Quantum Transport in Vertical and Lateral 2DMs-based Heterostructures

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Novel prospects for the quasi-perfect assembly of lateral (LHs) and vertical (VHs) heterostructures have been recently proposed by combining layers of two-dimensional materials (2DMs)[1]. Those 2DMs-based heterostructures are characterized by dangling-bond free surfaces and well controlled interfaces, enabling the inventive engineering of devices at the atomic scale when combined with the large number of existing 2DMs. From a theoretical perspective, an in-depth understanding of charge transport across a stacking of 2D layers is essential in the design of VHs, whereas the coupling between 2DMs and interfacial effects need to be explored in the case of LHs.
The present research consists in investigating VHs constructed from multi-layer graphene (MLG) encapsulated in metallic materials (Fig.1) as well as LHs composed of transition metal dichalcogenides (TMDs) (Fig.2). The corresponding transport properties are investigated using the Landauer-Büttiker formalism implemented within a Green's function approach. In the case of VHs, different metals, crystallographic transport directions and surface orientations are considered to accurately understand vertical tunneling transport. In addition, the electronic structures (band alignment, charge exchange, …) of TMDs-based LHs are explored for different strain profiles in the aim of proposing novel functionalities in straintronics[2].
The main goal of the present work is on the one hand to address the crucial importance of materials engineering in stacked systems[3] and on the other hand to fill in the lack of electronic transport characterization in TMDs-based LHs.

References

[1] Iannaccone G. et al., Nature Nanotechnology **13.3** (2018): **183**.
[2] Ávalos-Ovando O. et al., Journal of Physics: Cond. Matter **31.21** (2019): **213001**.
[3] Dechamps S., Nguyen V.-H. and Charlier J.-C., in preparation (2020)

Figures

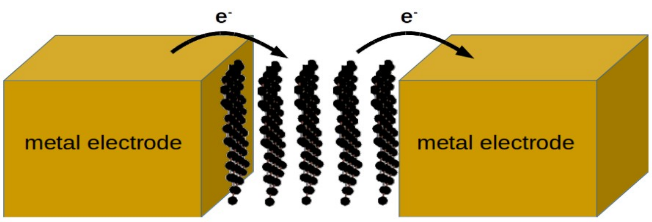

Figure 1: Modeling quantum transport through graphene-based VHs. Charge carriers are transmitted between the two metallic leads through a sequence of stacked graphene layers (in black) by tunneling effect, as schematized by the arrows

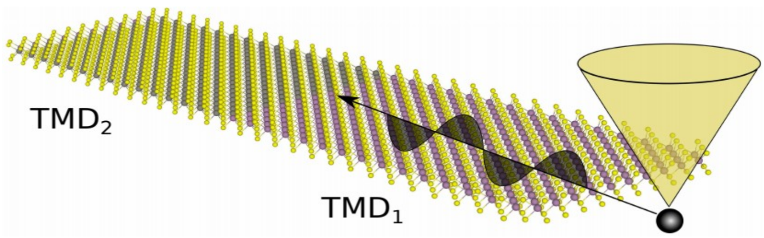

Figure 2: Modelling quantum transport through TMDs-based LHs. Charge carriers are injected in TMD_1 and collected in TMD_2