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Fermi Energy-Dependent Structural Deformation of Single-Wall Chiral Carbon Nanotubes[1] EDUARDO BARROS, UFC/MIT, BRUNO VIEIRA, ANTONIO SOUZA FILHO, UFC, MILDRED DRESSELHAUS, MIT — In this work, we investigate structural deformation of single wall carbon nanotubes as a function of the Fermi Energy by calculating the structural and electronic properties of charged carbon nanotubes within an extended tight-binding approach. Density-Functional-Theory-based tight-binding parameters were used, following the procedure introduced by Vercosa *et al.* [2] The total energy of the nanotube is calculated assuming that the electron population follows the Fermi-Dirac distribution for a given Fermi-Energy (E_F). As the Fermi energy is varied, the total charge of the nanotube changes, thereby simulating a charging effect. Our results show that the relaxation of the electronic stress generated by an extra charge on the nanotube causes axial, radial and torsional strains which directly affect the electronic band structure of carbon nanotubes. The electron-electron Coulomb repulsion further increases this effect, leading to extremely high torsional strains and considerable changes to the electronic structure of the nanotubes. For example, torsional strains of up to 2% were obtained for an (8,7) nanotube for a Fermi energy of about 1 eV, causing changes of more than 0.5 eV to the interband transition energies.

[1] Yang et al. PRL, 85(1), 2000. [2] Vercosa, et al. PRB, 81:165430, 2010.

[1]CSF-CNPq

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