

High-temperature superconductivity in M_2BH_6 hydrides under near ambient pressure

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Hydrogen-rich compounds that exhibit high-temperature superconductivity typically require extreme pressures, which severely limits their practical applicability. Recent theoretical predictions of the complex hydride Mg_2IrH_6 have introduced a new family of M_2XH_6 -type hydrides, highlighting the potential for high-temperature superconductivity at near-ambient pressure. Motivated by this, we have performed high-throughput first-principles investigations of the M_2XH_6 family ($M = \text{IA, IIA, IIIA, IIB metals}$; $X = \text{B, C, N}$) to identify dynamically stable hydrides and explore their superconducting properties. Eleven boron-based hydrides, M_2BH_6 ($M = \text{Li, Na, K, Rb, Cs, Ca, Sr, Ba, Sc, Y, La}$), featuring BH_6 octahedral units have been identified. Notably, Li_2BH_6 is dynamically stable down to 16 GPa and exhibits a superconducting critical temperature of 121.25 K. Electronic structure and phonon analyses indicate that high-frequency hydrogen vibrations from strong B–H covalent bonding, reinforced by light Li atoms, dominate the electron–phonon coupling. In contrast, noble-metal-based Li_2XH_6 compounds ($X = \text{Cu, Ag, Au}$) exhibit distinct superconducting mechanisms, driven by d electrons at the Fermi level and low-frequency metal vibrations. These findings expand the compositional space of the M_2XH_6 family and highlight Li_2BH_6 as a promising candidate for near-ambient-pressure high- T_c superconductivity.

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I. INTRODUCTION

The discovery of superconductivity critical temperature (T_c) exceeding 250 K in H_3S [1], LaH_{10} [2,3], and CaH_6 [4] has stimulated intense interest in high-pressure metallic hydrides. Guided by Ashcroft’s proposal of chemically pre-compressed hydrides [5], recent advances in crystal structure prediction (CSP) and experimental synthesis have focused extensively on this class of hydrogen-rich compounds [6–9]. Despite record-high T_c values, typically realized only at pressures above 150 GPa, the requirement of such extreme conditions poses a major obstacle for practical applications. A key challenge is to reduce the synthesis pressure of hydrogen-rich compounds while preserving their high- T_c superconducting properties [9–11]. Guest-element doping and covalent stabilization have emerged as effective strategies. For example, doping to introduce a third element offers a promising route, as ternary hydrides expand the structural landscape and provide additional degrees of freedom for stabilizing superconductivity under more moderate pressures.

High-pressure experiments suggest that ternary hydrides formed solely from metallic or solely from nonmetallic

elements do not significantly enhance T_c . For example, systems such as $(La,Y)H_{10}$ [12], $(La,Y)H_4$ [13], $(La,Ca)H_{10}$ [14], $(La,Sc)H_{12}$ [15], and $LaBeH_8$ [16,17] have not surpassed the T_c record of LaH_{10} [14]. Recently suggested $LaSc_2H_{24}$ shows a moderate increase over LaH_{10} by 10–40 K but at 200 GPa and above [18,19]. By contrast, ternary hydrides incorporating both metallic and nonmetallic elements can be synthesized at relatively lower pressures while retaining high T_c . A representative case is LaB_2H_8 , which exhibits a sizable T_c of 106 K at 90 GPa [20]. Light nonmetallic elements such as B, C, and N possess high electronegativity and form strong covalent bonds with hydrogen (e.g., B–H, C–H) [21–27]. These covalent units reinforce lattice rigidity, suppress hydrogen molecularization, thereby lowering the pressure required for metallization. Thus, incorporating nonmetallic elements into high-temperature superconducting hydrides realizes the “chemical precompression” effect, offering an effective strategy to lower synthesis pressures and facilitating the theoretical design of ternary hydrogen-rich superconductors.

Recently, several reports [28–30] have proposed the M_2XH_6 family hydrides, in which an electropositive cation M and a main-group element X are coordinated octahedrally by hydrogen. Notably, the Mg_2IrH_6 hydride has been predicted to exhibit conventional high-temperature superconductivity at ambient pressure [28–30]. Its elevated T_c (160 K at ambient pressure) arises from the cooperative effects of IrH_6 vibrational modes and a van Hove singularity (vHS) near the Fermi

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level [28]. Subsequent high-throughput density functional theory (DFT) calculations and machine-learning approaches have identified numerous Mg_2XH_6 compounds as potential ambient-pressure superconductors, many with predicted T_c values above 50 K [29,31–35]. These include systems featuring MH_6 octahedra, such as M_2XH_6 (where $M = Li, Na$; and $X = Fe, Rh, Ir, Pd, Pt$) [29,31–35]. More recently, reported compounds like KB_2H_8 [36] and Rb/CsB_2H_8 [37], which incorporate the B–H metallic σ bond in BH_4 motifs, are predicted to exhibit superconducting transition temperatures of 134 K and 100 K at 12 GPa and 25 GPa, respectively.

Inspired by the nonmetallic BH_4 structural motif, we have performed high-throughput computational searches targeting M_2XH_6 compounds, where M represents elements from groups IA, IIA, IIIA, and IIB, and X corresponds to B, C, or N. We identify 11 dynamically stable boron-based hydrides containing BH_6 octahedra, namely M_2BH_6 with $M = Li, Na, K, Cs, Rb, Ca, Sr, Ba, Sc, Y$, and La . Detailed first-principles calculations demonstrate that Li_2BH_6 is dynamically stable down to 16 GPa and exhibits a T_c as high as 121.25 K. These findings establish Li_2BH_6 as a promising candidate for realizing high-temperature superconductivity at near-ambient pressures.

II. COMPUTATIONAL DETAILS

Geometry optimizations and electronic structure calculations were carried out within the framework of density functional theory (DFT) using the Vienna *ab initio* simulation package (VASP) [38]. The generalized gradient approximation (GGA) in the form proposed by Perdew-Burke-Ernzerhof (PBE) [39,40] was employed for the exchange-correlation functional. A plane-wave kinetic energy cutoff of 800 eV and a Monkhorst-Pack k -point mesh with a reciprocal-space resolution of $2\pi \times 0.03 \text{ \AA}^{-1}$ were adopted to ensure convergence of the total energy and atomic forces. Phonon dispersion curves were obtained within density functional perturbation theory (DFPT) as implemented in the PHONOPY package [41]. The bonding characteristics were analyzed by the crystal orbital Hamilton population (COHP) method using the LOBSTER code [42,43]. Electron-phonon coupling (EPC) and superconductivity calculations were investigated using DFPT as implemented in the QUANTUM ESPRESSO package [44], employing optimized norm-conserving Vanderbilt (ONCV) pseudopotentials [45] (Table S1 in the Supplemental Material (SM) [46]). The kinetic energy cutoff for the wavefunctions and the charge density cutoff were set to 80 Ry and 600 Ry, respectively. A dense $24 \times 24 \times 24$ k -point mesh and a $6 \times 6 \times 6$ q -point grid were used to achieve convergence of EPC properties.

The EPC-derived superconducting critical temperature T_c was estimated using both the Allen-Dynes modified McMillan equation [47,48] and the numerical solution of the Eliashberg equations. The Allen-Dynes equation is given by

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

where λ is the EPC constant, and $\omega_{\log}$ is the logarithmic average phonon frequency. The μ^* is the effective Coulomb pseudopotential parameter, which have a chosen typical value

M \ X	B	C	N
Li	✓	✗	✗
Na	✓	✗	✗
K	✓	✗	✗
Rb	✓	✗	✗
Cs	✓	✗	✗
Ca	✓	✗	✗
Sr	✓	✗	✗
Ba	✓	✗	✗
Sc	✓	✗	✗
Y	✓	✗	✗
La	✓	✗	✗

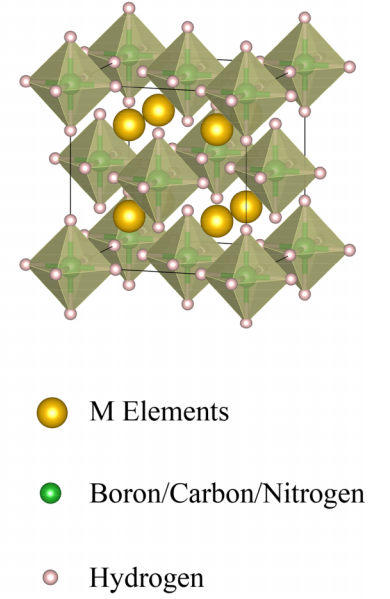


FIG. 1. Screening results for various combinations of M and X elements in M_2XH_6 compounds, along with the prototype structures in the pressure range of 0–50 GPa. The checkmarks (✓) represent compounds that are both dynamically stable and metallic.

of 0.1. The electron-phonon coupling constant λ and $\omega_{\log}$ were calculated from

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

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

with $\alpha^2 F(\omega)$ being the Eliashberg spectral function.

III. RESULTS AND DISCUSSION

We have performed screening calculations for the M_2XH_6 family, where M represents the metal elements from groups IA, IIA, IIIA, and IIB, and X corresponds to light nonmetallic elements (B, C, and N). The compounds adopt a cubic structure with space group $Fm\bar{3}m$ (No. 225), featuring XH_6 octahedra in which H atoms occupy the $24e$ ($1/2, 1/2, z$) Wyckoff sites, X occupies the $4a$ (0, 0, 0) site, and M occupies the $8c$ ($1/4, 1/4, 1/4$) site. Structural optimizations have been carried out from 0 to 50 GPa in steps of 10 GPa, and the structural parameters of M_2BH_6 at selected pressures have been collected in Table S2. After the structures are fully optimized, phonon dispersion calculations are subsequently performed to evaluate the dynamical stability of the optimized M_2XH_6 ($X = B, C, N$) structures (Figs. S2–S9). The results indicate that Li_2BH_6 is dynamically stable above 16 GPa, Na_2BH_6 above 5 GPa, Ca_2BH_6 above 10 GPa, and Sc_2BH_6 above 12 GPa. By contrast, M_2BH_6 compounds with $M = Na, K, Rb, Cs, Sr, Ba$, and La are stable at ambient or near-ambient pressure. As summarized in Fig. 1, the 11 dynamically stable M_2BH_6 ($M = Li, Na, K, Rb, Cs, Ca, Sr, Ba, Sc, Y, La$) compounds are identified within the pressure range 0–50 GPa.

TABLE I. Superconducting properties of the predicted M_2XH_6 compounds, including the electron-phonon coupling constant (λ), logarithmic average phonon frequency ($\omega_{\log}$), and estimated T_c from both the Allen-Dynes modified McMillan equation and the numerical solution of the isotropic Eliashberg equations.

Compound	Pressure (GPa)	λ	$\omega_{\log}$ (K)	T_c , McMillan (K)	T_c , Eliashberg (K)
Li_2BH_6	16	1.48	854.91	96.25	121.25
	25	1.31	1022.15	101.39	121.66
	50	1.07	1295.81	99.61	121.52
	100	0.94	1551	98 [26]	
	200	0.76	1940	81 [26]	
Li_2CuH_6	0	2.07	677.11	99.65	
	0	2.30	500.1	80 [30]	
	0	1.96	491	86 [31]	
Li_2AgH_6	0			83.0/108.8 [35]	
	5	2.46	416.21	67.95	
	10	2.82	496.71	87.78	
Li_2AuH_6	0	2.532	485.13	80.48	
	0			140, 116.1 [34,35]	
Na_2BH_6	5	1.27	368.65	35.38	
	10	1.08	496.45	38.66	
	50	1.14	554.54	46.32	
K_2BH_6	0	0.76	299.21	12.43	
Rb_2BH_6	0	0.62	275.33	6.85	
Cs_2BH_6	0	0.76	194.67	8.15	
Ca_2BH_6	10	1.48	197.55	22.22	
Sr_2BH_6	1	1.89	219.70	30.33	
	5	1.39	257.98	45.27	
Ba_2BH_6	0	0.54	274.80	4.35	
Sc_2BH_6	12	1.50	204.66	23.40	
	15	1.74	82.28	10.67	
Y_2BH_6	5	1.63	153.19	18.80	
La_2BH_6	0	0.47	228.98	2.10	

Unfortunately, phonon dispersion calculations revealed that neither the M_2CH_6 nor the M_2NH_6 phases exhibit dynamic stability below 50 GPa. This instability is attributed to the high electronegativity of the carbon and nitrogen atoms. The superconducting transition temperatures of the M_2BH_6 compounds were evaluated using QUANTUM ESPRESSO, and all are found to be superconducting phases. Notably, Li_2BH_6 reaches a T_c of 121.25 K at 16 GPa, exceeding the liquid-nitrogen boiling point of 77 K. The superconducting parameters for the eleven stable M_2BH_6 compounds, together with the reported values for Li_2CuH_6 [30,31], Li_2AgH_6 [35], and Li_2AuH_6 [34], are summarized in Table 1. To clarify the origin of high-temperature superconductivity in these compounds, we have performed detailed analyses of their electronic structures and EPC properties.

As shown in Fig. 2, we present the detailed structural motif of BH_6 , the electron localization function (ELF), and the electronic structure of Li_2BH_6 at 16 GPa. The optimized lattice parameter of Li_2BH_6 is determined to be 5.435 Å. Enthalpy-difference calculations further demonstrate that Li_2BH_6 remains thermodynamically stable down to 45 GPa, suggesting that it can be synthesized experimentally from suitable precursor compounds at around 45 GPa and subsequently quenched to lower pressures, where it remains dynamical stable to at least 16 GPa [Fig. S1(b)]. The B–H bond length in the BH_6 motif is 1.384 Å at 16 GPa [shown in Fig. 2(a)],

decreasing to 1.374 Å at 25 GPa, consistent with strong covalent bonding. For comparison, the B–H bonds in the BH_4 tetrahedra of alkali-metal AmB_2H_8 hydrides are typically 1.229–1.239 Å at 10 GPa [37], while the BH_8 backbone in $LaBH_8$ exhibits a B–H bond length of about 1.33 Å at 70 GPa [16,49]. The ELF map on the (001) plane shows localized charge around H atoms, corroborated by Bader charge analysis at 16 GPa: H atoms in BH_6 gain 0.474 $|e|$, while B and Li lose 1.081 $|e|$ and 0.883 $|e|$, respectively. The B–H bond is therefore best described as a polar covalent bond. In contrast, the isostructural Li_2XH_6 compounds with $X = Cu, Ag$, and Au exhibit different charge-transfer behavior, reflecting the influence of d -electron states (Table S3). The atom-projected electronic band structure and DOS [Fig. 2(c)] reveal two bands crossing the Fermi level, dominated by hybridization between H- s and B- p states, with Li acting primarily as an electron donor. Meanwhile, the detailed electronic band structures and DOS of Li_2BH_6 at 25 GPa and 50 GPa are presented in Fig. S10. The pronounced B–H covalent interactions, together with the substantial hydrogen-derived states at the Fermi level, indicate strong electron-phonon coupling, which is favorable for superconductivity.

We have calculated the projected and integrated crystal orbital Hamiltonian population (pCOHP, ICOHP) to investigate chemical bonding in M_2XH_6 hydrides, uncovering connections between superconductivity and structural configurations.

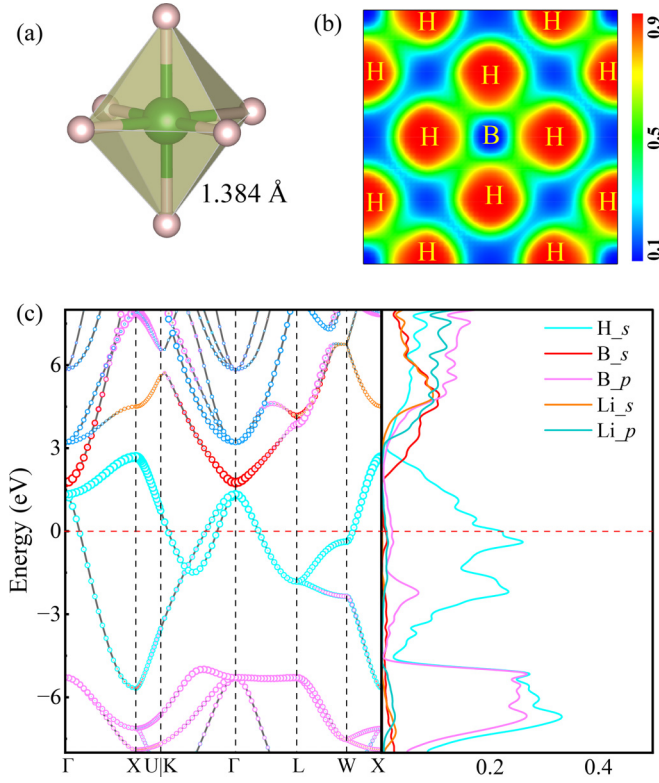


FIG. 2. (a) The octahedral structural motif of BH_6 . (b) Electron localization function (ELF) map in the (001) plane. (c) Atom-projected electronic band structure and density of states (DOS) of the Li_2BH_6 crystal structure at 16 GPa.

Figure 3 presents the pCOHP and ICOHP curves for B–H bonds in Li_2BH_6 and Na_2BH_6 , along with Cu–H and Au–H bonds in Li_2XH_6 ($X = \text{Cu}, \text{Au}$) at 0 GPa. The B–H bonds within the BH_6 octahedral motif exhibit pronounced covalent character due to occupied bonding states, confirming robust B–H bonding in Li_2BH_6 , with similar features in Na_2BH_6 at 5 GPa. In contrast, the isostructural Li_2AuH_6 and Li_2CuH_6 display longer Au–H (1.722 Å) and Cu–H (1.580 Å) bonds, attributed to the larger atomic radius of Au and Cu compared to B, resulting in weaker bonding, as evidenced by their ICOHP values (−1.316 and −1.097, respectively). ELF analysis (Fig. S11) further verifies weak bonding in Cu/Au-based Li_2XH_6 hydrides, highlighting the distinct superconducting mechanisms in B-based versus noble-metal-based hydrides. To elucidate the superconductivity and underlying mechanisms of $M_2\text{XH}_6$ hydrides, the superconducting parameters are summarized in Table 1. The phonon dispersion, atom-projected phonon density of states (phDOS), Eliashberg spectral function $\alpha^2F(\omega)$, and EPC integral $\lambda(\omega)$ for Li_2XH_6 ($X = \text{B}, \text{Cu}, \text{Ag}, \text{Au}$) under selected pressures are presented in Fig. 4 and Figs. S12–S14. The T_c of Li_2BH_6 are estimated using the Allen-Dynes modified McMillan equation and numerical solutions of the Eliashberg equations yields values of 96.25 K and 121.25 K at 16 GPa, respectively. Additionally, Kokail *et al.* have reported a T_c of approximately 98 K for Li_2BH_6 at 200 GPa [26]. The phonon dispersion of Li_2BH_6 reveals softening near the R point and along M– Γ , coinciding with large linewidths, indicating strong EPC contributions from

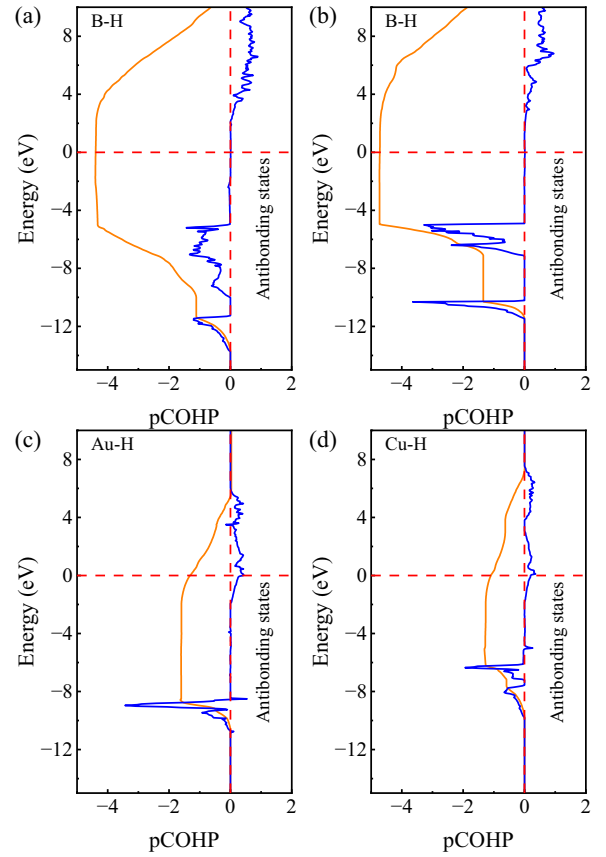


FIG. 3. The projected and integrated crystal orbital Hamiltonian population (blue: pCOHP, orange: ICOHP) of the X–H bonds in stable predicted $M_2\text{XH}_6$ compounds: (a) Li_2BH_6 at 16 GPa, (b) Na_2BH_6 at 5 GPa, (c) Li_2AuH_6 at 0 GPa, (d) Li_2CuH_6 at 0 GPa.

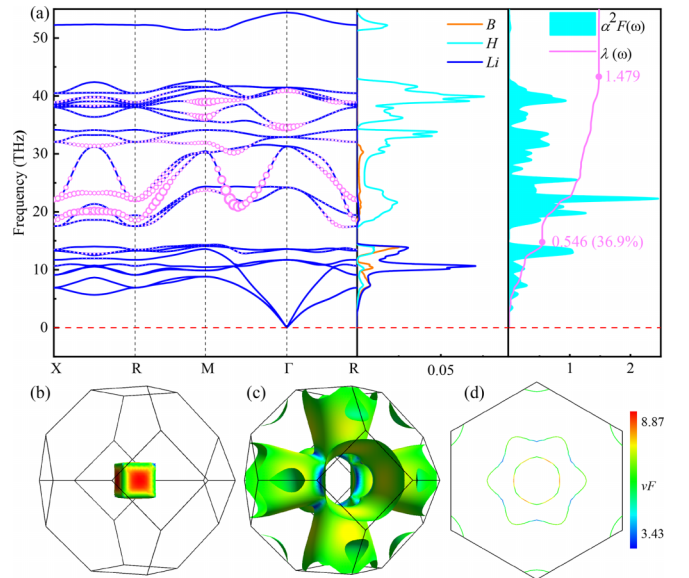


FIG. 4. Phonon dispersion curves (with pink circles proportional to the phonon linewidths), atom-projected phonon density of states (phDOS), and the Eliashberg spectral function $\alpha^2F(\omega)$ along with the electron-phonon coupling integral $\lambda(\omega)$, (b), (c) Fermi surface sheets, and (d) two-dimensional projection of the Fermi surface of Li_2BH_6 at 16 GPa.

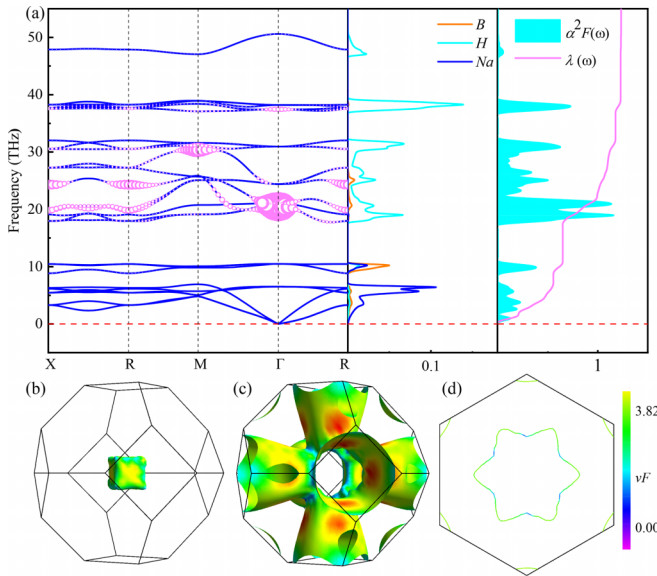


FIG. 5. Phonon dispersion curves (with pink circles proportional to the phonon linewidths), atom-projected phonon density of states (phDOS), and the Eliashberg spectral function $\alpha^2 F(\omega)$ along with the electron-phonon coupling integral $\lambda(\omega)$, (b), (c) Fermi surface sheets, and (d) two-dimensional projection of the Fermi surface of Na_2BH_6 at 5 GPa.

soft phonon modes. The phDOS together with the Eliashberg spectral function indicates that low-frequency (<15 THz) Li vibrations account for $\lambda = 0.546$ (36.9%), whereas high-frequency H vibrations dominate with 63.1% of the total coupling. This distribution emphasizes that the T_c is predominantly governed by the vibrations of light hydrogen atoms. The Fermi surface of Li_2BH_6 and Li_2XH_6 ($X = \text{Cu}, \text{Ag}, \text{Au}$) are depicted in Figures 4(b)–4(d) and Fig. S15, consisting of a central hole pocket at Γ and cross-shaped sheets extending toward the Brillouin-zone boundaries. A two-dimensional projection of the Fermi surface is provided in Fig. 4(d). To obtain more reliable superconducting T_c of Li_2BH_6 , anisotropic EPC calculations have been carried out by solving the Migdal-Eliashberg equations within the EPW code [50,51]. As shown in Fig. S16(a), the superconducting gap Δ is ~ 25 meV at 20 K and gradually vanishes at ~ 132 K under 16 GPa, yielding an anisotropic T_c of 132 K. At 50 GPa in Fig. S16(b), the anisotropic T_c is 112 K. The comparison indicates that anisotropic effects have a negligible influence on T_c relative to the isotropic results. Our predicted superconducting properties are robust and provide meaningful guidance for future experimental synthesis.

As shown in Fig. 5(a), Na_2BH_6 at 5 GPa exhibits behavior analogous to Li_2BH_6 , with the phonon band structure revealing softening at the Γ point and relatively large phonon linewidths. The Eliashberg spectral function shows significant contributions, with the phDOS indicating that vibrations below 8 THz are primarily driven by Na atoms, while those between 8–10 THz involve both Na and B atoms. At higher frequencies, H-atom vibrations predominantly con-

tribute to the electron-phonon coupling (EPC) constant λ . Consequently, Na_2BH_6 exhibits a T_c of 35.38 K at 5 GPa ($\lambda = 1.27$), significantly lower than that of Li_2BH_6 at comparable pressures. This reduction stems from the heavier Na atoms, which suppress the role of high-frequency H vibrations in the EPC, whereas the lighter Li atoms in Li_2BH_6 not only enhance the dominance of H-derived vibrations but also enable additional soft phonon modes, thereby supporting a substantially higher T_c . Meanwhile, we have also present the detailed electronic band structures and DOS of Na_2BH_6 at 5 GPa in Fig. S17.

Very recently, Ouyang, Gao, and co-workers have reported that the isostructural Li_2AuH_6 compound exhibits T_c values of ~ 140 K [30] and 116.1 K [35] at ambient pressure, whereas our calculations yield $T_c = 80.48$ K with $\lambda = 2.532$. The T_c values reported in this work display discernible discrepancies, predominantly arising from variations in the computational setup, including the pseudopotential schemes, q -point sampling densities, and the selected Coulomb pseudopotential (μ^*) parameters within the electron-phonon coupling framework [29]. Similar discrepancies have been documented for Mg_2IrH_6 , for which Dolui *et al.* predicted a T_c of approximately 160 K [28], whereas Sanna *et al.* reported a significantly lower value of about 80 K [29]. Gao *et al.* also reported that Li_2AgH_6 could approach the practical upper limit of conventional superconductivity at ambient pressure ($T_c \sim 108.8$ K) [35], suggesting its potential as a benchmark system within the Li_2XH_6 family.

To compare the role of precious metals (Cu, Ag, Au) with the nonmetal B in Li_2XH_6 compounds, we also calculated their electronic structures, phonon dispersions, and Eliashberg spectral functions. In contrast to Li_2BH_6 , the electronic band structures (Fig. S18) reveal that the d electrons of the noble metals dominate near the Fermi level, where strong hybridization between the Cu/Ag/Au d states and H- s states jointly contributes at the Fermi energy. The phonon spectra and EPC analyses demonstrate that in Li_2AuH_6 superconductivity originates primarily from low-frequency Au/Li vibrations (Fig. S14), which account for $\sim 63\%$ of the total EPC, significantly exceeding the contribution from Au–H octahedral vibrations. Comparable phonon and Eliashberg spectral function characteristics are observed in Li_2CuH_6 at 0 GPa (Fig. S12) and Li_2AgH_6 at 5 GPa (Fig. S13). These results highlight that the large mass disparity between noble metals (Cu/Ag/Au) and B, together with differences in the X–H bonding, generate distinct phonon modes within the same structural framework: in Li_2BH_6 , high-frequency H vibrations dominate the coupling and underpin the higher T_c , whereas in noble-metal systems, low-frequency vibrations play the leading role.

Notably, both Li_2BH_6 and Li_2XH_6 ($X = \text{Cu}, \text{Ag}, \text{Au}$) exhibit T_c values exceeding 77 K, with Li_2BH_6 reaching 121.25 K at 16 GPa. These results substantially broaden the compositional landscape of the $M_2\text{XH}_6$ hydride family and demonstrate that high-temperature superconductivity can be achieved not only in transition-metal-based $M_2\text{XH}_6$ compounds near ambient pressure, but also in Li_2BH_6 , which emerges as a particularly promising high- T_c superconductor.

IV. CONCLUSIONS

In summary, we have conducted high-throughput computational searches in the M_2XH_6 family and identified 11 dynamically stable boron-based hydrides containing BH_6 octahedra, namely M_2BH_6 with $M = Li, Na, K, Rb, Cs, Ca, Sr, Ba, Sc, Y$, and La . Among these, Li_2BH_6 is dynamically stable down to 16 GPa and exhibits a superconducting transition temperature $T_c = 121.25$ K. Analyses of the electronic structure and phonons indicate that high-frequency H vibrations and strong B–H covalent bonding, facilitated by light Li atoms and soft phonon modes, are primarily responsible for the strong electron-phonon coupling. In contrast, noble-metal Li_2XH_6 compounds ($X = Cu, Ag, Au$) exhibit distinct mechanisms, with d electrons dominating the Fermi level and low-frequency metal vibrations driving superconductivity. Our results significantly expand the compositional space of M_2XH_6 hydrides and demonstrate that high-temperature superconductivity can be realized in both nonmetallic and transition-metal-based systems. Li_2BH_6 , in particular, emerges as a promising candidate for near-ambient-pressure superconductivity, providing another pathway for the design of hydrogen-rich high- T_c materials.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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