THEORETICAL STUDY OF MAGNETO-ELECTRIC PROPERTIES OF MULTIFERROIC MATERIALS

Directeur de thèse : Mebarek Alouani et Daniel Stoeffler
UNIVERSITE DE STRASBOURG, IPCMS, 23 RUE DU LOESS, 67034 STRASBOURG
TEL : 03 88 10 70 06 ; E-MAIL : MEA@IPCMS.UNISTRA.FR

Multiferroic materials presenting both magnetic and dielectric properties are of great interests for the development of future multifunctional devices. In particular, magnetoelectric materials, where the magnetic and dielectric properties are coupled, are of importance for fundamental research and for potential technological devices and applications [1]. Indeed, an applied electric field or a magnetic field could control, respectively, the magnetic state and the ferroelectric state.

A few systems have been reported to exhibit a sizable magnetoelectric effect, among which $Ga_{1-x}Fe_xO_3$ (GFO) appears to be of a considerable significance. Several experiments performed at the IPCMS have demonstrated remarkable features of GFO such as a net ferrimagnetic order above room temperature for x=1.4 [2], as well as a large linear magnetoelectric effect, reported on single bulk crystals [3]. The electrical polarization has been determined with great accuracy when considering the variations of the polarization induced by small atomic displacements relative to a reference centrosymmetric structure [4].

The main goal of the present PhD thesis is to investigate the coupling between the electric polarization and the magnetization from an atomic viewpoint using Density Functional Theory based methods implemented into the VASP or the ABINIT codes. In a first step, the computation of the electric polarization and the magnetization variations will be conducted by means of an *ab initio* approach and the modern theory of polarization based on the Berry phase method. In a second step, the *ab initio* results will be employed to model the magneto-electric coupling, allowing the extension to inhomogeneous configurations using multiscale approaches, like the control of magnetic domain walls by an electric field.

The magneto-electric coupling can be decomposed into three main contributions resulting from three different mechanisms when an external magnetic or electric field is applied: (i) the purely spin-orbit coupling contribution (atomic positions frozen), which results from the redistribution of the electronic occupation of the spin-orbitals, (ii) the contribution which results from atomic motions inside the unit cell, and (iii) the contribution, which results from the deformation of the unit cell. All three contributions will be studied in order to quantify their magnitudes and their potential use in multifonctional devices. It is essential to notice that this study remains challenging for most real systems like GFO as a consequence of its complex structure. Less complex and more symmetric systems like $YFeO_3$ and Cr_2O_3 will be also considered.

Bibliography

[1] M. Bibes and A. Barthélémy, Nature Mater. **7**, 425 (2008).

[2] M. Trassin *et al*, J. Mater. Chem., **19**, 8876 (2009).

[3] G.T. Rado, Phys. Rev. Lett. **13**, 335 (1964).

[4] D. Stoeffler, J. Phys. : Condens. Matter **24**, 185502 (2012).