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Electronic structure of a linear carbon-atom chain inside single-walled carbon nanotubes[1] ROMEO DE COSS, ALEJANDRO TAPIA, CESAR CAB, Department of Applied Physics, CINVESTAV-Merida, Mexico, JORGE MEDINA, GABRIEL CANTO, CCMC-UNAM, Ensenada, Mexico, CESAR ACOSTA, FI-UADY, Yucatan, Mexico. — Recently has been reported a new type of one-dimensional carbon structures. Carbon nanowires formed by a linear carbon-atom chain inside an armchair (5,5) carbon nanotube has been observed using high-resolution transmission electron microscopy. In the present work we have studied the electronic structure of a linear carbon-atom chain inside the (5,5) and (8,0) single-walled carbon nanotubes (SWCN) using the Density Functional Theory. The calculations where performed with the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. We have analyzed the band structure, the local density of states (LDOS), and the local orbital population. We find charge transfer from the nanotube to the linear chain in both systems chain@(5,5) and chain@(8,0). However, the electronic character of the chain and nanotube sub-systems in chain@SWCN is the same that in the corresponding isolated chain or SWCN systems.

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Romeo de Coss
CINVESTAV-Merida

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