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Molecular Devices Based in 1D and 2D structures analogous to graphene with 5-6-7 carbon rings

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Abstract

The next generation of electronic devices is believed to be constructed through molecular level junctions. In the last decades, several devices in this scale and with varied functions have been proposed theoretically and experimentally. Recently, the construction of organic nanodevices with two-dimensional (2-D) materials has given rise to 2-D nanoelectronics which is one of the most interesting research focuses of the scientific community that aims to characterize high-performance 2-D electrodes. [1]. In this context, due to the unique properties of graphene [2] (GR) 2-D is a strong candidate for future applications to succeed in silicon-based technology [3]. However, pure GR 2-D is a null gap semiconductor, which limits its electronic applications. Theoretical and experimental studies have shown that one-dimensional (1-D) graphene nanoribbon (1-D NFGR) can induce an energy gap to suppress the on-off state in a GR-based field-effect transistor. Another way to tune the GR electronic gap is by doping [4] or topological defects in the GR structure by inserting rings with Cn (n = 5, 6, 7 and 8). In the literature, 2-D networks such as Phagraphene, Popgraphene and ψ-graphene, with (semi-) metallic and semiconductor properties [5] have been predicted. In 2017, X. Li et al. [6] using first principles calculations proposed Ψ-graphene (Ψ-GR) in which it is dynamically stable and has a metallic character with robust mechanism against external forces. Thus, the main objective of this work is to investigate the electron transport properties and the transition voltage spectroscopy (TVS) through spin less density functional theory (DFT) combined with the Green function of non-equilibrium (DFT / NEGF) [7] for Ψ-GR without (and with) hydrogen at the lower and upper edge. To obtain the geometry in its ground state of energy and the properties of electronic transport, we used DFT / GGA / PBE / SZP in Siesta [8] code and DFT / NEGF in TranSiesta code [9]. Our results showed that the signature of the I-V curve for the 2-D (non-hydrogen) device exhibits resonant tunnel diode (RTD) behavior with a (minimum) inflection point of ±0.6V for forward and reverse bias that is confirmed by Transition Voltage Spectroscopy- TVS (on the Fowler-Nordheim (FN) plot). In addition, there is a drop in current at ±0.2V, growing back from ±0.6V setting a negative differential resistance (NDR) is a nonlinear effect that occurs in quantum systems when current decreases as bias voltage increases, typical transistor behavior. For the 1-D device (with hydrogen), it presents less electric current compared to the 2-D. For voltages from -0.3V to 0.3V, the device has switching behavior and for higher voltages (-0.35V and 0.35V) the I-V curve has RTD behavior, where the RDN at ±0.5V for reverse bias and direct are evidenced by the minimum points on the FN plots, which is justified by the differential conductance result. This work opens great prospects for future electronic applications.

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