General objectives

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

Obj. 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. 2. New Perspective and Prospective Insights in lanthanide phosphor materials. Selected case studies.
Obj. 3. Multi-determinant wave function computations on cluster models with lanthanides.

Obj. 4. A new generation of ligand field models.

Obj. 5. A versatile model: the spherically mediated atom in the lattice, self-consistent treatment of the populations.

Stage 1. May – December 2022

Obj. 1. – part 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. 4. – part 1. A new generation of ligand field models.

Act. 1.1. - Non-standard plane wave (PW) calculations involving fractional orbital populations of f-type bands. PW calculations using codes like VASP, Abinit and similar. Methodologies for adjusting the interelectronic parameter DFT+U.

Act. 1.2. - Development of new ligand field models. Development and testing codes for DFT, WFT data processing and multilayer LF modeling, in Fortran, MATLAB-octave and/or Mathematica software.

- Conference participations.

Stage 2. January – December 2023

Obj. 1. – part 2. 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. 2. – part 1. New Perspective and Prospective Insights in lanthanide phosphor materials. Selected case studies.

Obj. 3. – part 1. Multi-determinant wave function computations on cluster models with lanthanides.

Act. 2.1. - Methodological developments in DFT & LF modelling strategies. DFT+U+J calculations, estimation of spin-orbit (SO) coupling effects in DFT&LF calculations.
Act. 2.2. - Plane-Wave calculations (PW) on lanthanide lattices selected from oxides, halides, silicates or phosphates. Corroboration of DFT results with LF-multilayer modelling of optical properties.
Act. 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

Stage 2. January – December 2024

Obj. 2. – part 2. New Perspective and Prospective Insights in lanthanide phosphor materials. Selected case studies.
Obj. 3. – part 2. Multi-determinant wave function computations on cluster models with lanthanides.

Obj. 4. – part 2. A new generation of ligand field models.

Obj. 5. A versatile model: the spherically mediated atom in the lattice, self-consistent treatment of the populations.

Act. 3.1. Calculations and models for lanthanide systems with high entropic organization. Effective modeling of disorder and structural variety in the condensed phase.

Act. 3.2. Complete Active Space (CAS) calculations on lanthanide systems and corroboration with extended Ligand Field models. Estimation of spin-orbit (SO) coupling in CAS calculations and LF model. Simulation of spectral states through original codes (in MATLAB or Fortran).

Act. 3.3. Modeling of the atom in the network with application in estimating the optical properties of phosphorescent materials based on lanthanides. Implementation of the spherically averaged free atom model – verification by CAS calculations. Developing a code for the Madelung potential of the network. Development of the algorithm and code for the spherical atom in the self-consistent Madelung potential.

- 4 ISI articles

- 1 book chapter

- Conference participations

- Workshop