

Sessions: Nanotechnology.

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## Title. POPGraphene: a New 2-D Carbon Allotrope and its Application in Molecular Electronics

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**Abstract:** The Popgraphene is a new 2-D carbon allotrope generate by inserting 5-8-5 defects in a graphene sheet [1]. Popgraphene has great features like great thermal stability and adsorption capacity of Li atoms, making enable to use it in batteries construction. In this work a unit cell of popgraphene was propose, and the theoretical electronic properties of popgraphene were study to propose a new nanodevice to be applied in the field of molecular electronics. The structure was building in Avogadro software and the unit cell was designed in Virtual NanoLab. The structure was optimized implementing the DFT methodology in SIESTA package [2], applying the GGA functional and the SZP basis set, and using the cell dimensions like boundary conditions. The electronic transport calculations were performed using in TranSIESTA package, implementing the DFT-NEGF methodology [3]. The results show that the Popgraphene has great features to the electronic conduction, because it presents high current values and a characteristic curve of a Field Effect Transistor, which makes possible its application in molecular electronics.

**Keywords:** DNA Nanodevice, DNA Sensor, Carbyne, DFT, NEGF.

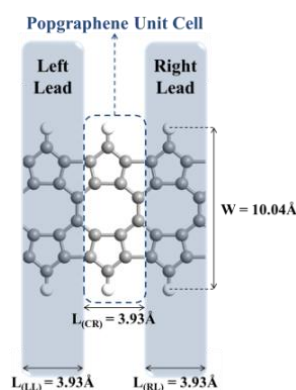


Figure 1: Popgraphene nanodevice.

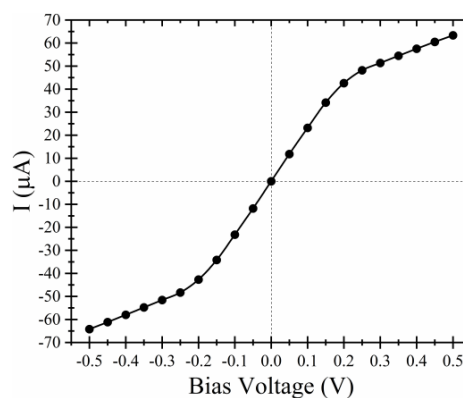


Figure 2: I-V curve of Popgraphene nanodevice.

### References:

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