Schottky barrier in Gold- and Palladium-contacted semiconducting carbon nanotubes

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Work on semiconducting carbon nanotubes (CNT's) has been intensified over the past few years in connection with their potential use as nanoscopic field-effect transistors [1]. Progress is, however, still hampered by the difficulties in understanding the contact between the metal electrodes and the CNT. Several groups are stepping up their efforts on the experimental side [2], progressively reaching a high degree of control on the contact formation and progressively gaining insight on this issue. To date, however, theoretical work lags behind, mostly focusing on developing simple microscopic models that can be handled at a reasonable computational cost [3], but with questionable prediction power.

Here we present work on the transport properties of semiconducting CNT coupled to metallic electrodes commonly used (such as Au and Pd) from a fully first-principles point of view. To this end we employ our code ALACANT (ALicante Ab initio Computation Applied to NanoTransport) [4]. Our preliminary results show that for simple contact geometries (see Figure 1) the Fermi level lies roughly in the middle of the gap for Pd-contacted CNT's, while this one is pinned at the bottom of the conduction band for Au-contacted CNT's. No appreciable band bending is observed for neither type of metal, although the charge transfer at the interface is larger in the case of Pd. Finally, the role of contact geometry and atomic relaxation will be considered.

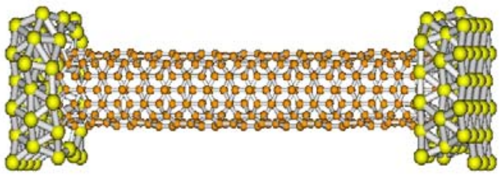

Figure 1. Relaxed structure of a CNT contacted by the open ends to Pd electrodes.

[1] J. Appenzeller, Y.-M. Lin, J. Knoch, and Ph. Avouris, Phys. Rev. Lett. 93, 196805 (2004).
[2] Harish M. Manohara, Eric W. Wong, Erich Schlecht, Brian D. Hunt, and Peter H. Siegel, Nano Letters (2006).
[3] N. Nemec, D. Tománek, and G. Cuniberti, Phys. Rev. Lett. 96, 076802 (2006).
[4] http://www.guirisystems.com/alacant.