Investigation of the crystal field in rare earth titanate pyrochlores by resonant inelsatic x-ray scattering

Octave Duros, Christian Brouder, Renaud Delaunay, Hebatalla Elnaggar, Romain Jarrier, Amelie Juhin, Gheorghe S Chiuzbaian

iMAT

Investigation of the crystal field in rare earth titanate pyrochlores by resonant inelastic x-ray scattering

Octave Duros[1,2] • Supervisors: Gheorghe Sorin Chiuzbăian[1], Amélie Juhin[2]

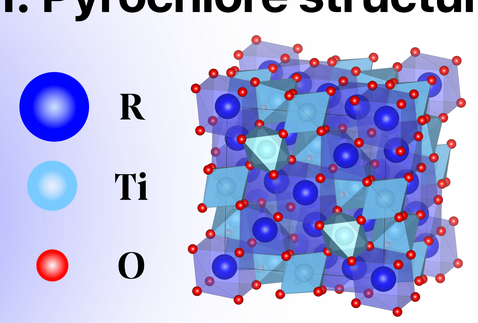
Context

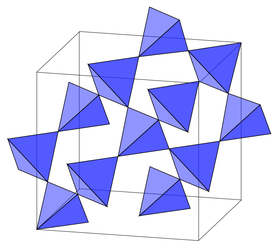
• Rare earth (R) titanate pyrochlores act as **geometrically frustrated magnets**, leading to a **wide variety of magnetic behaviors**.

• Frustated magnets are due to the presence of a **crystal electric field** (CEF) acting on the **R** sites.

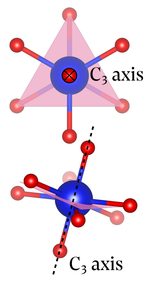
• Quantum spin liquids, spin ices and spin glasses can be observed depending on the rare-earth R.

1. Pyrochlore structure: $R_2Ti_2O_7$





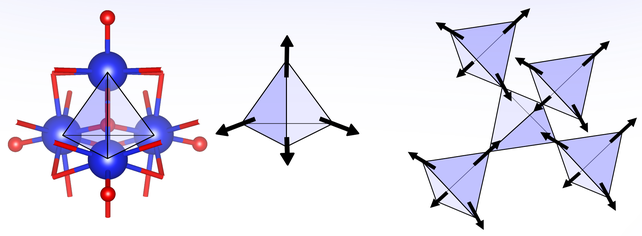
R atoms create a tetrahedra corner-sharing lattice



C_3 axis on the R site

• Crystal lattice with interpenetrating **corner-sharing sub-lattices**;
• **R** sites present a main **C3 axis**.

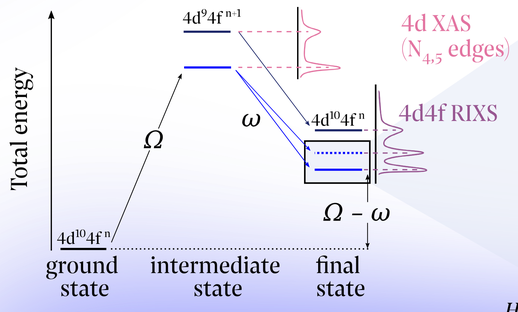
2. Crystal electric field

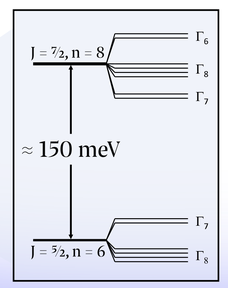


A tretrahedron element and its neighbors, with unaligned spins at the tops

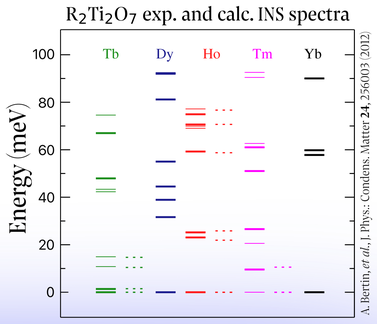
• CEF is a perturbation of the **R** electrons cloud by all the electrons of the system;
• It forces the magnetic moment J to **align along** the **C3 main axis** instead of the antiferromagnetic order.
• CEF potential can be defined as a sum of Stevens parameters: $H_{tri}^{CEF} = B_2^0 C_2^0 + B_4^0 C_4^0 + B_4^3 C_4^3 + B_6^0 C_6^0 + B_6^3 C_6^3 + B_6^6 C_6^6$

3. Resonant inelastic x-ray scattering (RIXS)



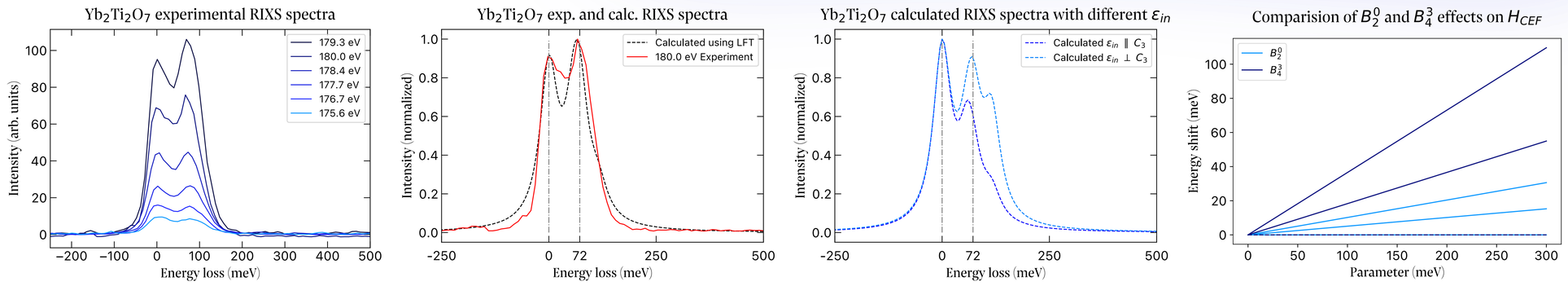


How CEF can split orbitals



• **High-resolution** RIXS allows **probing the CEF** for the first time;
• **Complementary** to Inelastic Neutrons Scattering (INS): RIXS can probe higher-lying excited states (few eV), eventually leading to a precise definition of H_{tri}^{CEF}.

4. Simulations, analysis



• Simulations run through **Quanty** software package: **Ligand Multiplet Theory** calculations with CEF contribution;
• Good agreement of the simulations with experimental data;
• RIXS spectra are **strongly dependent on the polarization** ε_{in}.

5. Conclusion and outlook

• First observation of the CEF effect in pyrochlore crystals at the $N_{4,5}$ resonances with RIXS.
• Promising results with first agreements between calculated and experimentally acquired spectra (RIXS and INS).
• Working on the precise parametrization of the Stevens Operators coefficients ($B_\mu^k C_\mu^k$).

Aknowledgments: Christian Brouder[2], Renaud Delaunay[1], Hebatalla Elnaggar[2], Romain Jarrier[1]

1: Laboratoire de Chimie Physique – Matière et Rayonnement, Sorbonne Université, UMR CNRS 7614, Paris, France
2: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université, UMR CNRS 7590, Paris, France

SCIENCES SORBONNE UNIVERSITÉ
cnrs
Institut de science des matériaux
ALLIANCE SORBONNE UNIVERSITÉ