ELECTRONIC TRANSPORT IN PHAGRAPHENE DOPED WITH BORON NITRIDE

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Since the discovery of graphene, several carbon allotropes have aroused the interest of the scientific community [1] due to their electronic properties and great potential for the synthesis of new devices [2]. Two-dimensional structures basead on carbon have recently attracted attention and have been extraordinarily promising in molecule-electrode junctions for current rectification [3]. Therefore, it was theoretically studied the electronic transport mechanism with a donor-acceptor system in a new two-dimensional material derived from the carbon called Phagrafeno [4], doped alternately with Boron and Nitrogen in the spreader region forming an arrangement analogous to the pair of spin and with carbon-only electrode. Was investigated by calculation with the density functional theory and the Green function nonequilibrium [5-7] (set of bases PBE and functional GGA) implemented by computacional package SIESTA [8] the structural conformation of the system, the properties of current-voltage curve, transmittance-energy, differential conductance negative, the density of states, the frontier molecular orbitals. The results revealed a diode-type device between 0.15V and 0.23V and an ohmic behavior of 0.25V to 0.5V. It was also observed a characteristic band gap of a semiconductor in the density of states, corroborated by analysis of the frontier molecular orbital. In this way, the system proves very interesting and promising for the development of electronic nanodevices.

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