B and N dopping effects in transport properties of Graphene allotrope nanoribbons

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The doping is an excellent approach to promotes differents properties in a structure. About 2D carbon allotropes, B and N are frequently implemented, because generates stable structures and behave like P and N semiconductors, making NDR regions appear. In this work, the doping effects of B, N, and BN in POPGraphene [1] nanoribbons are studied, to understand the changes of the electronic properties and propose applications in molecular electronics. The nanoribbons were optimized in SIESTA [2] package with Density Functional Theory at GGA/SZP approach, and the transport properties were obtained in TranSIESTA package [3] by DFT combined with Non-Equilibrium Green Functions method in the same approach. The results show that all nanodevices present a Field Effect Transistor behavior in the analyzed range, but with different operating range. Furthermore, the nanodevices doped with B and BN presents NDR regions, and a Resonant Tunneling Diode behavior.

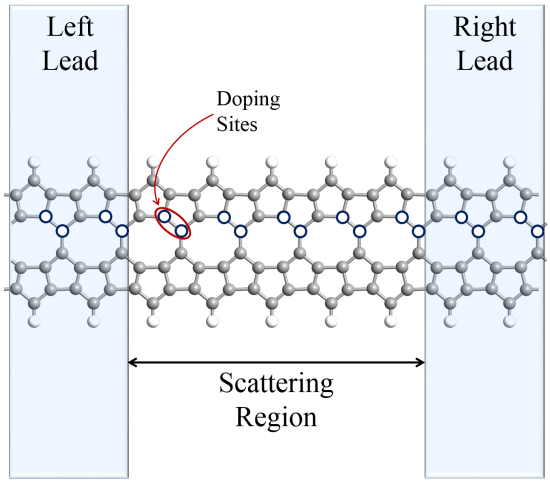

Figure 1: Proposed POPGraphene nanodevices. The fill white circles represents the doping site.

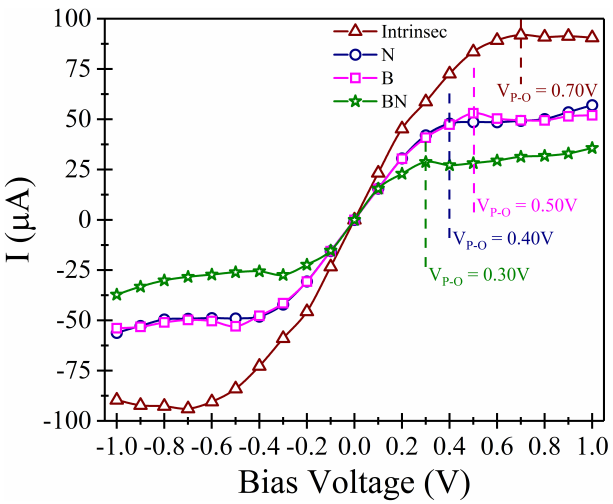

Figure 2: I-V for the intrinsec and doping nanodevices.

References

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[2] J. M. Soler *et al*, J. Phys.: Condens. Matter, 14, 2745 (2002).

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