Molecular Electronics Devices Composed by Nanoribbons ZigZag Graphene and Phagraphene Doped

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Abstract: Effect of doping of graphene either by boron (B) and Nitrogen (N) has already been studied by DFT where the calculations indicate that upon doping by N (electron doping), the Dirac point in the graphene band structure shifts bellow the Fermi level and an energy gap appears at the high symmetric K-point. On the other hand, by B (hole doping), the Dirac point band structure shifts above the Fermi level and an energy gap appears. In this work, we perform DFT and EHT/NEGF calculations to investigate the electronic transport in molecular junctions composed by NanoRibbons ZigZag Graphene (NRZZG) and PhaGraphene (NRZZPG) doped with, initially, 10% of boron (B) and Nitogen (N), i. e., p-type and n-type semiconducting. So, we exhibit the results of the I-V and G-V curves and LM and FN plots for characterize the device in molecular electronic.

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