

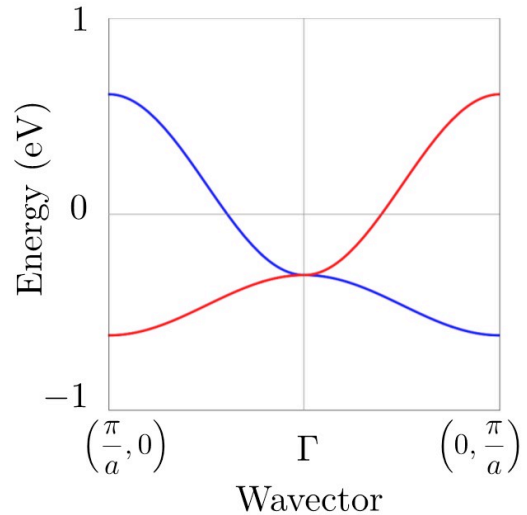
# INSTITUT NEEL Grenoble

## Proposition de stage Master 2 - Année universitaire 2024-2025

### Theoretical investigation of altermagnetic materials

Altermagnets represent a new class of antiferromagnets characterized by distinct electronic properties due to the splitting of the spin-up and spin-down electronic bands (see Figure 1). This band splitting leads to a variety of novel properties that make these materials highly promising for future spintronic applications, such as spin-charge conversion and the development of chiral magnons for magnonic devices [1].

The goal of this project is to investigate theoretically the altermagnetic phases that can emerge in perovskites and related materials. Magnetic members of the perovskite family typically exhibit antiferromagnetic ordering, and their natural inclination towards octahedral tilts provides an excellent platform for altermagnetism [2]. Through electronic structure calculations using density functional theory (DFT), we will investigate how different structural distortions and magnetic orders influence the altermagnetic spin splitting. One of the goals of the project is to establish a general set of design principles for identifying new altermagnetic materials within the perovskite family.



**Figure 1:** Electronic bands in an altermagnet, showing spin-up (red) and spin-down (blue) band splitting in different regions of the Brillouin zone

[1] L. Šmejkal, J. Sinova, and T. Jungwirth, Phys. Rev. X 12, 040501 (2022)

[2] Fabio Bernardini, Manfred Fiebig, and Andrés Cano, arXiv:2401.12910

#### Research topic and facilities available

The internship will be carried out at the Condensed Matter Theory (TMC) group at Institut NEEL. The available facilities include a HPC local cluster for the numerical calculations.

#### Possible collaboration and networking

The internship will be carried out in the framework of an ongoing national and international collaboration that includes theoreticians and experimentalists.

#### Possible extension as a PhD

Yes

#### Required skills

Theory. Solid state physics. Numerical calculations. Machine learning  
Starting date 1/10/2024 (tentative)

#### Contact

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