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N-doped carbon nanotubes and their behavior as ammonia sensors ANTONIO J.R. DA SILVA, MARIANA ROSSI, FREDERICO D. NOVAES, A. FAZZIO, Instituto de Fisica - Universidade de São Paulo — CNx nanotubes can display a measurable variation in resistance upon exposure to ammonia. We present a microscopic model for the origin of these variations. We studied, using Total Energy DFT calculations, a (5,5) CNT containing pyridine-like N atoms replacing C atoms, and how the NH_3 molecule binds to these sites. We also investigate how these defects affect the charge transport properties using a Non-Equilibrium Greens Function formalism. We initially studied a defect composed by a vacancy surrounded by 3 pyridine-like rings. The most stable adsorption configuration for the ammonia molecule adsorbed close to this defect is dissociative, with an amino group (NH_2) fragment bound to one of the nitrogens and a H atom bound to another. This configuration leads to an increase in the conductance and cannot, therefore, explain the increase of resistance that has been experimentally observed. We then investigate a variety of other configurations in order to propose possible causes for the resistance increase. We find that a divacancy surrounded by 4 pyridine-like defects is the most stable N-defect, instead of the previously proposed one. The ammonia also dissociates into NH_2 and H. Moreover, the calculated change in conductance after the NH_3 dissociation has the correct trend when compared to the experimental results. We acknowledge FAPESP, CNPq and CENAPAD-SP.

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