Ultrafast spin, charge and nuclear dynamics

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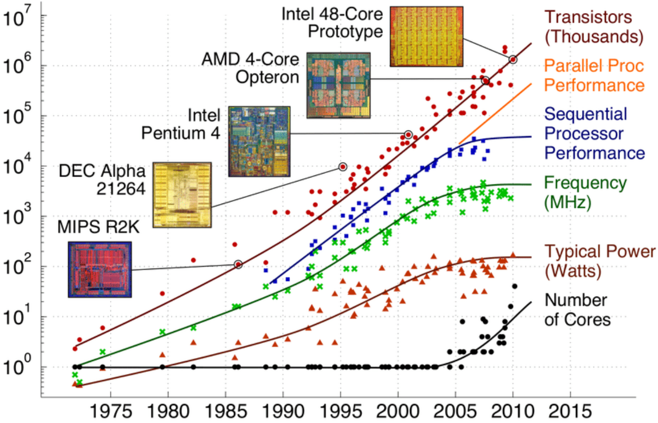
Theory collaborators: J.K. Dewhurst, E. K. U. Gross, K. Krieger, T. Müller, C. Wang, Q. Lee, P. Scheid, N. Singh, J. Krishna, P. Elliott, S. Shallcross.

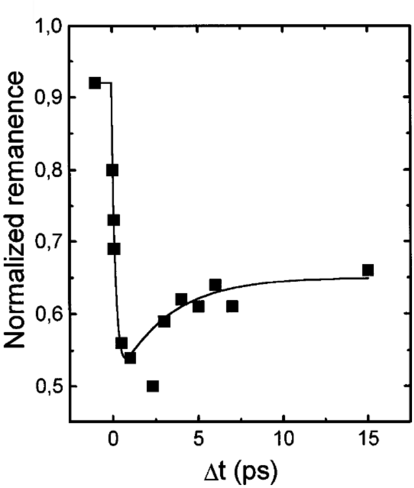
Experimental collaborators: M. Schultze, M. Münzenberg, S. Mathias, M. Aeschlimann, J. Chen, D. Steil, U. Bovensiepen, A. Eschenlohr, C. Von-Korff Schmising, S. Eisebitt, W. Kuch, J. Biegert, I. Radu, D. Schick

Funding: DFG TRR227 and SPP-QUTIF

Evolution of multi-core processors



Femto-magnetism



Laser-induced **demagnetization**

Expt: Beaurepair et al. PRL 76 4250 (1996)

Ultrafast manipulation of spins with light

- Efficient devices based in spin currents
- Fast (femtoseconds) operational times

Leading order terms in expansion of QED H

$$
\begin{aligned}
H = {} & \sum_i \frac{1}{2m}\mathbf{p}_i^2 - eV_{\text{ext}}(\mathbf{r}_i) + \sum_{i<j}\frac{e^2}{r_{ij}} + \frac{1}{c}\sum_i \frac{e}{m}\mathbf{p}_i\cdot\mathbf{A}_{\text{ext}}(\mathbf{r}_i) \\
& + \frac{1}{c}\sum_i \frac{e}{m}\mathbf{s}_i\cdot\mathbf{B}_{\text{ext}}(\mathbf{r}_i) + \frac{1}{c^2}\sum_i \frac{e}{2m^2}\mathbf{s}_i\cdot[\mathbf{E}_{\text{ext}}(\mathbf{r}_i)\times\mathbf{p}_i] \\
& + \frac{1}{c^2}\sum_i \frac{e^2}{2m}\mathbf{A}_{\text{ext}}^2(\mathbf{r}_i) - \frac{1}{c^2}\sum_i \frac{1}{8m^3}\mathbf{p}_i^4 + \frac{ie}{4m^2c^2}\mathbf{p}_i\cdot\mathbf{E}_{\text{ext}}(\mathbf{r}_i) \\
& - \frac{1}{c^2}\frac{e^2}{2m^2}\sum_{i<j}\mathbf{p}_i\cdot\left[\frac{(\mathbf{r}_i-\mathbf{r}_j)(\mathbf{r}_i-\mathbf{r}_j)}{r_{ij}^3} + \frac{1}{r_{ij}}\right]\cdot\mathbf{p}_j \\
& - \frac{1}{c^2}\frac{e^2}{m^2}\sum_{i<j}\mathbf{s}_i\cdot\left[\frac{3(\mathbf{r}_i-\mathbf{r}_j)(\mathbf{r}_i-\mathbf{r}_j)}{r_{ij}^5} - \frac{1}{r_{ij}^3}\right]\cdot\mathbf{s}_j \\
& - \frac{1}{c^2}\frac{e^2}{m^2}\sum_{i\neq j}\frac{1}{r_{ij}^3}\left(\mathbf{s}_i\cdot[(\mathbf{r}_j-\mathbf{r}_i)\times\mathbf{p}_j] + \frac{1}{2}\mathbf{s}_i\cdot[(\mathbf{r}_i-\mathbf{r}_j)\times\mathbf{p}_i]\right) \\
& + \dots
\end{aligned}
$$

Still only an approximation to QED...

Models to explain this demagnetisation

1. Elliott-Yafet mechanism: **electron-phonon or electron-impurity** mediated spin-flip causing a global demagnetization

   B. Koopmans, Nature Mater. 6, 715 (2007)

2. **Spin-lattice** relaxation causing global demagnetization

   W. Hübner and K. H. Bennemann, PRB 53, 3422 (1996)

3. Super-diffusive model: **Electron and spin current** flows causing a local demagnetization

   M. Battiato, K. Carva, and P. M. Oppeneer, PRL. 105, 027203 (2010)

4. **Electron -electron and -phonon** scattering causing global demagnetization

   B. Y. Mueller et al., PRL 111, 167204 (2013)

Method: *Ab-initio* theory

Our aim is to make quantitative predictions with a computer code knowing only the atomic species and crystal structure

No adjustable parameters

Theory: fully ab-initio approach

$$
\begin{aligned}
i\frac{\partial \psi_j(\mathbf{r},t)}{\partial t} &= \Bigg[\frac{1}{2}\left(i\nabla + \frac{1}{c}\mathbf{A}_{\mathrm{ext}}(t)\right)^2 + v_s(\mathbf{r},t) \\
&+ \frac{1}{2c}\vec{\sigma}\cdot\mathbf{B}_s(\mathbf{r},t) + \frac{1}{4c^2}\vec{\sigma}\cdot\left(\nabla v_s(\mathbf{r},t)\times i\nabla\right)\Bigg]\psi_j(\mathbf{r},t)
\end{aligned} \tag{1}
$$

Theory: fully ab-initio approach

$$
\begin{aligned}
i\frac{\partial \psi_j(\mathbf{r},t)}{\partial t} &= \left[\frac{1}{2}\left(i\nabla + \frac{1}{c}\mathbf{A}_{\text{ext}}(t)\right)^2 + v_s(\mathbf{r},t)\right. \qquad (1) \\
&+ \left.\frac{1}{2c}\vec{\sigma}\cdot\mathbf{B}_s(\mathbf{r},t) + \frac{1}{4c^2}\vec{\sigma}\cdot\left(\nabla v_s(\mathbf{r},t)\times i\nabla\right)\right]\psi_j(\mathbf{r},t)
\end{aligned}
$$

Effective potentials:

$$
\mathbf{B}_s[\rho,\mathbf{m}] = \mathbf{B}_{\text{ext}} + \mathbf{B}_{\text{xc}}[\rho,\mathbf{m}], \qquad v_s[\rho,\mathbf{m}] = v_{\text{cl}} + v_{\text{xc}}[\rho,\mathbf{m}] \quad (2)
$$

Theory: fully ab-initio approach

$$i\frac{\partial\psi_j(\mathbf{r},t)}{\partial t} = \left[\frac{1}{2}\left(i\nabla+\frac{1}{c}\mathbf{A}_{\rm ext}(t)\right)^2+v_s(\mathbf{r},t)\right. \quad (1)$$
$$\left. + \frac{1}{2c}\overrightarrow{\sigma}\cdot\mathbf{B}_s(\mathbf{r},t)+\frac{1}{4c^2}\overrightarrow{\sigma}\cdot(\nabla v_s(\mathbf{r},t)\times i\nabla)\right]\psi_j(\mathbf{r},t)$$

Effective potentials:

$$\mathbf{B}_s[\rho,\mathbf{m}]=\mathbf{B}_{\rm ext}+\mathbf{B}_{\rm xc}[\rho,\mathbf{m}], \qquad v_s[\rho,\mathbf{m}]=v_{\rm cl}+v_{\rm xc}[\rho,\mathbf{m}] \quad (2)$$

Density:

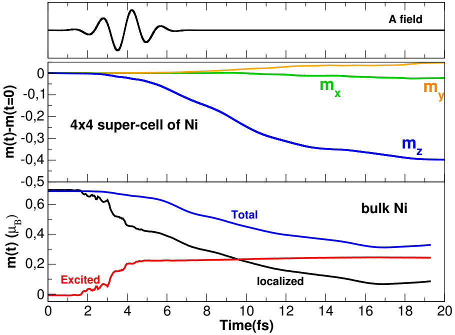
$$\rho(\mathbf{r},t)=\sum_j\psi_j^*(\mathbf{r},t)\psi_j(\mathbf{r},t) \quad (3)$$

Magnetization density(unconstrained vector field):

$$\mathbf{m}(\mathbf{r},t)=\sum_j\psi_j^*(\mathbf{r},t)\overrightarrow{\sigma}\psi_j^*(\mathbf{r},t) \quad (4)$$

E. Runge and E. K. U. Gross, Phys. Rev. Lett. **52**, 997 (1984)

Demagnetisation in supercell of fcc Ni



- Inter-site non-collinearity and magnons do not contribute in early times
- $\frac{1}{4c^2}\overrightarrow{\sigma} \cdot (\nabla v_s(\mathbf{r},t) \times i\nabla)$
- The physics is dominated by spin-orbit induced spin-flips

Krieger et al. JCTC **11**, 4870 (2015),
Elliott et al. New J. Phys. **18**, 013014 (2016),

Dewhurst et al. Computer Phys. Comm. **209**, 92 (2016)

How fast?–exchange and spin-orbit times in femto-seconds

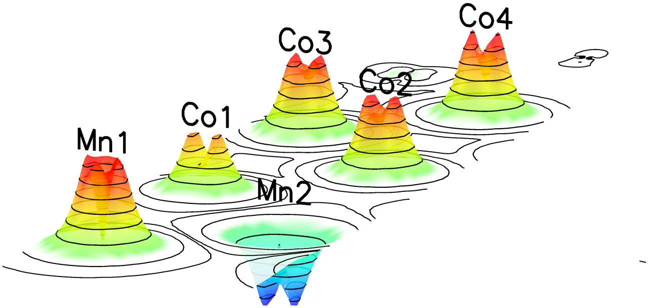
Metal	Exchange	Spin-orbit
Fe	52	50
Co	80	52
Ni	380	48

Table: Exchange time is Heisenberg exchange parameter converted to time. SO time is the time at which SO coupling causes spin flips in Fe/Mn, Co/Mn and Ni/Mn interfaces.

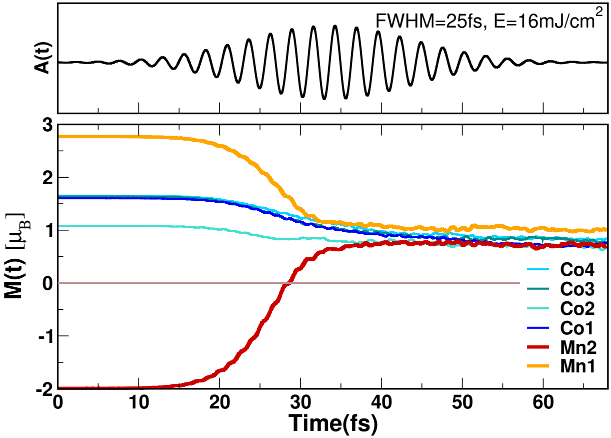
Faster than spin-orbit

1. A new ultrafast phenomena called OISTR.
   1.1 Spin manipulation faster than spin-orbit.
   1.2 Spin manipulation at sub-exchange time scales.
   1.3 Sub-exchange, sub-spin-orbit switching the magnetic order.
   1.4 Spin manipulation times coherently controlled by laser pulse.
2. Experimental demonstration of OISTR
3. What is missing and how we can try to change that

Ferri-magnetic layers: Mn2/Co4/Cu(001)



Magnetization dynamics in Mn2/Co4/Cu(001)



- Ground-state is Ferri-magnetic
- $\sim$ 29fs one of the Mn layers switches the direction of spin
- Stays in transient FM state at least till 150fs

Dewhurst, Elliott, Shallcross, Gross and Sharma, Nano Lett. **18**, 1842, (2018)

Spin-flips, spin current, charge current

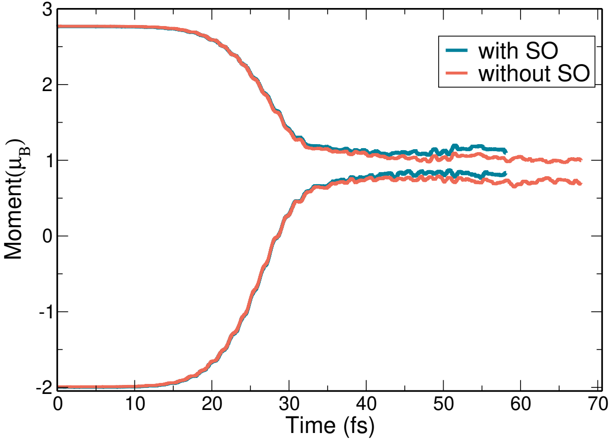
$$\hat{H}_s = \frac{1}{2}\left(i\nabla + \frac{1}{c}\mathbf{A}_{\rm ext}(t)\right)^2 + v_s(\mathbf{r},t) + \frac{1}{2c}\overrightarrow{\sigma}\cdot\mathbf{B}_{\rm xc}(\mathbf{r},t) \quad (5)$$
$$+ \frac{1}{4c^2}\overrightarrow{\sigma}(\nabla v_s(\mathbf{r},t)\times i\nabla)$$

$$\frac{\partial}{\partial t}\mathbf{m}(\mathbf{r},t) = i\langle[\hat{H}_s, \hat{\sigma}\hat{n}(\mathbf{r},t)]\rangle \quad (6)$$

$$\frac{\partial}{\partial t}\mathbf{m}(\mathbf{r},t) = - \boldsymbol{\nabla}\cdot\overleftrightarrow{\mathbf{J}}(\mathbf{r},t) + \frac{1}{c}[\mathbf{B}_{\rm xc}(\mathbf{r},t)\times\mathbf{m}(\mathbf{r},t)]$$
$$+ \frac{1}{4c^2}[\boldsymbol{\nabla}n(\mathbf{r},t)\times\boldsymbol{\nabla}v_s(\mathbf{r},t)]$$
$$+ \frac{1}{2c^2}[\overleftrightarrow{\mathbf{J}}^T(\mathbf{r},t) - Tr\{\overleftrightarrow{\mathbf{J}}(\mathbf{r},t)\}]\cdot\boldsymbol{\nabla}v_s(\mathbf{r},t) \quad (7)$$

Krieger et al. JPCM **29** , 224001 (2017),
Dewhurst et al. Computer Phys. Comm. **209**, 92 (2016)

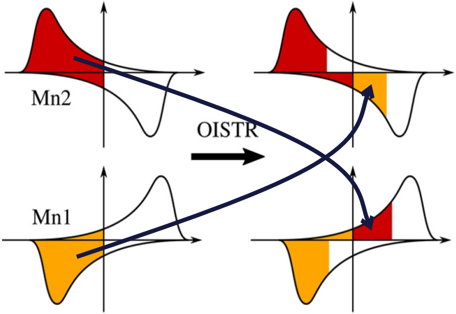
Magnetization dynamics in Mn2/Co4/Cu(001) without SO

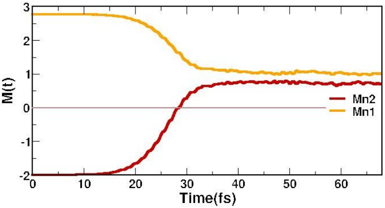


- Spin flips play no role in switching of magnetic order.

Dewhurst et al. Nano Lett. **18**, 1842, (2018)

Optical inter-site spin transfer (OISTR)





$$m = n_{\mathrm{up}} - n_{\mathrm{dn}}$$

Transient state density

$$\mathrm{DOS}(\omega, t) = \sum_{i=1}^{\infty} \int_{\mathrm{BZ}} \delta(\omega - \varepsilon_{i\mathbf{k}}) g_{i\mathbf{k}}(t), \tag{8}$$

with

$$g_{i\mathbf{k}}(t) = \sum_{j} n_{j\mathbf{k}} \left| O_{ij}^{\mathbf{k}}(t) \right|^2, \tag{9}$$

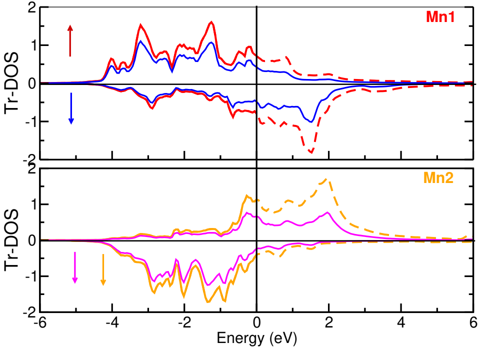
where $n_{j\mathbf{k}}$ is the occupation number of the j^{th} time-evolving orbital and

$$O_{ij}^{\mathbf{k}}(t) = \int d^3r \phi_{i\mathbf{k}}^{*}(\mathbf{r}) \psi_{j\mathbf{k}}(\mathbf{r}, t). \tag{10}$$

Here ϕ_i are the ground-state Kohn-Sham orbitals. In absence of any time-dependent perturbation $\psi_{j\mathbf{k}}(\mathbf{r}, t = 0) = \phi_{j\mathbf{k}}^{*}(\mathbf{r})$

Elliott et al. Sci. Rep. **6**, 38911 (2016)

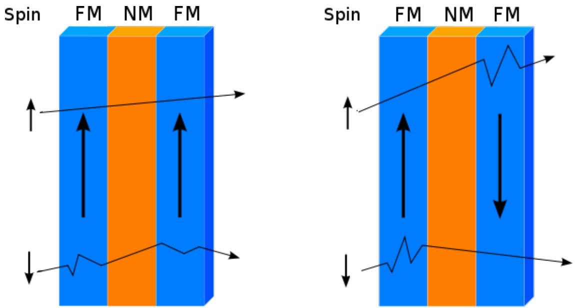
Transient occupied states



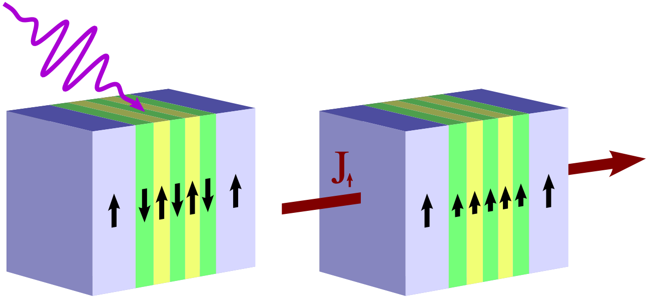
$$M = n_{\mathrm{up}} - n_{\mathrm{dn}}$$

- Optical inter-site spin transfer (OISTR) is responsible for switching
- Availability of states enforces OISTR

Outlook for OISTR: Ultrafast GMR

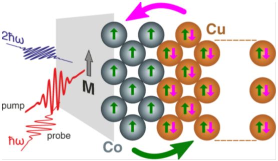


Laser induced transient OCMR device

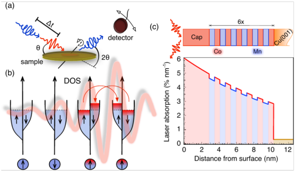


Resistance change of 385% in CuCoMn multilayers from Boltzmann simulations (Ingrid Mertig)

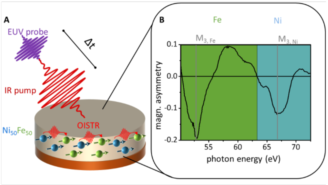
Experimental confirmation of OISTR



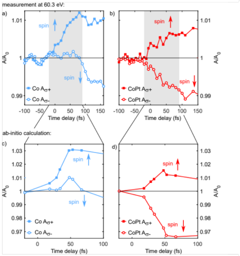
Chen *et al.*, Phys. Rev. Lett. **122**, 067202 (2019)



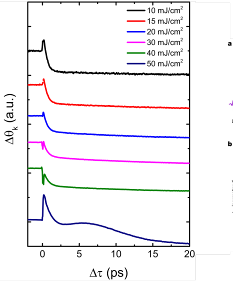
Golias et al., Phys. Rev. Lett. **126**, 107202 (2021)



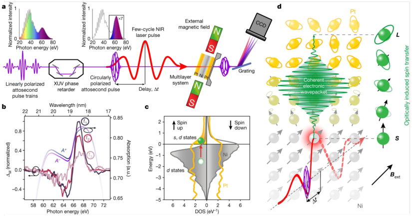
Hofherr *et al.* Science Advs. **6**, eaay8717 (2019)



F. Willems *et al.*, Nature Comm. **11**, 1 (2020)

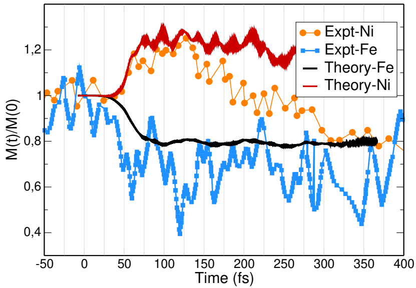


Steil *et al.*, Phys. Rev. Res. **2**, 023199 (2020)



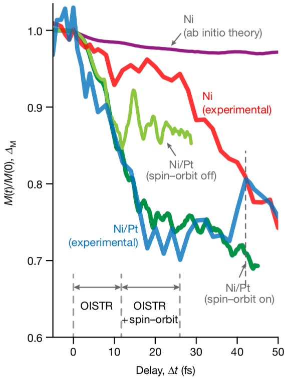
Siegrist *et al.* Nature **571**, 240 (2019)

Quantitative but indirect agreement with experiemnts



Laser-induced local **increase** in moment

Hofherr et al. Science Advs. **6**, eaay8717 (2019)



Attosecond dynamics via OISTR

Siegrist et al. Nature **571**, 240 (2019)

Linear response TDDFT

Interacting response function:

$$\varepsilon^{-1}(\mathbf{q},\omega) = 1 + \chi_0(\mathbf{q},\omega)\left[1 - (v_{\rm cl} + f_{\rm xc}(\mathbf{q},\omega))\chi_0(\mathbf{q},\omega)\right]^{-1} \quad (11)$$

Non-interacting response function:

$$\chi_0(\mathbf{r},\mathbf{r}',\omega) = \sum_{lmk}(n_{lk} - n_{mk})\frac{\phi^*_{lk}(\mathbf{r})\phi^*_{mk}(\mathbf{r}')\phi_{lk}(\mathbf{r}')\phi_{mk}(\mathbf{r})}{\omega - \epsilon_{lk} + \epsilon_{mk} + i\eta} \quad (12)$$

Linear response TDDFT

$$\varepsilon^{-1}(\mathbf{q},\omega) = 1 + \chi_0(\mathbf{q},\omega)\left[1 - (v_{\rm cl} + f_{\rm xc}(\mathbf{q},\omega))\chi_0(\mathbf{q},\omega)\right]^{-1} \quad (13)$$

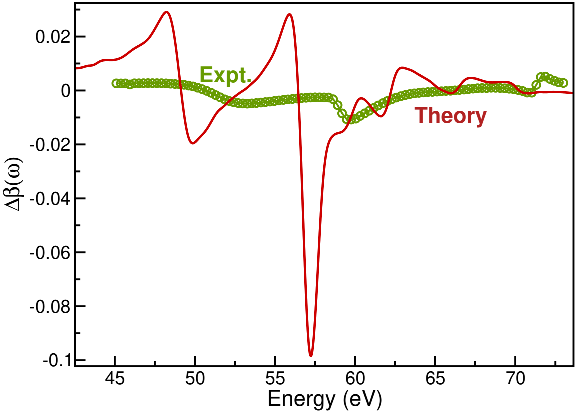
All quantities are treated as matrices in reciprocal space vectors **G**,**G'** to account for LFE.

Local field effects(LFE)– charge density rearrangement caused by the external perturbation leads to creation of local microscopic fields.

Light of the form $e^{i(\mathbf{G}+\mathbf{q}).\mathbf{r}}$ produces a response also of the form $e^{i(\mathbf{G}'+\mathbf{q}).\mathbf{r}}$

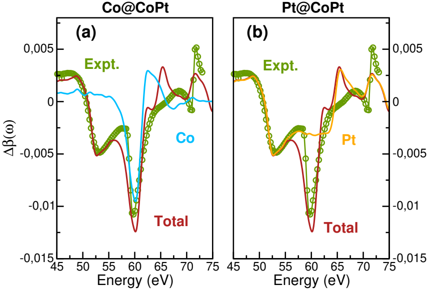
Simplest approximations:
$f_{\rm xc} = 0$ (RPA, i.e. no excitons) and **G**=**G'**=0 (no LFE)

CoPt: experimental response vs theoretical disaster



Disagreemet believed to be due to
(a) Missing many-body corrections and
(b) missing excitonic physics (i.e. $f_{\mathrm{xc}} \neq 0$).

Theory guiding experiments



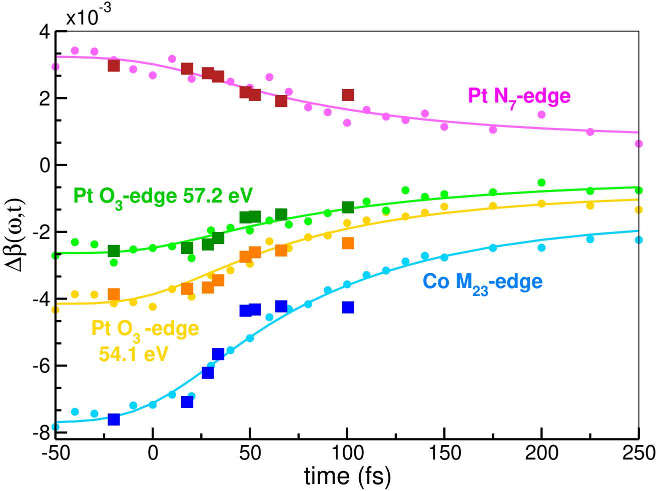
Agreement requires:

- Many-body correction via *GW*
- Excitonic physics included via bootstrap approximation
- Local field effects by solving matrix equation.

Dewhurst et al. Phys. Rev. Lett. **124**, 077203, (2020),
Willems et al. Phys. Rev. Lett. **122**, 217202, (2019),

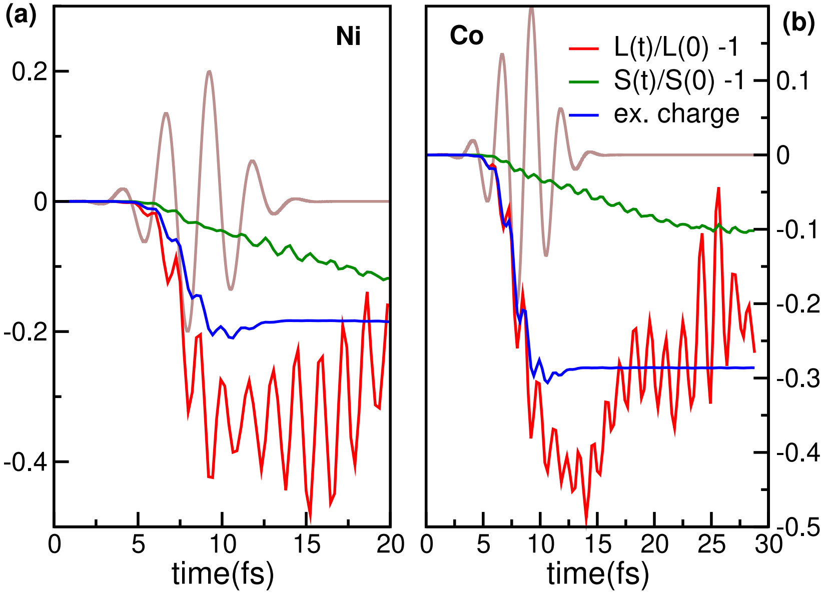
Willems et al. Nat. Comm. **11**, 1-7, (2020)

Transient response function in CoPt



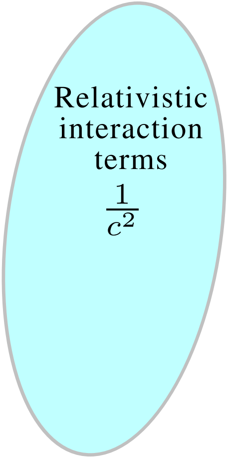
Dewhurst et al. Phys. Rev. Lett. **124**, 077203, (2020)

Where does the angular momentum go?
L+S+N is conserved



What is missing from the theory?

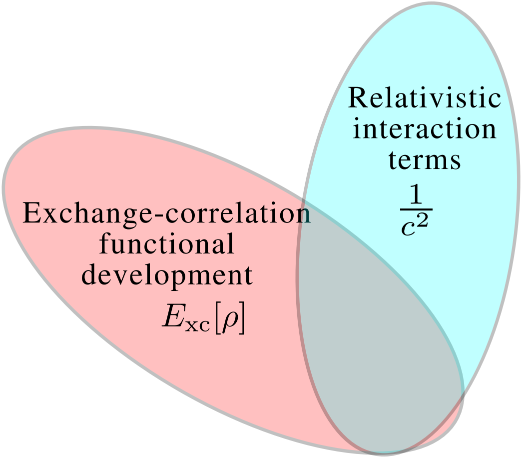
Even the exact functional will
not yield full predictiveness!


Relativistic
interaction
terms
$\frac{1}{c^2}$

Leading order terms in expansion of QED H

$$
\begin{aligned}
H = & \sum_i \frac{1}{2m}\mathbf{p}_i^2 - eV_{\text{ext}}(\mathbf{r}_i) + \sum_{i<j}\frac{e^2}{r_{ij}} + \frac{1}{c}\sum_i \frac{e}{m}\mathbf{p}_i\cdot\mathbf{A}_{\text{ext}}(\mathbf{r}_i) \\
& + \frac{1}{c}\sum_i \frac{e}{m}\mathbf{s}_i\cdot\mathbf{B}_{\text{ext}}(\mathbf{r}_i) + \frac{1}{c^2}\sum_i \frac{e}{2m^2}\mathbf{s}_i\cdot[\mathbf{E}_{\text{ext}}(\mathbf{r}_i)\times\mathbf{p}_i] \\
& + \frac{1}{c^2}\sum_i \frac{e^2}{2m}\mathbf{A}_{\text{ext}}^2(\mathbf{r}_i) - \frac{1}{c^2}\sum_i \frac{1}{8m^3}\mathbf{p}_i^4 + \frac{ie}{4m^2c^2}\mathbf{p}_i\cdot\mathbf{E}_{\text{ext}}(\mathbf{r}_i) \\
& - \frac{1}{c^2}\frac{e^2}{2m^2}\sum_{i<j}\mathbf{p}_i\cdot\left[\frac{(\mathbf{r}_i-\mathbf{r}_j)(\mathbf{r}_i-\mathbf{r}_j)}{r_{ij}^3} + \frac{1}{r_{ij}}\right]\cdot\mathbf{p}_j \\
& - \frac{1}{c^2}\frac{e^2}{m^2}\sum_{i<j}\mathbf{s}_i\cdot\left[\frac{3(\mathbf{r}_i-\mathbf{r}_j)(\mathbf{r}_i-\mathbf{r}_j)}{r_{ij}^5} - \frac{1}{r_{ij}^3}\right]\cdot\mathbf{s}_j \\
& - \frac{1}{c^2}\frac{e^2}{m^2}\sum_{i\neq j}\frac{1}{r_{ij}^3}\left(\mathbf{s}_i\cdot[(\mathbf{r}_j-\mathbf{r}_i)\times\mathbf{p}_j] + \frac{1}{2}\mathbf{s}_i\cdot[(\mathbf{r}_i-\mathbf{r}_j)\times\mathbf{p}_i]\right) \\
& + \ldots
\end{aligned}
$$

Still only an approximation to QED...


Relativistic
interaction
terms
$\frac{1}{c^2}$
Exchange-correlation
functional
development
$E_{\mathrm{xc}}[\rho]$

DFT of magnetic dipolar interactions

$$H_{\rm dip} = -\frac{1}{c^2}\frac{e^2}{m^2}\sum_{i<j}\mathbf{s}_i \cdot \left[\frac{3(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{r}_i - \mathbf{r}_j)}{r_{ij}^5} - \frac{1}{r_{ij}^3}\right] \cdot \mathbf{s}_j$$

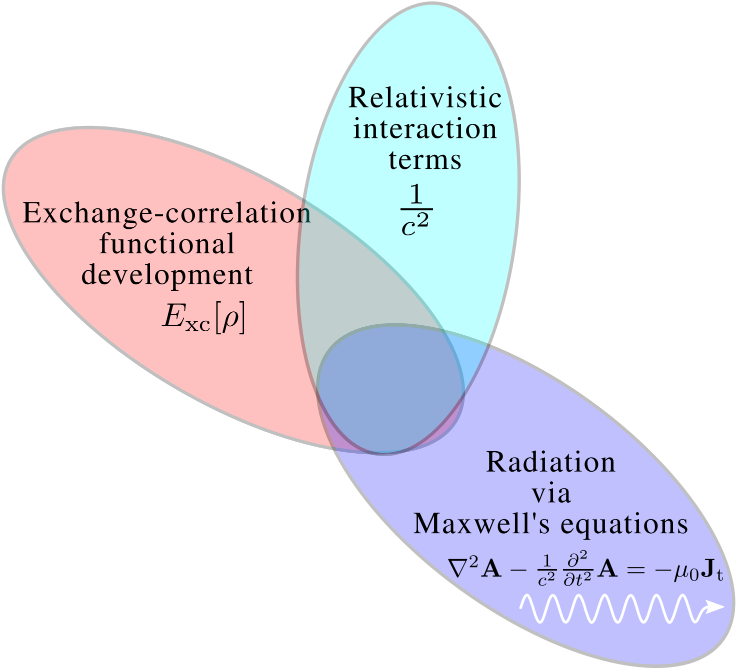
C. Pellegrini, T. Müller, JKD, S. Sharma, A. Sanna, E. K. U. Gross
Phys. Rev. B **101**, 144401 (2020)

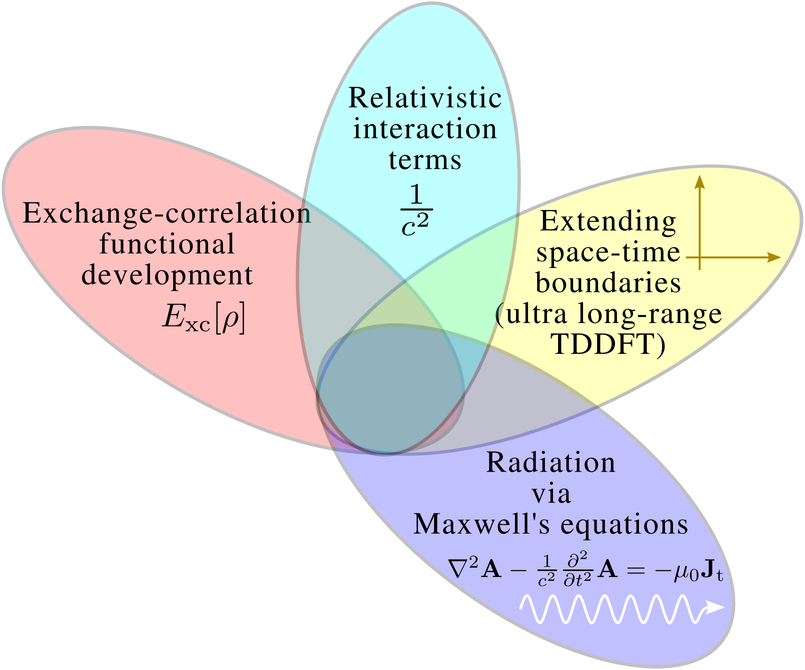
Direct and exchange dipole-dipole energy of the homogeneous electron gas is zero

Therefore no dipole LDA for exchange!

Instead we construct a functional from the response of the electron gas to a magnetic field:

$$E_x^{\rm dip} = \frac{\mu_B^2}{2}\int \frac{d^3q}{(2\pi)^3}\, K_{\rm x}^{ij}(\mathbf{q})\delta m_i(\mathbf{q})\delta m_j(-\mathbf{q})$$


Relativistic
interaction
terms
$\frac{1}{c^2}$
Exchange-correlation
functional
development
$E_{\mathrm{xc}}[\rho]$
Radiation
via
Maxwell's equations
$\nabla^2\mathbf{A} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{A} = -\mu_0\mathbf{J}_{\mathrm{t}}$



Relativistic interaction terms
$\frac{1}{c^2}$
Exchange-correlation functional development
$E_{\mathrm{xc}}[\rho]$
Extending space-time boundaries (ultra long-range TDDFT)
Radiation via Maxwell's equations
$\nabla^2 \mathbf{A} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{A} = -\mu_0 \mathbf{J}_{\mathrm{t}}$

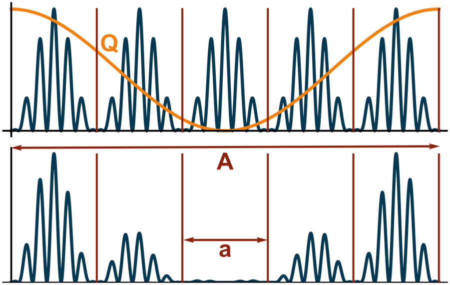
Long length scale physics

Spin-spiral ansatz

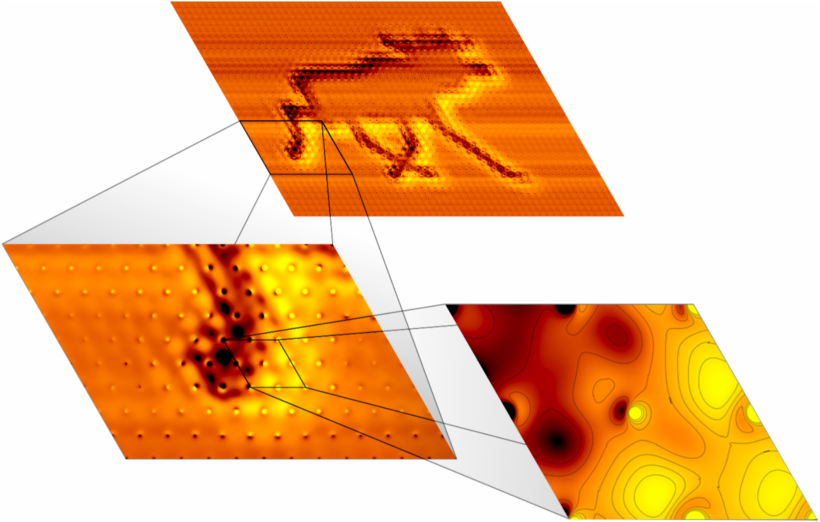
$$\Phi_n^{\mathbf{k}}(\boldsymbol{r}) = \begin{pmatrix} u_{n\mathbf{k}}^{\uparrow}(\boldsymbol{r})\, e^{i(\mathbf{q}/\mathbf{2})\cdot(\boldsymbol{r})} \\ u_{n\mathbf{k}}^{\downarrow}(\boldsymbol{r})\, e^{i(\mathbf{-q}/\mathbf{2})\cdot(\boldsymbol{r})} \end{pmatrix} e^{i\mathbf{k}\cdot\boldsymbol{r}} \tag{14}$$

Ultra long-range anstaz

$$\Phi_\alpha^{\mathbf{k}}(\boldsymbol{r}+\boldsymbol{R}) = \sum_{n\boldsymbol{\kappa}} c_{n\mathbf{k}+\boldsymbol{\kappa}}^{\alpha} \begin{pmatrix} u_{n\mathbf{k}}^{\uparrow}(\boldsymbol{r}) \\ u_{n\mathbf{k}}^{\downarrow}(\boldsymbol{r}) \end{pmatrix} e^{i(\mathbf{k}+\boldsymbol{\kappa})\cdot(\boldsymbol{r}+\boldsymbol{R})} \tag{15}$$

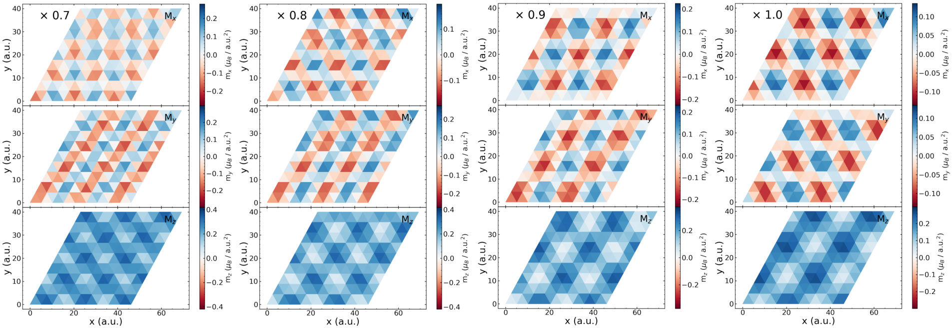


Self-consistent density for a 3456 atom cell of LiF

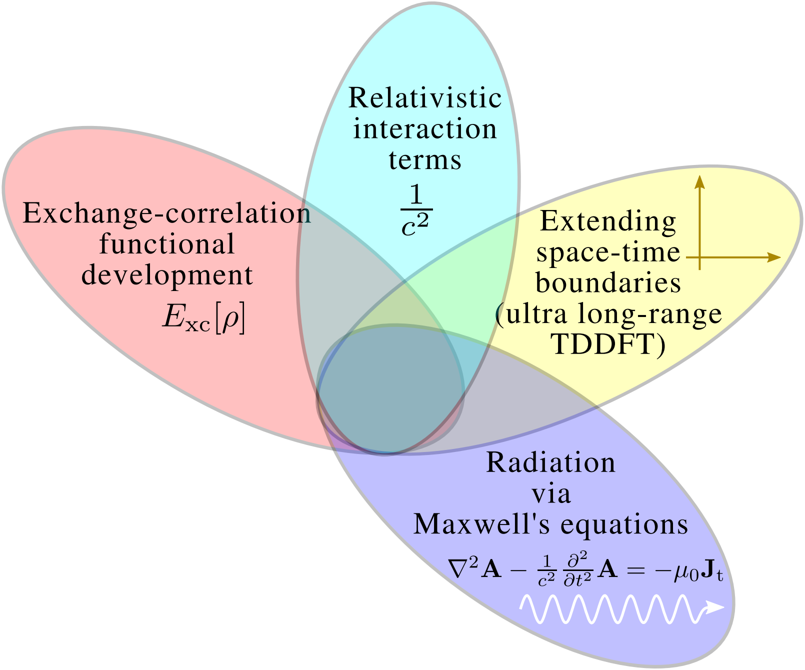


Müller, Sharma, Gross and Dewhurst, Phys. Rev. Lett. **125**, 256402 (2020)

Skyrmion in iron on iridium substrate



Plot of the surface magnetization density averaged in each unit cell in the Fe plane. Each triangle represents a unit cell and the ultracell vectors were scaled by 0.8, 0.9, 1.0 and 1.1.



Relativistic interaction terms
$\frac{1}{c^2}$
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$E_{\mathrm{xc}}[\rho]$
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Radiation via Maxwell's equations
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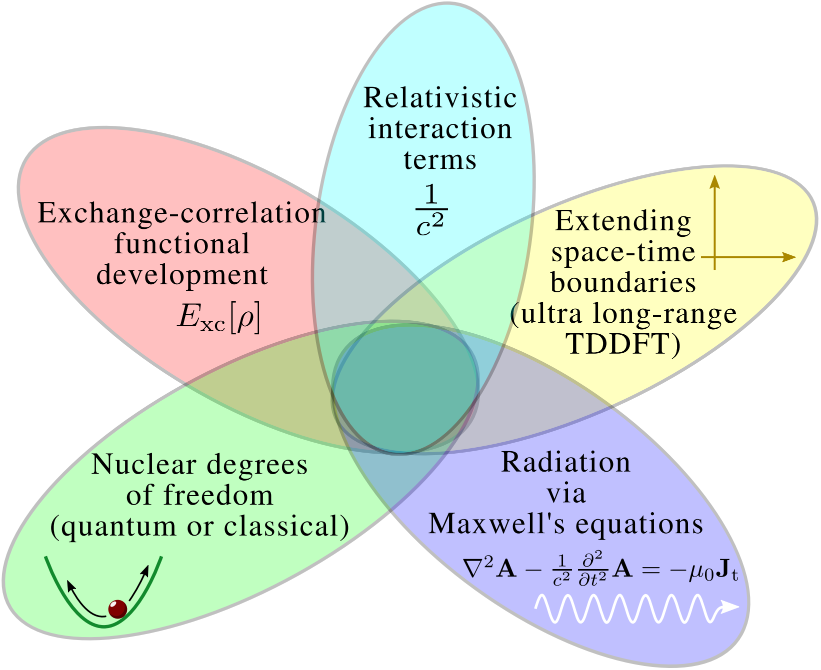
Relativistic
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Nuclear degrees
of freedom
(quantum or classical)
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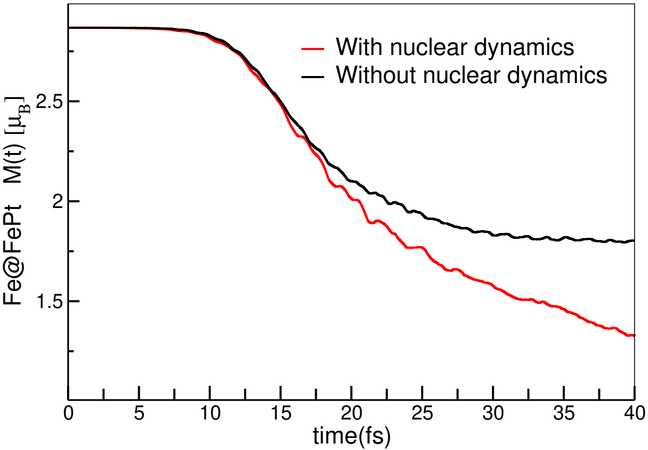
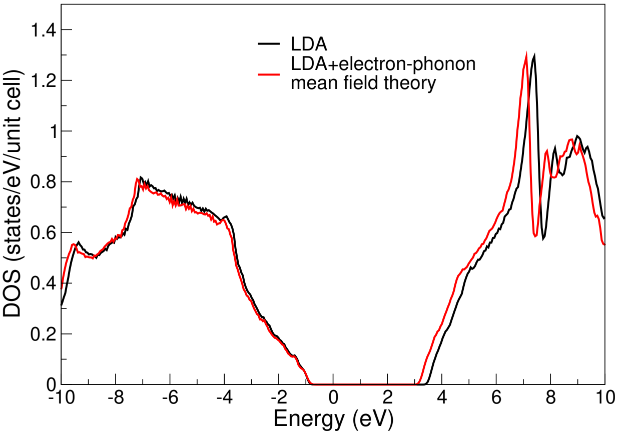
Nuclear degrees of freedom

Treat nuclei as classical point particles: Ehrenfest dynamics

Quantum nuclei required for superconductivity!

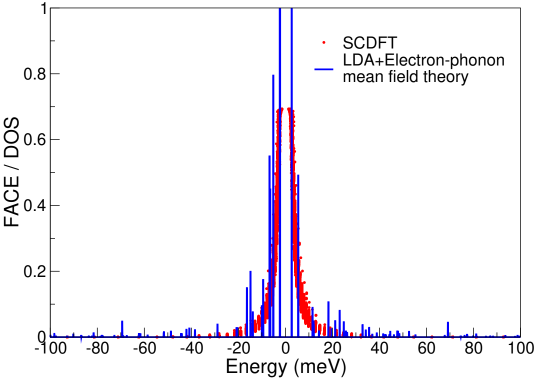
Coupled spin nuclear dynamics in FePt





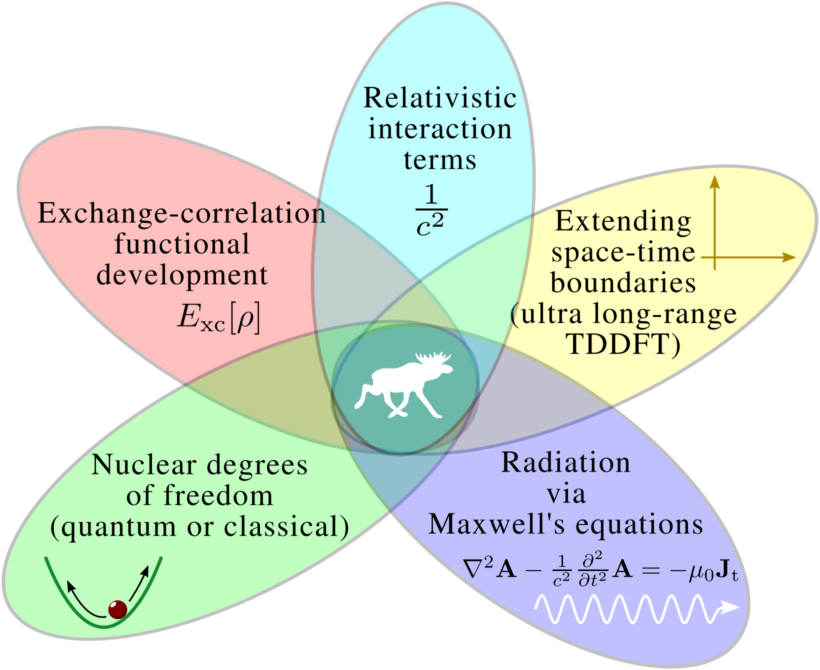
Change in the band gap

This work	-365 meV
S. Poncé *et al.*, *Comp. Mat. Sci.* **83**, 341 (2014)	-409 meV



Superconducting gap in niobium

This work	≈ 3.1 meV
Bonnet *et al.*, *Phys. Lett. A* **25**, 452 (1967)	2.32 meV



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Various combinations yield new predictiveness

$$\text{long-range} + \text{Maxwell's equations} + \text{TDDFT} \implies \begin{cases} \text{light propagation} \\ \text{density wave propagation} \end{cases}$$

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$$\text{long-range} + \text{superconductivity} + \frac{1}{c}\sum_i \frac{e}{m}\mathbf{p}_i \cdot \mathbf{A}_{\text{ext}}(\mathbf{r}_i) \implies \text{Abrikosov vortices}$$

New physics can be found at competing energy scales!

Elk code: full potential LAPW method

Science 351, 6280 (2016)

		AE							
		Elk	exciting	FHI-aims/tier2	FLEUR	FPLO/T+F+s	RSPt	WIEN2k/acc	average <Δ>
AE	Elk		0.3	0.3	0.6	1.0	0.9	0.3	0.6
AE	exciting	0.3		0.1	0.5	0.9	0.8	0.2	0.5
AE	FHI-aims/tier2	0.3	0.1		0.5	0.9	0.8	0.2	0.5
AE	FLEUR	0.6	0.5	0.5		0.8	0.6	0.4	0.6
AE	FPLO/T+F+s	1.0	0.9	0.9	0.8		0.9	0.9	0.9
AE	RSPt	0.9	0.8	0.8	0.6	0.9		0.8	0.8
AE	WIEN2k/acc	0.3	0.2	0.2	0.4	0.9	0.8		0.5
PAW	GBRV12/ABINIT	0.9	0.8	0.8	0.9	1.3	1.1	0.8	0.9
PAW	GPAW09/ABINIT	1.3	1.3	1.3	1.3	1.7	1.5	1.3	1.4
PAW	GPAW09/GPAW	1.5	1.5	1.5	1.5	1.8	1.7	1.5	1.6
PAW	JTH02/ABINIT	0.6	0.6	0.6	0.6	0.9	0.7	0.5	0.6
PAW	PSlib100/QE	0.9	0.8	0.8	0.8	1.3	1.1	0.8	0.9
PAW	VASPGW2015/VASP	0.5	0.4	0.4	0.6	1.0	0.9	0.4	0.6

Gold standard for electronic structure of solids. Features include:

- Ground state
- Most single particle observables
- Structural optimization
- Many-body methods: GW and beyond, RDMFT, BSE ...
- Response functions: magnons, phonons, plasmons, excitons ...
- Wannier90 interface
- Tensor moments
- Non-equilibrium spin dynamics
- Superconductivity: calculation of Tc, Eliashberg

J. K. Dewhurst, S. Sharma, L. Nordström and E. K. U. Gross ....

http://elk.sourceforge.net/