Internship offered in M2
2018-2019

Responsible for internship

Name: Amélie JUHIN

Location : IMPMC - 4 place Jussieu, 75005 Paris – Tower 23-24 4th floor, 413

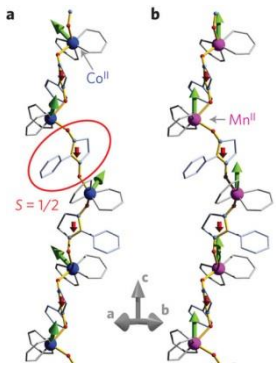
Group: Minéralogie et Magnétisme de Basses Dimensionnalités

E-mail: amelie.juhin@upmc.fr

Telephone : +33 (0)1 44 27 22 45

Group website: http://www.impmc.upmc.fr/fr/equipes/mineralogie-et-magnetisme-de-basses-dimensionnalites-mimabadi.html

Internship topic: Magnetic properties of chiral molecular magnets



This Master2 internship aims at applying a quantitative, magnetic spectroscopy to molecular magnets that currently focus a high interest in the community of molecular 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, single molecule magnets that show optical activity due to their chiral nature have been discovered **[2 and Figure]**. The experimental techniques used to characterize their electronic and magnetic properties are X-ray Absorption Spectroscopy (XAS), X-ray Magnetic Circular Dichroism (XMCD), X-ray Natural Circular Dichroism (XNCD) and X-ray Magneto-Chiral Dichroism (XMχD). These are synchrotron based element selective techniques that provide detailed information on the electronic and magnetic structures, but their fine interpretation requires advanced computational approaches.

We have recently implemented the semi-relativistic, ab-initio calculation of x-ray dichroisms in the XSpectra code (Quantum-Espresso distribution, based on Density Functional Theory) **[3]**. The program has already been benchmarked on simple compounds, and during the internship it will be used to calculate the XAS, XMCD, XNCD and XMχD spectra of chiral molecular magnets. Among the systems that will be studied are: *(i)* Co^{2+}-based molecular compounds that show a spin transition (from S=3/2 to S=1/2) by lowering the temperature or increasing the external pressure, *(ii)* chiral extended metal atom chains of Cobalt atoms.

[1] M. Mannini et al. Nature Materials 8, 194–197 (2009) and Nature 468, 417-421 (2010)
[2] R. Sessoli et al., Nature Physics 11, 69–74 (2015)
[3] N. Bouldi, A. Juhin et al., Phys. Rev. B 96, 085123 (2017) and Phys. Rev. B 98, 064430 (2018)

Techniques involved: XAS and associated dichroisms, calculations of spectra (Density Functional Theory).

Paid internship: Yes
Can this internship be continued for a PhD? Yes
If yes, type of PhD funding envisaged is: PhD fellowship Ecole Doctorale