



Research paper

Predicting the structural and electronic properties of two-dimensional single layer boron nitride sheets

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ABSTRACT

Three two-dimensional (2D) single layer boron nitride sheets have been predicted based on the first-principles calculations. These 2D boron nitride sheets are comprised of equivalent boron atoms and nitride atoms with sp^2 and sp bond hybridization. The geometry optimization reflects that they all possess stable planar crystal structures with the space group $P62m (D_{3h}^3)$ symmetry. The charge density distribution manifests that the B–N bonds in these boron nitride sheets are covalent in nature but with ionic characteristics. The tunable band gaps indicate their potential applications in nanoscale electronic and optoelectronic devices by changing the length of sp -bonded B–N linkages.

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1. Introduction

Since the successful isolation of freestanding graphene in experiment [1], there have been growing interests in exploring new structures of the two-dimensional (2D) carbon in recent years. Many 2D periodic carbon allotropes have been extensively predicted or investigated, such as graphyne [2], graphdiyne [3], graphtriyne [4], graphenylene [5], T graphene [6], C_4 [7] and so on. These 2D carbon structures possess rather fascinating physical properties [1,8,9] such as 2D electron-gas behavior, the anomalous quantum Hall effect, ballistic electronic conductivity, and the ambipolar effect. Therefore they are considered as revolutionary material for future generation of high-speed nanoelectronics [10], transparent electrodes [11], chemical sensors [12,13], hydrogen storage systems [14], etc. Graphyne, graphdiyne and graphtriyne belong to the same type of 2D carbon allotropes containing both sp^2 and sp hybridized carbon atoms [4]. The three carbon materials differ from each other with regard to the percentages of the acetylenic linkage ($-C\equiv C-$) [4]. The presence of sp carbon atoms is rather useful because of the structural linearity that does not suffer from fluctuation arising from cis–trans isomerization, it has small steric demands and the facility in connecting a sp carbon to a sp^2 or sp carbon center [15]. Because of the particular structure, the three monolayer carbon membranes possess many unique properties and applications [4,16–20]. Cranford et al. characterize the mechanical properties of graphyne sheets by ReaxFF molecular dynamics and find that unlike graphene, the fracture strain and

stress of graphyne depends strongly on the direction of the applied strain and the alignment with carbon triple-bond linkages [17]. Ma et al. have studied the high-temperature phase transition behavior of monolayer graphyne and graphdiyne using molecular dynamics simulations with the adaptive intermolecular reactive bond order potential [21]. Jiao et al. have theoretically extended the applications of graphdiyne to nanoelectronics and superior separation membrane for hydrogen purification [16]. Zhang et al. have explored the energetics and dynamics of Li in graphdiyne monolayers and proposed that graphdiyne is a promising anode material for lithium ion batteries with high capacity and rate capability [20]. In a clever synthetic attempt, graphdiyne has been successfully prepared by Li et al. in experiment [15].

Boron nitride (BN), being isoelectronic with the carbon polymorphs, can exist in the same structural forms as their carbon counterparts. Low dimensional BN nanomaterials are well-known for their excellent chemical inertness and thermal stabilities [22]. They provide excellent mechanical reinforcements and enhancement of thermal conductivity in diverse materials, such as polymers, ceramics, and metals [23–25]. Due to their wide energy band gaps (5–6 eV), low dimensional BN nanophases are the better choice than their C counterparts as electrically insulating substances [26,27]. Monolayer hexagonal boron nitride (h-BN), similar to graphene, is a typical 2D BN material which could be isolated from bulk BN or synthesized using chemical decomposition reactions of various precursors [28–31]. Many studies have been performed to investigate the properties and applications of monolayer h-BN and their similarities and differences with graphene [29,32,33]. However, studies on 2D BN nanostructures similar to graphyne are rarely reported. Based on the intriguing properties

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of graphyne, graphdiyne and graphtriyne, we expect that their BN counterparts could also possess particular properties and application in some field. In this respect, by means of the first principle calculation, we predicted three types of 2D BN nanomaterials with the similar structures to graphyne, graphdiyne and graphtriyne in this work. Here, we term the three 2D BN structures as BNyne, BNdiyne and BNtriyne which are corresponding to the graphyne, graphdiyne and graphtriyne, respectively.

2. Computational methods

The calculations are carried out using density functional theory within the generalized gradient approximation (GGA) in the form of Perdew–Burke–Ernzerhof function [34] for exchange–correlation potential. All the calculations are performed using the Vienna Ab-initio Simulation Package (VASP) [35]. Periodic boundary conditions were employed and vacuum slabs of 20 Å were used to isolate the replicas of BN layers. Geometrical optimizations are performed until the Hellmann–Feynman force on each ion is less than 0.001 eV/Å. The plane-wave basis is used with a cutoff of 400 eV and the energy convergence criterion is chosen as 10^{-7} eV between two ionic steps. The Brillouin zone is sampled using $17 \times 17 \times 1$ Monkhorst-Pack k-point scheme [36].

3. Results and discussion

To verify the reliability of the computational methods, the structural parameters of monolayer h-BN are optimized and compared with the experimental data. The in-plane lattice parameters of h-BN within the GGA were determined to $a = b = 2.51$ Å, which is very close to the experimental value of 2.505 Å [37]. Also, the B–N bond lengths (1.45 Å) here are consistent with the previous reported results [38,39]. The obtained geometrical structures of BNyne, BNdiyne and BNtriyne in 2×2 supercells are presented in Fig. 1(b)–(d). For comparison, the optimized structure of monolayer h-BN is also presented in Fig. 1(a). After being fully optimized, the three new BN sheets retain planar structure and their crystal structures all possess the space group $P\bar{6}2m$ (D_{3h}^3) symmetry. The primitive cells of three BN sheets are rhombic and they

respectively contain twelve, eighteen and twenty-four atoms: boron and nitrogen atoms stationing in half.

The equilibrium in-plane primitive cell length of BNyne, BNdiyne and BNtriyne are estimated to 7.01 Å, 9.63 Å and 12.26 Å with the acute angular separation of 60° and therefore they have the areal density of 0.28, 0.22 and 0.18 atoms per Å² respectively. As shown in Fig. 2, there exists five distinct bonds in three boron nitride sheets and the optimized bond lengths are depicted in Fig. 3. The bond lengths b1 and b3 are gradually increasing as the cell length increases, while the bond lengths b2 and b4 are slightly decreasing as the cell length increases. This is considered to be mainly caused by the effect of the conjugated bonds. On the other hand, the difference of the same bond length in three sheets is very small, which infers their same bond character in BNyne, BNdiyne and BNtriyne. At the same time, the bond lengths b3 and b5 that appear in BNtriyne are almost equivalent. In the same consideration, because the relative position of the nearest neighbor atoms is identical, the bonds with length b3 or b5 have the same bond character, too. Meanwhile, the two different types of bond angle ($\angle B-N-B$ and $\angle N-B-N$) in the hexatomic ring of these boron nitride sheets have the different angle values (listed in Fig. 2), which is differ from 120° in monolayer h-BN. Compared with monolayer h-BN, this difference is strong evidence of the presence of different B–N bonds. For monolayer h-BN, each boron (or nitride) atom is bonded with three identical sp^2 nitride (or boron) atoms through sp^2 hybridization [32]. However, for BNyne, BNdiyne and BNtriyne each boron (or nitride) atom in the hexatomic ring is bonded with two identical sp^2 nitride (or boron) atoms and one sp nitride (or boron) atom through sp^2 hybridization. Furthermore the unequal bond angle values in the hexatomic ring imply a strained state in three boron nitride sheets which probably leads to an enhancement in total energy with respect to monolayer h-BN. Actually, we have calculated the total energy as a function of the 2D crystal area for monolayer h-BN, BNyne, BNdiyne and BNtriyne, as depicted in Fig. 4. As shown in Fig. 4, we can see that the relative energetic stability order is monolayer h-BN > BNyne > BNdiyne > BNtriyne and the energy differences are 0.53 eV, 0.64 eV and 0.68 eV per atom for the other three 2D boron nitride sheets relative to monolayer h-BN, respectively. After initial structural relaxation, the atomic positions of three boron nitride

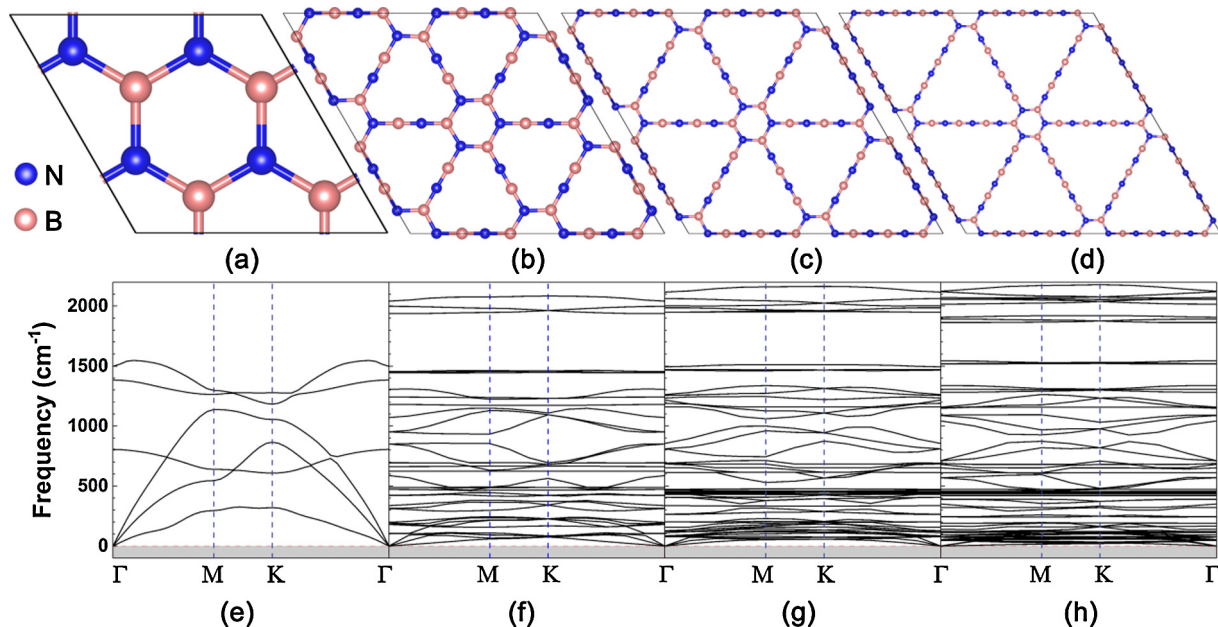


Fig. 1. The optimized geometrical structures and calculated phonon dispersions of (a, e) monolayer h-BN, (b, f) BNyne, (c, g) BNdiyne and (d, h) BNtriyne.

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