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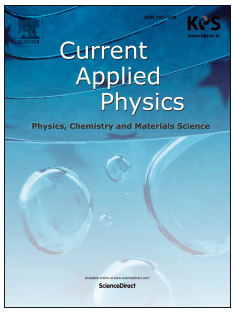

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Puspitapallab Chaudhuri, Angsula Ghosh, M.S. Gusmão, C. Mota, H.O. Frota

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Electronic structure and quantum transport properties of boron and nitrogen substituted graphene monolayers

Puspitapallab Chaudhuri[a], Angsula Ghosh[a], M. S. Gusmão[a,b], C. Mota[a], H. O. Frota[a,*]

[a] *Department of Physics, Federal University of Amazonas, 69077-000 Manaus-AM, Brazil*
[b] *Department of Physics,University of North Texas, 1155Union Circle 311427, Denton Texas 76203, USA*

Abstract

In this work we use *ab initio* density functional theory (DFT) and propose three new configurations of substituted graphene monolayers where the carbon atoms are replaced selectively by boron and nitrogen. The stable equilibrium geometries and corresponding structural, electronic and transport properties of the resulting graphene-like BC, NC and BN hexagonal single-atomic-layer compounds are determined. The characteristics of the NC and BC new compounds are found to be metallic. Our proposed boron-nitrogen hexagonal structure behaves as a semiconductor with gap of 0.52 eV, while the *h*-BN (alternating boron and nitrogen in graphene structure) studied so far widely is typically an insulator or a wide-band semiconductor. The value of electric current in BC structure is found to be higher than that in usual graphene for a given value of the bias voltage.

Keywords: Graphene, DFT, Transport properties
PACS: 73.63.Kv, 81.05.ue, 85.75.-d

1. Introduction

Graphene is a one-atom-thick two-dimensional sheet of sp^2-hybridized carbon atoms arranged in a hexagonal honeycomb lattice. Ever since its discovery by Novoselov *et al.* in 2004[1–3], graphene has always been a subject of intense research due to its unique structural features and remarkable physical properties. Extraordinary electrical and thermal conductivities and very high mechanical strength make graphene a promising candidate for a host of technological applications. A peculiar characteristic of graphene is the linear dispersion relation $\hbar v_F q$ of its band structure around the Dirac point (K). Another important characteristic is its lattice structure composed of two equivalent and independent triangular sublattices, giving rise to a chiral quantum number (pseudospin) in addition to the real electron spin. These two characteristics make the conduction electrons in graphene behave as massless ultra-relativistic Dirac fermions at low excitation energies, rendering it with exceptional carrier transport properties and creating possibility of its application in nanoscience and nanotechnology as a substitute for silicon-based electronics. However, there exists a basic technical barrier. The metallic behavior (zero band gap) of Graphene limits its application in electronic devices. So, scientists need to devise a way to make the material semiconducting. This has led to the ever increasing search of 2D systems beyond graphene.

A substantial amount of effort has been concentrated on the substitution of carbon (C) atoms with other chemical elements that allow sp^2 hybridization, such as, boron (B) and nitrogen (N) in order to obtain new useful graphene-like materials with a finite band-gap which is important for practical applications in electronics [4–6]. In fact, the investigations on the effect of substitution in graphite sheet, from which graphene had been isolated, preceded the discovery of graphene. In the experimental study of Kouvetakis *et. al.* [7], interaction of benzene with boron trichloride, resulted in the formation of a new material, a metallic solid of composition BC_3 with a graphite-like structure. Tománek *et. al.* [8] performed an *ab initio* calculation of this structure using density functional theory (DFT) with local density approximation (LDA). The hexagonal super cell was composed of eight atoms, where six of them are C, situated on the central hexagon, and two are B located symmetrically at the sites on the extremes of the super cell. They found that an isolated sheet of BC_3 behaved as a semiconductor and the metallic character of the bulk sample observed in [7] originated from the interaction between the neighboring layers with *AA* and *AB* stacking. Using the same technique, Liu *et al.* [9] analyzed three possible atomic arrangements and the respective electronic structures of BC_2N monolayers adopting a super cell of eight atoms. They observed that the two structures which lack the inversion symmetry presented semiconducting gap while the one with inversion symmetry behaved as metal. The last decade saw a large number of experimental and theoretical works on boron and nitrogen substituted graphene-like materials. Since the B-N

*Corresponding author
Email address: hfrota@ufam.edu.br (H. O. Frota)