Uniaxial and isotropic strain on carbon and boron nitride porous surfaces

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Abstract: The interest in graphene and its inorganic analogues has increased considerably, due to its potential scientific and applications. Nevertheless, in its pristine form, graphene is a zero gap semiconductor, and this brings restriction to its application in electronic devices. Consequently, developing approaches aimed at modifying the material in such a way to remove this band gap limitation has attracted considerable attention. Based on this fact, a few years ago a 2D structure derived from graphene was synthetized, known as porous graphene (PG) [1], which has a band gap over 3eV, later an intermediate structure called graphenylene (GP) [2] was proposed and recently synthetized, which has a band gap lower than 1eV. Also, an inorganic counterpart of these structures was proposed, called porous boron nitride (PBN) and inorganic graphenylene (IGP-BN) [3], in which is derived from the hexagonal boron nitride single-layer and both has a wide band gap. In this work the influence of uniaxial and isotropic strain on the band gap of PG, GP, PBN and IGP-BN single layer (see Figures 1 and 2) have been studied via periodic computational simulations based on density functional theory using a modified B3LYP functional (12% hybrid), and a triple-zeta plus polarization (TZVP) basis set. The hybrid percentage denotes the fraction of mixing of exact Hartree-Fock (HF) and DFT exchange contributions in the modified functional. This modified functional was chosen because of their good accuracy for bulk graphite, graphene, bulk hBN and hBN single layer. The calculated band gap of PG, GP, PBN and IGP-BN relaxed structures was 3.78, 0.83, 6.45 and 5.52eV, respectively, in a zero strain form. It seems that for the PG and PBN the band gap decreases as the strain grows and for the GP and IGP-BN the band gap decreases, changing the band gap up to three times the zero strain single layers. These calculations could bring us new insights to possible applications in electronic devices.

Figure 1: Porous single layers unit cell: (a) PG and (b) GP.
**Figure 2**: Porous single layers unit cell: (a) PBN and (b) IGP-BN.

**Key-words**: Strain, DFT, porous surfaces, porous graphene, graphenylene, porous boron nitride, inorganic graphenylene

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