Spin and Orbital magnetism by light in rutile altermagnets

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TOPOLOGICAL NANOELECTRONICS

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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]. In the field of optical magnetism, it is still unclear to which extend 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 altermagents from first-principles.

Computational methods

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$\mathcal{TB}$-basis set

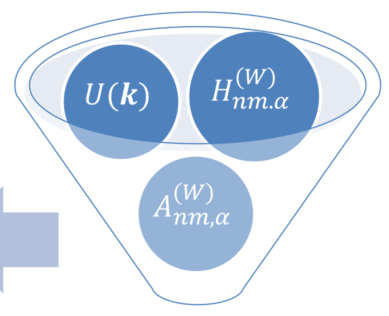
$\langle \mathbf{0}n|\hat{H}|\mathbf{R}m\rangle$

$\langle \mathbf{0}n|\hat{r}_\alpha|\mathbf{R}m\rangle$

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

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

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



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

Keldysh formalism

2nd order spin magnetization

- Response formula

LASER intensity — LASER polarization

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

- Response tensor

LASER frequency

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

- Retarded and Advanced Green's function

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

2nd order orbital magnetization

- Replace

$$\sigma_i \longrightarrow l_i$$

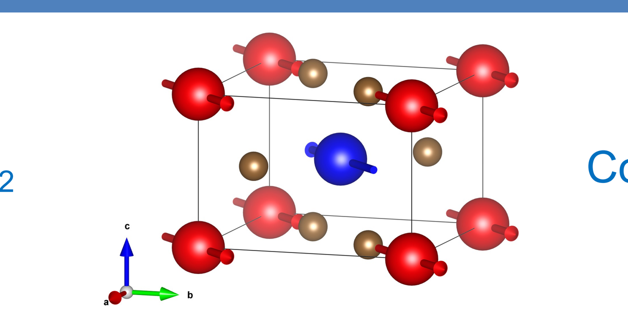
LASER

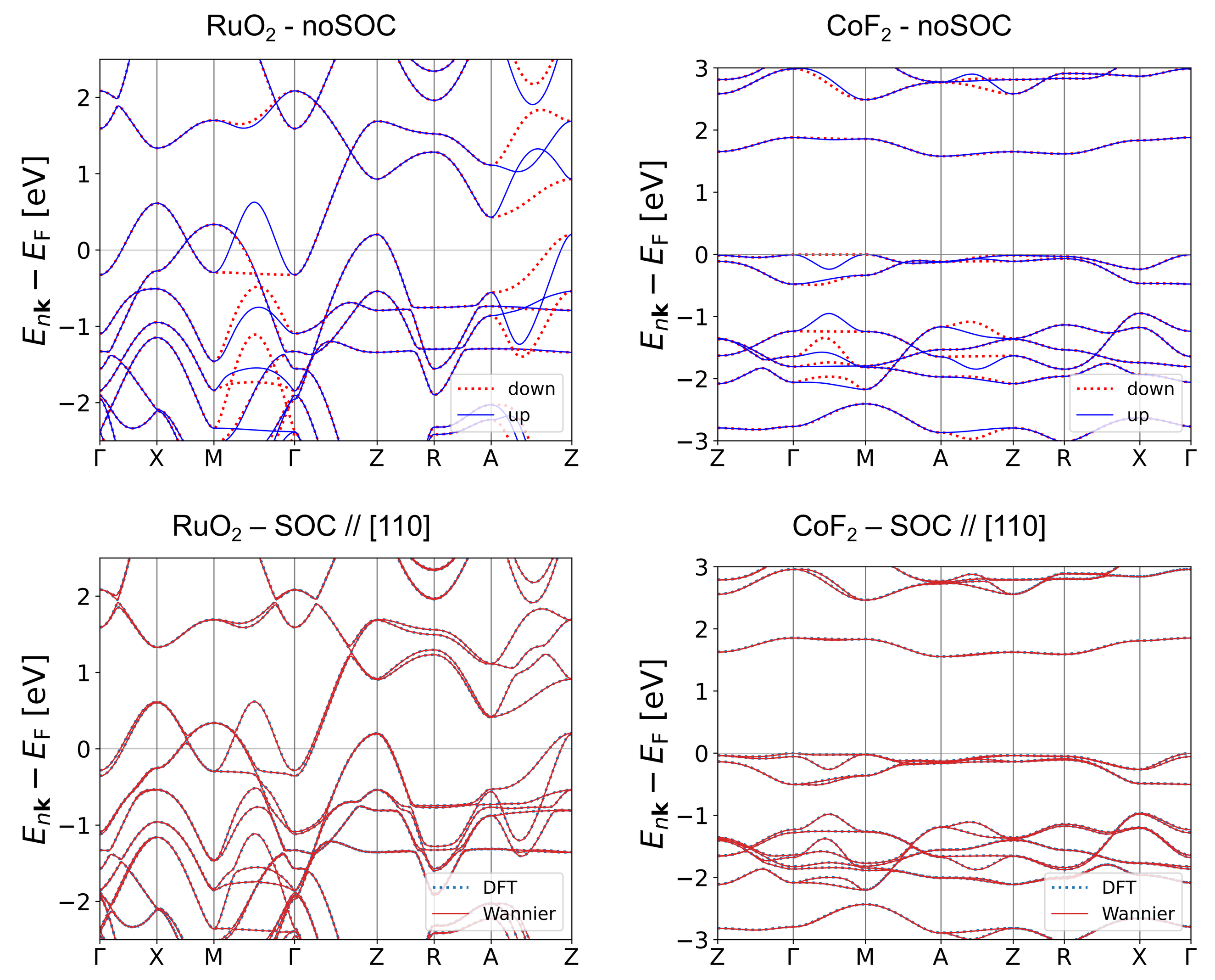
$\mathrm{I} = 10\ \mathrm{GWcm}^{-2}$

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

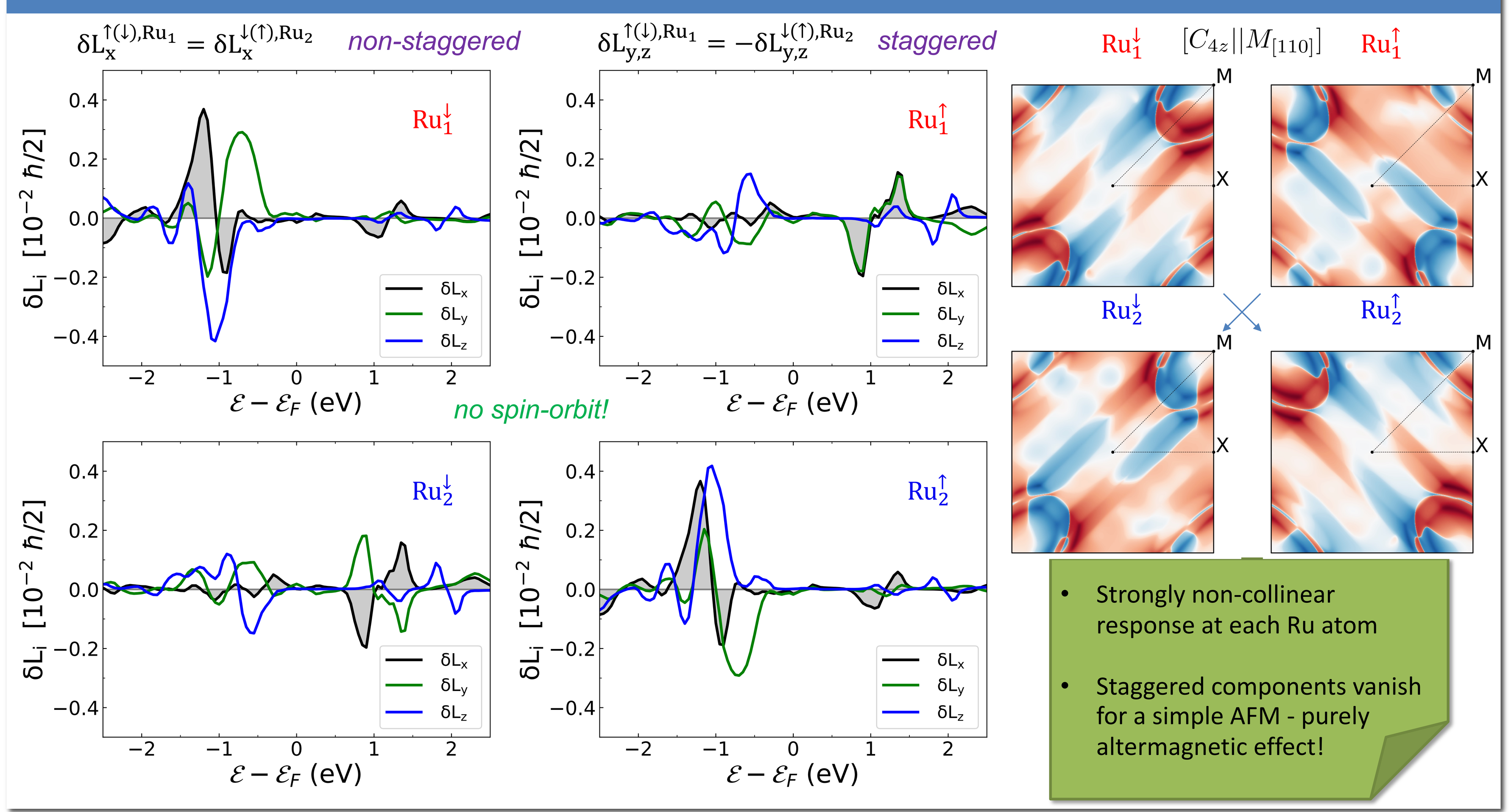
$\epsilon = (1, i\lambda, 0)/\sqrt{2}$

Studied systems



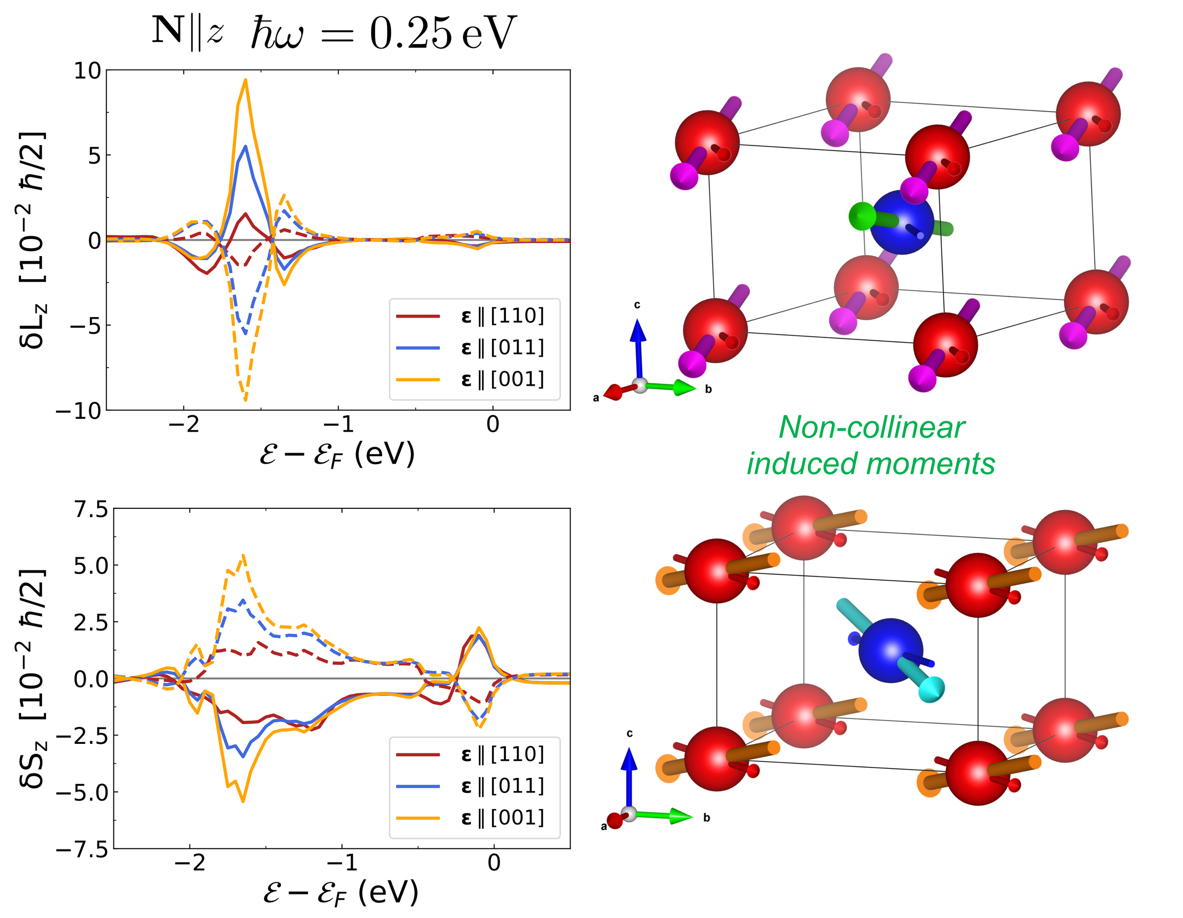


RuO_2 – non-relativistic orbital photomagnetization



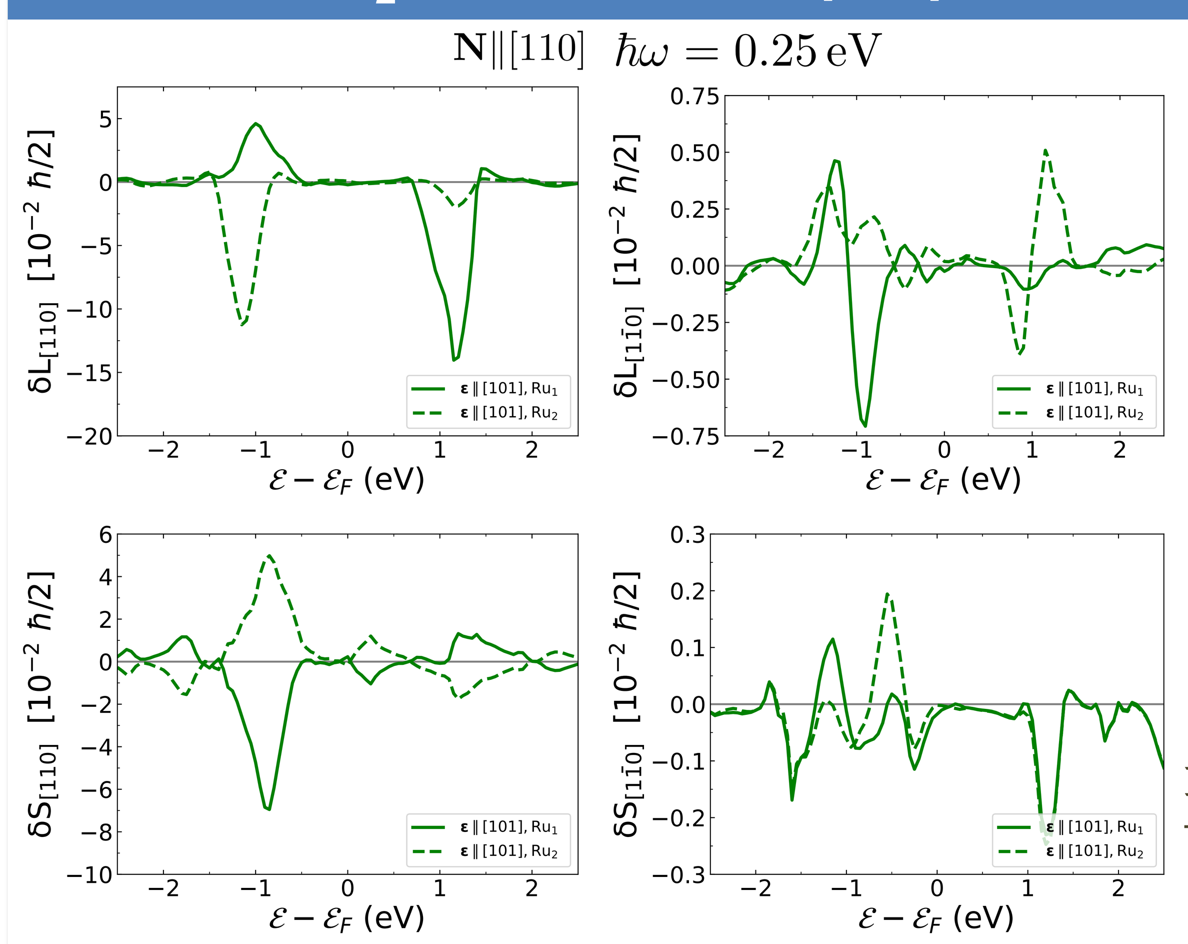
- Strongly non-collinear response at each Ru atom
- Staggered components vanish for a simple AFM - purely altermagnetic effect!

CoF_2 – orbital and spin photomagnetizations



- Similar values with RuO_2 – response independent of SOC
- Laser frequency tuned to match the altermagnetic splittings
- 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
- Universal results for all rutile altermagnets in term of symmetry of the response

RuO_2 – orbital and spin photomagnetizations



Colossal IFE along Néel vector: δL, δS ~ 0.1 μ_B ~ FePt

Enormous staggered IFE normal to Néel vector: δL, δS ~ **0.002** μ_B

FePt: 0.0003 μ_B
Mn_2Au : 10^{-6} μ_B

Large Torques expected!

$$\mathbf{N}\|[110] \rightarrow \delta\mathbf{M}\|[110]$$

Orbital ferri-altermagnetism

ground state

Atom	Spin moment	Orbital moment
Ru_1	1.11979	-0.00245
Ru_2	-1.12354	-0.01864

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

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