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Ab initio design of reallistic nanotube sensors ADALBERTO FAZZIO, ALEXANDRE ROCHA, MARIANA ROSSI, ANTONIO J.R. DA SILVA, Instituto de Física - USP Brazil — The understanding of the electronic transport properties of nanoscopic devices present tantalizing possibilities. In particular it has been demonstrated that carbon nanotubes can be used as sensors for hazardous gases. Large scale computer simulations have an important role to play in predicting the transport properties of such systems. In order to do so one must take into account devices which are a few hundred nanometers in length and present defects randomly distributed along the structure. These defects act as binding sites for the molecules one wishes to detect. In this work we initially use density functional theory (DFT) to determine the most likely defects in highly nitrogen-doped carbon nanotubes, and to calculate the dissociation path of ammonia and hydrogen sulphide molecules onto these defects. Finally we use a combination of DFT and recursive Green's functions techniques to first assemble and then calculte the electronic transport properties of nanotubes up to 200 nm in length and with defects randomly distributed along the structure. We demonstrate that these nanotubes present relatively large resistance changes even at low coverages which leads to highly sensitive devices. The result is a new paradigm in computer-aided sensor design, where one can simulate realistic sensors.

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