

## Ab-initio study of gas adsorption on carbon nanotubes

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Carbon nanotubes have recently been proposed as chemical sensors<sup>1</sup>, due to their fast response and high sensitivity towards environmental gaseous molecules. However, the chemical and physical interactions between molecules and sensing nanotubes are not yet completely understood. Within this framework, first principles calculations within the density functional theory have been performed for simple molecules (such as NO<sub>2</sub> and CO) adsorbed on (10,0) carbon nanotubes (CNT), using the Dmol<sup>3</sup> code. Our results show that the adsorption process of both CO and NO<sub>2</sub> is physisorption, with a pretty small binding energy. NO<sub>2</sub> and CO molecules are charge acceptor and donor, respectively. The CNT density of states is sensitive to the adsorption of NO<sub>2</sub>, with a strong peak close to the CNT valence band maximum, leading to a *p*-type conductivity. On the other hand, CO adsorption does not alter the CNT electronic properties. These findings are in excellent agreement with experimental conductivity measurements.

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<sup>1</sup>J.Kong *et al.*, *Science* **287**, 622 (2000).