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Transport properties of contaminated metal-graphene interfaces

BERNHARD KRETZ, Donostia International Physics Center (DIPC), Spain, CHRISTIAN S. PEDERSEN, DANIELE STRADI, MADS BRANDBYGE, Center for Nanostructured Graphene, Department of Micro- and Nanotechnology, DTU, Denmark, ARAN GARCIA-LEKUE, Donostia International Physics Center (DIPC) and IKERBASQUE, Basque Foundation for Science, Spain — Interfaces between 2D nanostructures and bulk materials play an important role for a wide range of nanotechnology applications. Recently, graphene-metal contacts have been extensively studied and built into devices. In the process of fabricating such graphene-metal devices, contamination of the contact, and thus, doping of the graphene, may occur. Theoretical and experimental studies have shown, that controlled edge doping can significantly change the electronic structure of graphene.[1] Nevertheless, when occurring in an uncontrolled manner, edge-contamination has the potential of hugely modifying the electronic properties of graphene-metal interfaces in unforeseen ways. In our work, we carry our first-principles transport calculations to systematically investigate the influence of different edge-contaminations on the electronic and transport properties of graphene-metal contacts. Our studies shed light on the impact of the contaminants, as well as of the metal and of the contact conformation, on the conductance properties of such interfaces.

[1] P. Wagner et al., J. Phys. Chem. C 117, 26790 (2013); J. Cai et al, Nat. Nano 9, 896 (2014).

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