



HAL
open science

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

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

► To cite this version:

Octave Duros, Christian Brouder, Renaud Delaunay, Hebatalla Elnaggar, Romain Jarrier, et al.. Investigation of the crystal field in rare earth titanate pyrochlores by resonant inelastic x-ray scattering. SUCCESS-2022, Aug 2022, Les Houches, France. . hal-03941780

HAL Id: hal-03941780

<https://hal.sorbonne-universite.fr/hal-03941780>

Submitted on 16 Jan 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

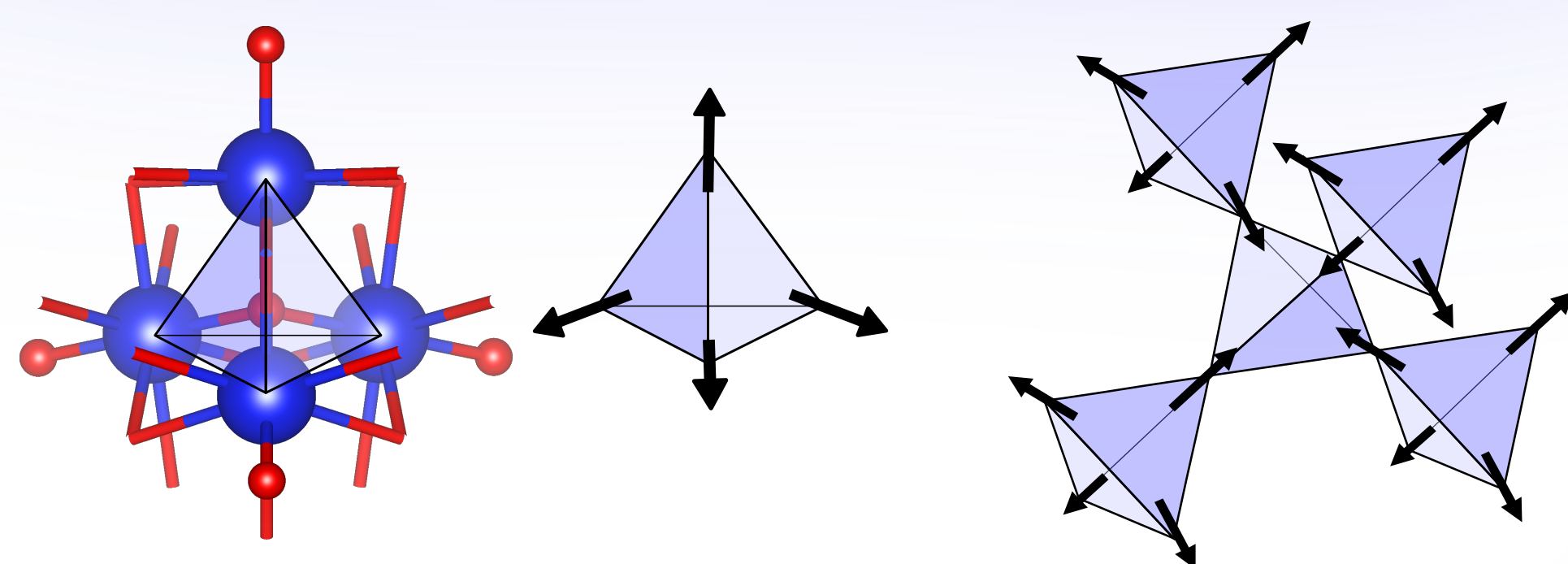
Investigation of the crystal field in rare earth titanate pyrochlores by resonant inelastic x-ray scattering

Octave Duros^{1,2} • Supervisors: Gheorghe Sorin Chiuzbăian¹, Amélie Juhin²

Context

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

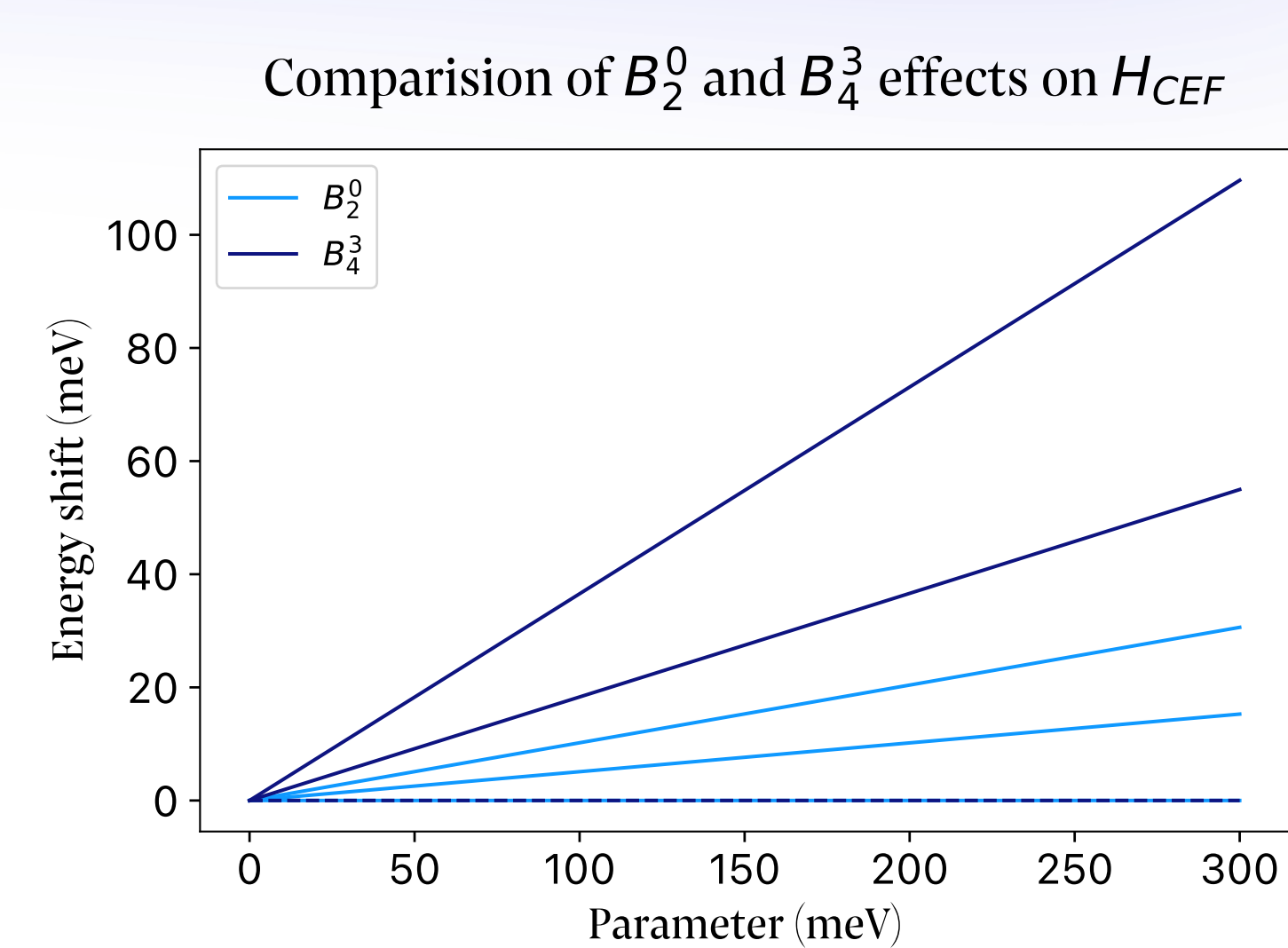
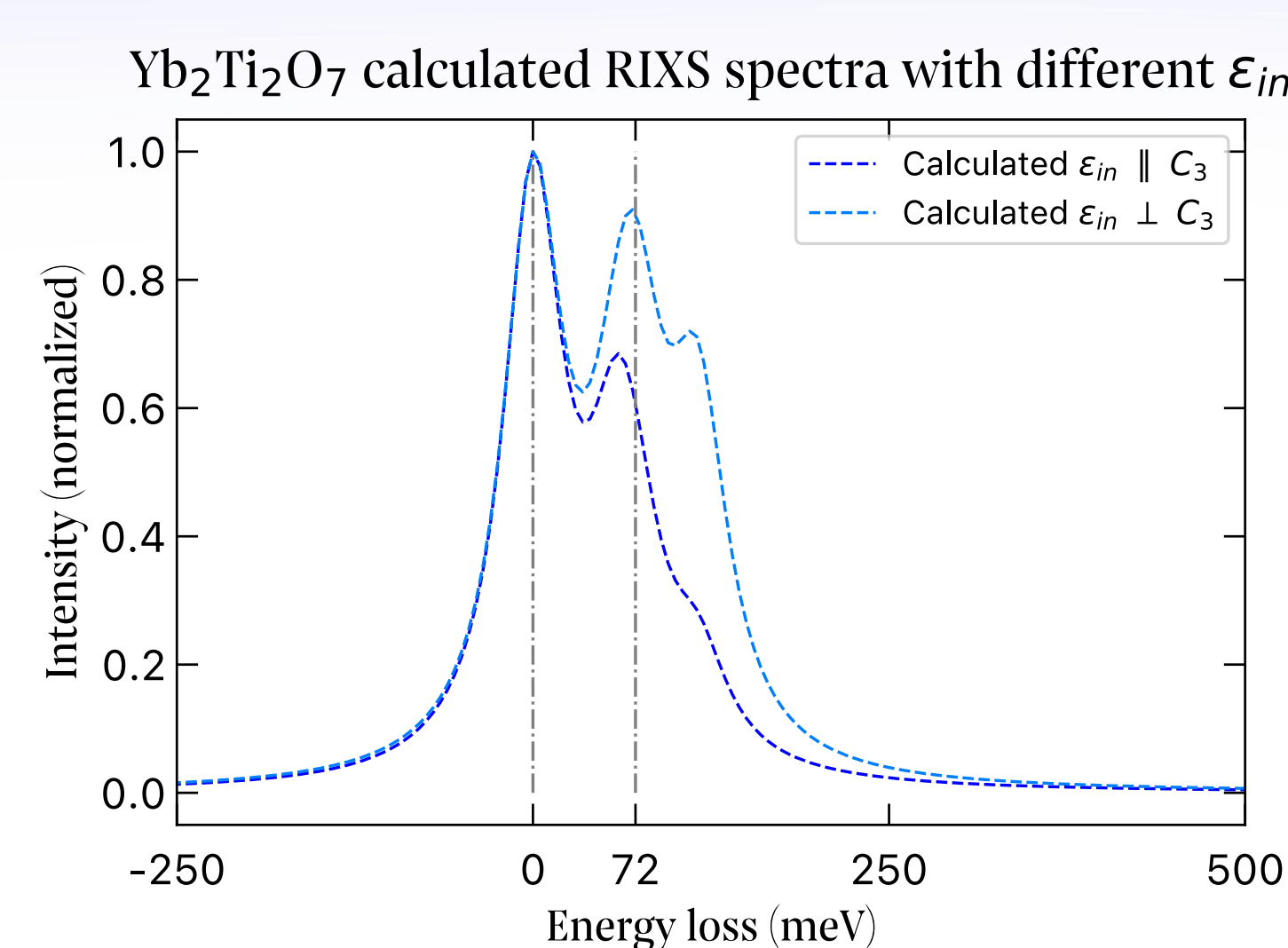
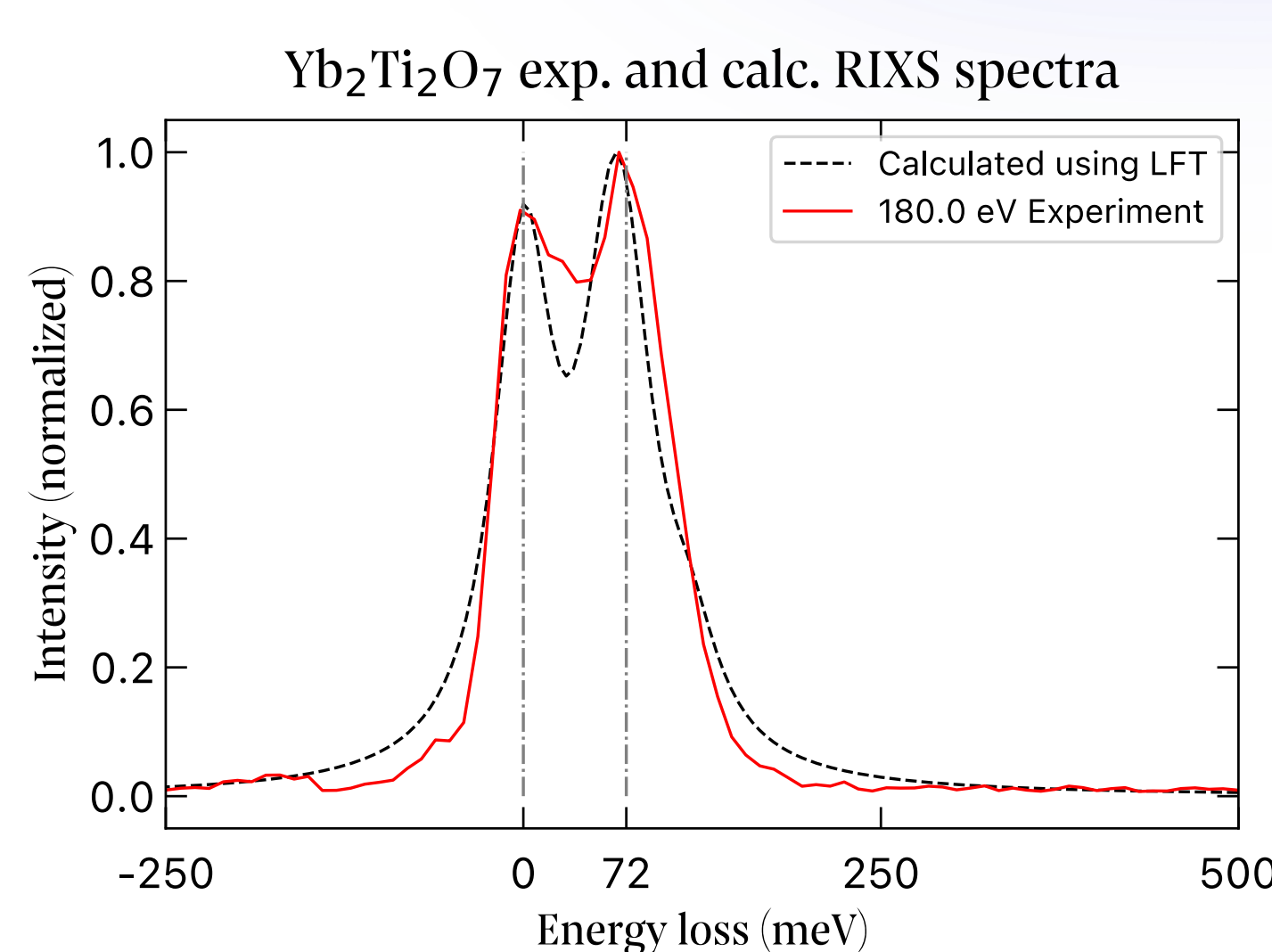
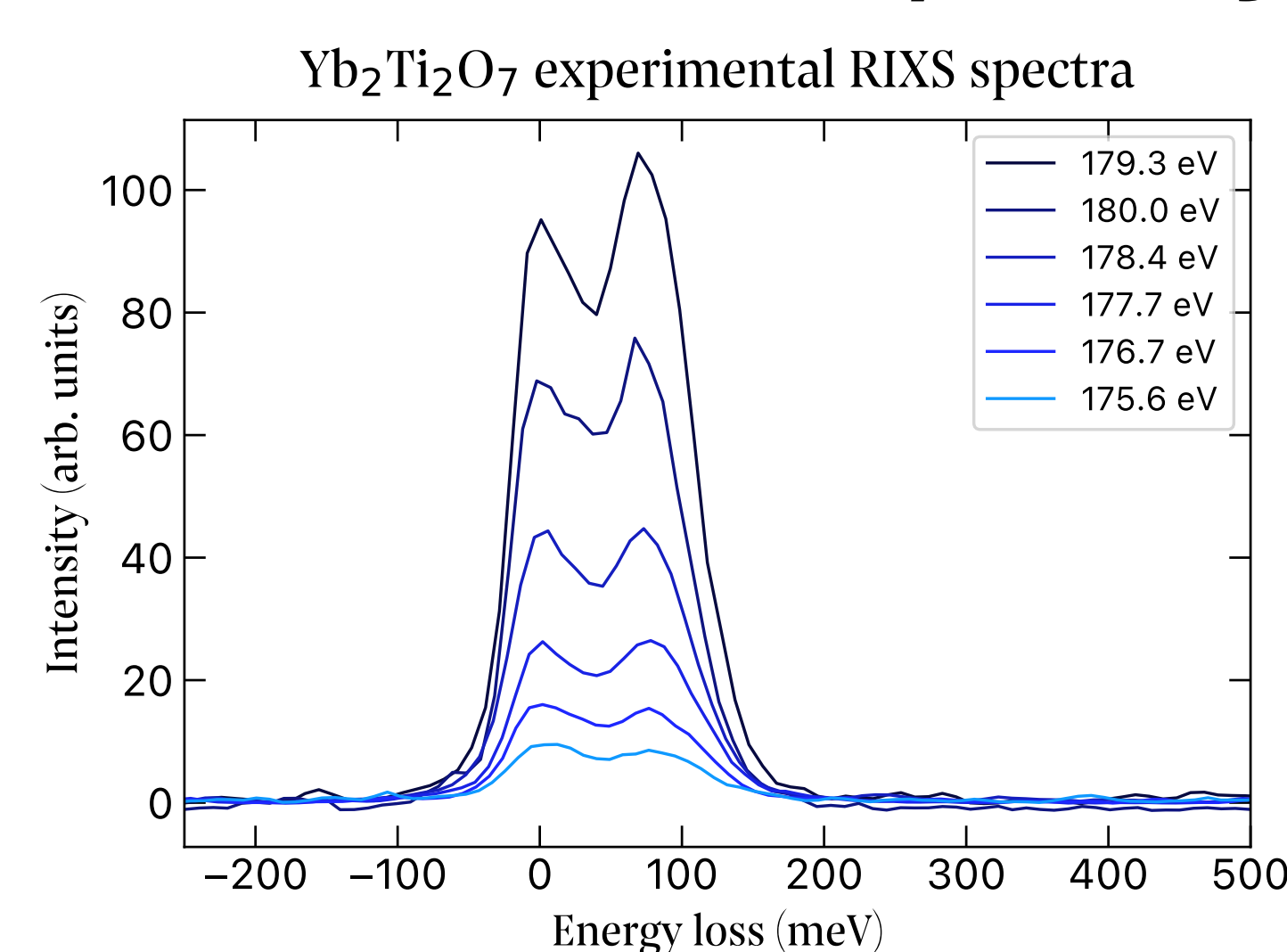
2. Crystal electric field



A tetrahedron 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: $H_{tri}^{CEF} = B_2^0 C_2^0 + B_4^0 C_4^0 + B_4^3 C_4^3 + B_6^0 C_6^0 + B_6^3 C_6^3 + B_6^6 C_6^6$

4. Simulations, analysis

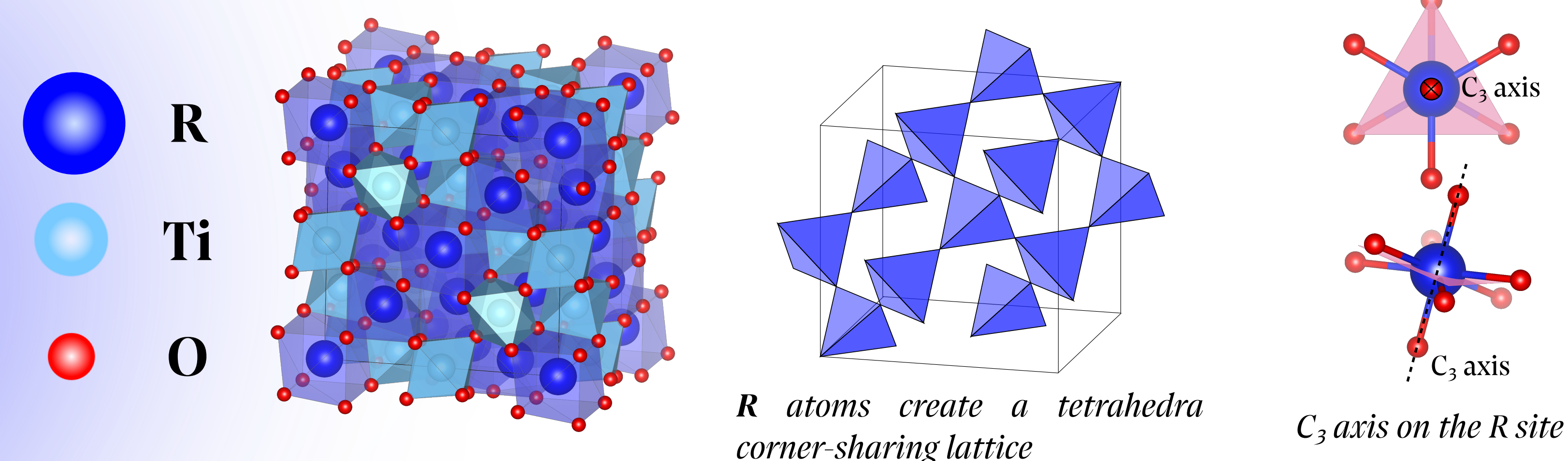


- Simulations run through **Quanty** software package: **Ligand Multiplet Theory** calculations with CEF contribution;
- Good agreement of the simulations with experimental data;
- RIXS spectra are **strongly dependent on the polarization ϵ_{in}** .

5. Conclusion and outlook

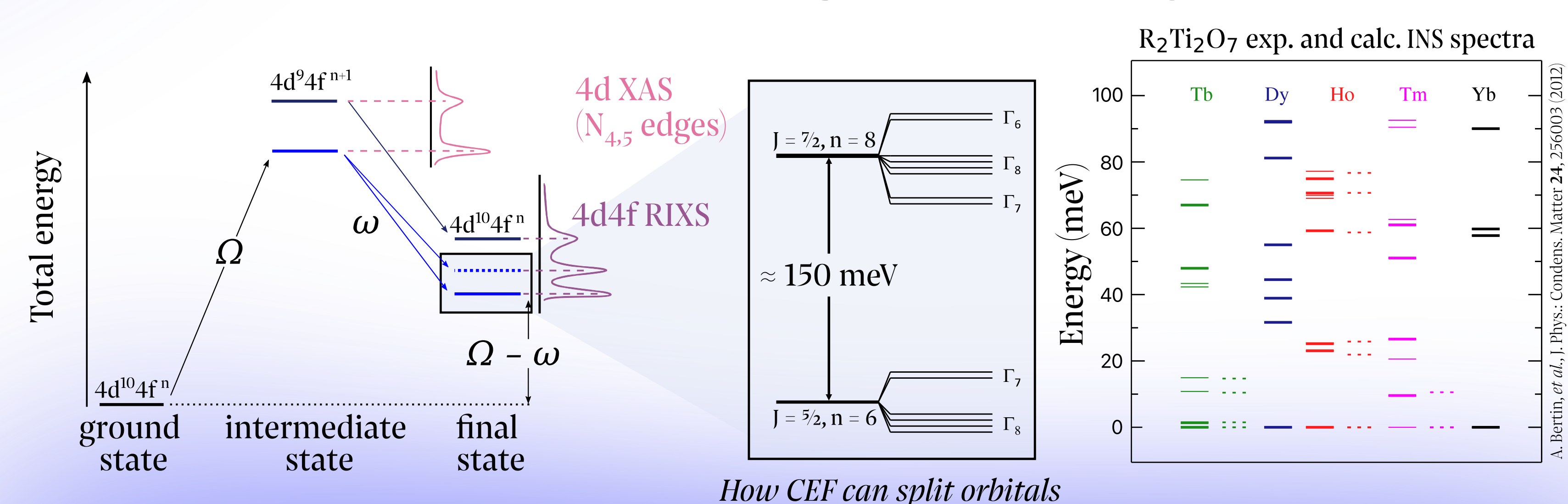
- First observation of the CEF effect in pyrochlore crystals at the N_{4,5} resonances with RIXS.
- Promising results with first agreements between calculated and experimentally acquired spectra (RIXS and INS).
- Working on the precise parametrization of the Stevens Operators coefficients ($B_{\mu}^k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

1. Pyrochlore structure: R₂Ti₂O₇



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

3. Resonant inelastic x-ray scattering (RIXS)



- **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} .

Aknowledgments: Christian Brouder², Renaud Delaunay¹, Hebatalla Elnaggar², Romain Jarrier¹

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