Internship proposal on "*Ab-initio* modeling of transport properties of van der Waals heterostructures of 2D materials"

Internship description: Nowadays, the two-dimensional (2-D) crystals and their van der Waals heterostructures (vdWHs) are deeply investigated by the scientific community due to the unique features such as the possibility to widely tune their band gap, the availability of heterojunction with neither dangling bonds or Fermi level pinning and their optimal electrostatic control [1]. However, vdWH have started to emerge only few years ago. Only a fraction of the almost infinite possibilities offered by them has been explored so far.

In this M2 internship, we will preliminarily investigate the electronic properties of 2D materials and their van der Waals heterojunctions by means of *ab-initio* methods such as density functional theory (DFT) [2,3]. By starting from this analysis, we will use state-of-the-art *ab-initio* quantum transport solvers, based on DFT Hamiltonians and the non-equilibrium Green's function formalism [4] to simulate nanoelectronic devices such as the metal-2D material interface sketched in the Figure as well as tunnel diodes based on heterostructures composed of transition metal dichalcogenides (TMDC). The validity of the models will be tested by comparing the results for vdWH-based devices with experimental data obtained from scientific partners involved in the "TUNNE2D" ANR project.

These results will advance our understanding of the physics involving electron transport in physical systems based on 2D materials. The continuation of this research in a PhD project is highly possible.

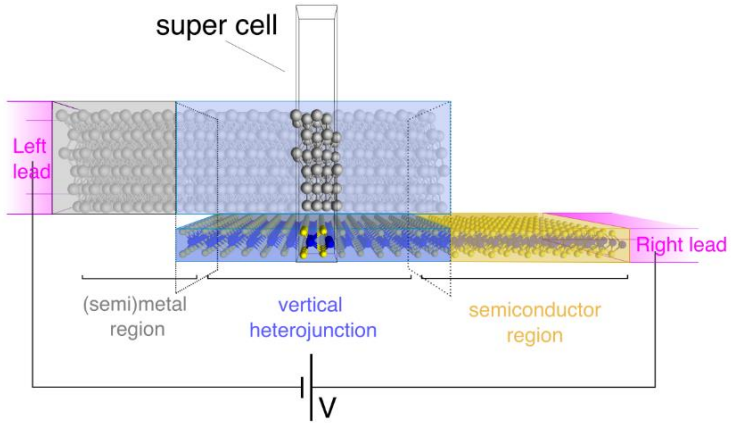

Figure: sketch of the atomistic structure representing the metal-2D material interface and consisting of the (semi)metal region at the left, the TMDC region at the right, and the actual metal-TMDC heterostructure in the center.

Objectives: The final objectives of the internship are: (i) to understand the physics and transport properties of 2D layered materials and their heterojunctions, (ii) to validate the physical models and numerical methods by comparing simulation results with experimental data.

Methods:

- DFT methods will be used for bandstructure calculations and the construction of the Hamiltonians used in the transport calculations.
- A first-principles approach will be used to simulate carrier transport within the framework of the non-equilibrium Green's function formalism coupled with Poisson's equation.

Candidate profile: The candidate should have a good knowledge of solid-state physics, electronic transport phenomena, and semiconductor devices, together with a good basis in quantum mechanics. He/she should have a taste for scientific calculation and computing. Knowledge of scientific programming language(s) is also appreciated (Matlab, C, Fortran).

Contact: In order to ask information and apply, please contact

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References

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[3] P. Giannozzi et al., J. Phys.: Condens. Matter vol. 29, p. 465901, (2017).

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