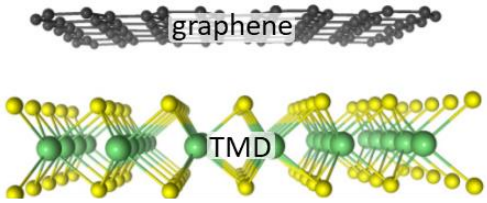
Spintronics in graphene over transition metal dichalcogenides: Simulations

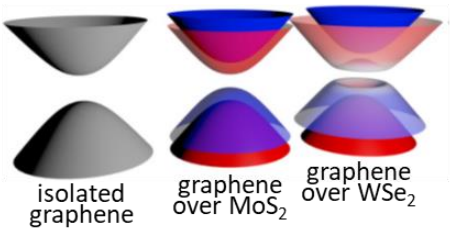
Context

In the context of **spintronics**, graphene is considered an ideal platform thanks to its very weak spin-orbit coupling (SOC), which allows spin scattering lengths of up to a few tens of micrometers [1]. For the same reason, however, spin manipulation is complicated. Transition metal dichalcogenides (TMDs), another class of two-dimensional materials, exhibit a considerable SOC due to the heavy metals they comprise. When graphene is over a TMD, a SOC is induced into graphene by proximity effect [2]. TMDs comprising a heavy metal element, such as WSe_2, give rise to a pronounced SOC, which in turn results in a topological insulator and a spin quantum Hall effect.



[1] "Graphene spintronics: the European Flagship perspective", S. Roche et al., ***2D Mater.*** 2, 030202 (2015)

[2] "Trivial and inverted Dirac bands and the emergence of quantum spin Hall states in graphene on transition-metal dichalcogenides", M. Gmitra et al., ***Phys. Rev. B*** 93, 155104 (2016)



Work program & Skills acquired during internship

This internship is jointly proposed by CROMA (Centre for Radiofrequencies, Optic and Micro-nanoelectronics in the Alps) and SPINTEC (SPINtronique et TEchnologie des Composants) research laboratories affiliated with Univ. Grenoble Alpes, Grenoble INP-UGA, CEA and CNRS. The objective is to study, through simulations based on the density functional theory, the effect of a **polycrystalline TMD on the band structure of the overlying graphene**. This is a common disorder in non-exfoliated TMDs, which warrants further study of how it affects the SOC induced in graphene. The different crystal orientations could lead to the formation of spin-polarized states in graphene at the grain boundaries, with important theoretical and application consequences. Thanks to the balance of **theory** and **numerical computation** that exists between our two labs, the intern student will develop important skills in the use of *ab initio* and tight-binding codes, thus enabling her or him to continue working in our labs with activities focused on magnetic or ferroelectric memories for low-power electronics and artificial intelligence.

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Requirement: (i) understanding of quantum mechanics and solid state physics, (ii) basic knowledge in computers with Linux operating system and/or basis in programming languages, (iii) previous experience in density functional theory is a plus.

Requested background: Master 2
Duration: 6 months
Start period: February/ March 2025
Possibility of PhD thesis : YES