Quantum Capacitance Effects in Carbon Nanotube Field-Effect Devices

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Conventional silicon MOSFET channel length continues to shrink rapidly towards few nanometers dimensions. These ultra-small devices are studied in view of application in ultra-large scale integrated circuits. New transport mechanisms different from those of conventional devices are involved when the channel length reduces to the ballistic limit. Beside the exploration of these conventional nanoscale transistors performances, theoretical studies and recent experimental realizations have been imposing molecular transistors as a challenging alternative to solid state field-effect devices.

Carbon nanotube (CNT) based transistors, for example, are especially interesting for both fundamentals of quantum transport and technology. They are quasi one-dimensional organic conductors in which electrons can propagate ballistically over very long distances. A CNT can be used as a nanometric channel for a device in which electron transmission can be modulated by a suitable gate potential, just like in standard FET devices.

Many examples of CNTFET have been realized using a conventional metal-oxide-semiconductor field-effect transistor (MOSFET) structure. In this kind of devices the gate contact modulating the CNT channel has a planar configuration. An important alternative to these structures is the possibility of growing a vertical CNT comprised between two metallic contacts and surrounded by a coaxial gate, from which it is separated by a coaxial insulating layer.

In this work we calculate the coherent transport properties of a coaxially gated semiconducting CNT using an *ab-initio* approach based on a self-consistent density-functional tight-binding method and the non-equilibrium Green's function formalism we have previously implemented.

Using a self-consistent non-equilibrium charge computation coupled to a three-dimensional real-space Poisson solver, we can fully account for the effects that the quantum capacitance of the one-dimensional CNT has on the modulation of the channel conductance. The quantum capacitance is added to the gate oxide capacitance to model the penetration of the external gate field inside the channel. We find that in the quantum capacitance limit (i.e., when the quantum capacitance is smaller than the geometrical one, which occurs for very thin gate oxides or high k gate dielectrics), the gate modulation is limited because of the poor screening properties of the one-dimensional CNT, which are particularly evident when the CNT dimensions become smaller than its screening length. Both limitations and new interesting operational modes can arise for such ultra-short one-dimensional field-effect devices, and a particular attention in the design of the gate electrostatics is required.

A full journal publication of this work will be published in the Journal of Computational Electronics.

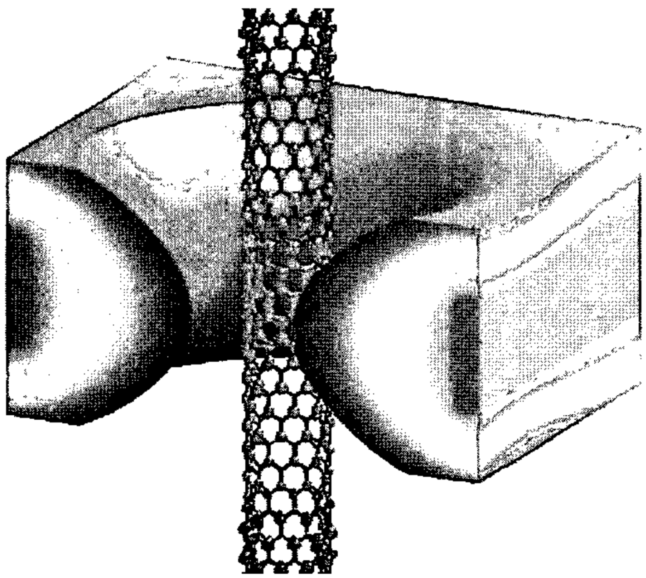

Figure 1: potential and charge density isosurfaces of a coaxially gated (10,0) semiconducting CNT in equilibrium conditions (V_{ds}=0.0V), when a potential of 0.2V is applied to the gate contact causing a local negative charge accumulation.

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