Superconducting boron allotropes

Shoutao Zhang, Xin Du, Jianyan Lin, Aitor Bergara, Xin Chen, Xiaobing Liu, Guochun Yang

1Centre for Advanced Optoelectronic Functional Materials Research and Laboratory for UV Light-Emitting Materials and Technology of Ministry of Education, Northeast Normal University, Changchun 130024, China
2Laboratory of High Pressure Physics and Material Science, School of Physics and Physical Engineering, Qufu Normal University, Qufu, Shandong Province 273165, China
3Departamento de Física de la Materia Condensada, Universidad del País Vasco-Euskal Herrikno Unibertsitatea, UPV/EHU, 48080 Bilbao, Spain
4Donostia International Physics Center (DIPC), 20018 Donostia, Spain
5Centro de Física de Materiales CFM, Centro Mixto CSIC-UPV/EHU, 20018 Donostia, Spain

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The search for elemental allotropes is an active research field to get unusual structures with unique properties. The removal of metal atoms from pressure-induced stable binary compounds has become a useful method for obtaining elemental allotropes with interesting properties that otherwise would not be accessible at ambient pressure. Although three-dimensional boron allotropes have been studied extensively, none of those found so far are superconducting at ambient pressure. Here we propose that NaB4 and Na2B17 can be used as precursors to achieve superconducting boron allotropes at ambient pressure. First-principle swarm-intelligence structure search calculations identify several novel sodium borides (e.g., Na3B2, Na2B3, and Na2B17) under high pressure. Interestingly, the B atoms in I4/mmm NaB4 and Pm Na2B17 form three-dimensional frameworks with open channels, where Na atoms are located. After the removal of Na atoms, two hitherto unknown boron allotropes, named as I4/mmm B4 and Pm B17, are stable at ambient pressure. They are metallic with superconducting critical temperatures of 19.8 and 15.4 K, respectively, becoming the highest ones among bulk boron allotropes. In addition, considering their predicted Vickers hardness of 27.3 and 26.8 GPa, they are also potential hard materials.

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I. INTRODUCTION

The preparation of high-temperature superconductors is of great importance for fundamental research and practical applications [1–6]. Recently discovered pressure-induced stable H-rich compounds (e.g., H2S [7] and LaH10 [8,9]) broke the superconducting transition temperature record of 164 K in cuprates [10]. Notably, theoretical predictions play a leading role in accelerating these innovative discoveries [11–13]. Very recently, room-temperature or even higher-temperature superconductivity has been predicted through doping lithium into MgH16, forming a novel ternary compound, Li2MgH16 [14]. However, a common characteristic of these hydrides is that their superconductivity emerges at more than one million times the atmospheric pressure. Therefore, the search for stable or metastable superconducting materials at ambient pressure is highly needed for practical application [15].

Some of pressure-induced stable compounds are recoverable to ambient pressure with interesting properties, especially for light mass elements, such as boron, carbon, and nitrogen. They can be synthesized, since pressure allows them to overcome the required reaction barriers to be formed. For example, well-known superhard materials, such as BC3 [16] and diamond [17], are synthesized at high pressures and become metastable at ambient pressure. On the other hand, pressure-induced stable binary compounds are also used as precursors to achieve elemental allotropes. For instance, two silicon allotropes, Si24 [18] and P6/m-Si6 [19], are obtained through a two-step synthesis methodology, removing the Na atoms from the pressure-induced stable Na2Si24 and P6/m-NaSi6 via a thermal “degassing” process. More interestingly, Si24 has a proper band gap of 1.3 eV, showing broad applications as photovoltaic cells [18]. P6/m-Si6 becomes a superconductor with a critical transition temperature of 12 K at ambient pressure [19]. In both structures the Si atoms form a three-dimensional frame with open channels, where the Na atoms are located, which makes it easy for them to escape.

The study of boron allotropes has attracted great attention because of their electron deficiency, structural complexity, and unusual bonding pattern [20,21]. Up to now, at least 14 boron allotropes have been reported [22]. Most of them consist of B12 icosahedra [23]. However, the arrangement of the icosahedra strongly modifies their electronic properties. For instance, I212121-B60, where B12 icosahedra are linked by helical boron chains, is a metal, whereas Pnma-B60, in

*Corresponding author: a.bergara@ehu.eus
†Corresponding author: yanggc468@nenu.edu.cn
‡Corresponding author: xiaobing.phy@qfnu.edu.cn
§Corresponding author: a.bergara@ehu.eus
which $B_{12}$ icosahedra are interconnected by two-atom wide $B$ ribbons, is a semimetal [24]. After compression, boron allotropes undergo complex structural transitions, caused by the appearance of novel boron units, which also modify their electronic properties [23,25–29]. So far, no bulk superconducting boron allotrope has been found at ambient pressure.

Having in mind that pressure can stabilize unusual stoichiometric compounds [30–32] and that known sodium borides consist of covalent $B$ frames [33–35], we consider the binary Na-B system to explore stable B-rich Na-B compounds with open channel frames, then to obtain metastable boron allotropes after releasing Na atoms. In this work, first-principle swarm-intelligence structural search method was employed to identify stable Na-B compounds at high pressures. Besides reproducing the known Na-B compounds (e.g., $Na_3B_{20}$ [33] and $NaB_{15}$ [35]) at ambient pressure, four new Na-B compositions (e.g., $Na_3B_2$, $Na_2B_3$, $NaB_4$, and $Na_2B_{17}$) become stable under high pressure. As expected, two metastable $I4/mmm$ $B_4$ and $Pm$ $B_{17}$ allotropes are obtained from $I4/mmm$ $NaB_4$ and $Pm$ $NaB_{17}$ precursors. Interestingly, these new compounds are predicted to be highly stable and even superconductors, becoming the first superconducting bulk boron allotropes at ambient pressure.

II. COMPUTATIONAL METHODS

To explore the stable Na-B phases under high pressure, we employ a swarm-intelligence based CALYPSO structure search method [36,37], which can find stable structures just depending on the chemical compositions. The geometry optimization and calculations of the electronic properties are performed with the Vienna $ab$ initio simulation package (VASP) code [38] within the framework of density functional theory (DFT) [39,40]. The all-electron projector augmented-wave (PAW) [41] pseudopotentials with $2s^22p^63s^1$ and $2s^22p^1$ valence electrons for Na and B atoms, respectively, are used to describe the interactions between electrons and ions. The full-potential all-electron calculations of the equation of states for NaB$_4$ compound were performed with the full-potential linearized augmented plane-wave method as implemented in the WIEN2k code [42] to examine the validity of the selected PAW pseudopotentials under high pressure (Fig. S0). The Perdew-Burke-Ernzerhof (PBE) [43] functional within the generalized gradient approximation (GGA) [44] is used to account for the exchange-correlation energy. A cutoff energy of 800 eV and a Monkhorst-Pack [45] $k$-point grid with a reciprocal space resolution of $2\pi \times 0.03 \text{Å}^{-1}$ in the Brillouin zone yield an excellent convergence for the Gibbs free energy. Electron-phonon coupling calculations within the density functional perturbation theory and the plane-wave pseudopotential method with ultrasoft pseudopotentials are implemented in the QUANTUM ESPRESSO package [46]. More detailed illustrations of structure search and computational details can be found in the Supplemental Material [47].

III. RESULTS AND DISCUSSION

A. Phase stability

Here we mainly focused on B-rich Na-B compounds, which have a tendency to form three-dimensional $B$ frames. We mainly focus on the phases of NaB$_4$ and Na$_2$B$_{17}$, consisting of three-dimensional $B$ frames. The structures and electron properties of the other predicted Na$_3$B$_2$ and Na$_2$B$_3$ can be found in Figs. S5 and S6. The low-pressure NaB$_4$

![FIG. 1. Pressure-composition phase stability diagram of the Na-B system between 1 atm and 100 GPa.](Image 301x598 to 547x730)

We conduct an extensive structure search on Na-B compounds with a variety of $Na_mB_n$ ($m = 1, n = 1–20$; $m = 2, n = 1, 3, 5, 7, 9, 11, 13, 15, 17, 19$; $m = 3, n = 2–10$) compositions at 0 K and the following pressures, 1 atm and 10, 25, 50, and 100 GPa. The relative thermodynamic stabilities of the considered $Na_mB_n$ compounds are shown in the convex hull diagram [48] (Fig. S1). The thermodynamic stable phases sitting at the solid line are denoted by solid spheres, whereas the metastable phases, represented by open spheres, decompose into elemental Na [49,50] and B [23] solids or other Na$_m$B$_n$ phases. At ambient pressure, the already known $Cmmm$ $Na_3B_{20}$ and $I2_12_22_1$ $NaB_{15}$ are reproduced in our structure search [35]. As can be seen in Fig. 1, $I2_12_22_1$ $NaB_{15}$ shows a much larger stable pressure range than $Cmmm$ $Na_3B_{20}$. On the other hand, the predicted phases and phase transition pressures for NaB$_3$ are in excellent agreement with the results of Zhou et al. (Fig. S2) [34]. All these results demonstrate that our adopted structure search method and pseudopotentials are suitable for the Na-B system.

At higher pressures, several new B-rich stoichiometries (i.e., Na$_3$B$_2$, Na$_4$B$_4$, and Na$_2$B$_{17}$) emerge on the convex hull (Fig. S1). Their stable pressure ranges are shown in Fig. 1. In more detail, $I4/mmm$ Na$_3$B$_2$ is predicted to be stable above 15.4 GPa. For NaB$_4$, there are two stable phases in the pressure range considered: $I4/mmm$ Na$_3$B$_2$ becomes stable at 38.4 GPa and then transforms into $I4/mmm$ Na$_3$B$_2$ above 78.1 GPa. Na$_2$B$_3$, with a higher B content, stabilizes above 75.6 GPa. Na-rich $C2/m$ Na$_3$B$_2$ begins to be stable above 67.5 GPa. For compounds containing light elements, zero-point energy (ZPE) potentially has a large contribution to the total Gibbs free energy, which might influence their relative stability [51–53]. However, the inclusion of ZPE for the predicted sodium borides at the selected pressure of 100 GPa did not change their relative stabilities (Fig. S3). Phonon spectra calculations [54,55] demonstrate that all Na$_m$B$_n$ compounds are dynamically stable, with no imaginary frequency modes at any high-symmetry direction in the whole Brillouin zone (Fig. S4).

B. Crystal structures

![Graphical representation of crystal structures associated with Na$_m$B$_n$ compounds.]

We mainly focus on the phases of NaB$_4$ and Na$_2$B$_{17}$, consisting of three-dimensional $B$ frames. The structures and electron properties of the other predicted Na$_3$B$_2$ and Na$_2$B$_3$ can be found in Figs. S5 and S6. The low-pressure NaB$_4$
phase is predicted to have an orthorhombic structure [space group Immm, 4 f.u. per cell, Fig. 2(a)]. There appears B₁₇ pentahedrons with B-B bond lengths of 1.65–1.80 Å at 50 GPa, and these pentahedrons make a B network via edge and face sharing. Each Na atom is 12-fold coordinated, with B forming a face-sharing Na-B polyhedra with Na-B bond lengths of 2.30–2.49 Å [Fig. 2(b)]. The high-pressure NaB₄ phase has a tetragonal structure [space group I4/mmm, 4 f.u. per cell, Fig. 2(c)], which is isostructural to LiB₄ [56]. Strikingly, it shows B₁₈ icosahedrons [Fig. 2(g)], which are interconnected to form an open-channel frame with a B-B distance of 1.70–1.96 Å at 100 GPa. Notably, Na atoms sit at the center of the open channel and coordinate with 16 B atoms [Fig. 2(d)].

Na₂B₁₇ stabilizes into a monoclinic structure [space group Pm, 1 f.u. per cell, Fig. 2(e)], consisting of three kinds of face-sharing B units, dubbed as B₁₁-I, B₁₄, and B₁₁-II [Fig. 2(h)]. The three B units interconnect with each other to form a three-dimensional framework with an open channel along the b direction. The B-B bond length is 1.53–1.96 Å at 100 GPa. More interestingly, Na atoms form linear chains located in the skeletal channels. Notably, Na atom in Na₂B₁₇ exhibits the highest coordination numbers (up to 19) among sodium borides. Electron localization function (ELF) [57] analysis shows that B-B bonds in three-dimensional frameworks of NaB₄ and Na₂B₁₇ are covalent (Fig. S7); while the Na-B bonding is weakly ionic, which is also supported by the Bader charge analysis (Table S3). To analyze the relative bond strength between Na-B and B-B bonds, the integrated crystal orbital Hamilton populations (ICOHP) are employed as implemented in the LOBSTER package [58,59]. The resulting ICOHPs of Na-B and B-B pairs in I4/mmm NaB₄ are −0.033 and −3.410 eV/pair, respectively, indicating that the Na-B interaction is much weaker than that of B-B. A silicon allotrope, Si₂₄, has been obtained from Na₄Si₂₄ through removing Na...
structures clearly indicate that to verify their thermal stability. The snapshots of the resulting B10 phase presents a linear atomic chain combined with an interpenetrating icosahedra and $\alpha$-B12 above 74 GPa, which is regarded as the modification of B12 icosahedra [27], is a superhard material. Under higher pressure (>375 GPa) B10 phase presents an linear atomic chain combined with an isoceles triangle, exhibiting a high-$T_c$ superconductivity of 44 K at 400 GPa [29]. Recently, several new metallic and hard B allotropes, termed as $\alpha$-B24 (20.0 GPa), c-B56 (26.6 GPa), $m$-B16 (56.2 GPa), and $o$-B16 (60.7 GPa) from ambient to high pressure up 120 GPa have been found, in which $o$-B24 has B12 icosahedra units, whereas B12 icosahedra in c-B56, $m$-B16, and $o$-B16 are absent [62]. More recently, it has been reported that $t$-B106 at ambient conditions is just slightly less stable than $\beta$-B [63], consisting of interstitial B atoms and interpenetrating icosahedra and $\alpha$-B12 [64]. However, compared with boron units of the known B allotropes at ambient and high pressures that we have briefly described above, the clathrate boron structural units in $I4/mmmm$ B4 and $Pm$ B17 are predicted to be also mechanically stable (Table S6) [60]. In addition, we have also performed molecular dynamical simulations [61] at 1000 and 1500 K with a time step of 1.0 fs to verify their thermal stability. The snapshots of the resulting structures clearly indicate that $I4/mmmm$ B4 and $Pm$ B17 also remain stable at these temperatures (Fig. S8), which supports their practical applicability.

Already known B allotropes at ambient and high pressures present a myriad of different structural characteristics with various interesting properties. For example, $\alpha$-B12, consisting of edging-sharing 20 boron trigons, is nonmetallic at ambient pressure [23]. High-pressure insulating ionic $\gamma$-B28 phase consists of cationic B2 pairs and anionic icosahedral B12 containing 20 boron trigons, shows a reduction of the band gap with pressure similar to that of $\alpha$-B12 [23]. Metallic $\alpha$-Ga-type B, transformed from $\alpha$-B12 above 74 GPa, which is regarded as the modification of B12 icosahedra [27], is a superhard material. Under higher pressure (>375 GPa) B10 phase presents an linear atomic chain combined with an isoceles triangle, exhibiting a high-$T_c$ superconductivity of 44 K at 400 GPa [29]. Recently, several new metallic and hard B allotropes, termed as $\alpha$-B24 (20.0 GPa), c-B56 (26.6 GPa), $m$-B16 (56.2 GPa), and $o$-B16 (60.7 GPa) from ambient to high pressure up 120 GPa have been found, in which $o$-B24 has B12 icosahedra units, whereas B12 icosahedra in c-B56, $m$-B16, and $o$-B16 are absent [62]. More recently, it has been reported that $t$-B106 at ambient conditions is just slightly less stable than $\beta$-B [63], consisting of interstitial B atoms and interpenetrating icosahedra and $\alpha$-B12 [64]. However, compared with boron units of the known B allotropes at ambient and high pressures that we have briefly described above, the clathrate boron structural units in $I4/mmmm$ B4 and $Pm$ B17 are predicted to be also mechanically stable (Table S6) [60]. In addition, we have also performed molecular dynamical simulations [61] at 1000 and 1500 K with a time step of 1.0 fs to verify their thermal stability. The snapshots of the resulting structures clearly indicate that $I4/mmmm$ B4 and $Pm$ B17 also remain stable at these temperatures (Fig. S8), which supports their practical applicability.

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FIG. 3. Electronic and superconducting properties of $I4/mmmm$ B4 and $Pm$ B17 at 1 atm. Phonon dispersion curves of (a) $I4/mmmm$ B4 and (b) $Pm$ B17. (c) Electronic band structure of $I4/mmmm$ B4. The horizontal dashed line indicates the Fermi level $E_F$. (d) PDOS of $I4/mmmm$ B4. The vertical dashed line indicates the Fermi level. (e) The Fermi surface for $I4/mmmm$ B4. The Fermi surface associated with each band crossing the Fermi energy is displayed in Fig. S10. (f) PDOS of $Pm$ B17. A close up of the PDOS around the van Hove singularity (vHs) near the $E_F$ is illustrated in the inset of (f). Eliashberg spectral function $\alpha^2F(\omega)$ (red area) and frequency-dependent electron-phonon coupling parameters $\lambda(\omega)$ (blue line) of (g) $I4/mmmm$ B4 and (h) $Pm$ B17.

Considering the strong B-B covalent bonding, the three-dimensional B framework in $I4/mmmm$ B4 and $Pm$ B17 and the excellent hardness in B-based compounds [65–68], we have also explored the hardness of the predicted new boron allotropes with the strain-stress method [69] and the Voigt-Reuss-Hill approximation [70]. Based on the empirical Vickers hardness model $H_v = 2.0 (k^2G)^{0.585} - 3.0$, $k = G/B$, where G and B are the shear and bulk modulus [71], the calculated hardness values of $I4/mmmm$ B4 and $Pm$ B17 are 27.3 and 26.8 GPa, respectively, indicating that they are good candidates as hard materials.

C. Electronic and superconducting properties

Much effort has been made to explore the superconductivity of B allotropes [72–75]. To be noted, two-dimensional
superconducting boron allotropes become superconducting due to their unique structure and inherent metallicity [72,73]. \(14/mmm\) \(B_4\) and \(Pm\) \(B_{17}\) allotropes are metallic at ambient pressure, as shown in the electronic band structures and PDOS [Fig. S9 and Figs. 3(c), 3(d), and 3(f)]. Similar to \(14/mmm\) \(NaB_4\) and \(Pm\) \(Na_2B_{17}\), \(B_{12}\) in \(14/mmm\) \(B_4\) and \(Pm\) \(B_{17}\) allotropes has also a large contribution to their metallic character, with a strong hybridization between \(B\) 2s and \(B\) 2p orbitals [Figs. 3(d) and 3(f)], which plays a key role in stabilizing the covalent B networks. Additionally, there is a clear Fermi surface nesting in \(14/mmm\) \(B_4\) along \(Z\) \(\rightarrow\) \(A\) and \(M\) \(\rightarrow\) \(\Gamma\) directions [Fig. 3(e)], with flatter bands along \(A\) \(\rightarrow\) \(M\) and \(R\) \(\rightarrow\) \(X\) [Fig. 3(c)], which induces high electronic density of states near the Fermi level [Figs. 3(d) and 3(f)]. There appears van Hove singularity [Fig. 3(f)] in \(Pm\) \(Na_2B_{17}\). On the other hand, \(14/mmm\) \(B_4\) and \(Pm\) \(B_{17}\) allotropes contain the novel B structural units, as described above. As these features might support the superconducting transition in these compounds, we have estimated their superconducting critical temperatures \(T_c\) using the Allen-Dynes modified McMillan equation [76–81] on the basis of Bardeen-Cooper-Schrieffer (BCS) [82] theory with adopting a typical Coulomb pseudopotential of \(\mu^* = 0.1\). The superconducting temperatures of \(14/mmm\) \(B_4\) and \(Pm\) \(B_{17}\) are predicted to be 19.8 and 15.4 K at ambient pressure, which are comparable to 2D B polymorphs (e.g., 18.7 K for \(\beta_1\) [74], 24.7 K for \(\chi_3\) [74], and 17.9 K for 2D boron layer [75]). The calculated electron-phonon coupling parameters \(\lambda\) of \(14/mmm\) \(B_4\) and \(Pm\) \(B_{17}\) at 1 atm are 0.65 and 0.67, respectively, comparable to 0.61 in \(MgB_2\) [83]. As clearly revealed in Fig. 3(g), the electron-phonon coupling (EPC) constant of \(14/mmm\) \(B_4\) mainly arises from the contribution of low-frequency phonon modes below 23.9 THz, giving the dominant contribution (97.8%) to the integral EPC constant \(\lambda\). The same is observed in \(Pm\) \(B_{17}\), in which low-frequency vibrations below 27.1 THz contribute 96.7% of the total \(\lambda\) [Fig. 3(h)]. Therefore, the superconducting mechanism is quite similar to that of the superconducting \(Li_3P\) electrode [84], but different from the high-frequency H-derived vibrations of high-\(T\) \(H_3S\) [7,12], \(H_2Se\) [85], and \(CaYH_{12}\) [86] superconductors and intermediate-frequency H-derived vibrations of \(H_4Te\) [87].

IV. CONCLUSIONS

In summary, four hitherto unknown Na-B compounds (i.e., \(NaB_2\), \(NaB_3\), \(NaB_4\), and \(NaB_{17}\)) are identified with first-principle swarm-intelligence structural search calculations. The arrangements of B atoms in these compounds evolve sequentially with increasing the B content from one-dimensional B linear chains to \(B_6\) octahedra, \(B_7\) pentahedra, and three-dimensional B frameworks. Removing Na atoms from \(14/mmm\) \(NaB_4\) and \(Pm\) \(NaB_{17}\), two metallic \(14/mmm\) \(B_4\) and \(Pm\) \(B_{17}\) allotropes become very stable at ambient conditions. Besides being potential hard compounds, among the already known three-dimensional boron allotropes, they show the highest superconducting transition temperatures of 19.8 and 15.4 K. Our work provides an effective way to get superconducting boron allotropes.

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