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Electronic Transport in Graphene Analogous with 5-6-7 Carbon Rings

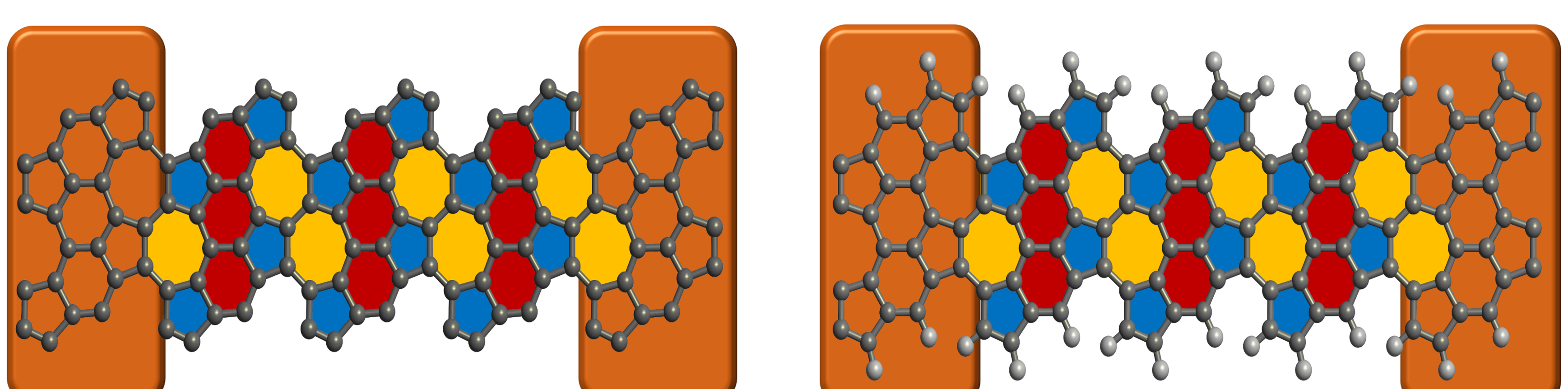
J. C. da S. dos Santos[1], D. F. S. Ferreira[1] C. A. B. da Silva Jr[2], and J. Del Nero[1,3]

[1]*Programa de Pós-Graduação em Engenharia Elétrica, Universidade Federal do Pará, Belém, 66075-110, Brasil;*
[2]*Faculdade de Física, Universidade Federal do Pará, Ananindeua, Belém, 67113-901, Brasil;*
[3]*Programa de Pós- Graduação em Física, Universidade Federal do Pará, Belém, 66075-110, Brasil.*

Introduction

The construction of organic nanodevices with two-dimensional (2-D) materials gave 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 2017, X. Li et al. [2] using first principle calculations proposed Ψ-graphene 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 unbalanced green function (DFT/NEGF) [3] for Ψ-graphene without (and with) hydrogen at the edge (bottom and top) as shown in figure 1 (a-b).



(a) (b)

Figure 1: (a) and (b) represent the configurations of 2D and 1D nanoribbon devices, respectively.

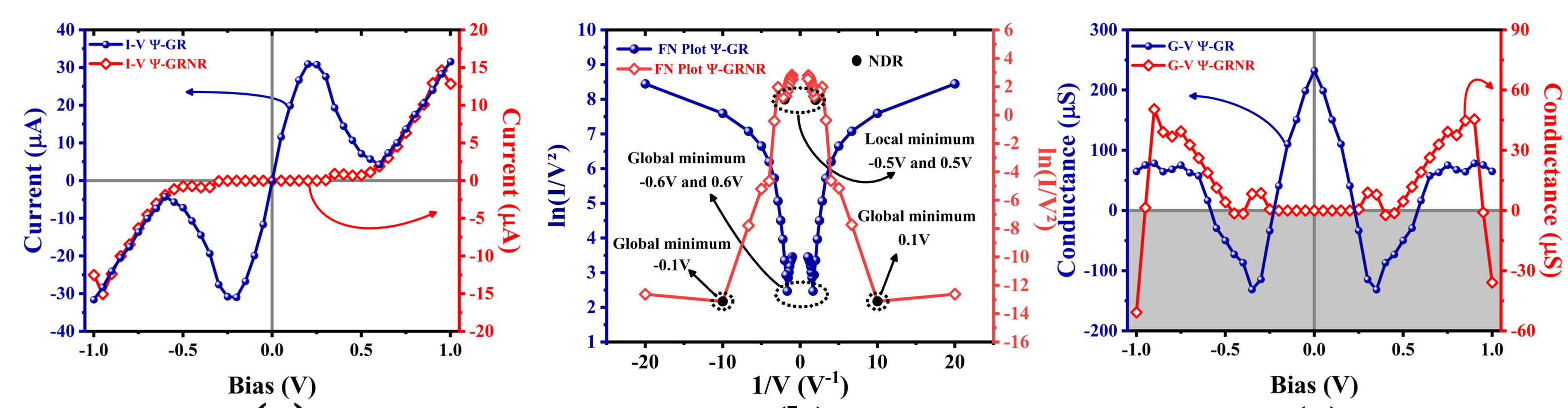
Methodology

Using first-principle methods based on Density Functional Theory (DFT) [3], the solution for the generalized gradient approximation (GGA) based on the PBE with the solution for the exchange-correlation potential [4], with a base set SZP, as cutoff of 300 Ry implemented in the SIESTA package [5] and to investigate the molecular electronic transport, was used the non-equilibrium green function (NEGF) [6] method, based on the TRANSIESTA package [7, 8] was used as a basis.

Results

Our results showed that the signature of the I-V curve for the 2-D (non-hydrogen) device exhibits resonant tunnel diode (RTD) behavior [fig. (2a)] 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) [fig.(2b)]. In addition, there is a drop in current at ±0.2V, growing back from ±0.6V setting a negative differential resistance (NDR) [fig (2c)] 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 [fig. (2a)]. 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 [fig. (2b)], which is justified by the differential conductance result [fig. (2c).



(a) (b) (c)

Figure 2: (a-c) represent the curve I-V, FN plot and differential conductance, respectively.

Conclusion

In summary, we show from DFT/NEGF calculations that the 2-d Ψ-GR device displays regions of NDR for tenons ± 0.6 V that is confirmed by Plot FN and differential conductance, typical RTD behavior. For the Ψ-GRNR (1D) device, in the range of -0.3V to 0.3V it has switching behavior, at voltages ± 0.5V it exhibits RTD behavior that is confirmed by the FN plots and differential conductance. This work opens great prospects for future electronic applications.

References

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