Quantum confinement effect in transport properties of armchair TGraphene nanodevices

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In this work, we investigated the quantum confinement effect of armchair TGraphene [1] nanoribbons, proposing two unit cell nanoribbons with Hamada index (1,0) and (2,0) (Figure 1), to understand the influence of the size in the transport properties of this material. The TGraphene unit cell was optimized in SIESTA package [2] using the Density Functional Theory (DFT) with GGA/DZP approach and the transport properties were obtained in TranSIESTA package [3] using DFT combined with Non-Equilibrium Green function method, with the same approach. The results show that incresing size favor the Dirac cones formation in nanoribbons unit cell. The transport properties shows that, unlike the literature results of 2D carbon allotropes, the conductance of the system increases with the reduction of the size, as can be seen by the I-V values (Figure 2). Furthermore, the (0,1) device has characteristics that resemble a Field Effect Transistor in the range of -0.80 V to .80 V, and as high frequency oscilation devices in the range of -0.80 V (0.80 V) to -1.00 V (1.00 V) due to the NDR presence.

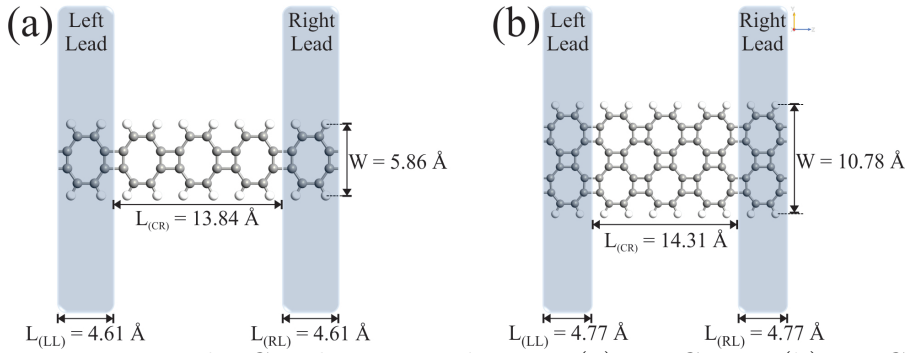

Figure 1: Proposed TGraphene nanodevices: (a) acTGH11. (b) acTGH12.

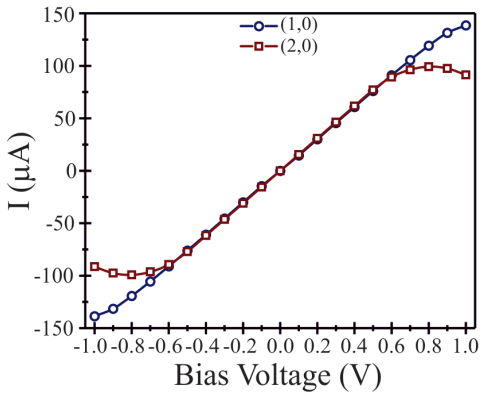

Figure 2: I-V for acTGH11 and acTGH12 nanodevices.

References

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