CENTRE D'ÉLABORATION DE MATÉRIAUX ET D'ÉTUDES STRUCTURALES

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Ab initio study of magnetic skyrmions in atomically thin 2D van der Waals layers

Internship supervisor(s)	name: Dr. Dongzhe Li e-mail: dongzhe.li@cemes.fr group: **M**aterials and devices for **E**lectronics and **M**agnetism (MEM)
Location	CEMES-CNRS 29 Rue Jeanne Marvig, 31055 Toulouse - FRANCE
This research master's degree research project could be followed by a PhD	☒ YES ☐ NO

Magnetic skyrmions – topologically protected quasi-particles with a whirling spin texture in real space – have raised great attention due to their rich physics and promising applications for future spintronic devices. With the recent discovery of 2D van der Waals (vdW) magnets [1], stabilizing and controlling magnetic skyrmions in atomically thin vdW materials has gained tremendous attention due to high tunability, enhanced functionality, and miniaturization [2]. The study of skyrmions in 2D magnets is still in its infancy stage. This leaves a timely and vast playground for investigating new mechanisms for skyrmion generation [3], detection [4], and manipulation [5] in the emerging area of vdW 2D magnets.

The purpose of this Master's project is to explore the generation and manipulation of magnetic skyrmions in novel 2D magnets and heterostructures. Fundamentally, chiral magnetic skyrmions have spin-orbit-driven non-collinear spin textures that result from a fine balance of different magnetic interactions. To capture these effects with sufficient accuracy, we will employ a multiscale approach that combines density functional theory (DFT) and atomistic spin simulations. Different magnetic interactions, such as Heisenberg exchange, Dzyaloshinskii-Moriya interaction, magnetocrystalline anisotropy energy, and higher-order exchange interactions (HOI), will be calculated by DFT. In particular, we will provide a deeper understanding of the interplay between DMI and HOI for skyrmion stability. Finally, we will investigate how external stimuli such as electric or magnetic fields tune topological spin textures (see Figure 1).

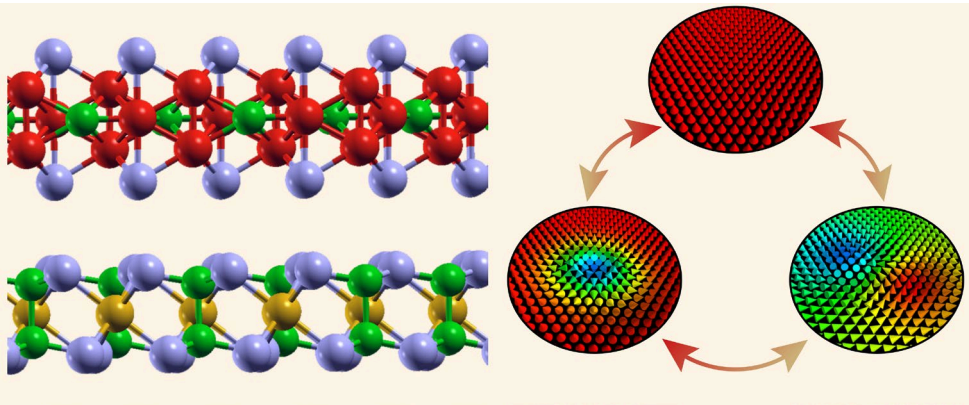

Figure 1: Topological spin texture transformation (skyrmions – bimerons - ferromagnetic) induced by external stimuli in an all-magnetic 2D van der Waals heterostructure.

This internship requires a taste for modeling. The numerical calculations will be performed using local and national HPC facilities. The results obtained will be analyzed with the possibility of publication in international scientific journals.

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References:

[1] B. Ding *et al.*, Nano Lett. 20, 868 (2020); Y. Wu *et al.*, Nat. Commun. 11, 3860 (2020);
[2] **Dongzhe Li** *et al.*, "Tuning the magnetic interactions in van der Waals Fe_3GeTe_2 heterostructures: A comparative study of *ab initio* methods", Phys. Rev. B 107, 104428 (2023).
[3] **Dongzhe Li** *et al.*, "Strain-driven zero-field near-10 nm skyrmions in two-dimensional van der Waals geterostructures", Nano Letters 22, 7706-7713 (2022).
[4] **Dongzhe Li** *et al.*, "Proposal for all-electrical skyrmion detection in van der Waals tunnel junctions", Nano Lett. 24, 2496-2502 (2024).
[5] **Dongzhe Li** *et al.*, "Stability and localization of nanoscale skyrmions and bimerons in an all-magnetic van der Waals heterostructure", arXiv:2408.15974 (2024).

Keywords, areas of expertise	Density functional theory, Spintronics, Magnetic Skyrmions, Dzyaloshinskii–Moriya interaction, Higher-order exchange interactions, 2D materials
Required skills for the internship	- Master in Physics, Nanosciences, Materials science, or any other equivalent majors. - Good background in quantum mechanics and solid-state physics. - Programming skills (Fortran, Python, or Bash) are not mandatory but will be considered an advantage.

How to apply?
Please send a CV, a copy of the last two years' transcripts (relevés de notes), and a letter of motivation to dongzhe.li@cemes.fr with the following title "M2 internship CNRS".

Starting date and work location
Master internship: 02/2025 – 08/2025
Lab: CEMES/CNRS, Toulouse, France

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