**Sessions:** Nanotechnology
**Preferred presentation Type**: Poster

# New 2D graphene allotrope with dirac cones

A. Sampaio-Silva[1], S.M. Correa[2], D.F.S. Ferreira[2],J. Del Nero[2].

[1]*University of State of Pará (UEPA), Brazil.*
[2]*Federal University of Pará (UFPA), Brazil.*
**Email:** alessandre@uepa.br

**Abstract:**

The three forms of carbon hybridization (*sp*, $sp^2$ and $sp^3$) indicate a wide variety of possibilities of allotropy for structures and devices derived from this matrix. Noteworthy are the fullerenes, nanotubes, carbynes and graphene as the most prominent allotropes electronically [1]. Graphene is a 2D allotropy of carbon admirably attractive for the transport of charge because of the amazing mobility tunneling of carrier and the quantum Hall effect from the $\pi$ and $\sigma$ bonds of the $sp^2$ hybridization. This extravagant behavior is evidenced by its band structure, which shows that graphene's electrons behave as massless Dirac fermions. [1,2]. From the graphene, several other allotroposes of the carbon in monolayer were proposed maintaining the dirac points, the graphynes and the phagraphene stand out [2,3]. In this work, the idea of the hexagonal graphyne was combined with the idea of the phagraphene, proposing multiple acetylated bonds in the rings of 5, 6 and 7 carbon atoms of sp2 bonds of the phagraphene forming a new two-dimensional graphene allotrope. The calculations of the electronic structure and mechanical properties were carried out from the Density Functional Theory (DFT) at the Generalized Gradient Approximation (GGA) with PBE functional using computational package SIESTA 4.0 [4]. The results showed that the band structure of the system maintains Dirac cones in the first zone of Brillioun, crossing four times the level of fermi, evidencing a typically metallic material. The dynamic stability was observed through the phonons spectrum, which converged without the existence of imaginary frequencies, which indicates good structural robustness in the vibrational modes, being according to the methodology, potentially stable and indicated for a future experimental approach.

**References:**

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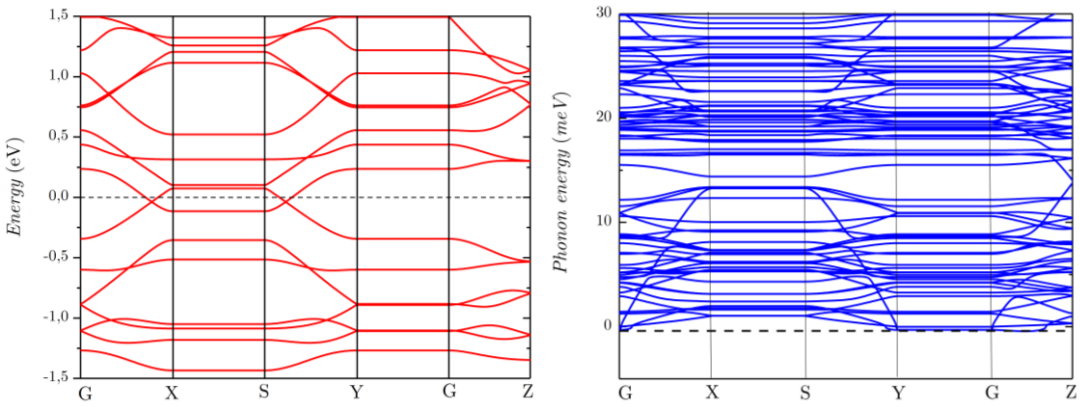


(a) (b)

**Fig.1.** (a) Band structure in DFT for the material and the respective high symmetry points. (b) Phonos dispersion and high symmetry points for the material.