Poster

SIMULATION OF CARBON NANOTUBE FIELD EFFECT TRANSISTORS WITH PALLADIUM CONTACTS

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The use of carbon nanotubes in field effect transistors (CNTFET) represents a promising way to develop new electronic devices. However, its development has raised a lot of questions regarding the contact with the electrodes and the electrostatic response of the nanotube. Actually, the fine structure of the interface between the metal and the nanotube and the chemical environment play an important role in the transport properties [1-3]. For instance, it has been proven that the use of Palladium contacts tends to reduce the Schottky barrier [1]. Moreover, the electrostatic influence of the gate over the nanotube is taking place over several ten or hundred nanometers. For these reasons, it is mandatory to use multiscale simulation in order to take into account the complexity of the interface at the atomic scale, and the geometry and electrostatics of the complete device.

The system considered to model the interface between the metal and the nanotube in the CNTFET is an infinite palladium nanowire connected to the nanotube (see figure). To model this interface, we start with a ground-state calculation of the system of interest using the SIESTA *ab-initio* package. The locality of the basis and the local density approximation lead to the partitioning of the system into "nearest-neighbor" sections so that the Hamiltonian H and overlap S matrices are tri-diagonal by blocks. This property allows to calculate with an O(N) scaling the Green's function of the system. We have thus been able to study the transmission across a semi-infinite metallic nanowire and a semiconducting carbon nanotube when different conformations for the contact are considered (flat connection or embedded nanotube into the metallic nanowire).

As the transport along the nanotube close to the Fermi level is mainly governed by the π-π^* bands, the *ab initio* calculation with a large orbital basis (used to model the contact between the metal and the nanotube) is unnecessary when we deal with the nanotube itself. Especially, the part of the tube submitted to the gate potential does not require such a large basis and a single orbital description is enough.

We have thus developed a technique to couple the *ab initio* calculations needed to describe the contact and the tight binding calculation for the part of the tube submitted to the gate potential. This has been performed by first computing with the *ab-initio* results the self-energy of a finite length nanotube connected to the palladium lead and then to use these self-energies to perform the self-consistent calculation of the influence of the gate on the nanotube using a simple π-π^* tight-binding basis. With this technique, the transmission properties of the contact are fully described without the inconvenience of the large basis used to model the contact.

Using this reduction of the tight-binding basis, quantum simulations of CNTFETs with coaxial gate have been performed. The Green's function formalism is used to compute the Landauer-Büttiker conductance and the charge on each orbital of the channel, similarly to the method used by Guo and co-workers [4]. The self-consistency is obtained iteratively by solving the Poisson equation, correcting the potential on the nanotube within the Hartree scheme, and recalculating the charge along the nanotube with the Green's function method. Once self-consistency is achieved, the Landauer-Büttiker conductance is computed. The

present study is performed at T = 300 K. It is limited to coherent transport in the low bias regime (V_{DS} smaller than kT). The current-gate voltage characteristics $I(V_G)$ are calculated. We study the influence of gate the parameters (distance to the contacts and to the channel). The results with "*ab initio*" Pd-CNT self-energies are compared to those obtained with a very simple model of metal contacts, in order to discriminate the contribution of the contacts in the $I(V_G)$ characteristics.

References:

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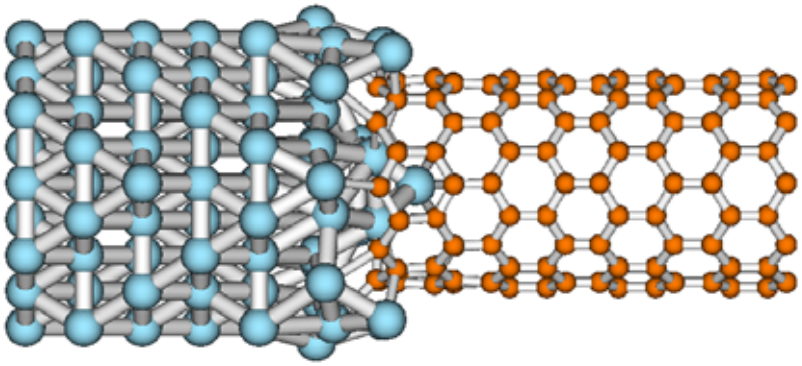
Figure:



Junction between a Pd nanowire and a (10,0) carbon nanotube