CONTACT DEPENDENCE OF CARRIER INJECTION IN CARBON NANOTUBES

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We combine *ab initio* density functional theory with transport calculations to provide a microscopic basis for distinguishing between "good" and "poor" metal contacts to nanotubes. Comparing Ti and Pd as examples of different contact metals, we trace back the observed superiority of Pd to the nature of the metal-nanotube hybridization. Based on large scale Landauer transport calculations, we suggest that the "optimum" metal-nanotube contact combines a weak hybridization with a large contact length between the metal and the nanotube.

Reference

N. Nemec, D. Tomanek, and G. Cuniberti, Phys. Rev. Lett. **96**, 076802 (2006).

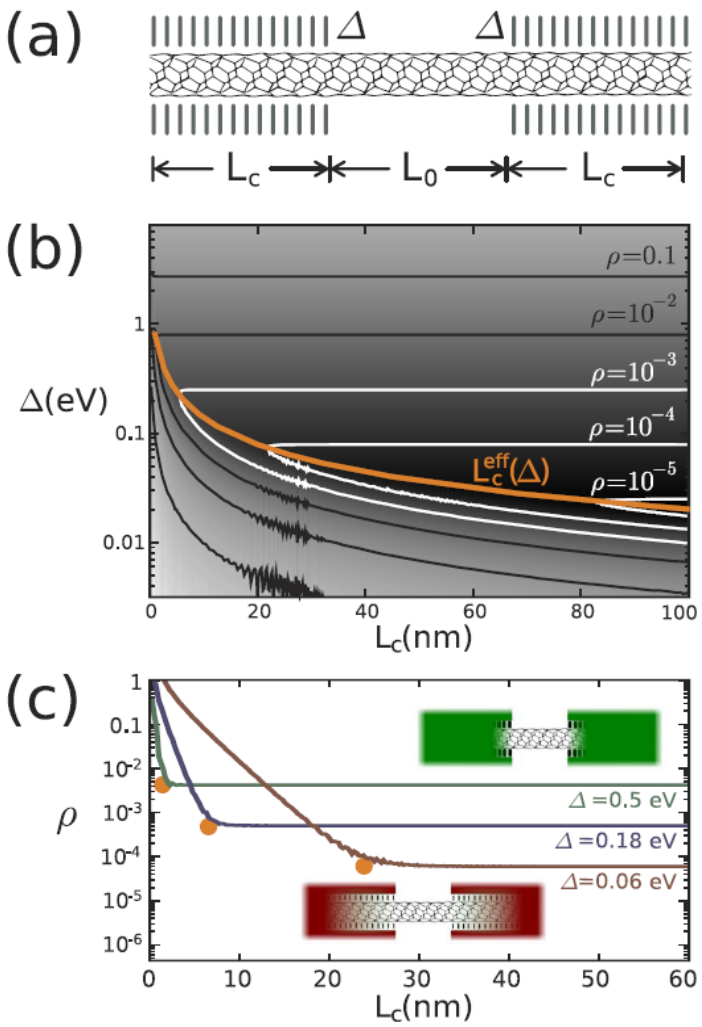

Figure
(a) Schematic geometry of the (6; 6) nanotube in contact with metal leads, used in the calculation of the contact reflection coefficient ρ. (b) Contact reflection coefficient ρ as a function of the nanotube-metal coupling Δ and the contact length L_c. (c) Cuts through the contour plot (b) at selected values of Δ, showing ρ as a function of L_c. The effective contact length L_c^{eff} is emphasized by a heavy solid line in (b) and by data points in (c).