Electron Transport in Graphene-Phagraphene Mixed Structures

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Abstract

The nanoelectronics is today a strong new front of development, providing findings about new properties in a large range of materials. Among different ways to approach nanodevices based technologies there is the molecular electronics [1]. The first design for molecular electronic device was attributed to Aviram and Ratner [2]. New nano materials that have similar properties as conventional electronic devices are the most interesting [3]. Among these materials, graphene based devices have called attention of researchers around the world, due electrical, mechanical and thermal properties and high Fermi velocity in low temperatures [4]. Recently, Z. Wang *et al.* have suggested a new allotropic form of carbon, the phagraphene, a bi-dimensional material composed by carbon rings with 5-6-7 atoms, with sp^2 hybridization and comparable in energy with graphene, but most favorable in energy than other allotropic forms [5]. In this work, we have proposed a phagraphene based nanoelectronic device with metallic graphene leads. To perform electron transport calculations we have used the DFT-NEGF methodology in the Landauer-Büttiker formalism as implemented in the TRANSIESTA [6] code. Properties as current-voltage, transmission through the system compared with molecular orbitals shows interesting results and suggests phagraphene as promising material in nanoelectronics.

Key-words: Electron Transport; Graphene; New allotropic forms; Phagraphene;

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