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Electronic structure and band gap engineering of bilayer graphene nanoflakes in the presence of nitrogen, boron and boron nitride impurities

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ABSTRACT

First-principles density functional theory (DFT) calculations were performed to study the electronic structure of pristine bilayer graphene nanoflakes (BGNFs) and nitrogen (N), boron(B) and boron nitride (BN) doped BGNFs. The pristine BGNTs displayed wide-band gap semiconducting properties. The effect of the bilayer spacing was studied by varying the distance between the flakes from 4 Å to 8 Å which showed an increase in the band gap value from 3.33 eV to 3.46 eV, respectively. By adding N, B and BN atoms at the center between the bilayer, the band gap of the BGNFs was narrowed to 0.09 eV − 1.9 eV. The aforementioned findings clearly reveal that the spacing between the bilayer along with the doping types changes significantly the induced band gap. The total energy and dipole moment were also shown to be affected by the spacing between the layers. In particular, total energy was decreased as the spacing between layers increased while the dipole moment was increased by increasing the distance between BGNFs layers comparing with pristine cases. The capability of manipulating the electronic properties of the BGNFs *via* changing bilayer spacing and doping atoms open up the opportunity of tuning the band gap as needed for many applications including a solar cell, photo, and gas sensor as well as energy storage nanodevices.

1. Introduction

Graphene and graphene-based nanostructures have established themselves as the excellent candidates for several applications owing to their novel physical and chemical properties initiating from their unique morphologies and large surface to volume ratio [1–7]. Although graphene exhibits an array of excellent properties including its electron transport, robust mechanical strength, and highest thermal conductivity yet measured, graphene has no band-gap which has limited its electronic applications. Numerous methods have been proposed to induce a band gap in graphene in order to overcome this fundamental limitation. One way is by cutting the edge of a graphene sheet to create graphene nanoribbons (GNRs) and/or graphene nanoflakes (GNFs). GNFs, a zero-dimensional form of graphene, have remarkable properties comparing with pristine two-dimensional graphene which offer great potential for series of the electronic and magnetic applications. GNFs is used in recent nanotechnology due to the fact that these nanomaterials are found to be stable, sensible, reproducible, and predictable for these applications [8–10].

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