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Superhard superconductor of hydrogen doped cubic BC₂N under ambient pressure

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ABSTRACT

The synthesis of superhard superconductor at ambient pressure remains a challenge in materials science. Here, we perform detailed high-throughput calculations to explore the feasibility of achieving concurrent superconductivity and superhardness in *c*-BC₂N at ambient pressure. The calculated results demonstrate that hydrogen (H), as the electron acceptor, occupies interstitial sites in the *c*-BC₂N lattice, causing local structure distortions. These distortions modify the electronic structures of *c*-BC₂N, transforming from an intrinsic indirect-gap semiconductor to a metallic state. Notably, the double H doping shifts the valence band of *c*-BC₂N upward and promotes the formation of a flat band from Y to T near the Fermi level, which effectively enhance the electron–phonon coupling (EPC) interactions, and ultimately achieve a relatively high superconducting transition temperature (*T*_c) of 37.6 K for (BC₂N)₃H₂ at ambient pressure. Interestingly, the double H doped *c*-BC₂N also exhibits a Vickers hardness of 44.2 GPa at ambient pressure, which is an outstanding superhard superconductor at ambient pressure. These findings indicate that H doping faultlessly regulates the structural and electronic properties of *c*-BC₂N, and provide novel insights for the design and synthesis of multifunctional materials at ambient conditions.

1. Introduction

Over the past century, the developments of superconducting materials have traversed from early metallic alloys, such as Nb₃Ge (*T*_c = 23 K) [1], to copper oxides like HgBa₂Ca₂Cu₃O_x (*T*_c = 150 K) [2], and more recently to nickel-based superconductors including (La,Pr)₃Ni₂O₇ (*T*_c > 40 K) [3]. Achieving higher *T*_c values typically requires extreme external conditions. In recent years, the hydrides are regarded as promising candidates for high temperature and even room temperature superconductors [4–9]. Previous reports confirm that H₃S exhibits superconductivity at 203 K under 155 GPa [10], while LaH₁₀ shows a *T*_c of about 250–260 K at 170–190 GPa [11–14]. Other H-rich compounds, including CaH₆ (*T*_c = 215 K at 175 GPa) [15,16] and YH₆ (*T*_c = 224 K at 166 GPa) [17–19], also demonstrate to be superconductor with superconductivity above 200 K. In these hydrides, electrons donated by guest metal atoms occupy the antibonding orbitals of H, leading to the formation of caged geometries through weak covalent interactions among the adjacent H atoms.

However, these H-rich compounds are stable only under ultra-high pressure up to 150 GPa. One design strategy to reduce required

pressures involves hydrogen-rich compounds with stronger covalent bonding. Compounds such as La(B,Be)H₈ and Mg₂IrH₆ feature metal–hydrogen coordination complexes that ensure dynamical stability, and moderately high *T*_c, to much lower pressures [20–24]. These compounds are not, at the lower pressures, energetically stable, but that is not necessarily problematic: copper oxide based superconductors are not the most energetically stable compounds either, in fact they are not superconducting without doping, a property they share with traditional transition metal hydrides MH_x (*x* ≤ 1) [25]. The search for superconductivity in hydrogen-doped metastable compounds holds promise for experimental verification.

In an alternative approach to address the pressure dependency, i.e. exploring superconductors at moderate or ambient pressures, light-element compounds come into the field of vision [26–30]. Recent efforts are focused on covalent caged frameworks composed of light-elements, like C, B, N, and Si elements [31–33]. For instance, SrB₃C₃ and BaB₃C₃ compounds are predicted to exhibit *T*_c values of 40 K and 43 K, respectively [34]. The high temperature superconductivities are driven by the strong coupling interactions between *sp*³-hybridized σ -bonding states and *E_g* phonon modes of boron (B) atoms [35]. Li et al.

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have reported that TiB_2C_8 exhibits a T_c of 96 K at ambient pressure, which is the highest T_c value among B–C caged compounds [36]. Moreover, metal doped BN cages, such as $\text{Na}(\text{BN})_5$, $\text{Al}(\text{BN})_5$, $\text{In}(\text{BN})_5$, and $\text{Tl}(\text{BN})_5$, are confirmed to be superconductors at ambient pressure with T_c values of 8 K, 22 K, 15 K, and 15 K, respectively [37]. Another example is RbB_3Si_3 compound, which shows a T_c value of ~ 14 K at ambient pressure, achieved through precise control of the sizes of alkali metal cations to stabilize the caged AB_3Si_3 geometries [38]. These findings suggest that combining strong covalent frameworks with metal doping provides an effective route to achieve the high T_c superconductors at ambient pressure. Nevertheless, many of these compounds suffer from the decrease of hardness and strength due to the presence of metallic elements, which may limit their utility under extreme mechanical stress.

Superhard materials, defined by a Vickers hardness (H_v) ≥ 40 GPa, play an irreplaceable role in industrial cutting, wear-resistant coatings, and extreme-condition devices [39–41]. Among these, $c\text{-BC}_2\text{N}$ has attracted significant attention. It is recognized as the third-generation superhard material following diamond and cubic boron nitride ($c\text{-BN}$) [42,43]. Its exceptional properties arise from the unique sp^3 -hybridized covalent bonding networks. The body-centered cubic (BCC) phase of $c\text{-BC}_2\text{N}$ (space group $Im\bar{3}m$) stands out due to its distinct atomic arrangements and chemical bonding patterns. The unit cell contains 12 atoms (3B, 6C, 3N), with carbon atoms occupying face-centered positions and B/N atoms alternating between body-centered and vertex sites. This configuration maximizes the number of C–C and B–N chemical bonds, with a C–C to B–N bond ratio of about 2:1, leading to enhanced mechanical strength. Solozhenko et al. have declared that BC_2N exhibits large bulk modulus (B_0) of 305–309 GPa, high Vickers hardness exceeding 60 GPa, and good thermal stability with a decomposition temperature ~ 200 K higher than diamond [44]. The $c\text{-BC}_2\text{N}$ has been synthesized via laser-heated diamond anvil cell (DAC) and multi-anvil press techniques, with graphite-like BC_2N serving as the precursor under pressures exceeding 18 GPa and temperatures above 2200 K. Its superhard feature is confirmed through Vickers and Knoop hardness measurements. The robust sp^3 -bonded frameworks in $\text{bc6-BC}_2\text{N}$ endow it with shear strength about 12 GPa, enabling resistance to extreme shear stress [45]. However, $\text{bc6-BC}_2\text{N}$ is an indirect-bandgap semiconductor with bandgap of ~ 0.6 eV. The highly delocalized covalent bonding leads to obvious electron localization, limiting its potential in the applications of electronic and quantum devices. Thus, the main challenge in the design of superhard superconductor is the intrinsic conflict between achieving strong covalent networks for superior hardness and promoting electronic delocalization for high carrier concentration. Normally, in superhard materials, strong bonding configurations usually result in highly localized electrons. A well-known example is diamond, which shows an ultra-wide bandgap of 5.5 eV. After doping other elements, such as B, the boron-doped diamond is a superconductor with T_c of 4 K [46]. However, this method often compromises mechanical properties, resulting in hardness values that fail to meet the 40 GPa threshold [47].

To address the above mentioned issues, we propose a strategy of fine-tuning the electronic structure of $c\text{-BC}_2\text{N}$ through precision H doping. The prototype structure is based on the $\text{bc6-BC}_2\text{N}$ configuration reported by Luo et al. [48]. Our calculations reveal that H atoms, insertion into caged voids or interstitial sites, still preserve the sp^3 -hybridized covalent frameworks of $c\text{-BC}_2\text{N}$. The single H doped $c\text{-BC}_2\text{N}$ exhibits a T_c of ~ 7 K at ambient pressure, while the double H doped $c\text{-BC}_2\text{N}$ achieves a T_c of 37 K. Remarkably, this $c\text{-BC}_2\text{N}\text{-H}_2$ compound exhibits a Vickers hardness of 44.2 GPa. In principle, H atoms occupy interstitial sites in the cubic BC_2N lattice, causing local lattice distortions. These distortions enhance the vibrational modes that mediate interactions between conduction electrons, which shift the valence band upward and promote the formation of a flat band from Y to T near the Fermi level. The flat band, with its high DOS near the Fermi level, enhances EPC and Cooper pair formation, thereby playing a critical role in mediating superconductivity. We will discuss the potential superconducting mechanism of double H doped $c\text{-BC}_2\text{N}$ in detail below.

2. Computational methods

The geometric optimizations and electronic structure calculations are carried out within the framework of density functional theory (DFT) using the Vienna Ab initio Simulation Package (VASP) [49–51]. The stable structures are rechecked by Crystal structure AnaLYsis by Particle Swarm Optimization (CALYPSO) structure prediction method [52, 53]. The interactions between electrons and ions are described using the projector augmented wave (PAW) method [54]. The exchange–correlation energy is treated using the Perdew–Burke–Ernzerhof (PBE) functional within the generalized gradient approximation (GGA) [55]. The plane-wave energy cutoff is set to 770 eV. The convergence criteria for total energy and atomic forces are 1×10^{-6} eV and 1×10^{-3} eV/Å, respectively. Brillouin zone integrations are conducted using Monkhorst–Pack (MP) k-point meshes with a density of $2\pi \times 0.02 \text{ \AA}^{-1}$ [56], ensuring that the total energy is converged to within 0.1 meV/atom. The crystal orbital Hamilton population (COHP) analyses are conducted using the LOBSTER package [57].

The EPC parameters and superconducting properties of H doped $c\text{-BC}_2\text{N}$ compound are calculated by using the QUANTUM ESPRESSO (QE) package [58,59]. The electron–ion interactions are described using ultrasoft pseudopotentials within the PBE framework. The plane-wave kinetic energy cutoff is set to 100 Ry and a charge density cutoff of 1000 Ry is employed. The electron–phonon interaction matrix elements are calculated using an irreducible $6 \times 6 \times 6$ q-point grid. The T_c values of H doped BC_2N compounds are estimated using the McMillan equation based on Bardeen–Cooper–Schrieffer (BCS) theory [60], which is expressed as follows:

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

The Coulomb pseudopotential μ^* is set to 0.1, and $\omega_{\log}$ is the logarithmic mean of phonons, which is expressed as:

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

The electron–phonon coupling constant λ is

$$\lambda = 2 \int_0^\infty \frac{\alpha^2 F(\omega)}{\omega} d\omega \quad (3)$$

To quantify Fermi surface nesting, which could support electron–phonon coupling, we determined the band-pair-resolved static dielectric susceptibility,

$$\chi_0^{ij}(\mathbf{q}) = - \sum_{\mathbf{k}} \frac{f_j(\mathbf{k}) - f_i(\mathbf{k} + \mathbf{q})}{\epsilon_j(\mathbf{k}) - \epsilon_i(\mathbf{k} + \mathbf{q}) + i\eta}, \quad (4)$$

where $f_i(\mathbf{k})$ is the Fermi–Dirac occupancy of band i at point $\mathbf{k}$ in the Brillouin zone (using a smearing width of 20 K), $\epsilon_i(\mathbf{k})$ the corresponding band energy, and $\eta = 1 \text{ } \mu\text{eV}$ a small energy broadening.

3. Results and discussions

To explore doping feasibility, we have evaluated the incorporation of numerous elements in the periodic table into the $c\text{-BC}_2\text{N}$ caged frameworks through high-throughput calculations. Unfortunately, all metal doped $c\text{-BC}_2\text{N}$ configurations, except Zn, Rh, Pd and Au, are unstable. These four metals doped $c\text{-BC}_2\text{N}$ configurations are also verified by CALYPSO structural prediction method [52,53]. Although these metals doped $c\text{-BC}_2\text{N}$ preserve metallic states, they fail to induce superconductivity. In contrast, $c\text{-BC}_2\text{N}$ doped with the majority of non-metallic elements exhibit dynamic stabilities at ambient pressure (Fig. 1).

Based on the above findings, we mainly focus on H element. On the one hand, the mass of H element is light which provide the high-frequency phonons required for high T_c but also enhance coupling strength through its electronic structure. On the other hand, the atomic

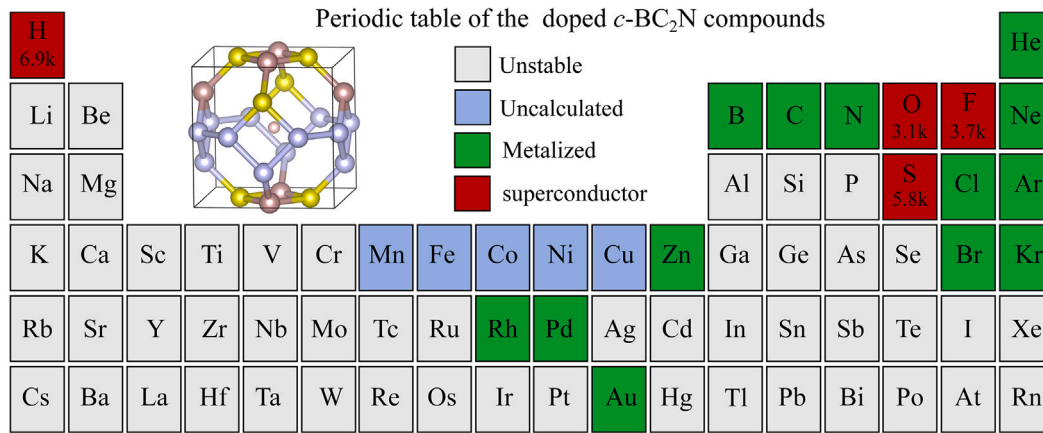


Fig. 1. Periodic table of the doped c -BC₂N compounds. Red squares denote superconducting structures, green squares denote metallic structures, gray represents dynamically unstable structures, and blue corresponds to the uncalculated structures. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

radius of H element is small, and the doped H atoms do not disrupt the sp^3 covalent frameworks of c -BC₂N compound. Three H doped c -BC₂N configurations are designed: (1) a single H atom at the body-center Wyckoff 1d (0.50, 0.50, 0.50) site; (2) a single H atom at the corner Wyckoff 1a (0.00, 0.00, 0.00) site; and (3) two H atoms co-occupying Wyckoff 1d (0.50, 0.50, 0.50) and 1a (0.00, 0.00, 0.00) sites. These configurations correspond to the chemical formulas B₃C₆N₃H₁ (denoted as c -BC₂N-H, encompassing single H atom doping at the two distinct positions) and B₃C₆N₃H₂ (denoted as c -BC₂N-H₂, for double H atoms doping). All three configurations are dynamic stable at ambient pressure. The c -BC₂N covalent cages are still intact after H incorporation. Among them, the c -BC₂N-H₂ configuration achieves the highest T_c value while also exhibits superhard feature. Consequently, in this work, we concentrate on the c -BC₂N-H₂ configuration. The details of the other configurations are shown in the Supplementary Material.

Fig. 2(a) shows double H doped c -BC₂N compound. The local BC₂N cages are presented in Fig. 2(b). H atom incorporation induces the geometric perturbations of bond lengths and angles in BC four-membered rings (4MRs) of BC₂N cages, whereas CN-4MRs and BC six-membered rings (6MRs) exhibit negligible variations. These observations confirm spatially confined lattice strain, which preserves the crystallographic integrity of the covalent frameworks in c -BC₂N. The angle B-C-B in BC-4MRs contracts progressively with increasing H concentration (Fig. S1), which is 88.39° (initial) → 86.42° (1H-center) → 84.39° (1H-corner) → 83.21° (double H doped). Concomitant adjustments in adjacent C-C-B and B-C-N angles further demonstrate the local elastic response to interstitial H atoms. By contrast, CN-4MRs and BC-6MRs show negligible angular variations, confirming structural robustness in the extended sp^3 -bonding networks. The lattice parameters of c -BC₂N-H₂ compound are $a = 4.4591$ Å, $b = 4.3108$ Å, and $c = 4.5155$ Å. However, the lattice parameters of undoped c -BC₂N are $a = 4.4079$ Å, $b = 4.4336$ Å, and $c = 4.3966$ Å. The ~2.8% contraction along the b -axis is originated from the compressed BC-4MRs, whereas the ~2.7% elongation along the c -axis reflects steric expansion to accommodate the inserted H atoms. Despite these anisotropic lattice distortions, the covalent skeleton remains continuous and structurally coherent.

To assess the influence of H doping on the mechanical properties of c -BC₂N, we calculate the elastic constants and moduli of the undoped and H doped c -BC₂N compounds. The calculated results are summarized in Table S1. All three configurations, i.e. undoped c -BC₂N, single H doped c -BC₂N-H, and double H doped c -BC₂N-H₂, satisfy the Born mechanical stability criteria ($C_{11} - C_{12} > 0$, $C_{11} + 2C_{12} > 0$, $C_{44} > 0$). Compared with undoped c -BC₂N, the elastic constants C_{11} , C_{12} , and C_{44} of double H doped c -BC₂N exhibit significant variations, indicating reduced crystal rigidity and hardness. The bulk modulus of

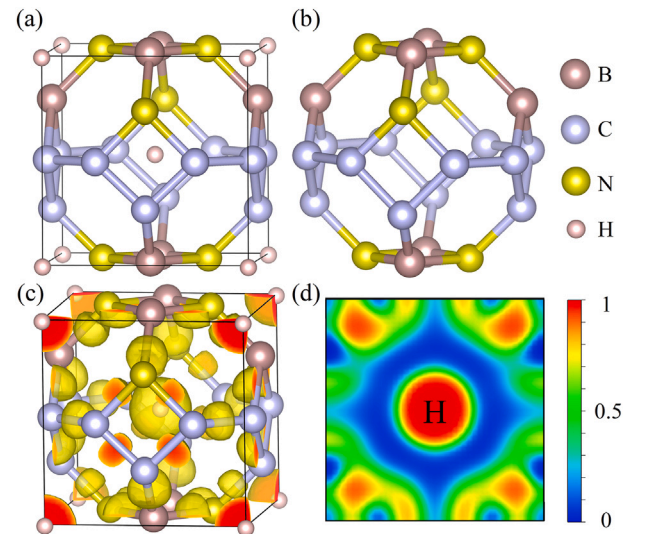


Fig. 2. (a) Crystal structure of double H doped c -BC₂N (c -BC₂N-H₂) compound, (b) BC₂N cage, (c) Electron localization function (ELF) of c -BC₂N-H₂ compound at an isovalue of 0.8, and (d) ELF distribution on the (100) plane of c -BC₂N-H₂ compound.

c -BC₂N-H₂ remains high, around 300 GPa, suggesting robust resistance to volume compression. Meanwhile, Pugh's ratio B/G and Poisson's ratio (ν) show slight increases, indicating enhanced ductility. Using the Voigt-Reuss-Hill approximation [61,62], the Vickers hardness H_v of (BC₂N)₃H₂ is estimated to be ~44 GPa, which is ~27% reduction from the ~60 GPa reported for undoped c -BC₂N [48]. Generally, H doping may introduce anisotropic lattice distortions for c -BC₂N. To quantitatively assess the anisotropy, we have calculated the universal elastic anisotropy index A^U and listed the results in Table S1. The results show that the A^U value of (BC₂N)₃H₂ is 0.25, which is higher than that of pristine BC₂N (0.12) and also higher than those of the single-H configurations (0.17 and 0.20), indicating that H doping indeed enhances the elastic anisotropy. In fact, double H doping leads to an approximately 2.8% contraction along the b -axis and an approximately 2.7% elongation along the c -axis for c -BC₂N. For simplicity, we have calculated the average Vickers hardness.

To elucidate bonding characteristics upon hydrogen incorporation, we perform electron localization function (ELF) analysis of the (BC₂N)₃H₂ compound. The detailed results are shown in Fig. 2(c) and

Fig. 2(d). In $(\text{BC}_2\text{N})_3\text{H}_2$, ELF distributions reveal robust contiguous lobes between B–C and C–N pairs, confirming the characteristic sp^3 covalent bonding in superhard materials. Upon H doping, these primary features persist with minimal modulation [Fig. 2(d)], confirming the intact covalent framework despite the presence of interstitial dopants. In contrast, each H atom exhibits a localized spherical region spatially isolated from adjacent electron clouds. This spatial isolation indicates absent directional electron sharing, indicating non-bonded anionic behavior, which is consistent with the reported hydridic H^- species [63], where dopants retain localized electron density without forming covalent bonds. Bader charge analysis provides definitive evidence of charge redistribution induced by H doping. In H-doped $c\text{-BC}_2\text{N}$, each interstitial H atom gains approximately 0.10–0.12 e, which indicates that H atom acts as an electron acceptor, essentially forming a hydride-like H^- anion [64]. As for double H doped $c\text{-BC}_2\text{N}$ compound, the two H atoms together accumulate roughly 0.20 e (about 0.10 e per H atom), further corroborating the anionic character. By contrast, the adjacent carbon atoms lose a comparable amount of electrons. In undoped $c\text{-BC}_2\text{N}$, each C atom possesses a Bader charge of ~ 3.8 e (just slightly below its valence of 4 e), whereas after H incorporation, this value decreases to ~ 3.7 e. The decrease of ~ 0.1 e per C atom confirms that electrons transfer from the C atoms to the interstitial H atoms, which induces distortions of BC 4MRs in $(\text{BC}_2\text{N})_3\text{H}_2$ compound.

These electronic reconstructions weaken the covalent interactions of neighboring C–C and B–C bonds and reduce the capacities to maintain cooperative structural responses under deformations. Notably, while bond weakening compromises mechanical strength, H doping simultaneously introduces additional localized states and mobile charge carriers, which enable the semiconductor-to-metal transition of $c\text{-BC}_2\text{N}$. In fact, H doping weakens C–C and B–C covalent bonds is also verified by the reduced absolute integrated crystal orbital Hamiltonian population (ICOHP) values (Table S2), which shows substantially weakened covalent interactions in these bonds. This weakening arises from H induced electron redistribution. H atoms acquire electrons from adjacent carbon atoms, reducing the valence electron density and bond-orbital occupation in C–C/B–C bonds. Additionally, H incorporation induces localized distortions (e.g., twisting of B/C 4MRs), further diminishing orbital overlap. These atomic-scale changes are consistent with macroscopic observations. The reduction in hardness correlates directly with decreased C–C and B–C bond energies, due to that high hardness is inherently associated with robust covalent frameworks. Notably, B–N and C–N bonds exhibit near-constant ICOHP values following hydrogenation, indicating that doping effects are localized to regions near H sites. The three-dimensional covalent network retains full connectivity.

Fig. 3 shows the projected band structures and projected density of states (PDOS) for $c\text{-BC}_2\text{N}$ and H doped $c\text{-BC}_2\text{N}$. Upon H doping, the electronic structure of $c\text{-BC}_2\text{N}$ is reconfigured significantly. The $c\text{-BC}_2\text{N}$ compound undergoes a distinct transition from semiconductor to metal with high electronic DOS near the Fermi level after H doping. In undoped $c\text{-BC}_2\text{N}$, the Fermi level lies within a bandgap between the valence and conduction bands, which is attributed to the strong sp^3 covalent bonding frameworks in $c\text{-BC}_2\text{N}$ compound. As a result, no electronic states are available near Fermi level [Fig. 3(a)]. The DOS around Fermi level approaches zero, with most electronic states localized in valence or conduction regions.

For single H doped $c\text{-BC}_2\text{N}$, the increased charge carrier concentration shifts the valence band upward and crosses the Fermi level, inducing the metallic state of $(\text{BC}_2\text{N})_3\text{H}$ compound [Fig. 3(b)]. However, the occupation of states at the Fermi level in the single H doped $c\text{-BC}_2\text{N}$ is not high, with a relatively low T_c value of 7 K. As for double H doped $c\text{-BC}_2\text{N}$, valence bands dominated by B–C/N sp^3 bonding undergo reconstruction, with a collective upward shift and crossing of the Fermi level. This shift is driven by occupation of hydrogenic states from an effective hole-doped covalent bond lattice, which leads to lattice distortions (e.g., B–C/N bond elongation), weakened covalent hybridization and reduced bond strength. The reduced bond strength

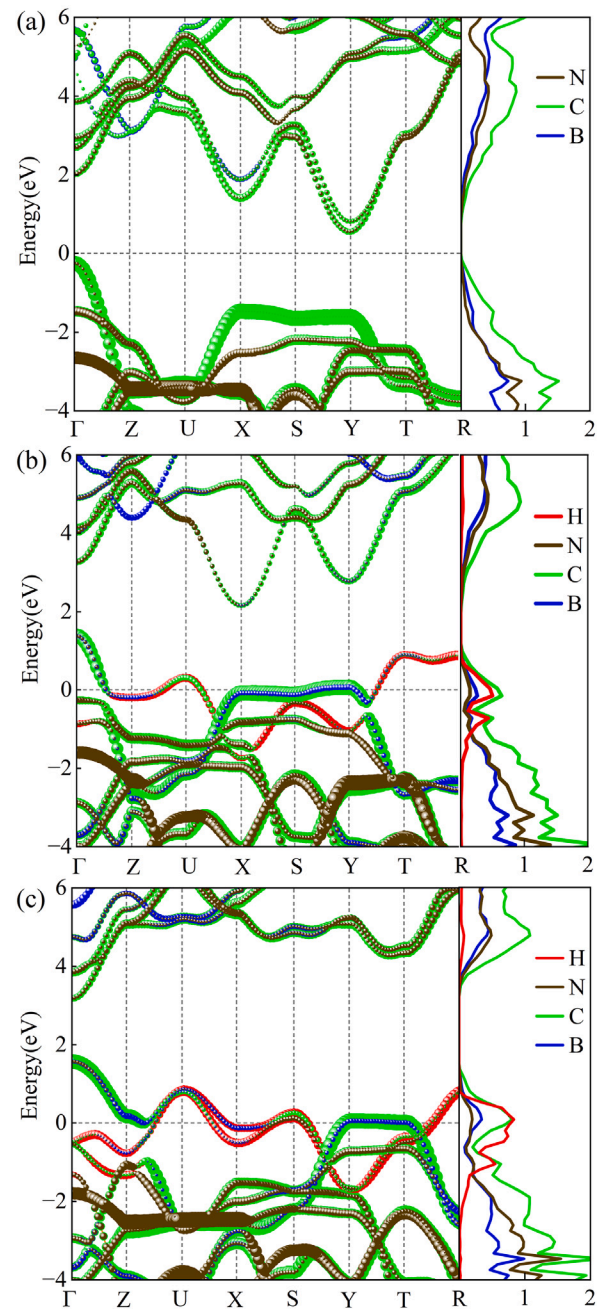


Fig. 3. Projected band structures and corresponding PDOS(State/eV/atom) for $c\text{-BC}_2\text{N}$ and $(\text{BC}_2\text{N})_3\text{H}_2$ under ambient pressure. (a) BC_2N ; (b) $(\text{BC}_2\text{N})_3\text{H}$ -center; (c) $(\text{BC}_2\text{N})_3\text{H}_2$. The size of the circles represents the magnitude of atomic orbital contributions. The Fermi level is indicated by a gray dashed line.

decreases bonding–antibonding splitting, destabilizing bonding states and raising their energies, which promotes the formation of a flat band near the Fermi level [Fig. 3(c)]. That flat band mainly originates from the orbitals of B and C atoms. Meanwhile, H atoms contribute a distinct localized DOS peak near the Fermi level. This behavior indicates that the highest bonding states from B–C bonds become partially unoccupied upon H doping. Although H atoms do not directly form strong covalent bonds with B atoms, their electronic states are effectively coupled with the orbitals of surrounding B, C, and N atoms. As shown in the PDOS, the hydrogenic states are primarily concentrated around the Fermi level. This phenomenon implies that H plays an important

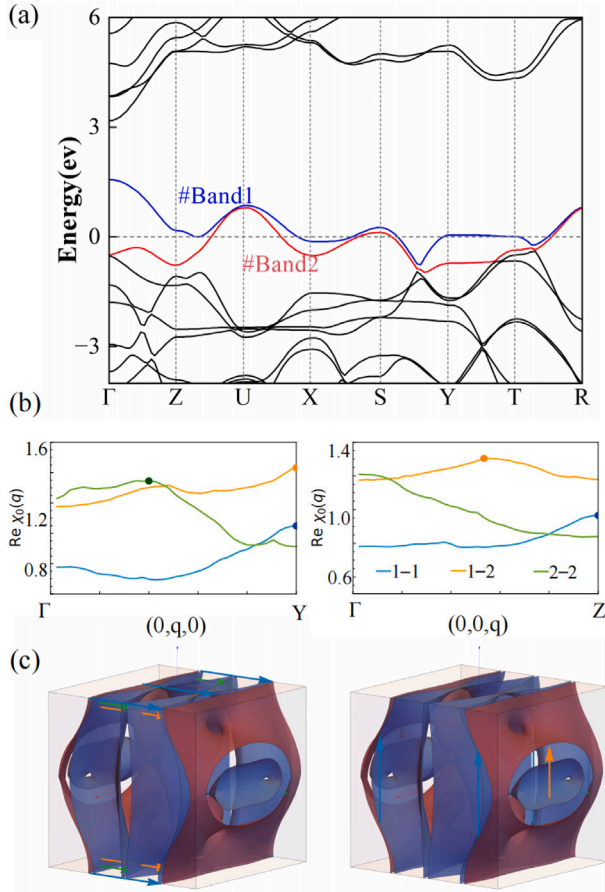


Fig. 4. (a) The band structure of $(\text{BC}_2\text{N})_3\text{H}_2$, highlighting the two bands crossing the Fermi level. (b) Static dielectric susceptibility $\chi_0^{ij}(\mathbf{q})$ for three different band combinations i, j and for $\mathbf{q} = (0, q, 0)$ (left) and $\mathbf{q} = (0, 0, q)$ (right). (c) Fermi surface of $(\text{BC}_2\text{N})_3\text{H}_2$, with colored arrows highlighting the strongest contributions to the maxima in $\chi_0^{ij}(\mathbf{q})$ highlighted in part (b).

role in the conduction behavior. The redistributions of multi-orbital electronic states results in a pronounced enhancement in the DOS near the Fermi level. A high occupation of DOS near the Fermi level is recognized to enhance EPC interactions, thereby increasing the T_c value [65].

Fig. 4 highlights the two energy bands that cross the Fermi level of $(\text{BC}_2\text{N})_3\text{H}_2$ and the corresponding Fermi surface (FS). The two FS sheets are distributed planes perpendicular to the k_y direction, with significant corrugation along k_z . Fig. 4(b) shows the magnitude of χ_0^{ij} along two high-symmetry directions, Γ -Y and Γ -Z, for the different band pair combinations. The most prominent nesting is for the interband term χ_0^{12} at $\mathbf{q} = (0, 1/2, 0)$, though other maxima appear as well. In Fig. 4(c) we show the Fermi surface of $(\text{BC}_2\text{N})_3\text{H}_2$ overlaid with arrows from the strongest contributions to the maxima in χ_0^{ij} (colors match the band pair coloring in Fig. 4(b)). As the nesting function is based purely on the Fermi surface geometry, electron-phonon coupling matrix elements are expected to renormalize χ_0^{ij} .

Fig. 5 shows phonon dispersion, phonon density of states (PhDOS), Eliashberg spectral function $\alpha^2F(\omega)$, and frequency-integrated EPC constant $\lambda(\omega)$ of $(\text{BC}_2\text{N})_3\text{H}_2$ at ambient pressure. Phonon dispersion and PhDOS of $(\text{BC}_2\text{N})_3\text{H}_2$ show that, in the low-frequency range (0–300 cm^{-1}), the acoustic branches are dominated by collective vibrations of the B–C–N covalent framework, with minimal contribution from H atoms. In the 300–950 cm^{-1} range, H derived modes appear as dominant components. These modes correspond to the cooperative vibrations of H coupled with the caged B–C–N covalent framework,

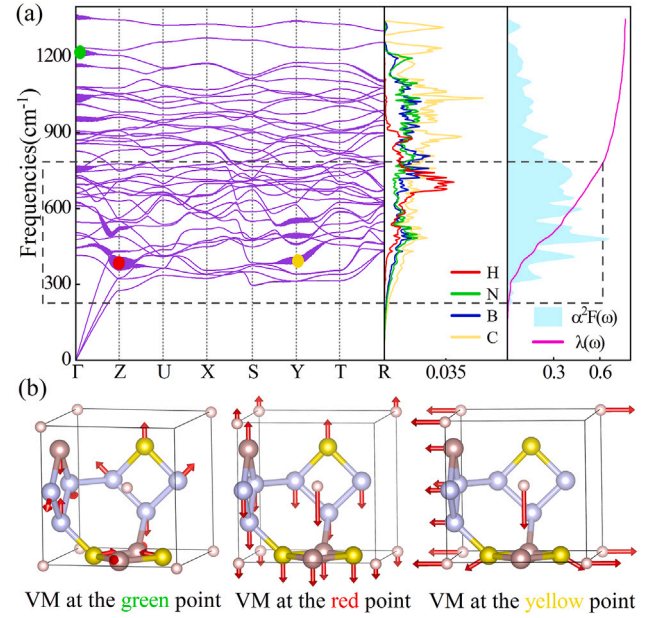


Fig. 5. (a) Phonon dispersion, projected phonon density of states (PhDOS), Eliashberg spectral function $\alpha^2F(\omega)$, and integrated electron-phonon coupling function $\lambda(\omega)$ of $(\text{BC}_2\text{N})_3\text{H}_2$ superconductor at ambient pressure. Phonon dispersion band widths correspond to mode-resolved EPC strength $\lambda_i(\mathbf{q})$. (b) Atomic vibration modes (VM) corresponding to the green, red, and yellow points. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

which are evidenced by pronounced H-projected weight in PhDOS. The bulk of the EPC (large $\alpha^2F(\omega)$ and steep slope of $\lambda(\omega)$) stems from the 300–750 cm^{-1} frequency range, highlighted by the dashed box in Fig. 5(a). We obtain a total electron-phonon coupling constant of $\lambda = 0.80$ and a logarithmic average frequency of $\omega_{\log} = 804$ K. Employing these values in the McMillan equation (with a Coulomb pseudopotential of $\mu^* = 0.1$) yields a superconducting critical temperature of $T_c = 37.7$ K. Using $\mu^* = 0.08$ – 0.13 , the calculated T_c of $(\text{BC}_2\text{N})_3\text{H}_2$ varies from 39.9 K to 34.8 K. Although the absolute T_c value shows moderate dependence on μ^* , the predicted superconductivity remains robust. The corresponding plots for $\text{B}_3\text{C}_6\text{N}_3\text{H}_1$, of phonon spectra, element-projected PhDOS, Eliashberg spectral function $\alpha^2F(\omega)$, and EPC integral $\lambda(\omega)$, are shown in Figs. S7–S8 of the Supplemental Material.

In contrast, no isolated H modes are observed in the 950–1400 cm^{-1} range, instead, it is characterized by C dominated local vibrations, with negligible H participation. These results are different from H-rich superconductors, where strong H–host covalent bonds generate distinct high-frequency modes. In $(\text{BC}_2\text{N})_3\text{H}_2$, H occupies nonbonding cage sites without forming strong covalent bonds, resulting in vibrational frequencies substantially lower than those in hydride superconductors. The vibrations of H atoms couple with the caged B–C–N covalent framework, undergoing a shift to mid-frequency range, without isolated high-frequency peaks [66]. Thus, cooperative vibrations of H atoms and the caged B–C–N covalent framework constitute the dominant EPC interactions, providing the major spectral weight of $\alpha^2F(\omega)$ and driving the rapid accumulation of $\lambda(\omega)$, which are critical to the realization of superconductivity.

The displacement vectors of the vibrational modes labeled in Fig. 5(a) are shown in Fig. 5(b). At the green point (corresponding to the Γ point in the high-frequency region), vibrations are dominated by the bond stretching motion of B, C, and N atoms in the caged covalent frameworks, whereas H atoms exhibit negligible displacement. In contrast, several phonon modes near the red point (Z point, mid-frequency region) and yellow point (Y point, mid-frequency region)

exhibit cooperative vibrations involving both H atoms and caged B–C–N frameworks. Crucially, the mode-resolved electron–phonon coupling constant $\lambda_v(\mathbf{q})$, visualized by the width of the phonon dispersion bands in Fig. 5(a), identifies these specific modes around the Y and Z points as those with the largest coupling strength. These points (especially at Y, where several phonon modes have large $\lambda_v(\mathbf{q})$) correspond to points of appreciable Fermi surface nesting, as established above. The dominance of these mid-frequency modes is quantitatively confirmed, as they contribute 78% of the total EPC strength λ . Although H atoms are light and typically produce high-frequency modes, their non-bonding confinement within the rigid B–C–N cages shifts these critical vibrations into the 300–750 cm^{-1} range. In contrast, in typical hydride superconductors, such as LaH_{10} , H atoms form strong covalent bonds with the host lattice, resulting in highly localized high-frequency phonon modes that are well separated from those of heavier elements. This distinction highlights the unique coupling mechanism in $(\text{BC}_2\text{N})_3\text{H}_2$ superconductor.

It is worth mentioning that H incorporation does not disrupt the inherent sp^3 covalent network; instead, H atoms occupy interstitial sites while the BC_2N cages remain intact. This observation implies that hydrogenation can proceed as an interstitial modification of the pre-existing $c\text{-BC}_2\text{N}$ framework. We have also evaluated the formation enthalpies of three distinct H-doped configurations relative to reference phases comprising $c\text{-BN}$, diamond, and H_2 . The calculated values show formation enthalpies of -288.8 meV/atom for the $(\text{BC}_2\text{N})_3\text{H}$ -center configuration and -289.9 meV/atom for the $(\text{BC}_2\text{N})_3\text{H}$ -corner configuration, whereas the $(\text{BC}_2\text{N})_3\text{H}_2$ double-H doped configuration shows a higher value of -81.3 meV/atom. These results indicate that the double-H configuration is likely stabilized only under more hydrogen-rich environments or high-temperature and high-pressure conditions. In fact, similar cases also exist, such as diamond and graphite. Metastable diamond can be synthesized from graphite under high-temperature and high-pressure conditions. More detailed experiments are needed to verify the present results.

4. Conclusions

In summary, we conduct high-throughput calculations to explore the feasibility of achieving concurrent superconductivity and superhardness in $c\text{-BC}_2\text{N}$ at ambient pressure. The calculated results reveal that the double H doped $c\text{-BC}_2\text{N}$, i.e., $(\text{BC}_2\text{N})_3\text{H}_2$, exhibits superconductivity of 37.6 K at ambient pressure while retaining a Vickers hardness of 44.2 GPa. It is an excellent superhard superconductor at ambient pressure. The doped H atom acting as electron acceptor and forming a hydride-like H^- anion, occupies interstitial sites within the $c\text{-BC}_2\text{N}$ lattice, inducing local lattice distortions. These distortions modify the electronic structure of $c\text{-BC}_2\text{N}$, transforming from an intrinsic semiconductor to a metal. Notably, the double H doping shifts the valence band of $c\text{-BC}_2\text{N}$ upward and promotes the formation of a flat band near the Fermi level, which effectively enhance the EPC interactions, and finally achieve high temperature superconductivity for $(\text{BC}_2\text{N})_3\text{H}_2$ at ambient pressure. The superhard characteristic of $(\text{BC}_2\text{N})_3\text{H}_2$ is primarily attributed to the intact and rigid B–C–N covalent framework. Our findings demonstrate that H doping precisely modulates the structural and electronic properties of $c\text{-BC}_2\text{N}$, and offer vital insights into the design and synthesis of multifunctional materials at ambient conditions.

CRediT authorship contribution statement

Wenrui Zhang: Writing – original draft, Investigation, Formal analysis, Data curation, Conceptualization. **Junyi Miao:** Formal analysis, Data curation. **Sarah Alnujaim:** Formal analysis. **Chen Chen:** Visualization, Formal analysis. **Xin Zhong:** Software, Resources. **Andreas Hermann:** Writing – review & editing, Methodology. **Cheng Lu:** Writing – review & editing, Supervision, Software, Resources, Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.actamat.2026.122292>.

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