# Effects of Metal Contacts on Electronic Transport through Two-Terminal Graphene Junctions

Salvador Barraza-Lopez*

*School of Physics, Georgia Institute of Technology*
*Atlanta, GA 30332, U.S.A.*

Graphene is a unique material with a linear energy dispersion around the $K$-point. A large amount of experimental and theoretical work has been carried out over the last five years in order to understand its properties, including many two- and four-terminal electrical measurements of graphene samples. Of particular interest is the role of metal contacts in modifying the transport properties. Although model calculations have been reported, first-principles studies are desirable in order to provide an unambiguous description of the effects of metal contacts. We have performed transport calculations at zero source-drain bias using the nonequilibrium Green's function SMEAGOL code,[1] which is interfaced with the density-functional theory (DFT) SIESTA package. Modifications to the transport code have been made to improve memory allocation and parallelization, making it possible to handle large-scale calculations that include metal leads in a two-terminal configuration. We have studied the conductance through graphene suspended between Al contacts as a function of junction length, width, and orientation.[2] The charge transfer at the leads and into the freestanding section gives rise to an electron-hole asymmetry in the conductance and in sufficiently long junctions induces two conductance minima at the energies of the Dirac points for suspended and clamped regions, respectively. We will discuss the potential profile along a junction caused by doping and provide parameters for effective model calculations of the junction conductance with weakly interacting metallic leads. We will also discuss the adsorption characteristics of different metal contacts on graphene.

*In collaboration with Mihajlo Vanević, Markus Kindermann, Lede Xian, and Mei-Yin Chou.

[1] A.R Rocha, V. M. Garcí a-Suárez, S. Bailey, C. Lambert, J. Ferrer, and S. Sanvito, Phys. Rev. B **73**, 085414 (2006).

[2] S. Barraza-Lopez, M. Vanević, M. Kindermann, and M. Y. Chou, Phys. Rev. Lett. **104**, 076807 (2010).