

# **Research line B: NANOTUBES Coherent quantum transport and phonons in nanotubes** Miriam del Valle, Norbert Nemec and Gianaurelio Cuniberti

### **Extended contacts**

Starting from microscopic *ab initio* calculations of a metal-CNT interface, we extract parameters for large-scale tight-binding transport calculations.



### **CNT junctions**

We have analyzed the conductance behavior of several threeterminal CNT junctions. Around the Fermi energy, resonances in the LDOS are encountered, associated to bounded states.



Such localized states are pinned by the defects and interact with the continuum of states, giving rise to Fano resonances.

The Fano-like characteristics are then observed in I-V curves; **the big change in current** for some of the junctions make them interesting for their use as circuit components.

M. del Valle, C. Tejedor and G. Cuniberti, Phys. Rev. B 71, 125306 (2005)

## **Gold nanotubes (AuNTs)**

The transport properties of the recently experimentally observed helical gold nanotubes [Kondo, Takayanagi, Science 289, 606 (2000)] are investigated in order to understand the role of chirality and of the different orbitals in the conductance characteristics.



Using an analytical model accounting only for s-orbitals, we can reproduce exactly the results of the numerical calculations, which show a slight decreasing trend in the conductance per atom row:

$$G = 2 \frac{e^2}{h} \left[ 2 \cdot Int \left( \sqrt{\frac{n^2 + m^2 + nm}{\pi \sqrt{3}}} \right) + 1 \right]$$





**Result:** for extended metal contacts, *weak metal-CNT coupling*, as found for Pd as contacting material, leads to *longer effective* contact regions and lower reflection at the

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





M. del Valle, C. Tejedor and G. Cuniberti, Phys. Rev. B 74, 045408 (2006)

