

PhD thesis at the University of Bordeaux from Fall 2022 (36 months)

ANR funding, in collaboration with IMPMC (Paris) and the SOLEIL and ESRF synchrotrons

Topic: Probing chirality with X-rays: Molecular materials for XNCD and RIXS-NCD spectroscopies

Thesis objectives: Synthesis and crystallization of chiral coordination compounds for the study of X-ray Natural Circular Dichroism and Resonant Inelastic X-ray Scattering Natural Circular Dichroism

Abstract: In the XIMTEX ANR project, we will develop tools to simulate XNCD (X-ray Natural Circular Dichroism) and RIXS-NCD (Resonant Inelastic X-ray Scattering Natural Circular Dichroism) spectra based on original experimental datasets collected on crystal-state chiral coordination complexes. The proposed systems have been designed to answer fundamental questions regarding the influence of electronic structure and local symmetry on the shape and intensity of XNCD and RIXS-NCD spectra.

XIMTEX assembles chemists and physicists from the ICMCB UMR 5026 and the IMPMC UMR 7590, as well as from the SOLEIL and ESRF synchrotrons, with the aim of unlocking the potential of XNCD and RIXS-NCD spectroscopy for materials characterization. This will be done by the selection and fabrication of model compounds, the collection of benchmark XNCD data, the use of these data to identify the important parameters in the simulation of the spectra, leading to software that can be used by the broader scientific community working in X-ray optical activity.

The focus of this thesis will be the preparation and crystallographic characterization of chiral coordination complexes in the solid state. The student will learn techniques in coordination chemistry synthesis and characterization, including synthesis under inert atmosphere. Mastery of X-ray diffraction and structure solution and refinement will be obtained during the thesis. The student will furthermore participate in experimental sessions at SOLEIL and the ESRF synchrotron for data collection and treatment.

Important references:

- [1] J. Goulon, A. Rogalev, C. Brouder, in *Comprehensive Chiroptical Spectroscopy*, John Wiley & Sons, Ltd 2011.
- [2] J. Goulon, A. Rogalev, F. Wilhelm, C. Goulon-Ginet, P. Carra, I. Marri, Ch. Brouder, *J. Exp. Theor. Phys.* 2003, 97 (2), 402–431. DOI: 10.1134/1.1609001.
- [3] C. R. Natoli, C. Brouder, P. Sainctavit, J. Goulon, C. Goulon-Ginet, A. Rogalev, *Eur. Phys. J. B.* 1998, 4 (1), 1–11. DOI: 10.1007/s100510050344.

Activities: Synthesis of compounds, some of them under inert atmosphere (glove box, Schlenk techniques), solution-based crystal growth, structural characterization by single crystal X-ray diffraction, routine characterization (IR, elemental analysis, UV-vis spectroscopy), advanced optical characterization by X-ray absorption and RIXS.

Required skills: Knowledge and/or experience in coordination chemistry, coursework in X-ray diffraction, fluency in French and/or English, good organization skills, and a respect for lab safety and teamwork.

Place: ICMCB – UMR5026, 87, Avenue du Docteur Schweitzer, 33600 PESSAC (France)
[ICMCB - Institut de Chimie de la Matière Condensée de Bordeaux - CNRS UMR 5026](#)

Dates: Start date between September and October 2022. Funding for 36 months.

Application requirements: Applicants should apply via the site [Portail Emploi CNRS - Job offer - H/F Doctorant.e sur les matériaux moléculaires pour les spectroscopies XNCD et RIXS-NCD](#)

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