Tunable gap in bilayer beta-graphyne

M. Pacheco[1], A. León[2]

[1]Universidad Santa María, Avda España 1680, Valparaíso, Chile
[2]Universidad Diego Portales, Ejército 441, Santiago, Chile
monica.pacheco@usm.cl

Abstract

Among the large variety of carbon allotropes there are graphene-like structures which can be constructed by replacing some bonds =C = C = in graphene by acetylenic linkages - C ≡ C -, called graphynes (GYs) [1], or by diacetylenic linkages - C ≡ C - C ≡ C, called graphdiynes (GDYs) [2]. These non-natural carbon allotropes include both, sp^2 - and sp^1 -hybridized carbon atoms. After the theoretical prediction of these flat structures, with exceptional electronic, thermal and mechanical properties, several experimental studies have been performed to achieve their large-scale synthesis [3]. Due to their intrinsic semiconducting properties, GYs and GDYs have been proposed as promising candidates in many electronic and photoelectronic applications and also with potential applications as membranes to separate molecules, hydrogen storage media, and anode materials in lithium-ion batteries [4,5].
According to first-principles calculations [6] some particular types of graphynes-like networks possess Dirac cones, as the case of graphene. One of these structure the so-called β-graphyne, has a Dirac cone not located at the K and K' points of the Brillouin zone but on lines between the high symmetry Γ and M points. In this work we show a theoretical study based on DFT of the electronic properties of bilayers of β-graphyne, for different stacking configurations. In Fig. 1 it is shown a scheme of the β-graphyne and the unit cell with the different stacking considered. Our results show that the bilayer is semimetal or semiconductor, depending on the staking mode. The system changes from a metal, for A-A stacking, to a semiconductor with a small gap of 0.15 eV for A-B stacking, being this most stable configuration according to the study of total energy and stability (Fig.2).
By applying an electric field perpendicular to the layers, the gap of semiconductors can be closed and a metallic state is obtained (Fig.3). This behavior is contrary to that reported for the case of α-graphyne [7] for which the semi-metallic systems become semiconductor with a gap that increases with the field intensity.

References

[1] Baughman RH, Eckhardt H, Kertesz M, J Chem Phys, **87** (1987) 6687.
[2] M. M. Haley, S. C. Brand and J. J. Pak, Angew. Chem., Int. Ed. Engl., **36** (1997) 836.
[3] G. Li, Y. Li, H. Liu, Y. Guo, Y. Li and D. Zhu, Chem. Commun., **46** (2010) 3256.
[4]Ivanovskii A. L. Progress in Solid State Chemistry **41** (2013) 1.
[5] Tang Q, Zhou Z, Chen Z. Nanoscale, 5 (2013) 4541.
[6] Malko D, Neiss C, Vines F, Gorling A. Phys. Rev. Lett., **108** (2012) 086804.
[7] O. Leenaerts, B. Partoens, and F. M. Peeters, Applied Physics Letters **103** (2013) 013105.

Figures

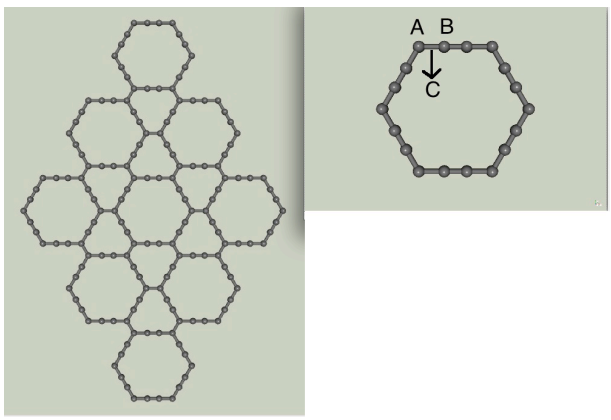

Fig.1 Scheme of a β-graphyne

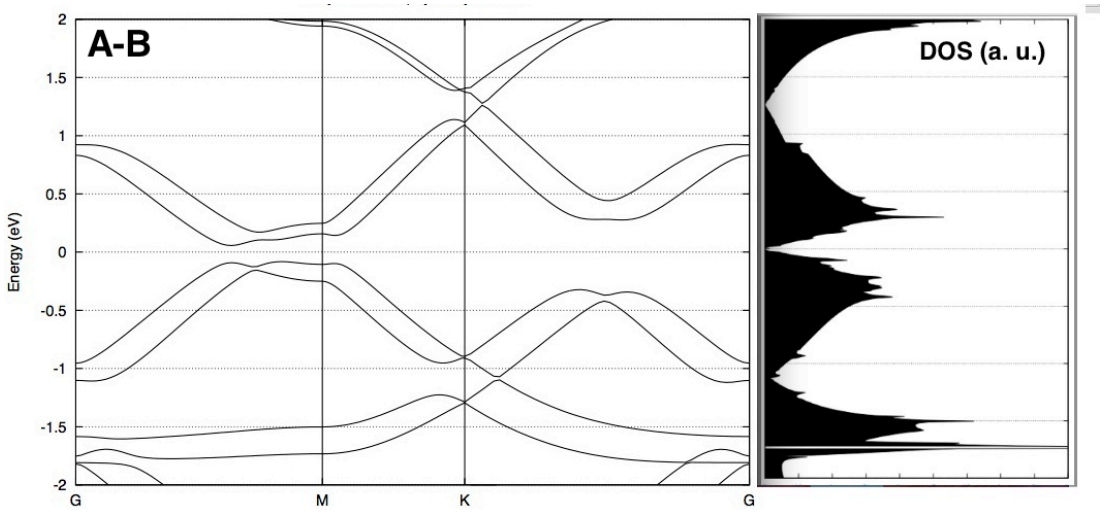

Fig.2 Band structure and DOS for a β-graphyne A-B bilayer (gap ~0.15 eV)

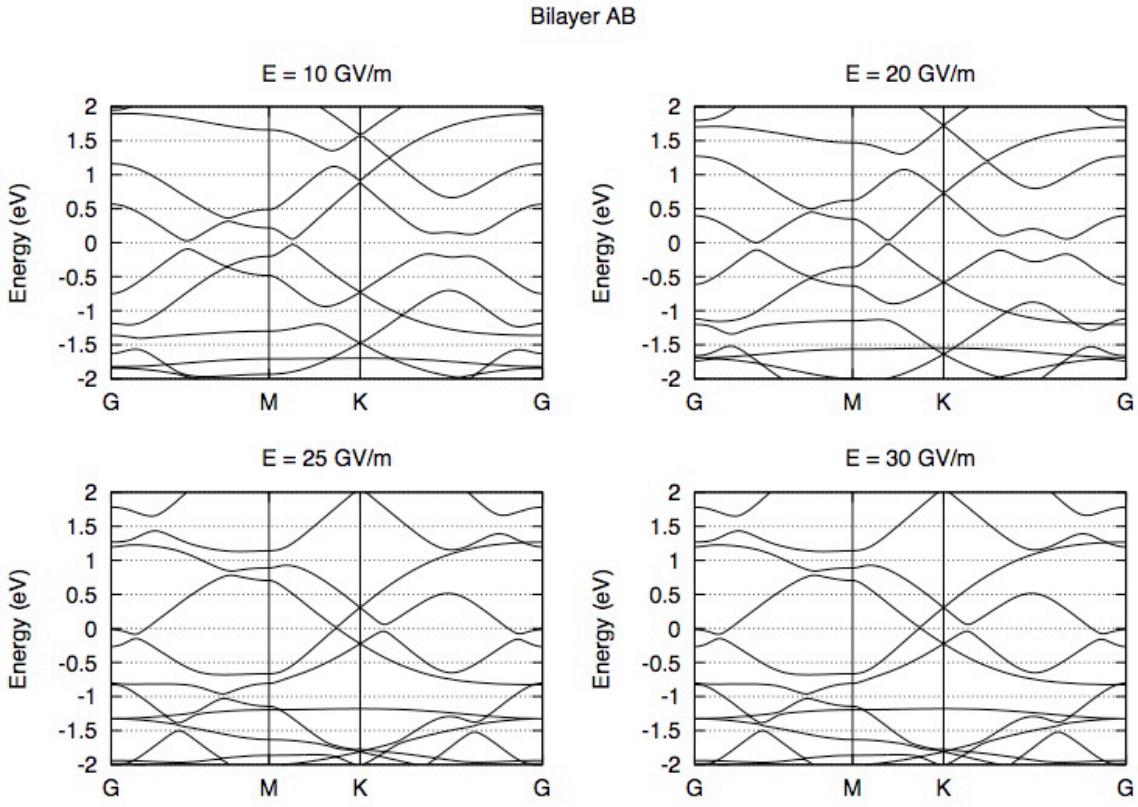

Fig.3 A β-graphyne A-B bilayer for different electric field intensities.