

Inverse Faraday Effect in altermagnets from first-principles

Theodoros Adamantopoulos^{1,2*}, M. Merte^{1,2,3}, F. Freimuth³, D. Go³, M. Ležaić¹, W. Feng⁴, Y. Yao⁴, L. Smejkal^{3,5}, J. Sinova^{3,5}, S. Blügel¹, and Y. Mokrousov^{1,3}

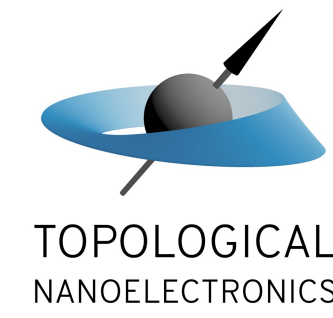
¹Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich GmbH and JARA, 52425 Jülich, Germany

²Department of Physics, RWTH Aachen University, 52056 Aachen, Germany

³Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

⁴Beijing Institute of Technology, Beijing, 100081, China

⁵Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6, Czech Republic



*t.adamantopoulos@fz-juelich.de

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]. In the field of optical magnetism, it is still unclear to which extent altermagnets as a class can exhibit a distinct behavior. Here we choose RuO₂, a prototype metallic altermagnet with a giant spin splitting, and CoF₂, an experimentally known insulating altermagnet, to study the light-induced magnetism in rutile altermagnets from first-principles.

Computational methods

www.flapw.de
Fleur FZ-Jülich

WANNIER90

$\mathcal{T}\mathcal{B}$ -basis set

$$\begin{cases} \langle 0n | \hat{H} | Rm \rangle \\ \langle 0n | \hat{p}_\alpha | Rm \rangle \end{cases} \begin{cases} H_{nm}^{(W)}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle 0n | \hat{H} | Rm \rangle \\ H_{nm,\alpha}^{(W)}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} iR_\alpha \langle 0n | \hat{H} | Rm \rangle \\ A_{nm,\alpha}^{(W)}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle 0n | \hat{p}_\alpha | Rm \rangle \end{cases}$$

$v_{nm,\alpha}^{(H)} = \frac{1}{\hbar} \bar{H}_{nm,\alpha}^{(H)} - \frac{i}{\hbar} (\epsilon_m^{(H)} - \epsilon_n^{(H)}) \bar{A}_{nm,\alpha}^{(H)}$

Keldysh formalism

2nd order spin magnetization

• Response formula

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

• Response tensor

$$\tilde{\chi}_{ijk} = \frac{2}{N\hbar a_0^3} \sum_{\mathbf{k}} \int d\mathcal{E} \times \text{Tr} [f(\mathcal{E}) \sigma_i G_{\mathbf{k}}^R(\mathcal{E}) v_j G_{\mathbf{k}}^R(\mathcal{E} - \hbar\omega) v_k G_{\mathbf{k}}^R(\mathcal{E}) - f(\mathcal{E}) \sigma_i G_{\mathbf{k}}^R(\mathcal{E}) v_j G_{\mathbf{k}}^R(\mathcal{E} - \hbar\omega) v_k G_{\mathbf{k}}^A(\mathcal{E}) + f(\mathcal{E}) \sigma_i G_{\mathbf{k}}^R(\mathcal{E}) v_j G_{\mathbf{k}}^R(\mathcal{E} + \hbar\omega) v_k G_{\mathbf{k}}^R(\mathcal{E}) - f(\mathcal{E}) \sigma_i G_{\mathbf{k}}^R(\mathcal{E}) v_k G_{\mathbf{k}}^R(\mathcal{E} + \hbar\omega) v_j G_{\mathbf{k}}^R(\mathcal{E}) + f(\mathcal{E} - \hbar\omega) \sigma_i G_{\mathbf{k}}^R(\mathcal{E}) v_j G_{\mathbf{k}}^R(\mathcal{E} - \hbar\omega) v_k G_{\mathbf{k}}^A(\mathcal{E}) + f(\mathcal{E} + \hbar\omega) \sigma_i G_{\mathbf{k}}^R(\mathcal{E}) v_k G_{\mathbf{k}}^R(\mathcal{E} + \hbar\omega) v_j G_{\mathbf{k}}^A(\mathcal{E})]$$

• Retarded and Advanced Green's function

$$G_{\mathbf{k}}^R(\mathcal{E}) = \hbar \sum_n \frac{|kn\rangle \langle kn|}{\mathcal{E} - \epsilon_{kn} + i\Gamma} \quad \text{and} \quad G_{\mathbf{k}}^A(\mathcal{E}) = [G_{\mathbf{k}}^R(\mathcal{E})]^\dagger$$

2nd order orbital magnetization

• Replace

$$\sigma_i \rightarrow l_i$$

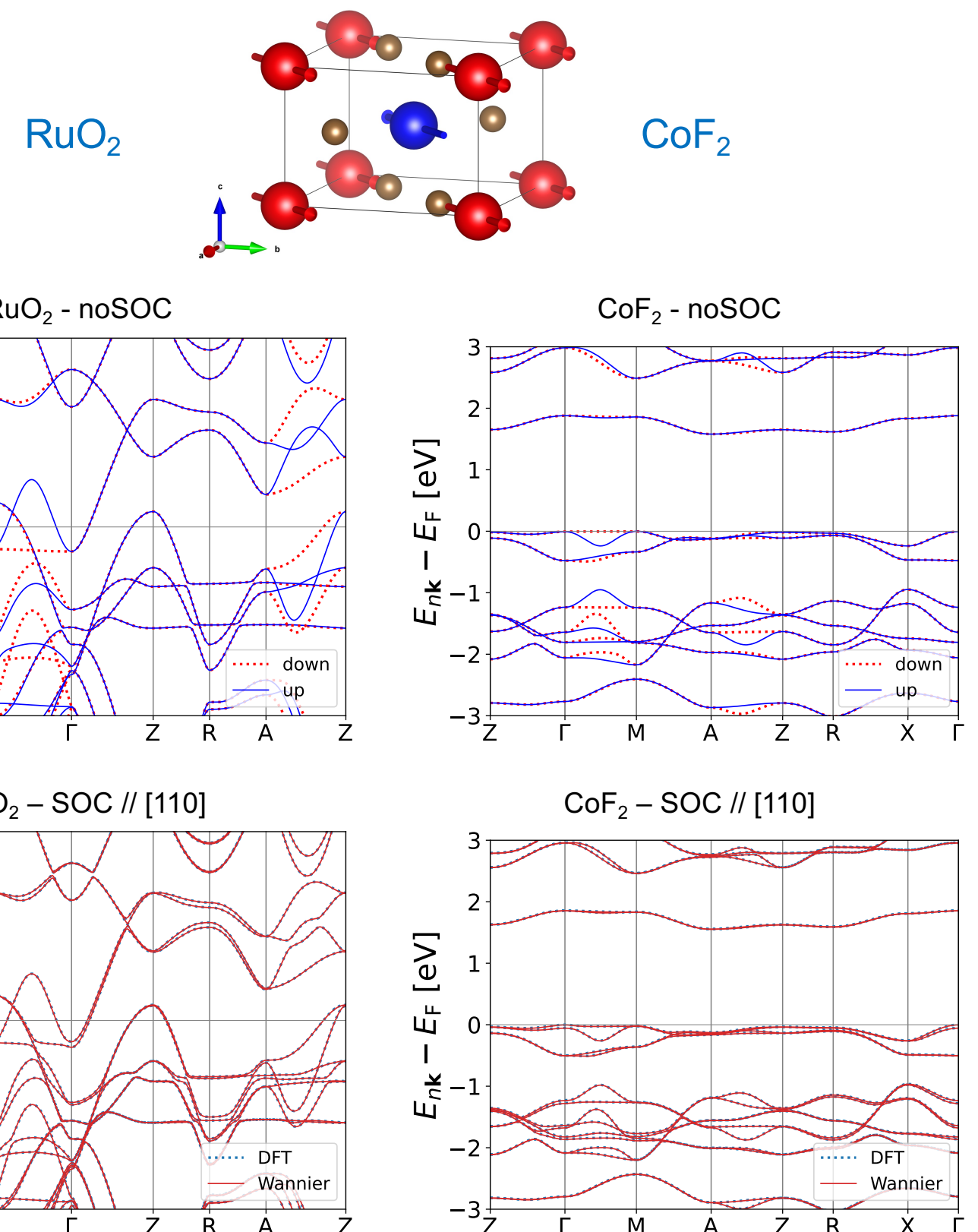
LASER

$$I = 10 \text{ GW cm}^{-2}$$

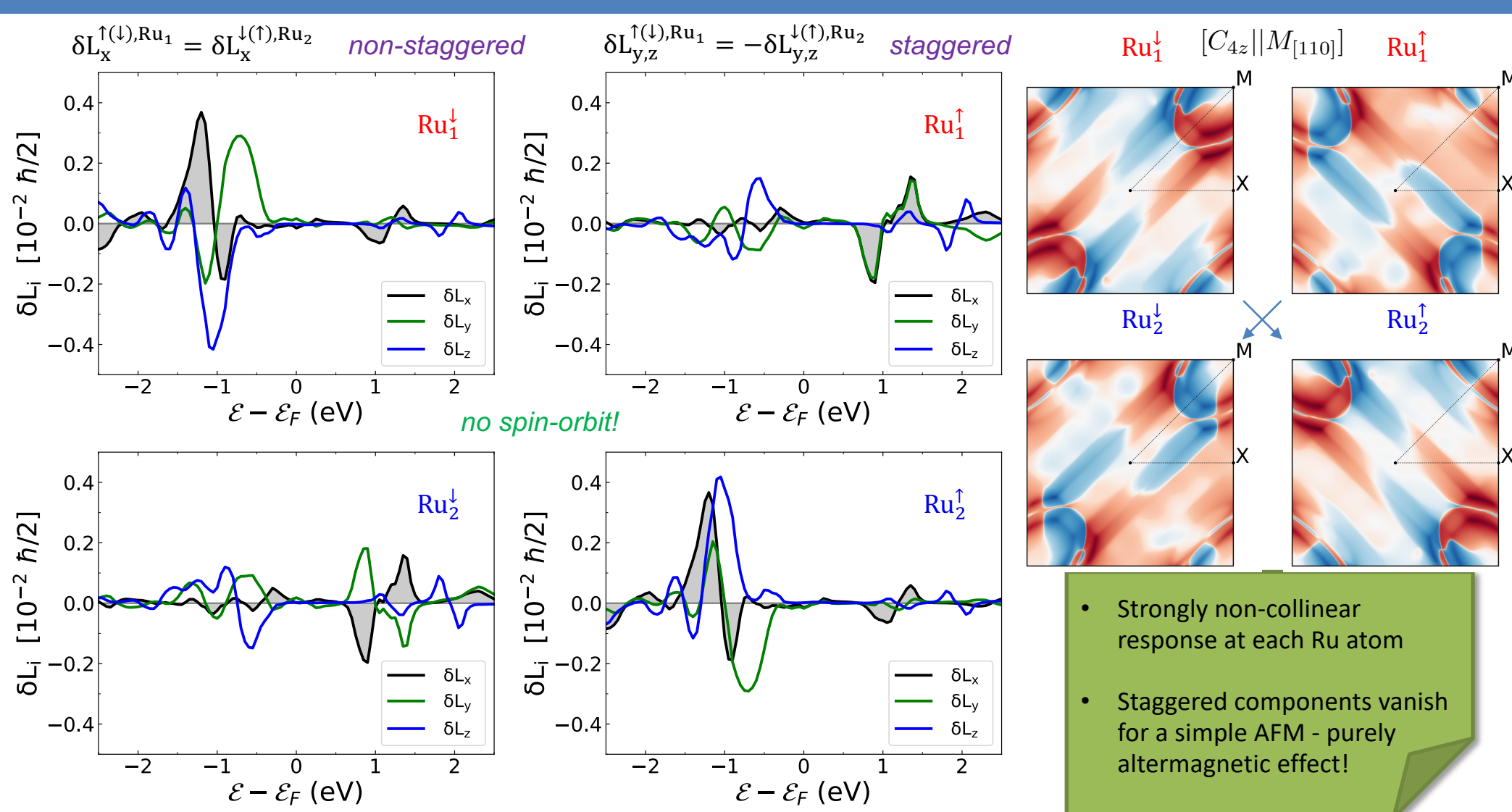
$$\epsilon_j \epsilon_k^* = \begin{pmatrix} 1/2 & -i\lambda/2 \\ i\lambda/2 & \lambda^2/2 \end{pmatrix}$$

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

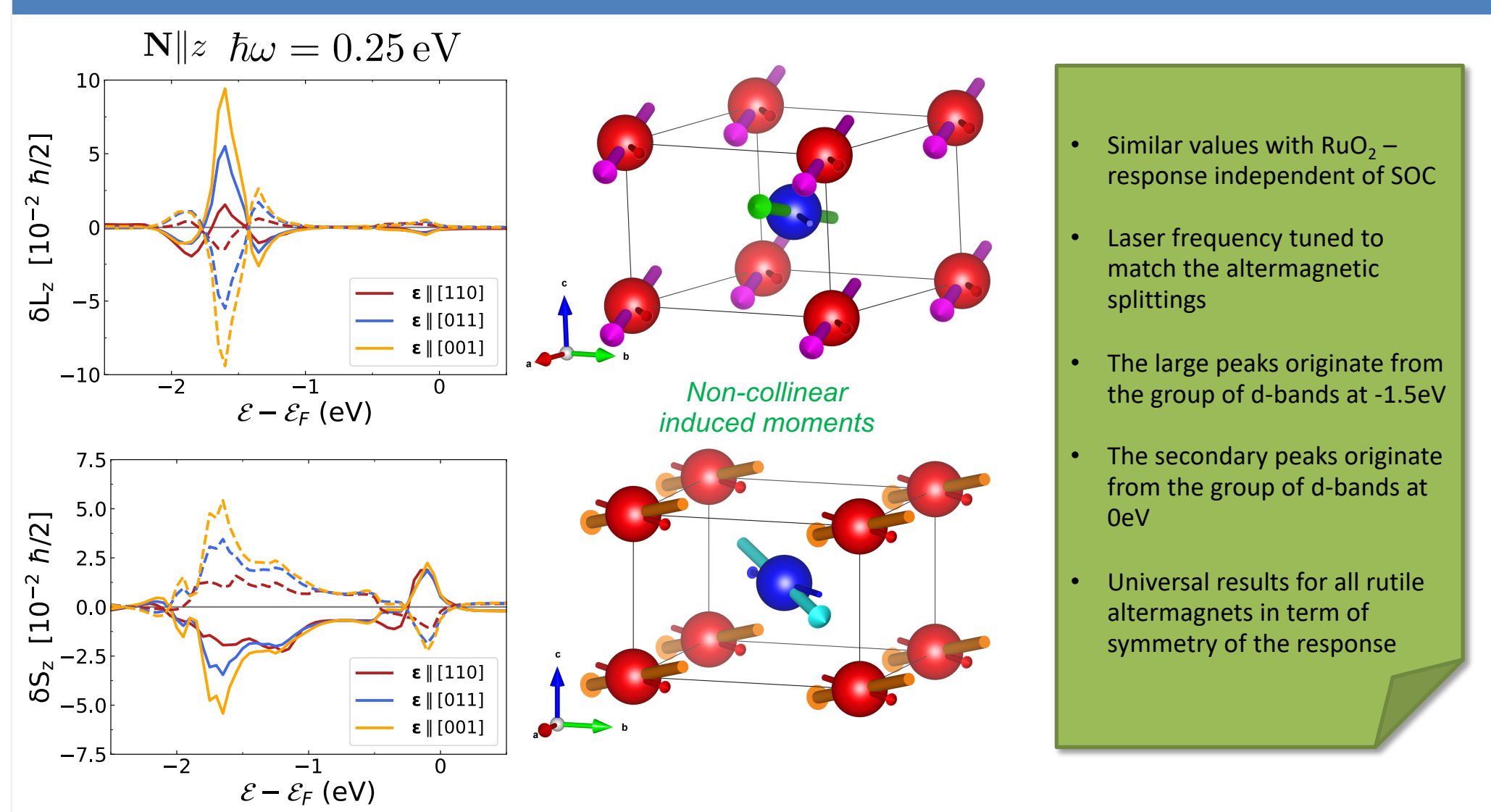
Studied systems



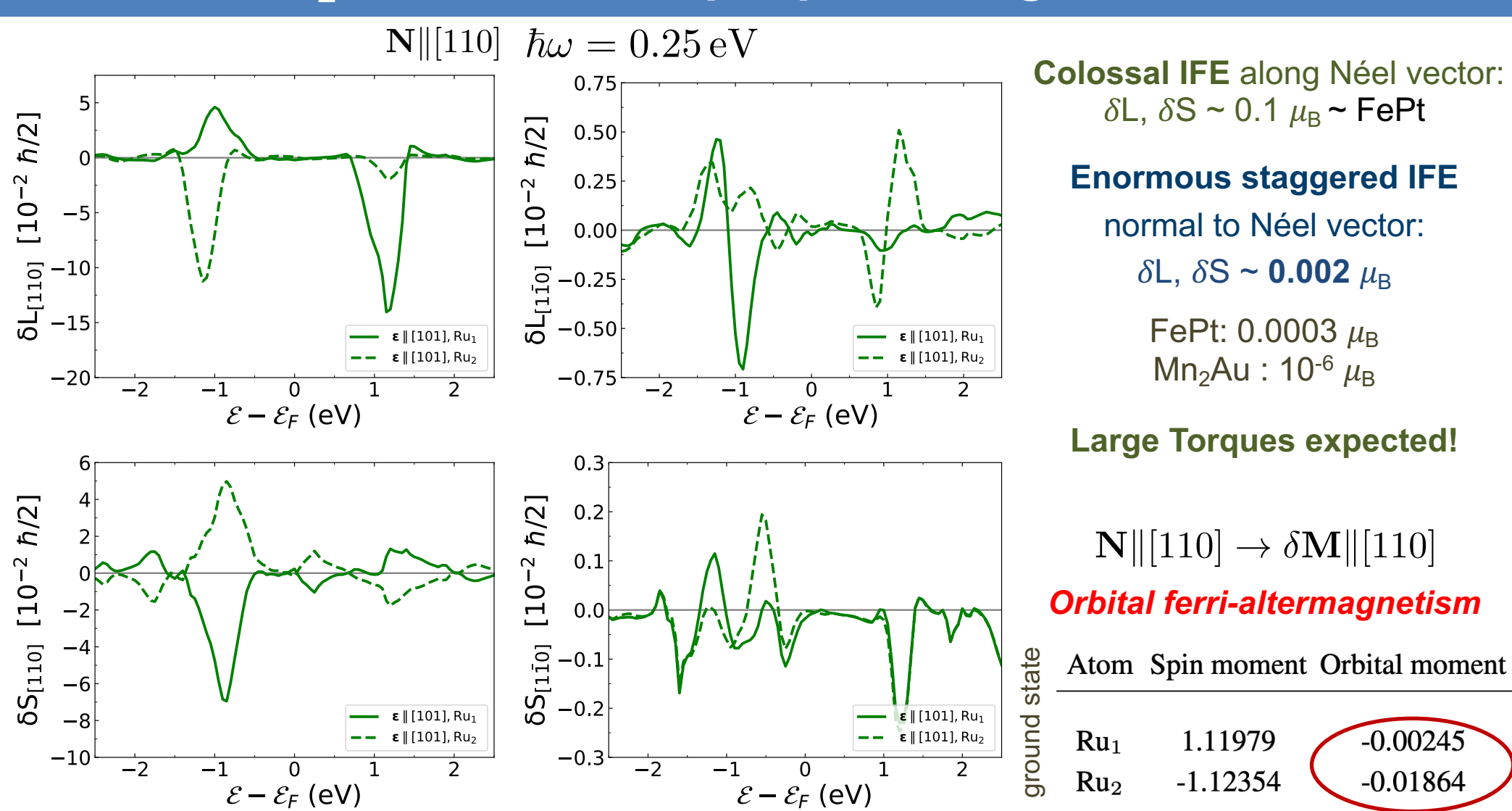
RuO₂ – non-relativistic orbital photomagnetization



CoF₂ – orbital and spin photomagnetizations



RuO₂ – orbital and spin photomagnetizations



Conclusions

- ✓ Altermagnets are a fruitful platform for exploiting the complexity of IFE
- ✓ The colossal magnitude of IFE can be further manipulated by the application magnetic fields or used for angular momentum injection
- ✓ The large IFE normal to the Néel vector may give rise to significant optical torques
- ✓ Orbital ferri-altermagnetism: the colossal light-induced orbital magnetism may be used for Néel order manipulation

References

- [1] L. Smejkal et al. PRX **12**, 040501 (2022)
- [2] Fleur code, see www.flapw.de
- [3] Wannier90, G. Pizzi et al., arXiv:1907.09788 (2019)
- [4] M. Merte et al., APL Mater. **11**, 071106 (2023)
- [5] F. Freimuth et al. PRB **94**, 144432 (2016)
- [6] T. Adamantopoulos et al., arXiv:2403.10235 (2024)