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Ceramics International 42 (2016) 4026–4032

CERAMICS INTERNATIONAL

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# Exciton and piezoelectricity in insulating 2-dimensional boron carbide

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Received 20 September 2015; received in revised form 14 November 2015; accepted 15 November 2015
Available online 22 November 2015

## Abstract

Using first-principles density functional theory, we predict a hexagonal structure of boron carbide with two shells, which consists of the $sp^2$ hybridized boron and carbon in (001) plane and the pz–pz ($\sigma$) bonding carbon along [001] direction. The calculated results show that the structure is thermodynamically stable and possesses lower formation energy than other candidates. In addition, the quasiparticle calculations within the *GW* approximation reveal that the boron carbide, which is a two dimensional insulator, exhibits the indirect band gap of 2.4 eV and large exciton bonding energy of 1.35 eV. In optical absorption spectra, a bright Frenkel class bound exciton has been discovered at about 2.98 eV, which is desirable for light emitting applications. Besides, the piezoelectric coefficient ($e_{22}$) of $-2.38 \times 10^{-10}\,\mathrm{Cm}^{-1}$ is predicted for monolayer boron carbide, which indicates that the monolayer boron carbide is a potential candidate for piezoelectric applications in the nanoelectromechanical systems.

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*Keywords:* First principles; Boron carbide; Optical absorption spectra; Piezoelectricity

## 1. Introduction

The low-dimensional materials [1–6], such as $MoS_2$, ZnO nanowire, graphene, and Boron nitride, have attracted more attentions in recent decades due to their unique properties. Especially, graphene with two-dimensional (2D) structure opens up a new era in the fields of physics, chemistry and material science. It was known that graphene has a relatively strong $\pi$-conjugated bonding that stabilizes its planar configuration, thus graphene often exhibits metallicity. There was a contradiction between larger $\pi$–$\pi$ bonding and a band-gap opening in graphene, which greatly hindered the technological applications of graphene based electronic devices in the fields of semiconductor, optics and piezoelectrics. Although the numerous attempts [7–9] were devoted to open its band-gap, the obtained band-gap was still small due to its intrinsic metallic characteristic. Moreover, the complexity of those attempts makes it difficult to practically apply the optical property of graphene to the photoelectric device. Another particularly interesting property of 2D and bulk materials was piezoelectricity [10–21], which permits the energy conversion between electrical and mechanical energy. Recently, the experimental evidence of piezoelectricity was reported in a single layer of $MoS_2$ and graphene nitride nanosheets [4,22,23]. The theoretical studies have predicted piezoelectricity for transition metal dichalcogenides [6], doped graphene, single-layer hexagonal BN [24], graphene oxide [25] and two-dimensional graphene nitride nanosheets [23]. Most 2D materials were made of III–V, IV–VI elements and metal oxides, while III–IV 2D monolayer compounds have rarely been reported in the literature, which prompted us to search for new 2D monolayer materials with an intrinsic gap and made of III–IV elements.

In this work, we performed an intensive simulation search for new two-dimensional structures made of III–IV elements using first-principles method. A 2D structure of boron carbide with the two shells and hexagonal unit has been found. Our results revealed that the monolayer BC with space group C2 was the most stable structure among all candidates that investigated in this study, which was made of $sp^2$ hybridized boron and carbon in the (001) plane and pz–pz ($\sigma$) bonding

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http://dx.doi.org/10.1016/j.ceramint.2015.11.072
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carbon along the [001] direction. Then it was found that this 2D material had an indirect band gap of 2.4 eV and a bright bound exciton in optical absorption spectra at 2.98 eV, which were predicted using the quasiparticle scheme within the *GW* approximation by solving the many-body Bethe–Salpeter equation (BSE). Furthermore, a predicted $e_{22}$ piezoelectric coefficient about $-2.38\ \mathrm{Cm}^{-1}$ was exhibited. This finding revealed that it was a promising piezoelectric material for nano-electromechanical systems.

## 2. Calculation details

In order to obtain the preferable crystal structures of BC, we built the candidate structures using the arranging method, and then the first-principles calculations method was carried out using the QUANTUM-ESPRESSO package [26]. The first-principles method could well predict the friction and piezoelectric properties [6,23–25,27,28]. By breaking the symmetry, a starting point was provided for the structure optimization, which enables us to look for the minimum energy. The local density approximation and the Troullier–Martins norm conserving pseudo-potentials [29] were used to describe the exchange correlation potential. We treated three valence electrons for B ($2s^22p^1$) and four for C ($2s^22p^2$). A plane-wave energy cutoff of 2249 eV was used in total energy calculations, and the convergence for energy and force was set as $6.8\times10^{-3}$ meV and $1.3\times10^{-4}$ eV/Å, respectively. Meanwhile, the dense Monkhorst–Pack meshes were applied to ensure the energy differences converge to 2 meV/atom. Phonon dispersions and piezoelectric coefficients were directly obtained through density functional perturbation theory (DFPT) implemented in the ABINIT [30]. The quasiparticle energy band calculations of monolayer BC were performed by solving the *GW*-Bethe–Salpeter equation and using the BerkeleyGW [31–33]. A plasmon pole model was adopted to mimic the frequency dependence of the dielectric matrix. The kinetic energy of G-vectors (epsilon_cutoff), screened coulomb energy cutoff and bare coulomb energy cutoff were set as 109 eV, 109 eV and 612 eV, respectively. The cell slab truncation was used in order to improve the convergence of Coulomb potential. The symmetry of the candidate structures was decided by Aflow [34]. The schematic images of the crystal structure and electronic localization function were depicted using VESTA [35], and the Wannier function was visualized using VMD program [36].

Table 1
Calculated lattice parameter of monolayer BC with space group C2.

| Struct. | Wyc. | Lattice parameters (Å and degree) | | |
|---|---|---|---|---|
| BC (C2) | | $a$=2.7358 | $b$=4.6749 | $c$=17.8052 |
| | | $\alpha$=90 | $\beta$=90 | $\gamma$=120 |
| B | 4c | 0.86662 | 0.41565 | 0.54894 |
| C | 4c | 0.62216 | 0.25035 | 0.4552 |

## 3. Structure and bonding analysis

The obtained lattice parameter of the ground state monolayer BC is listed in Table 1. The structure with the space group C2 and hexagonal unit cell has a two-atom-thick honeycomb-like sheet as shown in Fig. 1(a) and (b); the height of the structure is about 1.67 Å; each C atom exists three B nearest neighbors in the 2D plane (i.e. (001) plane), and both C and B atoms form $sp^2$ bonding in this plane. In the vertical [001] direction (i.e. *c* axis), the bond distance of C–C (1.73 Å) is comparable to that of single bonds of C–C (1.0–1.7 Å), but smaller than the interlayer distance (3 Å) of graphene, implying that this structure is not a simple stacking of the monolayer BC; the pz states of C form a $\sigma$-bonding state along the [001] direction, which is further confirmed by the calculated electronic localization function and the Wannier function as shown in Fig. 3. Moreover, the formation energy calculations indicate the C2-type phase is the most stable structure for monolayer BC.

We also calculated the interlayer binding energy between two sheets of BC with AB- and AA-type stacking and compared to that of graphite and BN (see Fig. 2). The results show that a van der Waals (vdW) interaction of AB-type BC is stronger than that of AA-type, implying that the AB-type stacking is energetically favorable. Compared to graphite and BN, the vdW interaction of AB-type BC is also stronger because of its intrinsic bilayer-like structure that contributes more to the vdW interaction, leading to a smaller separation about 2.96 Å.

The C atom usually exhibits $sp^3$ or $sp^2$ bonding in its compound, and B usually has a $sp^2$ bonding with another

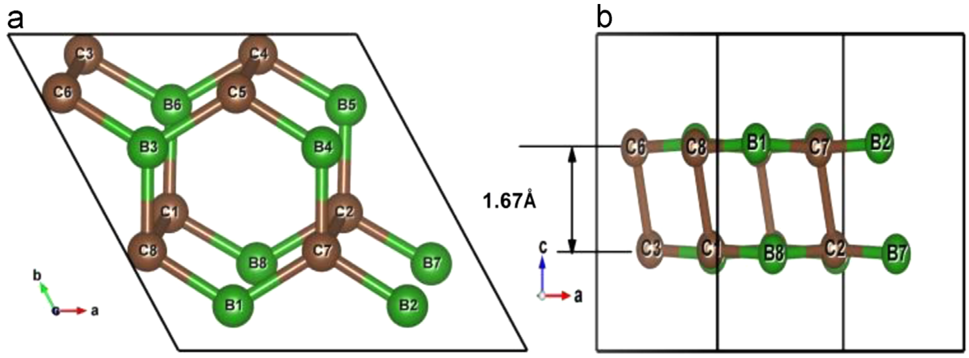

Fig. 1. (a, b) The predicted ground state structure of monolayer BC with space group of C2 in this work.

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