Quantum confinement effect in transport properties of armchair TGraphene nanodevices

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INTRODUCTION

Graphene is a bidimensional (2D) carbon allotrope with hexagonal symmetry which has great properties like mechanical resistance, and high thermal and electronic transport. When the hexagonal graphene symmetry is broken, another 2D carbon allotrope with different properties emerges, for instance the TGraphene (TG) sheet (Figure 1)[1].

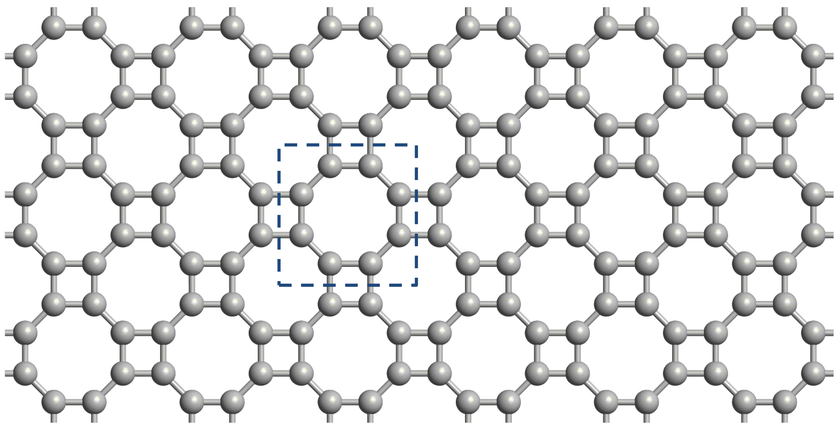

Figure 1: TG structure. In detail, its unit cell.

According to literature, when a ribbon is tailored and its width is reduced, the electronic properties changes and the conductivity of the nanoribbon decreases. In cases of metallic ribbons, can be occurs a metal-semiconductor transition, where the gap energy will be depend of the ribbon width. This is named Quantum Confinement Effect (QCE).

In this work we investigates the influence of tailoring in the electronic and transport properties of a planar nanoribbon hydrogenated of TG armchair (TGH), to propose applications for this structure (nanodevice) in molecular electronics.

METHODOLOGY

The TG unit cell was designed as in Figure 1, and was optimized in y- and z-directions using DFT methodology in SIESTA package [2] with GGA/DZP approach, to find the TG unit cell of minimum energy (Figure 2).

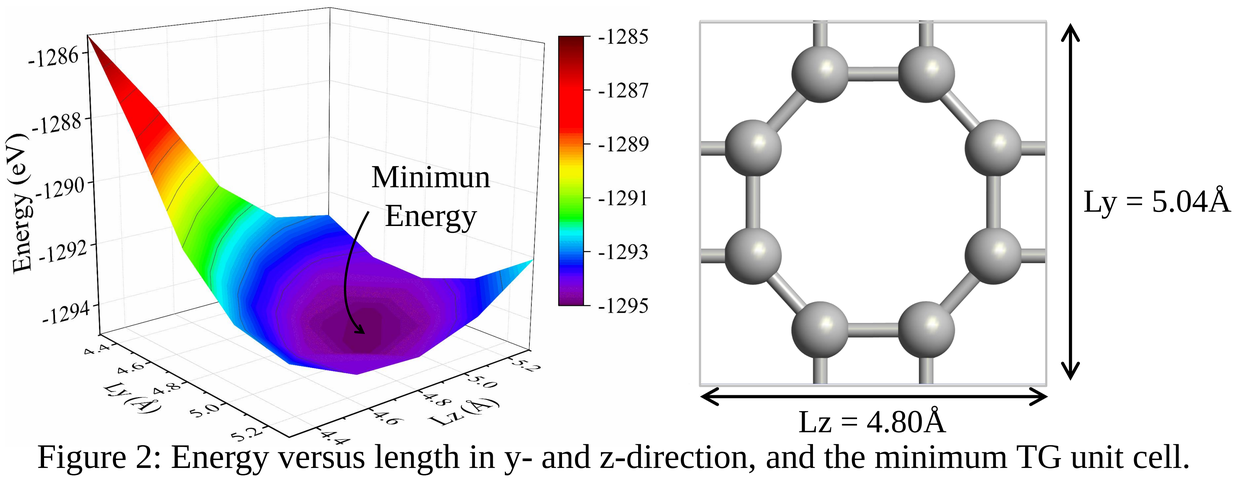

Figure 2: Energy versus length in y- and z-direction, and the minimum TG unit cell.

Two unit cells were proposed: with one and two unit cells in y-direction. The first one (TGH(0,0)) was designed hydrogenating the edges of a TG unit cell. The second one (TGH(0,1)) was designed replicating the TG unit cell one time in y-direction and hydrogenating their edges. As the transport was carried out in z-direction, in both cases (TGH(0,0) and TGH(0,1)) the unit cell was optimized in this direction, and in transversal directions (x e y) a vacuum distance of 10 Å was used, to avoid reflection and taking account the edge effects in optimization (Figure 3). Using TGH(0,0) and TGH(0,1) unit cell, the nanodevices based on TG were designed (Figure 4), and the electronic transport was performed in TranSIESTA package [3].

Figure 3: Optimized unit cells of: (a) TGH(0,1) and (b) TGH(0,0).

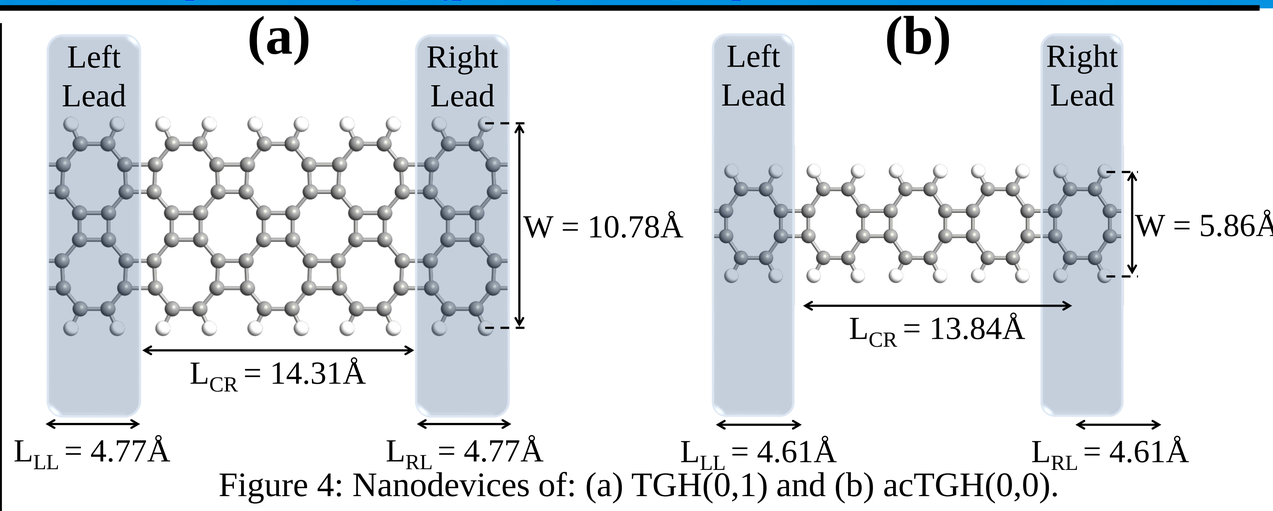

Figure 4: Nanodevices of: (a) TGH(0,1) and (b) acTGH(0,0).

RESULTS AND DISCUSSION

The I-V results (Figure 5a) shows that TGH(0,0) has an ohmic behavior in approximately all the range, just having a smaller decrease after ±0.80 V. The TGH(0,1) one has an ohmic behavior between -0.40 V to 0.40 V, presenting a smaller saturation between 0.60 V to 0.80V. These results are corroborated by the differential conductance (Figure 5b), where we can see the ohmic behavior of both devices. Furthermore, the TGH(0,1) presents a Negative Differential Resistance (NDR) region after ±0.80 V.

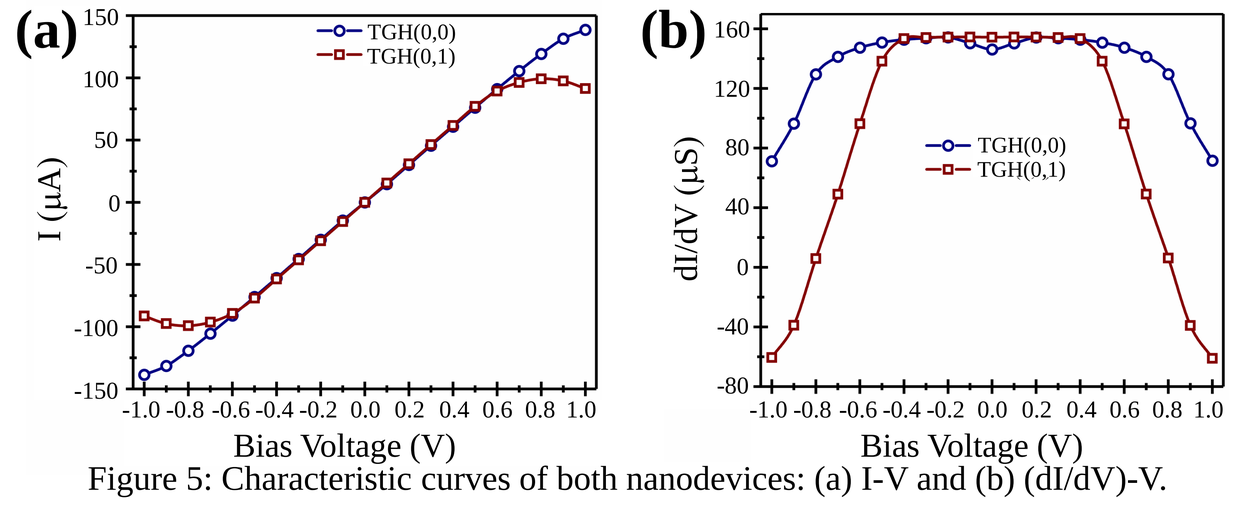

Figure 5: Characteristic curves of both nanodevices: (a) I-V and (b) (dI/dV)-V.

Figure 6a shows that the quasi-linear aspect in the I-V curve of TGH(0,0) is due to a higher and equal contributions of states with positive and negative energy in all range. Figure 6a shows that the ohmic behavior of TGH(0,1) happens due to an equal contribution of states with positive and negative energy, and its starts to decrease due to a suppression in the states with a negative energy after ±0.40 V. The NDR region appear due to states with positive that starts to being suppressed in 0.80 V together with the states with negative ones.

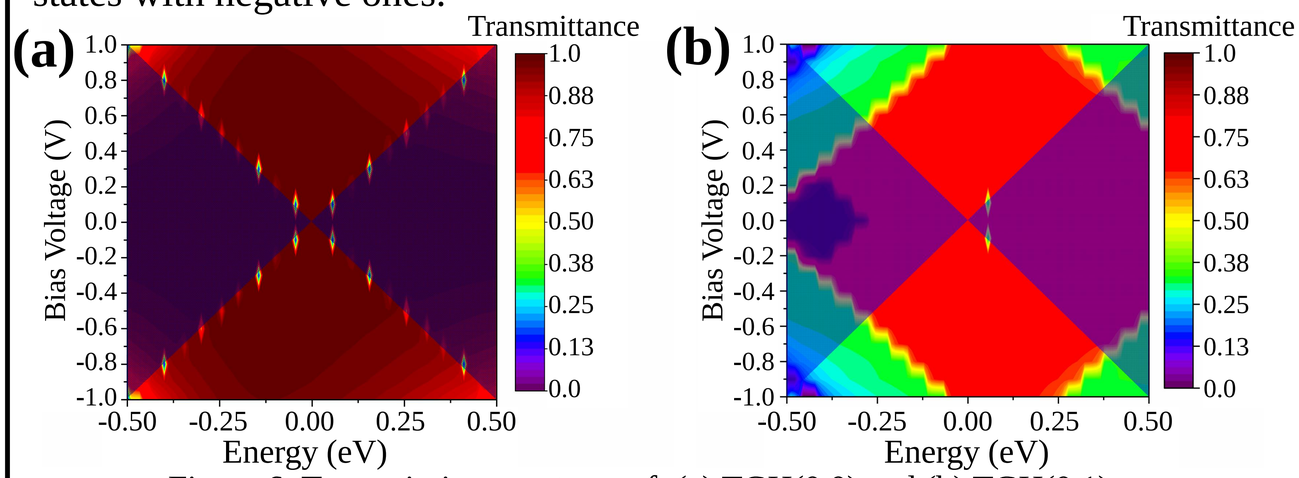

Figure 6: Transmission spectrum of: (a) TGH(0,0) and (b) TGH(0,1).

CONCLUSIONS

The results show that QCE are not valid to TGH, since the conductivity decreases with the nanoribbon width. The TGH(0,1) can be applied as a FET in the range of -0.80 V to 0.80 V and as high frequency oscillation devices in the range of 0.80 V (-0.80 V) to 1.00 V (-1.00 V).

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