Master 2 Physics – Condensed Matter and Nanophysics

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Ab initio multiferroics properties of materials

Multiferroic materials, coupling both magnetic and electric degrees of freedom, are of great interests. The so-called magnetoelectric effect, beside its importance from a fundamental point of view, can be exploited in potential technological devices and applications [1]. Indeed, a few materials have been reported to exhibit a sizable magnetoelectric effect, among which $Ga_{2-x}Fe_xO3$ (GFO) appears to be of a considerable significance. Several experiments have demonstrated remarkable features of GFO such as a net ferrimagnetic order above room temperature for x=1.4 composition [2], as well as the large linear magnetoelectric effect reported on single bulk crystals [3]. Nevertheless, it was until Kim et al. work that a microscopic investigation of GFO's magnetic properties was provided [4]. As an unexpectedly large orbital moment was measured in this half-filled d^5 system, it was attributed to the anisotropic Fe-O hybridization caused by the off-center movements of the Fe ions. Such information about the orbital and electronic anisotropy are the keywords for a better microscopic description of the spin-orbit coupling driven properties of GFO [5]. The electrical polarization is an important property of as multiferroic materials. It should be determined precisely when considering variations of the polarization induced by small atomic displacements and its effect on the magnetic properties [6].

In this internship, the student will first learn how to use and run an ab initio program to compute the magnetoelectric properties of materials, the so called VASP package [7], which is written in modern Fortran 95 and runs on parallel machines. The student will then determine how the spin-orbit coupling can affect the magnetic and electronic structure of multiferroics materials such as GFO, YFeO3, and Cr2O3. The student will then address the calculation of the electric polarization in a polar structure in several ways: (i) using a model of constant formal charges during atomic displacements, (ii) using the VASP package and the Berry phase method to make a direct calculation [8], -(iii) using the Born effective charge model to determine the transition path. The student will have the opportunity to write small programs to implement simple models.

References

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