EFEITO DA TENSÃO MECÂNICA NO TRANSPORTE ELETRÔNICO EM SISTEMAS 1D E QUASI-1D

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Abstract

In the present work we have studied mechanical properties of ballistic and inelastic electron transport in molecules of carbyne connected between Single-Wall carbon nanotubes closed on tips. Electrical current, conductance and transmission through the system were analyzed under compression, equilibrium and mechanical distension. The results shows that while the mechanical tension displace the energy levels and change the band gaps in the closed tips of the nanotubes, the applied voltage break the degeneracy in the states of nanotube tips and define the electrical conductance along the system. The analysis of Projected Density of States (PDOS) suggests that the higher contribution to electrical current comes from the superposition between closed nanotube tip states, which is in agreement with the calculated transmission. The current? voltage curve let consider the observed system as a transistor. The Inelastic Electron Tunneling Spectroscopy (IETS) shows that the distension decreases the energy of phonons, in agreement with the decreasing of interactions intensity between neighbor atoms. For regions in lower frequencies the IETS intensity increases, while for higher frequencies the compression generates blue shifts. These last results provide information about the mechanical vibrations of the system during the electron transport and let us analyze the dynamics of electron-phonon interactions.