Title: Theoretical study of excitations in the magneto-electric RMn$_2$O$_5$ compounds

General Scope: Multiferroic materials are multifunctional systems that couple multiple orders and in particular magnetism and ferroelectricity. Their interest is double. First the possibility to control magnetism with an electric field has many potential applications in the domains of energy saving in microelectronics or for data storage and processing. Second, the properties of these systems raise a large number of fundamental questions. For instance, the origin or the amplitude of the magneto-electric coupling remains to be fully understood. The complexity arises from the numerous degrees of freedom involved that are all intrinsically interdependent. One can cite for the static aspects the structural (atomic organisation), magnetic (spins amplitude and orientation) and dielectric (spatial distribution of charges) parameters, while phonons and magnons may also be coupled in excited states.

Research topic and facilities available: In this internship proposal, we propose to investigate the properties of a particular family of magneto-electric multiferroics: the RMn$_2$O$_5$ (R=Rare Earth). Studying these materials is motivated by their very strong magneto-electric coupling (a field of only 2 Tesla can reverse the polarization [1]) and by the microscopic mechanism which is at work in this case (exchange-striction)[2,3,4].

For this purpose the student will perform ab-initio calculations, learn how to map them into Fermi level effective models and to solve the latter to compare with experimental results. She/he will thus

- learn the basis of electronic and magnetic structure calculations
- learn how to use the supercomputers accessible in the national/regional computation centers
- learn how to extract the important information from the calculation in order to built a model.

For this purpose he/she will have access not only to the lab. computer facilities but also to supercomputer centers.

Possible collaboration and networking: The student will collaborate with the experimentalists working on this systems, namely members of the P. Foury group from the LPS (Orsay), specialists of neutrons scattering from the LLB (Saclay) and ILL (Grenoble) neutron facilities. The student will also collaborate with theoreticians from ILL in particular E. Rebolini.

Possible extension as a PhD

Required skills: The student should have a good knowledge of quantum mechanics, as well as knowledge of computers usage.

Starting date: between January and March 2019, end date not after July 31st.

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