# Contact resistance in metal/two-dimensional material junctions from first principles

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In order for graphene and other two-dimensional materials to become competitive players amongst the myriads of electronic devices, one of the main technological hurdles that must be overcome is achieving a low contact resistance ($R_c$) so that high frequency performance is not compromised [1]. For graphene, it is often quoted that an Rc value lower than 100 Ω•μm is desirable, while larger values are thought to be a limiting factor on the graphene field effect transistor performance [2,3]. Recent experiments have achieved this landmark value with a top contact geometry [4].

On the other hand, an edge contact has been shown experimentally to achieve contact resistances with similar or lower values than most top contacts [5], challenging the conventional wisdom that having a large contact area will result in a decreased value of the contact resistance. Attempts at explaining this behavior resort to the perceived need of electrons to scatter from a value with $k_z \neq 0$ to $k_z = 0$ when entering the graphene layer.

We will argue that ballistic electron injection into graphene (or any other 2D material) is basically a perimeter-dependent phenomenon, dependent only on the atomistic details of the graphene-metal configuration at the edge of the metal. 2D materials have a low current carrying capacity per unit width —related to the number of available orbitals in a given energy window—, which is easily saturated by one or a few orbitals with a good overlap in the metal edge – graphene region. This is clearly illustrated in an imaginary graphene-graphene contact, where there is no backscattering and hence a null Rc is obtained (of course, these junctions are not advisable for realistic devices due to the higher value of the resistance in graphene with respect to a bulk metal).

Our arguments are supported by first principles calculations of a model Al/Graphene flake contact, showing a square root dependence of the transmitted current with the contact area (Fig. 1), and graphene with a varying overlap on top of a Ni(111) surface [6], where it is shown that a large fraction of the theoretical maximum of the conductance per unit width is achieved even with a very small overlapping region between the graphene and the Ni(111) surface (Figs. 2 and 3). We will also show that these conclusions are similar for physisorbed graphene.

From these results it can be concluded that the experimentally observed high contact resistances in metal – 2D material junctions may be amendable if proper care is taken that the edge region has an intimate contact with the metal. In fact, having a large overlapping region between the metal and the 2D material may be detrimental to the goal of a low contact resistance.

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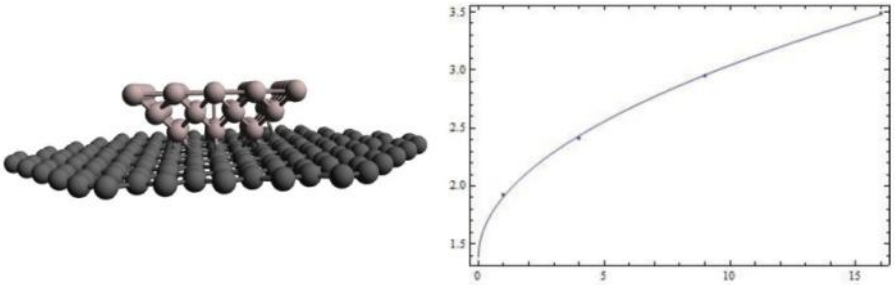

**Figure 1.** Left: Metal-graphene flake contact. Right: Current vs number of atoms in the contact (points), and a fit of a square root dependence (line).

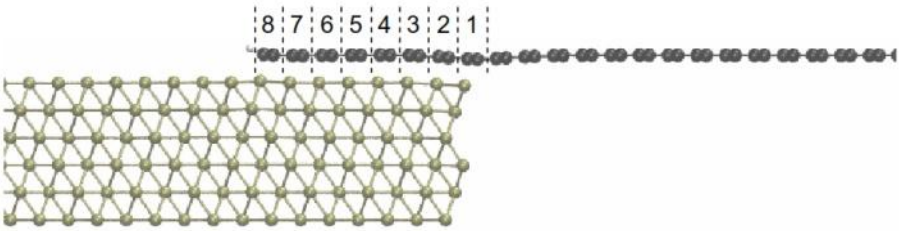


**Figure 2.** Relaxed Graphene / Ni(111) structure with the amount of overlapping zigzag chains indicated

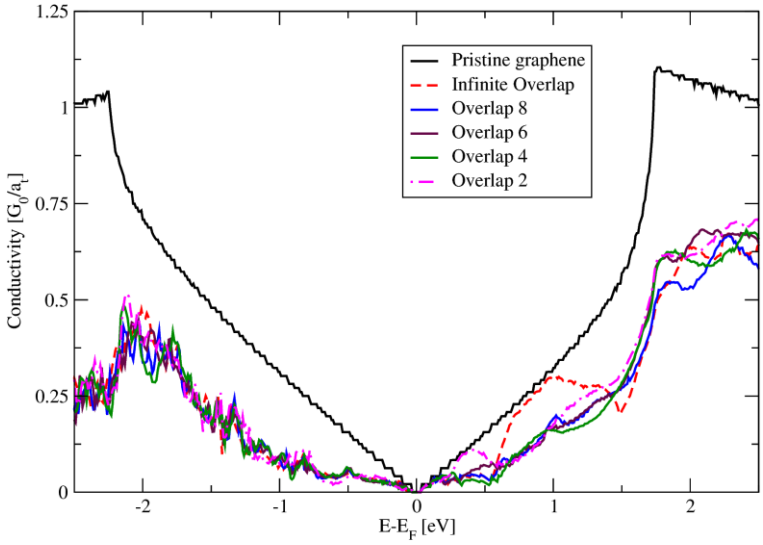


**Figure 3.** Minority spin line conductivity corresponding to the structure in Fig. 2.