Carbon Nanotubes as gas sensors: a first-principles study
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One promising application of carbon nanotubes is the fabrication of chemistry sensors for gas detection. Recently [1] it was experimentally shown that the effect of the interaction between distinct gases and the nanotube on the system capacitance is specific and may be used to build a capacitive sensor device. In this work we have applied first-principles calculations based on the Density Functional Theory (DFT) in order to analyse the interaction of carbon nanotubes with distinct molecules (benzene and oxygen, for instance) and determine the effect of the interaction on the nanotube capacitance. For each molecule we first determine the equilibrium geometry close to the nanotube wall, then we do calculations in distinct charge states to obtain the capacitance. Our results show that there is a definite relationship between the change of the density of states (DOS) close to the Fermi level upon interaction of the nanotube with the oxygen molecule and the change of the capacitance, which means that the quantum contribution to the capacitance may be used to sense oxygen molecules. As for the benzene, the effect on the capacitance is null, as well as the change in the DOS close to the Fermi level. We employ the SIESTA [2] implementation of the DFT formalism, which makes use of pseudopotentials and a basis set composed of pseudo atomic orbitals of finite range.