Time-dependent density functional theory

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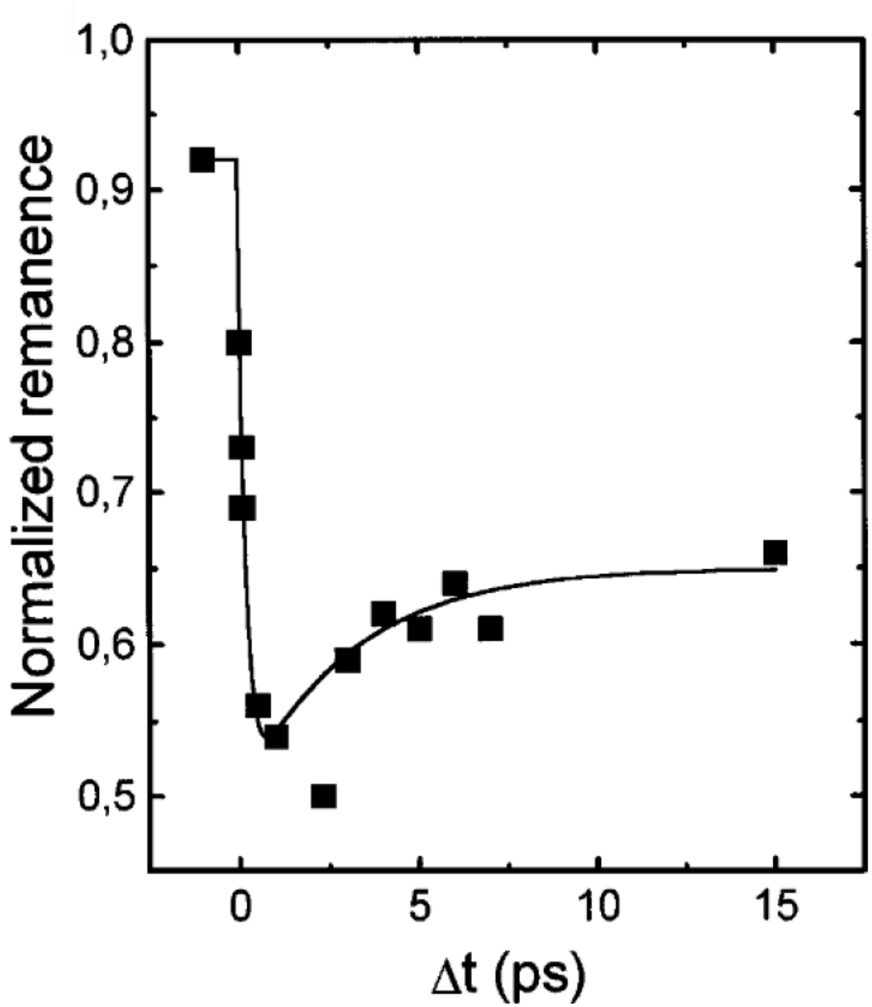
האוניברסיטה העברית בירושלים
THE HEBREW UNIVERSITY OF JERUSALEM
الجامعة العبرية في اورشليم القدس

<u>DAY 2</u>: Real-time TDDFT beyond the linear regime: Ultrafast laser-driven spin dynamics in solids

First experiment on ultrafast laser induced demagnetization



Beaurepaire et al, PRL 76, 4250 (1996)

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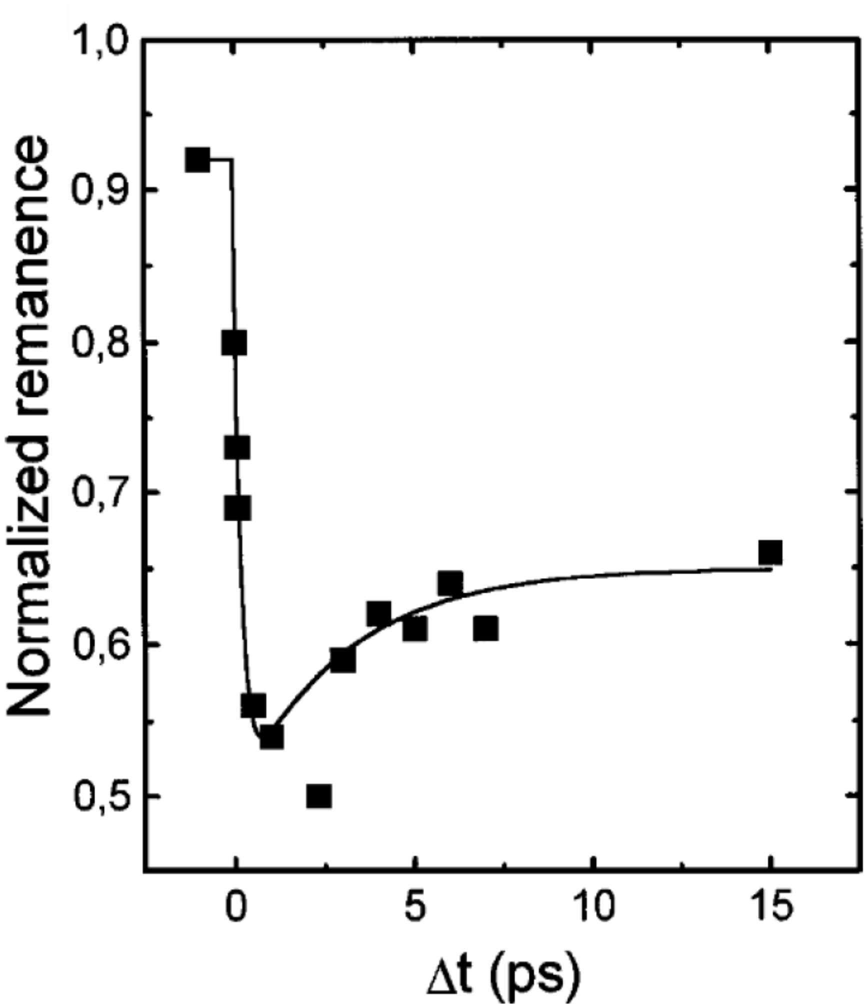

Beaurepaire et al, PRL 76, 4250 (1996)

Demagnetization in less than 100 fs has been demonstrated experimentally

Non-collinear-Spin TDDFT with Spin-Orbit-Coupling (weakly relativistic limit of relativistic TDDFT)

$$i\frac{\partial}{\partial t}\varphi_k(r,t)=\Big[\frac{1}{2}\big(-i\nabla-A_{laser}(t)\big)^2+v_S[\rho,\boldsymbol{m}](r,t)-\mu_B\sigma\cdot B_S[\rho,\boldsymbol{m}](r,t)+\frac{\mu_B}{2c}\sigma\cdot\big(\nabla v_S[\rho,\boldsymbol{m}](r,t)\big)\times\big(-i\nabla\big)\Big]\varphi_k(r,t)$$

$$v_S[\rho,\boldsymbol{m}](r,t)=v_{lattice}(r)+\int\frac{\rho(r',t)}{|r-r'|}d^3r'+v_{xc}[\rho,\boldsymbol{m}](r,t)$$

$$B_S[\rho,\boldsymbol{m}](r,t)=B_{external}(r,t)+B_{xc}[\rho,\boldsymbol{m}](r,t)$$

where $\varphi_k(r,t)$ are Pauli spinors

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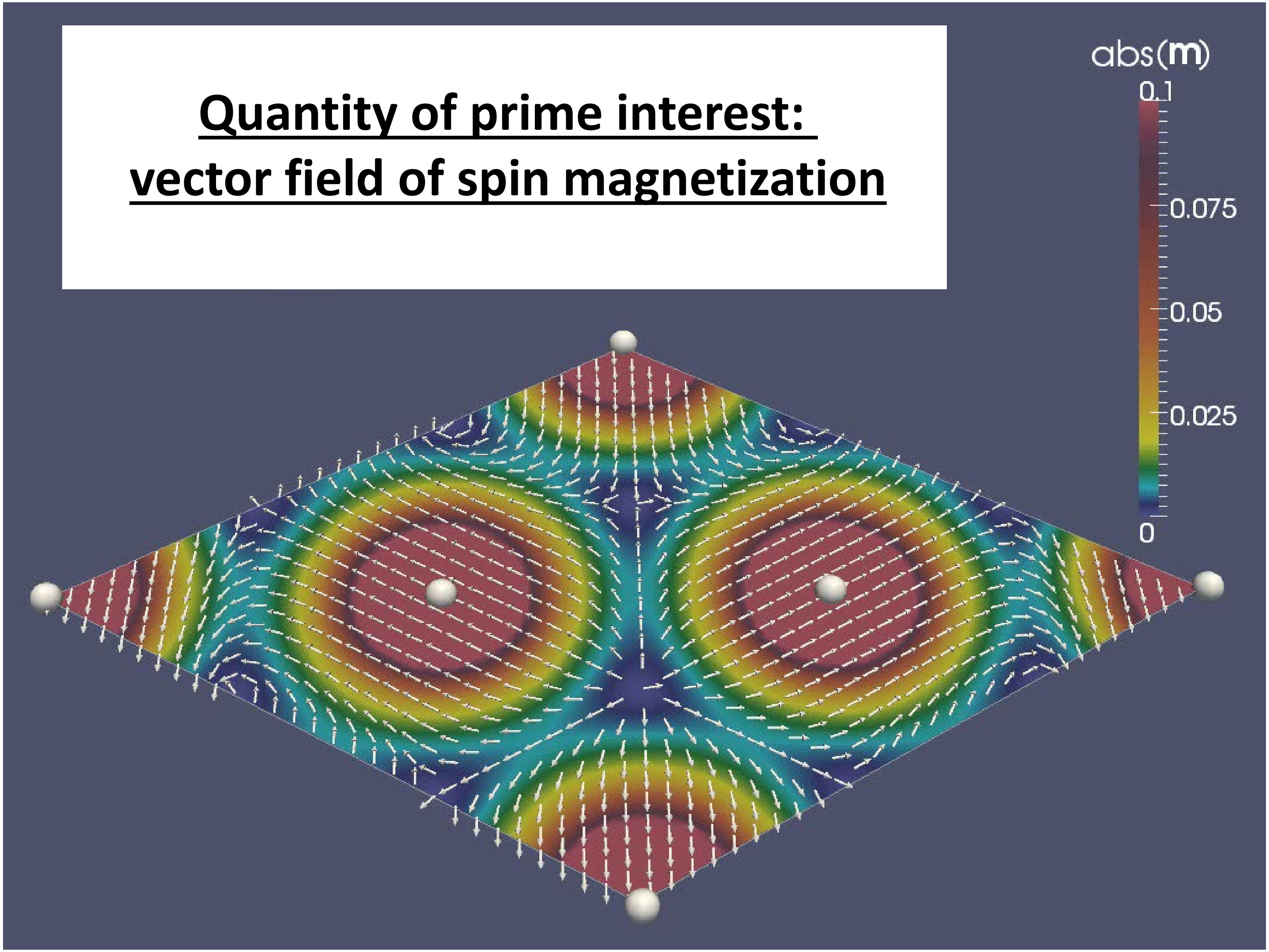
Universal functionals of ρ and m

where $\varphi_k(r,t)$ are Pauli spinors

$$n\left(\boldsymbol{r},t\right)=\sum_{j=1}^{N}\varphi_j^{\dagger}\left(\boldsymbol{r},t\right)\,\varphi_j\left(\boldsymbol{r},t\right)$$

$$\vec{\mathbf{m}}\left(\boldsymbol{r},t\right)=\sum_{j=1}^{N}\varphi_j^{\dagger}\left(\boldsymbol{r},t\right)\vec{\boldsymbol{\sigma}}\,\varphi_j\left(\boldsymbol{r},t\right)$$

Quantity of prime interest: vector field of spin magnetization



Cr monolayer in ground state

Aspects of the numerical implementation

- Wave length of laser in the visible regime
  (very large compared to unit cell)

  ⇒ Dipole approximation is made
  (i.e. electric field of laser is assumed to be spatially constant)

  ⇒ Laser can be described by a purely time-dependent vector potential

- **Periodicity of the TDKS Hamiltonian is preserved!**

- **Implementation in ELK code (FLAPW) (http://elk.sourceforge.net/)**

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Kay Dewhurst

ELK = Electrons in K-Space
or
Electrons in Kay's Space

Sangeeta Sharma

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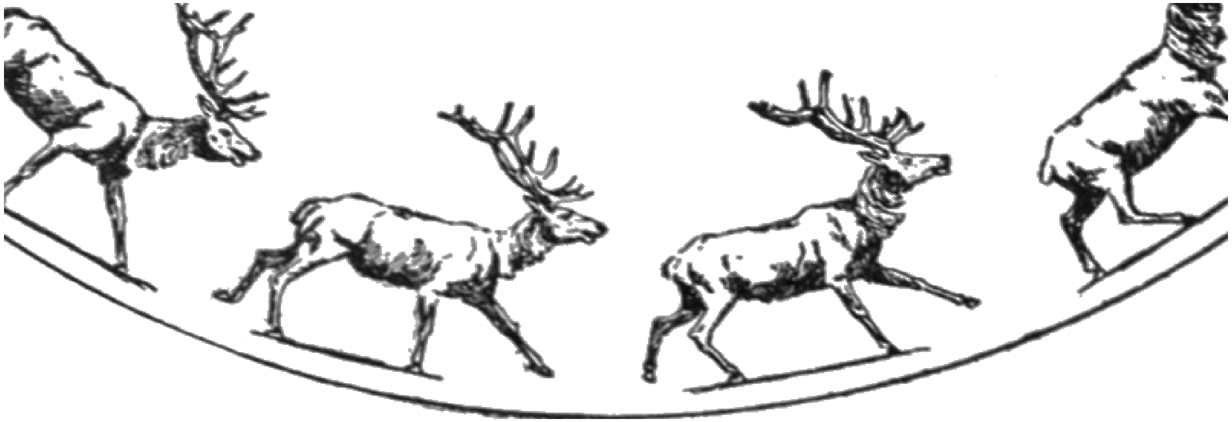
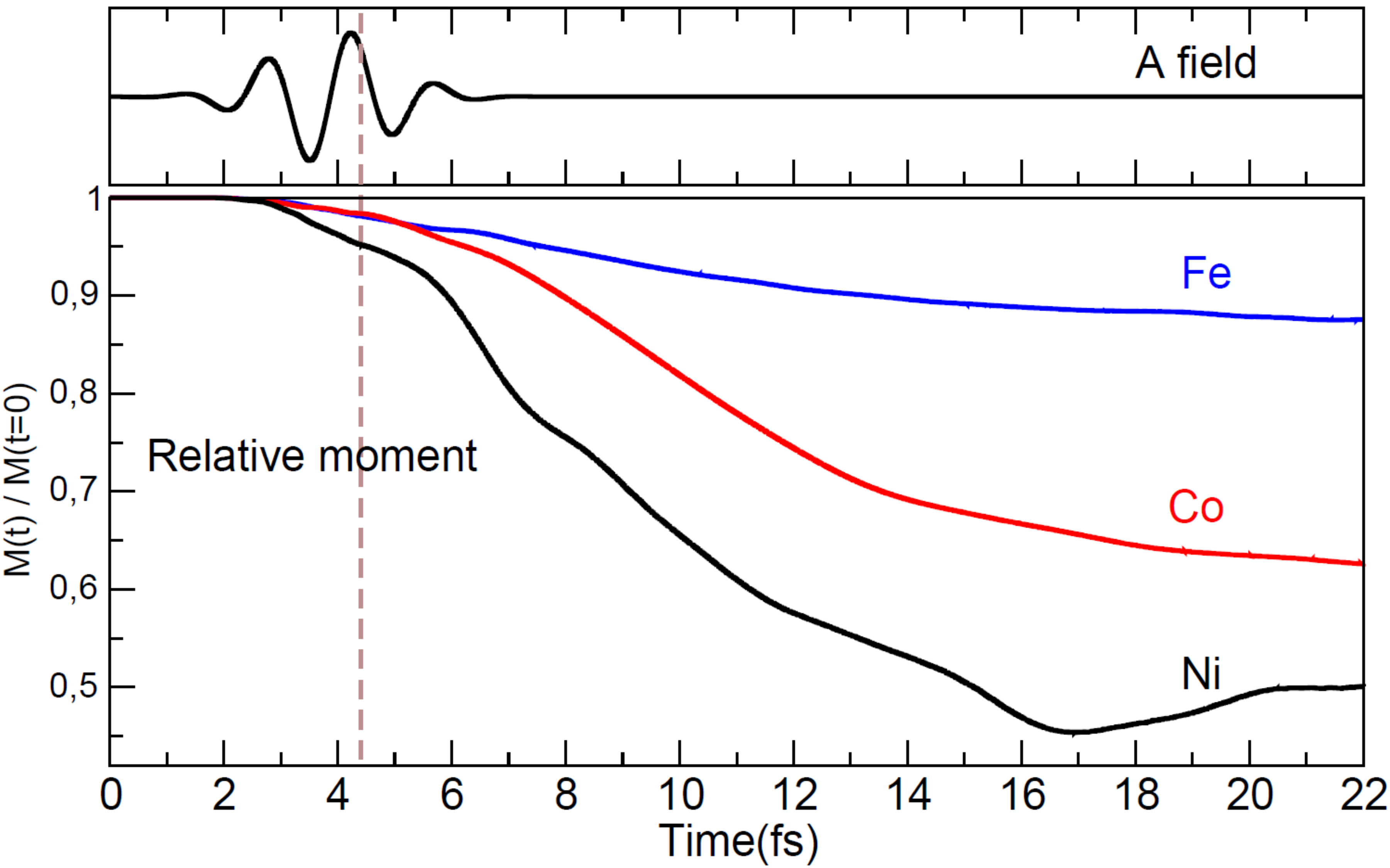


Demagnetisation in Fe, Co and Ni

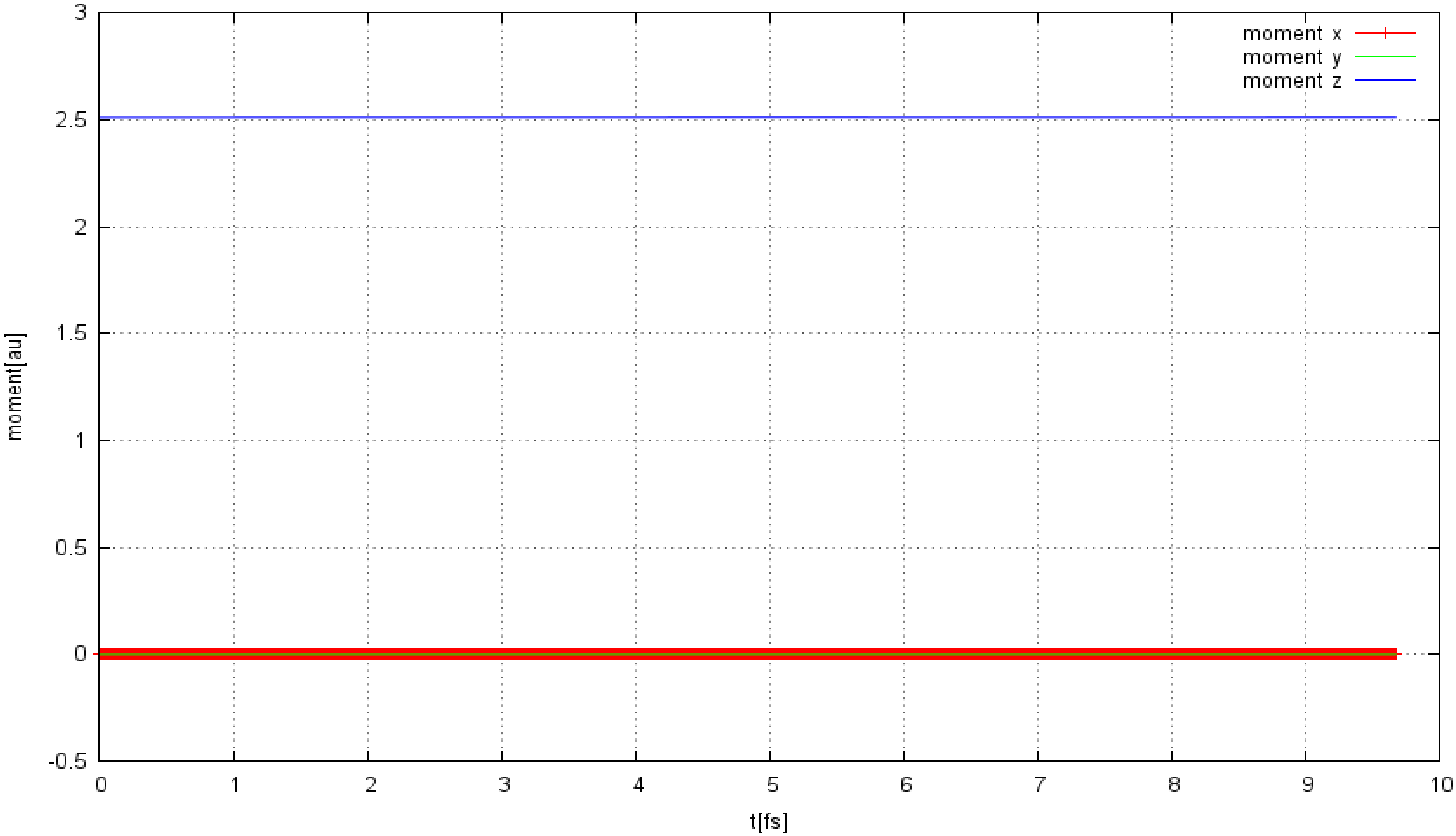


K. Krieger, K. Dewhurst, P. Elliott, S. Sharma, E.K.U.G., JCTC 11, 4870 (2015)

Analysis of the results

Calculation without spin-orbit coupling

components of spin moment



Exact equation of motion

$$\frac{\partial}{\partial t} m_z(r,t) = \frac{i}{\hbar} \left\langle \Phi_{KS}^{det}(t) \,|\left[\hat{H}_{KS}, \hat{m}_z(r) \right]|\, \Phi_{KS}^{det}(t) \right\rangle$$

$$= \left\{ m_x(r,t) B_{xc,y}(rt) - m_y(r,t) B_{xc,x}(rt) \right\}$$

$$+ \frac{1}{2c^2} \left\{ \hat{x} \cdot \left[\nabla v_s(r,t) \times j_y(r,t) \right] - \hat{y} \cdot \left[\nabla v_s(r,t) \times j_z(r,t) \right] \right\}$$

$$-\nabla \cdot j_z(r,t)$$

$$\overset{\leftrightarrow}{j}(r,t) = \left\langle \hat{\sigma} \otimes \hat{j}(r) \right\rangle$$ spin current tensor

Exact equation of motion

$$\frac{\partial}{\partial t} m_z(r,t) = \frac{i}{\hbar}\left\langle \Phi_{KS}^{det}(t) \,|\left[\hat{H}_{KS}, \hat{m}_z(r)\right]|\, \Phi_{KS}^{det}(t)\right\rangle$$ **local spin torque** $(m \times B_{xc})_z$

$$= \left\{ m_x(r,t) B_{xc,y}(rt) - m_y(r,t) B_{xc,x}(rt) \right\}$$

$$+ \frac{1}{2c^2}\left\{ \hat{x}\cdot\left[\nabla v_s(r,t) \times j_y(r,t)\right] - \hat{y}\cdot\left[\nabla v_s(r,t)\times j_z(r,t)\right]\right\}$$ **SOC**

$$-\nabla \cdot j_z(r,t)$$ **"continuity"**

$$\overleftrightarrow{j}(r,t) = \left\langle \hat{\sigma} \otimes \hat{\vec{j}}(r) \right\rangle$$ spin current tensor

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local spin torque **$(m \times B_{xc})_z$**

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$$\overset{\leftrightarrow}{j}(\mathbf{r},t) = \left\langle \hat{\sigma} \otimes \hat{j}(\mathbf{r}) \right\rangle$$ spin current tensor

Dynamics of **total** moment: Integrate over the unit cell

Exact equation of motion for total moment

$$\frac{\partial}{\partial t} M_z(t) = \frac{i}{\hbar} \int d^3r \left\langle \Phi_{KS}^{det}(t) \,|\, \left[\hat{H}_{KS}, \hat{m}_z(r) \right] |\, \Phi_{KS}^{det}(t) \right\rangle$$

$$= \int d^3r \left\{ m_x(r,t) B_{xc,y}(rt) - m_y(r,t) B_{xc,x}(rt) \right\}$$

$$+ \int d^3r \frac{1}{2c^2} \left\{ \hat{x} \cdot \left[\nabla v_s(r,t) \times j_y(r,t) \right] - \hat{y} \cdot \left[\nabla v_s(r,t) \times j_z(r,t) \right] \right\}$$ **SOC**

$$- \int d^3r \left\{ \nabla \cdot j_z(r,t) \right\}$$ **=0**

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Exact equation of motion for total moment

$$\frac{\partial}{\partial t} M_z(t) = \frac{i}{\hbar} \int d^3r \left\langle \Phi_{KS}^{det}(t) \,|\, \left[\hat{H}_{KS}, \hat{m}_z(r) \right] |\, \Phi_{KS}^{det}(t) \right\rangle$$

$$= \int d^3r \left\{ m_x(r,t) B_{xc,y}(rt) - m_y(r,t) B_{xc,x}(rt) \right\}$$

Global torque exerted by B_{xc} = 0 (zero torque theorem)

$$+ \int d^3r \frac{1}{2c^2} \left\{ \hat{x} \cdot \left[\nabla v_s(r,t) \times j_y(r,t) \right] - \hat{y} \cdot \left[\nabla v_s(r,t) \times j_z(r,t) \right] \right\}$$

SOC

$$- \int d^3r \left\{ \nabla \cdot j_z(r,t) \right\}$$

=0

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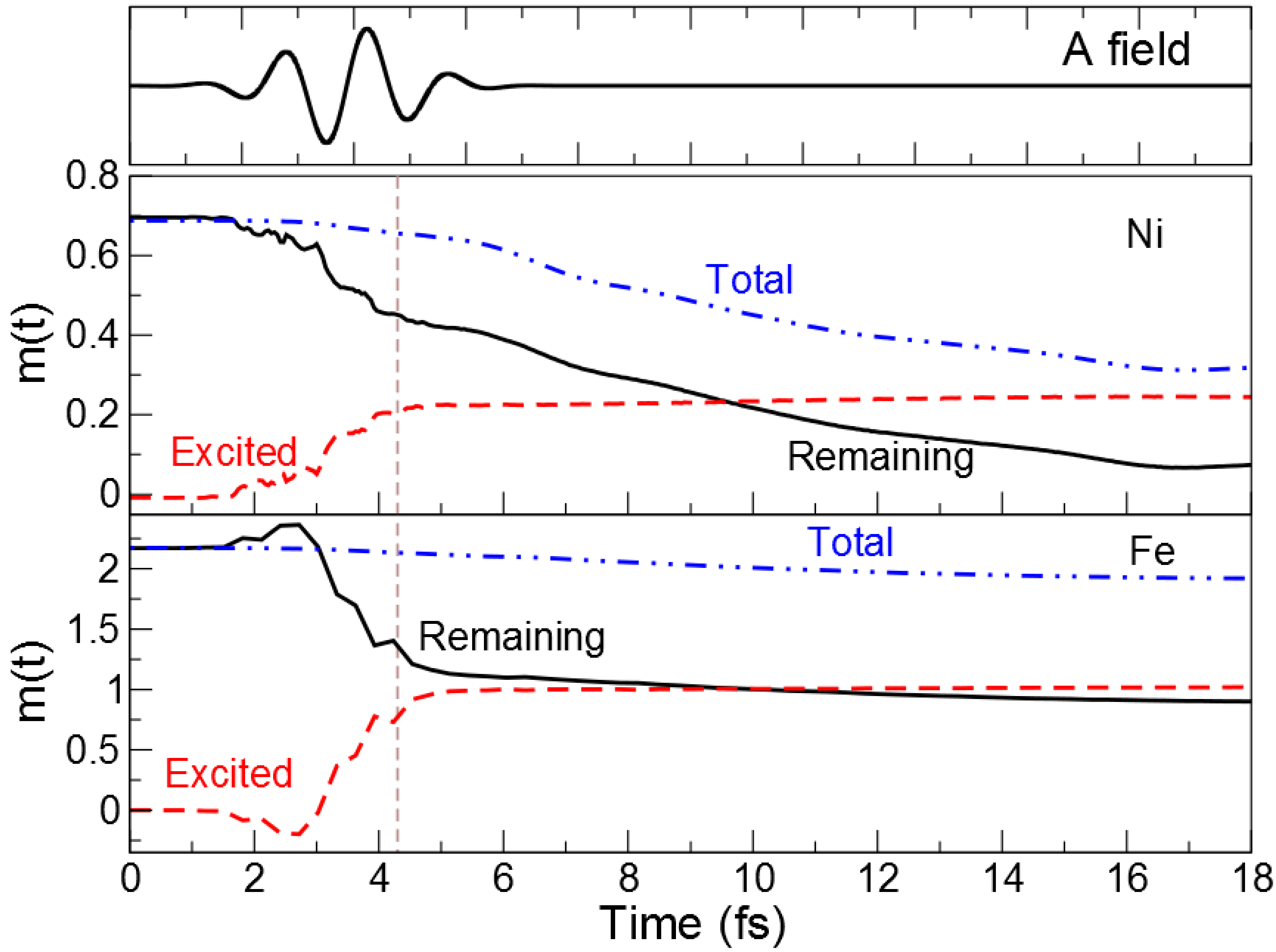
$$\overleftrightarrow{j}(r,t) = \left\langle \hat{\sigma} \otimes \hat{j}(r) \right\rangle$$ spin current tensor

SOC is the only term which can change the total moment!


A field
0.8
0.6
0.4
0.2
0
m(t)
Ni
Total
Excited
Remaining
Fe
Total
Remaining
Excited
2
1.5
1
0.5
0
m(t)
0
2
4
6
8
10
12
14
16
18
Time (fs)

Demagnetization occurs in two steps:

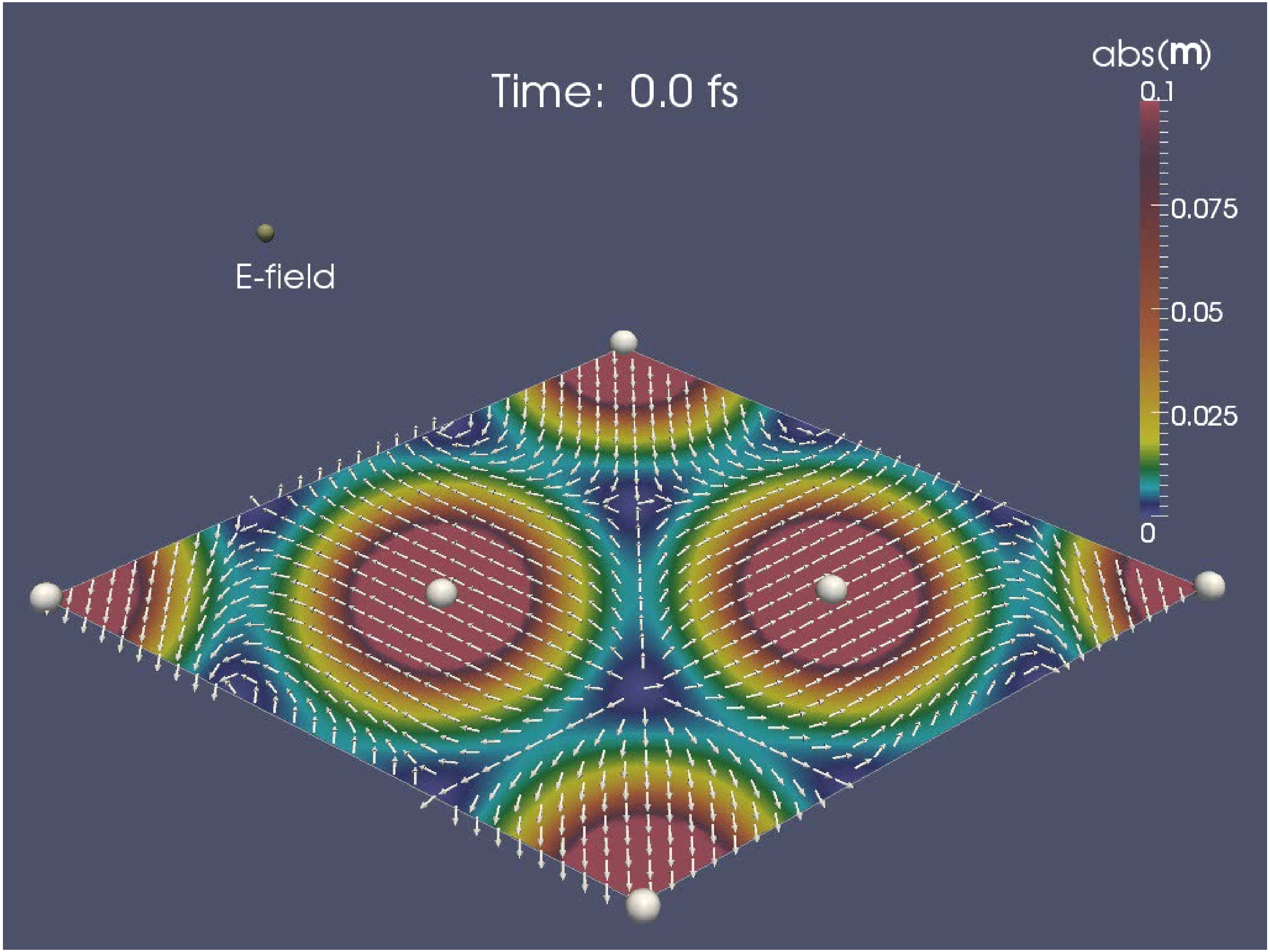
- Initial excitation by laser *moves* magnetization from atomic region into interstitial region. Total Moment is basically conserved during this phase.

- Spin-Orbit term drives demagnetization of the more localized electrons until stabilization at lower moment is achieved

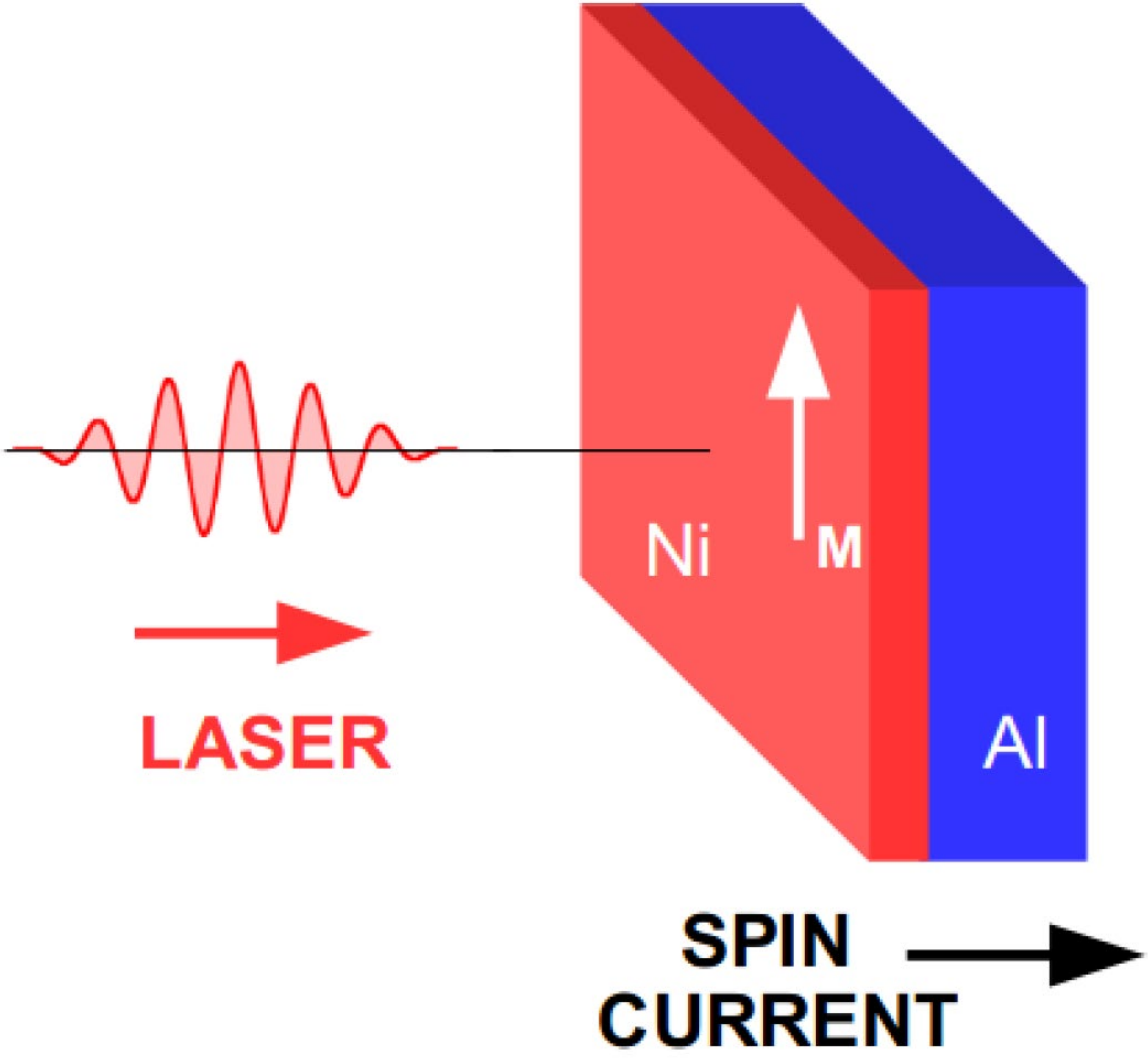
- This is a local mechanism, hence occurs in this form in essentially all systems, e.g. magnetic clusters (Sanvito group, Dublin) or magnetic mono-layer / few-layer systems

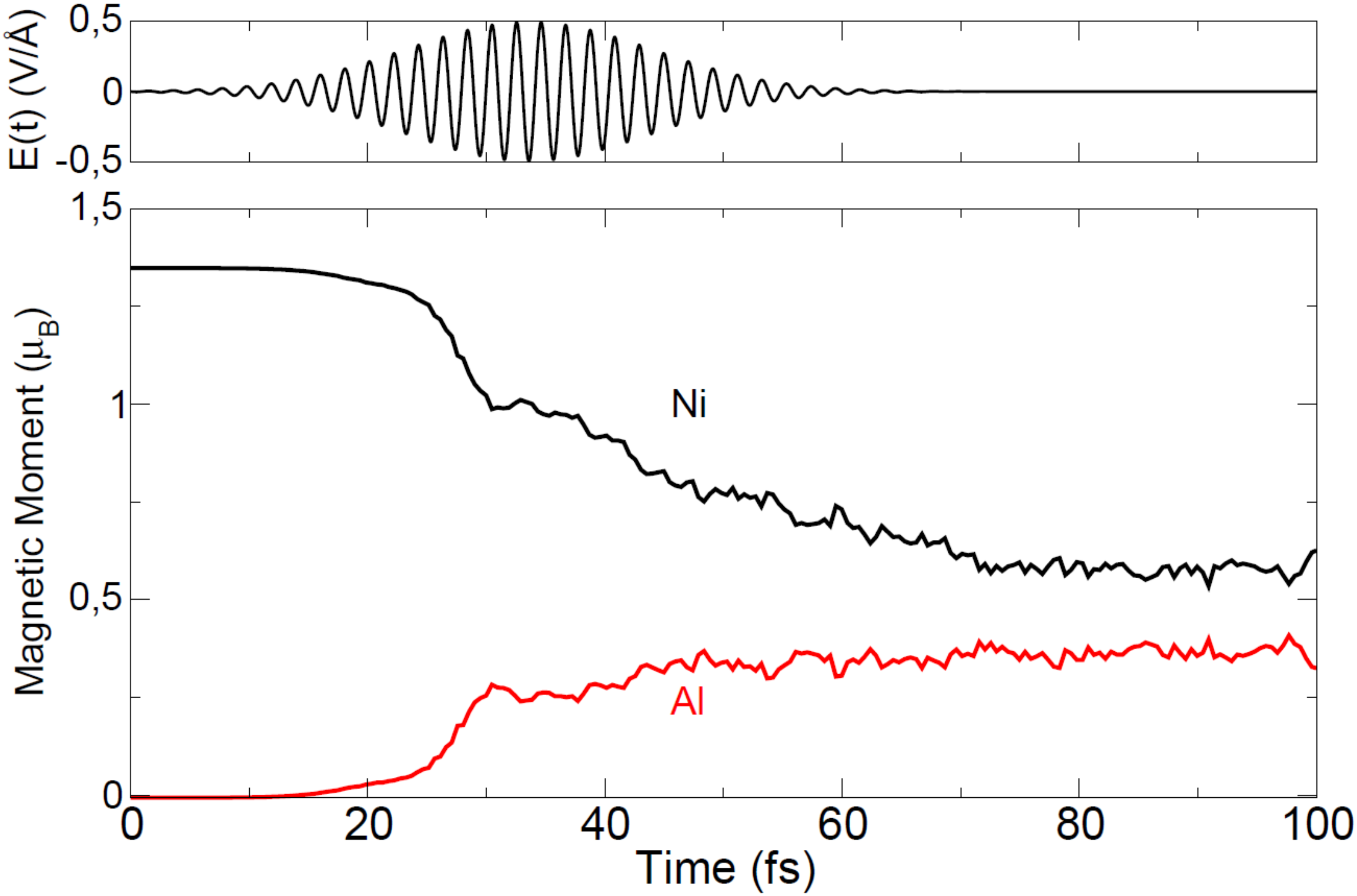
- **K. Krieger, J.K. Dewhurst, P. Elliott, S. Sharma, E.K.U. Gross, JCTC 11, 4870 (2015).**
- **K. Krieger, P. Elliott, T. Müller, N. Singh, J. K. Dewhurst, E.K.U. Gross, S. Sharma, J. Phys. Cond. Matter 29, 224001 (2017).**
- **V. Shokeen, M. Sanchez Piaia, J.Y. Bigot, T. Mueller, P. Elliott, J.K. Dewhurst, S. Sharma, E.K.U. Gross, Phys. Rev. Lett. 119, 107203 (2017).**

Beyond 3D bulk

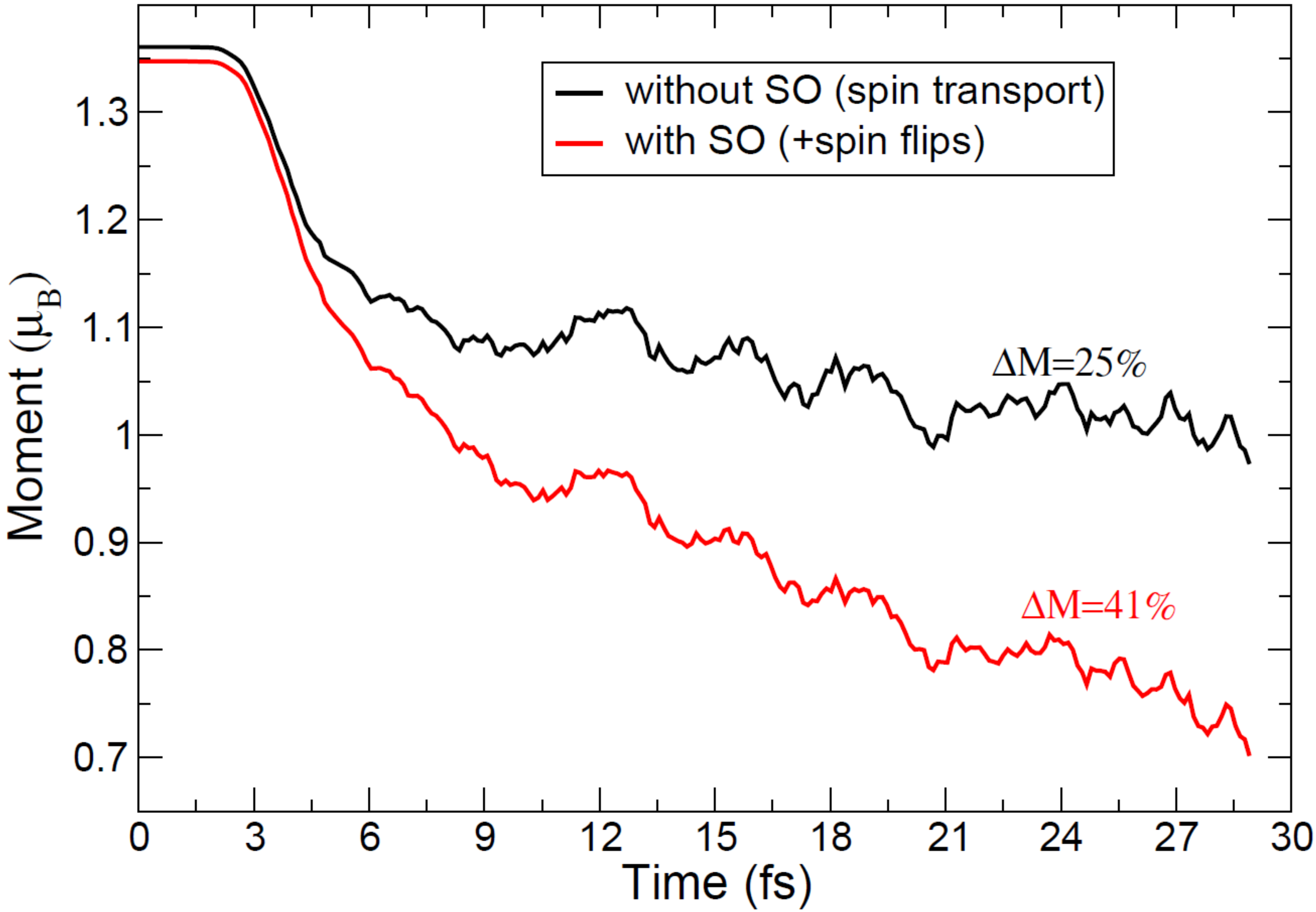


Cr monolayer


Ni
M
Al
LASER
SPIN
CURRENT



E(t) (V/Å)
0,5
0
-0,5
1,5
1
0,5
0
Magnetic Moment (μ_B)
Ni
Al
0
20
40
60
80
100
Time (fs)



without SO (spin transport)
with SO (+spin flips)
ΔM=25%
ΔM=41%
Moment (μB)
Time (fs)
0
3
6
9
12
15
18
21
24
27
30
0.7
0.8
0.9
1
1.1
1.2
1.3

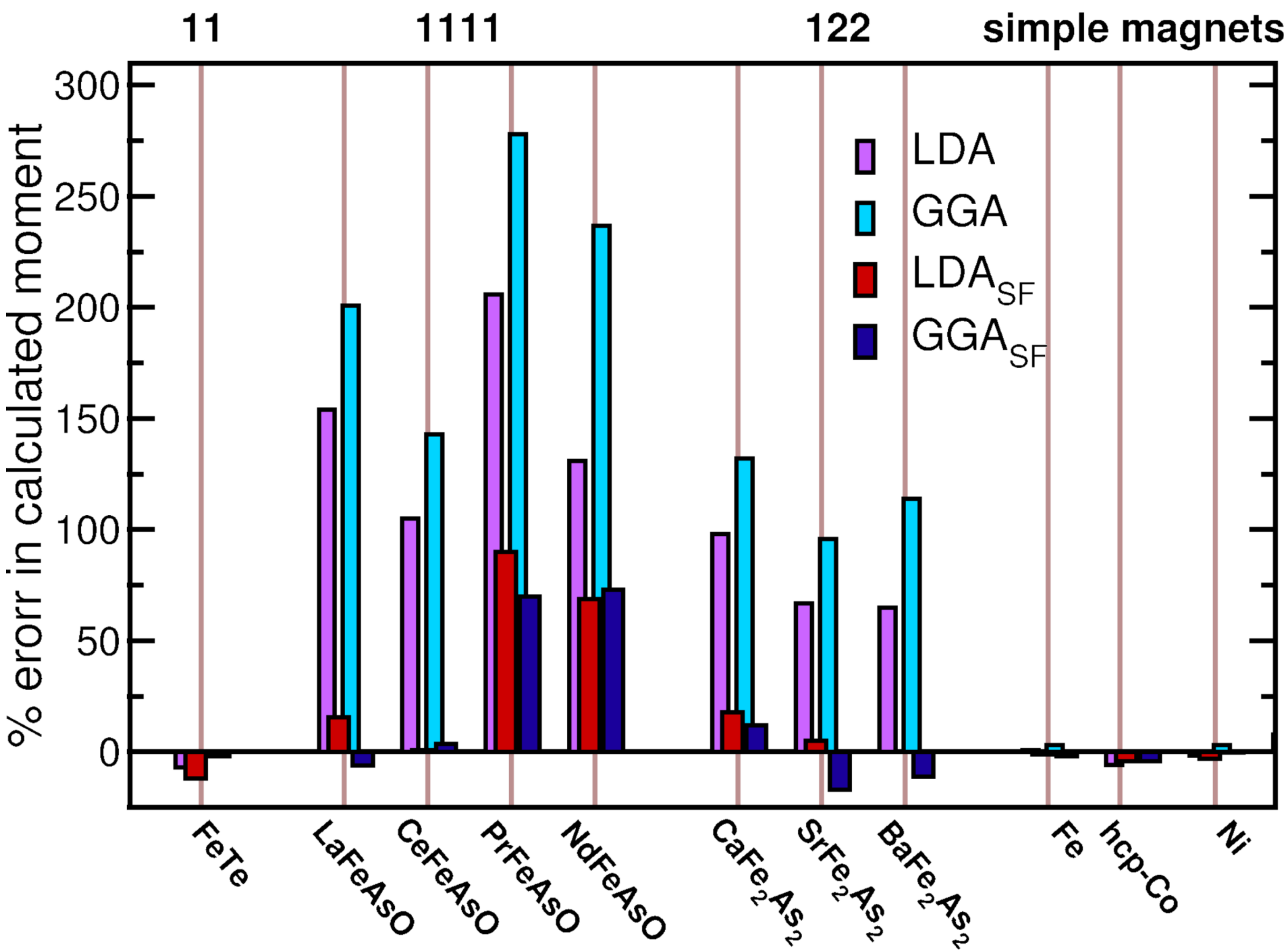
Experimental confirmation:

Spin Flips versus Spin Transport in Nonthermal Electrons Excited by Ultrashort Optical Pulses in Transition Metals,
V. Shokeen, M. Sanchez Piaia, J.-Y. Bigot, T. Mueller, P. Elliott, J.K. Dewhurst, S. Sharma, E. K. U. Gross, Phys. Rev. Lett. 119, 107203 (2017).

Review article:

Time-Dependent Density Functional Theory for Spin Dynamics,
P. Elliott, M. Stamenova, J. Simoni, S. Sharma, S. Sanvito, and E.K.U. Gross, in: Handbook of Materials Modeling, W. Andreoni, S. Yip eds, Springer (2020), p. 841

xc-functional in SDFT


11
1111
122
simple magnets
% erorr in calculated moment
300
250
200
150
100
50
0
LDA
GGA
LDA$_{SF}$
GGA$_{SF}$
FeTe
LaFeAsO
CeFeAsO
PrFeAsO
NdFeAsO
$CaFe_2As_2$
$SrFe_2As_2$
$BaFe_2As_2$
Fe
hcp-Co
Ni

Construction of a novel xc functional for non-collinear magnetism

Enforce property of the exact xc functional:

$$\boldsymbol{B}_{xc}^{exact}\left(\boldsymbol{r}\right)=\nabla\times A_{xc}^{exact}\left(\boldsymbol{r}\right)$$

K. Capelle, E.K.U. Gross, PRL 78, 1872 (1997)

By virtue of Helmholtz' theorem, any vector field can be decomposed as:

$$\boldsymbol{B}_{xc}^{GGA}\left(\boldsymbol{r}\right)=\nabla\times A_{xc}\left(\boldsymbol{r}\right)+\nabla\phi(r)$$

Enforce exact property by subtracting source term!

Explicit construction:

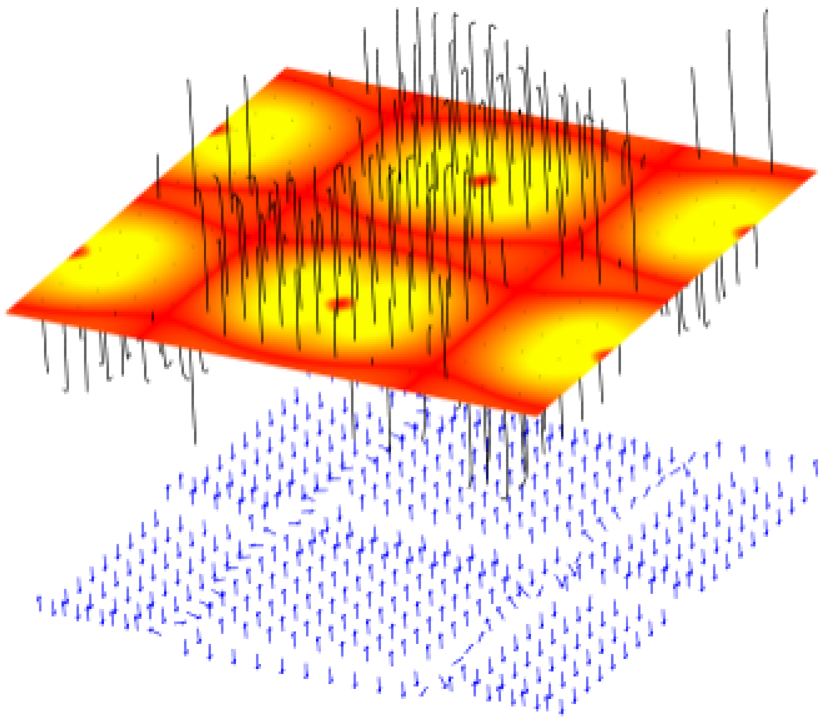
S. Sharma, E.K.U. Gross, A. Sanna, K. Dewhurst, JCTC14, 1247 (2018)

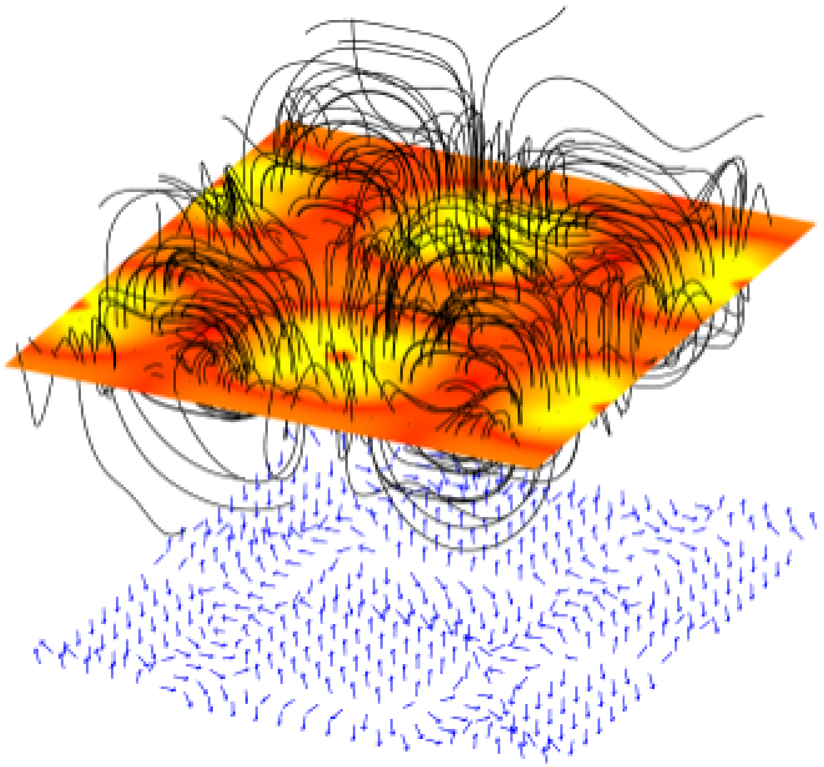
$$\nabla^2 \phi(\boldsymbol{r}) = 4\pi \nabla \cdot B_{xc}^{GGA}(\boldsymbol{r})$$

$$\tilde{B}_{xc}(\boldsymbol{r}) \cong B_{xc}^{GGA}(\boldsymbol{r}) - \frac{1}{4\pi} \nabla \phi(\boldsymbol{r})$$

$$B_{xc}^{SF}(\boldsymbol{r}) = s\, \tilde{B}_{xc}(\boldsymbol{r})$$

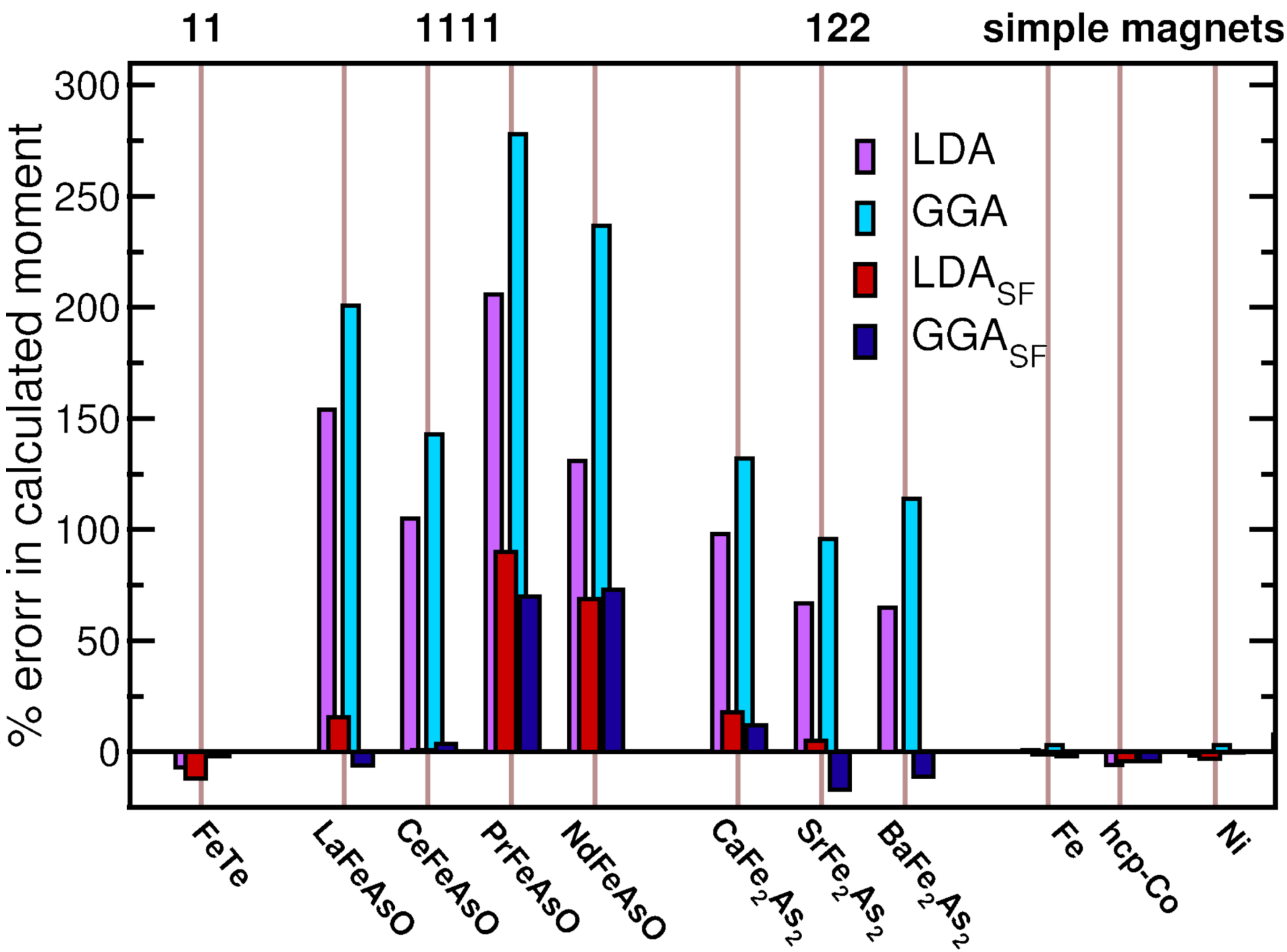
Scaling factor, s, only depends on underlying functional (GGA/LSDA), nothing else. (s = 1.14 for GGAs)



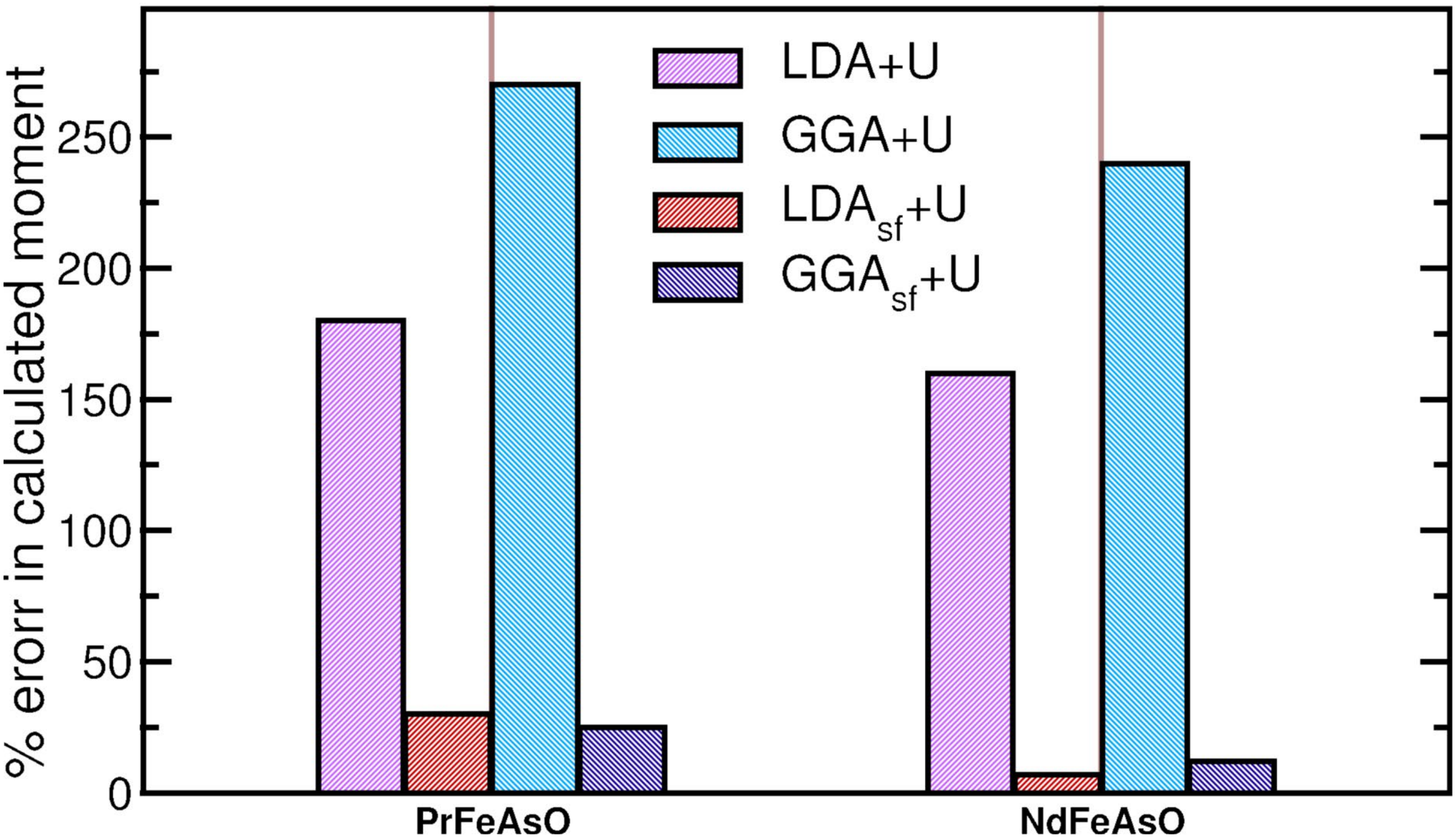


LSDA **Source-free LSDA**

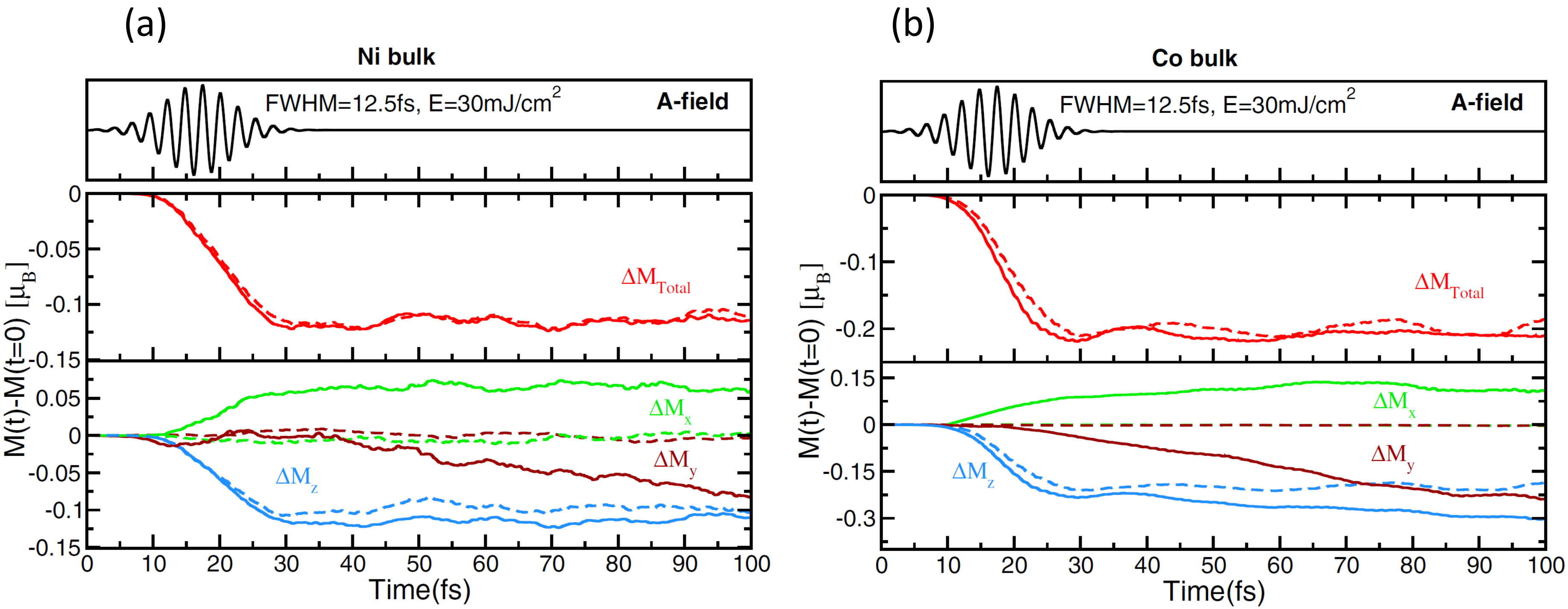
Vector field B_{xc} for $BaFe_2As_2$ on a plane containing the Fe atoms. Colors indicate the magnitude of B_{xc} while arrows show the direction. The black field lines originate from a regular grid in the plane and follow the vector field B_{xc}. The removal of the source term leads to an enhancement ofnon-collinearity.



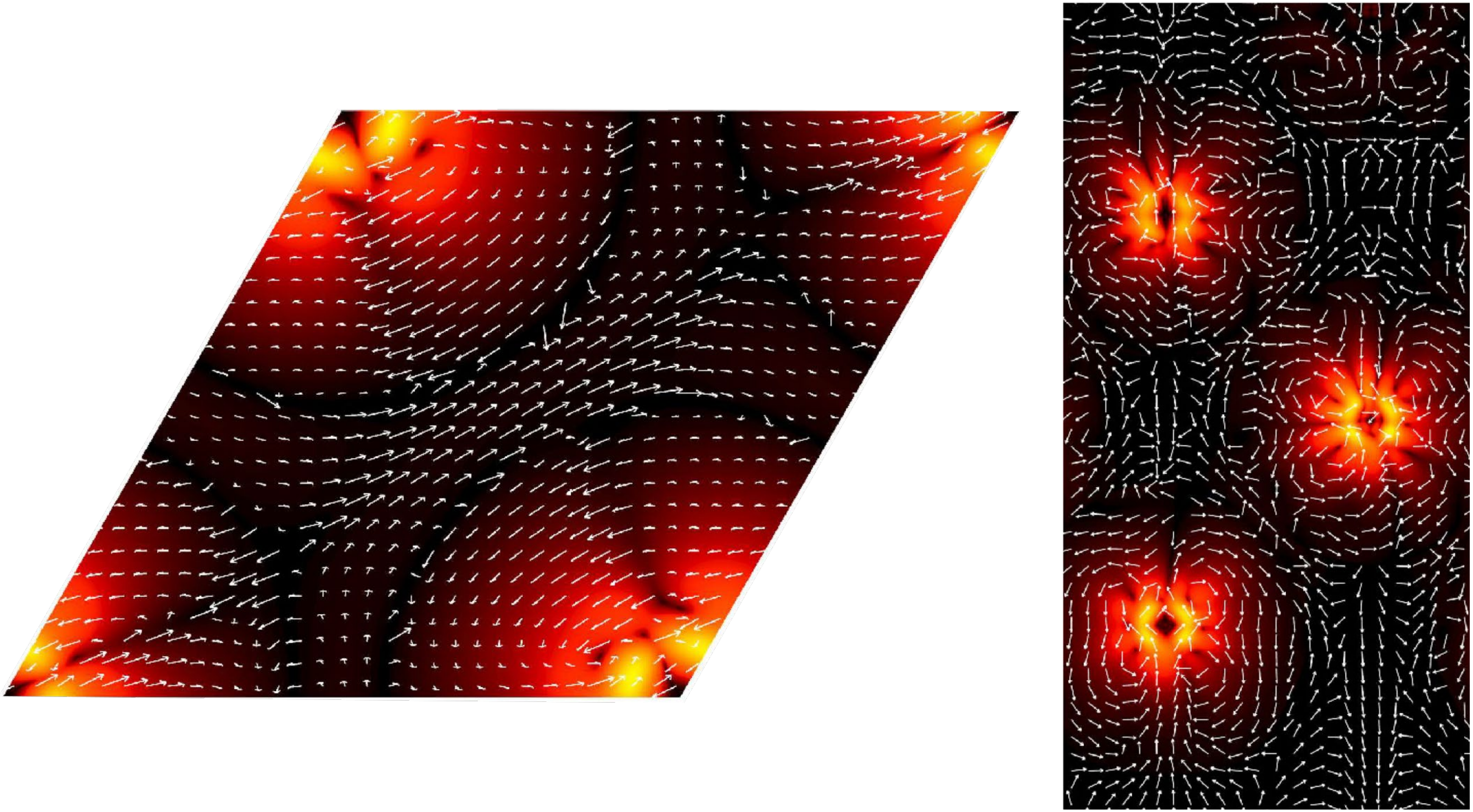
11
1111
122
simple magnets
% erorr in calculated moment
300
250
200
150
100
50
0
LDA
GGA
LDA$_{SF}$
GGA$_{SF}$
FeTe
LaFeAsO
CeFeAsO
PrFeAsO
NdFeAsO
CaFe$_2$As$_2$
SrFe$_2$As$_2$
BaFe$_2$As$_2$
Fe
hcp-Co
Ni



LDA+U
GGA+U
LDA$_{sf}$+U
GGA$_{sf}$+U
% erorr in calculated moment
0
50
100
150
200
250
PrFeAsO
NdFeAsO



(a) Middle panel shows the total moment (red) and the bottom panel x (green), y (brown) and z (blue) projected moments for bulk Ni as a function of time. Dashed lines are the results obtained using the ALSDA and full lines the results obtained using the source-free functional. (b) The same as (a) but for bulk Co.



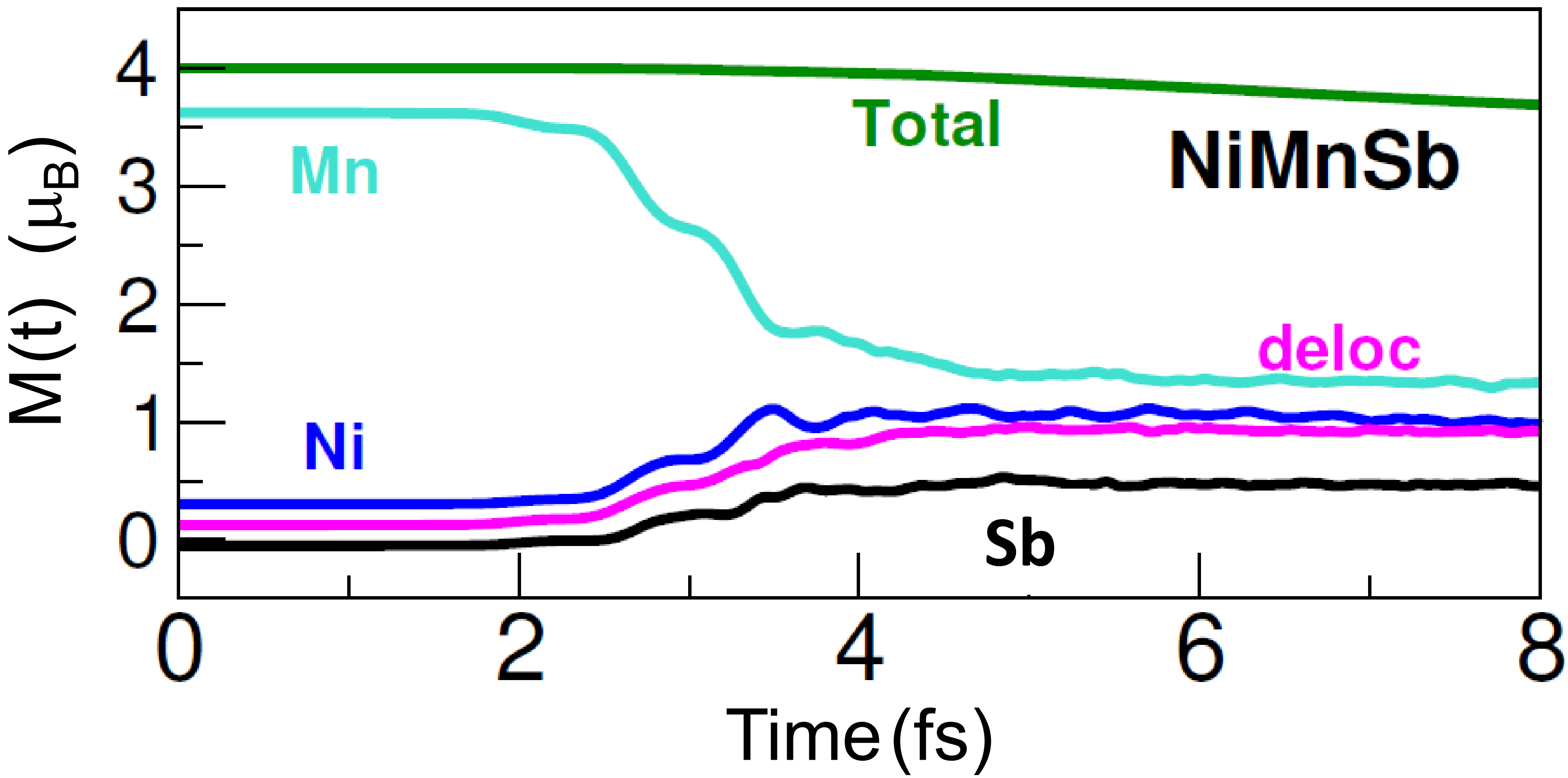
Left panel: Local xc torque for bulk Ni in (111) plane. Right panel: Local xc torque for 3ML Ni@5ML Pt in the (110) plane. The arrows indicate the direction and colors the magnitude.

Optical intersublattice spin transfer (OISTR)

P. Elliott, T. Mueller, K. Dewhurst, S. Sharma, E.K.U.Gross,
Scientific Reports 6, 38911 (2016)

K. Dewhurst, P. Elliott, S. Shallcross, E.K.U. Gross, S. Sharma,
Nano Lett. 18, 1842 (2018)

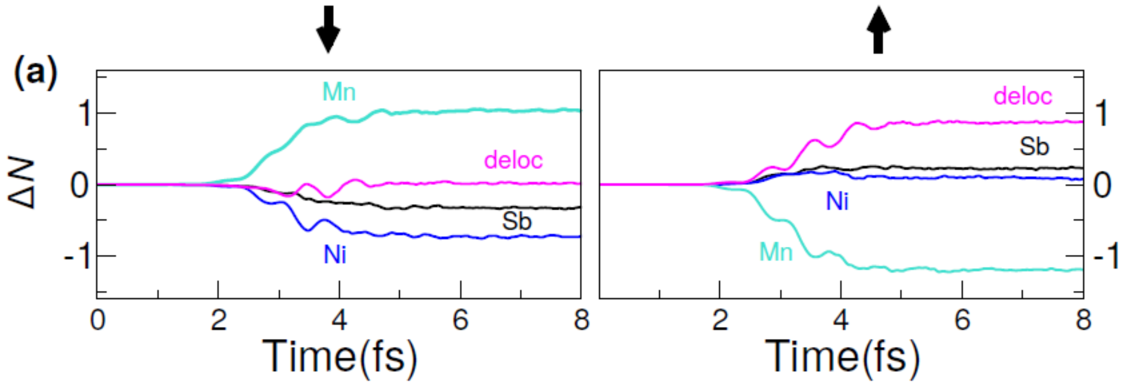
OISTR was first predicted with TDDFT and later found experimentally (Aeschlimann group, Kaiserslautern, 2018)



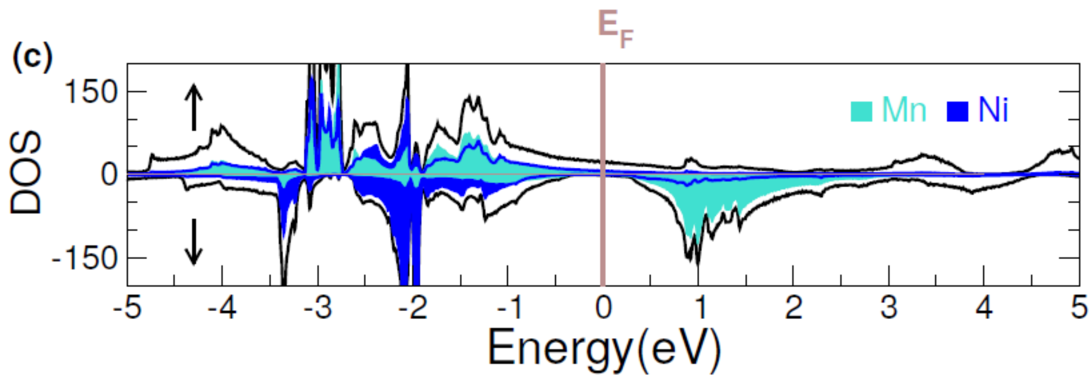
Global moment |M(t)| nearly preserved. Local moments change.

Laser parameters: ω= 2.72 eV, a FWHM of 2.42 fs, and fluence of 93.5 mJ/cm2, giving a peak intensity of 1 × 1014 W/cm2.

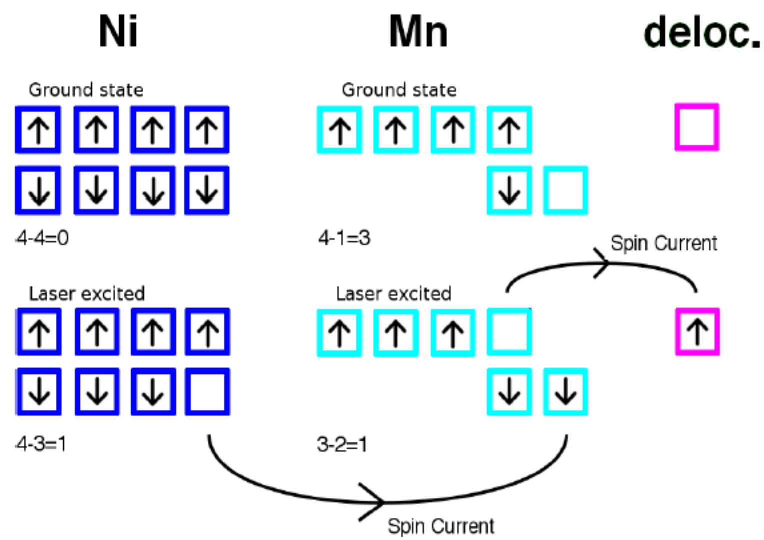
NiMnSb



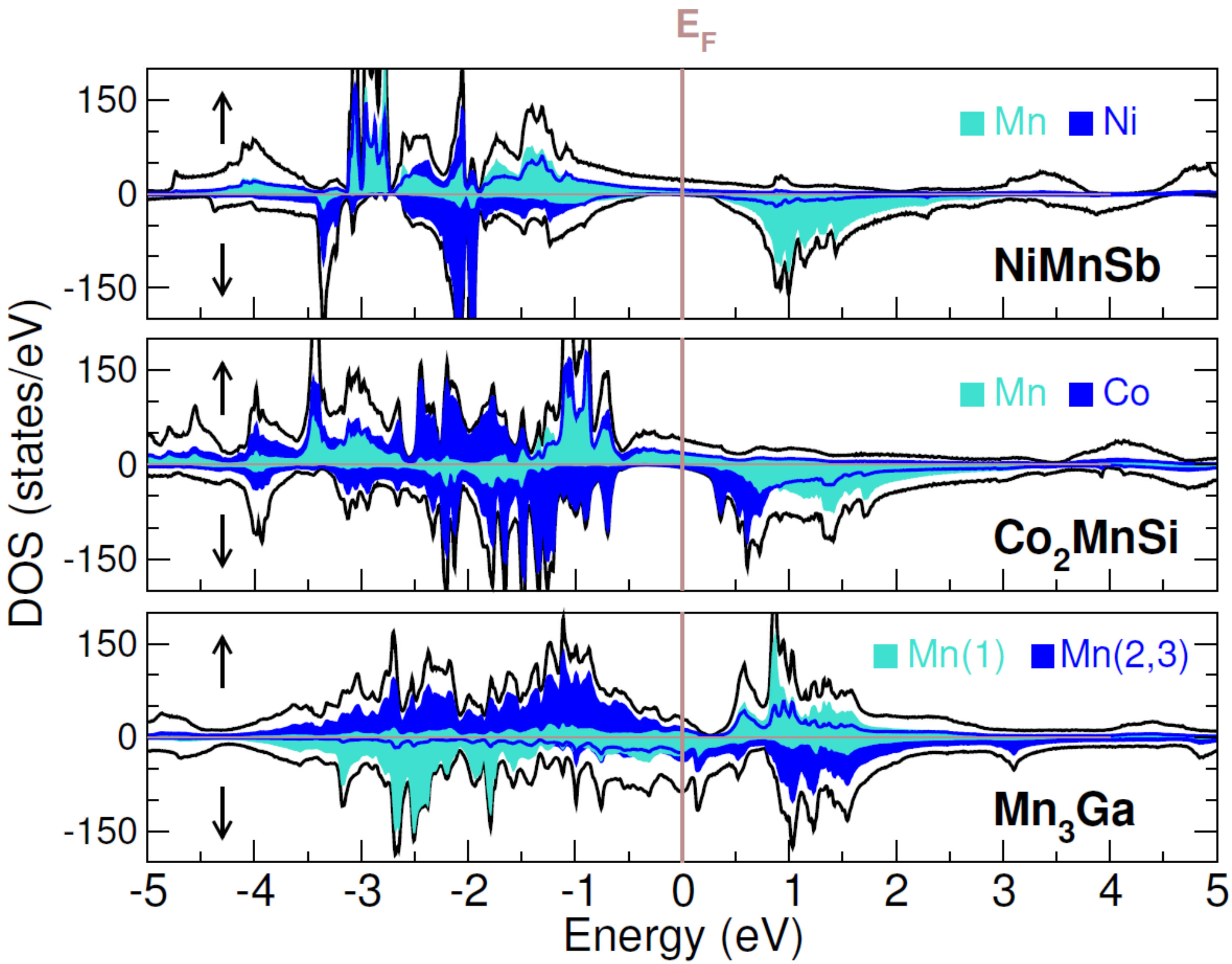
(a)
ΔN
Mn
deloc
Sb
Ni
Time(fs)



(c)
E_F
DOS
Mn
Ni
Energy(eV)

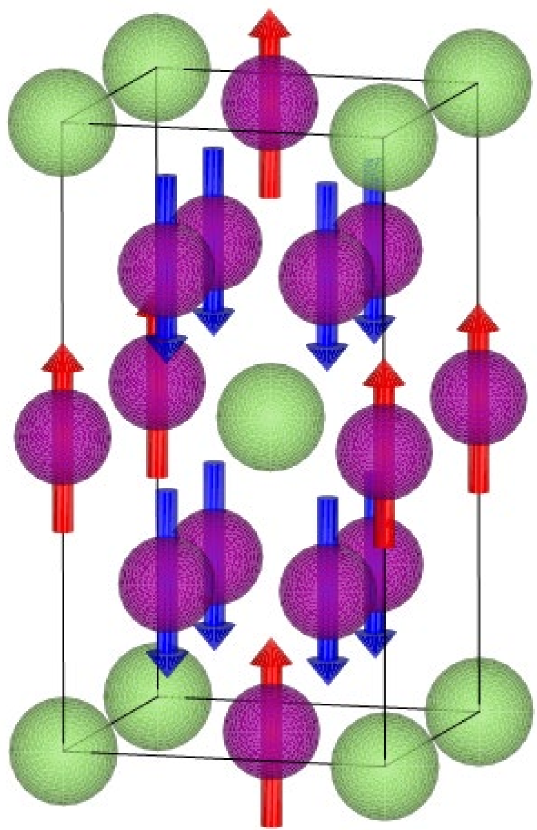


Ni
Mn
deloc.
Ground state
Ground state
4-4=0
4-1=3
Spin Current
Laser excited
Laser excited
4-3=1
3-2=1
Spin Current



E_F
DOS (states/eV)
150
0
-150
↑
↓
Mn
Ni
NiMnSb
Co
Co2MnSi
Mn(1)
Mn(2,3)
Mn3Ga
-5
-4
-3
-2
-1
0
1
2
3
4
5
Energy (eV)

Mn_3Ga (ferri-magnet)



Ga
Mn

TDDFT prediction for Mn_3Ga: ferri → ferro transition within 4 fs

PHYSICS

Ultrafast optically induced spin transfer in ferromagnetic alloys

M. Hofherr[1,2], S. Häuser[1], J. K. Dewhurst[3], P. Tengdin[4], S. Sakshath[1], H. T. Nembach[4,5], S. T. Weber[1], J. M. Shaw[5], T. J. Silva[5], H. C. Kapteyn[4], M. Cinchetti[6], B. Rethfeld[1], M. M. Murnane[4], D. Steil[7], B. Stadtmüller[1,2], S. Sharma[8], M. Aeschlimann[1], S. Mathias[7]*

The vision of using light to manipulate electronic and spin excitations in materials on their fundamental time and length scales requires new approaches in experiment and theory to observe and understand these excitations. The ultimate speed limit for all-optical manipulation requires control schemes for which the electronic or magnetic subsystems of the materials are coherently manipulated on the time scale of the laser excitation pulse. In our work, we provide experimental evidence of such a direct, ultrafast, and coherent spin transfer between two magnetic subsystems of an alloy of Fe and Ni. Our experimental findings are fully supported by time-dependent density functional theory simulations and, hence, suggest the possibility of coherently controlling spin dynamics on subfemtosecond time scales, i.e., the birth of the research area of attomagnetism.

INTRODUCTION

Next-generation quantum materials will make it possible to surpass the speed and efficiency limits of current devices to generate faster, smaller, and more energy-efficient technological implementations (*1*–*8*). A promising approach to enhance data processing speed is to use ever shorter external stimuli for the manipulation and control of the state of matter. In this context, light represents the fastest means to alter the state of a material since laser pulses can now be generated with extremely short temporal duration down to a few tens of attoseconds. Visible lasers can deliver pulses with few-femtosecond durations that can be used to excite matter, while attosecond pulses can be generated in the extreme ultraviolet (EUV) and soft x-ray regions to probe the resulting dynamics (*9*–*12*). When combined with advanced spectroscopies, these new light sources are enabling comprehensive views into material results in a nonequilibrium hot charge distribution, which subsequently triggers a series of cascaded incoherent secondary processes including transport, (spin-flip) scattering, and quasiparticle generation, ultimately leading to macroscopic demagnetization of the magnetic material within <500 fs (*18*–*22*).

The fastest manipulation of the magnetic state should occur, however, through the direct (possibly coherent) interaction between the spin system of the material and the light field itself (*23*–*25*). While the first experiments have provided indications that such a direct manipulation scheme might be possible (*26*–*29*), to our knowledge, only one experimental study on magnetic metallic systems to date has focused on this challenging aspect of coherent ultrafast magnetism induced by femtosecond laser pulses (*24*). One particularly interesting and previously unknown scheme for the ultrafast

PHYSICS

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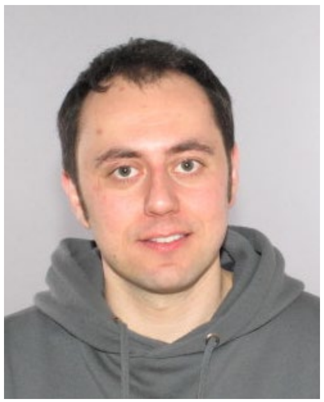
What's missing:

- **Include relaxation processes due to el-el scattering**
  - in principle contained in TDDFT,
  - but not with adiabatic xc functionals
  - need xc functional approximations with memory or CDFT functional
- **Include relaxation processes due to electron-nuclear interaction**
  - decoherence
- **Include relaxation due to radiative effects**
  - simultaneous propagation of TDKS and Maxwell equations
- **Include dipole-dipole interaction to describe motion of domains**
  - construct approximate xc functionals associated with dipole dipole interaction

Thanks!

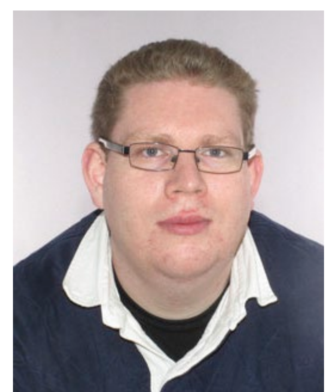


Kevin Krieger

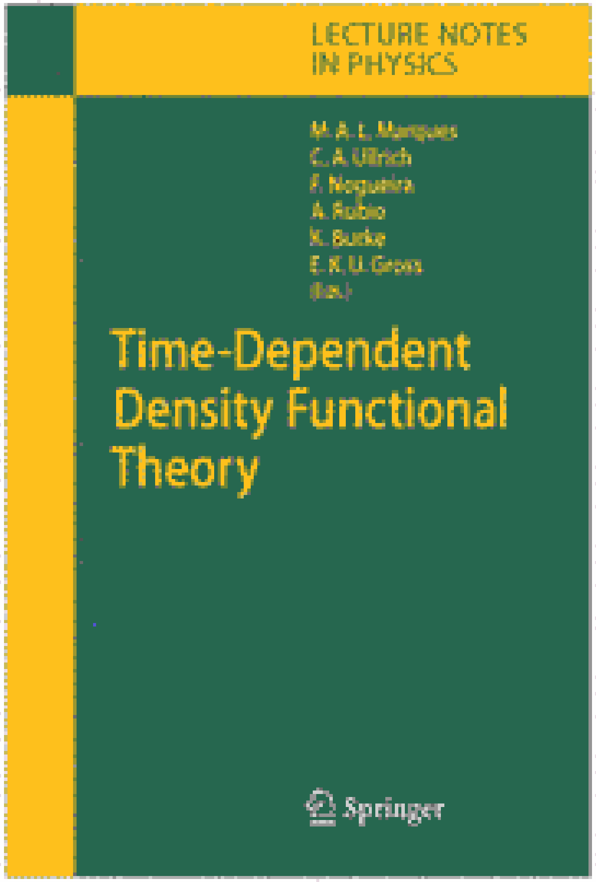
Sangeeta Sharma

Florian Eich

Kay Dewhurst



Peter Elliott



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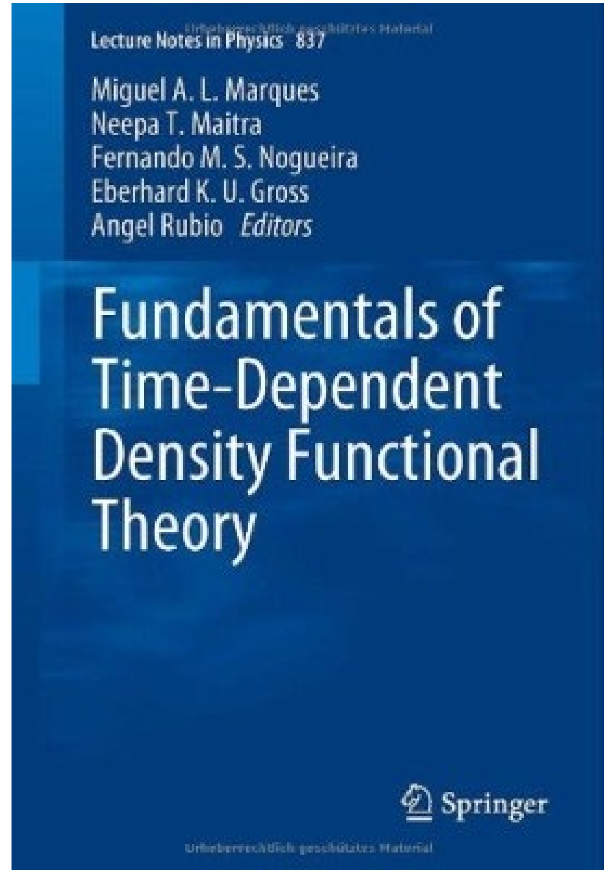

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