Spin-orbit torques in antiferromagnetic CuMnAs and its band structure

Karel Výborný
Fyzikální ústav AV ČR (IoP, Academy of Sciences)

People involved:

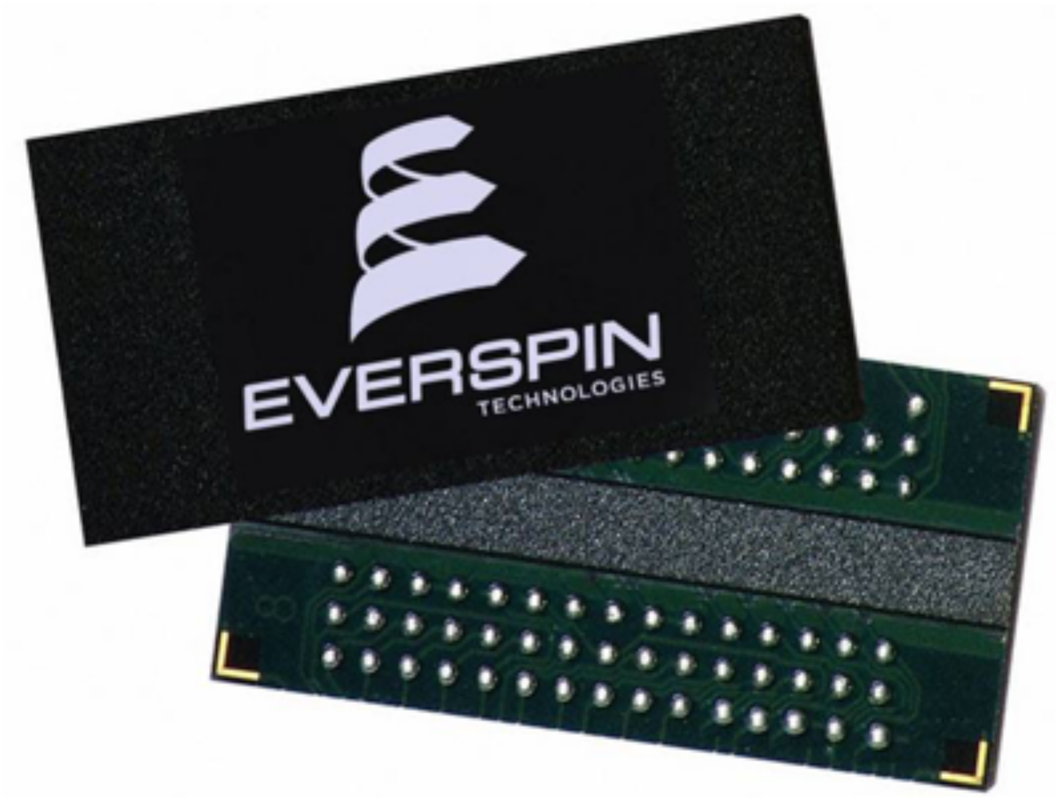
Martin Veis (Karlova Univerzita, Praha)
Ján Minár (Západočeská U., Plzeň)
Vít Novák (Akademie věd ČR, Praha)

Further input:

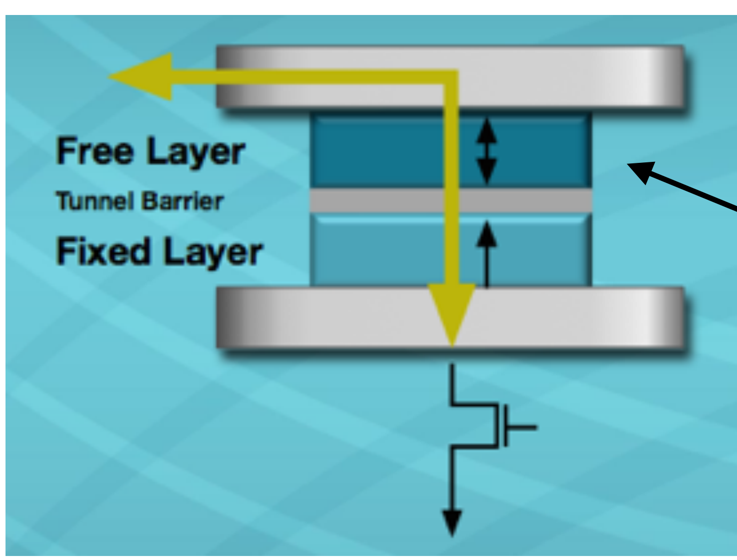
Tomáš Jungwirth (Praha/Nottingham)
Jakub Železný (Dresden)

Magnetic memories: beyond HDD

ferromagnets:



MTJ-based MRAM

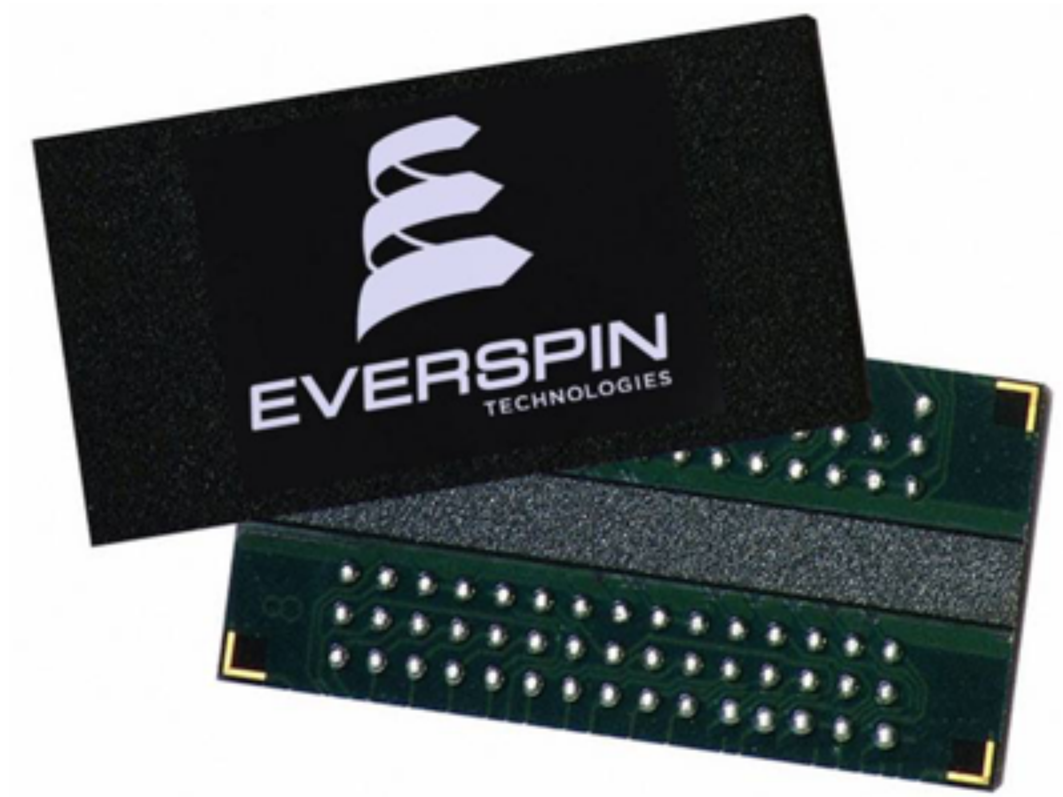


0 or 1: free layer magnetisation direction

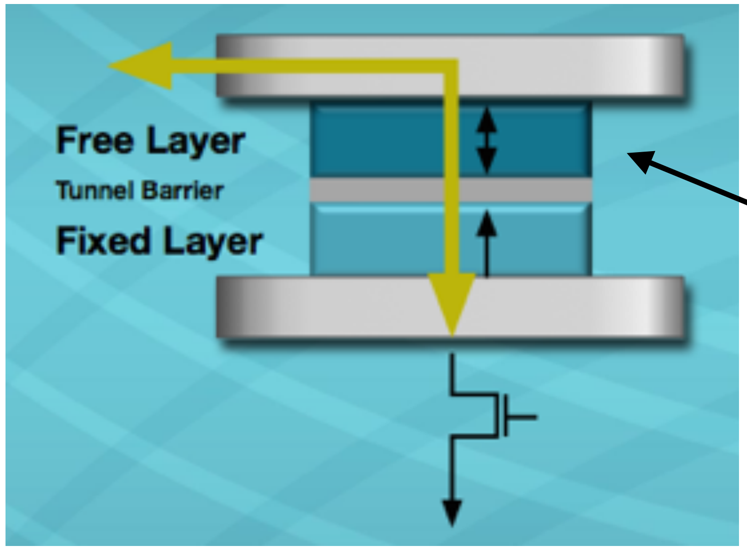
any new ideas?

Magnetic memories: beyond HDD

ferromagnets:



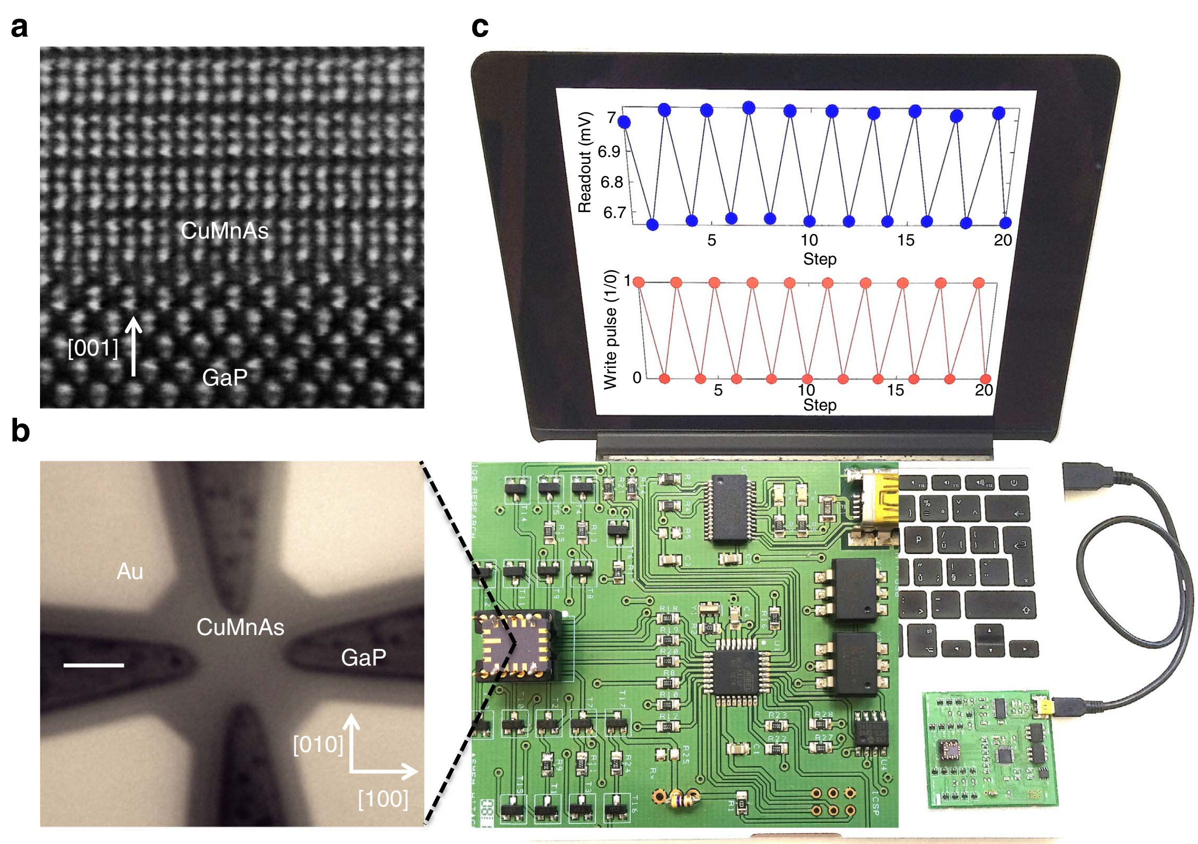
MTJ-based MRAM



0 or 1: free layer magnetisation direction

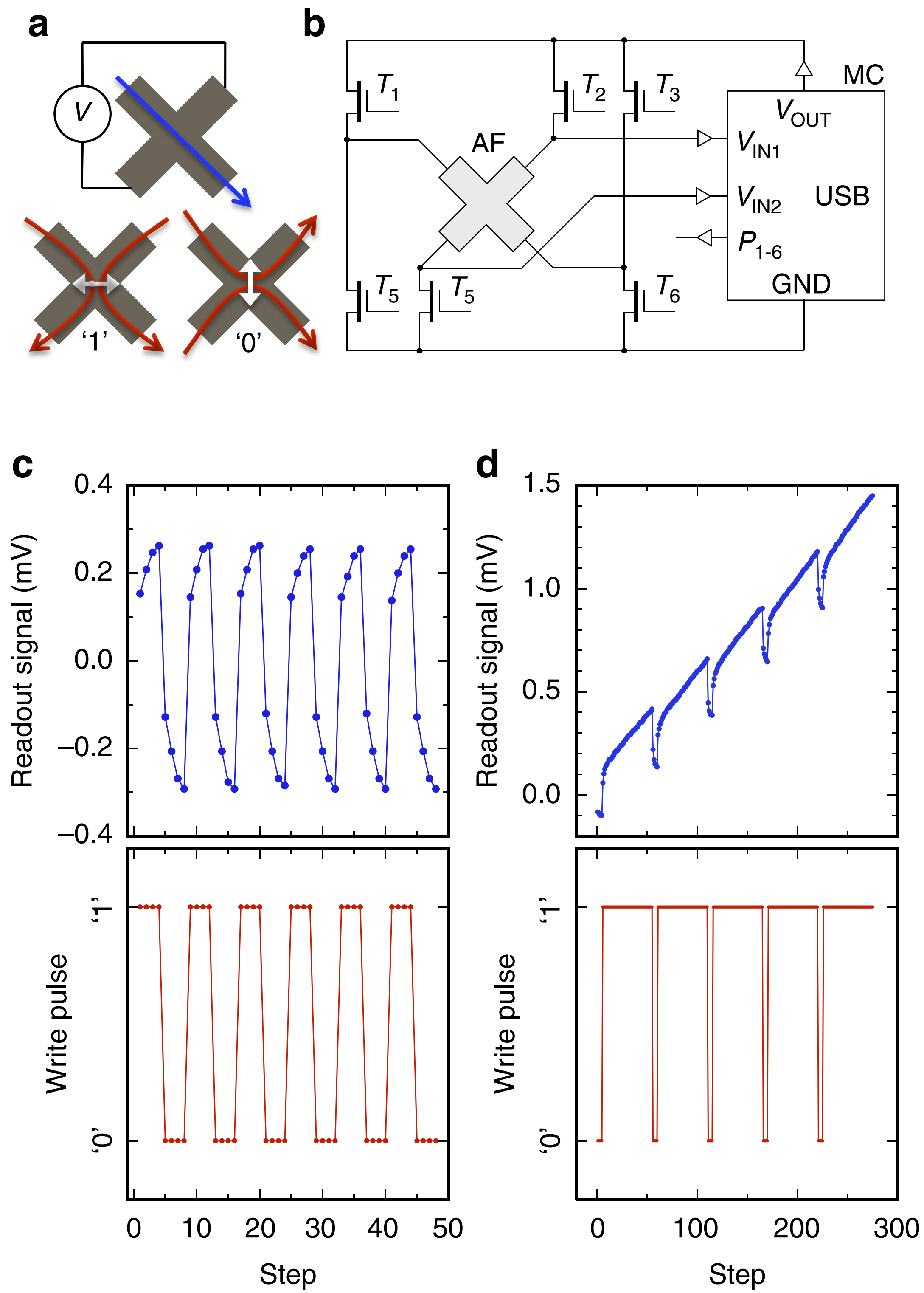
any new ideas? Yes!

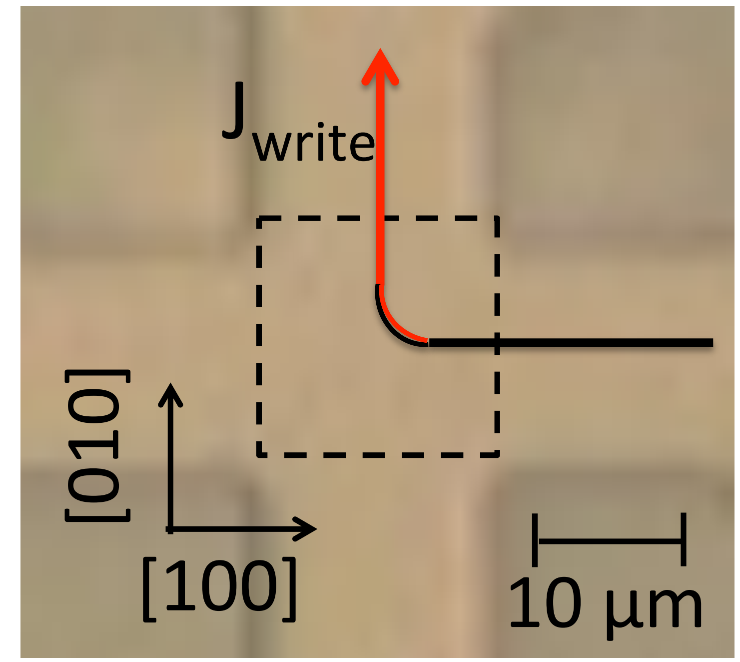
Antiferromagnetic memory based on CuMnAs



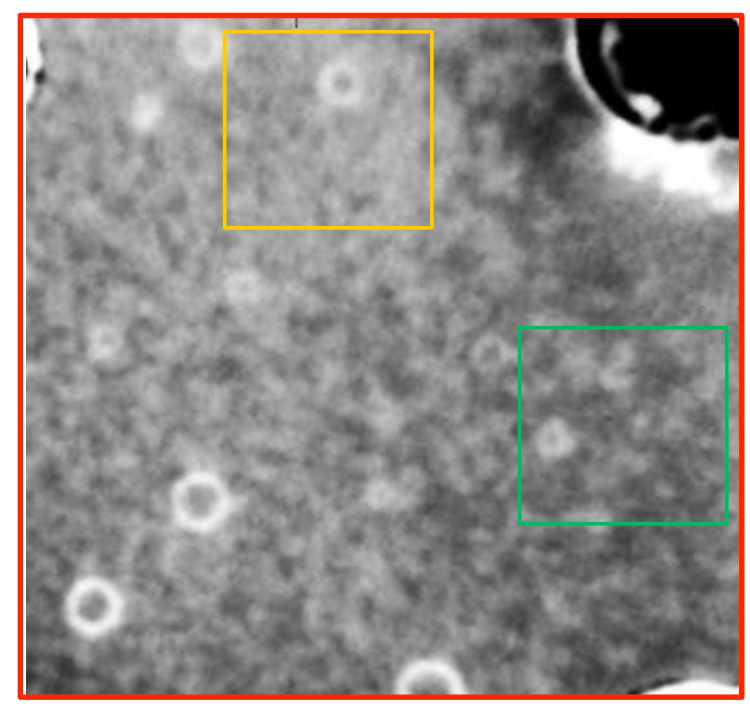
Olejník et al. ’17
[10.1038/ncomms15434]

… so what's behind that AFM memory? (experimentally)





small domains seen by PEEM

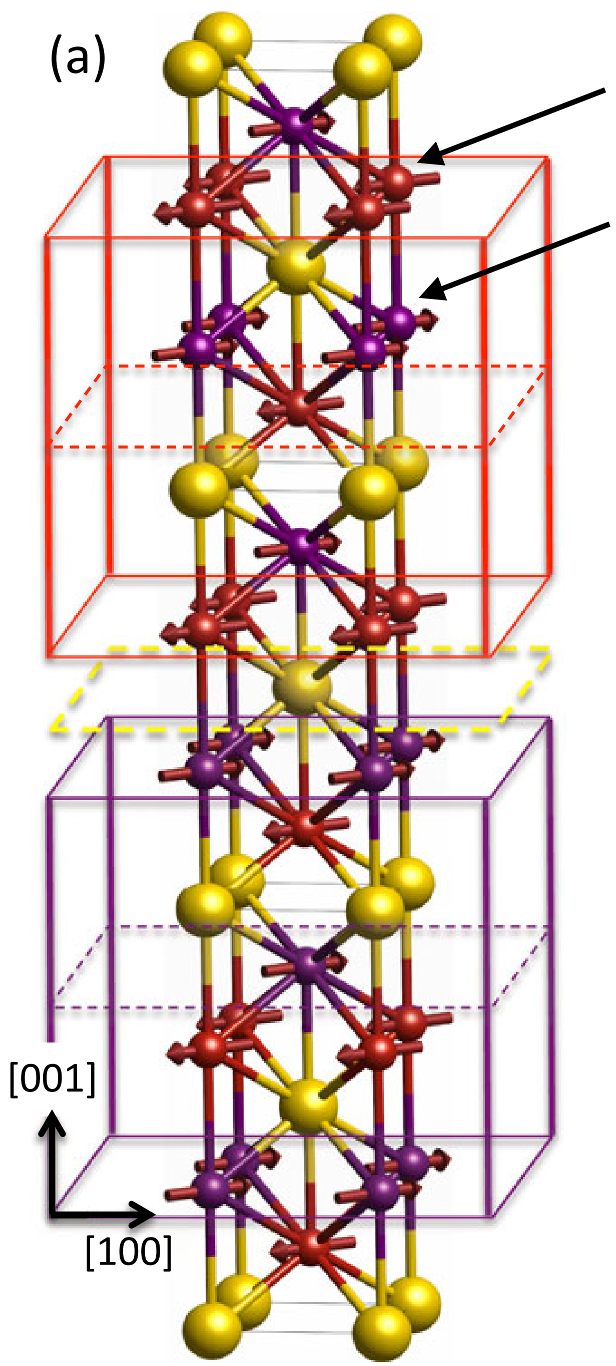


… actually a memristor

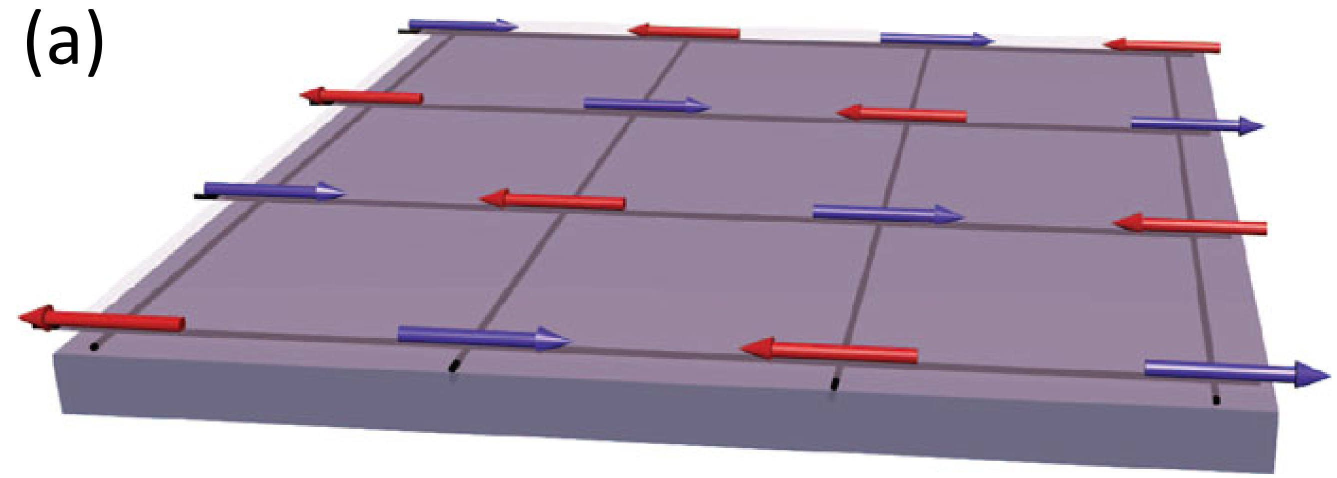
Olejník et al. '17
[10.1038/ncomms15434]

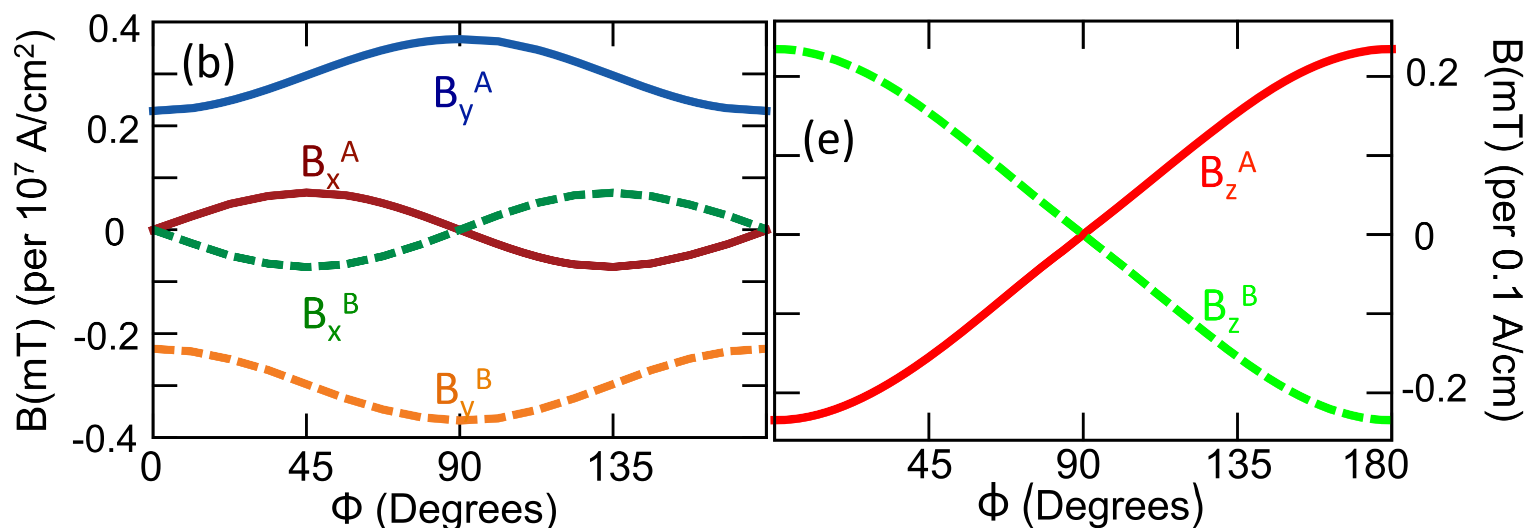
Wadley et al. '16
Science 351, 587

… so what's behind that AFM memory? (theoretically)



Mn_2Au





Železný et al. '14
Phys Rev Lett 113, 157201

Spin-orbit torques in antiferromagnets

Torques acting on magnetic moments

Solid state:

$$\frac{d\vec{M}}{dt} = \gamma \vec{M} \times \vec{B}$$

Torques acting on magnetic moments

Basics:

mechanical torque: $$\vec{T} = \frac{d\vec{L}}{dt}$$

magnetic field acting on a dipole: $$\vec{T} = \vec{\mu} \times \vec{B}$$

gyromagnetic ratio: $$\vec{\mu} = \gamma \vec{L}$$

total magnetisation: $$\vec{M} = \frac{1}{V} \sum_i \vec{\mu}_i$$

Solid state:

$$\frac{d\vec{M}}{dt} = \gamma \vec{M} \times \vec{B}$$

Torques acting on magnetic moments

Basics:

mechanical torque: $$\vec{T} = \frac{d\vec{L}}{dt}$$

magnetic field acting on a dipole: $$\vec{T} = \vec{\mu} \times \vec{B}$$

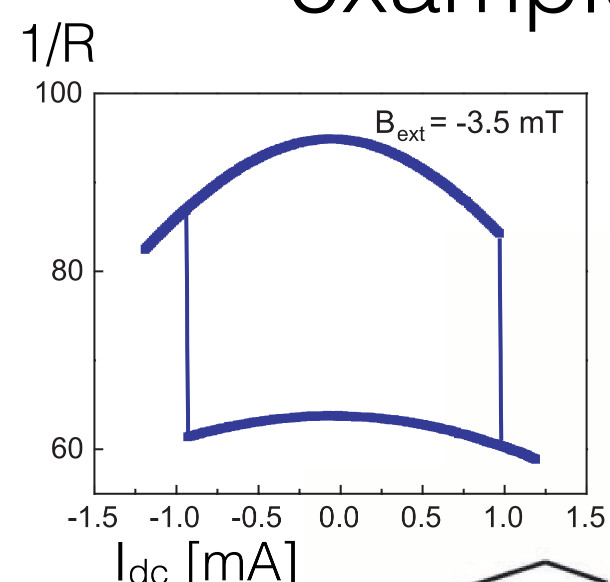
gyromagnetic ratio: $$\vec{\mu} = \gamma \vec{L}$$

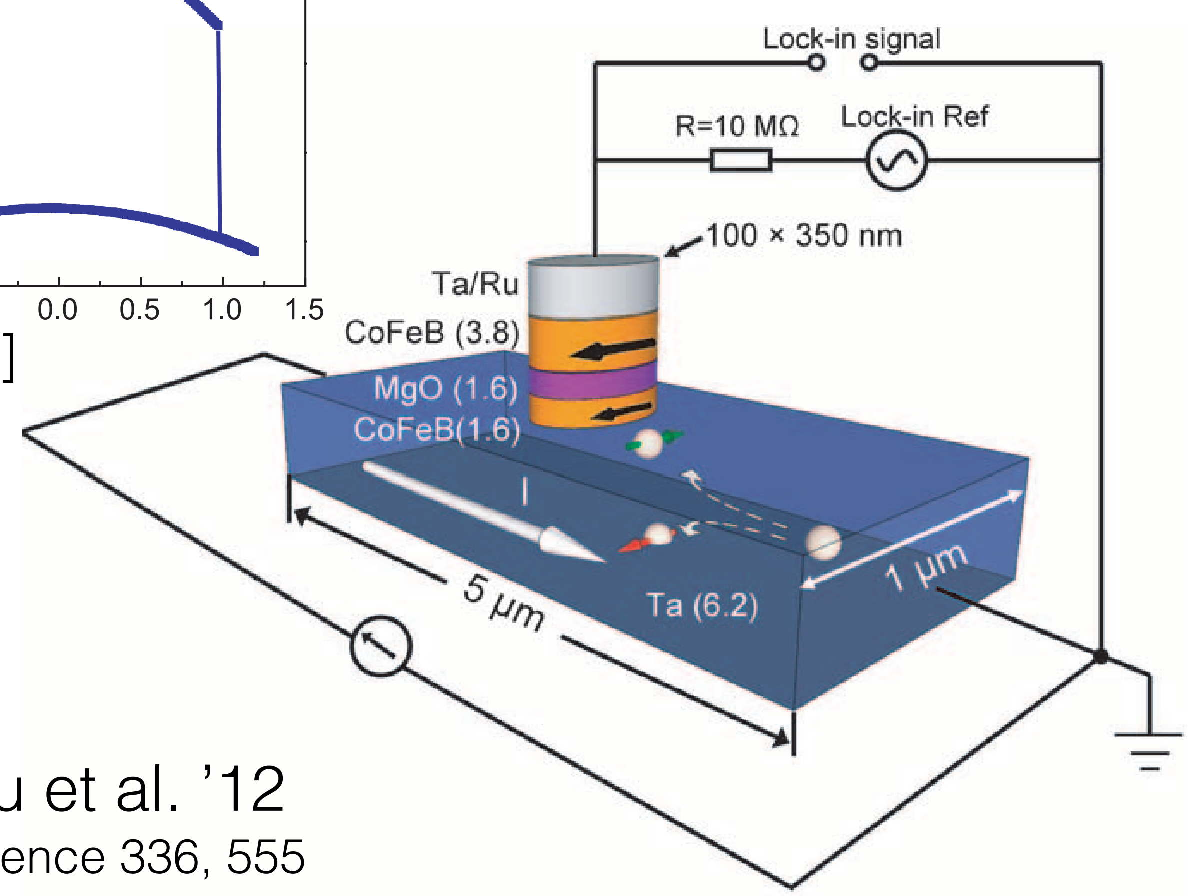
total magnetisation: $$\vec{M} = \frac{1}{V} \sum_i \vec{\mu}_i$$

Solid state:

$$\frac{d\vec{M}}{dt} = \gamma \vec{M} \times \vec{B}$$

example: SHE-SOT





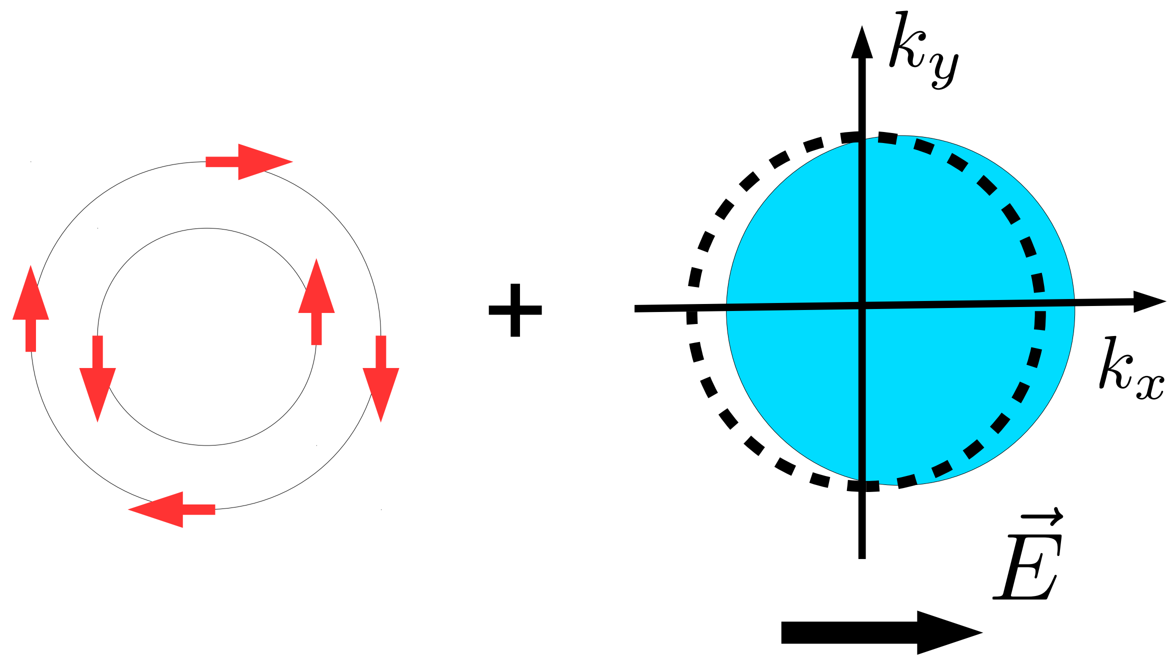
Liu et al. ’12
Science 336, 555

Current-induced spin-orbit torque - for ferromagnets

Edelstein effect…

$$\delta\mathbf{S} = \chi\,\mathbf{E}$$

simplest example: Rashba-Bychkov spin-orbit int. (sol. st. comm. 73, 233)



$$\delta\mathbf{S} = \int S\delta f\ dk + \int f\delta S\ dk$$

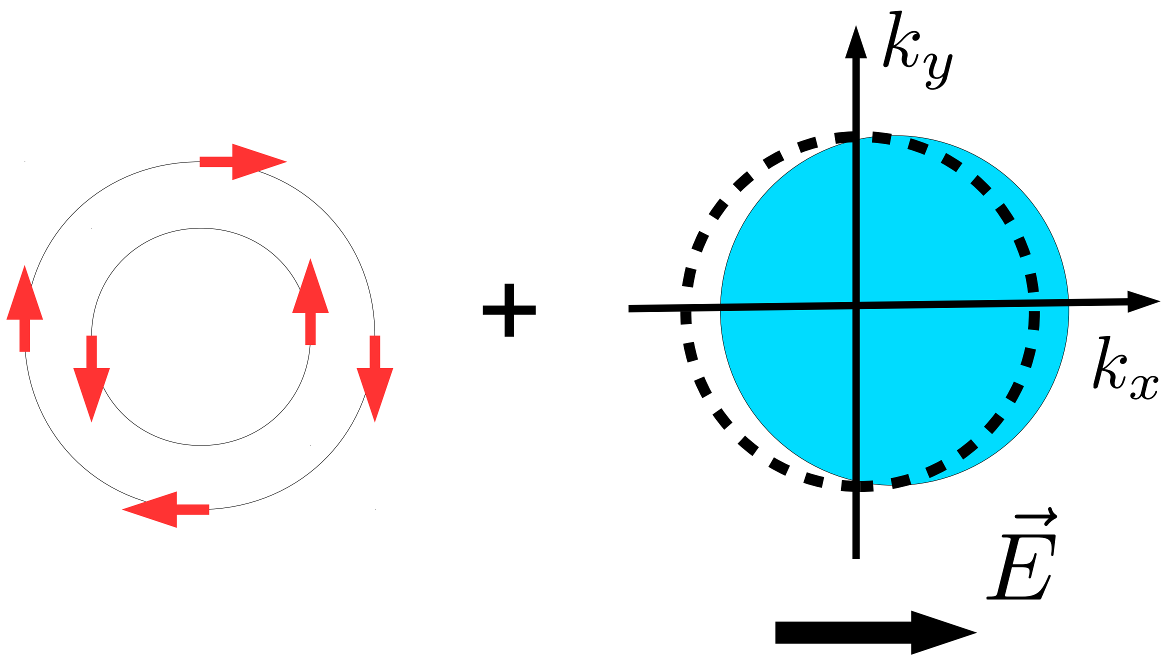
"intraband" "interband"

Current-induced spin-orbit torque - for ferromagnets

Edelstein effect…

$$\delta\mathbf{S} = \chi\,\mathbf{E}$$

simplest example: Rashba-Bychkov spin-orbit int. (sol. st. comm. 73, 233)



$$\delta\mathbf{S} = \int S\delta f\ dk + \int f\delta S\ dk$$

… action on magnetic moments

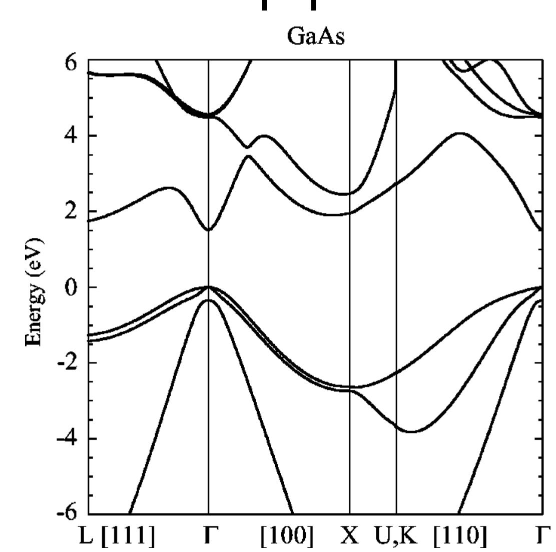
Phil. Tr. R. Soc. London A 369, 3175

$$\vec{T} = \frac{h}{M}\delta\vec{S} \times \vec{M}$$

in the context of p-d type Hamiltonian

$$H = H_{KL} + h\hat{e}_M \cdot \mathbf{s}$$

… applicable to (Ga,Mn)As



- ferromagnetism induced by carriers
- Mn d-states coupled to hole p-states (carriers) [RMP 78, 809]

$$H = H_{KL} + J_{pd}\sum_{i,I} \vec{S}_I \cdot \vec{s}_i \delta(\vec{r}_i - \vec{R}_I)$$

after mean field: $h \propto J_{pd}$ [PRB 80, 165204]

Current-induced spin-orbit torque - ferromagnetic (Ga,Mn)As

$$\delta\mathbf{S} = \chi\,\mathbf{E}$$
$$S_i = \chi_{ij} E_j$$

Current-induced (non-equilibrium) spin polarisation - in linear response

Current-induced spin-orbit torque - ferromagnetic (Ga,Mn)As

$$\delta\mathbf{S} = \chi\,\mathbf{E}$$

$$S_i = \chi_{ij} E_j$$

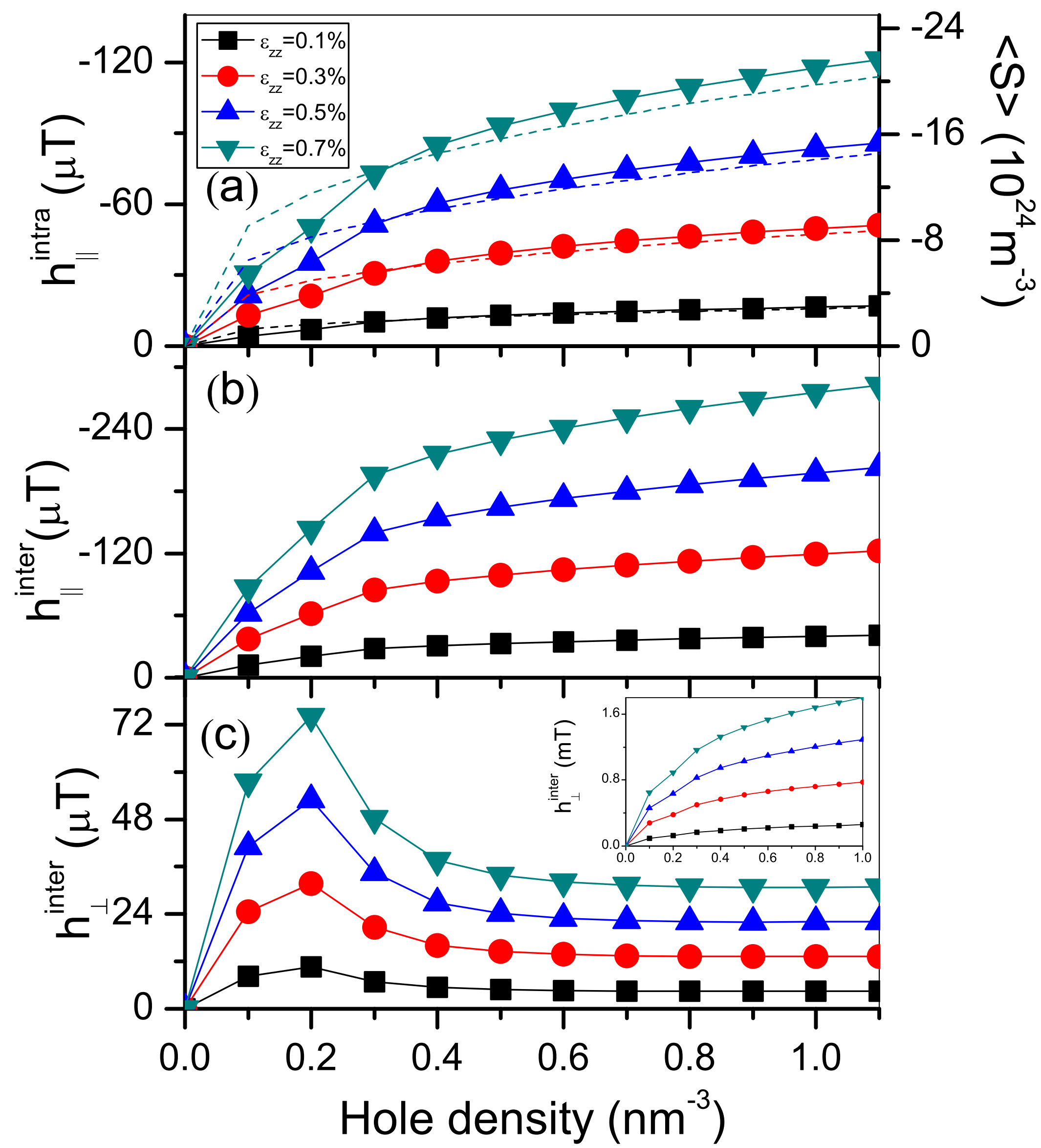
CISP - in linear response

$$\delta\mathbf{S} = \delta\mathbf{S}^{\mathrm{intra}} + \delta\mathbf{S}_1^{\mathrm{inter}} + \delta\mathbf{S}_2^{\mathrm{inter}}$$

$$\delta\mathbf{S}^{\mathrm{intra}} = \frac{1}{V}\frac{e\hbar}{2\Gamma}\sum_{\mathbf{k},a}\langle\psi_{\mathbf{k}a}|\hat{\mathbf{s}}|\psi_{\mathbf{k}a}\rangle\langle\psi_{\mathbf{k}a}|\mathbf{E}\cdot\hat{\mathbf{v}}|\psi_{\mathbf{k}a}\rangle \times \delta(E_{\mathbf{k}a}-E_F), \tag{3}$$

$$\delta\mathbf{S}_1^{\mathrm{inter}} = -\frac{e\hbar}{V}\sum_{\mathbf{k},a\neq b} 2\mathrm{Re}[\langle\psi_{a\mathbf{k}}|\hat{\mathbf{s}}|\psi_{b\mathbf{k}}\rangle\langle\psi_{b\mathbf{k}}|\mathbf{E}\cdot\hat{\mathbf{v}}|\psi_{a\mathbf{k}}\rangle] \times \frac{\Gamma(E_{\mathbf{k}a}-E_{\mathbf{k}b})}{[(E_{\mathbf{k}a}-E_{\mathbf{k}b})^2+\Gamma^2]^2}(f_{\mathbf{k}a}-f_{\mathbf{k}b}), \tag{4}$$

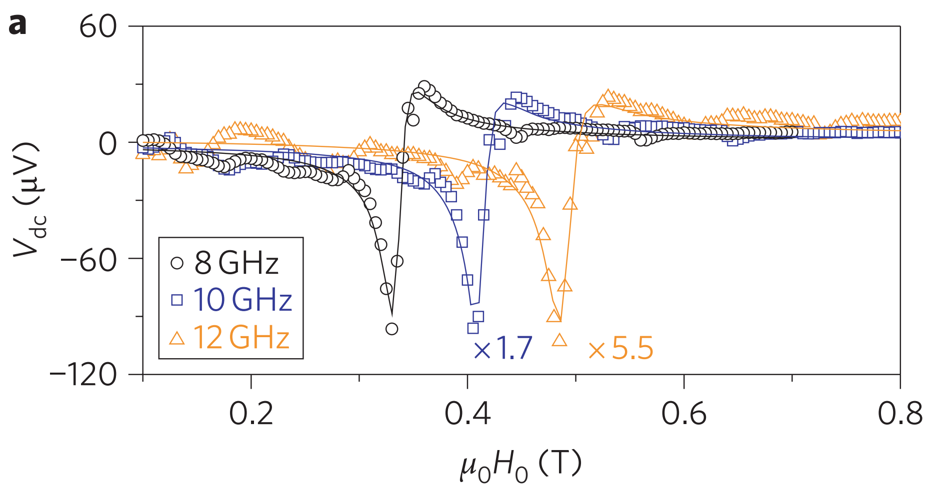
$$\delta\mathbf{S}_2^{\mathrm{inter}} = -\frac{e\hbar}{V}\sum_{\mathbf{k},a\neq b} \mathrm{Im}[\langle\psi_{\mathbf{k}a}|\hat{\mathbf{s}}|\psi_{\mathbf{k}b}\rangle\langle\psi_{\mathbf{k}b}|\mathbf{E}\cdot\hat{\mathbf{v}}|\psi_{\mathbf{k}a}\rangle] \times \frac{\Gamma^2-(E_{\mathbf{k}a}-E_{\mathbf{k}b})^2}{[(E_{\mathbf{k}a}-E_{\mathbf{k}b})^2+\Gamma^2]^2}(f_{\mathbf{k}a}-f_{\mathbf{k}b}). \tag{5}$$



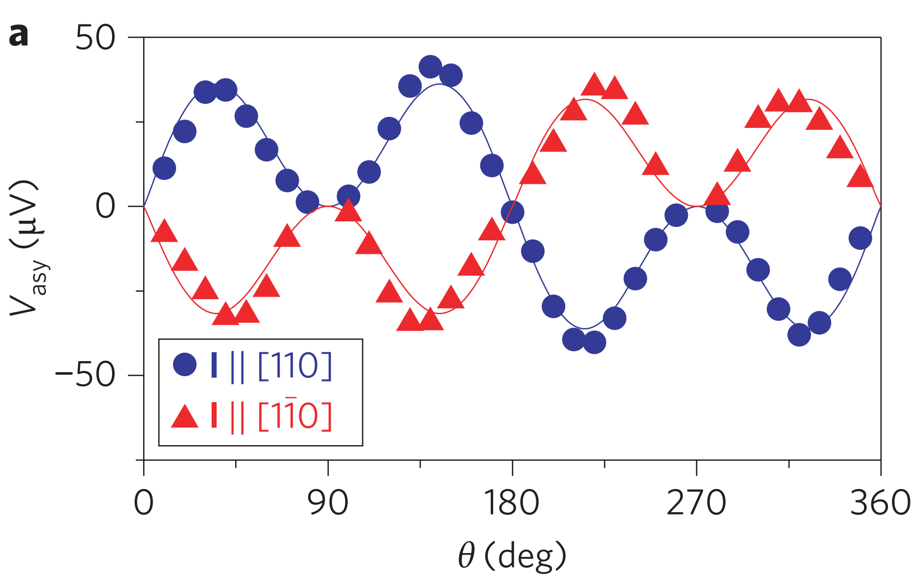
Li et al. ’15
Phys Rev B 91, 134402

Current-induced spin-orbit torque - ferromagnetic (Ga,Mn)As

intraband

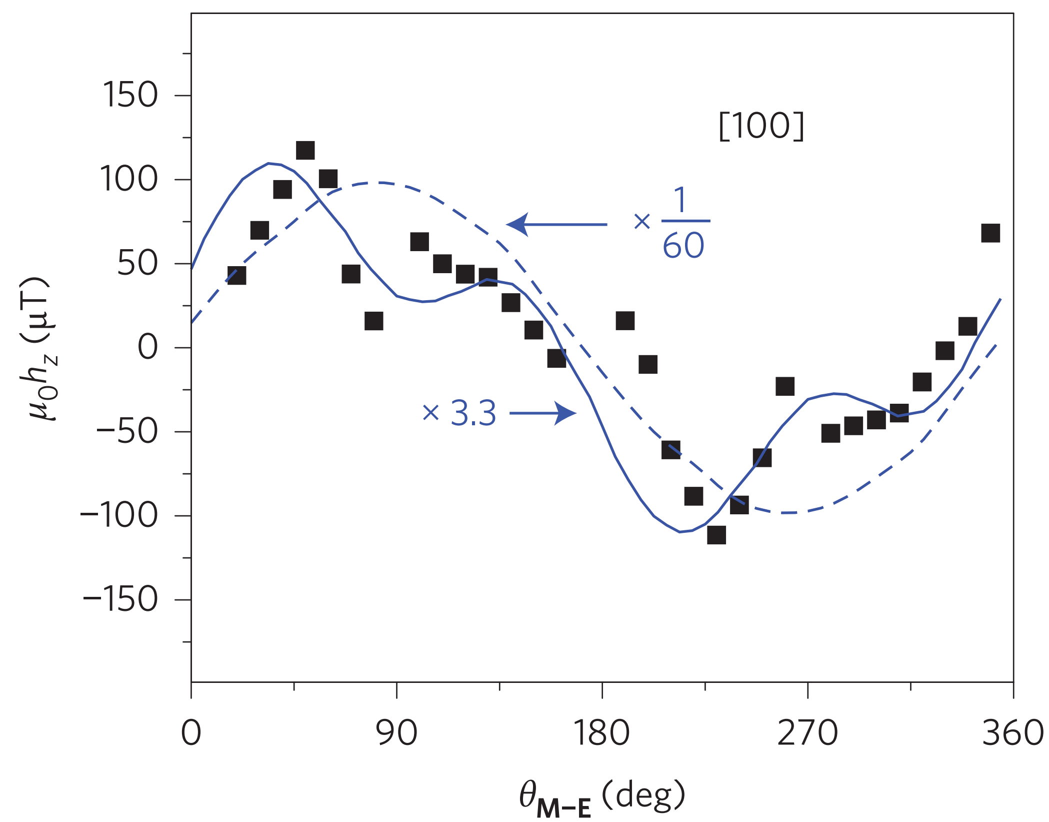


$$\mathrm{Re}\{V_{\mathrm{dc}}\} = V_{\mathrm{sym}} \frac{\Delta H^2}{(H_0 - H_{\mathrm{res}})^2 + \Delta H^2} + + V_{\mathrm{asy}} \frac{\Delta H (H_0 - \Delta H)}{(H_0 - H_{\mathrm{res}})^2 + \Delta H^2}$$



Fang et al. ’11
[10.1038/nnano.2011.68]

interband



Berry-curvature type expressions…

$$S_z = \frac{\hbar}{V} \sum_{\mathbf{k}, a \neq b} (f_{\mathbf{k},a} - f_{\mathbf{k},b}) \frac{\mathrm{Im}[\langle \mathbf{k}, a | s_z | \mathbf{k}, b \rangle \langle \mathbf{k}, b | e\boldsymbol{E} \cdot \mathbf{v} | \mathbf{k}, a \rangle]}{(E_{\mathbf{k},a} - E_{\mathbf{k},b})^2}$$

$$S_z = ieE \sum_{\text{occ. states}} \left[\left\langle \frac{\partial \psi}{\partial h_z} \middle| \frac{\partial \psi}{\partial k_x} \right\rangle - \left\langle \frac{\partial \psi}{\partial k_x} \middle| \frac{\partial \psi}{\partial h_z} \right\rangle \right]$$

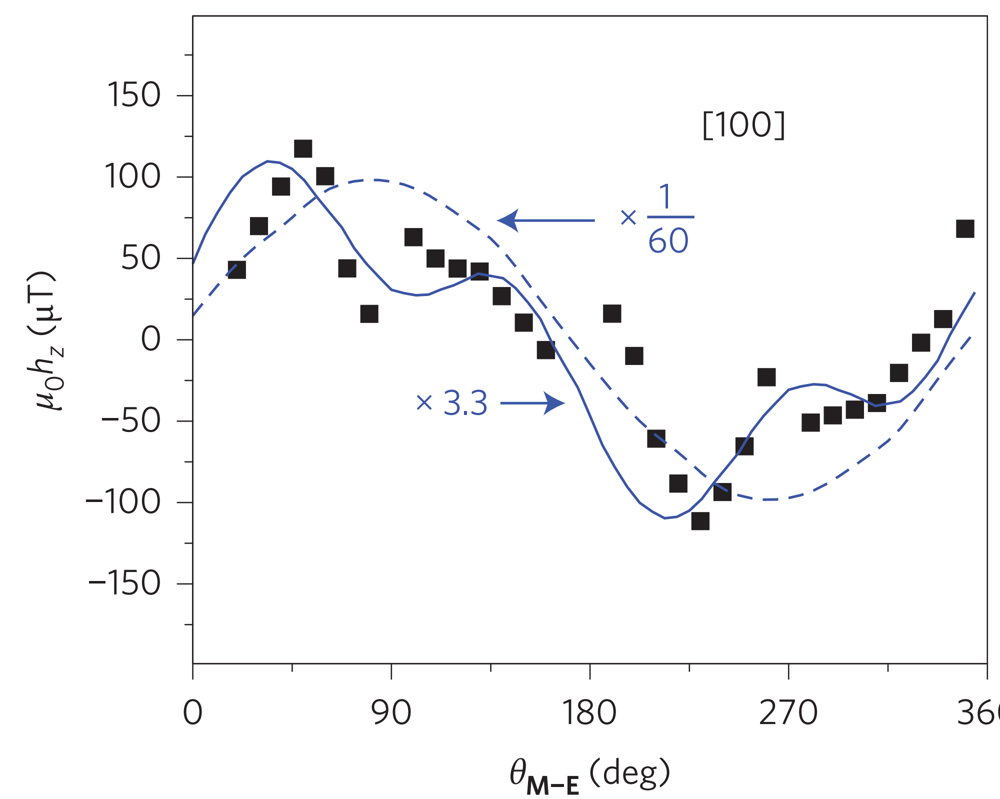
Kurebayashi et al. ’14
[10.1038/nnano.2014.15]

Two basic types of SOTs (spin-orbit torques)

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma \mathbf{M} \times (\mathbf{H}_{\text{tot}} + \mathbf{h}_{\text{eff}}) + \frac{\alpha}{M_s} \left(\mathbf{M} \times \frac{\partial \mathbf{M}}{\partial t} \right)$$

(Landau-Lifshitz-Gilbert)

- on the mean-field level, magnetisation feels the effective field: $\mu_0 \mathbf{h}_{\text{eff}} \propto J_{pd} \langle \mathbf{s} \rangle$
- depending on how $\mathbf{h}_{\text{eff}}$ depends on $\mathbf{M}$:
  - **field-like** torque:
    $\mathbf{h}_{\text{eff}}$ constant
  - **(anti)damping-like** torque:
    $\mathbf{h}_{\text{eff}}$ perpendicular to $\mathbf{M}$



Kurebayashi et al. '14
[10.1038/nnano.2014.15]

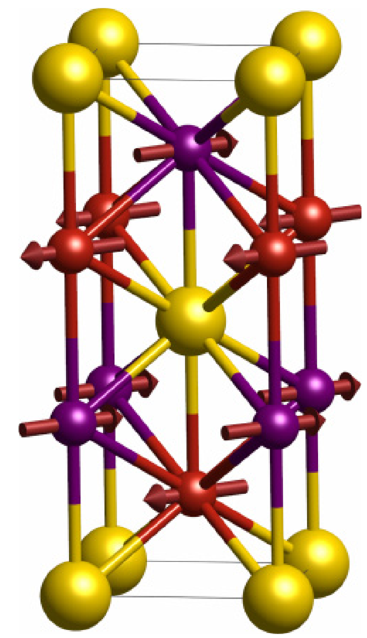
Current-induced spin-orbit torque - for antiferromagnets

Edelstein effect…

$$\delta \mathbf{S}_a = \chi_a \mathbf{E} \qquad \text{(CISP)}$$

(sublattice-resolved)

… staggered CISP



Mn_2Au

$$\chi_A^{\text{even}} = -\chi_B^{\text{even}}$$
$$\chi_A^{\text{odd}} = \chi_B^{\text{odd}},$$

Symmetry considerations:

$$\chi_{a,ij}(\hat{\mathbf{n}}) = \chi^{(0)}_{a,ij} + \chi^{(1)}_{a,ij,k}\hat{n}_k + \chi^{(2)}_{a,ij,kl}\hat{n}_k\hat{n}_l + \cdots$$

where n is the Néel vector, $\mathbf{L} = L\hat{\mathbf{n}} = \mathbf{M}_1 - \mathbf{M}_2$

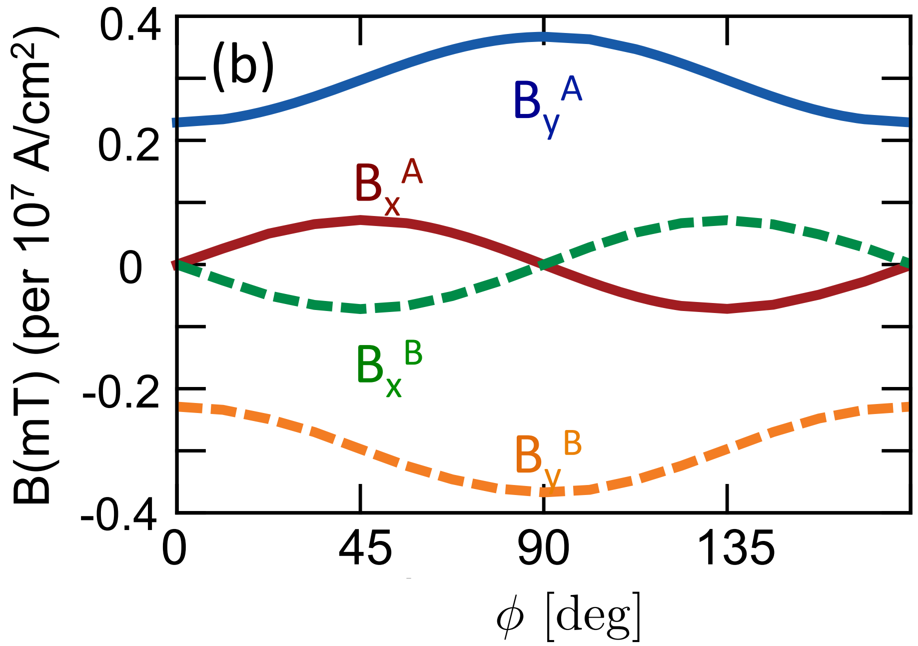
Železný et al. '17
Phys Rev B 95, 014403

Crystal system	Point group	$\chi^{(0)}$	$\chi^{(1)}$
tetragonal	4	$\begin{pmatrix} x_{11} & -x_{21} & 0 \\ x_{21} & x_{11} & 0 \\ 0 & 0 & x_{33} \end{pmatrix}$	$\begin{pmatrix} \hat{n}_z x_6 & -\hat{n}_z x_2 & \hat{n}_x x_5 - \hat{n}_y x_7 \\ \hat{n}_z x_2 & \hat{n}_z x_6 & \hat{n}_x x_7 + \hat{n}_y x_5 \\ \hat{n}_x x_4 - \hat{n}_y x_3 & \hat{n}_x x_3 + \hat{n}_y x_4 & \hat{n}_z x_1 \end{pmatrix}$

…

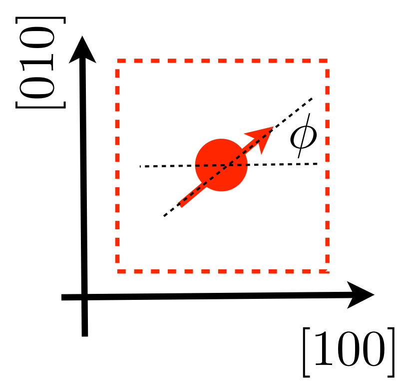
Spin-orbit torque in model systems

Železný et al. '14
Phys Rev Lett 113, 157201



	intra	inter
Mn_2Au	staggered field-like	normal anti-damping
Rashba	normal field-like	staggered antidamping

- **intraband non-equilibrium spin polarization**
- **projected to sublattice A/B**



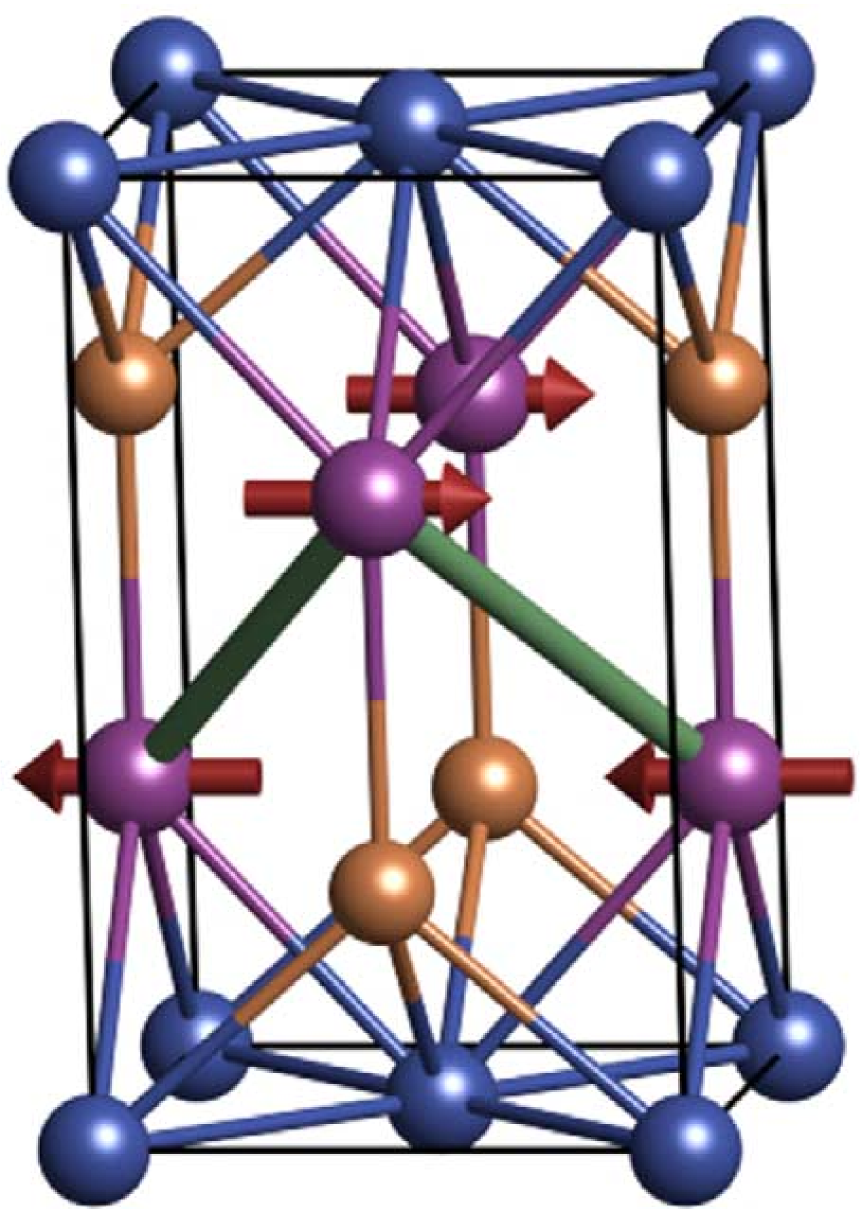
- interband part
- both extrinsic and intrinsic contributions, e.g.

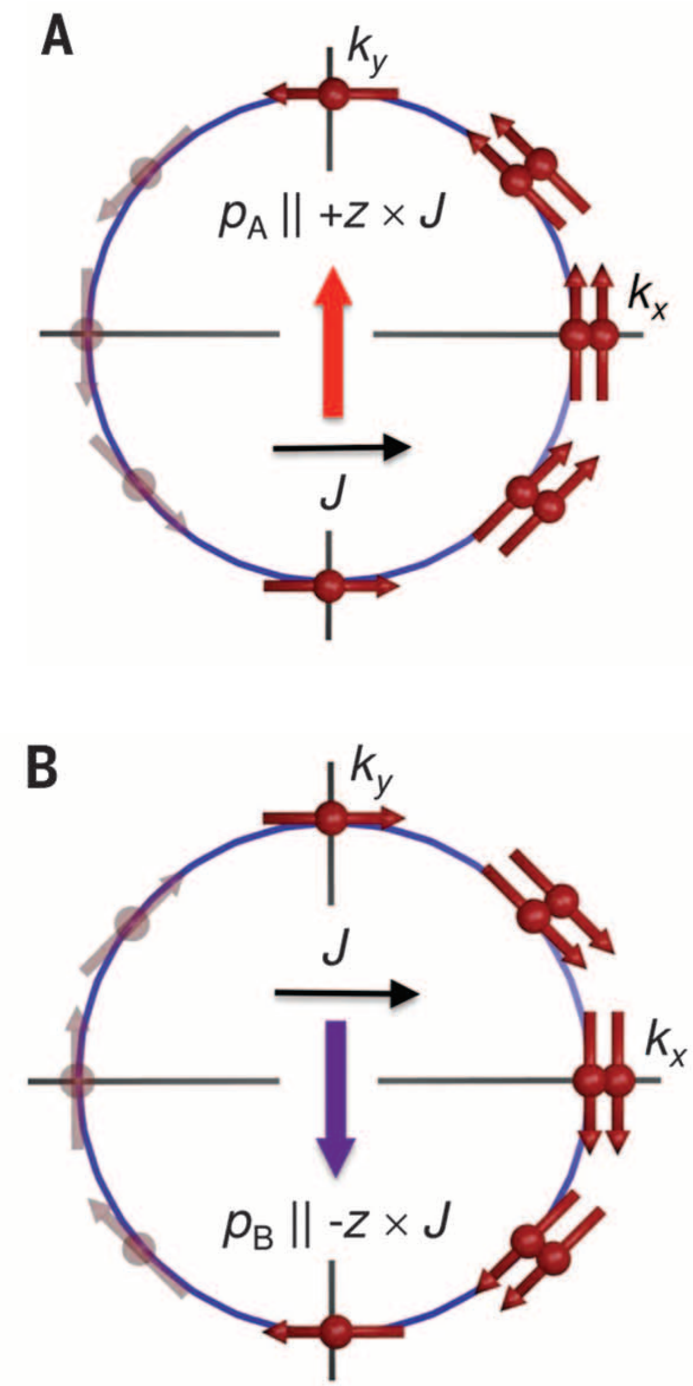
$$\delta\vec{s}^{\text{intra}} = \frac{eE\hbar}{2\Gamma}\int\frac{d^3k}{(2\pi)^3}\sum_{\alpha}(\vec{s})^{\mathsf{A}}_{\vec{k}\alpha}(v_I)_{\vec{k}\alpha}\delta(E_{\vec{k}\alpha}-E_F)$$

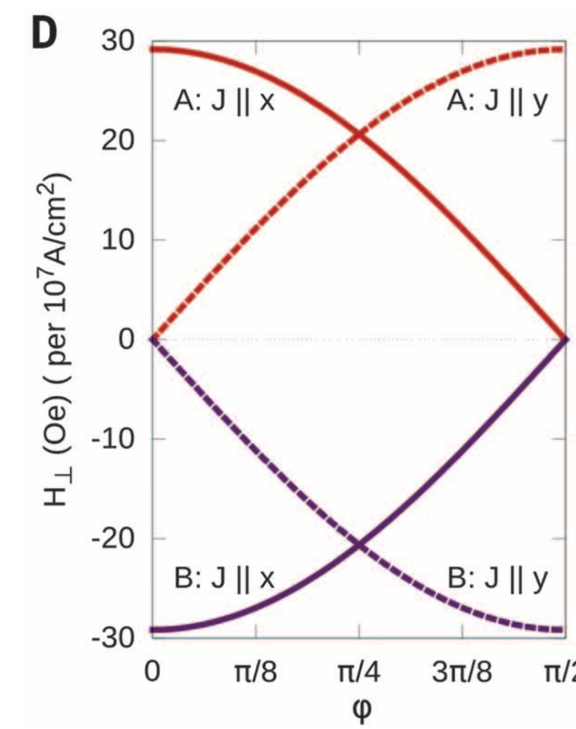
$$\delta\vec{s}^{\text{inter}} = \frac{\hbar}{L^2}\sum_{\vec{k}\alpha\neq\beta}(f_{\vec{k}\alpha}-f_{\vec{k}\beta})\,\frac{\text{Im}[(\vec{s})^{\mathsf{A}}_{\alpha\beta}(e\vec{E}\cdot\vec{v})_{\beta\alpha}]}{(E_{\vec{k}\alpha}-E_{\vec{k}\beta})^2}$$

Spin-orbit torque in CuMnAs

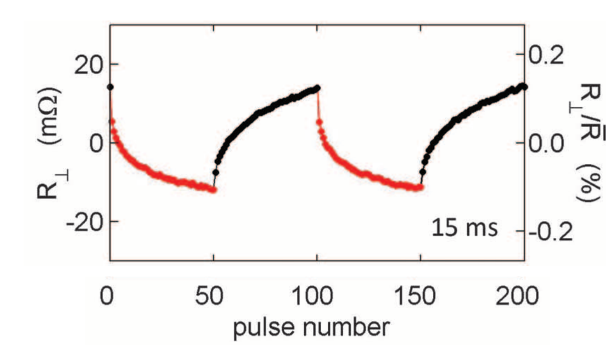
CuMnAs tetragonal







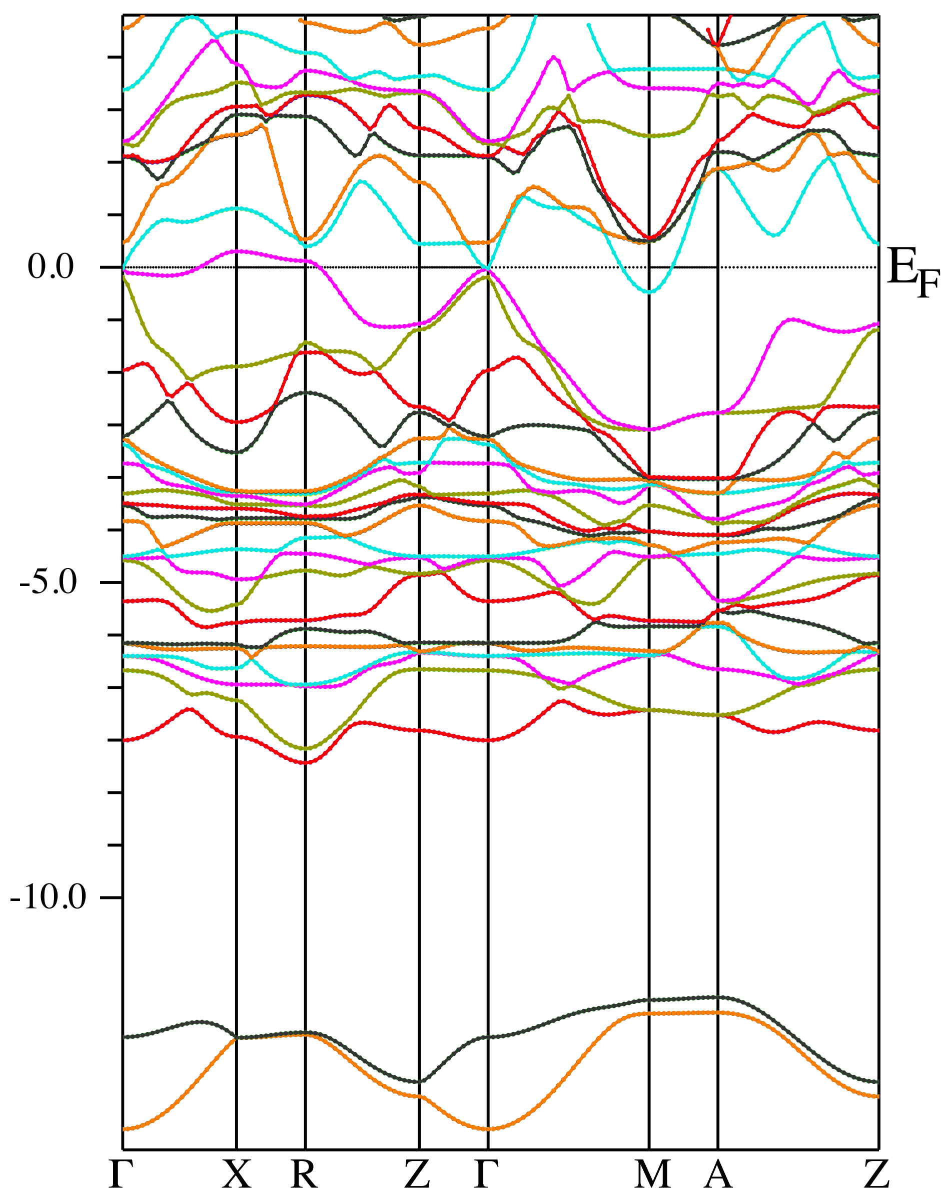
train of 'write' pulses:



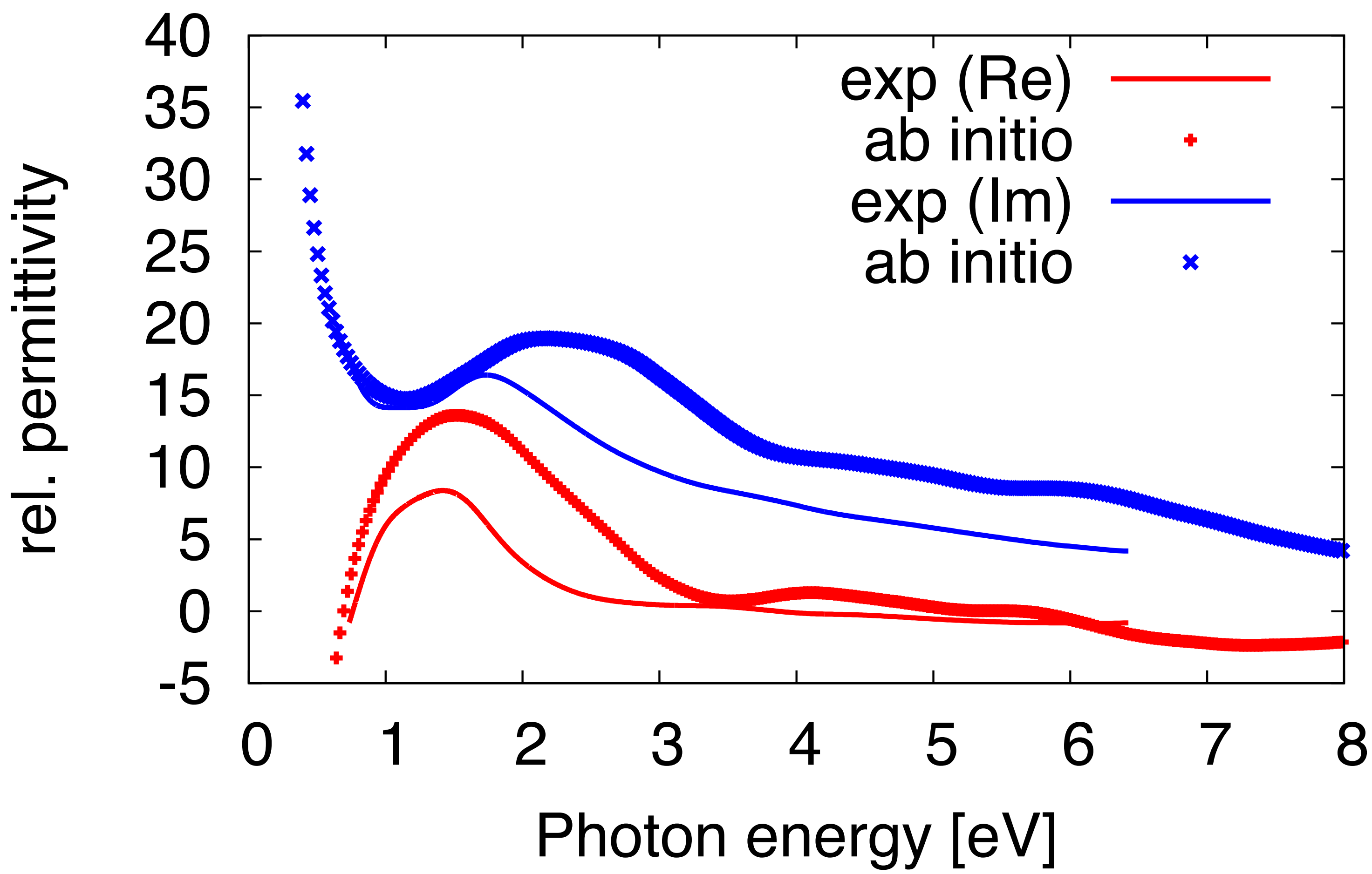
Wadley et al. '16
Science 351, 587

Band structure of CuMnAs

CuMnAs



- (semi)metallic antiferromagnet
- AC permittivity in optical range



… what does *ab initio* actually mean here

$$\epsilon(\omega)/\epsilon_0 = \epsilon_{\mathrm{b}} - \underbrace{\frac{\omega_{\mathrm{p}}^2}{\omega^2 + 1/\tau^2} + \frac{\mathrm{i}\omega_{\mathrm{p}}^2/\omega\tau}{\omega^2 + 1/\tau^2}}_{\text{intra-band}} + \frac{\mathrm{i}\sigma_{\mathrm{inter}}(\omega)}{\epsilon_0\omega}$$

- calculate interband part
- plasma frequency
- relaxation time from DC conductivity

Saidl et al. '16
New J Phys 18, 083017

$$\sigma_0 = \frac{ne^2\tau}{m} = \omega_p^2\epsilon\tau$$

well, frankly, it is not really ab initio

Hubbard U

$$\Delta E = \frac{1}{2} \sum_{m,s \neq m',s'} (U - \delta_{s,s'} J) n_{ms} n_{m's'}$$

- choose orbital
- think about values of U & J

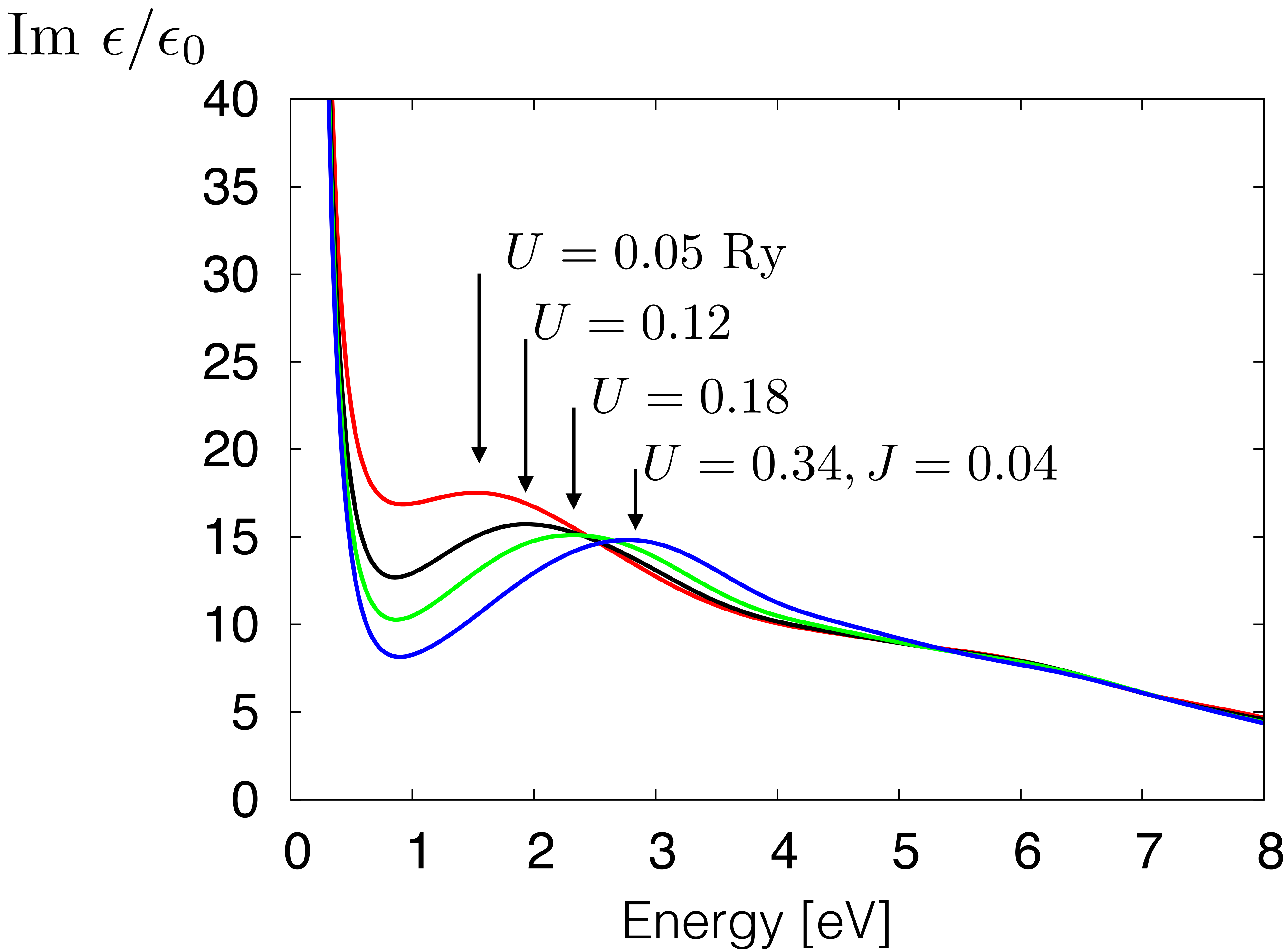
TABLE I. Calculated values of U for transition-metal oxides, compared to values of Anisimov, Zaanen, and Andersen (AZA) (Ref. 6). Empirical values include representative values from the literature.

Ref.	VO	MnO	FeO	CoO	NiO
This work	2.7	3.6	4.6	5.0	5.1
AZA	6.7	6.9	6.8	7.8	8.0
Empirical	4.0–4.8 [a]	7.8–8.8 [a]	3.5–5.1 [a]	4.9–5.3 [a]	6.1–6.7 [a]
		7.0 [d]	3.9 [c], 7.0 [d]	4.9 [c]	7.9,[b] 6.1,[c] 7.5[d]

Pickett et al. '98

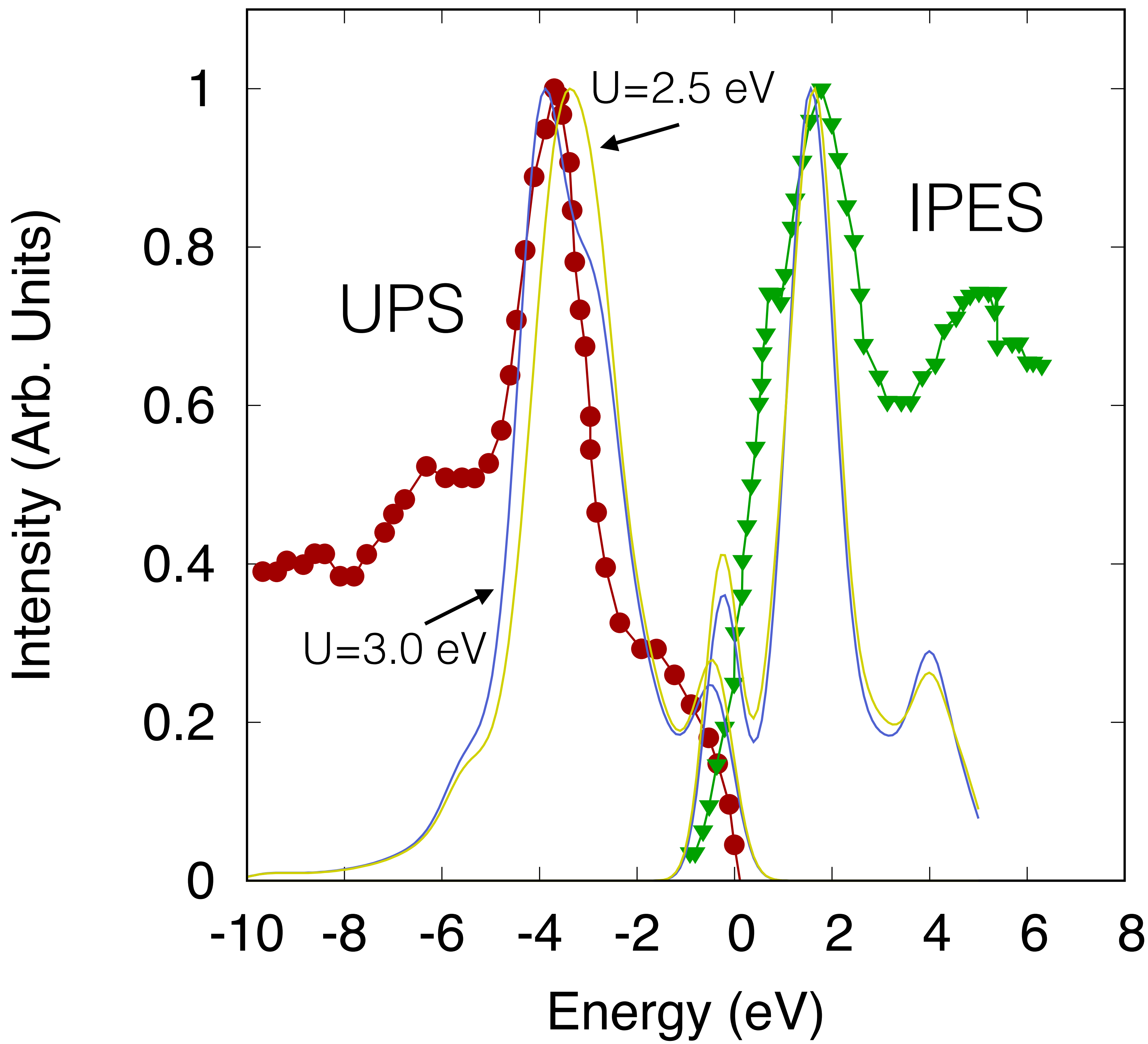
Phys Rev B 58, 1201

Empirical values of U (CuMnAs)



… in this way, U is effectively a fitting parameter

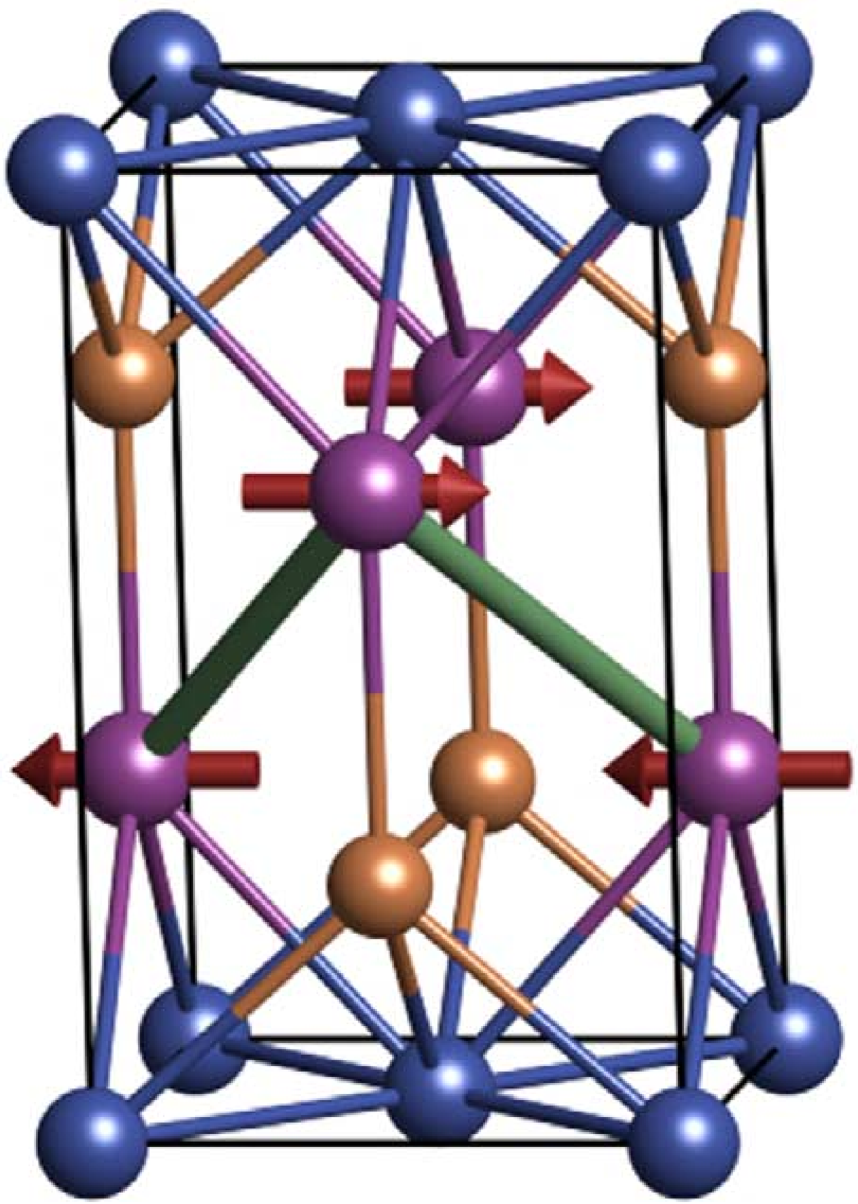
Another measurable quantity: UPS - cross check



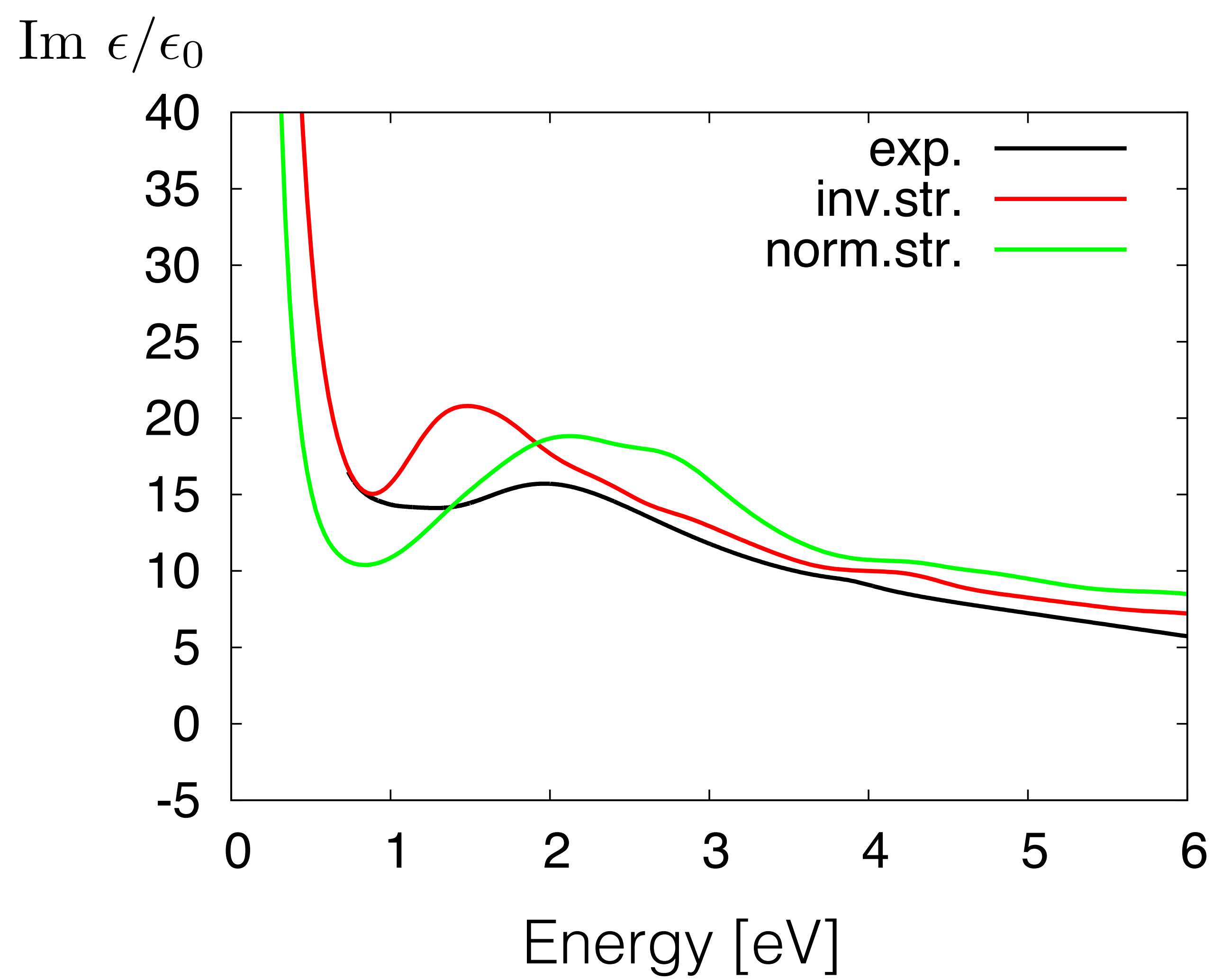
What if…

“normal structure”

CuMnAs tetragonal

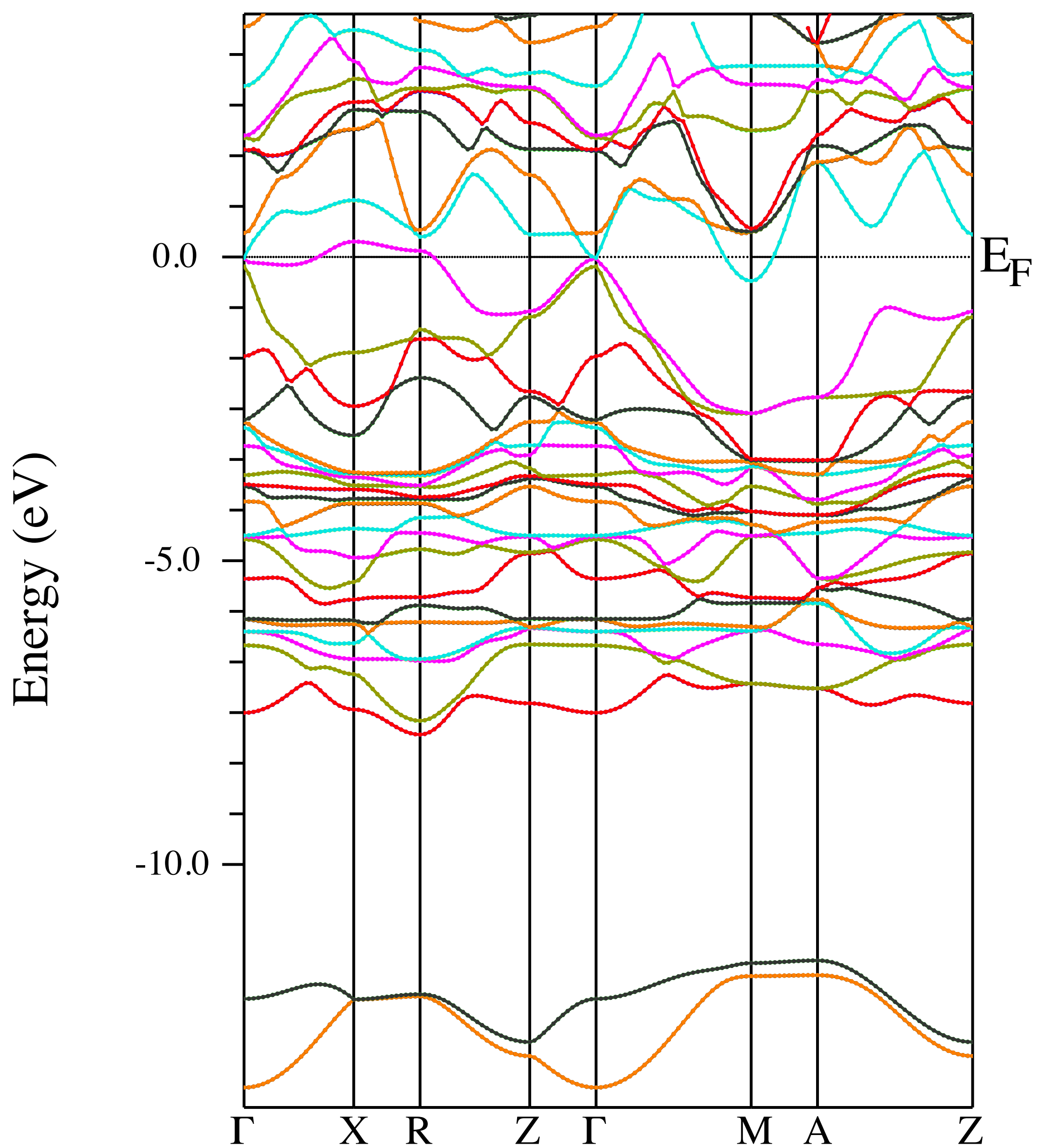


… positions of Cu and Mn are in fact swapped

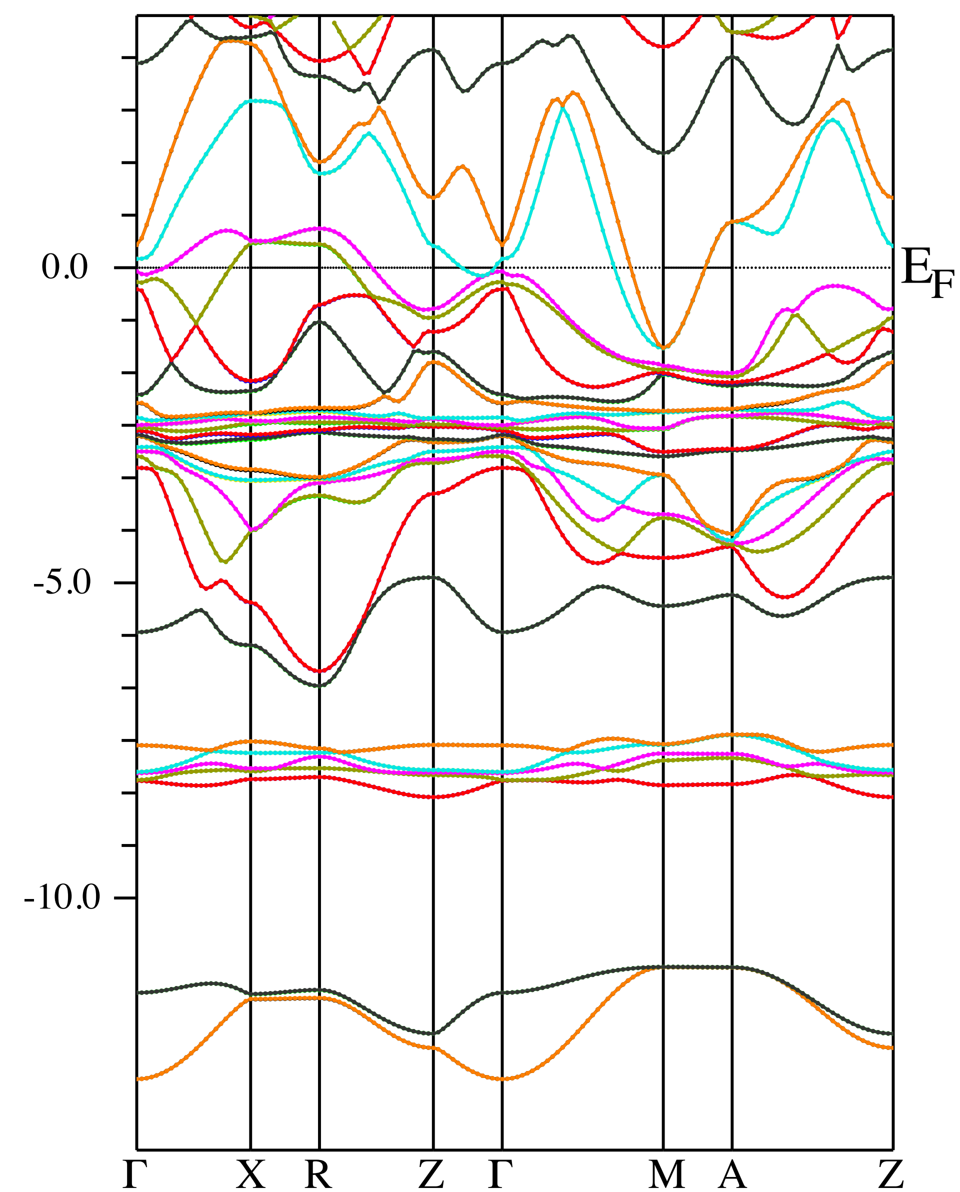


CuMnAs band structure

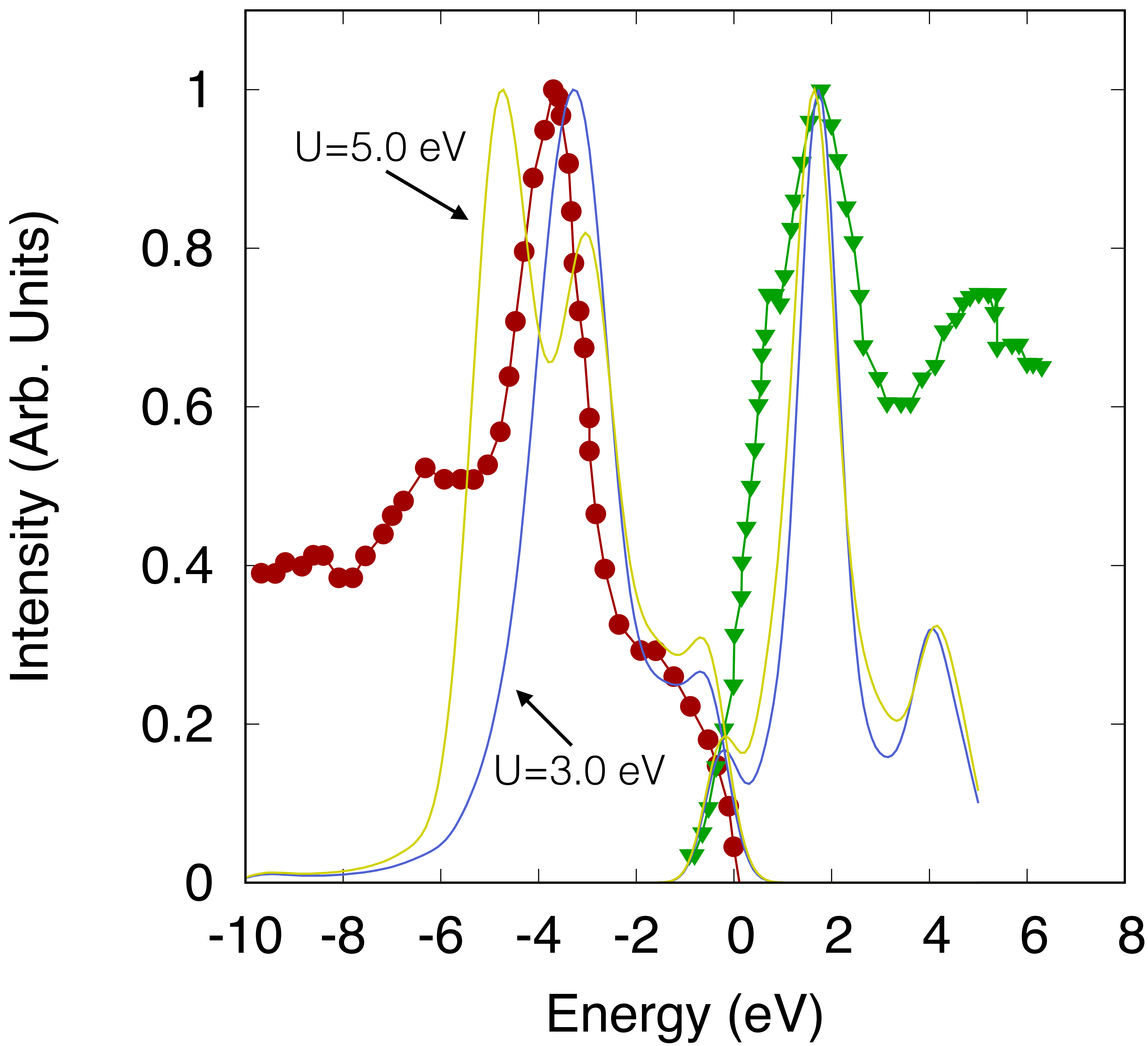
Mn+As tetrahedra
(normal, U=0.2 Ry)



Cu+As tetrahedra
(inverted, U=0.4 Ry)

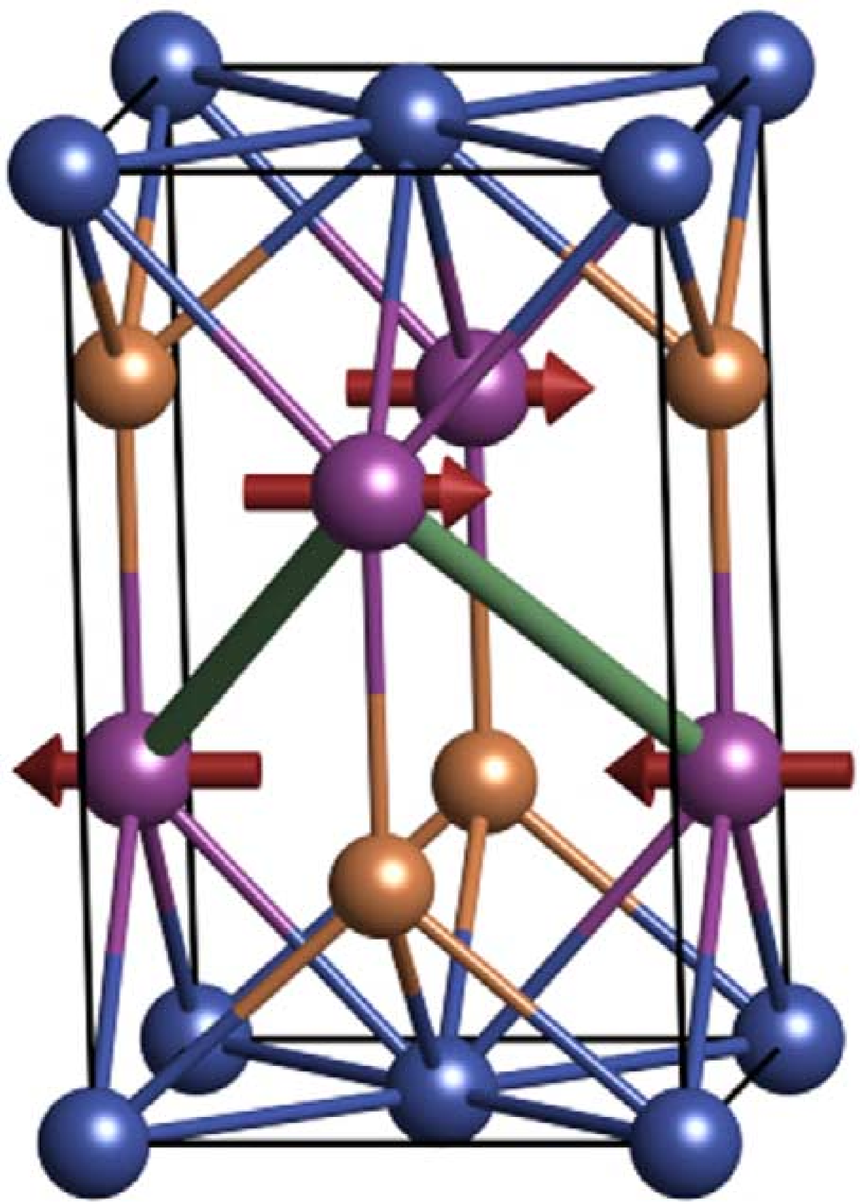


Back to UPS - cross check



So what's out there in CuMnAs…

CuMnAs tetragonal



- "inverted" structure unlikely
- in DFT+U, reasonable values are $U \approx 0.1 - 0.2\ \mathrm{Ry}$
- based on combined evidence from UPS and ellipsometry

Summary

- not only in ferromagnets, magnetic moments can be manipulated electrically by **spin-orbit torques**
- in **antiferromagnets**, this is a very efficient means of “writing information”

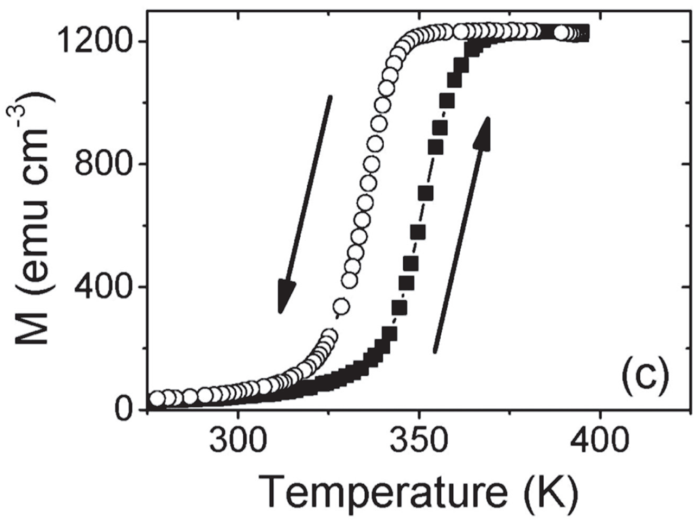
Summary

- not only in ferromagnets, magnetic moments can be manipulated electrically by spin-orbit torques
- in antiferromagnets, this is a very efficient means of "writing information"
- microscopically, the effect is simply just **linear response:** $\delta \mathbf{S} = \chi \, \mathbf{E}$
- in a given material, it requires spin-orbit interaction and depends on the band structure…

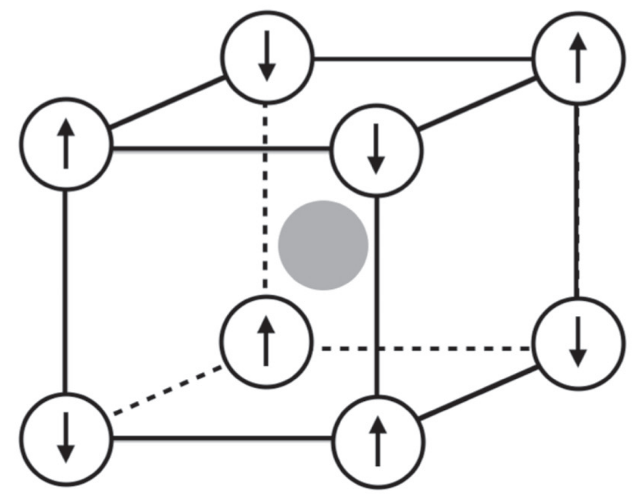
Summary

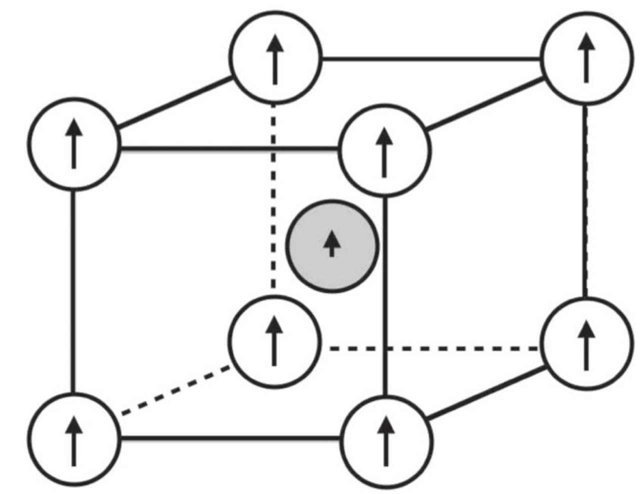
- not only in ferromagnets, magnetic moments can be manipulated electrically by spin-orbit torques
- in antiferromagnets, this is a very efficient means of “writing information”
- microscopically, the effect is simply just linear response - $\delta\mathbf{S} = \chi\,\mathbf{E}$
- in a given material, it requires spin-orbit interaction and depends on the band structure…
- … which one should **check against experiments** such as “optics” (ellipsometric determination of permittivity in optical part of spectrum)

Antiferromagnet/ferromagnet transition in FeRh

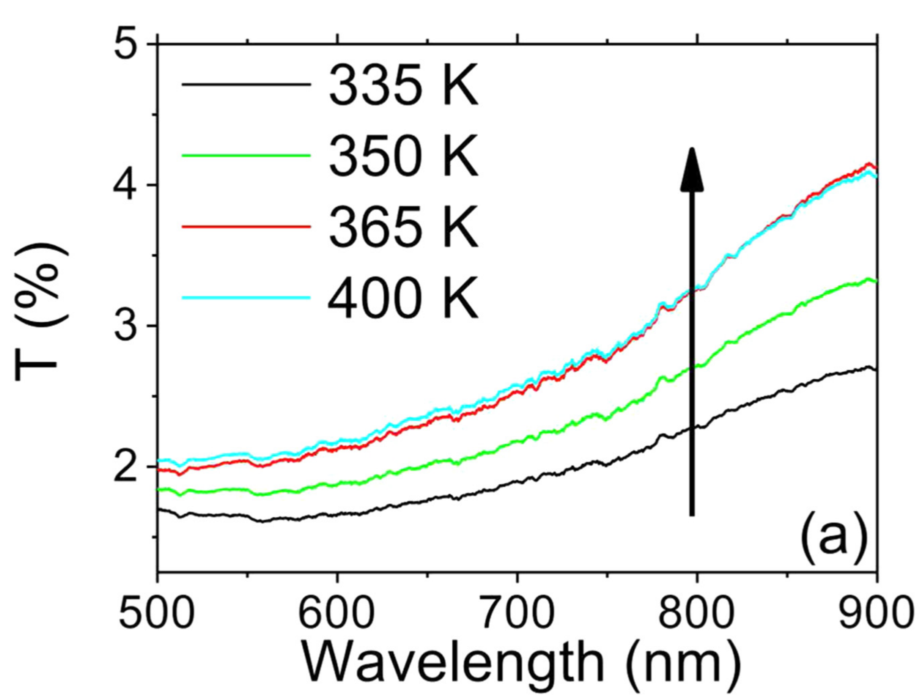


Saidl et al. '16
New J Phys 18, 083017

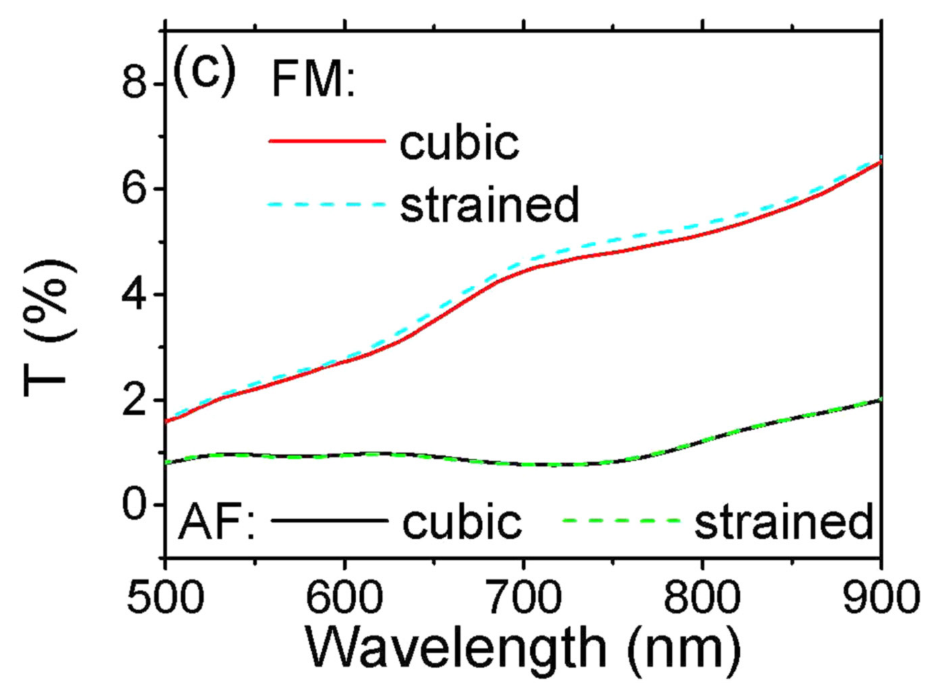




experiment



model



How to calculate the torque due to CISP

… when the magnetism
and CISP can be separated

Gambardella & Miron '11
[10.1098/rsta.2010.0336]

$$H = H_{KL} + J_{pd} \sum_{i,I} \vec{S}_I \cdot \vec{s}_i \delta(\vec{r}_i - \vec{R}_I)$$

$$\vec{T} = \frac{h}{M} \delta\vec{S} \times \vec{M}$$

where *h* is obtained from the above Hamiltonian by mean-field treatment

Výborný et al. '09
Phys Rev B 80, 165204

II. COMPUTATIONAL METHOD

A. Kubo linear-response formalism for the torkance tensor

Within the local spin density approximation to DFT the Hamiltonian H can be decomposed as [23]

$$H = H_0 + \mu_B \boldsymbol{\sigma} \cdot \boldsymbol{\Omega}^{\mathrm{xc}}, \qquad (1)$$

where H_0 contains kinetic energy, scalar potential, and SOI. μ_B is the Bohr magneton, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)^{\mathrm{T}}$ is the vector of Pauli spin matrices, and $\boldsymbol{\Omega}^{\mathrm{xc}}$ is the exchange field. We consider only ferromagnetic systems, where the exchange field $\boldsymbol{\Omega}^{\mathrm{xc}}(\mathbf{r}) = \Omega^{\mathrm{xc}}(\mathbf{r})\hat{\mathbf{M}}$ is characterized by a position-independent direction $\hat{\mathbf{M}}$ and a position-dependent amplitude $\Omega^{\mathrm{xc}}(\mathbf{r})$. The relation to the Kohn-Sham effective potentials $V^{\mathrm{eff}}_{\mathrm{majority}}(\mathbf{r})$ and $V^{\mathrm{eff}}_{\mathrm{minority}}(\mathbf{r})$ of majority and minority electrons is given by $\Omega^{\mathrm{xc}}(\mathbf{r}) = \frac{1}{2\mu_B}[V^{\mathrm{eff}}_{\mathrm{minority}}(\mathbf{r}) - V^{\mathrm{eff}}_{\mathrm{majority}}(\mathbf{r})]$. In response to an applied electric field a magnetization $\delta\mathbf{M}(\mathbf{r})$ is induced at position $\mathbf{r}$. As a consequence, the exchange field $\boldsymbol{\Omega}^{\mathrm{xc}}(\mathbf{r})$ is modified by $\delta\boldsymbol{\Omega}^{\mathrm{xc}}(\mathbf{r}) = \Omega^{\mathrm{xc}}(\mathbf{r})\delta\mathbf{M}(\mathbf{r})/M(\mathbf{r})$. The resulting torque $\mathbf{T}$ on the magnetization within one unit cell is given by [24,25]

$$\mathbf{T} = \int d^3r\, \mathbf{M}(\mathbf{r}) \times \delta\boldsymbol{\Omega}^{\mathrm{xc}}(\mathbf{r}) = \int d^3r\, \boldsymbol{\Omega}^{\mathrm{xc}}(\mathbf{r}) \times \delta\mathbf{M}(\mathbf{r}), \quad (2)$$

where the integration is over the unit cell volume. Thus, the torque on the magnetization arises from the component of $\delta\mathbf{M}(\mathbf{r})$ that is perpendicular to $\boldsymbol{\Omega}^{\mathrm{xc}}(\mathbf{r})$. Within linear-response theory the torque $\mathbf{T}$ arising due to an applied electric field $\mathbf{E}$ can be written as $\mathbf{T} = \mathbf{tE}$, which defines the torkance tensor $\mathbf{t}$.

Freimuth et al. '14
Phys Rev B 90, 174423