Abstract Submitted
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Electro-optical properties of a bilayer β-graphyne[1] MÓNICA PACHECO, UNIVERSIDAD TECNICA FEDERICO SANTA MARIA, ALEJANDRO LEÓN, UNIVERSIDAD DIEGO PORTALES — Graphynes (GYs) are graphene-like structures that can be constructed by replacing some bonds = C = C = in graphene by acetylenic linkages, - C ≡ C - [1]. According to first-principles calculations [2] 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 a previous work we show that a bilayer of β-graphyne can be metal or semiconductor, depending on the staking. An electric field applied perpendicular to the layers has remarkable effects on the electronic properties of this structure. We have found that the field can close the gap in the case of semiconductor bilayers [3]. In this work we perform a theoretical study of the electro-optical properties of a bilayer β-graphyne. Calculations are based on density functional theory (DFT) method. The indirect and direct band gap of the optimized lattice parameters is calculated by ABINIT. Finally, the dielectric function of the bilayer β-graphyne is calculated. Our results show that the optical properties of this type of graphyne are strongly anisotropic and that the optical band gap can be tuned by means of an external electric field. [1] Baughman RH et al., Chem. Phys., 87 (1987) 6687. [2] Malko D et al., Phys. Rev. Lett., 108 (2012) 086804 [3] León A, Pacheco M, Chem. Phys. Lett., 620 (2015) 67

[1]FONDECYT N 1151316

MÓNICA PACHECO
UNIVERSIDAD TECNICA FEDERICO SANTA MARIA

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