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PAPER

Theoretical prediction of high-temperature superconductivity above 80 K in boron carbide at ambient pressure

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E-mail: M592847073jy@cug.edu.cn, a.hermann@ed.ac.uk and lucheng@cug.edu.cn**Keywords:** boron carbide, superconductivity properties, CALYPSO method, first-principles calculationsSupplementary material for this article is available [online](#)RECEIVED
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5 March 2026**Abstract**

The pursuit of room-temperature superconductors remains a critical challenge in modern science. Here, we perform comprehensive high-throughput structure searches for boron carbide (BC) at ambient pressure using CALYPSO method and first-principles calculations. The structure searches rapidly identify the ground state and two new stable phases, $P6_3mc$ and $Pmm2$, of BC compounds at ambient pressure. The $P6_3mc$ phase shows remarkable superconductivity with high superconducting transition temperature (T_c) up to 86 K, exceeding the boiling point of liquid nitrogen. Our calculations indicate that the high T_c value of the $P6_3mc$ phase of BC arises from its metalized σ -bands and dominant hole-like pockets crossing the Fermi level. Moreover, the $Pmm2$ phase of BC compound is verified as a superhard superconductor, with T_c of 24 K and Vickers hardness of 44 GPa. These theoretical findings not only enrich the understanding of potential ambient superconductors but also offer promising avenues for the design and synthesis of advanced high-temperature superconductors at ambient pressure.

1. Introduction

Superconductivity is one of the most compelling areas in condensed matter physics since its discovery in 1911 [1]. Superconductors are materials that conduct electricity without resistance when cooled below a T_c , which have potential applications in areas ranging from energy transmission to advanced medical imaging systems [2]. While much progress has been made in developing superconducting materials [3, 4], most conventional superconductors work at extremely low temperatures and require significant cooling, typically through the use of liquid helium. This presents practical limitations on their widespread adoption, especially in terms of cost and accessibility. However, since MgB_2 was experimentally confirmed to have a T_c of ~ 39 K at ambient pressure [5], achieving superconductivity with even higher T_c under ambient conditions has remained a long-standing dream in materials science.

Carbon (C), a fundamental element of life, plays a significant role in the evolutionary processes of the universe [6]. Chemically, C exhibits diverse bonding configurations, including single, double and triple chemical bonds [7]. These various bonding modes within its crystal lattice give rise to distinct carbon-based materials, such as diamond, graphite, fullerenes, and carbon nanotubes, each characterized by unique physical and chemical properties [8–11]. Boron (B), positioned between the metal beryllium (Be) and the non-metal C in the periodic table, exhibits an electron configuration of $1s^2 2s^2 2p^2$ [12]. B shows both metallic and non-metallic properties. Its metallicity originates from a single $2p$ electron, while its non-metallicity is attributed to the fact that the orbital radius of $2p$ state is similar to that of the $2s$ state, allowing it to reach sufficient electron localization [13]. B shares similarities in nonmetallic properties with C, and shows roughly analogous applications, including their use in superhard [14],

superconducting [15, 16], and thermoelectric materials [17, 18]. Due to its electron deficiency, B often engages in intriguing multicenter chemical bonding, giving rise to a wide variety of bonding geometries. The structure and physical properties of B and C are thus both highly distinctive. Thus, it is no doubt that the compounds formed by B and C must be excellent.

Boron carbide (BC) was first synthesized in 1883 by Suri *et al* [19]. However, it was not until 1934 that Rigdway determined its stoichiometric ratio [20]. The most commonly accepted stable stoichiometric ratio of BC is B_4C , which corresponds to 20% carbon and 80% boron by weight. B_4C is a non-metallic material. Its high hardness, combined with low density, excellent thermal stability, and chemical inertness, makes it a promising material for a range of applications, including lightweight armor, cutting tools, and neutron absorbers in nuclear reactors [21]. These exceptional properties and broad range of applications of B_4C have inspired extensive studies on B–C systems. In fact, BC exhibits other stoichiometries, and the actual boron-to-carbon ratio is varied, depending on the synthesis methods and conditions [21–38]. One notable development in this field was the synthesis of the diamond-like BC_5 compound by Solozhenko *et al* [22]. The diamond-like BC_5 was synthesized at 24 GPa and 2200 K. It is a superhard material with a Vickers hardness of 71 GPa [22], surpassing the hardness of cubic boron nitride (c-BN) (62 GPa) [39].

Beyond its extraordinary hardness, the BC_5 compound is predicted to be a superconductor, although experimental confirmation of its superconductivity remains absent to date. The calculated T_c of BC_5 at ambient pressure is about 45 K [23], which is comparable to the T_c of MgB_2 (39 K) [5]. Furthermore, Zinin *et al* discovered the cubic BC_3 compound, synthesized through the direct transformation from a graphite phase at 39 GPa and 2200 K [24]. Using first-principles calculations, Liu *et al* reported three low-energy phases of diamond-like BC_3 . All these low-energy phases are superhard and superconductive [25]. In 2008, Moussa and Cohen declared that the T_c of B–C compounds could be significantly increased by adjusting the stoichiometric ratio of B and C. Specifically, they suggested that a boron content of 50% in the B–C systems could result in a high T_c value [34]. Saha *et al* supported this inference, and discovered a series of metallic structures with stoichiometric ratio of 1:1. Many of them were predicted to be superconductors. The T_c value of $F-43m$ phase of BC is about 75 K [40]. These theoretical researches highlight the potential for B–C compounds to serve as high temperature superconductors, particularly if their transition temperatures can be further increased.

In this work, we carry out high-throughput structure searches of BC compounds with stoichiometric ratio of 1:1 at ambient pressure using the CALYPSO method and first-principles calculations. We fleetly identify the lowest-energy $Imm2$ phase and uncover two novel metastable phases, $Pmm2$ and $P6_3mc$ structures. Both the $Pmm2$ and $P6_3mc$ phases exhibit metallic properties. Notably, the $P6_3mc$ phase of BC shows excellent superconductivity with a high T_c of 86 K, which is the highest among all known BC compounds. Additionally, the $Pmm2$ phase of BC is a superhard superconductor with Vickers hardness of 44 GPa and T_c value of 24 K.

2. Methods

The high-throughput structure searches of BC compounds at ambient pressure are performed by using the CALYPSO method [41, 42] and first-principles calculations. The effectiveness of the CALYPSO method in crystal structure prediction has been validated by numerous theoretical and experimental studies [43–51]. We conducted a comprehensive structural search for BC compounds at ambient pressure by integrating the CALYPSO crystal structure prediction framework with first-principles calculations. The exploration protocol combined fixed-cell (1, 2, 4, and 6 formula units) and variable-cell (1–6 formula units) simulations. Each independent search consisted of 50 generations, with 30 candidate structures produced per generation. Among these structures, 30% were generated via random sampling, while the remaining 70% were produced using particle-swarm optimization. After applying a selection strategy that favors low energy, high symmetry, and structural diversity, we screened approximately 1500 initial structures down to 20 promising candidates for high-precision optimization. From these, three stable and metastable phases were ultimately identified, as illustrated in figure 1. Total energy calculations, mechanical and electronic properties are carried out by using the generalized gradient approximation [52], as implemented in the Vienna *ab initio* simulation package (VASP) code [53]. The Perdew–Burke–Ernzerh (PBE) functionals [54] with $2s^22p^1$ and $2s^22p^2$ valence electrons for B and C atoms are adopted to calculate the exchange–correlation interactions. The projector-augmented wave (PAW) method [55] is used to describe for the electron–ion potential. The cutoff energy for plane-wave bases and the dense k -point mesh are set to 380 eV and $2\pi \times 0.02 \text{ \AA}^{-1}$, respectively, ensuring excellent convergence of total energies and energy differences. The dynamical properties of the crystal structures are analyzed using the PHONOPY code [56]. The electron–phonon coupling (EPC) and superconductivities of the

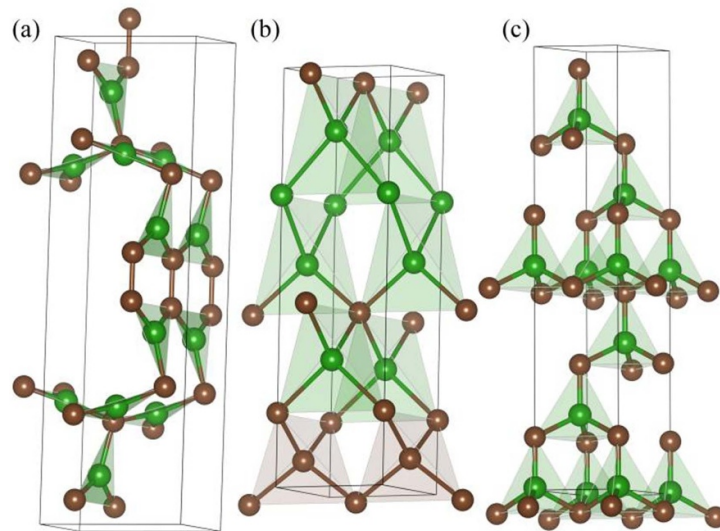


Figure 1. The ground state and two metastable structures of BC compounds at ambient pressure. The B and C atoms are represented by green and brown balls, respectively. (a) The ground state *Imm2* phase (-7.8 eV/atom), (b) the metastable *Pmm2* phase (-7.6 eV/atom), and (c) the metastable *P63mc* phase (-7.5 eV/atom).

BC compounds are calculated using the QUANTUM ESPRESSO code [57]. Based on convergence tests, we select the PAW pseudopotentials based on the PBE functional to describe the electron–ion interactions. The cutoff energy is set to 100 Ry. For the *P63mc* and *Pmm2* phases, q-point grids of $8 \times 8 \times 2$ and $6 \times 6 \times 2$ were adopted, respectively, together with corresponding *k*-point grids of $32 \times 32 \times 8$ and $24 \times 24 \times 8$. The superconducting properties are evaluated by solving the McMillan equation modified by Allen–Dynes (McAD) [58], with a Coulomb shielding constant μ^* of 0.10.

3. Results and discussions

Comprehensive crystal structure searches are conducted on BC at ambient pressure. The ground state structure of the BC compounds at ambient pressure is quickly identified, which is the *Imm2* phase and in good agreement with the results of Saha *et al* [40]. The convex hulls of the B–C compounds at ambient pressure indicate that the *Imm2* phase is metastable relative to graphite, but thermodynamically stable when other amorphous carbon is used as a reference state [40]. Finally, we have searched a series of metastable structures. Two new metastable phases of BC compounds are uncovered which possess *Pmm2* and *P63mc* symmetries, respectively. The calculated formation energies of these BC compounds range from 0.1 to 1.0 eV/atom, as listed table S1, which remain within the thermodynamic limit of synthesizability for polycrystalline carbon [59]. Thus, by selecting an appropriate carbon precursor, it is possible to experimentally synthesize these metastable BC compounds [40]. We further calculate the phonon dispersion curves of these phases to confirm their dynamic stabilities. No imaginary frequencies are observed across the entire Brillouin zone at ambient pressure (see figure S1). The calculated elastic constants of these phases at ambient pressure are listed in table S2. Their mechanical stabilities are further validated by using the Born–Huang criterion [60], as all elastic constants satisfy the required stability conditions.

The crystal structures of the *Imm2*, *Pmm2* and *P63mc* phases of BC are illustrated in figure 1. Their detailed structural parameters are listed in table S3. Figure 1(a) shows the ground state structure of *Imm2* phase of BC at ambient pressure. The structure includes both sp^2 -hybridized and sp^3 -hybridized chemical bonds. Among them, the B atom is sp^2 -bonded, forming a trigonal planar configuration with three neighboring C atoms. The C atoms exhibit a mixed bonding environment: some are sp^2 -bonded in a similar trigonal planar arrangement, while others are sp^3 -bonded to B atoms, forming tetrahedral geometries. The B–C bond length lengths are 1.559 Å, 1.570 Å, 1.580 Å, and 1.591 Å, respectively, and the C–C bond length is 1.376 Å, which form a tubular three-dimensional covalent network. Figure 1(b) presents the crystal structure of the metastable *Pmm2* phase of BC at ambient pressure. The B–C, B–B, and C–C chemical bonds form four distinct types of tetrahedra. The B-centered tetrahedra (B3C2) exist in two configurations, with bond lengths of B–B: 1.798/1.815 Å and B–C: 1.638/1.604 Å, respectively. The B–C bond lengths in the B-centered tetrahedron of BC4 are 1.625 Å and 1.644 Å, while the C–C bond lengths in the C-centered tetrahedron (C5) are 1.513 Å and 1.523 Å. Figure 1(c) illustrates the

crystal structure of the metastable $P6_3mc$ phase of BC at ambient pressure. The structure is exclusively composed of sp^3 -hybridized B–C chemical bonds, forming the B-centered tetrahedra (BC4). The two distinct bond lengths between B and C atoms in triangular pyramids are 1.565 Å and 1.673 Å, respectively.

To determine the electronic properties of these phases of BC compounds, we calculate their projected energy bands and projected electronic density of states (PDOSs). The results are shown in figure 2. From figure 2(a), it can be seen that the metallic behavior at the Fermi level (FEL) for the $P6_3mc$ phase is primarily derived by the contributions from the C-2p orbitals. There are significant overlaps between the p_y orbitals of C atoms and the p_y orbitals of B atoms, indicating the strong covalent interactions between B and C atoms, which enhances the structural stability of the $P6_3mc$ phase. Interestingly, no electrons occupy the orbitals in the energy range from 2.59 eV to 4.71 eV, resulting in a 2.12 eV energy gap in the conduction bands. This is because of the electron deficiency in BC. It needs one more electron per BC to be isoelectronic to C-diamond. The integrated DOS from the FEL to the band gap adds up to one electron per BC. In figure 2(b), the $Pmm2$ phase shows four σ -bands crossing the FEL, suggesting its metallicity. Figure 2(b) clearly shows that no dispersion is found along KZ direction (Γ –Z, T–Y, X–U paths). The bands cross the FEL are all in-plane (xy) p -orbitals. As can be seen in figure 2(c), visible overlaps of the p_y and p_z orbitals of B atoms and the p_y and p_z orbitals of C atoms are found at the FEL. The metallic character of the $Imm2$ phase at the FEL is equally contributed by the p_x orbitals of both B and C atoms. On the whole, the $Imm2$, $Pmm2$ and $P6_3mc$ phases of BC compounds exhibit obviously electronic occupation at the FEL, confirming their metallic characteristics.

Previous reports [40, 46, 61, 62] indicate that most of BC compounds are potential high temperature superconductors. We then explore the superconductivities of the metallic $P6_3mc$, $Pmm2$, and $Imm2$ phases of BC compounds. The T_c values are simulated by solving the McAD equation based on the Bardeen–Cooper–Schrieffer theory [58], which are listed as follows:

$$T_c = \frac{\omega_{\log}}{1.2} \exp \left[\frac{-1.04(1 + \lambda)}{\lambda(1 - 0.62\mu^* - \mu^*)} \right]. \quad (1)$$

Coulomb repulsion pseudopotentials μ^* with widely accepted values of 0.10 is adopted. The EPC parameter λ and the logarithmic average phonon frequency $\omega_{\log}$ are calculated from the Eliashberg spectral function $\alpha^2F(\omega)$ as:

$$\lambda = 2 \int_0^\infty \frac{\alpha^2F(\omega)}{\omega} d\omega \quad (2)$$

$$\omega_{\log} = \exp \left[\frac{\lambda}{2} \int_0^\infty \frac{d\omega}{\omega} \alpha^2F(\omega) \ln(\omega) \right]. \quad (3)$$

We first calculate the superconductivity for the $Imm2$ phase of BC. The calculated T_c value of the $Imm2$ phase at ambient pressure is 0 K, which is consistent with previous results [40], confirming the reliability of currently computational method. Notably, our calculations also reveal the high T_c values of $P6_3mc$ and $Pmm2$ phases at ambient pressure. Specifically, the T_c of the $P6_3mc$ phase at ambient pressure is 86 K (figure S2). As shown in the PDOS of BC compounds in figures 2(a) and (b), the DOS at the FEL for the $Pmm2$ phase (0.68 states eV⁻¹/atom) is obviously higher than that of the $P6_3mc$ phase (0.37 states eV⁻¹/atom). According to conventional understanding of light-element based superconductors, such as the hydrogen-rich superconductors, the higher electron density at the FEL corresponds to stronger EPC and higher T_c values [63, 64].

Based on this inference, we initially hypothesize that the T_c of the $Pmm2$ phase maybe surpasses that of the $P6_3mc$ phase at ambient pressure. However, the succedent calculations indicate that the T_c of the $Pmm2$ phase is just 24 K (figure S3) at ambient pressure, with $\lambda = 0.707$ and $\omega_{\log} = 670.274$ K. Thus, the generally accepted high DOS of light elements at the FEL is not directly related to the high T_c value of BC compounds. We will discuss the underlying origins for this discrepancy in detail later. Of course, both B and C atoms in the $P6_3mc$ and $Pmm2$ phases adopt sp^3 -hybridized, forming strong σ chemical bonds. The metallic σ -bands, which cross the FEL, couple with phonons to facilitate the formation of the Cooper electron pair, contributing to the large T_c values. Additionally, the electron deficiencies of B atoms facilitate electron transfer from B to C atoms results in the formation of hole-like pockets at the FEL. This behavior increases the probability of the formation of the Cooper electron pair near the Fermi surface and enhances the EPC, which further supports their relatively high T_c values at ambient pressure [25, 46, 61]. These are essences why the T_c values of the $P6_3mc$ and $Pmm2$ phases of BC are obviously higher than those of many transition metal borides and carbides.

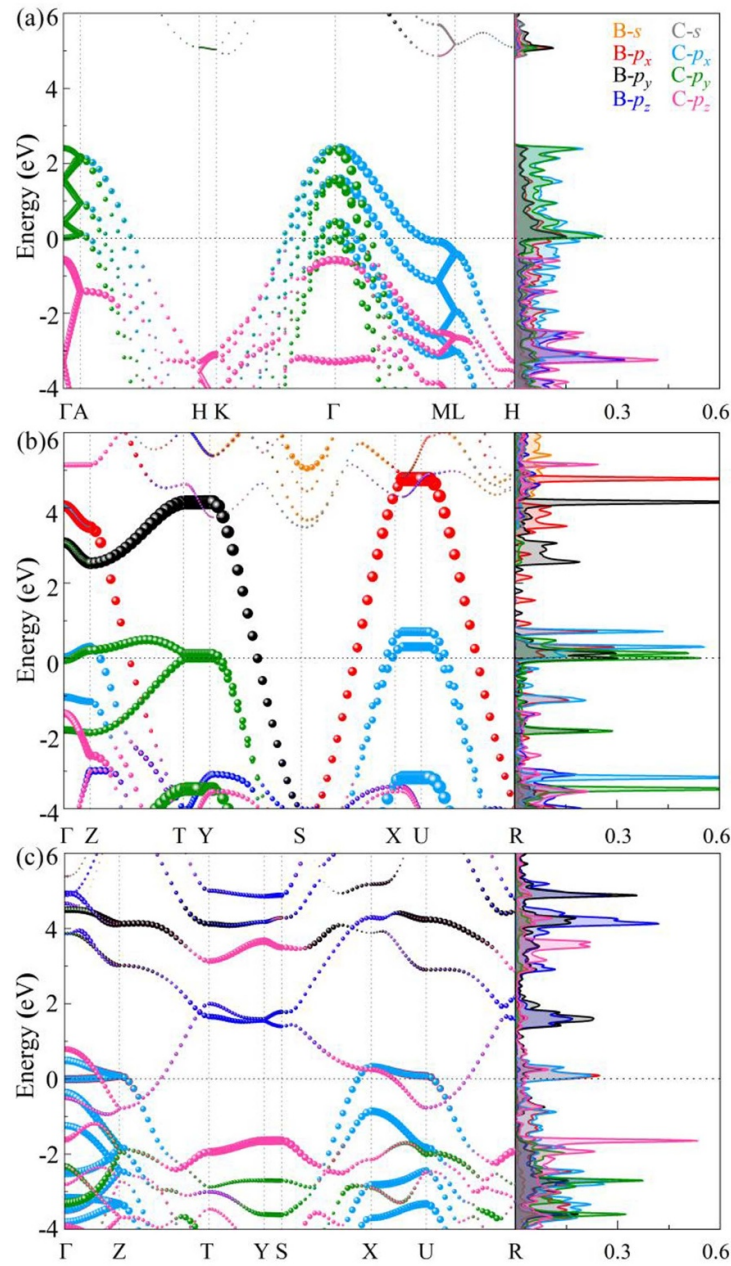


Figure 2. The projected energy bands and corresponding PDOS for BC compounds at ambient pressure. (a) $P6_3mc$ phase, (b) $Pmm2$ phase, and (c) $Imm2$ phase. The size of the balls represents the magnitude of the contributions of B and C atoms.

To gain a deeper understanding of the superconducting mechanism of the high T_c value of $P6_3mc$ phase, we conduct a comprehensive analysis of its phonon dispersion curves, PhDOS, and EPC. Figure 3(a) displays the λ_{qv} -weighted phonon dispersion curves, PhDOS, $\alpha^2F(\omega)$, and λ for the $P6_3mc$ phase at ambient pressure. The phonon vibrational modes corresponding to the black, blue and green dots in the phonon dispersion curves are shown in figures 3(b)–(d), respectively. From figure 3(a), it can be seen that the EPC parameter λ shows a rapid increase in the regions near the black, blue and green dots. The PhDOS of the $P6_3mc$ phase indicate that both B and C atoms contribute equally to the PhDOS in the low-frequency phonon range from 100 cm^{-1} to 300 cm^{-1} , which primarily originates from the out-of-plane displacements of B and C atoms. The phonon vibrational mode at the black dot (136 cm^{-1}) is depicted in figure 3(b), where the atoms in the lattice exhibit synchronous movement with similar amplitudes in the same direction. The weighted phonon spectrum, as shown in figure 3(a), clearly shows that the mid-frequency region ($300\text{--}770\text{ cm}^{-1}$) contributes the most to the EPC. This is due to the increase in the degrees of freedom of atomic vibrations after the release of quantum constraints, enhancing the EPC effect [65, 66]. Within this frequency range, the contributions to the PhDOS from B and C atoms are evenly distributed, with half of the contributions coming from B atoms and the

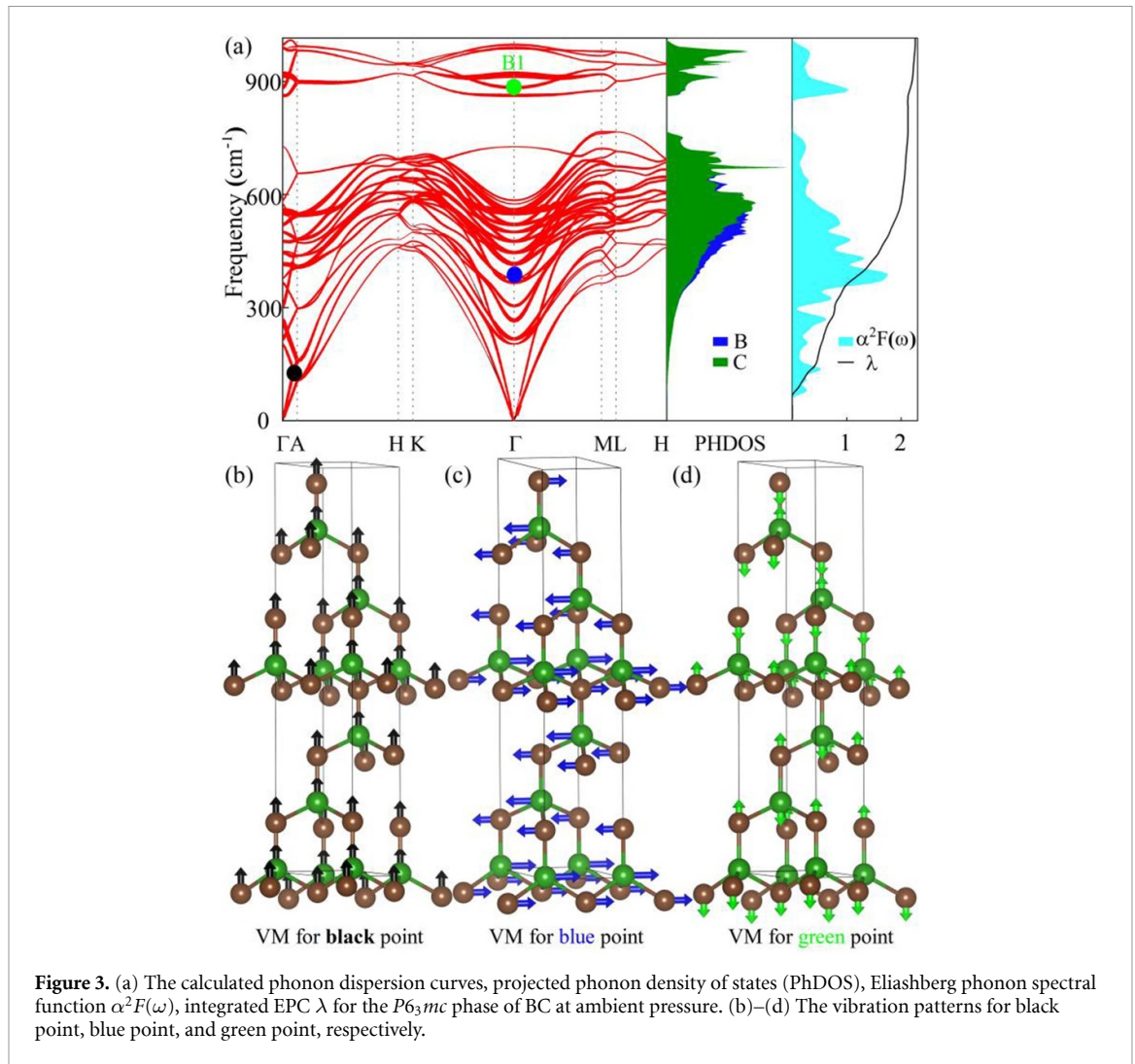


Figure 3. (a) The calculated phonon dispersion curves, projected phonon density of states (PhDOS), Eliashberg phonon spectral function $\alpha^2F(\omega)$, integrated EPC λ for the $P6_3mc$ phase of BC at ambient pressure. (b)–(d) The vibration patterns for black point, blue point, and green point, respectively.

other half from C atoms. The phonon mode at the blue dot (370 cm⁻¹) exhibits a double degeneracy, as shown in figure 3(c). In this mode, the atoms in the lattice are more active. Most of the B and C atoms vibrate along the *a*-axis, with a small fraction vibrating in the opposite direction. The amplitudes of B atoms are higher than those of C atoms, which are in consistent with the PhDOS results.

Under the influence of the EPC effect, a phonon vibrational anomaly appears in the high-frequency range (770–860 cm⁻¹), suggesting the strong σ -band coupling between B and C atoms. In the optical modes above 860 cm⁻¹, the B and C atoms undergo compressive vibrations along the *c*-axis under the B1 vibrational mode (green dot: 884 cm⁻¹), with the B atoms in the lattice remaining stationary (figure 3(d)). These strong interactions among the electrons in the sp^3 -hybridized orbitals of B and C atoms play an important role in the enhancement T_c of the $P6_3mc$ phase.

To further understand the discrepancies in T_c values between the $P6_3mc$ and $Pmm2$ phases of BC compounds, we perform an additional analysis of their electronic band structures. As for $P6_3mc$ phase, there are twelve σ -bands crossing the FEL, by contrast, only four σ -bands cross the FEL for $Pmm2$ phase. To confirm these deductions, we calculate the Fermi-surface (FS) sheets of the $P6_3mc$ and $Pmm2$ phases of BC compounds. The calculated results are shown in figure 4. In $P6_3mc$ phase, the σ -bands form electronlike pockets near the H point and hole-like pockets near the Γ point along the K – Γ – M direction. The nine blue σ -bands in figure 4(a) generate complex FS sheets with both hole and electron characteristics (figure 4(c)), while the three red σ -bands form hole-like FS sheets (figure 4(d)). The FS along the (001) plane of the $P6_3mc$ phase of BC, as shown in Figure 4(e), consists of hole-like rings surrounding the Γ point, along with intricate hole and electron contours. These FS sheets, particularly the hole-like features, suggest that holes are conducive to the formation of the Cooper electron pair, indicating that the $P6_3mc$ phase of BC is a hole-type superconductor. In contrast, the σ -bands crossing the FEL in $Pmm2$ phase of BC form electronlike pockets near the S point and hole-like pockets near the X and

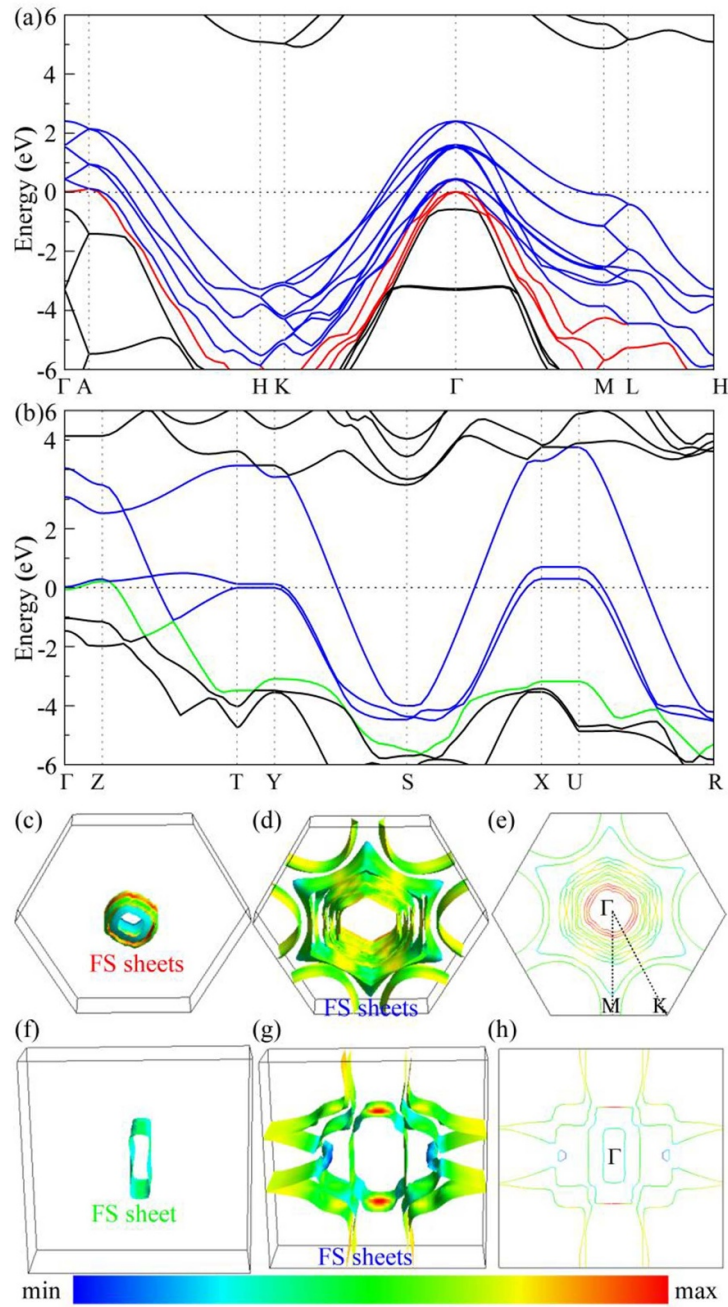


Figure 4. The calculated electronic band structure and FS sheets of BC compounds. (a) The electronic band structure of $P6_3mc$ phase, (b) the electronic band structure of $Pmm2$ phase, (c)–(e) the FS sheets of $P6_3mc$ phase and (f)–(h) the FS sheets of $Pmm2$ phase.

U points (figure 4(b)). Three of the blue σ -bands form the complex FS sheets with both hole and electron features (figure 4(f)), while a green σ -band forms a near-electron FS sheet (figure 4(g)). Figure 4(h) shows the FS along the (001) plane of the $Pmm2$ phase of BC, which are the electronlike rings around the Γ point and intricate hole–electron contours. The electron-like FS sheets are dominated, implying that the electron-like features, which indicates that the $Pmm2$ phase of BC is an electron-type superconductor. The hole-like FS sheets are mainly composed of unoccupied states carrying positively charged carriers, while the electron-like FS sheets are consisted of occupied states carrying negatively charged carriers. We also calculated the Fermi velocities of both $P6_3mc$ and $Pmm2$ phases of BC by the formula of $v_F = h(3\pi^2 n)^{1/3}/m$, which correspond to the color intensities on the FS sheets. The v_F of the $P6_3mc$ phase is obviously higher than that of the $Pmm2$ phase, leading to the higher T_c for the $P6_3mc$ phase. Thus, the high T_c of 86 K in the $P6_3mc$ phase of BC is attributed to the prominent of hole-type superconducting behavior.

Although the T_c value of the $Pmm2$ phase is just 24 K, it is a superhard superconductor, displaying both superconductivity and superhardness. It combines mechanical robustness with superconductivity, which is a rare and valuable combination in materials. Based on the semi-empirical model ($H_v = 2(G^3/B^2)^{0.585} - 3$) proposed by Chen *et al* [67], we calculate the Vickers hardness of the $Pmm2$ phase. The Vickers hardness of the $Pmm2$ phase of BC is 44 GPa, and exceeds the threshold value of 40 GPa for superhard materials [68]. In fact, in $Pmm2$ phase of BC, both B and C atoms adopt sp^3 -hybridized, forming robust covalent networks including C–C, B–B, and B–C bonds, which are the typical characteristic of superhard material. The metallicity of the $Pmm2$ phase mainly arises from covalent bonds formed by localized valence electrons of B and C atoms. Consequently, the $Pmm2$ phase of BC is a multifunctional material, which is an excellent superhard superconductor. It holds significant potential in several advanced technological areas requiring both high mechanical strength and superconducting efficiency, such as in future energy storage systems or high-efficiency superconducting cables.

4. Conclusions

In summary, we conduct high-throughput structure searches of BC compounds at ambient pressure by CALYPSO method and first-principles calculations. We successfully identify the ground state $Imm2$ phase and two novel metastable phases of $P6_3mc$ and $Pmm2$, which are both mechanically and dynamically stable at ambient pressure. Our calculations indicate both $P6_3mc$ and $Pmm2$ phases of BC are metallic. Interestingly, the $P6_3mc$ phase of BC exhibits high T_c value of 86 K, exceeding the liquid nitrogen boiling temperature. The high T_c of $P6_3mc$ phase of BC is attributed to its special electronic structures, i.e. metallized σ -bands, hole-like pockets and empty bands near the FEL, enhance of the EPC interactions. Furthermore, the $Pmm2$ phase of BC is identified as a superhard superconductor, exhibiting T_c of 24 K and Vickers hardness of 44 GPa. The robust σ -bonds between B and C atoms contribute to the superhard feature of $Pmm2$ phase of BC. These findings offer important insights into the superconducting behavior of BC compounds, which provide powerful guidance for design and synthesis of light-element-based superconductors at ambient pressure.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors. Supplementary Material available at <https://doi.org/10.1088/1361-648X/ae49d0/data1>.

Conflict of interest

The authors declare that they have no conflict of interest.

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