

Prediction of the structural stability and superconducting properties of RbSc_2 hydrides under high pressure

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Ternary hydrides, owing to their chemical diversity and structural tunability, are considered important candidate systems for the exploration of high-temperature superconductivity. In this work, we performed systematic structure searches and superconductivity calculations on the RbSc_2H_x ternary system over pressures ranging from 150 to 300 GPa. Our results reveal that $\text{RbSc}_2\text{H}_{16}$ adopts a highly symmetric cubic structure with space group $Fd-3m$, which is both dynamically and thermodynamically stable down to 150 GPa, featuring a hydrogen-based cage framework. Upon increasing hydrogen content, $\text{RbSc}_2\text{H}_{17}$ forms a fully occupied cage structure with enhanced H-H interactions and strengthened Sc-H hybridization. Electron localization function, crystal orbital Hamilton population, and Bader charge analysis collectively indicate that the bonding is dominated by strong H-H covalent interactions, supported by ionic contributions from Sc-H bonds. Electronic structure calculations show pronounced metallicity with Sc-3d and H-1s hybridization dominating near the Fermi level, facilitating strong electron-phonon coupling. The superconducting critical temperatures estimated using the Allen-Dynes modified McMillan formula reach 140 K for $\text{RbSc}_2\text{H}_{16}$ at 150 GPa and 190.7 K for $\text{RbSc}_2\text{H}_{17}$ at 200 GPa, underscoring the crucial role of hydrogen occupancy in optimizing superconducting behavior. The results indicate that variations in hydrogen content have a noticeable effect on the stability and superconducting characteristics of the RbSc_2H_x system.

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I. INTRODUCTION

Since the discovery of superconductivity, the pursuit of materials with high superconducting critical temperatures (T_c) has never ceased. Based on the Bardeen-Cooper-Schrieffer theory [1], hydrogen (the lightest element) was predicted to become metallic and exhibit high-temperature superconductivity under extremely high pressures [2]. However, achieving metallic hydrogen requires enormous pressures (>500 GPa), posing significant experimental challenges. Ashcroft's concept of "chemical precompression" offers a promising solution by introducing other elements to form hydrides, effectively lowering the pressure required for hydrogen metallization [3]. Guided by this theory, a series of high-performance binary hydride superconductors have been successfully predicted and synthesized. Notably, the covalent hydride H_3S [4,5] with $Im-3m$ symmetry exhibits a T_c of 203 K at 155 GPa, and a series of clathratelike hydrides, such as CaH_6 (215 K, 172 GPa) [6,7], LaH_{10} (250 K, 170 GPa) [8–10], YH_9 (243 K, 201 GPa) [11], and YH_6 (220 K, 183 GPa)

[11,12], show even higher T_c values, with some binary hydrides exceeding 200 K.

In recent years, the research focus has gradually shifted from binary hydrogen-rich superconductors to ternary systems. The incorporation of a third element expands the accessible phase space and structural diversity of ternary hydrides, providing insights into the design of hydrogen-rich phases stable at lower pressures [13,14]. Experimentally, substitutional ternary hydrides have made significant progress. Partial replacement of metal elements allows tuning of the lattice parameters and electronic structure of hydrides, thereby optimizing their superconducting performance, such as $(\text{La}, \text{Ca})\text{H}_{10}$ (247 K, 173 GPa) [15], $(\text{La}, \text{Ce})\text{H}_9$ (148–178 K, 97–72 GPa) [16], $(\text{La}, \text{Y})\text{H}_{10}$ (253 K, 183 GPa) [17], and $(\text{La}, \text{Al})\text{H}_{10}$ (223 K, 164 GPa) [18]. Although these substitutional hydrides exhibit considerable T_c , they have not provided ternary structural prototypes capable of supporting higher superconducting temperatures. Theoretical predictions have proposed a design strategy: doping metals into binary superhydride to introduce additional electrons, thereby producing an electronic density of states at the Fermi level mainly from hydrogen. For example, systems such as $\text{Li}_2\text{MgH}_{16}$ (space group $Fd-3m$) achieve a cagelike structure by lithium atom doping that converts H_2 molecules into atomic hydrogen, with a predicted T_c of 473 K at 250 GPa [19]. Similarly, in the Li-Na-H system, I-type and II-type cagelike ternary hydrides exhibit thermodynamically stable room-temperature superconductivity, among which the II-type $\text{Li}_2\text{NaH}_{17}$ structure is predicted to reach a T_c of 357 K at 220 GPa [20]. Guided by

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theoretical predictions, the stoichiometric ternary superhydride LaBeH_8 (110 K, 80 GPa) was recently synthesized, exhibiting a characteristic interstitial-type ternary structure that serves as a structural template for high-temperature superconductivity [21,22]. Subsequently, a hexagonal-phase superhydride with a stoichiometry of $\text{LaSc}_2\text{H}_{24}$ was successfully synthesized, exhibiting a superconducting critical temperature of 271–298 K under pressures of 195–266 GPa, representing a further step toward achieving room-temperature superconductivity [23,24].

To identify ternary hydrides that are stable at lower pressures than $\text{Li}_2\text{MgH}_{16}$ [19] and $\text{Li}_2\text{NaH}_{17}$ [20], we first selected $\text{Li}_2\text{MgH}_{16}$ with the cubic $Fd-3m$ structure as prototype frameworks. We then performed systematic A- and B-site substitutions (elements from groups I–III, excluding previously reported combinations [25–27]) to generate candidate compositions. The dynamical stability of these candidates was further evaluated via phonon calculations. Through this screening process, the Rb-Sc-H system was identified as a promising target, and the primary lattice was further restricted to RbSc_2 . On the one hand, AB_2 -type hydrides such as $\text{Li}_2\text{MgH}_{16}$ and $\text{Li}_2\text{NaH}_{17}$ have been demonstrated to possess structural advantages for achieving high T_c . On the other hand, phonon spectra of Rb_2Sc hydrides exhibit distinct imaginary modes, indicating dynamical instability within the studied pressure range (see Fig. S3 in the Supplemental Material [28]). Therefore, this work focuses on the structural and superconducting properties of the RbSc_2H_x family. In this study, we conducted systematic structural predictions for RbSc_2H_x ($x = 9$ –18) under pressures of 150, 200, and 300 GPa. The most stable phases with the lowest free energies at each pressure were identified through structure searches, and convex hull diagrams were constructed to determine the thermodynamically stable phase compositions. The lattice dynamical stability of the candidate structures was further verified by phonon dispersion calculations. On this basis, the superconducting critical temperatures (T_c) of the most stable RbSc_2H_x compounds were predicted within the framework of electron-phonon coupling (EPC) theory. The results indicate that at a relatively low pressure of 150 GPa, the thermodynamically stable phase $\text{RbSc}_2\text{H}_{16}$ already exhibits a superconducting critical temperature as high as 140 K. Furthermore, a metastable phase $\text{RbSc}_2\text{H}_{17}$ is predicted to emerge at 200 GPa, with its T_c further enhanced to 190.7 K, thereby demonstrating even greater potential for high-temperature superconductivity.

II. COMPUTATIONAL DETAILS

We employed the CALYPSO software [31,32] package to search for crystal structures of RbSc_2H_x ($x = 9$ –18) under pressures of 150, 200, and 300 GPa. During the structure search, each generated structure was fully relaxed using the Vienna *Ab initio* Simulation Package (VASP) [33] within the framework of density functional theory. Both atomic positions and lattice vectors were optimized iteratively until the total energy converged. For each stoichiometry, the five lowest-energy structures were selected as candidates and subsequently subjected to fine structural optimization. The projector augmented-wave [34] method was used to describe the electron-ion interactions, and the exchange-correlation

effects were treated with the Perdew-Burke-Ernzerhof functional within the generalized gradient approximation [35,36]. The valence electron configurations were set as follows: Rb-4s4p5s, Sc-3p4s3d, and H-1s. The plane-wave cutoff energy was 400 eV, and the Brillouin zone was sampled using a Monkhorst-Pack scheme with a k -point spacing of $2\pi \times 0.03 \text{ \AA}^{-1}$, ensuring energy convergence within 1 meV/atom. The lowest-energy structures were then selected to calculate relative formation enthalpies. For preliminary screening of dynamical stability, phonon spectra were computed using the density functional perturbation method implemented in PHONOPY [37], with structures modeled in $2 \times 2 \times 2$ supercells. A denser k -point mesh of $2\pi \times 0.02 \text{ \AA}^{-1}$ was used for electronic structure calculations. Chemical bonding characteristics were analyzed using the LOBSTER package [38] to compute crystal orbital Hamilton population (COHP) [39] distributions, while Bader [40] charge analysis was employed to determine charge transfer. Electron localization function (ELF) [41] calculations were performed to visualize bonding features [42].

The electron phonon coupling parameters were calculated using density functional perturbation theory as implemented in the QUANTUM ESPRESSO (QE) code [43], and phonon spectra from QE were used to verify dynamical stability. For $\text{RbSc}_2\text{H}_{16}$, $\text{RbSc}_2\text{H}_{16.5}$, and $\text{RbSc}_2\text{H}_{17}$, ultrasoft pseudopotentials [44] were employed with a kinetic energy cutoff of 80 Ry and a charge density and potential cutoff of 800 Ry. EPC matrix elements were computed on a $16 \times 16 \times 16$ k -point grid and a $4 \times 4 \times 4$ q -point grid. The superconducting critical temperature (T_c) was estimated using the Allen-Dynes modified McMillan formula [45]:

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

where μ^* represents the effective Coulomb pseudopotential, generally assigned a value of 0.1, and λ is the electron-phonon coupling constant, obtained from

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

$\omega_{\log}$ denotes the logarithmic average of the phonon vibration frequencies, which is given by

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

III. RESULTS AND DISCUSSION

To evaluate the dynamical feasibility of the $Fd-3m$ structural type for different alkali-metal combinations, we systematically calculated the phonon dispersion relations of the AB_2H_{16} and AB_2H_{17} compounds ($A = \text{Na, Mg, K, Ca, Rb}$; $B = \text{Sc, Y}$), as shown in Figs. S1–S3 in the Supplemental Material [28]. The results show that $\text{RbSc}_2\text{H}_{16}$ remains dynamically stable without phonon softening in the pressure range of 150–300 GPa, whereas most of the other AB_2H_{16} and AB_2H_{17} systems exhibit pronounced imaginary phonon modes. This stability can be attributed to both chemical and electronic factors. Compared with other alkali metals, Rb possesses a larger ionic radius and lower electronegativity, which help expand the hydrogen cages and donate more electrons to

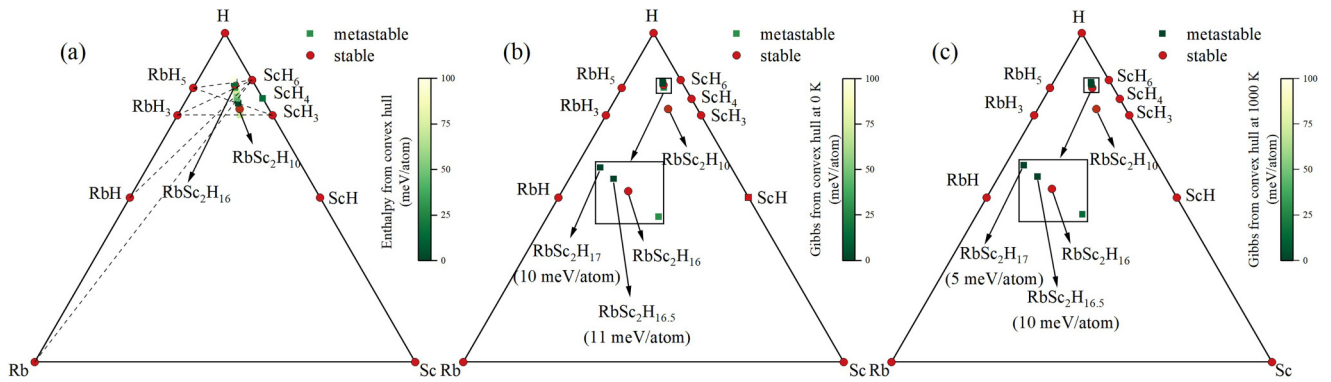


FIG. 1. Convex hulls of the RbSc_2H_x system at 200 GPa. Formation enthalpies (a) without ZPE, (b) at 0 K including ZPE, and (c) at 1000 K including vibrational entropy. Red circles indicate stable phases, while green squares denote metastable or unstable phases, with the color scale representing the energy offset from the convex hull. Insets show enlarged views of the $\text{RbSc}_2\text{H}_{16}$, $\text{RbSc}_2\text{H}_{16.5}$, and $\text{RbSc}_2\text{H}_{17}$ phases.

the hydrogen framework, thereby enhancing structural stability. Moreover, the effective hybridization between the Sc-3d and H-1s orbitals further reinforces this stability. Based on these findings, we performed a detailed investigation of the RbSc_2 hydrides.

The RbSc_2 metallic framework forms three-dimensional hydrogen cages, enabling hydrogen atoms to arrange into a dense and continuous network, thereby exhibiting excellent structural stability under high pressure. We performed crystal structure predictions for RbSc_2H_x ($x = 9-18$) in the pressure range of 150–300 GPa. The thermodynamic stability of the compounds was evaluated by calculating the formation enthalpy, and the corresponding convex hulls were constructed with the inclusion of zero-point energy (ZPE). Since hydrogen atoms exhibit very high lattice vibrational frequencies, the ZPE makes a significant contribution to the formation enthalpy. Considering that most hydrogen-rich compounds are experimentally synthesized under laser-heating conditions (~ 1000 K), where finite-temperature entropy may modify the Gibbs free-energy landscape and stabilize phases that are unstable at 0 K, we further evaluated the formation enthalpy including both ZPE and vibrational entropy at 1000 K. Accordingly, three convex hulls at 200 GPa were constructed under different thermodynamic conditions, as shown in Fig. 1, while the corresponding data at 150 and 300 GPa are provided in the Supplemental Material [28]. Analysis of the convex hulls reveals that $\text{RbSc}_2\text{H}_{16}$ remains thermodynamically stable throughout the entire pressure range of 150–300 GPa. In contrast, $\text{RbSc}_2\text{H}_{16.5}$ always lies slightly above the convex hull, with formation-enthalpy deviations of approximately 5–15 meV/atom, indicating that it remains metastable within this pressure range. We attribute this metastability to the presence of hydrogen vacancies in its lattice. When all hydrogen sites are fully occupied (corresponding to $\text{RbSc}_2\text{H}_{17}$; see Fig. 1), the inclusion of the entropy contribution at 1000 K further reduces its formation-enthalpy deviation from the convex hull from 10 to 5 meV/atom. In addition, at 0 K the inclusion of ZPE renders the binary ScH_4 phase thermodynamically stable, consistent with previous reports [27]. It is generally accepted that metastable materials with energy deviations below 50 meV/atom can be experimentally synthesized [46]. Notably, at 300 GPa the inclusion of ZPE alone is sufficient to stabilize $\text{RbSc}_2\text{H}_{17}$, driving it from a metastable to a stable phase (see

Fig. S6 in the Supplemental Material [28]), indicating that its stability is significantly enhanced with increasing pressure. As the pressure increases, the H-H distances are further reduced, strengthening the H-H interactions and the metal-hydrogen hybridization, which lowers the formation enthalpy and ultimately places $\text{RbSc}_2\text{H}_{17}$ onto the convex hull. The three crystal structures, shown in Fig. 2, form highly symmetric cubic lattices under the $Fd-3m$ space group. Hydrogen atoms occupy the 96g, 32e, and 8b sites to form cage-like frameworks. In $\text{RbSc}_2\text{H}_{16}$, the 8b sites are vacant, resulting in an incompletely filled hydrogen cage and the presence of systematic vacancy sites, which may give rise to localized electronic states. In $\text{RbSc}_2\text{H}_{16.5}$, the 8b sites are partially occupied, reducing the number of vacancies, slightly shortening the average H-H distances, and enhancing covalent interactions. In $\text{RbSc}_2\text{H}_{17}$, the 8b sites are fully occupied, forming a complete hydrogen cage framework with the strongest H-H interactions, yielding the highest overall symmetry and structural stability. As the hydrogen content increases, the H-H covalent interactions are strengthened, making the hydrogen cages more rigid and thereby contributing to the maintenance of crystal structure stability under high pressure. To further examine their stability at finite temperatures, we performed *ab initio* molecular dynamics simulations for $\text{RbSc}_2\text{H}_{16}$ and $\text{RbSc}_2\text{H}_{17}$ at 300 K (see Fig. S4 in the Supplemental Material [28]). The results show that all atoms vibrate around their equilibrium positions, with only minor fluctuations in the total energy and temperature throughout the simulations, and no changes in the solid phase were observed. This indicates that $\text{RbSc}_2\text{H}_{16}$ and $\text{RbSc}_2\text{H}_{17}$ exhibit strong stability against thermal fluctuations.

To explore the bonding characteristics of RbSc_2 hydrides under pressure, we calculated the electron localization function (ELF), as shown in Fig. 3 and Figs. S7 and S8 in the Supplemental Material [28]. The results indicate that the ELF values between metal and hydrogen atoms are nearly zero, suggesting that Rb-H and Sc-H bonds exhibit ionic interactions. The electron localization is mainly concentrated around H atoms, while the ELF value between H-H atoms is approximately 0.65, showing partial overlap of the electron clouds and implying the presence of covalent interactions. Such moderate H-H covalent bonding plays an important role in stabilizing the hydrogen framework under high pressure. To further quantify the bonding characteristics, COHP

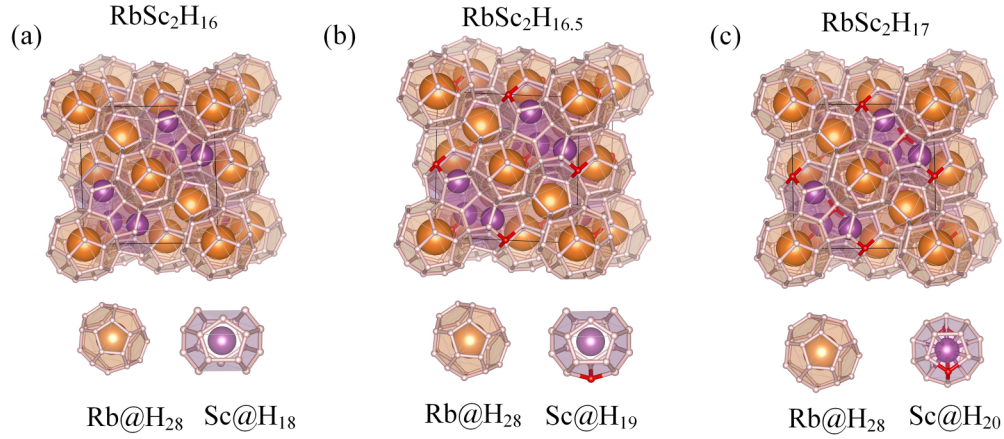


FIG. 2. Crystal structures and hydrogen cage configurations of (a) $\text{RbSc}_2\text{H}_{16}$, (b) $\text{RbSc}_2\text{H}_{16.5}$, and (c) $\text{RbSc}_2\text{H}_{17}$. Orange, purple, and pink spheres represent Rb, Sc, and H atoms, respectively. The red spheres represent the Wyckoff 8b sites.

calculations were performed to decompose the orbital interactions between atoms. As shown in Fig. 3(c), the positive and negative values of -COHP correspond to bonding and antibonding features, respectively. In the energy range from -15 to -5 eV, H-H bonds contribute the largest proportion of bonding states. The integrated COHP (ICOHP) below the Fermi level reveals that the -ICOHP value of H-H bonds is 1.09 eV/pair, which is much larger than those of Sc-H (0.07 eV/pair), Rb-Sc (0.27 eV/pair), and Rb-H (0.18 eV/pair) bonds, indicating that H-H covalent interactions dominate the bonding of the system. This suggests that hydrogen-derived electronic states may play an important role in electron-phonon coupling, which is consistent with the ELF results. Further Bader charge analysis (see Table S5 in the Supplemental Material [28]) reveals how the transferred electronic charge is distributed among different hydrogen sites. Sc atoms donate approximately one electron to the hydrogen framework, whereas Rb atoms donate about half an electron, indicating a much stronger ionic interaction between Sc and H. At 300 GPa, as the hydrogen content increases from $\text{RbSc}_2\text{H}_{16}$ to $\text{RbSc}_2\text{H}_{17}$, the H_3 (8b) site carries a

larger negative charge of $-0.25 e^-$, while H_2 (32e) decreases from -0.20 to $-0.09 e^-$, indicating electron redistribution within the hydrogen framework. In contrast, Rb primarily behaves as a typical alkali cation, making a relatively minor contribution. Overall, the combined ELF, COHP, and Bader analyses demonstrate that H-H interactions play a crucial role in bonding, stabilizing the crystal structure under pressure, and potentially influencing the superconducting properties of the system.

By calculating the electronic band structures and PDOS in the pressure range of 150–300 GPa, the evolution of the electronic structure can be clearly revealed. As shown in Fig. 4 and Fig. S10 in the Supplemental Material [28], all systems exhibit electronic states crossing the Fermi level, indicating pronounced metallic behavior. The Sc-3d orbitals dominate near the Fermi level, while the contribution of H-1s orbitals increases with higher hydrogen content, reflecting strong Sc-3d and H-1s hybridization, whereas the contribution from Rb remains negligible. Notably, a flat band is clearly observed along the Γ -L direction, which enhances the electronic occupation of Sc states near the Fermi level. At 150 GPa,

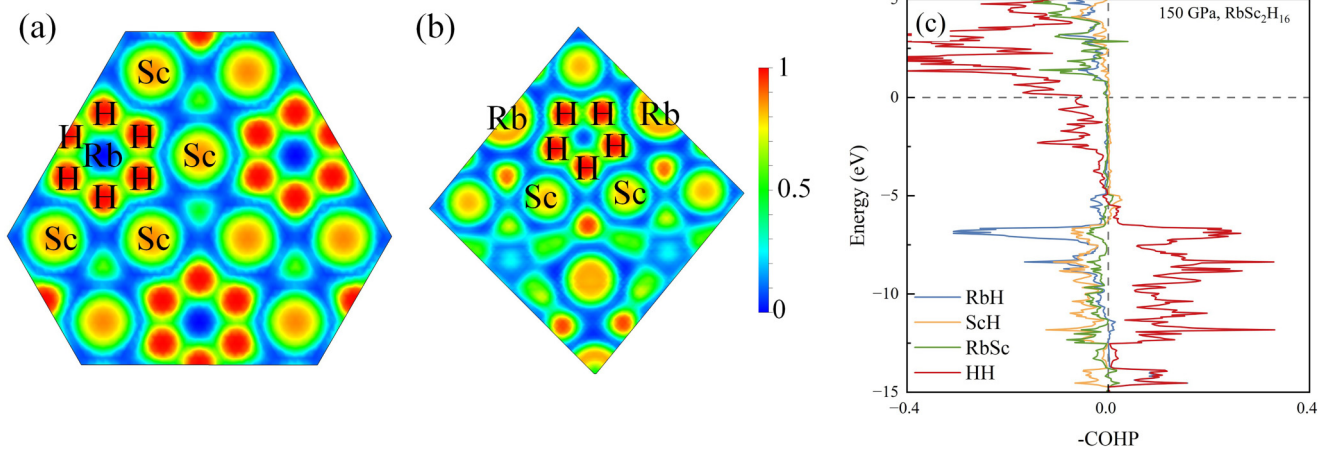


FIG. 3. Two-dimensional (2D) cross section of the ELF for $Fd\text{-}3m$ $\text{RbSc}_2\text{H}_{16}$ on the (a) (111) and (b) (-131) plane at 150 GPa. COHP distributions for (c) $\text{RbSc}_2\text{H}_{16}$ at 150 GPa. The inset in the top right corner presents the -ICOHP values at the Fermi level along with the corresponding bond lengths.

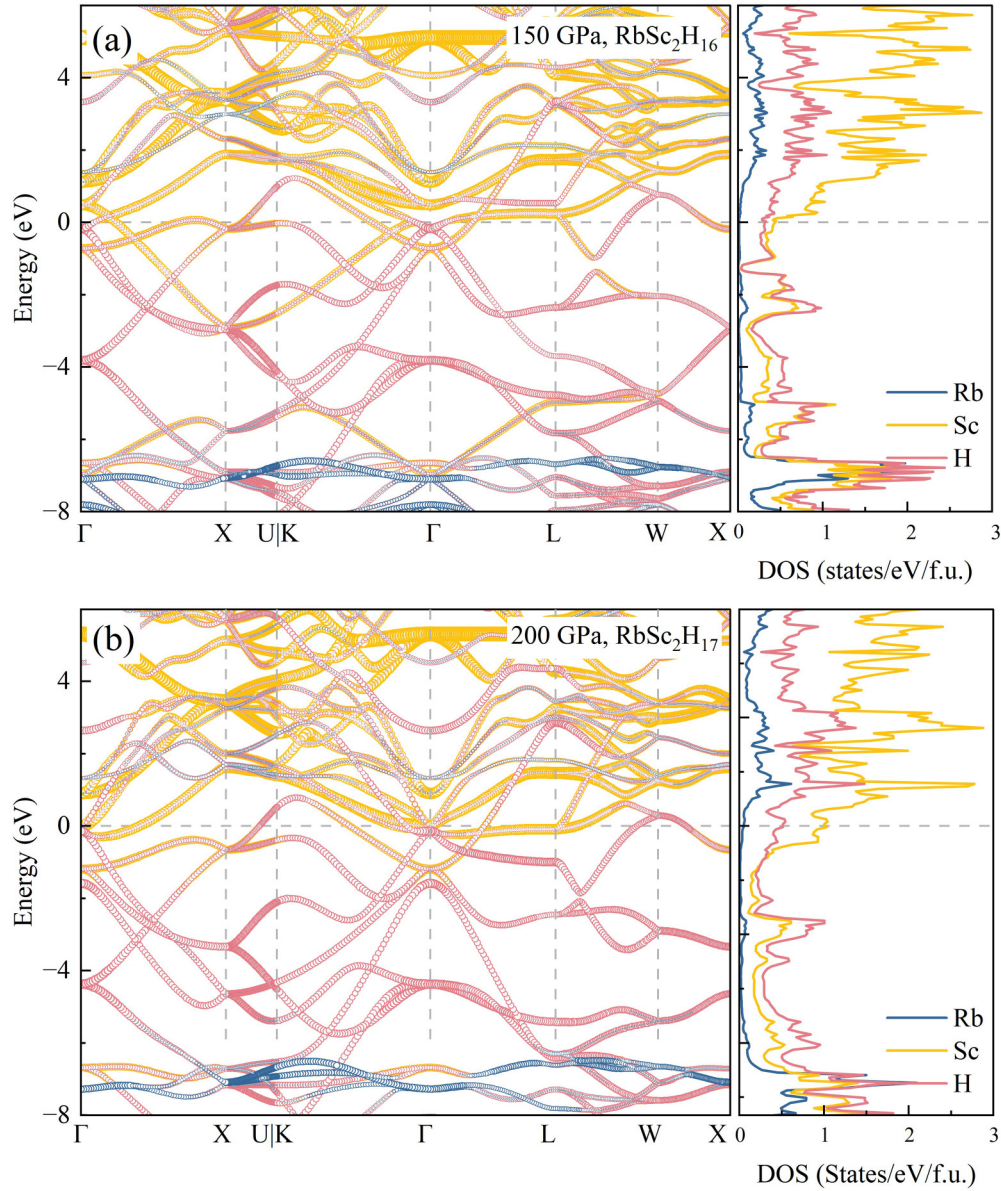


FIG. 4. Electronic band structures and atom-projected electronic density of states (PDOS) of (a) $\text{RbSc}_2\text{H}_{16}$ at 150 GPa and (b) $\text{RbSc}_2\text{H}_{17}$ at 200 GPa. The Fermi level is set at 0 eV, and the PDOS contributions from Rb, Sc, and H atoms are shown as blue, yellow, and red lines, respectively.

$\text{RbSc}_2\text{H}_{16}$ exhibits three band crossings near the Γ point, with a hydrogen PDOS at the Fermi level of approximately 0.31 states/eV/f.u. When the hydrogen content increases to $\text{RbSc}_2\text{H}_{17}$, the bottom of the conduction band pocket shifts down to the Fermi level, resulting in six band crossings and an increased hydrogen PDOS of about 0.51 states/eV/f.u. at 200 GPa. Meanwhile, the relative contribution of the H-1s orbit in the total density of states decreased from 41.5% in $\text{RbSc}_2\text{H}_{16}$ (150 GPa) to 27.6% in $\text{RbSc}_2\text{H}_{17}$ (200 GPa); this relative reduction arises primarily because the additional band crossings are predominantly Sc-3d in character, causing the total $N(E_F)$ to increase faster than the hydrogen-projected DOS. Nevertheless, the absolute DOS of hydrogen near the Fermi level increases substantially, which significantly enhances the hydrogen-derived EPC and thus favors an increase in the superconducting critical temperature T_c .

We systematically calculated the phonon spectra, PhDOS, Eliashberg spectral function $\alpha^2F(\omega)$, and frequency-dependent electron-phonon coupling integral $\lambda(\omega)$ of $\text{RbSc}_2\text{H}_{16}$, $\text{RbSc}_2\text{H}_{16.5}$, and $\text{RbSc}_2\text{H}_{17}$ under 150–300 GPa (see Fig. 5 and Figs. S11–S13 in the Supplemental Material [28]). No imaginary phonon frequencies were observed throughout the Brillouin zone, confirming their dynamical stability under high pressure. Across all pressures, the phonon spectra of these hydrides can be consistently divided into three regions, namely, low frequency (<15 THz), mid-frequency (15–30 THz), and high frequency (>30 THz). The low-frequency modes are dominated by Rb and Sc vibrations. Due to their heavier atomic masses, these modes contribute only weakly to λ . In contrast, the mid- and high-frequency regions are almost entirely derived from hydrogen vibrations. Owing to the light mass of H, these

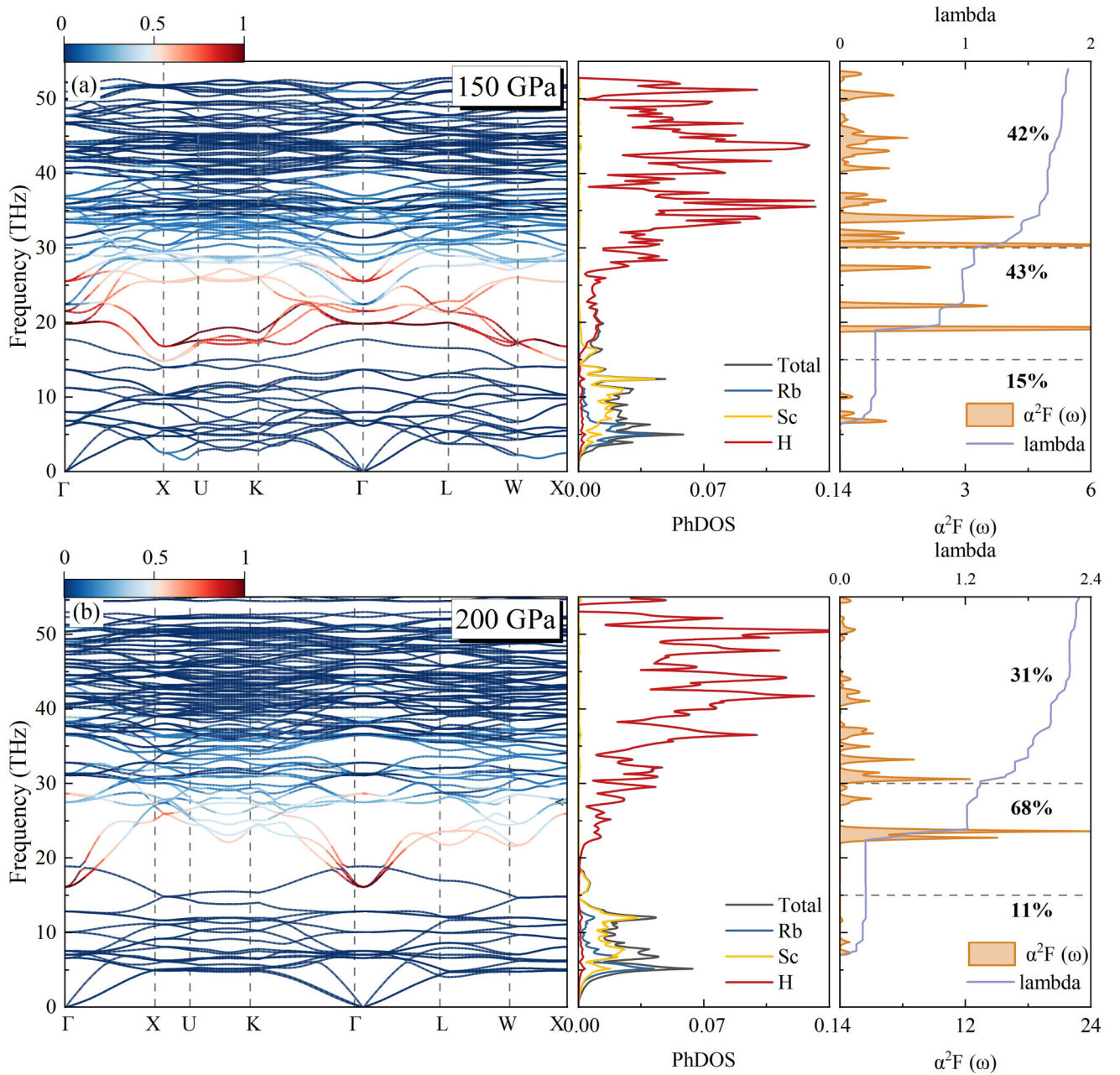


FIG. 5. Phonon dispersion (left), phonon density of states (PhDOS, middle), Eliashberg spectral function $\alpha^2F(\omega)$ and electron-phonon coupling parameter (λ , right) for (a) RbSc₂H₁₆ at 150 GPa and (b) RbSc₂H₁₇ at 200 GPa. The color scale indicates the phonon linewidth.

modes extend to higher frequencies and strongly couple to electronic states near the Fermi level, thus serving as the primary contributors to electron-phonon coupling. This trend is consistent with previous findings in prototypical hydrides such as LaH₁₀ and Li₂MgH₁₆ [9,19], further confirming the central role of H modes in the superconductivity of high-pressure hydrides. At 300 GPa, a comparison of the $\alpha^2F(\omega)$ functions of RbSc₂H_{16.5} and RbSc₂H₁₇ in Figs. S12 and S13 in the Supplemental Material [28] shows that, when the 8b site is not fully occupied, hydrogen vacancies disrupt the integrity of the Sc-centered hydrogen cages, thereby weakening the coupling between high-frequency hydrogen modes and electrons. In RbSc₂H_{16.5}, partial occupancy introduces hydrogen vacancies, weakening local H-H bonding

and their coupling to electronic states, thereby limiting the high-frequency contribution to λ to about 68%. In contrast, full occupancy in RbSc₂H₁₇ restores a dense hydrogen sublattice, enhances bonding rigidity and electron-phonon coupling, and increases the high-frequency contribution to 71%. These results demonstrate that 8b site occupancy provides a microscopic mechanism for tuning the frequency distribution of λ . The mode-resolved phonon linewidths were mapped onto the phonon spectrum, thereby indicating the contribution of each vibrational mode to the electron-phonon coupling. At 150 GPa, the λ value of RbSc₂H₁₆ arises predominantly from the mid- and high-frequency H modes (43% and 42%, respectively), while the low-frequency metallic modes contribute only $\sim 15\%$. This indicates that

TABLE I. Calculated EPC parameter (λ), logarithmic average phonon frequency $\omega_{\log}$ (K), electronic density of states at the Fermi level $N(E_F)$ (states/eV/f.u.), and superconducting critical temperature (T_c) of RbSc_2H_x under different pressures, with $\mu^* = 0.1$ and 0.13. For comparison, the corresponding data for $\text{Li}_2\text{NaH}_{17}$ and $\text{Li}_2\text{LaH}_{17}$ with the same $Fd-3m$ structure, as well as the recently reported $\text{LaSc}_2\text{H}_{24}$, are also included.

	P (GPa)	λ	$\omega_{\log}$ (K)	$N(E_F)$ (states/eV/f.u.)	T_c^{AD} (K), $\mu^* = 0.1$	T_c^{AD} (K), $\mu^* = 0.13$	Reference
$\text{RbSc}_2\text{H}_{16}$	150	1.81	1043	0.56	140	130	This work
	300	0.69	933	0.51	31.1	23.6	This work
$\text{RbSc}_2\text{H}_{17}$	200	2.30	1215	0.83	190.7	180	This work
	300	1.21	1128	0.78	102.2	90.8	This work
$\text{RbSc}_2\text{H}_{16.5}$	300	0.92	1294	0.62	78.66	66.1	This work
$\text{Li}_2\text{NaH}_{17}$	220	5.92	623	0.57	268	294	[24]
$\text{Li}_2\text{LaH}_{17}$	160	1.8	1274	0.34	156	142	[49]
$\text{LaSc}_2\text{H}_{24}$	300	3.34	968	1.27	329	–	[23]

although metallic atoms stabilize the lattice, their vibrational modes play a limited role in enhancing the coupling strength. With increased hydrogen content, $\text{RbSc}_2\text{H}_{17}$ at 200 GPa exhibits pronounced phonon softening, particularly in mid-frequency modes near the Γ point. This softening significantly increases the mid-frequency contribution to 68%, driving λ to rise sharply from 0.24 to 1.22, and consequently enhancing T_c . However, at 300 GPa, the phonon softening in $\text{RbSc}_2\text{H}_{17}$ is strongly suppressed. A phonon gap emerges in the mid-frequency region, causing $\alpha^2F(\omega)$ to vanish in this range. As a result, λ originates mainly from low-frequency metallic and high-frequency H modes, but the loss of mid-frequency contributions leads to an overall reduction in λ and T_c . This trend highlights that pressure not only stabilizes the lattice but also reshapes the phonon spectrum, thereby tuning the electron-phonon interaction strength. In summary, hydrogen vibrations consistently dominate the electron-phonon coupling across all pressures and structures, while phonon softening plays a critical role in enhancing λ and T_c at intermediate pressures. The suppression of softening at higher pressures reduces the coupling strength and superconducting performance. This “enhancement-suppression” dual effect is also observed in other hydrides, indicating a general feature of high-pressure superconductivity and providing valuable guidance for designing high- T_c materials [20,47,48].

We calculated the superconducting critical temperature (T_c) by solving the Allen-Dynes modified McMillan equation. Typically, the Coulomb pseudopotential μ^* is taken to lie in the range of 0.1–0.13. The T_c values obtained in this work, together with the relevant data for other reported ternary hydrogen-rich compounds such as $\text{Li}_2\text{NaH}_{17}$, $\text{Li}_2\text{LaH}_{17}$, and $\text{LaSc}_2\text{H}_{24}$, are summarized in Table I. At 150 GPa, $\text{RbSc}_2\text{H}_{16}$ exhibits strong electron-phonon coupling ($\lambda = 1.81$) combined with a high logarithmic average phonon frequency ($\omega_{\log} = 1043$ K), resulting in a superconducting critical temperature (T_c) of approximately 130–140 K. This indicates that, at relatively low pressure, the $\text{RbSc}_2\text{H}_{16}$ can simultaneously sustain strong electron-phonon interactions and high lattice vibrational energy, thereby ensuring favorable superconducting properties. However, as pressure increases to 300 GPa, the λ value of $\text{RbSc}_2\text{H}_{16}$ decreases significantly to 0.69, leading to a sharp reduction in T_c to ~ 31 K. This behavior reflects the fact that lattice com-

pression at high pressure suppresses the effective coupling between electrons and phonons, thereby weakening superconductivity. In contrast, the fully hydrogen-occupied $\text{RbSc}_2\text{H}_{17}$ already demonstrates superior superconducting properties at 200 GPa, with a T_c as high as 190.7 K ($\lambda = 2.3$). The incorporation of additional hydrogen atoms increases the electronic density of states at the Fermi level while simultaneously enhancing the phonon modes associated with H-H vibrations, thus reinforcing the electron-phonon coupling. As a result, $\text{RbSc}_2\text{H}_{17}$ maintains relatively higher T_c values over a broader pressure range, clearly demonstrating its superior robustness against pressure-induced suppression. Even at 300 GPa, $\text{RbSc}_2\text{H}_{17}$ sustains a T_c of ~ 102 K, far exceeding that of $\text{RbSc}_2\text{H}_{16}$, underscoring the critical role of hydrogen content in stabilizing high-temperature superconductivity. Interestingly, the intermediate hydrogen-vacancy phase $\text{RbSc}_2\text{H}_{16.5}$ exhibits T_c values between those of $\text{RbSc}_2\text{H}_{16}$ and $\text{RbSc}_2\text{H}_{17}$ (approximately 78–66 K) at 300 GPa. This result suggests that the introduction of hydrogen vacancies weakens electron-phonon interactions by reducing the λ value. Nevertheless, the local lattice distortions associated with vacancies also promote contributions from certain high-frequency phonon modes, enabling the system to sustain a moderate T_c . Overall, the comparison of $\text{RbSc}_2\text{H}_{16}$, $\text{RbSc}_2\text{H}_{16.5}$, and $\text{RbSc}_2\text{H}_{17}$ indicates that hydrogen content and occupancy significantly influence the superconducting behavior. The $\text{RbSc}_2\text{H}_{16}$ exhibits promising superconductivity at low pressure but experiences a rapid decline under compression. The $\text{RbSc}_2\text{H}_{17}$ remains robust, with high T_c values, even at high pressures. The intermediate $\text{RbSc}_2\text{H}_{16.5}$ lies between the two, reflecting the subtle and complex influence of hydrogen vacancies. These findings provide valuable insights into the intrinsic relationship between hydrogen content, lattice dynamics, and superconducting properties in hydrogen-rich hydrides.

IV. CONCLUSION

In summary, the RbSc_2H_x ternary system exhibits excellent potential for achieving high-temperature superconductivity at moderate pressures. Structural predictions reveal that $\text{RbSc}_2\text{H}_{16}$ and $\text{RbSc}_2\text{H}_{17}$ crystallize in a cubic $Fd-3m$ symmetry with hydrogen-based cage frameworks. Effective charge transfer from Rb and Sc to the hydrogen network,

together with strong H-H covalent bonding, endows these frameworks with excellent stability and provides a basis for superconductivity. $\text{RbSc}_2\text{H}_{16}$ has a T_c of 140 K at 150 GPa, while $\text{RbSc}_2\text{H}_{17}$ reaches 190.7 K at 200 GPa and maintains significant superconductivity even at 300 GPa. Further analysis shows that the variation in T_c is mainly determined by hydrogen-derived vibrational modes. In the $\text{RbSc}_2\text{H}_{17}$ phase, pronounced mid-frequency phonon softening occurs at 200 GPa, enhancing electron-phonon coupling and increasing T_c . However, at 300 GPa, this softening is suppressed and accompanied by a phonon gap, leading to a decrease in T_c . These results demonstrate that even in structurally similar hydrogen cage frameworks,

hydrogen occupancy can significantly modulate phonon dynamics and superconducting behavior, providing a physical strategy for designing high-pressure ternary hydride superconductors.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [50].

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