INSTITUT NEEL Grenoble

Post-doctoral position

Ab-initio calculations of the magnetic spectrum and the magneto-electric coupling in multiferroic materials

Context : Magnetoelectric (ME) multiferroics materials present the peculiar property to couple electric and magnetic ordersi. As a result it is possible to toggle the electric polarisation using a magnetic field and reversely to modify the magnetic order using an electric field. These multifunctional materials thus present a high potential in new technologies.
Two classes of multiferroics have been defined based on the mechanism promoting the spontaneous polar order. In type I multiferroics the polarisation originates in displacive mechanism and may be large. However the ME coupling is usually weak. The type II multiferroics, also named spin-driven ferroelectrics (SDF), are improper ferroelectrics in the sense that the polar state is driven by a magnetic transition. In these systems the ME coupling may be large (complete polarisation reversal under an applied magnetic field as in TbMn2O5) however the polarisation remains usually weak.
The conditions for the existence of a ME coupling start to be understood and different mechanisms at the origin of the latter have been identified. Generally, ME compounds are systems presenting a complex magnetic structure, characterized by spatial variations of the magnetization. The microscopic model proposed to explain this spin induced ferroelectricity is associated with the antisymmetric Dzyaloshinskii-Moriya (DM) interaction. Unfortunately, as the amplitude of the spin-orbit coupling is generally weak, so is the polarisation, and those systems are inappropriate for technological applications. More recently several families with larger effects have been identified. In these systems the microscopic mechanisms at the origin of the ME coupling are rather related with the release of magnetic frustration by exchange-striction.

Objectives and means available : The objectives of the present post-doc is to decipher the degrees of freedom responsible nor only for the existence but also for the amplitude of the magneto-electric coupling. For this purpose one needs to to have the knowledge of the ME coupling tensor for real systems under external stresses or chemical doping. We recently developed a method to compute the ME coupling tensor from first principle calculations. This method requires only the crystal and magnetic structures of the compound under consideration. The candidate will thus be expected to participate to the method and code development and/or study the ME coupling on different families of compounds.

Possible collaboration and networking : As neutrons scattering is a key method for the experimental investigation of multiferroics systems the candidate will collaborate with the Institut Laue Langevin (ILL: European neutrons source) Theory Group, as well as ILL the experimentalists and users working on the subject.

Required profile : the candidate should have a PhD in theoretical condensed matter Physics or Quantum Chemistry and experience in of ab-initio calculations.

Foreseen start for the position : october 2019
Salary : Standard university grids
Duration : 12 months

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