'Physique et Chimie des Matériaux' – ED 397 – année 2022

PhD project for funding, to send by 28/02/2022 to

nadine.witkowski@sorbonne-universite.fr under PDF form « acronyme labo_nom PI.pdf »

Research unit (full name + acronym) : Institut de minéralogie, de physique des matériaux et de

Team if applicable : Mimabadi

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Project leader (PI): Philippe Sainctavit HDR? yes Position : Researcher CNRS

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Nber of phD under supervision 1 Participation to supervisor training? no Year

Co-supervisor : Edwige Otero HDR? no Position : select

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Research unit : Synchrotron Soleil

International co-supervision ? select

Keyword 1 : Chirality Keyword 2 : X-ray absorption spectroscopy

Keyword 3 : Synchrotron Keyword 4 : X-ray optical activity

Select co-funding programme if applicable : Other ANR + SOLEIL

Project title : Chiral Molecular Magnets for Symmetry Induced Magnetism

Project Description :

Molecular magnets currently focus a high interest in the community of magnetism, in a context of increasing technologic efforts for the development of nanostructured magnets and for the magnetic storage of information in recording devices [1]. Recently, chiral molecular crystals have been extensively studied because of the interplay between magnetism and optical activity. Chiral crystals [see Figure] break point symmetry and magnetic crystals break time reversal so that coupling both magnetism and chirality results in creating systems for which exotic states of matter such as toroidal momenta exist [2].

In most cases, the electronic and magnetic properties of chiral magnets have been explored by experimental techniques such as MCD in the UV-Vis range for which the lack of chemical selectivity prevented the understanding of the coupling between the localized nature of magnetism and the extended nature of chirality.

Recently, we and co-workers applied chemically selective spectroscopies performed at the K-edges of 3d ions to tackle the coupling between chirality and magnetism [2,3]. These are synchrotron based spectroscopies such as X-ray Absorption Spectroscopy (XAS), X-ray Magnetic Circular Dichroism (XMCD), X-ray Natural Circular Dichroism (XNCD) and X-ray Magneto-Chiral Dichroism (XMChiD). Unfortunately, up to now none of these experimental results have received any theoretical interpretation that requires advanced computational approaches.

We have recently implemented a semi-relativistic, ab initio code to calculate such X-ray dichroic signals at K-edges(XMCD, XNCD, and XMChiD) within the XSpectra code (Quantum-Espresso distribution, based on Density Functional Theory) [4] and the program has already been benchmarked on simple compounds [5].The main target of the Ph.D. thesis will be to determine how the topology and the geometry of molecular systems can promote original magnetic properties. The main focus will be on calculating and measuring magnetic tensors that are governed by time reversal symmetry and/orelectric quadrupole anisotropy. At K-edges, this is for the instance the case for the still enigmatic anapole moment or the numerous octupolar magnetic moments.

Required skills : This is a mainly theoretical subject with a possible, additional experimental part on synchrotron so that a fine understanding of solid state physics and solid-state chemistry is a necessary pre-requisite.

Ph.D. Grant: The Ph.D.thesis will be financed by a government grantfollowing ED397 selection procedures or an already acquired ANR grant.

[1] Mannini, Arrio, Sainctavit et al.NATURE(2010) 468, 417-19;
[2] Sessoli, Mannini et al. NATURE PHYSICS(2015) 11, 69-74;
[3] Srinavasan, Sainctavit et al.CHEMICAL SCIENCE (2018)9, 1136-43;
[4] Bouldi, Juhin, Sainctavit et al.PHYS. REV. B (2017), 96, 085123;
[5] Bouldi, Juhin, Sainctavit et al. PHYS. REV. B (2018), 98, 06443