

**Estudo teórico de sensores baseados em nanotubos de  $CN_x$  utilizando cálculos *ab initio***

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Recently, it has been experimentally shown that  $CN_x$  nanotubes (NTs) display a measurable variation in resistance upon exposure to ammonia. Our objective is to understand, from a microscopic point of view, the origins of this variation. To this end, we studied a (5,5) metallic carbon NT containing a defect composed of a vacancy surrounded by three pyridine-like rings, and how the  $NH_3$  molecule binded to this defect. We also studied the charge transport through the NT with and without the  $NH_3$ . We have used Total Energy Density Functional Theory (DFT) calculations for the adsorption studies, and the conductances were calculated using a DFT-based non-equilibrium Greens function formalism. We have found that the  $NH_3$  adsorbed close to the defect prefers to fragment into a  $NH_2$  and a H atom, with a binding energy of approximately 0.2 eV. However, the change in conductance was contrary to experimental results. Therefore, we made a systematic study of  $CN_x$  structures, found the one with lowest formation energy, which is a defect composed of four pyridine-like rings and two vacancies, and calculated how the ammonia molecule binded to it. Again, it fragments itself in two parts but its binding energy is around 0.02 eV. The charge transport calculations for this configuration shows that the transmittance is lower if compared to the tube with the defect and without the  $NH_3$ , which is in accordance with experimental results.