Ab initio theory for coherent magnetic switching

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MŰEGYETEM 1782

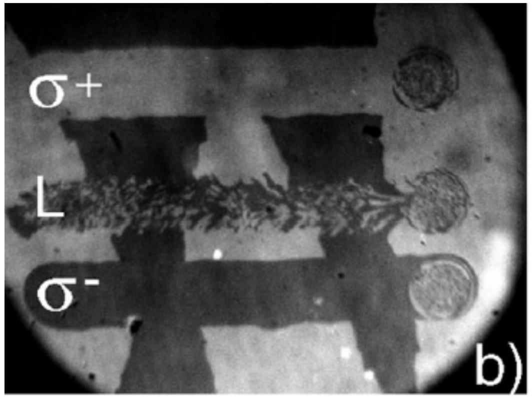
Karel Carva

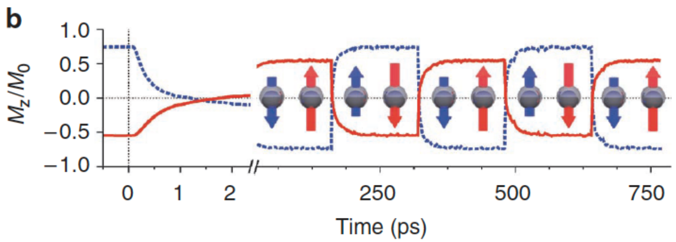
General ways to switch AFMs or ferrimagnets

Incoherent processes ⟷ Coherent processes

Heating, “destroy & rebuild”

E.g., GdFeCo



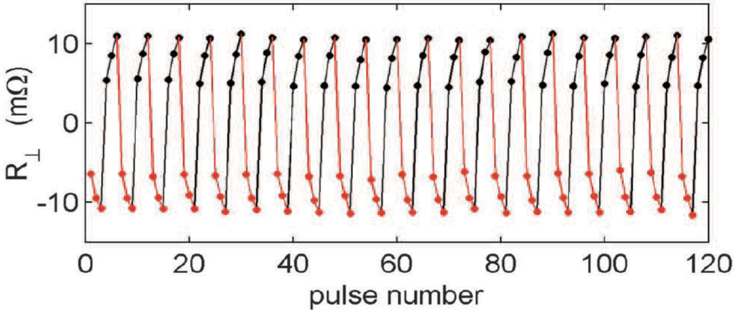


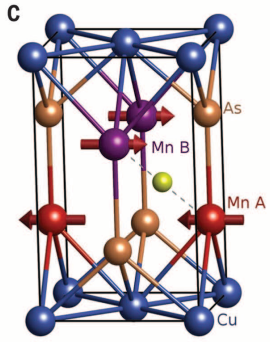
Stanciu et al, PRL **99**, 047601 (2007)

Ostler et al, Nat. Comm. **3**, 666 (2012)

E.g. (Rashba -) Edelstein effect

“staggered torque in AFMs”





CuMnAs

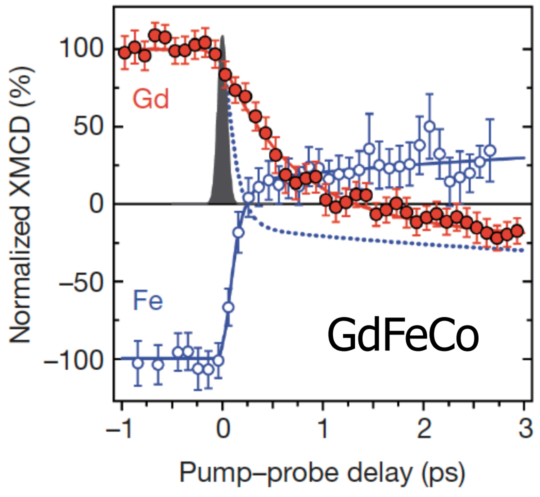
Zelezny et al, PRL **113**, 157201 (2014)

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

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

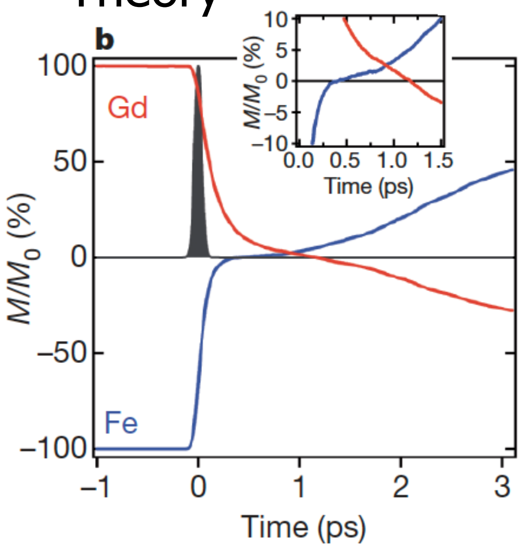
Switching in ferrimagnets

Experiment



Radu et al, Nature **472**, 205 (2011)

Theory



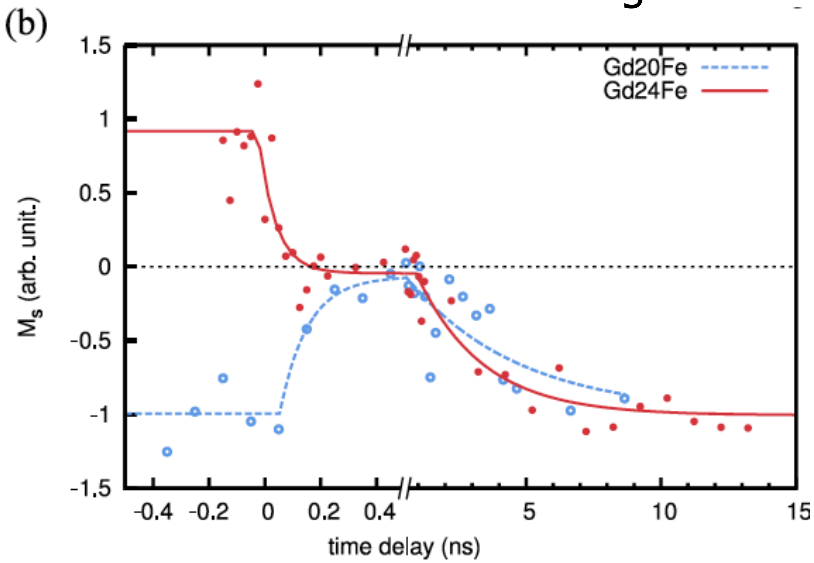
"Destroy & rebuild"

Nearly fully demagnetized ~ 1 ps

Very long *restoring* time ~ 1 ns of incoherent process

Re-writable at > 0.5 ns

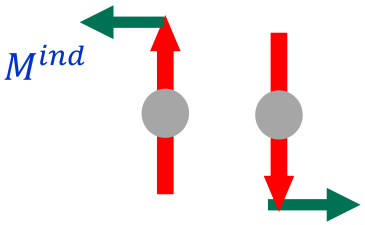
XMCD PEEM Fe L3 edge



LeGuyader et al, PRB **93**, 134402 (2016)

Possible *coherent* processes

- (Rashba -) Edelstein effect $\vec{M}^{ind}(\omega) = \chi(\omega)\vec{E}(\omega)$ Current or THz field (ps)



Staggered torques

Requires local symmetry breaking

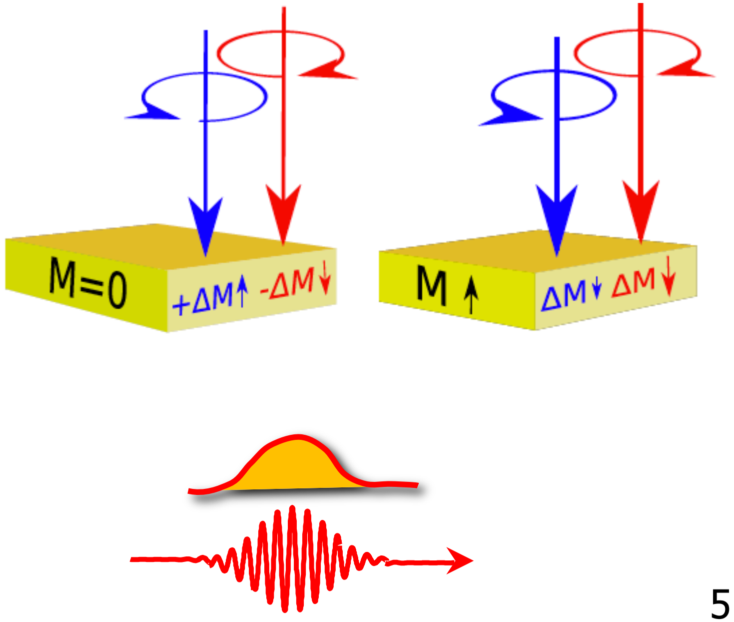
Zelezny et al, PRL **113**, 157201 (2014)
Wadley et al, Science **351**, 587 (2016)

- Inverse Faraday effect $\vec{M}^{ind}(0) = \kappa^{IFE}(\omega)\vec{E}^{*}\times\vec{E} = K^{IFE}(\omega)E^{2}(\omega)$ fs-laser field

Kimel et al, Nature **435,** 655 (2005)
Berritta, Mondal, Carva, PMO, PRL **117**, 137203 (2016)
John et al, Sci.Rep. **7**, 4114 (2017)

symmetry breaking not required

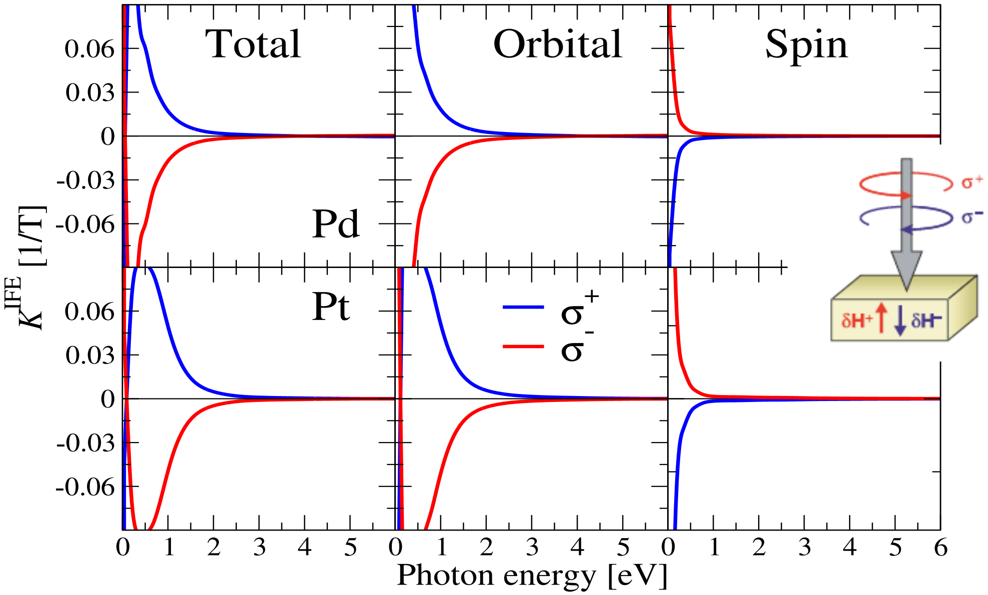
Disadvantage: not much known about it

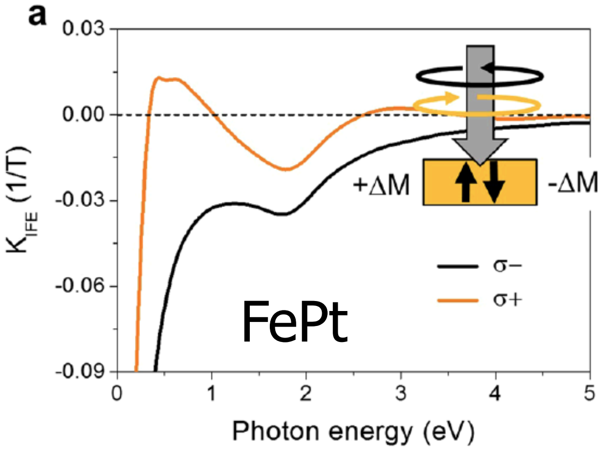


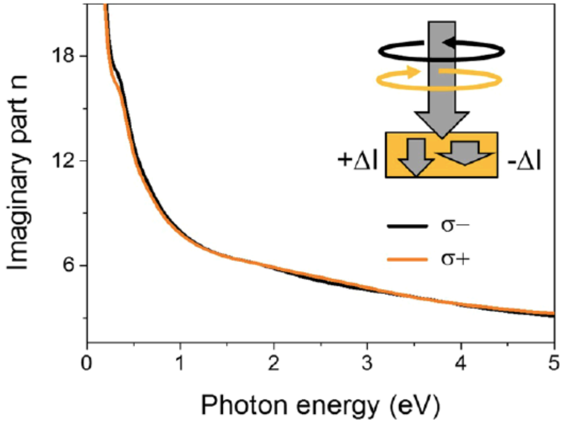
Nonmagnetic metals / ferromagnets

$$M^{ind}(0) = [K_L^{IFE}(\omega) + K_S^{IFE}(\omega)]\, I/c,\; I = \varepsilon_0 c\, E^2/2 \qquad (\hbar\Gamma = 0.03\ Ry)$$

2nd order response theory







Dichroic absorption

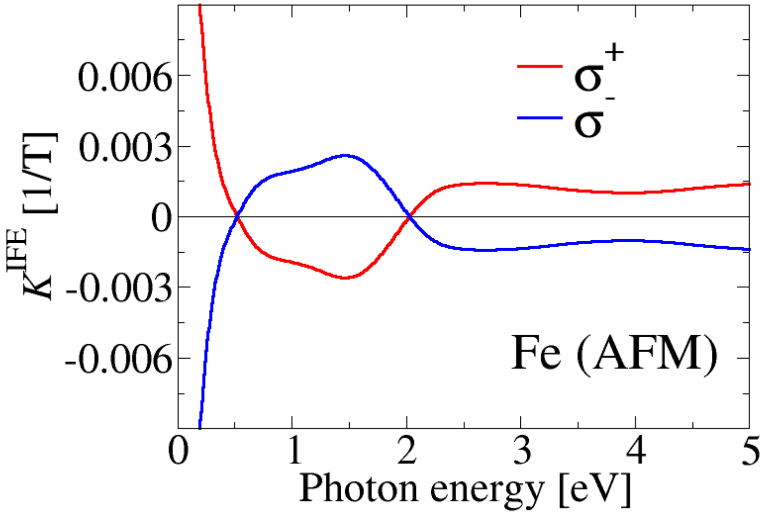
- *Antisymmetric* in helicity for nonmagnetic materials
- Opposite effect of spin and orbital IFE contributions possible
- Asymmetric for ferromagnets

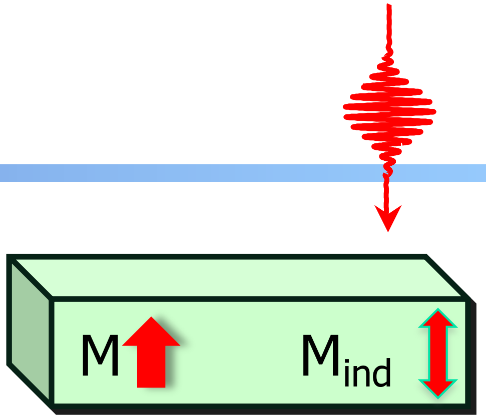
Berritta, Mondal, Carva, PMO, PRL **117**, 137203 (2016)

Freimuth, Blügel, Mokrousov, PRB **94**, 144432 (2016)

John et al, Sci.Rep. **7**, 4114 (2017)

Antiferromagnetic materials

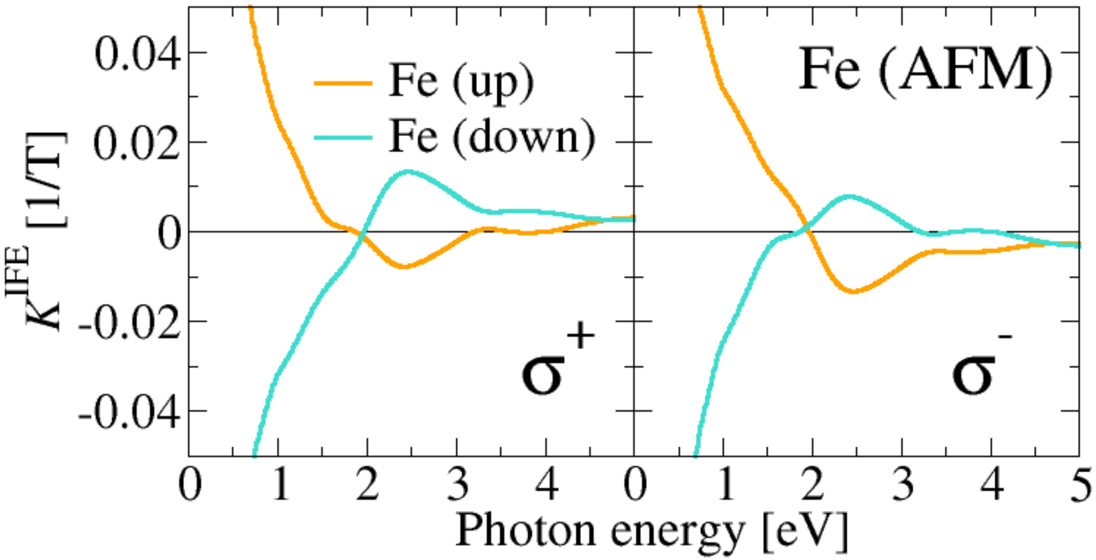




Fe (AFM)

$$M^{Fe} = \pm 1.635 \mu_B$$

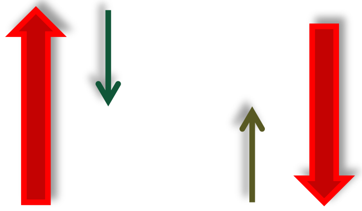
Small effect, antisymmetric?



I=1 GW/cm^2 ω=2.5 eV

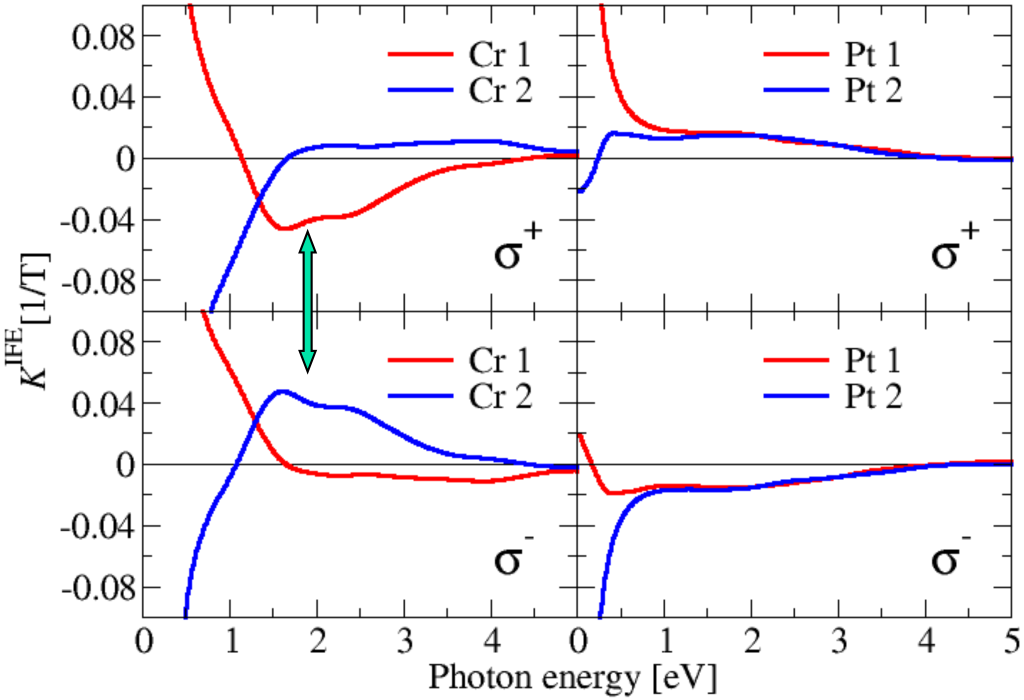
$$M_{ind}^{\Uparrow}(\sigma^+) = -6.4 \times 10^{-4} \mu_B$$

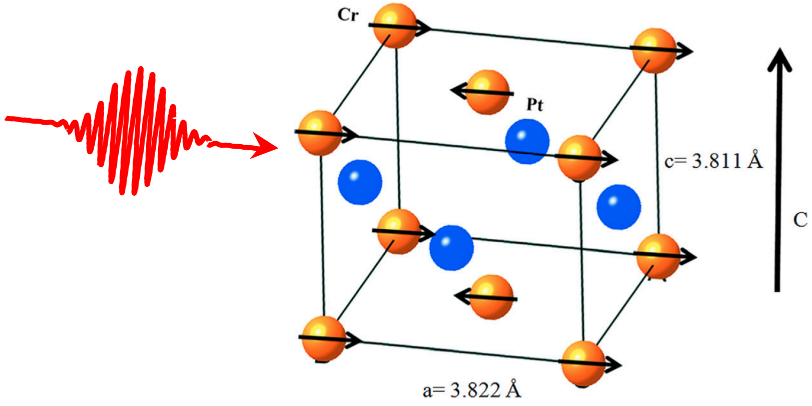
$$M_{ind}^{\Downarrow}(\sigma^+) = 1.1 \times 10^{-3} \mu_B$$



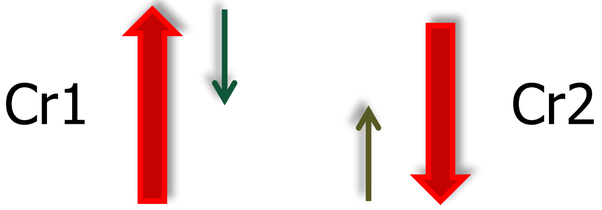
Gives staggered induced moments

Antiferromagnetic CrPt





$T_N \sim 760$ K



Staggered induced moments, not equal size

ω =2.26 eV

I= 1 GW/cm²

Cr_1 $M^{ind}(\sigma^+)=-0.08\mu_B$

Cr_2 $M^{ind}(\sigma^+)= 0.014\mu_B$

Pt_1 $M^{ind}(\sigma^+)= 0.03\mu_B$

Pt_2 $M^{ind}(\sigma^+)= 0.03\mu_B$

Dannegger, Berritta, Carva, Selzer, Ritzmann, PMO, Nowak, PRB **104**, L060413 (2021)

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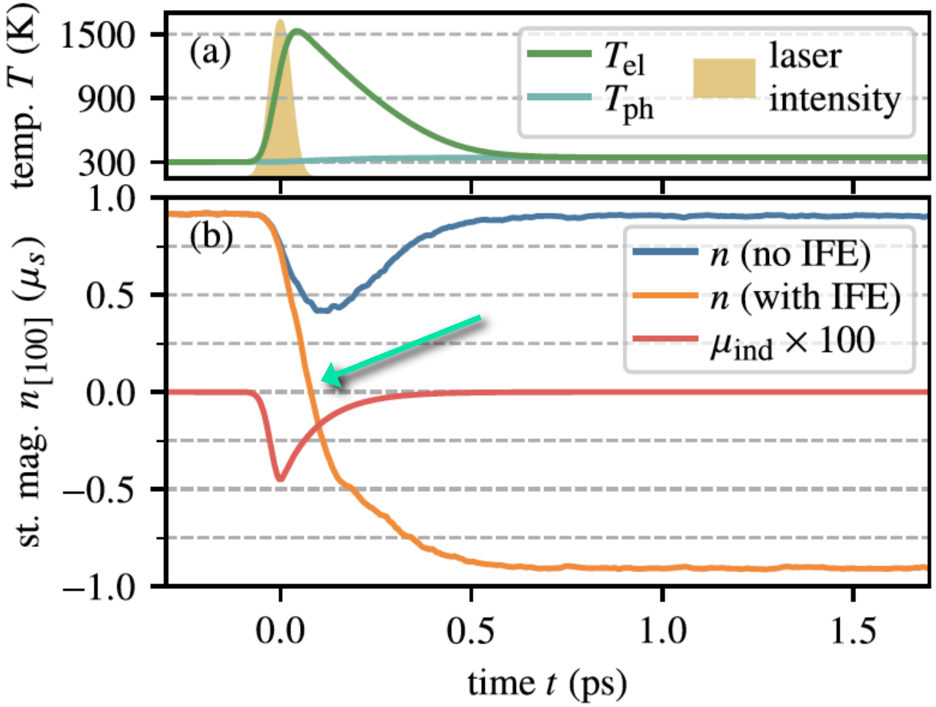
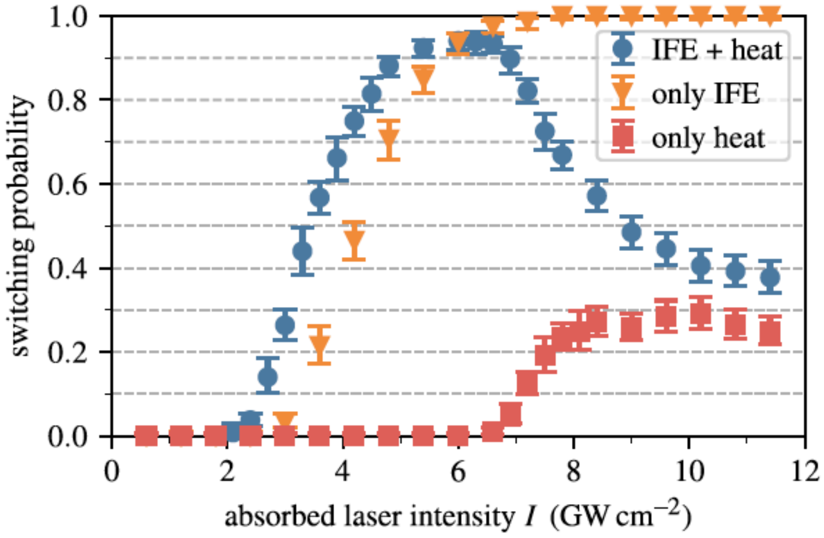
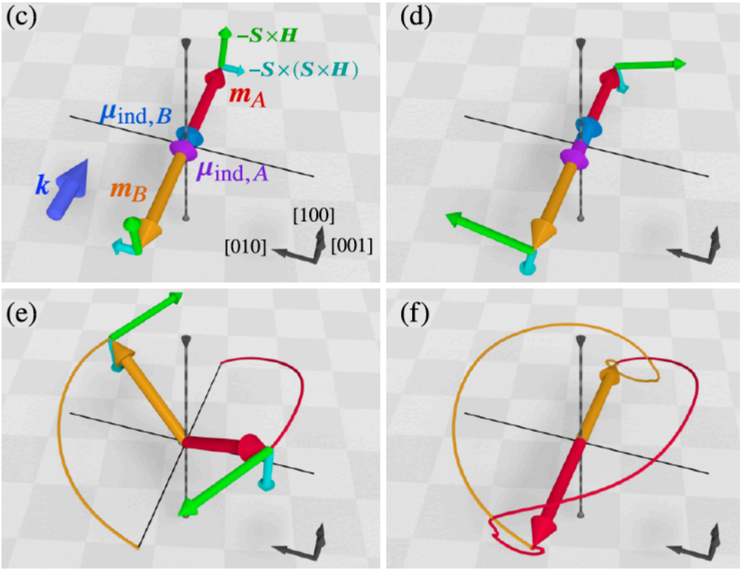
Atomistic spin dynamics simulations

⇨ Talk of Uli Nowak, poster Tobias Dannegger



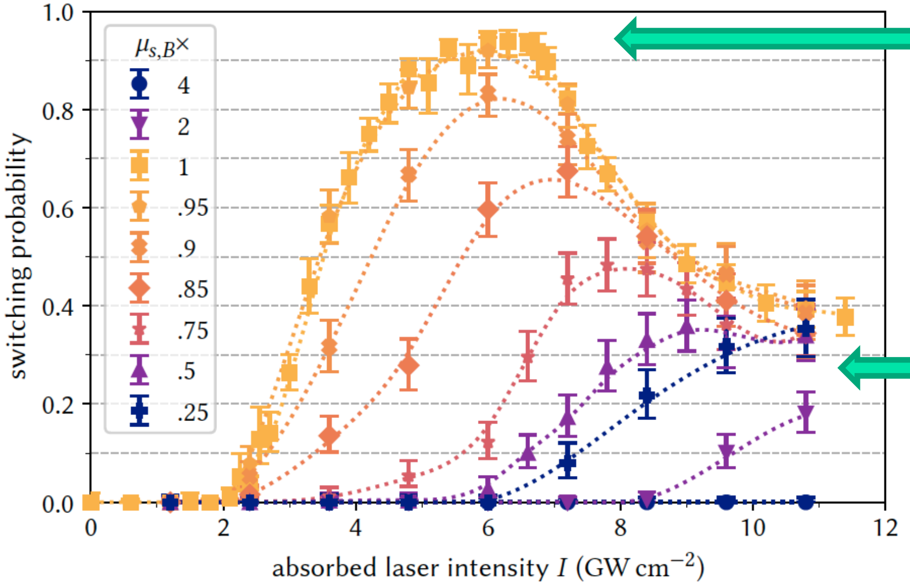




- ➢ *Switches in ~200 fs, completed at 500 fs*
- ➢ Nonthermal switching, much heat works against switching probability
- ➢ 90° coherent switching possible
- ➢ AFM exchange enhanced switching

From AFM to ferrimagnet

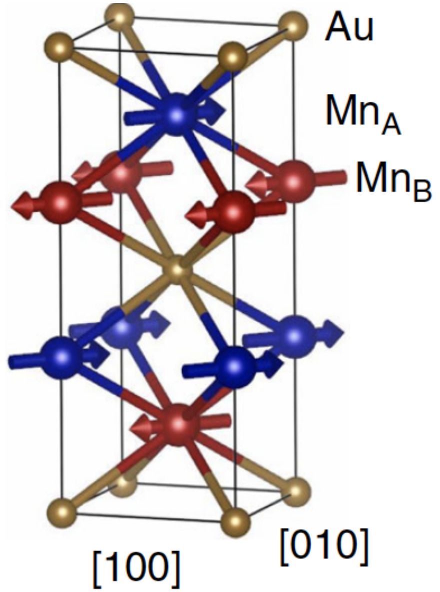
Ferrimagnetic order – unequal sublat. moments

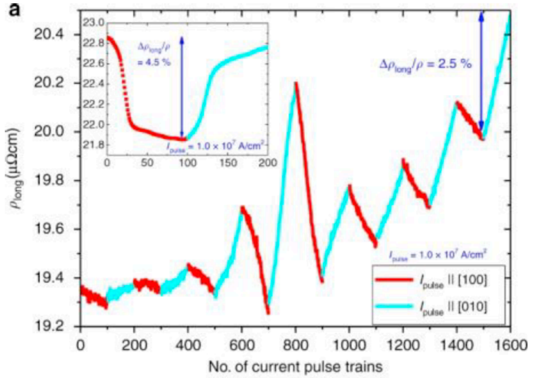


AFM

Ferrimagnet

Current induced switching in Mn_2Au





Bodnar et al, Nat. Commun. **9**, 348 (2018)

Orb. Edelstein effect

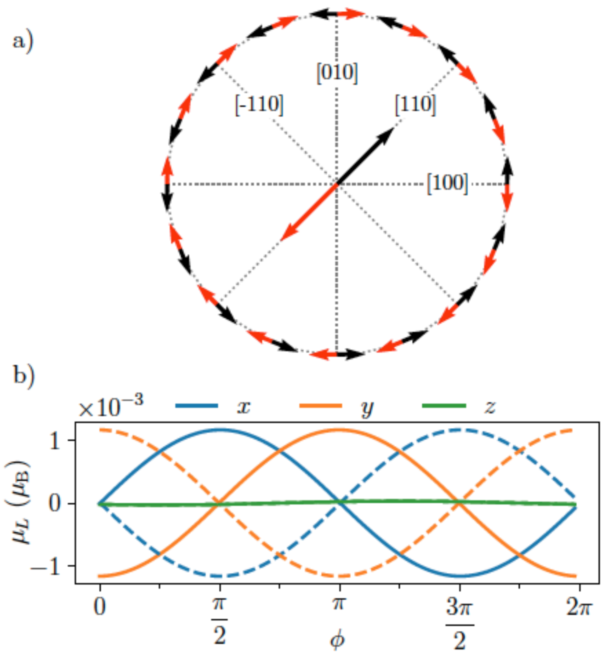
Spin Edelstein effect

$$M_i^{ind} = \chi_{ij} \cdot E_j$$

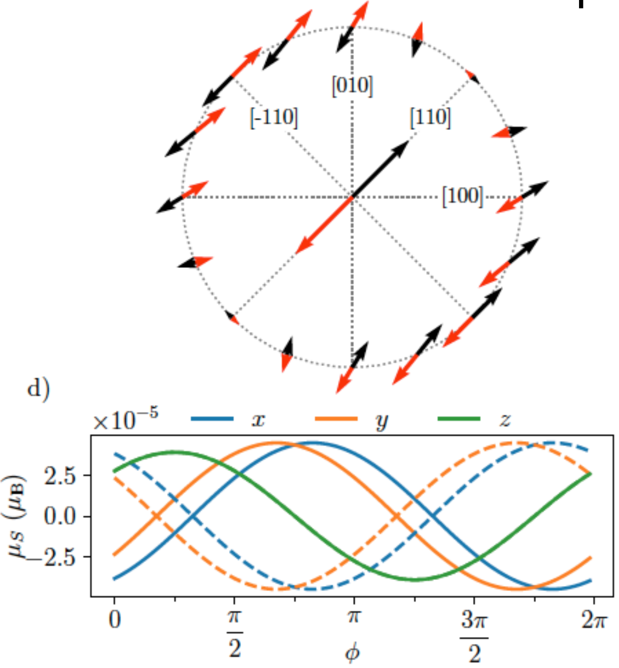
Lin. response

Mn1

Mn2



10^{-3} μ_B “Rashba”



10^{-5} μ_B “Dresselhaus”

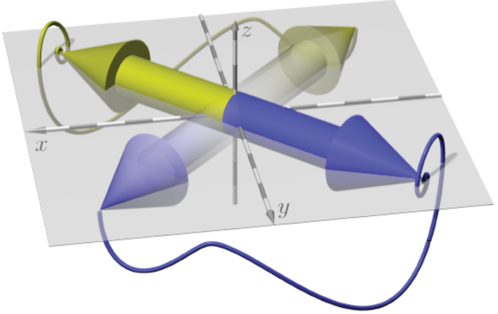
- Orbital REE dominant (not due to SOC)
- Large non-Néel elements present (spin)
- Orbital polarization is staggered

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

Atomistic spin dynamics simulations

$$\mathcal{H} = -\frac{1}{2}\sum_{i\neq j} J_{ij}(\boldsymbol{S}_i+\boldsymbol{s}_i)\cdot(\boldsymbol{S}_j+\boldsymbol{s}_j) - \sum_i J^{\mathrm{sd}}\boldsymbol{S}_i\cdot\boldsymbol{s}_i + \sum_i \xi \boldsymbol{S}_i\cdot\boldsymbol{l}_i - \sum_i d_z S_{i,z}^2 - \sum_i d_{xy} S_{i,x}^2 S_{i,y}^2 ,$$

With *ab initio* input

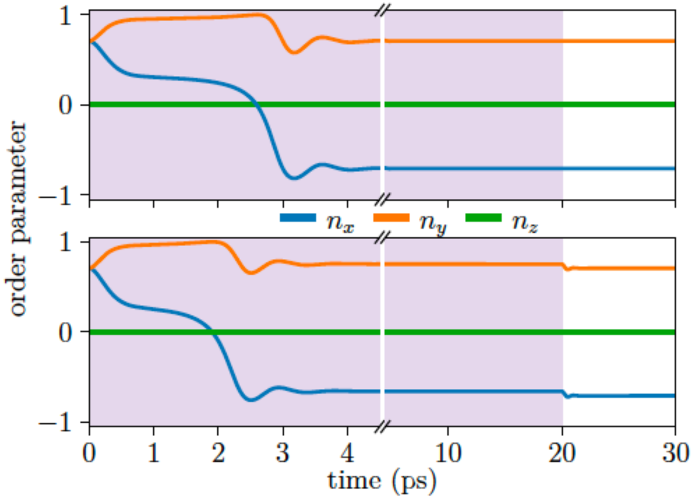


Switching path

AFM exchange enhanced

$$T \sim (E_{ani}E_{xch})^{-1/2}$$

Roy, Otxoa, Wunderlich, PRB **94**, 014439 (2016)



$E \parallel [110]$

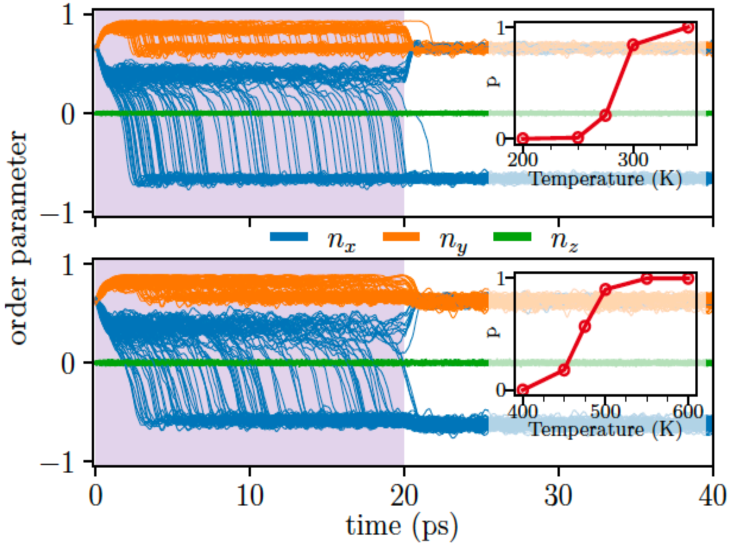
E =1.9 10^7 V/m

$E \parallel [100]$

E =3.1 10^7 V/m

90° switching simulation for 20 ps pulse (T=0 K, high E field)

=> Fast switching ~4 ps



$E \parallel [110]$

E = 10^7 V/m, T = 300 K

Switching assisted by temperature !

$E \parallel [100]$

E = 10^7 V/m, T = 500 K

Selzer, Salemi, Deak, Simon, Szunyogh, PMO, Nowak, PRB in press

Other possible coherent torques?

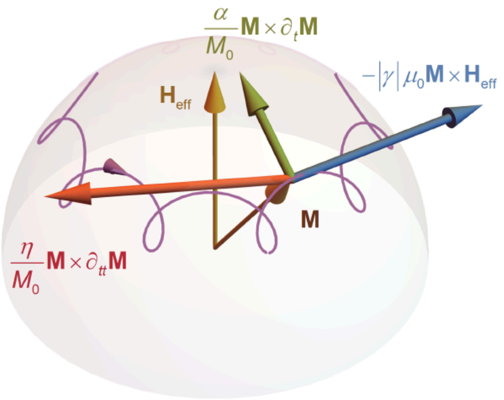
$$\boxed{\frac{\partial \boldsymbol{M}}{\partial t} = -\gamma\, \boldsymbol{M} \times \boldsymbol{H}_{\text{eff}} + \alpha\, \boldsymbol{M} \times \frac{\partial \boldsymbol{M}}{\partial t} + \boldsymbol{T}}$$

- Inertial torque $T^{inert} = M \times \left[I \cdot \frac{\partial^2 M}{\partial t^2} \right]$

Short time scale (fs-ps), but intrinsic I – *how to steer it?*

Mondal, Berritta, Nandy, PMO, PRB **96**, 024425 (2017)
Cherkasskii et al, PRB **102**, 184432 (2020)
Neeraj et al, Nat. Phys. **17**, 245 (2021)
Mondal, Großenbach, Rozsa, Nowak, PRB **103**, 104404 (2021)

$$I \propto -\bar{\tau}\, \alpha \qquad \bar{\tau} \approx 700\ fs$$



- Optical spin-orbit torque $T^{OSOT} = -\frac{e^2}{2m^2c^2\varepsilon_0} M \times j_s$

$$\boldsymbol{j}_s = -2\boldsymbol{E} \times \boldsymbol{A}\ (\epsilon_0 = 1)$$

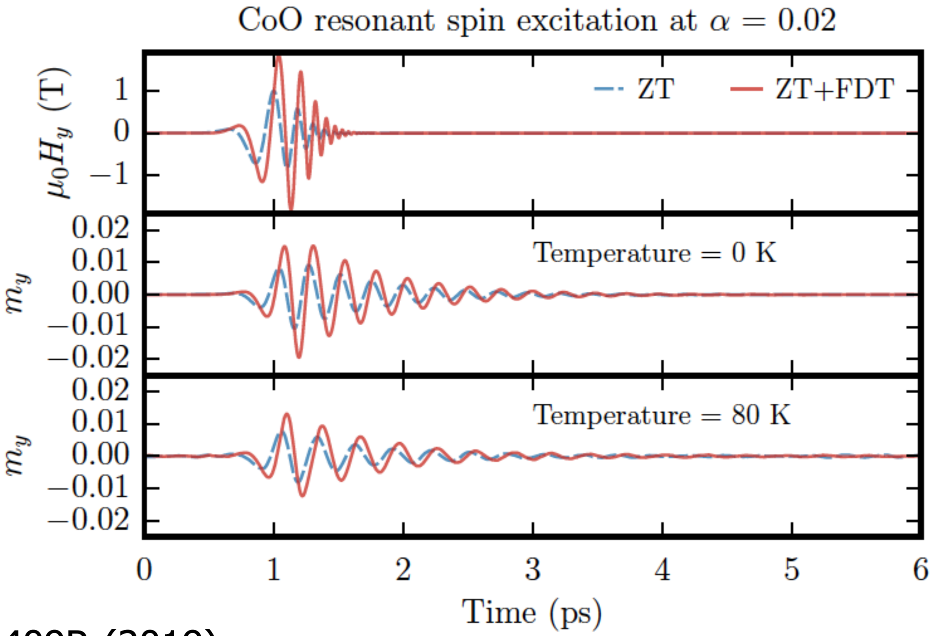
Photon spin angular moment

Mondal, Berritta, Paillard et al, PRB **92**, 100402R (2015)
Mondal, Berritta, Oppeneer, JPCM **29**, 194002 (2017)
Mondal, Donges, Nowak, PRRes **3**, 023116 (20121)

Some possible observations (?)

Other possible torques?

- Field-derivative torque $T^{FDT} \propto M \times \frac{\partial H}{\partial t}$ (non-relativistic)



- for THz pulses FDT could be important
- phase difference between Zeeman torque and FDT
- No experimental observation so far

Mondal, Berritta, PMO, PRB **94**, 144419 (2016)

Mondal, Donges, Ritzmann, PMO, Nowak, PRB **100**, 060409R (2019)

Conclusions

- Inverse Faraday effect can give staggered induced moments in AFMs
  (no symmetry-breaking needed)
- Can initiate fast AFM switching process (~200fs) in CrPt *w/o incoherent heating*
- Electric-field induced switching in Mn_2Au possible in ~ 4 ps
- Heating by current pulses strongly assists the AFM switching in Mn_2Au
- Other possible torques for ultrafast switching:
  Inertial torque, FDT, and OSOT – not enough known and possibly too small

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