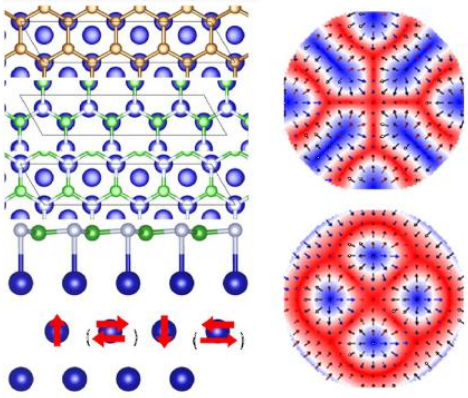
Spin-orbit phenomena in heterostructures with two-dimensional materials

Context

Spin electronics, or spintronics, is a rapidly expanding field of high interest for both scientists and engineers since its breakthrough research discoveries give rise to novel development of industrial applications in the fields of magnetic recording, sensors and memory devices. Spin-orbit phenomena such as perpendicular magnetic anisotropy (PMA) or Dzyaloshinskii-Moriya interaction (DMI) have become of tremendous interest since they play a major role in particular for magnetic random access memories based on spin transfer (STT-MRAM) and spin-orbit torques (SOT-MRAM) as well as emergence of spin-orbitronics [1,2]. At the same time, 2D materials such as graphene, transition metal dichalcogenides and associated van der Waals heterostructures including 2D magnets have become of major interest in recent years since they may serve as an efficient alternatives for these and next generation of spintronic devices, thus giving rise to emergence of graphene and 2D spintronics[3,4,5].



Gr/Co, h-BN(AB)/Co and h-BN(AC)/Co structures and relaxed magnetization distributions of h-BN(AC)/Co(3ML) with domains transformed into skyrmion states (From Ref. [6]).

This internship project aims on unveiling microscopic mechanisms of spin-orbit phenomena including DMI, PMA as well as spin-charge interconversion (Rashba and Rashba-Edelstein effects) in heterostructures comprising traditional materials (transition metals, oxides) and van der Waals 2D (transition metal dichalcogenides, 2D magnets, graphene…) in order to help optimizing spintronic devices. In particular, the mechanisms of their control via external stimuli (strain, external electric and magnetic fields) and possibility of inducing chiral magnetic structures such as skyrmions will be investigated [6].

Work program & Skills acquired during internship

The selected candidate will set up supercells combining various van der Waals 2D materials with oxides and/or metals and will primarily perform *ab initio* calculations in order to find optimal material combinations ensuring optimal values of aforementioned phenomena. The calculations will be performed on Spintec computational cluster nodes using first-principles packages based on density functional theory (DFT) combined with other simulation techniques. Results obtained will be carefully analyzed with possibility of publication in international scientific journals. Strong collaboration with labs in France (CEA/LETI, Univ. of Montpellier, Aix-Marseille Univ…) and abroad (ICN2/Spain, Nanjing Univ. China…) is previewed.

[1]B. Dieny and M. Chshiev, ***Rev. Mod. Phys.*** 89, 025008 (2017) [url]
[2] A. Fert, M. Chshiev, A. Thiaville and H.-X. Yang, ***J. Phys. Soc. Jpn.*** 92, 081001 (2023) [url]
[3] S. Roche et al., ***2D Mater.*** 2, 030202 (2015) [url]
[4] Q. H. Wang et al, ***ACS Nano*** 16, 6960 (2022) [url]
[5] H. Yang et al, ***Nature*** 606, 663 (2022) [url]
[6] A. Hallal et al, ***Nano Lett.*** 21, 7138 (2021) [url]

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Requested background: Master 2
Duration: 6 months
Start period: Feb/ March 2024
Possibility of PhD thesis : YES