Defective carbon nanotubes: magnetism, spin transport and gas sensing applications

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Carbon nanotubes (CNTs) are renowed in the scientific community for being both a playground for studying fundamental physical properties and for applications in, to mention a few, electronic, spintronic and gas sensing technologies. However, despite the progresses in growth techniques, CNTs always exhibit structural defects [1] and their electronic and transport properties will be affected accordingly [2]. In addition, the presence of defects in carbon-based nanostructures has been seen as source of magnetism [3]. Hence, mastering the physics underlying defected CNTs is crucial not only to model realistic systems but also to design new devices.

The spin-polarized electron transport properties of carbon nanotubes with vacancies are investigated using first principles and non-equilibrium Greens function techniques [4]. Carbon atoms with unsaturated bonds are found to behave as quasi-localized magnetic impurities, coupled by long range interactions. The magnetism of carbon nanotubes with reconstructed mono- and tri-vacancies results in spin dependent contuctances and, hence, can be exploited in spintronic devices such as nano-spin valves.

Clarified the properties of CNTs with vacancies, the sensing ability of defected CNTs towards several molecules (NO_2, NH_3, CO, CO_2, H_2O) has also been investigated *ab initio* . Since the adsorption/desorption of molecules induces modulations on the electrical conductivity of the tube, quantum conductances of the CNT-based sensors are predicted, finding that defective nanotubes are sensitive to NO_2, NH_3, CO, and H_2O while molecular selectivity is provided by the nature of the charge transfer.

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