NÉEL INSTITUTE Grenoble

PhD Project – Academic year 2024-2025

First-principles theory of multiferroicity in magnetic spinels

General Scope

One of the most pressing topics of modern research in physics and materials science is the discovery of materials that can be used in the next generation of more energy-efficient electronic devices. Magnetoelectric multiferroics provide a promising class of materials (see e.g. [1]). They exhibit both magnetic and ferroelectric orders and show a strong cross-coupling between the two, allowing for the electric control of magnetism and vice versa. In this project, we aim to understand and tune multiferroicity and magnetoelectricity in magnetic spinels.

Research Topic and Facilities Available

Magnetic spinels have a cubic crystal structure, with two sublattices (see the crystal structure in Fig. 1). They are promising multiferroics since the ferroelectricity is induced by the complex magnetic orders in the materials, and thus the coupling between the two can be significant (this is called type II multiferroicity). However, the exact coupling mechanism between the magnetic orders and the electric dipole moments remains puzzling [2].

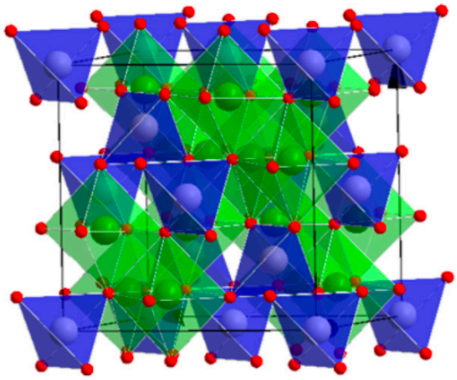

Fig 1: Spinel crystal structure [2]

In this project, The PhD student will perform quantum mechanical calculations using density functional theory to explore the nature of magnetoelectric coupling and to elucidate the physical mechanism that enables the coupling between the magnetic structure, ferroelectricity, and crystal structure. She/He will use a combination of first-principles-based phenomenological modeling (see e.g. [3,4]) as well as novel machine-learning methods.

Possible Collaboration and Networking

The project is a joint effort between the theory group (Théorie de la matière condensée) and the MagSup (Magnetisme et supraconductivité) team at Institut Néel. While the project is purely theoretical, it is carried out in close collaboration with experimentalists.

Required skills: Background in Solid Physics and Magnetism.

Starting date: Spring 2025

Contact

Name: Quintin MEIER / Sophie DE BRION
Institut Néel - CNRS
e-mail: quintin.meier@neel.cnrs.fr sophie.debrion@neel.cnrs.fr

References

[1] N.A Spaldin and R. Ramesh, *Nat. Mater.*, **volume 18**, pages 203–212 (2019)
[2] A. Sundaresan and N. V. Ter-Oganessian, J. Appl. Phys. 129, 060901 (2021)
[3] M. Giraldo, Q.N. Meier, et al, Nat. comm.12 (1), 3093 (2021)
[4] TN Tošić, Q. N. Meier, NA Spaldin, Phys. Rev. Research 4 (3), 033204 (2022)