Ab initio quantum transport in metal-graphene-metal junctions

Samuel Dechamps, Viet-Hung Nguyen, and Jean-Christophe Charlier

Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, 1348 Louvain-la-Neuve, Belgium.

samuel.dechamps@uclouvain.be

The emergence of van der Waals (vdW) materials offers novel prospects for the quasi-perfect assembly of heterostructures, using two-dimensional (2D) materials. Such 2D-based vdW systems are characterized by dangling-bond free surfaces stacked together with well controlled interfaces, enabling the realization of next-generation electronics including resonant tunneling diodes, tunnel field effect transistors, optoelectronic devices as well as spintronic applications [1].

An essential issue in designing heterostructures consists in understanding the basis of vertical transport of charge carriers by tunneling effect across a stacking of 2D layers. Although most of the 2D materials considered are insulators, a tunneling barrier based on graphene would be nearly transparent and could act as a lateral conductor with a tunable barrier potential.

In the present research, vertical junctions composed of multi-layers graphene (MLG) encapsulated in a metallic bulk material are considered (see Fig.1). The corresponding transport properties are investigated using the Landauer-Büttiker formalism implemented within a non-equilibrium Green's function approach. In order to accurately describe the out-of-plane transport, vdW interactions are included within either semi-empirical models or density dependent functionals [2]. Moreover, different crystallographic transport directions and surface orientations are considered.

Various distinct transmissions are observed, depending on the nature of the metallic material. Concurrently, a simple model based on the matching between the metal and graphene electronic structures is developed. The qualitative agreement between DFT and this simple model suggests that the electronic correspondence is the dominant factor for out-of-plane transport, indicating that crystallographic engineering in stacked systems is of crucial importance for the next-generation electronics and spintronic applications.

References

[1] Zhu, Xiaodan, et al., Nano Letters **18**, 682-688 (2018)

[2] Jiří Klimeš and Angelos Michaelides, The Journal of Chemical Physics **137**, 120901 (2012)

Figures

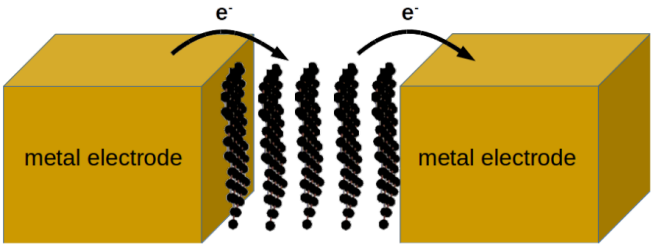

Figure 1. Modelling quantum transport through graphene-based vertical heterostructures. Charge carriers are transmitted between the two metallic leads through a sequence of stacked graphene layers (in black) by tunneling effect, as indicated by the arrows.