# Realistic simulations of electronic transport at the nanoscale: from gas sensors to spintronics

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The possible application to electronics of nanoscale devices presents tantalizing perspectives. The possibility of using an ever smaller number of atoms in the same tasks of today's silicon-based devices with improved performance and lower power consumption is driving much of the scientific research effort.

At the nanoscale, even a single defect can cause significant changes to the electronic transport properties of a device. Our lack of control over fabrication processes has led to a situation whereby defects are unavoidable. Furthermore, it is not possible to determine *a priori* the position of such defects. From the theoretical perspective, up until now it was only possible, using *ab initio* methods, to consider a small number of defects. This has hindered theoretical efforts thus far.

In this work we present electronic transport calculations of large disordered systems. We will outline our methodology which is based on a combination of density functional theory (DFT) and recursive non-equilibrium Green's functions (NEGF). This powerful combination enables one to calculate the electronic transport properties of systems up to 450 nm long with up to 20,000 atoms using *ab initio* methods.

As some examples we will show how one can use nitrogen-doped carbon nanotubes as gas sensors for a variety of molecules such as ammonia [1,2], carbon monoxide, oxygen and water. In particular we will show the possible dissociation paths for these molecules and how a large number of dissociated molecules onto the nanotube will alter the electronic transport properties.

Finally we will also demonstrate how one can use one-dimensional disordered carbon-based systems such as carbon nanotubes [3] and graphene nanoribbons [4] within the Anderson localization regime to design spintronics devices. In these systemsthe current through the system is either perfectly spin polarized or a giant magnetoresistance effect, with values up to 7000 %, is obtained. In all cases there is no need to inject polarized electrons.

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