# DOPING OF SEMICONDUCTING CARBON NANOTUBES WITH ACID MOLECULES

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A significant challenge for the use of carbon nanotube (CNT) thin films as transparent electrodes is the low conductivity due to semiconducting nanotubes. To improve the conductance of CNTs, they can be doped with various atoms and molecules. A p-type doping effect has been observed in CNTs treated by gold chloride molecules [1, 2]. Moreover, nitric acid results in a similar effect lowering remarkably the CNT Fermi level [3].

We have investigated computationally the influence of gold chloride and nitric acid doping on single-walled semiconducting (10,0) CNTs. We consider $AuCl_4$ and $NO_3$ molecules placed on top of a (10,0) CNT. The effect of $H_2O$ molecules attached to $NO_3$ is also investigated. Calculations are performed with the FHI-aims code package based on the density functional theory [4]. The band structures of doped CNTs are calculated with the hybrid functional HSE06. Electron transfer takes place from the nanotube to the adsorbed molecules. The doping effect is around $1.07$ and $0.73$ electrons per $AuCl_4$ and $NO_3$ molecules, respectively. Attached $H_2O$ molecules increase the effect to $0.89$ electrons per $NO_3$ molecule. We have also performed calculations using the partial self-interaction corrected formalism [5] implemented to the GPAW code [6]. The SIC and HSE06 results are consistent.

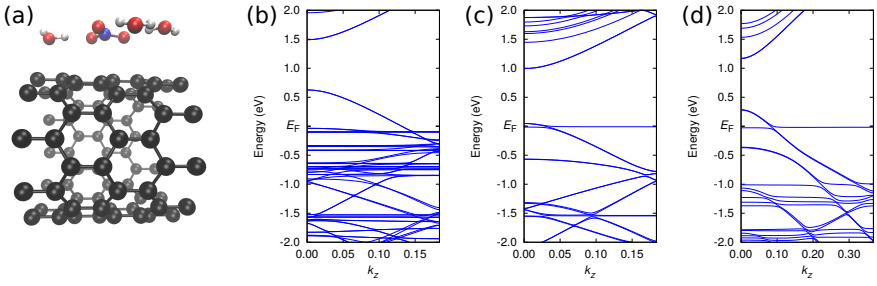


Figure 1: (a) (10,0) CNT with a $NO_3$ molecule surrounded by $H_2O$ molecules. Band structures for the CNTs doped with (b) (a high concentration of) $AuCl_4$ molecules, (c) (a low concentration of) $NO_3$ molecules, and (d) $NO_3$ molecules with attached $H_2O$.

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