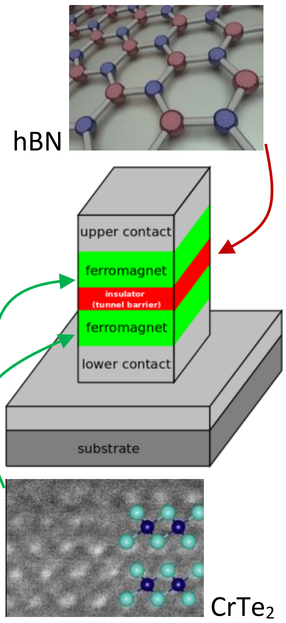
Quantum simulation of magnetic memories based on 2D materials

Context - One of the central goals for future nanoelectronics concerns the fabrication of low-power devices based on sustainable materials. In this context, both spintronics and 2D materials (2DMs) represent a springboard to cutting-edge research and the future development of durable technologies. The recent experimental demonstration of 2D ferromagnets ignited significant interest in non-volatile memories based on Magnetic Tunnel Junctions (MTJs) consisting of 2DM van der Waals (vdW) heterostructures, where a 2D nonmagnetic material acts as a barrier sandwiched between two 2D ferromagnets. The vdW coupling between different 2DMs entails challenges at the interface level, including reduced interlayer tunneling and a more difficult control over the orientation of the layers. To address these challenges, an accurate numerical study of structural, electronic and transport properties of vdW heterostructures is imperative for elucidating the transmission behavior in a 2DM-based MTJ.

Project - To calculate the tunnel magnetoresistance (TMR) and its dependence and stability on interfacial stacking and disorder, we will combine DFT calculations and quantum transport simulations based on the atomistic quantum Green's function approach. The plan includes: (i) the DFT calculations for monolayer or multilayer graphene, h-BN and TMDs as barrier layers, and for Fe_3GeTe_2, Fe_5GeTe_2, VSe_2 and $CrTe_2$ as ferromagnets (obtained experimentally and with a relatively high Curie temperature), (ii) DFT calculations for MTJs composed of monolayer or multilayer barrier material sandwiched between two ferromagnets, (iii) extracting the Hamiltonian and simulating quantum transport for the considered MTJs, (iv) considering the presence of defects (vacancy, substitutional doping or grain boundaries) and studying their effects on the transport properties of MTJs. Our calculations will benefit from and guide experiments at Spintec MRAM and 2D teams, thus aiding in the identification of specific materials of interest. The expected outcomes are important for the realization of 2D MTJ-based sustainable electronics. In particular, they will indicate the best material combinations, within those tested, and the expected performances.



Required skills – Background in solid-state physics and materials science, interest in coding and performing numerical simulations and working in a collaborative team.

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Further reading

- M. Chshiev et al., *Analytical description of ballistic spin currents and torques in magnetic tunnel junctions*, Phys. Rev. B 92, 104422 (2015)
- Q. H. Wang et al., *The Magnetic Genome of Two-Dimensional van der Waals Materials*, ACS Nano 16, 6960 (2022)
- H. Yang et al., *Two-dimensional materials prospects for non-volatile spintronic memories*, Nature 606, 663 (2022)