General objectives

Calculations and methodological developments in modeling the optical properties of lanthanide systems.

Objectives for 2022 stage:

Stage 1 – From models to materials

Mutations and extensions in hybrid DFT computational strategies (DFT – Density Functional Theory) and plane waves (PW), towards a new generation of ligand field models (LF).
Obj 1.1. - Non-standard plane wave (PW) calculations involving fractional orbital populations of f-type bands.
Obj 1.2. - Development of new ligand field models.

- Conference participations

Objectives for 2023 stage:

Stage 2 - New Perspective and Prospective Insights in lanthanide phosphor materials. Selected case studies. Multi-determinant Wave Function calculations on lanthanide cluster models. A new generation of Ligand Field models. Non-holohedral LF effective Hamiltonians.

Obj 2.1. - Methodological developments in DFT & LF modeling strategies. DFT+U+J calculations, estimation of spin-orbit (SO) coupling effects in DFT&LF calculations.
Obj 2.2. - Plane-Wave calculations (PW) on lanthanide lattices selected from oxides, halides, silicates or phosphates. Corroboration of DFT results with LF-multilayer modeling of optical properties.
Obj 2.3. - Multiconfigurational WFT calculations on molecular and cluster structures. Adaptation of cluster systems according to phosphorescent lanthanide material networks. Non-routine procedures for assembling molecular orbitals from fragment components.

- 4 ISI articles

- 1 book chapter

- Conference participations