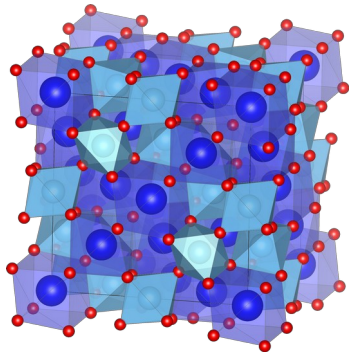


# Investigation of the crystal field in exotic spin phase materials by resonant inelastic x-ray scattering

Octave Duros

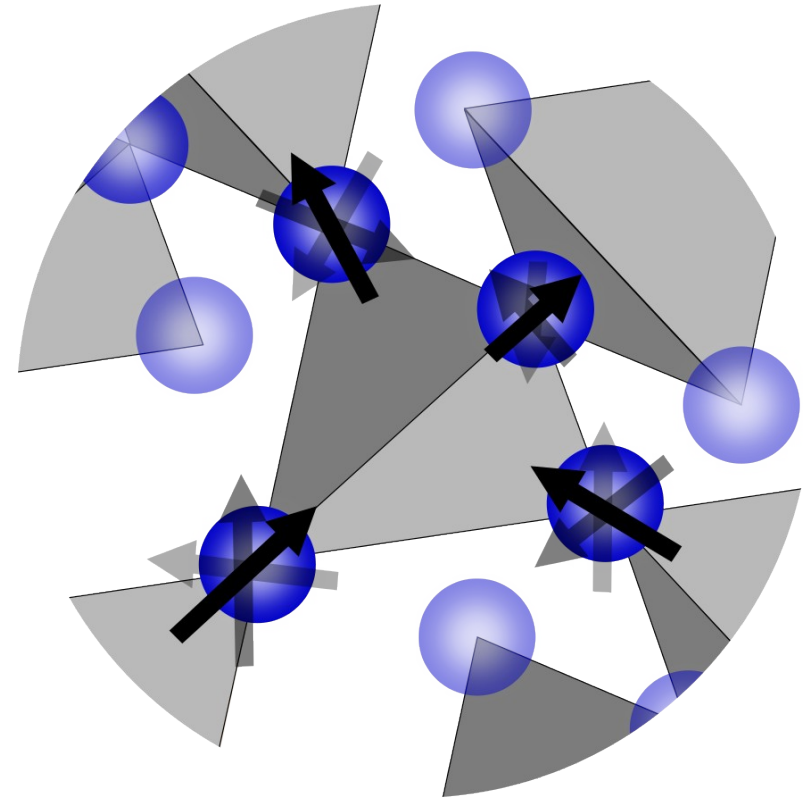
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# Context



- $R$  ion (metal)
- Titanium
- Oxygen (ligands)

- $R_2Ti_2O_7$  ( $R = \text{Sm, Tb, Dy, Ho, Er, Yb}$ ):  $Fd\bar{3}m$
- **Fascinating magnetic states:** spin liquid, spin glass or quantum spin ice<sup>[1, 2]</sup>
- Key ingredient: **crystal electric field (CEF)** acting on the  $R$  sites
- Objective: extract a precise description of CEF



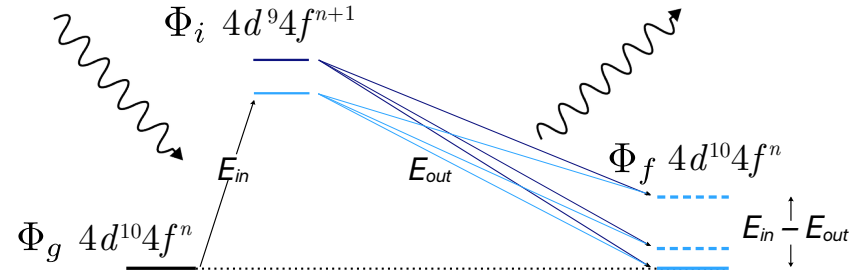
Close-up representation of the  $R$  sublattice

[1] S. T. Bramwell, Nat. Comm. **8**, 2088 (2017)

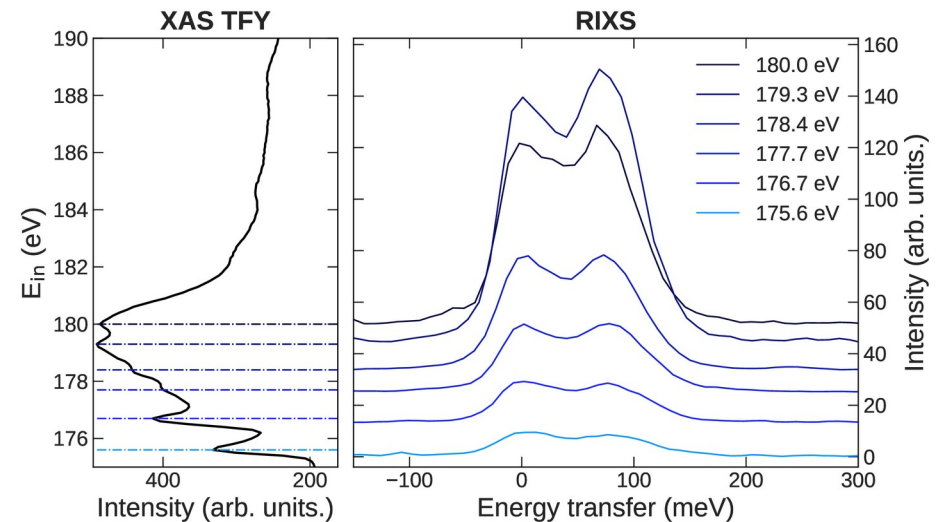
[2] S. R. Giblin *et al.*, Phys. Rev. Lett. **121**, 067202 (2018)

# Experimental observations

- $N_{4,5}$ -edge of rare earths: **first resonant inelastic x-ray scattering (RIXS) observation** of the CEF effect, acquired at SOLEIL (SEXTANTS beamline)<sup>[3,4]</sup>
- Complementary data recorded at the rare-earths  $M_5$  edge at MAX IV (Veritas beamline)
- Interpretation through **ligand field multiplet (LFM)** calculations with QUANTY program<sup>[5]</sup>:
  - Multiplet states  $\Phi_g$ ,  $\Phi_i$  and  $\Phi_f$  computation with **spin-orbit coupling** and **CEF**



CEF effect on  $\text{Yb}_2\text{Ti}_2\text{O}_7$  4f states



[3] M. Sacchi *et al.*, J. Phys.: Conf. Ser. **425**, 072018 (2013)

[4] G.S. Chiuzbăian *et al.*, Rev. Sci. Instrum. **85**, 4, 043108 (2014)

[5] M.W. Haverkort *et al.*, Phys. Rev. B **85**, 165113 (2012)

# Multiplet calculations

- Inclusion of the effective RIXS measurement conditions:

sample orientation, polarization, temperature

- Definition of the CEF as:

$$H_{\text{CEF}}^{D_{3d}} = B_0^2 C_0^2 + B_0^4 C_0^4 + B_3^4 (C_{-3}^4 - C_3^4) + B_0^6 C_0^6 + B_3^6 (C_{-3}^6 - C_3^6) + B_6^6 (C_{-6}^6 + C_6^6)$$

Parameter	Bertin $A_q^k$ (meV)	Duros $A_q^k$ (meV)
$A_0^2$	55	115
$A_0^4$	222	275
$A_3^4$	-84	6
$A_0^6$	71	122
$A_3^6$	57	50
$A_6^6$	63	50

- Want to know more? Have a chat with us at our poster!

CEF effect on  $\text{Yb}_2\text{Ti}_2\text{O}_7$  4f states

