INSTITUT Laue Langevin Grenoble, France

Topic for Master 2 internship – Academic year 2022-2023

Magnetic exchange : what are the orbitals bridging the interaction?

General Scope :
Magnetic materials and in the recent years multiferroic materials (coupling spin and electronic degrees of freedom) have been extensively studied. Indeed, their properties are fascinating and the understanding of the microscopic origin (nature of the atoms, geometry) of their magnetic orders or their magneto-electric couplings is a crucial subject of research for material design with specific properties.

The structure/properties relationship is thus a fundamental research subject to which the present internship belongs.

At the beginning are the nature of the atoms and their positions. From these pieces of information alone, quantum mechanics provides a Hamiltonian and a Schrödinger equation (so-called ab-initio) entirely describing the system under consideration. Magnetism is however a property of the Fermi level electrons. One thus usually describes it using effective Hamiltonians focused on only the magnetic degrees of freedom. The parameters of such models are effective magnetic interactions.

Research topic and facilities available :
In transition metal oxides, these effective interactions can be direct, or mediated by ligands, bridging the magnetic atoms. What are the ligand orbitals bridging the magnetic interactions ? How can we define them and compute them ? That is the question we plan to tackle during this internship.

For this purpose we will explore several tracks and use different quantum mechanical tools. We will study the impact of the choice of the bridging orbitals on the quantum description of the effective magnetic interactions.

The student will have to use different quantum mechanics codes, as well as get acquainted with super-calculators. He/She will have to analyse his/her results on the basis of physical considerations by comparing them with reference ones. She/He will then include the best method to the RelaxSE code for magnetic interactions calculations.

Possible collaboration and networking :
This work will be done in collaboration with MB Lepetit from the ILL theory group and E. Rebolini for the scientific computing group.

Possible extension as a PhD : yes but with a subject change

Required skills: A good knowledge of quantum mechanics is required as well as basic knowledge of linux operating system.

Starting date : Anytime between february and april 2023

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