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FIRST PRINCIPLES DFT/NEGF ANALYSIS IN LINEAR CARBON CHAIN

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ABSTRACT

The studies experimental and theoretical targeted with Carbon or organic-metals growing a number of discoveries and applications of allotropes, such as Fullerens, Graphene, wires as Carbon nanotubes (CNTs) and Carbynes (*Polyynes* or *Cumulenes*), that proved promising in technological applications [1-3]. One of the allotropes of carbon include electronic devices the materials of one dimension (1D) such as CNTs and Carbynes, classified molecular wires present, electrical and optical properties of high strength [1-4]. That research consisted in the study of electronic properties of linear device coupling of a Carbyne with 10 Carbons atoms bound between two electrodes of CNTs *single-wall* with Chiral indexes $n = 9$ and $m = 0$ duly closed. For computational theoretical calculations of electronic transport using the density functional theory (DFT) getting energy balance of the system in conjunction with Non-Equilibrium Green Function (NEGF) implemented in computational packages SIESTA [5-6] using set of bases (PBE) [7]. The results, in the search for E_{min} (eV), those results showed the lengths of their links the central region with variations of ~ 1.2A and ~1.4A [1,8,9] in alternation for all molecular wire which features triple and single bonds alternating respectively featuring a polyyne [8,9]. In electronic transport detected in current-voltage graph with a variation for 0V to 0.5 V, Ohmic behavior consistent with Cretu et al. [10], indicating semiconductor by presenting gap in the Density of States (DoS). Conclusion it was the current variation with increasing of structure compression, which significantly altered the behavior I-V, being displayed on the change of (E, V_b) and Transmission T(V_b).

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