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Ab initio simulations of the eletronic and transport properties of nanotube bundles used as gas sensors ALEXANDRE ROCHA, RODRIGO AMORIM, Universidade Federal do ABC, Brazil, ADALBERTO FAZZIO, ANTÔNIO J.R. DA SILVA, Instituto de Física, Universidade de São Paulo, Brazil — Carbon nanotubes (CNT) have exceptional mechanical and - particularly - electronic properties that make this material of great potential interest for applications in different areas of materials science. One of the possibilities which raises the highest hopes is the area of nanotube-based gas sensors. From the fabrication point of view, one is probably going to use bundles of CNTs instead of a single tube. In this work we initially use density functional theory (DFT) calculations to determine the electronic structure properties of different molecules interstitially positioned between the nanotubes in a bundle. From the most stable structures we couple the DFT calculations to a recursive Green's function method to simulate. The electronic transport properties of a disordered nanotube bundle containing a large number of molecules randomly distributed along the different tubes forming the ropes. This way one is able to simulate a realistic sensor based on three-dimensional nanotube bundles taking into consideration the effects of disorder.

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