M2 internship: High-throughput screening of 2D spintronic materials

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

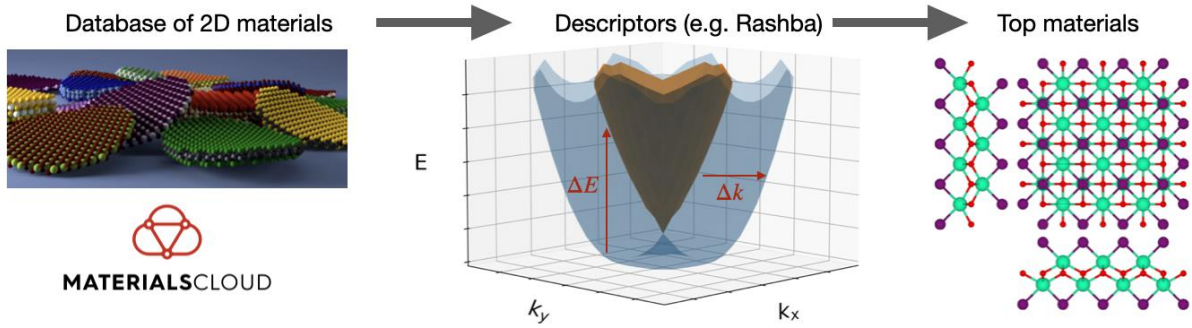
In contrast with conventional electronics using the electrons' charge, spintronics uses the spin of electrons to design devices for sensing, communications, memory, computing and other technological applications. The physical mechanisms used to operate those devices (spin-Hall effect, spin-orbit torque, Rashba-Edelstein effect...) rely on some specific material properties like spin-orbit coupling [1,2].

2D materials have shown great promise in tailoring the properties of matter for technological applications. The aim of this internship project is to identify a set of 2D materials with interesting features for spintronics from a database of about 2000 candidates [3]. This will be done using AiiDA [4], a sophisticated tool for automation and data management in computational materials science.

The internship takes place at Laboratoire Charles Coulomb in the University of Montpellier, under the supervision of T. Sohier (L2C Montpellier) and M. Chshiev (Spintec Grenoble). Possibility of continuing with a PhD starting in Fall 2024, funded by the French national program PEPR SPIN.

Profile of the student:

Excellent coding skills (mostly python) and a strong interest for computational physics are required. The background to understand the quantum physical mechanisms involved in spintronic devices is necessary. Experience with ab initio codes and supercomputers is also useful.



[1] B. Dieny and M. Chshiev, *Perpendicular Magnetic Anisotropy at Transition Metal/Oxide Interfaces and Applications*, Rev. Mod. Phys. **89**, 025008 (2017).

[2] A. Manchon, J. Železný, I. M. Miron, T. Jungwirth, J. Sinova, A. Thiaville, K. Garello, and P. Gambardella, *Current-Induced Spin-Orbit Torques in Ferromagnetic and Antiferromagnetic Systems*, Reviews of Modern Physics **91**, 035004 (2019).

[3] https://www.materialscloud.org/discover/mc2d, N. Mounet et al., *Two-Dimensional Materials from High-Throughput Computational Exfoliation of Experimentally Known Compounds*, Nature Nanotechnology **13**, 246 (2018).

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