MOLECULAR ELECTRONICS DEVICES COMPOSED BY GRAPHENE AND PHAGRAPHENE

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ABSTRACT

In the last two decades, the researchers have attracted great attention in the investigation of the electronic properties of two-dimensional (2D) materials, composed of a one-atom-thick layer with aim for future electronic applications [1]. The first of these materials, graphene, was rediscovered, isolated and characterized in 2004 by A. Geim and K. Novoselov [2]. Last year, Oganov *et al*. using the ab initio evolutionary algorithm USPEX (Universal Structure Predictor: Evolutionary Xtallography) discovered a new graphene allotrope composed of 5-6-7 Carbon rings with low-energy called phagraphene that is a 2D material in which Dirac cones appear in the first Brillioun zone (BZ), but distorted due to the different number of atoms in the rings and electrons behave similarly to particles without mass traveling with velocity in it depends on the direction [3]. This is not the case in graphene. This planar carbon allotrope is energetically comparable to graphene and more favorable than other carbon allotropes proposed in previous works [4-9], due to its sp^2 hybridization and dense atomic packing. Phagraphene possesses all the other properties of graphene that allows it to be considered an advanced material for flexible electronic devices, transistors, solar batteries, display units and many other things [3]. So, we investigate the electronic transport in molecular junctions composed of: *(i)* graphene and *(ii)* phagraphene.

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