Electronic Transport in Graphene / Ni(111) contacts from first principles

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Abstract

Graphene microwave applications require an ultralow graphene-metal contact resistance in order to reduce extrinsic RC times that impact on the intrinsic performance of graphene field effect transistors (GFETs) [1]. For device applications, it is desirable to have a contact resistance (R_c) lower than 100 Ω·μm, while larger values are thought to be a limiting factor on the GFET performance [2,3]. Recent experimental developments have achieved this landmark value [4].

Injection of electrons from the metal into the GFET channel can be thought of as a succession of two steps: 1) injection from the metal into the graphene in contact with the metal, and 2) injection from the graphene in contact with the metal into the channel. Both steps will give rise to contributions towards R_c termed R_i (for interface, step 1) and R_g (for graphene, step 2). First principles calculations can provide insight on the fundamental processes at hand, identifying the limiting factors for efficient electron transfer from the contact into graphene.

We will present *ab initio* calculations of ballistic transport in a Graphene / Ni(111) junction. It has been shown experimentally that graphene can be grown epitaxially on such a metal surface [5], thus providing an ideal testbed for first-principle calculations.

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References

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Figures

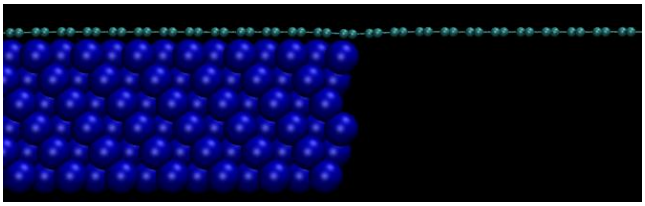

Fig. 1: Relaxed Graphene / Ni(111) structure to study R_g.

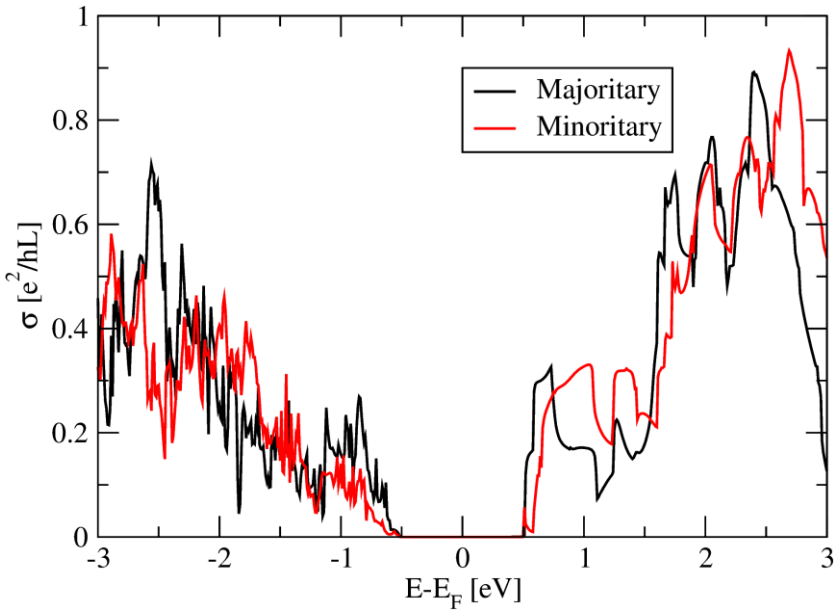

Fig. 2: Spin-resolved line conductivity corresponding to the structure in Fig. 1.