2D-iron based Materials: a platform for exotic spin states, spin-clusters and domains and their dynamics.

This PhD project is part of a three-year collaboration between the University of Lille and the Institut Laue Langevin. The candidate will be based in each institution for a period of 1.5 years and will be attached to the Doctoral School - 104 of the University of Lille (*Ecole Doctorale-104, Sciences de la Matière du Rayonnement et de l'Environnement*).

During the 3 years of this project, the PhD student will be responsible for sample preparation using solid state and solvothermal techniques, and physical characterisation of the sample using laboratory techniques (powder and single crystal X-ray diffraction, electron microscopy, magnetometry measurements and surface analysis among others) as well as advanced techniques such as magnetic force microscopy, unpolarised and polarised neutron diffraction (powder and single crystal), synchrotron measurements and inelastic neutron measurements. Measurements using neutron techniques will be carried out mainly at the ILL, while others will be developed at other large facilities in Europe or in collaborating laboratories. The ultimate goal is to have an in-depth knowledge of the interplay between crystal structure and magnetic and magnetoelectric properties of 2D iron-based compounds.

The chemical tailoring of the proposed 2D platform will allow us to set new paradigms on exotic magnetic states/excitations/dynamics of spins/clusters/magnetic domains. For this PhD project, we have selected three promising series of layered Fe-based materials ($BaFe_2(PO_4)_2$, Fe-based mica compounds and Fe-based Aurivillius oxyfluorides). Preliminary studies on these systems have been developed at the UCCS (Univ. Lille) and show great potential in terms of magnetic (-electric) behaviour.

From a chemical point of view, these systems offer different degrees of freedom and chemical/lattice/redox flexibility towards tuneable magnetic components (direct exchange, spin, anisotropy or correlation lengths). The academic supervisors have a strong background in sample preparation, so most of the synthetic work will be carried out during the time at the University of Lille.

The PhD student will start the project (1 year) in Olivier Mentre's group (UCCS, Lille) where the inorganic synthesis, crystallographic studies and physical characterisation will be carried out. During this period, the student will also be introduced to the basics of diffraction and first-principles theoretical methods. Short stays to receive specific training necessary for the development of the PhD will also be carried out during this period. In addition, the candidate should attend some doctoral courses at the University of Lille. During the next 1.5 years, the PhD student will be based at the ILL (Grenoble) and will focus on neutron diffraction experiments and data treatment. For the last 6 months of the project, the PhD student will return to the UCCS to complete the writing of the thesis and the PhD defence.

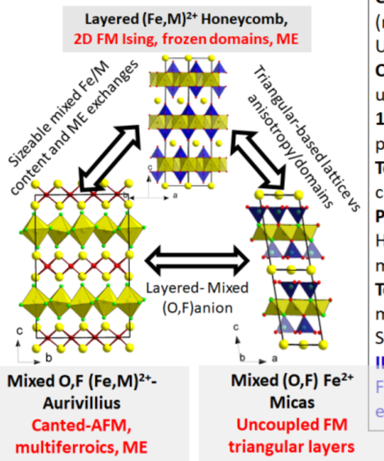
We are looking for a highly motivated candidate with a degree in physics, chemistry or materials science. The candidate must hold an MSc degree in an affine field and meet the requirements to be enrolled in the Doctoral School of the University of Lille.

How to apply: email to Olivier Mentré/Angel Arevalo-Lopez + Oscar Fabello/Clemens Ritter
(olivier.mentre@univ-lille.fr; angel.arevalo-lopez@univ-lille.fr; fabelo@ill.fr; ritter@ill.fr)
with the subject “Thesis-MAG-2023_17-your name”. Attach a CV, a brief motivation letter and the contact person for a reference.
For additional details about the specific conditions for the PhD and the application procedure, please consult the following link: https://www.ill.eu/careers/all-our-vacancies/phd-recruitment/open-phd-position

The topic of the Thesis is sketched below

Context : $BaM_2(XO_4)_2$ series, low-D magn, (M=Fe^{2+} : UCCS).
Questions to be raised : How chemical and lattice defects will modify the domain wall topology and dynamics ? Modification of the magneto-Crystalline anisotropy in mixed Fe/M compounds, Investigation of the 2D FM ising → 2D AFM ?
1) Chemistry : **Well Mastered** : powder and crystals of Fe and mixed M,Fe phases, reversible implantation of sizeable Fe vacancies.
To Do : prepare large amount of samples for neutron experiments
2) Properties : **Known :** Magnetism + DFT + MFM (domains) + Magneto-E couplings of the parent Fe phases, FM of Fe-rich mixed phases. Evidence of blocked domains in mixed Fe/M compounds. Magn excitation in BFPO (Ising gap, etc) + determination of magneto-crystalline anisotropy by INS
To Do : accurate magn + magn structure of Fe-depleted phases. Blocked domains + magneto-crystalline anisotropy +MFM+ ME in mixed and Fe-deficient phases.
ILL job : • Vacancies and mixed Fe/M and magn structure distribution in mixed Fe/M/□ phases • Magnetic excitation (INS) • aniso in the most pertinent samples • spin up/down analyzis in bluk samples by polarized neutrons (understanding the shift of M(H) to full saturation …

Context : all magnetic slabs in (O,F) Aurivillius compounds (M=Fe^{2+},Ni^{2+},Mn^{2+} : UCCS).
Questions to be raised : struct/properties varying the anionic content and mixed, Multi-ferro, polarity, Fe^{2+}/Fe^{3+} valence
1) Chemistry: Well Mastered : powder in solvothermal conditions with changing M redox (water *vs* ethanol). Topochemical transformation.
To Do : scale up, mixed Fe/M, larger single-cryst, high-pressure synthesis of novel phases.
2) Properties: Known : Magnetism + multiferroism in single metal materials, magn struct
To Do: full charact. of mixed and anion-defficient phase, FM component vs polarity, increase $T_{N.}$ towards FM/metallic layers (mixed Mn^{3+}, Mn^{4+}) , e.g. $[Bi_2O_2][MnF_{3-\delta}O_{1+\delta}]$
ILL job : • anionic Structure • magnetic ordering
• in-situ survey of the topochemical transformation
• high-pressure NPD …



Context : (O, OH) Micas well-known family, (recent results on rare Fe^{2+} magnetic Micas UCCS).
Questions to be raised : extend the family + understanding the Low-D FM
1) Chemistry: **Well-mastered** : Single phase Fe,Ga,OH,O in autoclave
To Do: F^- for OH^- subtstitution, larger single crystals, mixed Fe/M
Properties: for Fe^{2+}, FM layers decoupled (?) Huge magnetic anisotropy expected (uniaxial magn) = ideal for ME exchanges.
To do :almost everything … for instance no magn structure reported for MICAS…
Study of magn domains.
ILL job : • magnetic ordering or not in mixed Fe/M • PND under field • Magnetic excitation in decoupled FM units (IS) …