

## Local strains and gap formation in graphene

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Graphene is a novel two-dimensional material [1,2] that, due to its exceptional mechanical and electronic properties, has attracted a great deal of attention in the last year. Despite having an extremely high carrier mobility [3], its straightforward use in the electronics industry is precluded, among other factors, by its semimetallic character. Thus, great efforts have been made in order to open a gap in graphene and render it a semiconductor. These include adding an extra dimension of confinement, obtaining graphene nanoribbons (GNRs) [4], electrostatic patterning [5], chemical decoration [6], etc.

Band crossings, such as the one present at the graphene charge neutrality point (CNP), typically reflect an underlying lattice symmetry that forbids the coupling of the different participating states. Therefore, a common route for introducing such couplings is to apply a uniaxial strain to the system, thereby reducing the crystal symmetry. This approach has been followed by Zhong *et al.* and Farjam *et al.* [7,8], who have observed that, in isolated graphene, the application of a uniaxial strain is not sufficient to induce the opening of a gap. However, in that study the strain was applied uniformly, whereas, in some experimental situations, such as bent graphene [9], strain might be applied only to a limited region of the material.

Thus, we have investigated the band structure of graphene under several types of local strain that aim to isolate the different strain components that can be present when undergoing an experiment where graphene is strained in a limited region.

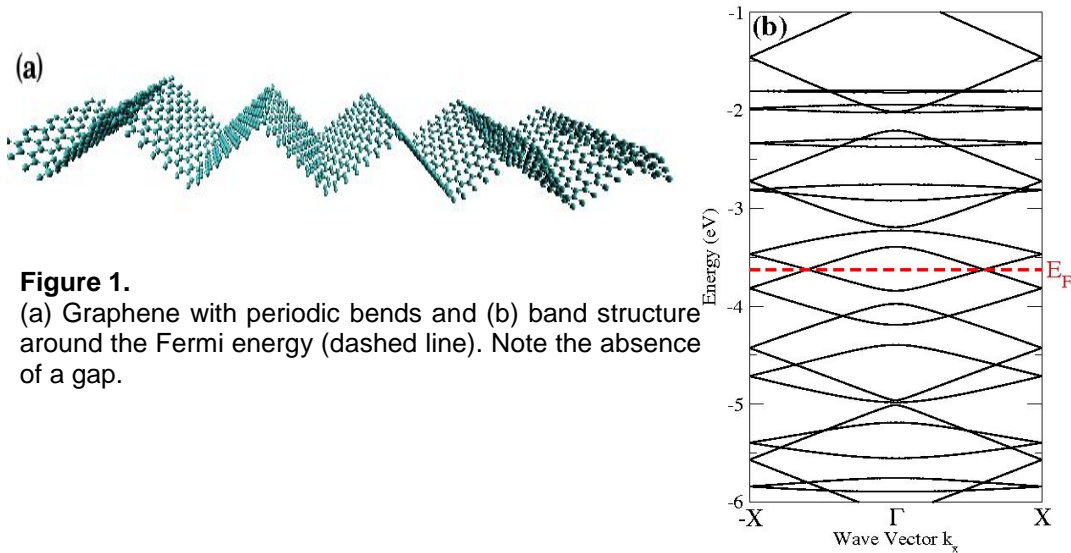
First we have studied the effect of a pure torsion of graphene (Fig. 1.a), while keeping all bond distances intact. We have observed that, no matter the width  $w$  of resulting "pseudoribbons" and the crystallographic direction (zigzag vs. armchair) along which the bending is applied, the band crossing remains at the CNP (Fig. 1.b).

We have also studied the effect of stretching one or two lines of bonds along an armchair direction, simulating the local stretching that can take place in the region with finite curvature when a graphene sheet is bent. For one stretched line of bonds, when account is taken of the periodic boundary conditions needed for ab-initio calculations, the resulting structure resembles an array of laterally coupled armchair GNRs (aGNRs) (Fig. 2.a). There are well known rules that determine the semimetallic or semiconductor character of isolated aGNRs, and we find that these rules are not modified by the introduction of the lateral coupling (Figs. 2.b and 2.c). Finally, we extend the area of application of the local strain by allowing two bond lines to stretch (Fig. 3.a). We observe that, now, electrons propagating along the  $y$  axis observe a gap, but those moving along  $x$  are still subject to a band crossing (Fig. 3.b). However, if the bond stretching occurs asymmetrically, as would be the case for a non-uniform strain, a gap does appear over the whole Brillouin zone.

We acknowledge financial support by the Spanish Ministerio de Ciencia e Innovación under Project No. TEC2009-06986.

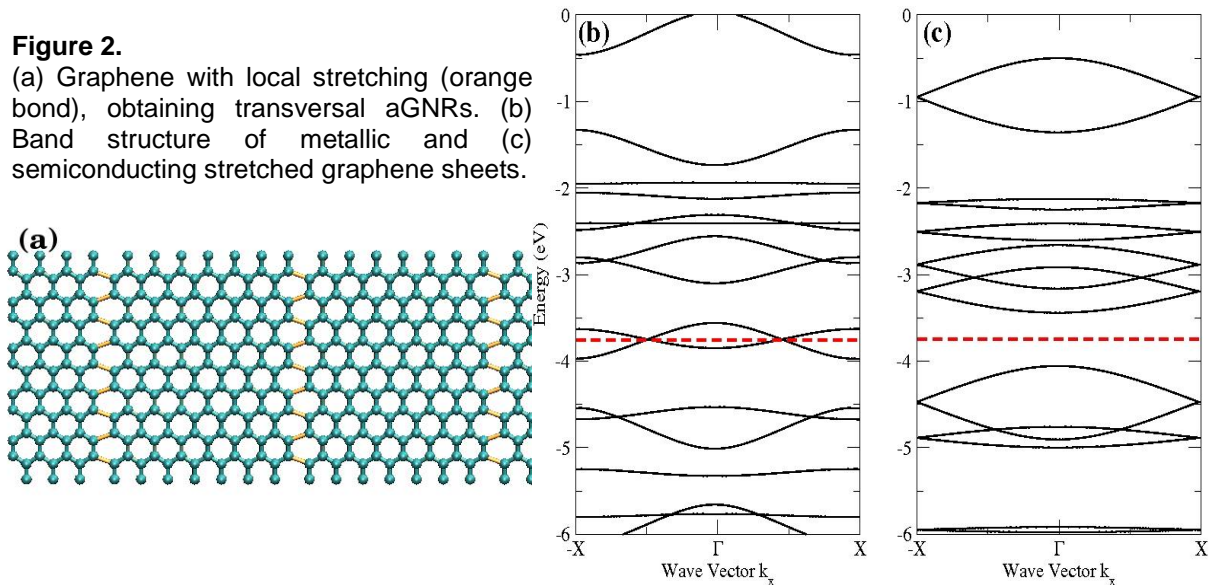
## References

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**Figure 1.**  
 (a) Graphene with periodic bends and (b) band structure around the Fermi energy (dashed line). Note the absence of a gap.

**Figure 2.**  
 (a) Graphene with local stretching (orange bond), obtaining transversal aGNRs. (b) Band structure of metallic and (c) semiconducting stretched graphene sheets.



**Figure 3**  
 (a) Graphene with two stretched bonds (in orange). (b) Band structure and Brillouin zone (inset).

