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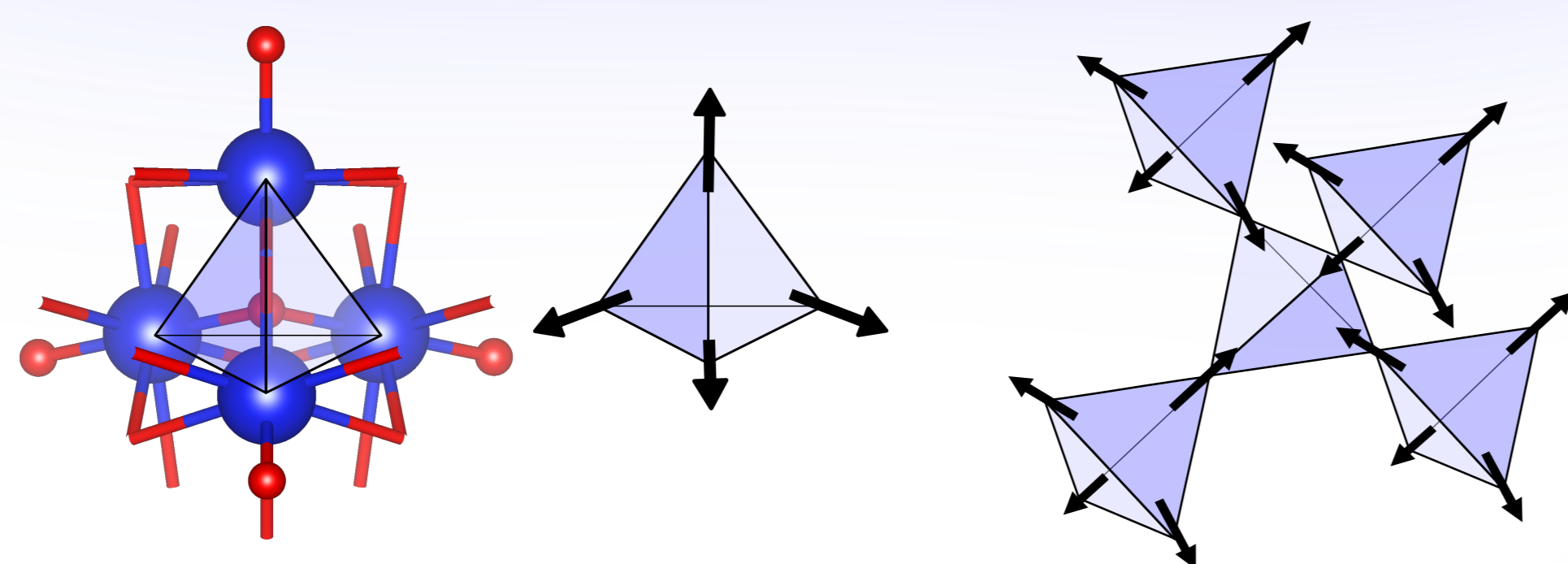
Investigation of the crystal field in rare earth titanate pyrochlores by resonant inelastic x-ray scattering

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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.

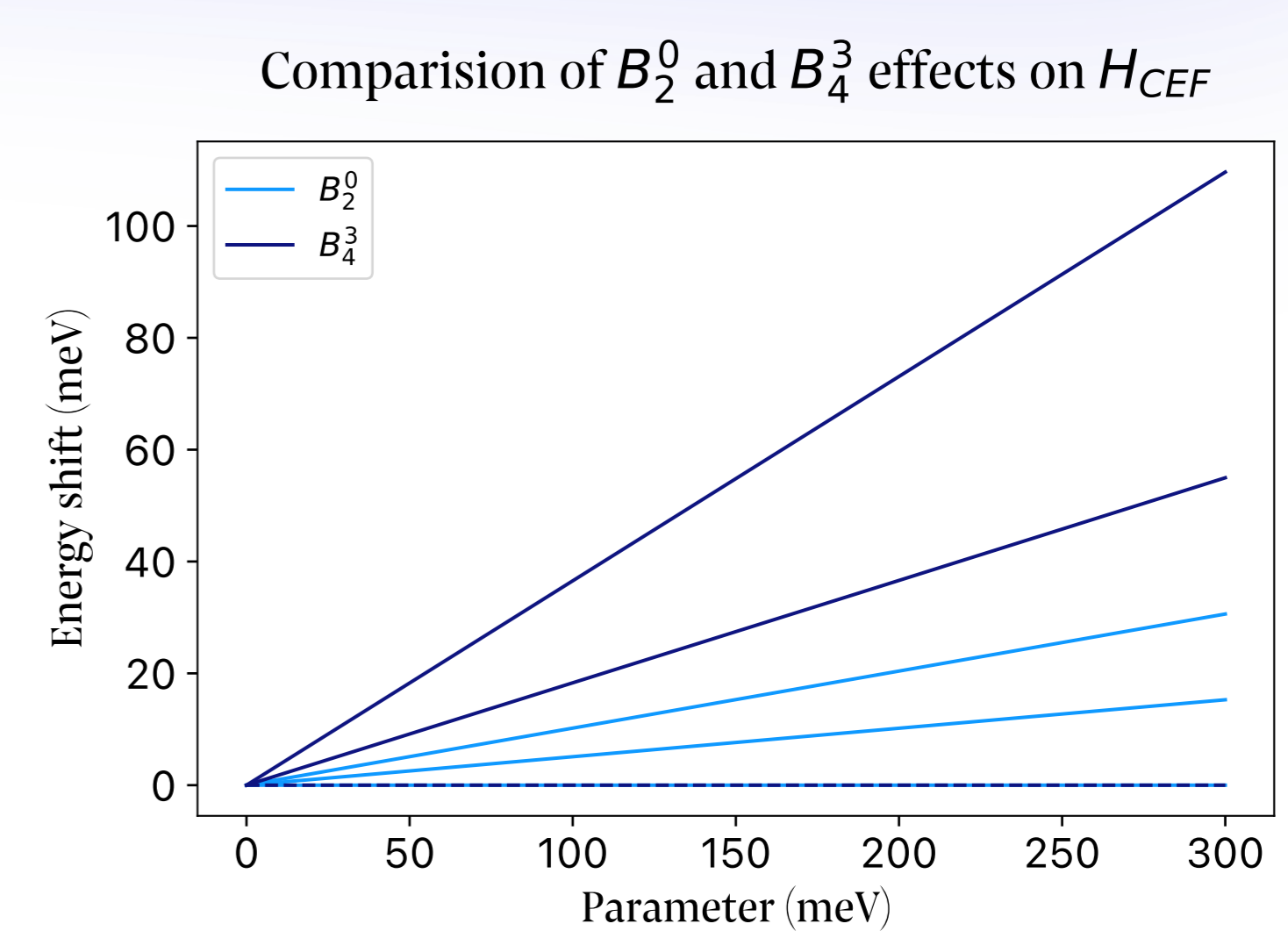
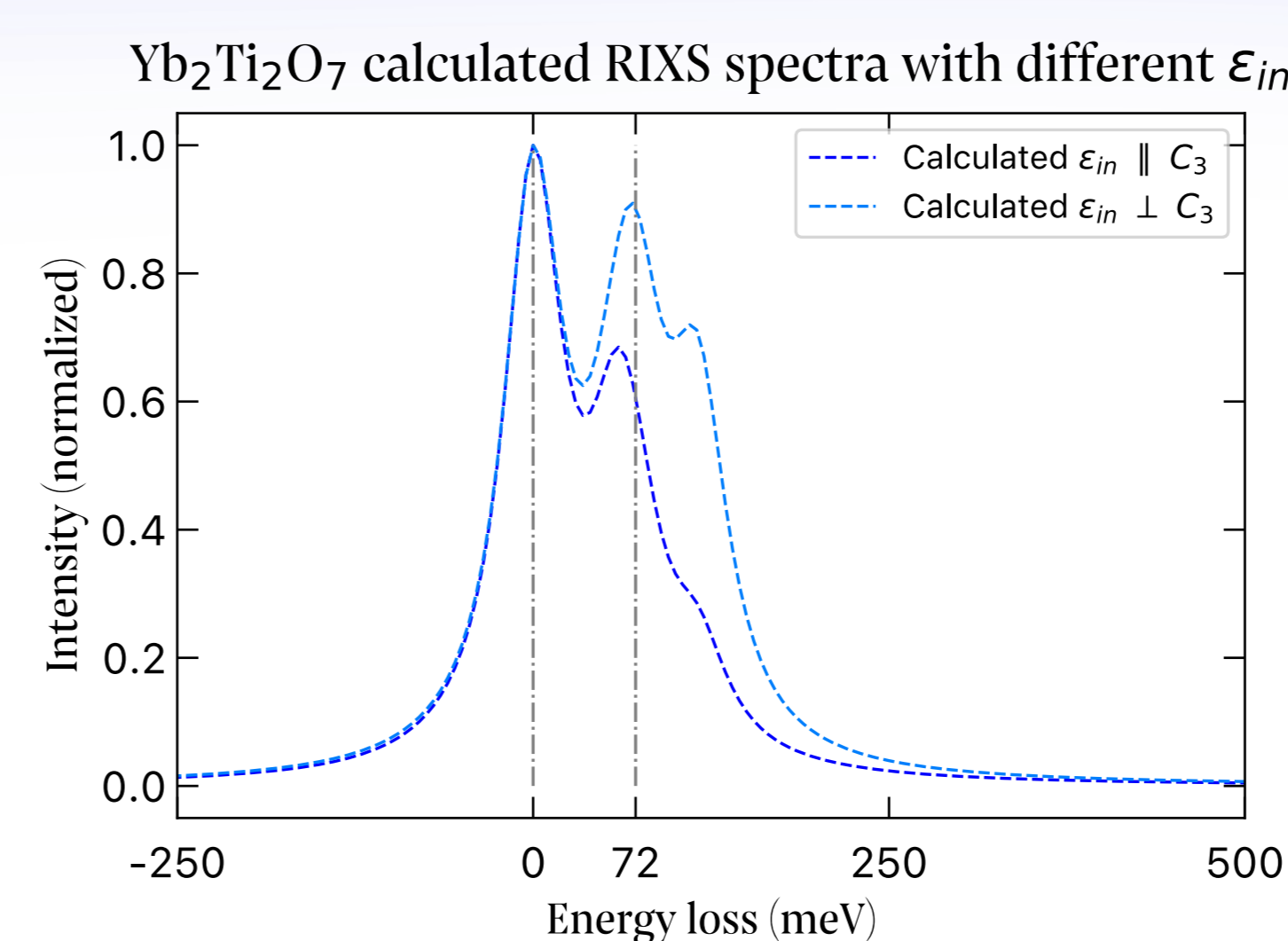
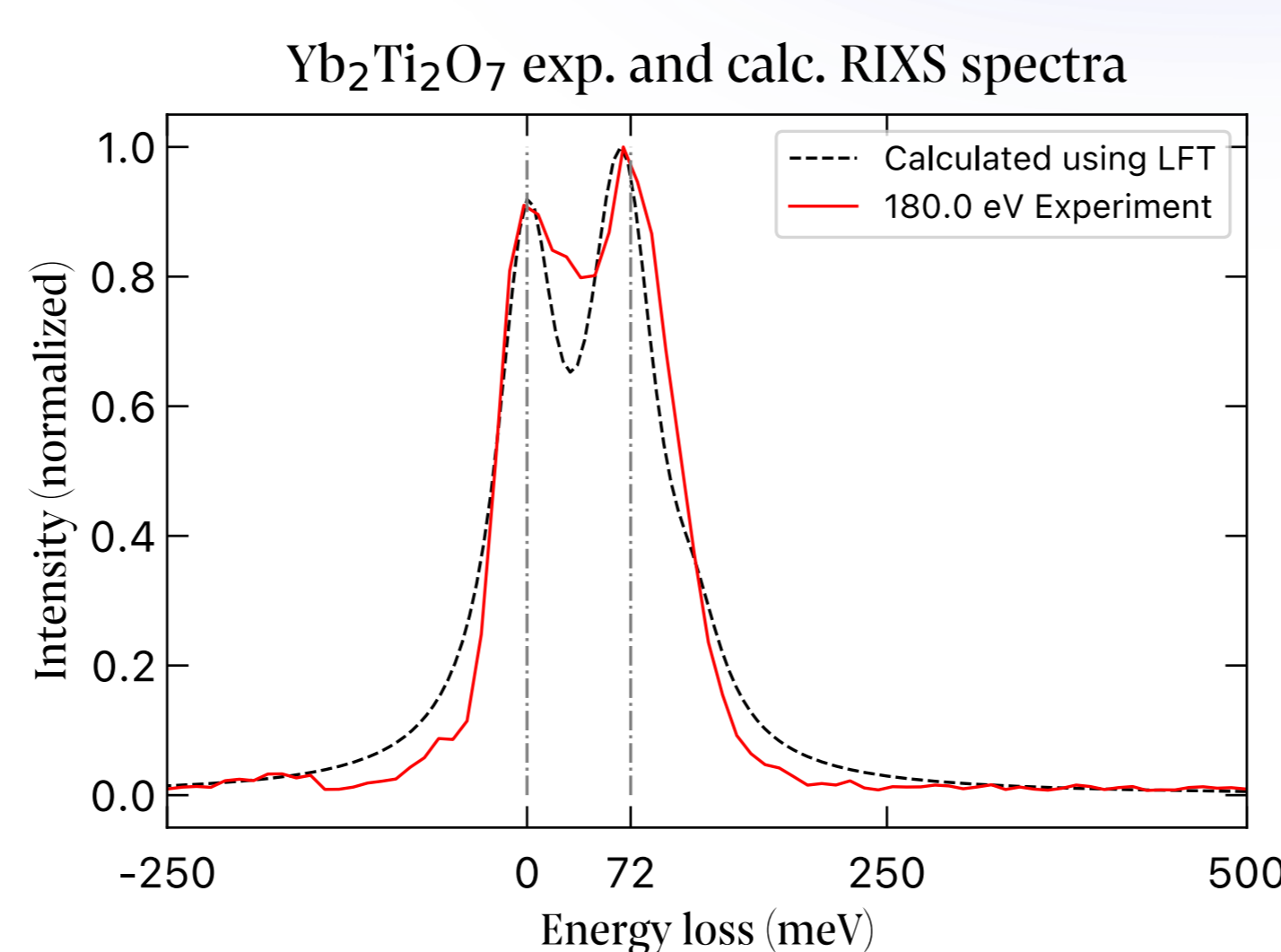
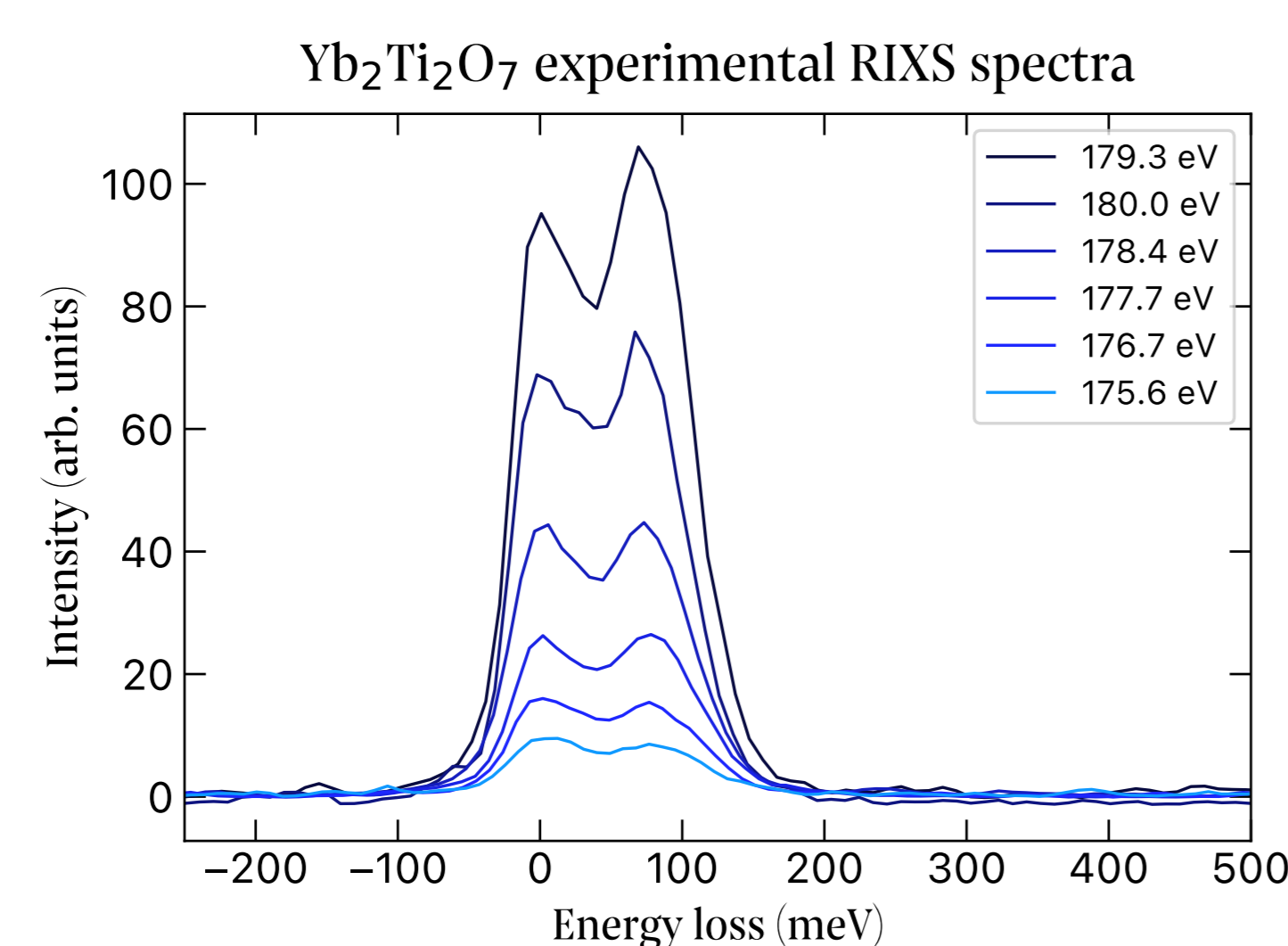
2. Crystal electric field



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

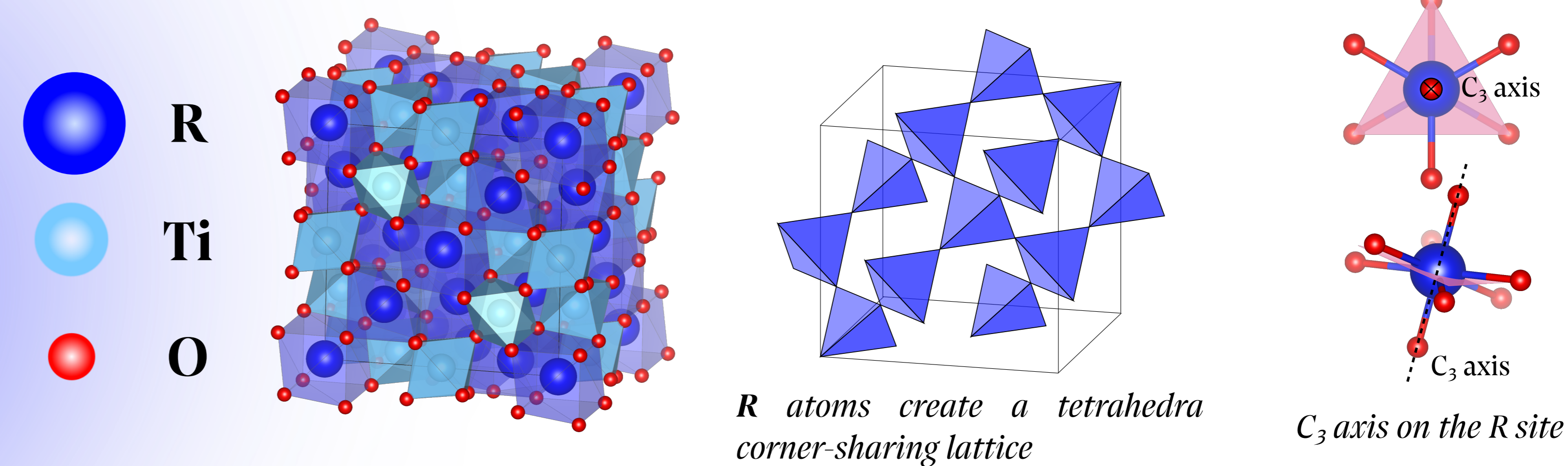


- Simulations run through **Quanty** software package: **Ligand Multiplet Theory** calculations with CEF contribution;
- Good agreement of the simulations with experimental data;
- RIXS spectra are **strongly dependent on the polarization ϵ_{in}** .

5. Conclusion and outlook

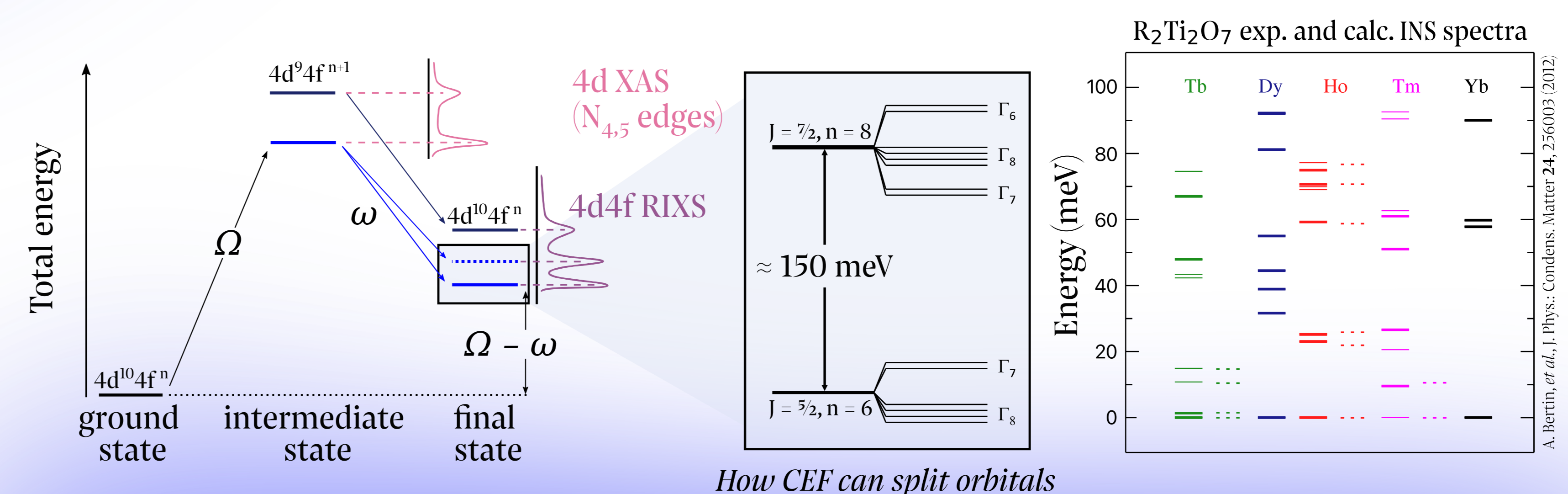
- First observation of the CEF effect in pyrochlore crystals at the $N_{4,5}$ resonances with RIXS.
- Promising results with first agreements between calculated and experimentally acquired spectra (RIXS and INS).
- Working on the precise parametrization of the Stevens Operators coefficients ($B_{\mu}^k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

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

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