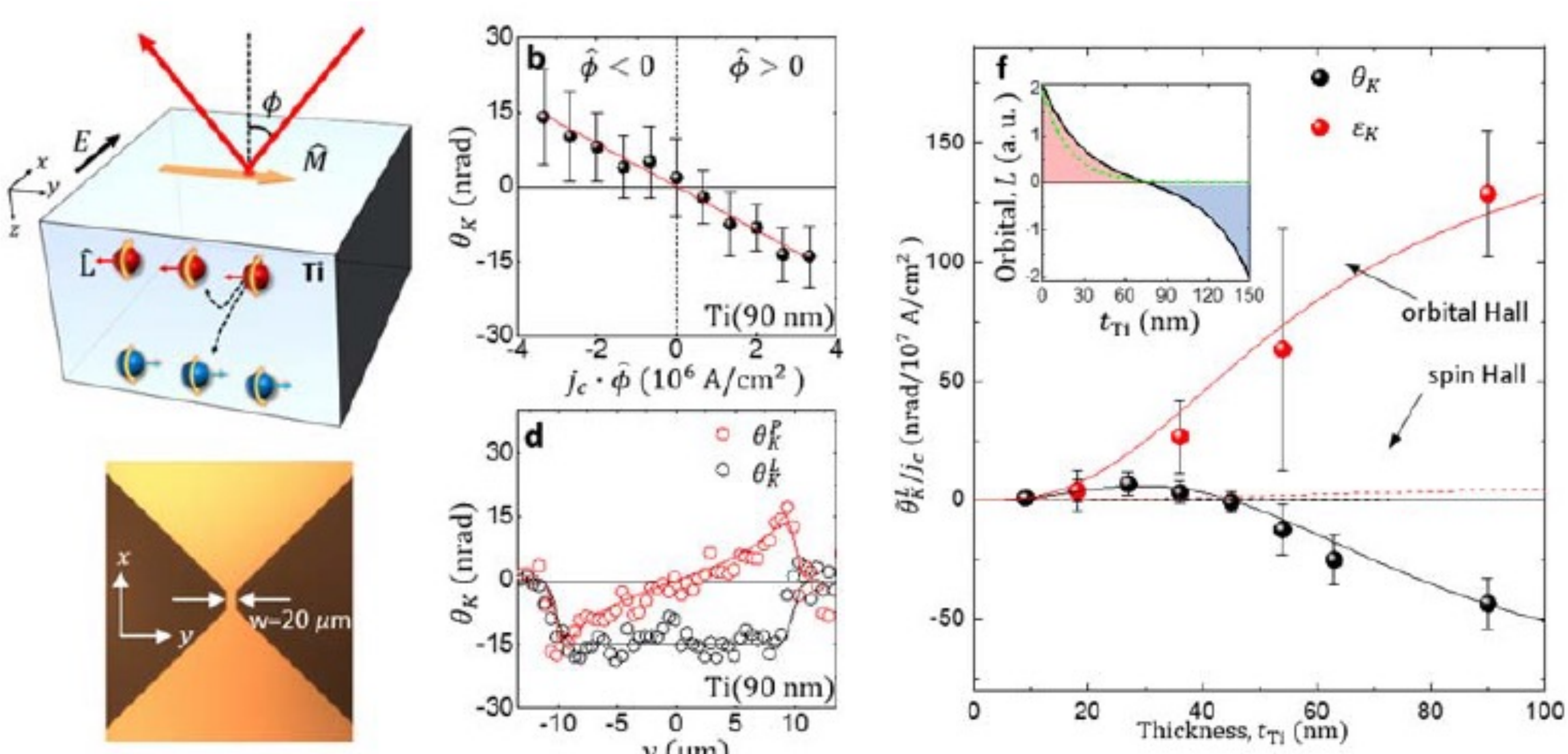
Elements

- Large OHE in light 3d metals predicted
- First evidence of very large OHE in Cr

Vetenskapsrådet
H2020
SEVENTH FRAMEWORK PROGRAMME
FEMTO TERABYTE
S·NEBULA
Knut och Alice Wallenbergs Stiftelse

Magneto-optical detection of OHE in Ti

L-MOKE



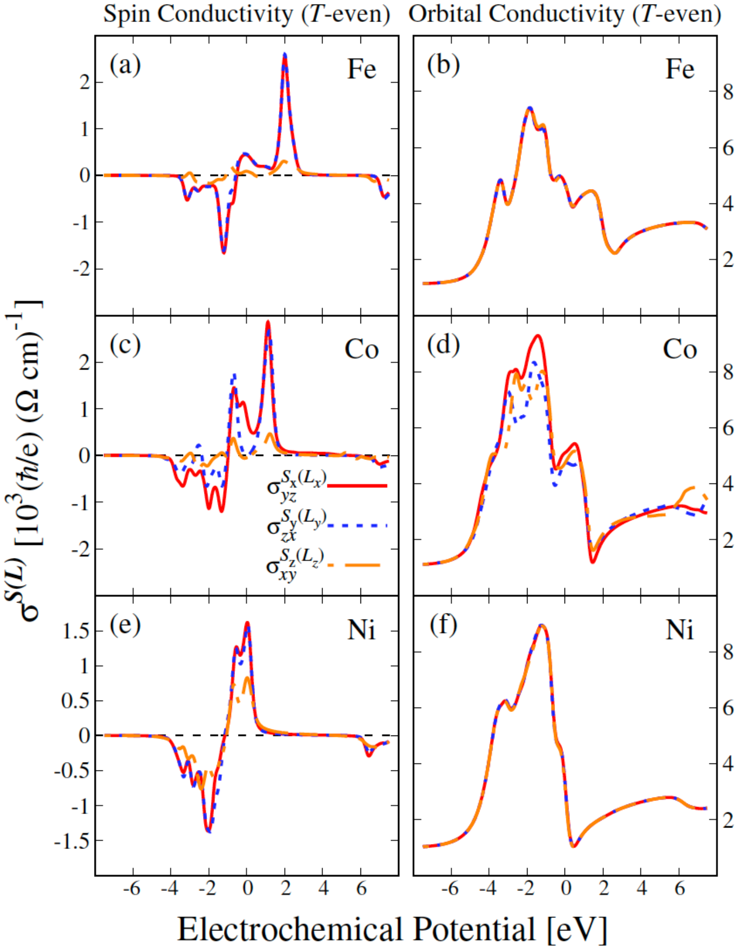
Orbital diffusion length l_o ~ 60 – 70 nm

But had to scale σ^{OH} by a factor of 1/100

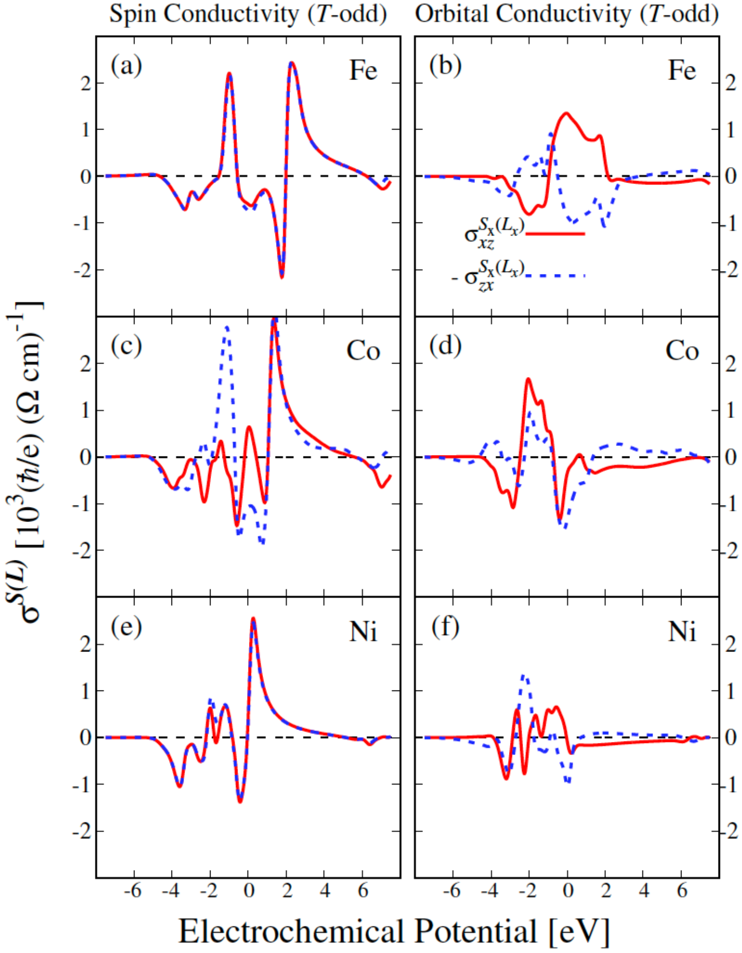
Choi, Jo et al., Nature, in press (2023)

Ab initio calculated results Fe, Co, Ni

SHE-like OHE



MSHE-like MOHE



lifetime

$\hbar\tau^{-1} = 40$ meV

OHE ⋙ SHE

SHE *M*-anisotropic

MOHE ~ MSHE

MSHE ~ isotropic

MSHE ~ SHE

MOHE < OHE

Salemi and PMO, PRB 106, 024410 (2022)

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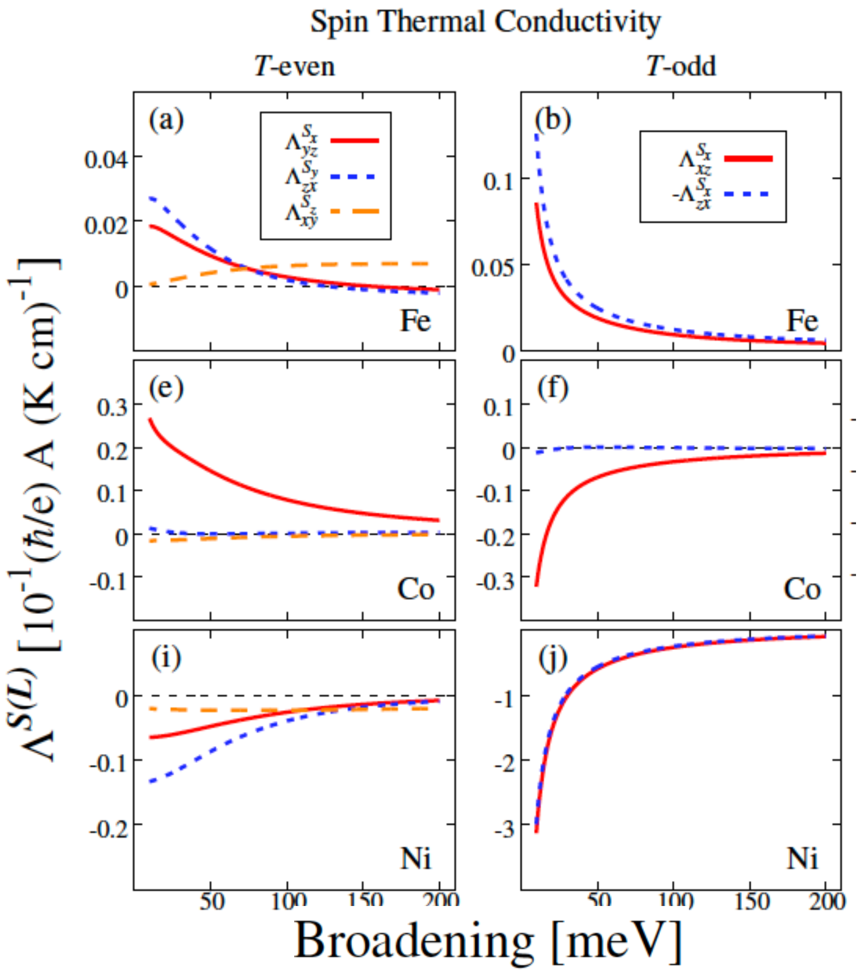
Magnetic spin and orbital Nernst effects

$$J_i^{S_k} = \sigma_{ij}^{S_k} E_j - \Lambda_{ij}^{S_k} \frac{dT}{dr_j} \qquad \Lambda_{ij}^{S_k(L_k)} = \frac{\pi^2 k_B^2 T}{-3e} \left(\frac{d}{dE} \sigma_{ij}^{S_k(L_k)}(E) \right)_{E=E_F} \qquad \alpha_{ij}^{S_k(L_k)} = \frac{\Lambda_{ij}^{S_k(L_k)}}{\sigma_{ij}^{S_k(L_k)}}$$


Spin Thermal Conductivity

“interband” “intraband”

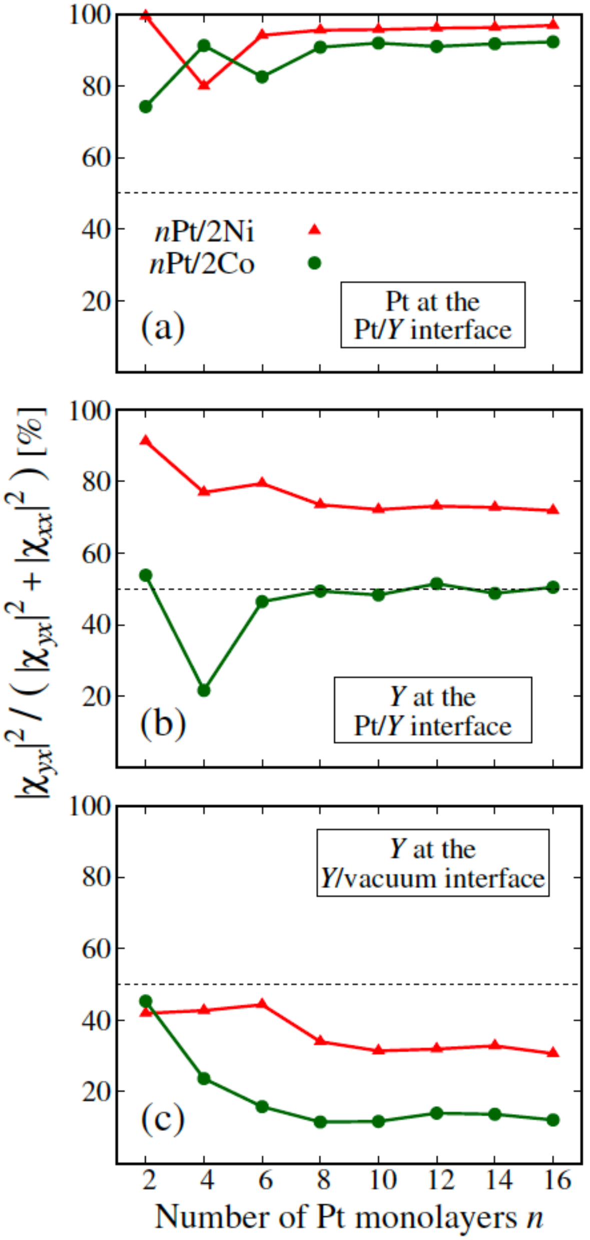
μVK^{-1}	SNC			MSNC	
	$\alpha_{yz}^{S_x}$	$\alpha_{zx}^{S_y}$	$\alpha_{xy}^{S_z}$	$\alpha_{xz}^{S_x}$	$\alpha_{zx}^{S_x}$
Fe	2.63	3.32	3.57	-3.94	-4.18
Co	19.72	1.10	28.74	-14.12	2.91
Ni	-3.35	-6.50	-2.80	-192.55	-248.60

$T = 300$ K

	ONC			MONC	
	$\alpha_{yz}^{L_x}$	$\alpha_{zx}^{L_y}$	$\alpha_{xy}^{L_z}$	$\alpha_{xz}^{L_x}$	$\alpha_{zx}^{L_x}$
Fe	2.87	3.02	2.93	1.07	-6.10
Co	-0.77	-0.83	-1.75	33.48	9.67
Ni	18.22	18.85	19.26	-253.57	-5.61

- Large MSNC and MONC predicted *T*-odd

Sizes of torques & Influence of SOC

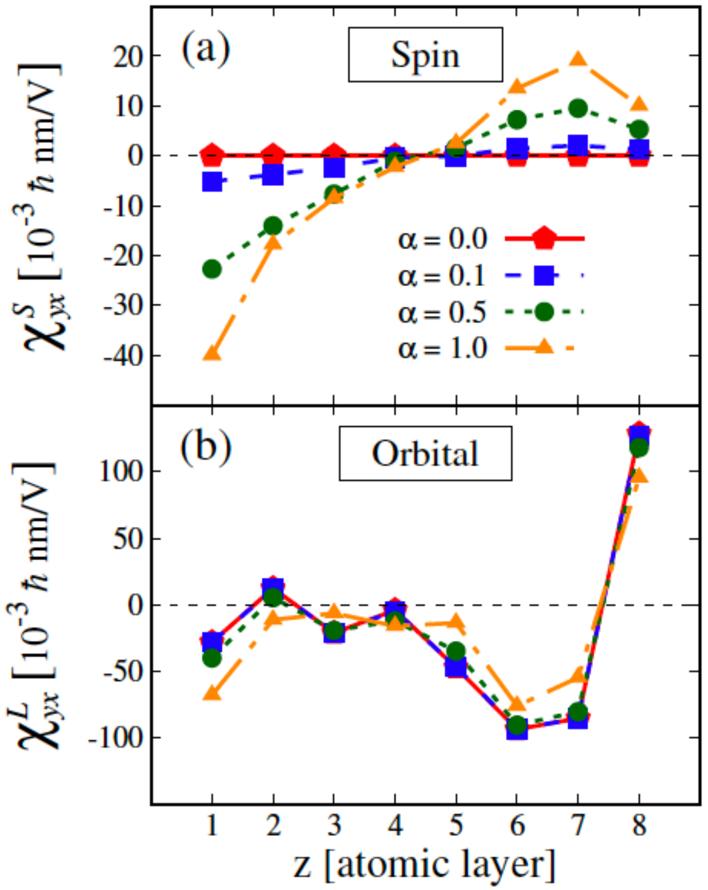


$$\frac{|\chi_{xy}^{S(L)}|^2}{|\chi_{xy}^{S(L)}|^2+|\chi_{xx}^{S(L)}|^2}$$

Spin accum.

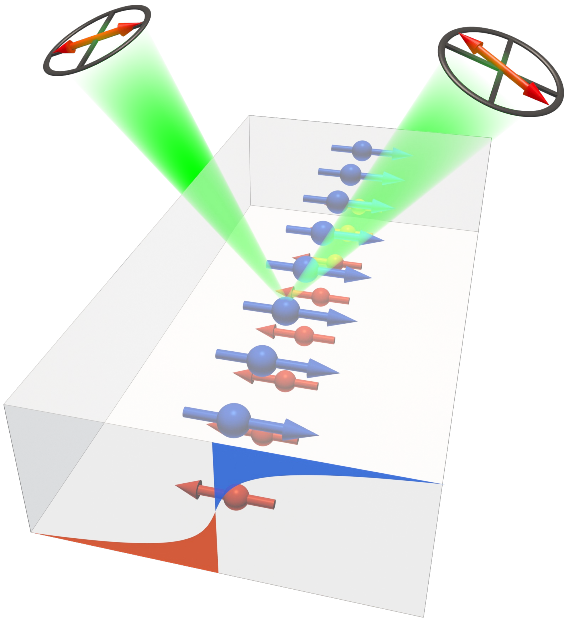
Magn. SHE

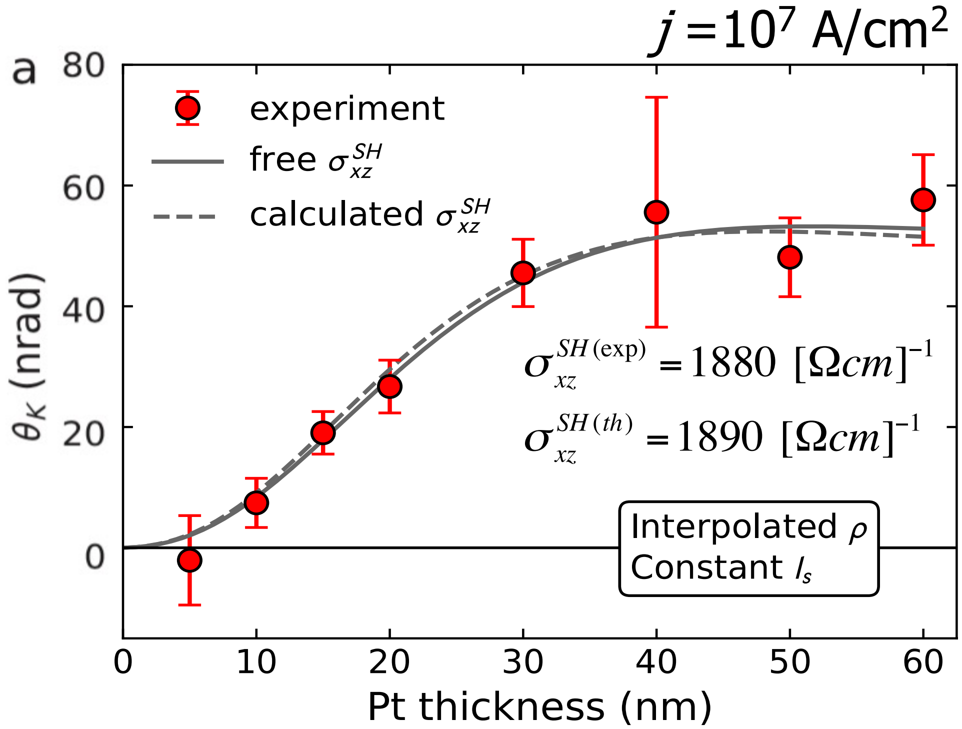
Influence of SOC



T-even orb. accumulation and OHE not due to SOC, all others SOC induced

Magneto-optical detection of SHE





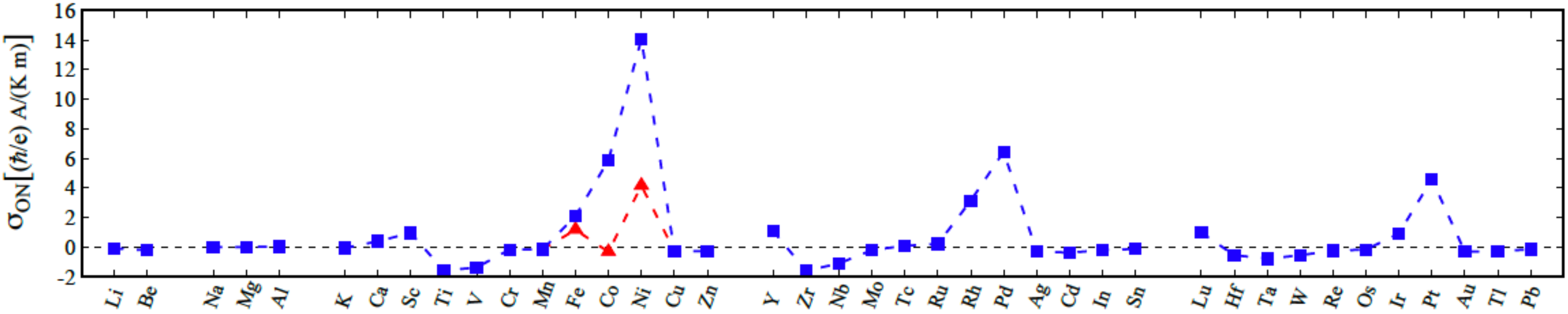
Stamm, Murer, Berritta, Feng, Gabureac, Oppeneer & Gambardella, PRL **119**, 087203 (2017)

Excellent agreement with experiment!

Estimated l_s=11.4±2 nm for pure Pt

- Accurate *ab initio* predictions of spin Hall effect possible
- Direct MOKE measurement of SH conductivity in heavy metals feasible

Orbital Nernst effect



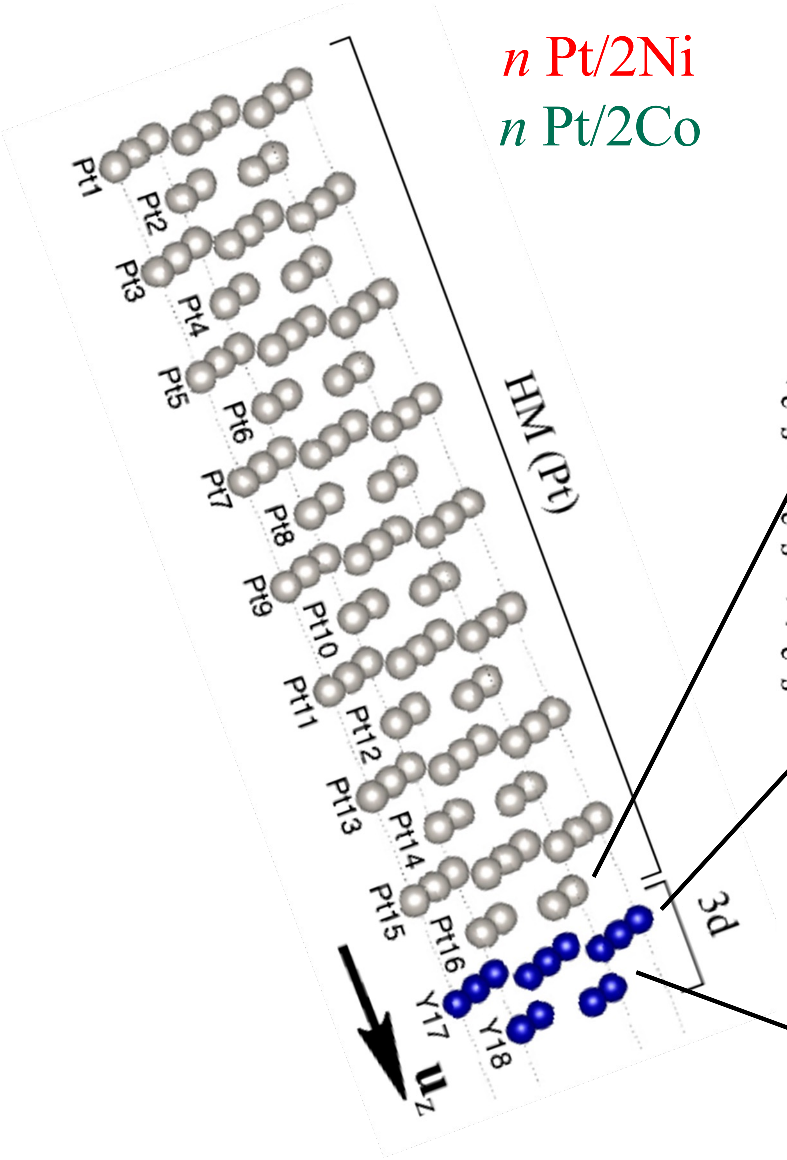
Large for nonmagnetic Ni, Pd & Pt

$$J_i^{S_k} = \sigma_{ij}^{S_k} E_j - \Lambda_{ij}^{S_k} \frac{dT}{dr_j}$$

Salemi and Oppeneer, arxiv2203.17037

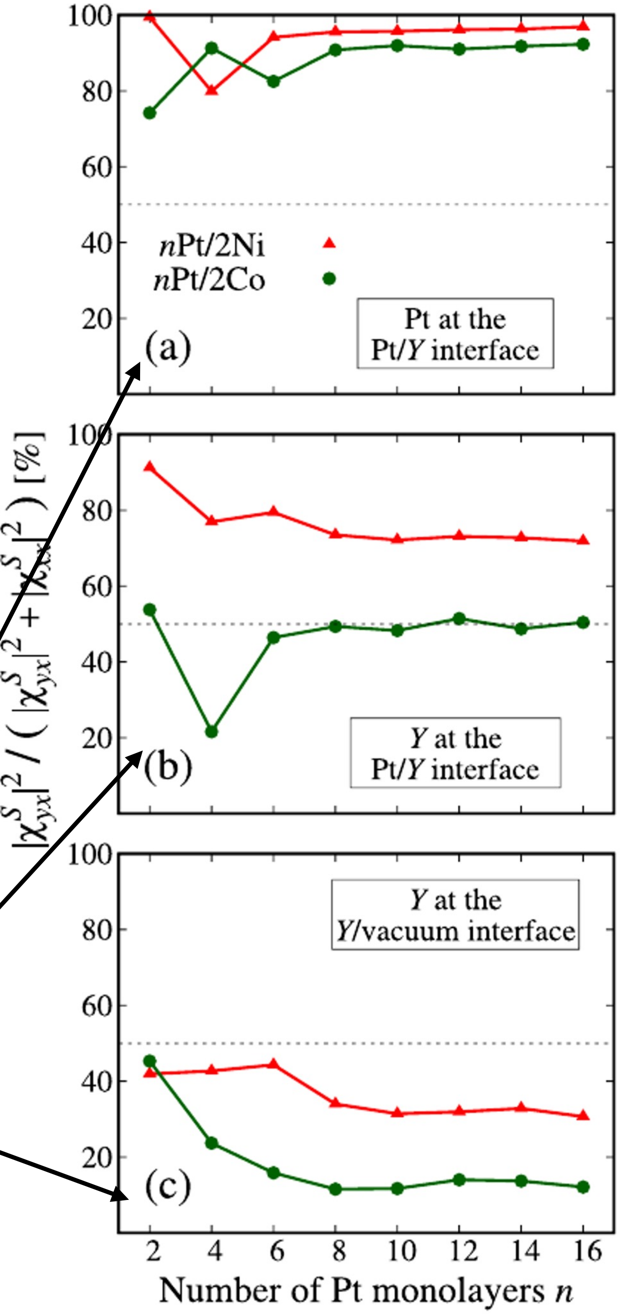
Layer-resolved comparison of spin accumulation

$$\mathcal{T} = -2\mu_B|\boldsymbol{B}_{\rm XC}| \left[\boldsymbol{\mathcal{M}} \times \left(\chi^S \boldsymbol{E}\right)\right]$$



n Pt/2Ni

n Pt/2Co



$$|\chi^S_{yx}|^2 / (|\chi^S_{yx}|^2 + |\chi^S_{xx}|^2)$$

SHE dominated

$$\mathcal{T}_{\rm odd} \gg \mathcal{T}_{\rm even}$$

$$\mathcal{T}_{\rm odd} \gtrsim \mathcal{T}_{\rm even}$$

$$\mathcal{T}_{\rm odd} \lesssim \mathcal{T}_{\rm even}$$

Magn. SHE larger

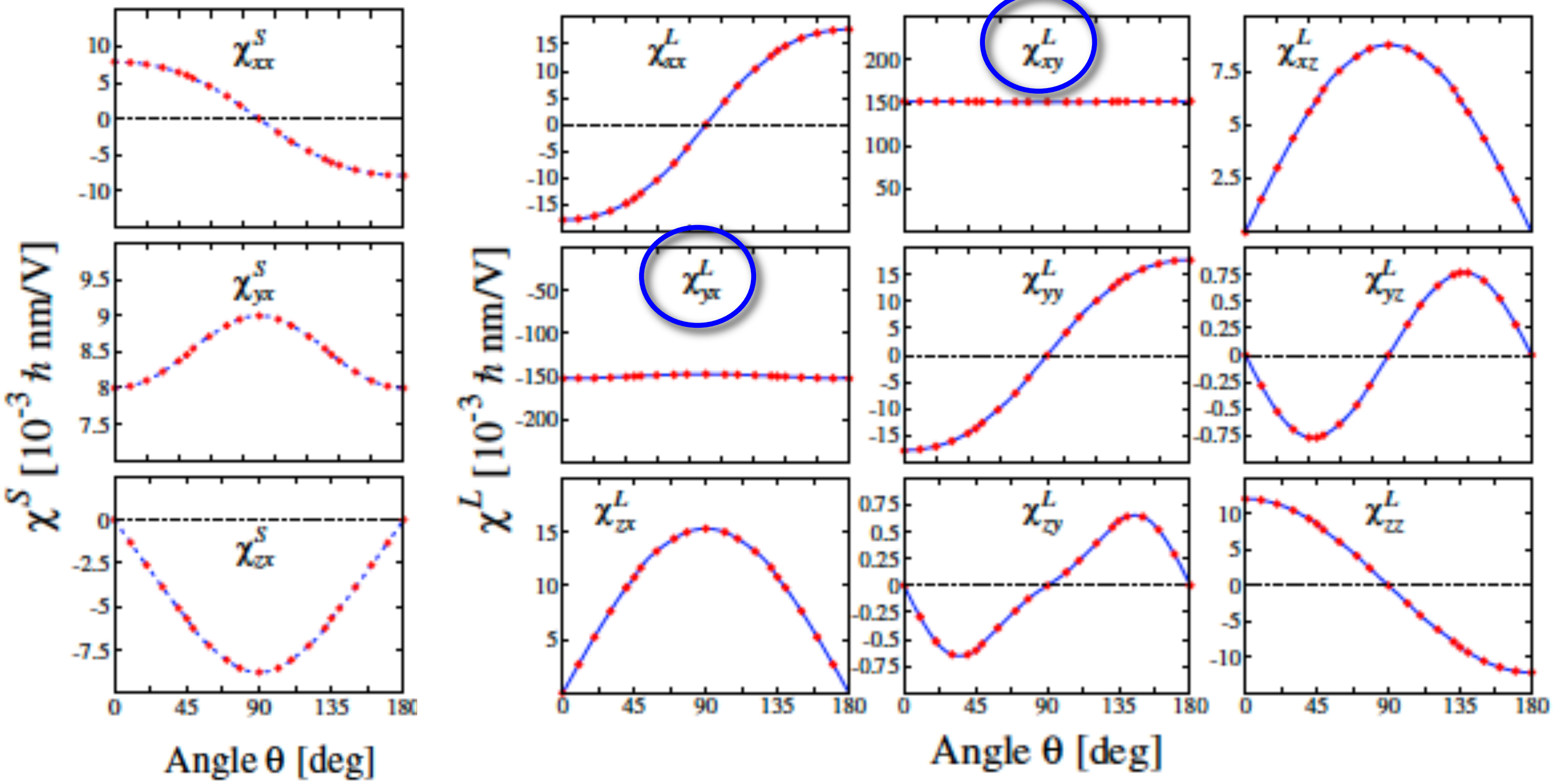
But: lifetime dependent,
χ_{xy} intraband

Induced orbital polarization – *M* direction dependence

12Pt/2Co, 1st Co

ORBITAL SUSCEPTIBILITY

$z - x$ plane



- Orbital χ_{xy} is *nonrelativistic* and antisymmetric $\chi^L_{xy} \approx -\chi^L_{yx}$
- All other components due to SOC

Spin-charge angle tensor θ

$$\boldsymbol{J}^{S_k} = \boldsymbol{\sigma}^{S_k}\boldsymbol{\sigma}^{-1}\boldsymbol{J} = \underbrace{\boldsymbol{\sigma}^{S_k}\boldsymbol{\rho}}\boldsymbol{J} = \frac{\hbar}{2e}\boldsymbol{\theta}^{S_k}\boldsymbol{J} \qquad \boldsymbol{\rho} = \begin{pmatrix} \rho_1 & \rho_A & 0 \\ -\rho_A & \rho_1 & 0 \\ 0 & 0 & \rho_2 \end{pmatrix}$$

$\mathbf{M} \parallel \mathbf{u}_z$

$$\boldsymbol{\theta}^{S_x} = \frac{2e}{\hbar}\begin{pmatrix} 0 & 0 & \sigma^{S_x}_{xz}\rho_2 \\ 0 & 0 & \sigma^{S_x}_{yz}\rho_2 \\ \sigma^{S_x}_{zx}\rho_1 - \sigma^{S_x}_{zy}\rho_A & \boxed{\sigma^{S_x}_{zx}\rho_A + \sigma^{S_x}_{zy}\rho_1} & 0 \end{pmatrix}$$

Mixing of effects

$$\boldsymbol{\theta}^{S_y} = \frac{2e}{\hbar}\begin{pmatrix} 0 & 0 & \sigma^{S_y}_{xz}\rho_2 \\ 0 & 0 & \sigma^{S_y}_{yz}\rho_2 \\ \sigma^{S_y}_{zx}\rho_1 - \sigma^{S_y}_{zy}\rho_A & \sigma^{S_y}_{zx}\rho_A + \sigma^{S_y}_{zy}\rho_1 & 0 \end{pmatrix}$$

Spin-filtering on AHE

$$\boldsymbol{\theta}^{S_z} = \frac{2e}{\hbar}\begin{pmatrix} \sigma^{S_z}_{xx}\rho_1 - \sigma^{S_z}_{xy}\rho_A & \boxed{\sigma^{S_z}_{xx}\rho_A + \sigma^{S_z}_{xy}\rho_1} & 0 \\ \sigma^{S_z}_{yx}\rho_1 - \sigma^{S_z}_{yy}\rho_A & \sigma^{S_z}_{yx}\rho_A + \sigma^{S_z}_{yy}\rho_1 & 0 \\ 0 & 0 & \sigma^{S_z}_{zz}\rho_2 \end{pmatrix}$$

Salemi and PMO, arXiv:2203.17025