High-throughput screening of 2D spintronic materials

Keywords: 2D materials, spintronics, computational material science, high-throughput, database

In contrast with conventional electronics using the electrons' charge, spintronics uses the spin of electrons to design devices for sensing, communications, memory, computing and other technological applications. Exploring spin-orbit phenomena such as perpendicular magnetic anisotropy, DMI, Rashba effects and spin-orbit torques for next generations of spintronic applications have become of tremendous interest in recent years and led to the creation of emerging field of spin-orbitronics[1,2]. At the same time, 2D materials such as graphene, transition metal dichalcogenides and associated van der Waals heterostructures have been intensely studied in recent years since they may serve as an efficient alternative for next generation of spintronic devices [3,4,5].

In the context of the PEPR Spin aiming at the development of spintronics at the French national level, we are offering funding for a PhD thesis in the fields of computational materials science, condensed matter theory and device physics applied to spintronics.

The aim of the PhD project is to identify and characterise useful 2D materials for various spin-orbitronics applications relevant to the PEPR Spin, based on *ab initio* simulations. We will use high-performance computing and high-throughput techniques to screen a database of exfoliable 2D materials [6] and compute a set of relevant parameters for the most promising candidates.

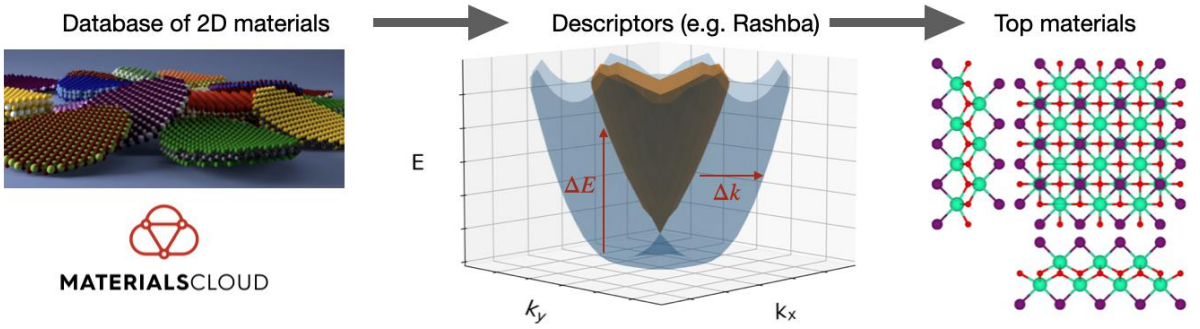
The first step will be to collect a list of useful properties and study current models of the corresponding mechanisms. From there, we will determine how to use already available data [6] or easily computed properties to pre-select prospective candidates. The spin-orbitronic properties of a selected subset of 2D materials will be further characterised (spin texture, Rashba effect, anisotropy, exchange parameters...). This will require the establishment of a meaningful set of descriptors and the development of *ab initio* workflows to compute them, using the AiiDA (https://www.aiida.net) code. Finally, the 2D materials combining the best properties for targeted applications will be studied in full with state-of-the-art *ab initio* simulations.

Throughout the project, we will pay special attention to enabling valuable exchanges with different work packages of the whole PEPR Spin consortium. This includes taking inputs from other experimental and theoretical work packages and disseminating the results of our work through a simple interface.

The motivated candidate is expected to have a strong background in computational science and condensed matter theory. Computational skills are a must, as the PhD will involve a significant amount of coding (mostly in Python). Experience with supercomputers and ab initio calculation is a plus. This should be combined with the ability to absorb complex quantum physical concepts to develop meaningful *ab initio* models. A good understanding of the mechanisms involved in prospective spintronic devices will be preferable to identify the best materials.

The PhD takes place at Laboratoire Charles Coulomb in the University of Montpellier, under the supervision of T. Sohier (L2C Montpellier) and M. Chshiev (Spintec Grenoble).

Contacts: thibault.sohier@umontpellier.fr - mair.chshiev@cea.fr



[1] B. Dieny and M. Chshiev, Reviews of Modern Physics **89**, 025008 (2017).

[2] A. Manchon, et al., Reviews of Modern Physics **91**, 035004 (2019).

[3] S. Roche et al, 2D Materials **2**, 030202 (2015)

[4] Q. H. Wang et al, ACS Nano **16**, 6960 (2022)

[5] H. Yang, S. O. Valenzuela, M. Chshiev et al, Nature **606**, 663 (2022)

[6] https://www.materialscloud.org/discover/mc2d, N. Mounet et al., Nature Nanotechnology **13**, 246 (2018).