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Ab initio charge transport through N-doped carbon nanotubes: microscopic understanding of carbon nanotube sensors FREDERICO D. NOVAES, MARIANA ROSSI, ANTÔNIO J. R. DA SILVA, A. FAZZIO, Instituto de Física, Universidade de São Paulo — We calculate, using an ab initio non-equilibrium Green's function formalism, the conductance of metallic carbon nanotubes with pyridine-like defects. We show that there is a decrease of the conductance at the Fermi energy due to these defects, which is caused by nitrogen related levels within an energy window of 1.5 eV below the Fermi energy. We then investigate how exposure to NH₃ can affect the conductance. At the pyridine-like structure the NH₃ dissociated into NH₂ and H, with both molecules binding to nitrogen atoms. This configuration leads to an increase of the conductance, and cannot, therefore, explain the increase of resistance that has been experimentally observed. We then investigate other configurations, and suggest that a possible cause of the resistance increase is adsorption of atomic or molecular species at the wall of pristine nanotubes.

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