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Transport properties of single vacancies in nanotubes ALEXANDRE R. ROCHA, J.E. PADILHA, ADALBERTO FAZZIO, ANTONIO J.R. DA SILVA, Instituto de Física - USP Brazil — We present transport, density of states and electronic transport calculations of single vacancies in carbon nanotubes. We confirm that the defect reconstructs into a pentagon and a nonagon following the removal of a single carbon atom. This leads to the formation of a dangling bond. Finally we demonstrate that care must be taken when calculating the density of states of impurities in one dimensional systems in general. We show that obtaining information about the transport properties of such systems with defects solely from the density of states of a periodic DFT calculation can be misleading. The appearance of mini-gaps and oscillations, even in the limit of large unit cells, can be erroneously associated with changes induced by the defect itself instead of a figment of the procedure. In fact, we demonstrate that those mini-gaps vanish if the appropriate approach is taken, namely a Green's function method where the effects of semi-infinite electrodes are considered and a true open system is calculated.

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