

Abstract Submitted
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First principles study of energetic interaction of a carbon chain inside carbon nanotubes¹ LUIS AGUILERA, CINVESTAV, ALEJANDRO TAPIA, UADY, ROMEO DE COSS, CINVESTAV, CINVESTAV-UADY TEAM, MATERIAL SIMULATION TEAM — Recently has been reported a new type of one-dimensional carbon nanostructure. Carbon nanowires formed by a linear carbon-atom chain inside a carbon-nanotube have been observed using high-resolution transmission electron microscopy (HRTEM). In the present work, we have studied the energetic interaction and atomics forces inside of the (5,5) and (8,0) carbon nanowires, using the Density Functional Theory. The calculations were performed by the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange- correlation potential. Analyzing the energetic interaction inside the carbon nanowires, we found that the linear carbon chain obtains a preferential position inside of the carbon nanowires.

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