Inverse Faraday Effect in altermagnets from first-principles

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Abstract

While the understanding of altermagnetism is still in a very early stage, it is expected to play a role in various fields of condensed matter research, for example spintronics, caloritronics and superconductivity [1]. Concerning the field of optical magnetism, it is intriguing to study whether altermagnets can host magnetization dynamic effects with different properties from ferromagnets and antiferromagnets. Here we choose RuO2, a prototype metallic altermagnet with a giant spin splitting, and CoF2, an experimentally well studied insulating altermagnet, and calculate the inverse Faraday effect (IFE), i.e., laser-induced spin and orbital magnetizations, from first-principles.

Computational methods

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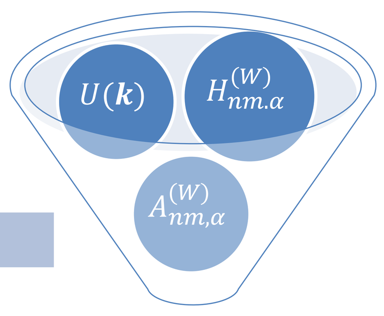
$\mathcal{TB}$-basis set: $\langle 0n|\hat{H}|\mathbf{R}m\rangle$, $\langle 0n|\hat{r}_\alpha|\mathbf{R}m\rangle$

$$H^{(W)}_{nm}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\,\mathbf{k}\cdot\mathbf{R}} \langle 0n|\hat{H}|\mathbf{R}m\rangle$$

$$H^{(W)}_{nm,\alpha}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\,\mathbf{k}\cdot\mathbf{R}}\, iR_\alpha \langle 0n|\hat{H}|\mathbf{R}m\rangle$$

$$A^{(W)}_{nm,\alpha}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\,\mathbf{k}\cdot\mathbf{R}} \langle 0n|\hat{r}_\alpha|\mathbf{R}m\rangle$$



$$v^{(H)}_{nm,\alpha} = \frac{1}{\hbar}\bar{H}^{(H)}_{nm,\alpha} - \frac{i}{\hbar}(\epsilon^{(H)}_m - \epsilon^{(H)}_n)\bar{A}^{(H)}_{nm,\alpha}$$

Keldysh formalism

2nd order spin magnetization

- Response formula

$$\delta S_i = -\frac{\hbar}{2}\frac{a_0^3 I}{c}\frac{\mathcal{E}_H}{(\hbar\omega)^2}\mathrm{Im}\sum_{jk}\epsilon_j\epsilon_k^*\tilde{\chi}_{ijk}$$

LASER intensity; LASER polarization; LASER frequency

- Response tensor

$$\tilde{\chi}_{ijk} = \frac{2}{N\hbar a_0^2}\sum_{\mathbf{k}}\int d\mathcal{E}$$
$$\times \mathrm{Tr}\big[f(\mathcal{E})\sigma_i G^R_{\mathbf{k}}(\mathcal{E})v_j G^R_{\mathbf{k}}(\mathcal{E}-\hbar\omega)v_k G^R_{\mathbf{k}}(\mathcal{E})$$
$$- f(\mathcal{E})\sigma_i G^R_{\mathbf{k}}(\mathcal{E})v_j G^R_{\mathbf{k}}(\mathcal{E}-\hbar\omega)v_k G^A_{\mathbf{k}}(\mathcal{E})$$
$$+ f(\mathcal{E})\sigma_i G^R_{\mathbf{k}}(\mathcal{E})v_k G^R_{\mathbf{k}}(\mathcal{E}+\hbar\omega)v_j G^R_{\mathbf{k}}(\mathcal{E})$$
$$- f(\mathcal{E})\sigma_i G^R_{\mathbf{k}}(\mathcal{E})v_k G^R_{\mathbf{k}}(\mathcal{E}+\hbar\omega)v_j G^A_{\mathbf{k}}(\mathcal{E})$$
$$+ f(\mathcal{E}-\hbar\omega)\sigma_i G^R_{\mathbf{k}}(\mathcal{E})v_j G^R_{\mathbf{k}}(\mathcal{E}-\hbar\omega)v_k G^A_{\mathbf{k}}(\mathcal{E})$$
$$+ f(\mathcal{E}+\hbar\omega)\sigma_i G^R_{\mathbf{k}}(\mathcal{E})v_k G^R_{\mathbf{k}}(\mathcal{E}+\hbar\omega)v_j G^A_{\mathbf{k}}(\mathcal{E})\big]$$

- Retarded and Advanced Green's function

$$G^R_{\mathbf{k}}(\mathcal{E}) = \hbar\sum_n \frac{|kn\rangle\langle kn|}{\mathcal{E}-\mathcal{E}_{kn}+i\Gamma} \quad\text{and}\quad G^A_{\mathbf{k}}(\mathcal{E}) = [G^R_{\mathbf{k}}(\mathcal{E})]^\dagger$$

2nd order orbital magnetization

- Replace

$$\sigma_i \longrightarrow l_i$$

LASER

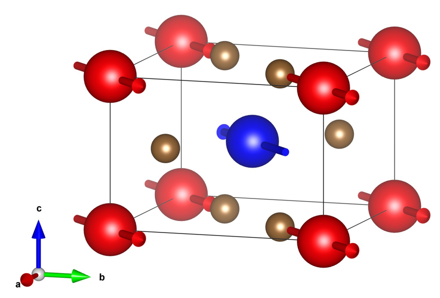
$$I = 10\ \mathrm{GWcm^{-2}}$$

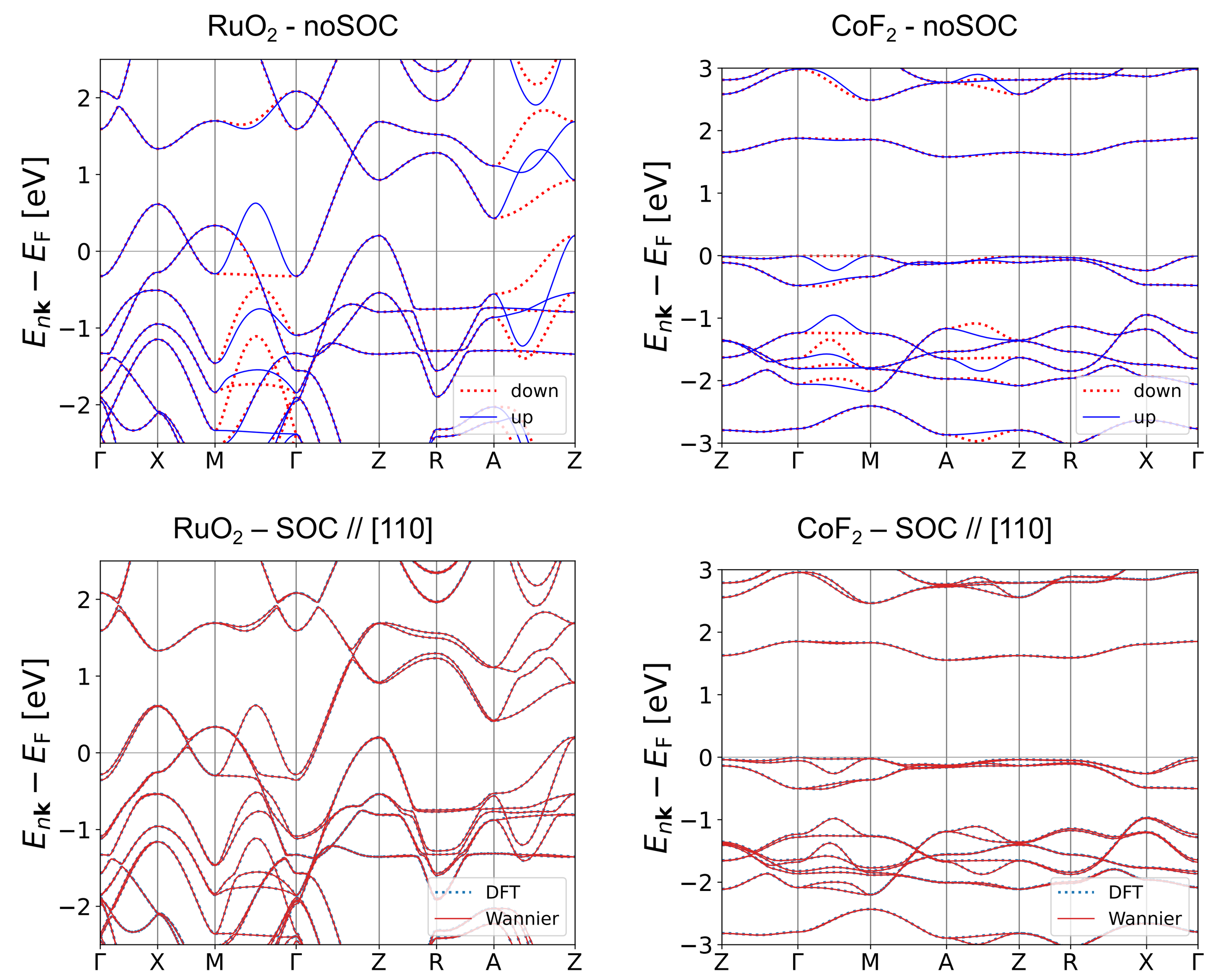
$$\epsilon_j\epsilon_k^* = \begin{pmatrix} 1/2 & -i\lambda/2 \\ i\lambda/2 & \lambda^2/2 \end{pmatrix}$$

$$\epsilon = (1, i\lambda, 0)/\sqrt{2}$$

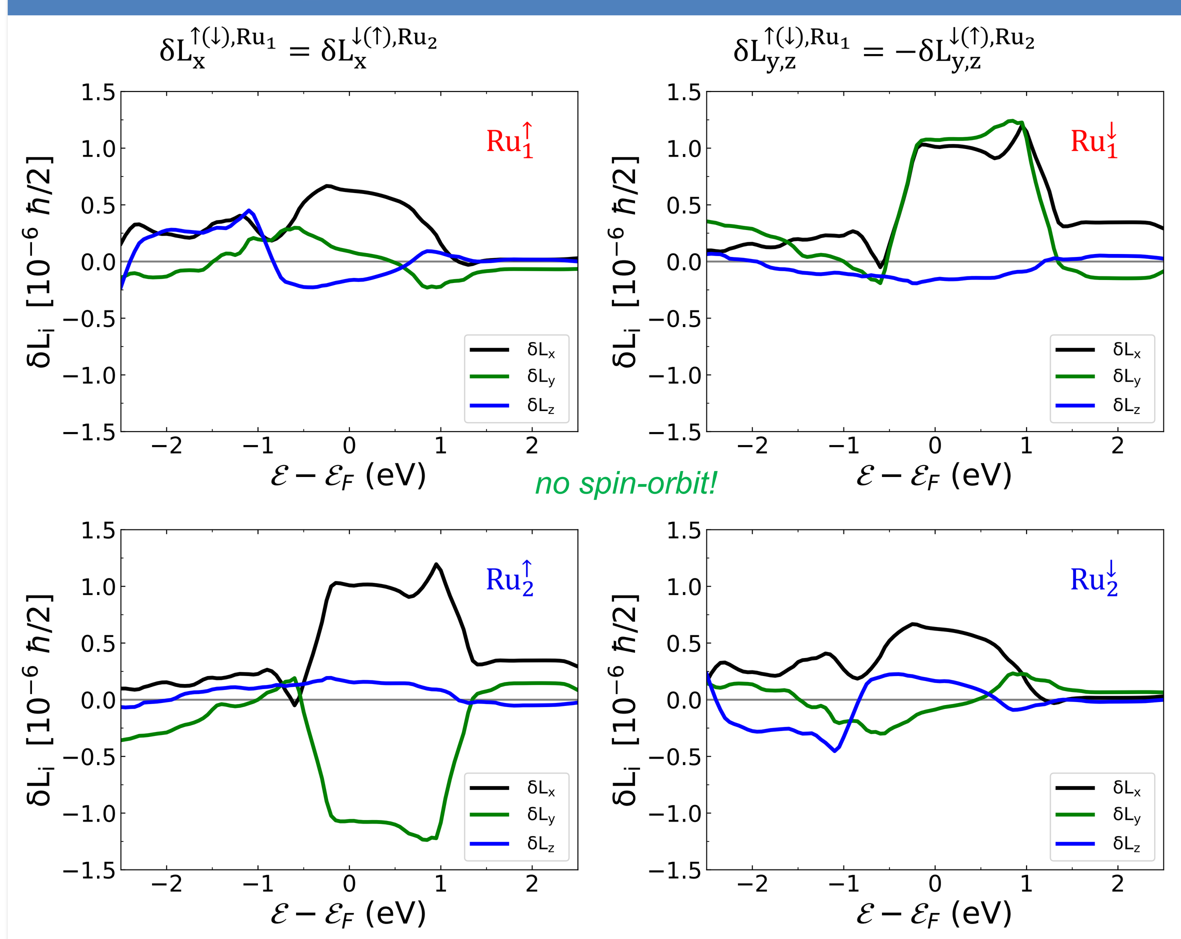
Studied systems

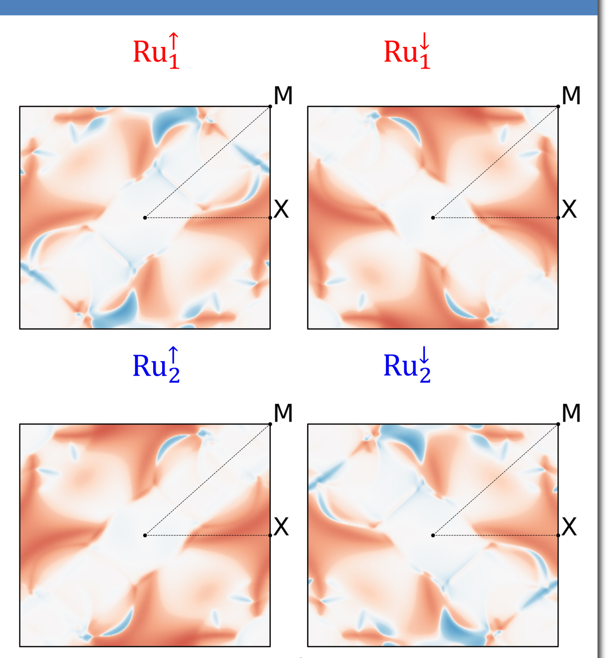
RuO$_2$ — CoF$_2$





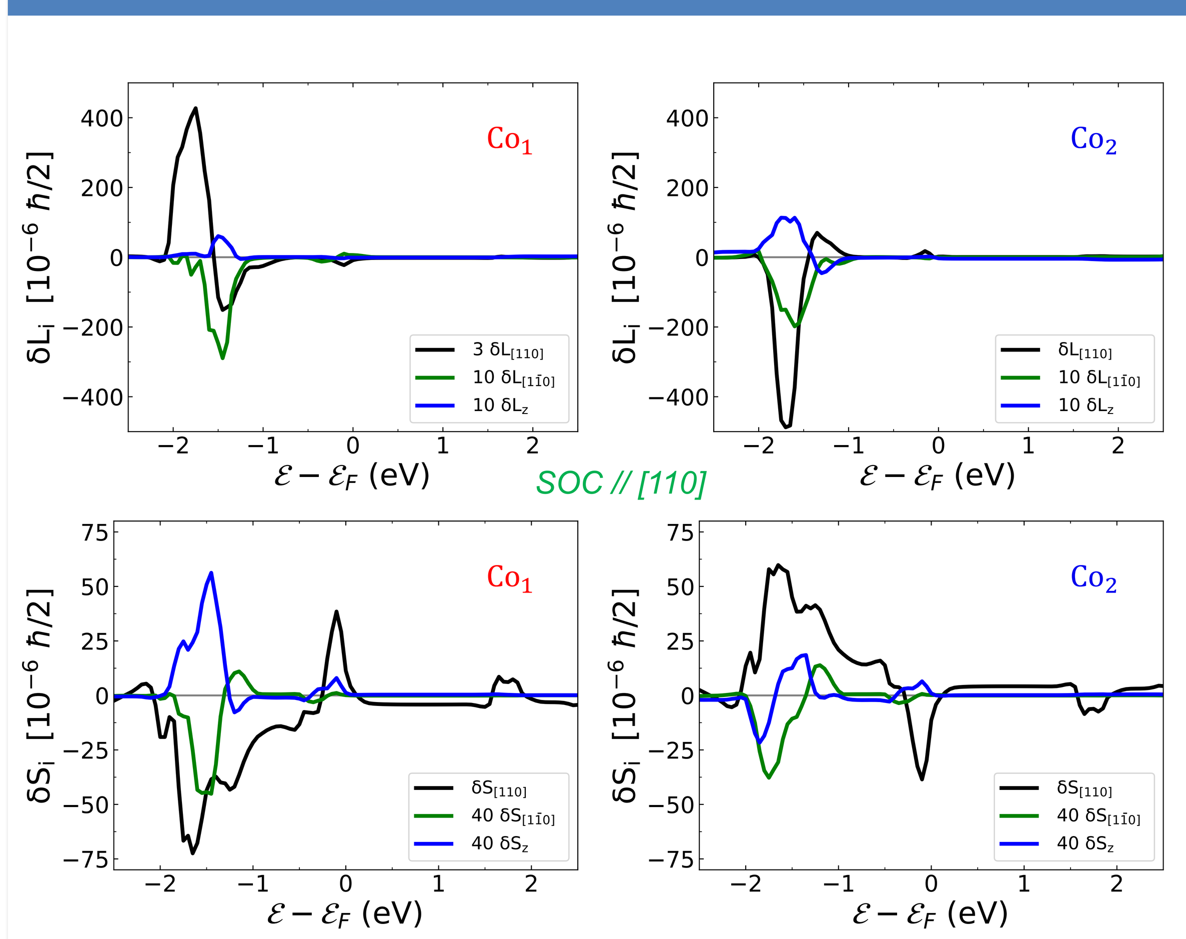
RuO$_2$ – non-relativistic orbital photomagnetization





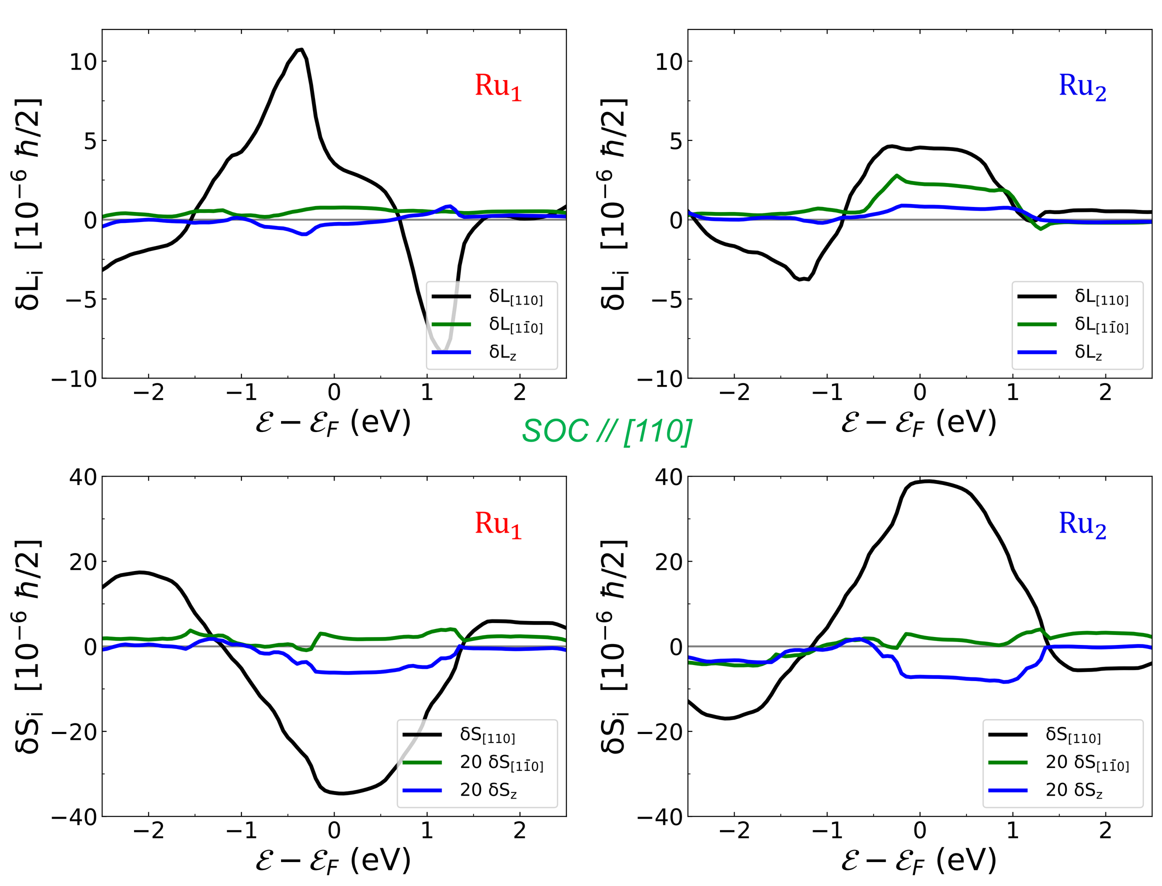
- Distinct behavior for each Ru atom and spin polarization
- 90° degrees rotation of the signal in reciprocal space

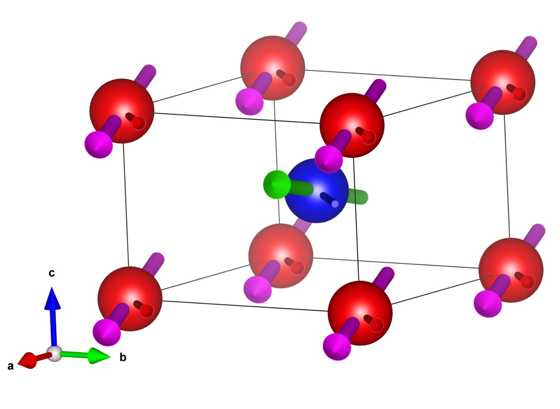
CoF$_2$ – orbital and spin photomagnetizations



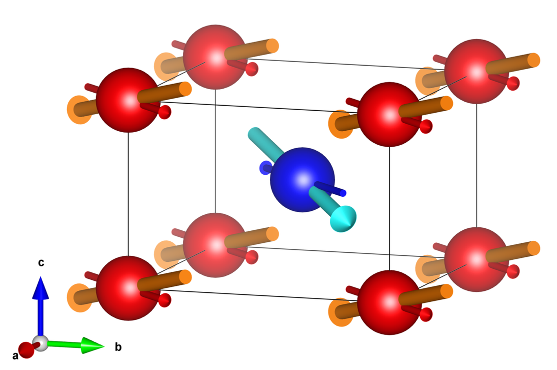
- Very large induced orbital moments, with difference in magnitude even among the Co atoms
- The induced spin moments are sizeable but one order of magnitude smaller than the orbital
- The large peaks originate from the group of d-bands at -1.5eV
- The secondary peaks originate from the group of d-bands at 0eV

RuO$_2$ – orbital and spin photomagnetizations





Non-collinear induced moments



Conclusions

- ✓ Laser light can induce non-collinear orbital and spin moments in altermagnets
- ✓ Peaks in the signal can be related to the altermagnetic splittings in the bandstructure
- ✓ In RuO$_2$ the induced moments are sizeable with spin larger than the orbital
- ✓ In CoF$_2$ the induced orbital moments are one order of magnitude larger than the spin
- ✓ Tempting to study the demagnetization and switching behavior of these altermagnets

References

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