Electronic and transport properties of phosphorus and boron nanoribbons

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The nanometric materials, such as 1D and 2D structures, display many intriguing properties which are not found in bulk ones. This is because the original electronic structure is substantially altered from its 3D characteristics [1]. Black phosphorene (BP) and β12 borophene (β12BR) are both interesting structures, the first one shows anisotropic electrical [2] and optical [3] properties, while the second shows unique anisotropic flexibility and metallicity [4]. From the structural point of view, unlike in graphene and β12BR, the BP layers are not perfectly flat; instead, they form a buckled surface due to the sp^3 hybridization, this structural disparity will definitely result in different properties. In this work is evaluated the structural, electronic, magnetic and transport properties of H-passivated BP, graphene, and β12BR nanoribbons for biosensor applications. Since BP is a semiconductor with a large band gap, we also analyse the effect of Si doping in its structure, which can promote a conductance along the phosphorene-based devices [5]. First-principles calculations based on Density Functional Theory [6,7] were performed using the SIESTA code [8]. The transport properties were investigated by the quantum transport code TranSIESTA [9] within the NEGF approach. At first we performed the unit cell size tests along the periodic axis for H-BP and H-β12BR nanoribbons. Si-doped H-BP nanoribbon was the only system we performed a supercell size test given that the structure has a single Si atom substitutional doping for the whole supercell. We observe that, unlike the H-BP, Si-doped H-BP nanoribbon presents a spin polarization effect due to the Si-doping. Moreover, it is possible to notice that the Si-doping creates a transport channel at Fermi level, while H-BP nanoribbons present large band gap between conductance and valence regions. The zigzag and armchair graphene nanoribbons can show metallic (like H-β12BR nanoribbon) and semiconductor behaviour, respectively, but no significant changes happen for the semiconductor case.

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