B and N doping effects in transport properties of graphene allotrope nanoribbons

E. A. V. Mota[1], C. A. B. da Silva Jr[2] and J. Del Nero[3]

[1] Programa de Pós-Graduação em Física, UFPA, Belém, PA, Brazil

[2] Faculdade de Física, UFPA, Ananindeua, PA, Brazil.

[3] Faculdade de Física, UFPA, Belém, PA, Brazil

E-mail: elder.mota@icen.ufpa.br, *cabsjr@ufpa.br*, jordan@ufpa.br

INTRODUCTION

Carbon allotropes are highlighting in the last years due to their great mechanical, thermal and electronics properties. Among the carbon allotropes, graphene receives a special attention since their experimental achievement in 2004 by Geim *et al.* This fact encourage the scientific community to researcher and propose new 2D carbon allotropes, among then we have the POPGraphene (POPG) structure [1](Figure 1).

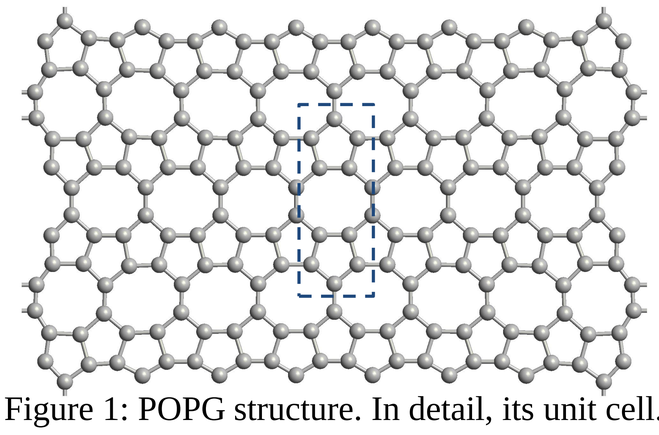

Figure 1: POPG structure. In detail, its unit cell.

The doping is an excellent way to change and insert new properties in a structure. In 2D carbon allotropes case, the B and N atoms are highlighting in this role [2], because the resulting structure is stable, and they acts in it like a “p-type” or “n-type” semiconductor, respectively, possibly creating NDR regions in the device operation.

In this work we investigates the influence of B, N and BN doping in the electronic and transport properties of a POPG nanoribbon hydrogenated (POPGH), to propose applications for these structure (nanodevice) in molecular electronics.

METHODOLOGY

The POPG unit cell was designed as in Figure 1, and was hydrogenated to saturate the carbon edges. Since the electronic transport was carry in z-direction, the unit cell was optimized in this direction using DFT methodology in SIESTA package [3] with GGA/DZP approach, to find the minimum z-length which correspond to a unit cell of minimum energy (Figure 2a). In the transversal direction, a vacuum distance of 10 Å was take, to avoid a neighboring cell interaction and include the edges effect (Figure 2b). The doping was made in a substitutional way, using the optimized POPGH unit cell, with a dopant concentration of about 14% (two atoms).

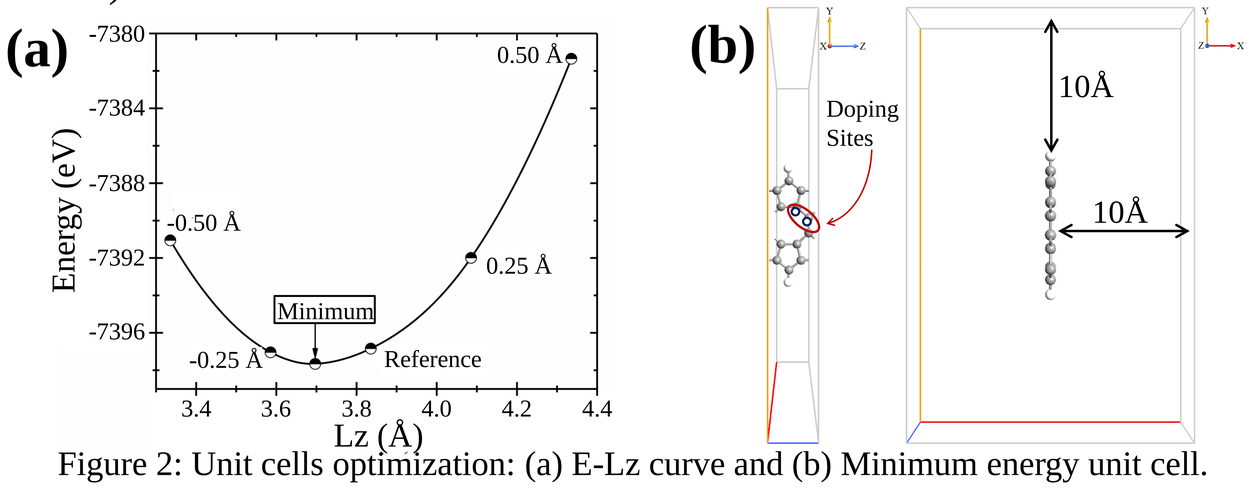

Figure 2: Unit cells optimization: (a) E-Lz curve and (b) Minimum energy unit cell.

Using the intrinsic (POPGH) and the doping optimized unit cells, the nanodevices based on POPG were designed (Figure 3), using two unit cells in each electrode and five in the scattering region. The electronic transport was performed in TranSIESTA package [4] in a bias range from -1.0V to 1.0V.

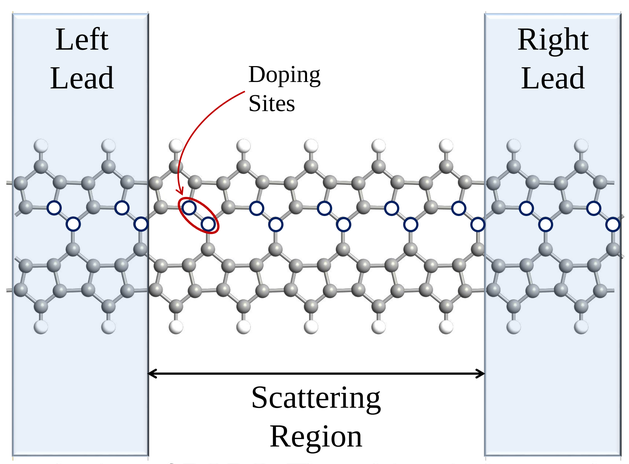

Figure 3: Nanodevice of POPG. The white circles are the doping site.

RESULTS AND DISCUSSION

The I-V results (Figure 4a) shows that all proposed nanodevices has characteristics curves that resemble a behavior of a Field Effect Transistors (FET), but with different operation range. This can be seen by the different peak values to the currents, which is higher for the intrinsic ones, and by the pinch-off bias ($V_{P\text{-}O}$), that has different values for each nanodevice. Furthermore, by the differential conductance (Figure 4b) we can see that the N-doping one do not present NDR, having a FET behavior in all biase range.

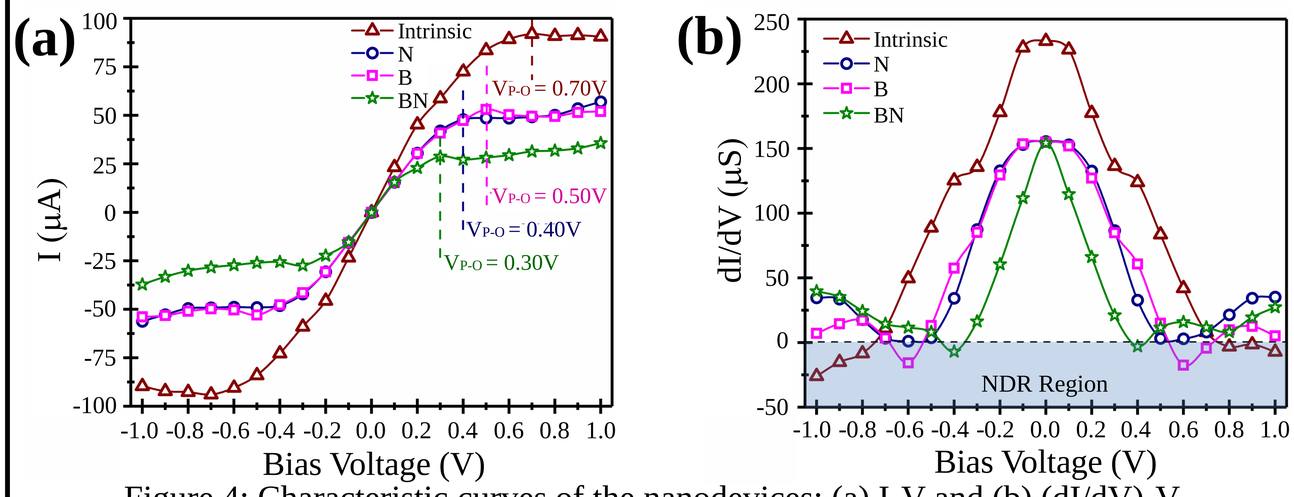

Figure 4: Characteristic curves of the nanodevices: (a) I-V and (b) (dI/dV)-V.

For the others nanodevices, Figure 4b shows that due to the NDR region, they can be applied as high frequency oscillation devices (HFOD), but Figure 4a, shows that the B-doping has a local maximum of 53.0 μA at 0.50 V and a local minimum of 49.5 μA at 0.80 V, and then we have a Peak-to-Valley Ratio (PVR) of 3.5 μA, and the B-doping nanodevice can also be applied as a Resonant Tunneling Diode (RTD) in this range. The same approach can be applied to the BN-doping ones, which presents a peak value of 28,8 μA in 0.30 V and a valley value of 27,2 μA in 0.40V, presenting a PVR value of 1.6 μA. This also suggesting applications of RTD for the BN-doping device in this range.

The minimum value of both nanodevices can be explained by the TVS analysis (Figure 5), where we can see that the Lauritsen-Millikan (LM) curve presents minimum values in the bias of -0.70 V and 0.80 V (Figure 5a) for the B-doping case, and in the bias of -0.40 V and 0.40 V for the BN-doping ones.

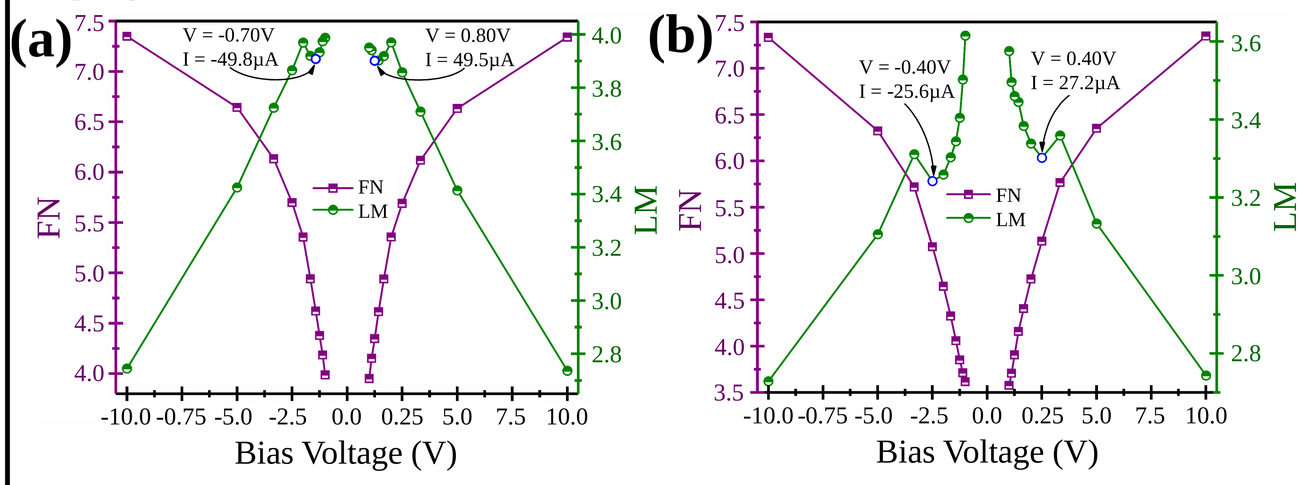

Figure 4: TVS analysis of: (a) B-doping and (b) BN-doping device.

CONCLUSIONS

The results show that all nanodevices can be applied as a FET, but with different operation ranges. The intrinsic, B and BN-doping as HFOD in the NDR range, and the B and BN-doping as RTD in the PVR range. Furthermore, the BN-doping is the more efficiency, because NDR appear in low bias values.

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