Eletronic transport of monolayer of α-graphyne in armchair orientation non-doped and doped with Phosphorus and Nitrogen using DFT-NEGF theory

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ABSTRACT

Recently interests in two-dimensional (2D) structures of carbon allotropes have a growing search for having very interesting physical and electronic characteristics for applications in nanoelectronics [1]. Given the recent searches, a new allotrope has been proposed known as α-graphyne [1, 2] presenting an organizational structure similar to that of graphene a honeycomb, however in its unit cell there are more atoms with sp bonds, or forms of acetylene bonds at the edges of the geometry. The results were obtained through the use of the DFT / NEGF formalism based on the Landauer-Buttiker equations [4]. Thus, a brief analysis of the behavior of the current with increase of the tapes is analyzed, analyzing the different behaviors and similarities with electronic devices. (A), without doping behaves as a semiconductor device with gap ~ 0.35 eV, similar behavior with armchair-type graphene sheets that present in the density of states Fig.), the signatures of Van Hoff's singularities [5].

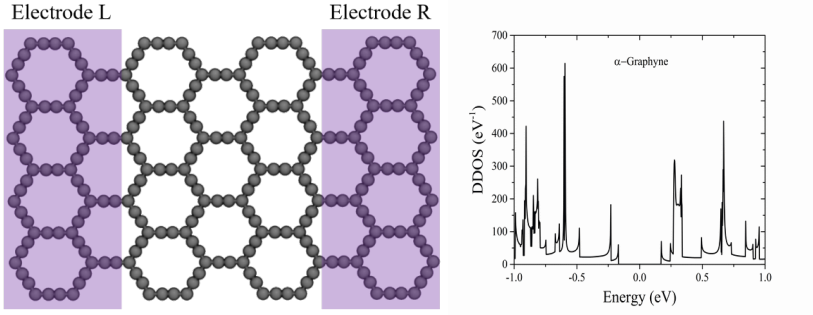

Fig. 1. (a) Configuração espacial do dispositivo estudado (b)

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