

Metastability and high- T_c superconductivity in A15-type ternary hydride YSbH₆ at moderate pressure

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(Received 22 December 2025; accepted 18 February 2026; published 23 March 2026)

The discovery of high-temperature superconductors remains a central challenge in materials science. Hydrogen-rich compounds are among the most promising candidates, as they can exhibit phonon-mediated superconductivity at elevated critical temperatures, though their stabilization typically requires extreme pressures. Here, we report the identification of YSbH₆ as a promising superconductor by a multistage high-throughput screening on ternary A15-type hydrides, followed by a high-throughput computational search of the Y-Sb-H system, accelerated by ephemeral data derived potentials. The cubic $Pm\bar{3}$ YSbH₆ phase exhibits a predicted critical temperature of 118 K at 50 GPa, among the highest T_c reported to date for an A15 hydride at this pressure. Thermodynamic analysis shows that YSbH₆ lies ~ 100 meV/atom above the convex hull at 50 GPa, but only 26 meV/atom above the hull at 120 GPa, suggesting possible metastability and synthesis at similar high-pressure conditions. The phase is dynamically stable over a wide pressure range (20–120 GPa), displays kinetic stability at 50 GPa, and elastic stability at 20 and 50 GPa, key ingredients for long-lived metastable behavior at moderate pressures. These results highlight YSbH₆ as a benchmark case illustrating the balance between high- T_c performance and limited thermodynamic stability in ternary hydrides, and underscore the importance of combined dynamic, thermodynamic, kinetic, and elastic stability analyses for guiding experimental synthesis of metastable superconductors.

DOI: [10.1103/9f4v-4bvs](https://doi.org/10.1103/9f4v-4bvs)

I. INTRODUCTION

The quest for room-temperature superconductors has driven intense theoretical and experimental efforts, motivated by their transformative potential for energy transmission, magnetic technologies, and quantum devices. Among the most promising candidates are hydrogen-rich materials, which, under high pressure, can exhibit phonon-mediated superconductivity with high critical temperatures (T_c), even approaching room temperature, such as in LaH₁₀ with a T_c of 250–260 K [1,2]. First-principles calculations have played a central role in these discoveries, accurately predicting several compounds later confirmed experimentally [3–8].

However, their practical use is constrained by the high pressures required to stabilize them, which can often exceed 200 GPa. This limitation has directed the focus of the search to ternary hydrides with stabilization pressures within the megabar range (below 100 GPa) [7,9,10]. Indeed, superconducting ternary hydrides that are thermodynamically stable at high pressures could remain metastable at a lower pressure, and could potentially be quenched to ambient pressure. Di Cataldo *et al.* identified LaBH₈ as a high- T_c superconductor

thermodynamically stable at pressures above one megabar (100 GPa), and dynamically stable down to 40 GPa [7]. Liang *et al.* likewise predicted LaBH₈ [11] to be a promising system. Similarly, Zhang *et al.* predicted the $Fm\bar{3}m$ phase of LaBeH₈, characterized by a fluorite-type H-Be alloy backbone, to be metastable and superconducting with a T_c of 191 K at 50 GPa. Later work resulted in the successful experimental synthesis of LaBeH₈ at 110 GPa, which remained metastable down to 80 GPa [12]. Recently, two independent studies predicted Mg₂IrH₆ would exhibit a superconducting transition temperature in the 80–160 K range [9,10]. Dolui *et al.* reported that the compound was metastable at ambient pressure and proposed a synthesis pathway *via* Mg₂IrH₇. This latter phase is thermodynamically stable above 15 GPa, and becomes thermodynamically unfavorable compared to the superconducting Mg₂IrH₆ phase at ambient pressure. However, attempts to synthesize this structure have so far been unsuccessful, with the disordered Mg₂IrH₅ phase being formed instead. Mg₂IrH₅ is isostructural with Mg₂IrH₆ but has a 5/6 site occupancy for hydrogen [13].

Quenching has been achieved for a ternary hydride Y₃Fe₄H₂₀, which was synthesized at 80 GPa from a Laves phase hydride YFe₂H₇, and recovered at ambient pressure and in ambient air for a few hours [14,15]. However, this success did not translate to superconductivity at ambient pressure, and other predicted metastable structures have not been successful [13]. It is considerably more challenging to predict materials that both feature a superconducting transition and that are possible to fabricate and quench to ambient pressure.

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Recent years have seen remarkable progress in the search for hydrogen-rich superconductors, including ternary hydrides that range from perovskite-like to A15-derived frameworks [16–20], which are suggested to combine high- T_c behavior with potentially reduced stabilization pressures, in some cases down to ambient pressure for perovskites [21–27]. However, although many of the theoretically reported phases are dynamically stable, their thermodynamic and kinetic stability remains to be confirmed [21,22,28–35]. This raises an open question about the likelihood of experimental realization of these predicted superconductors. As highlighted in Ref. [36], dynamic stability alone is an insufficient criteria to guide synthesis; a robust assessment of thermodynamic and kinetic stability is equally crucial.

Thermodynamic stability corresponds to the system having the lowest Gibbs free energy among all the species existing in the same convex hull (products and reactants) at a given pressure and temperature. It can be evaluated via the Maxwell construction, which measures the distance from the convex hull in free energy-composition space [37]. Structures lying on the hull are thermodynamically stable, whereas those slightly above it may be metastable if they also satisfy dynamic and kinetic criteria. Dynamic stability can be inferred from phonon dispersions and requires the absence of imaginary phonon modes, ensuring that the structure is robust against infinitesimal atomic displacements. Kinetic stability, in contrast, reflects resistance to large-scale structural transformations (e.g., lattice distortions or reconstructive phase transitions), typically governed by activation barriers at finite temperature, which can trap metastable states over long timescales. Elastic stability, as determined by the Born stability criteria [38] derived from the elastic constants, is a key yet often overlooked assessment criterion. It reflects a material's response to infinitesimal strains and constitutes a necessary, though not sufficient, condition for mechanical stability under finite stresses. Together, these four criteria determine the likelihood that a theoretically predicted compound can be synthesized and persist experimentally.

Since metastable states vastly outnumber thermodynamically stable ones, a large pool of energetically plausible metastable high- T_c hydrides can be expected. However, only a fraction of these may be experimentally accessible. Incorporating synthetic feasibility into predictive frameworks could therefore significantly improve the realization of theoretically promising candidates. Recent advances in *ab initio* structure prediction, accelerated by machine learning, now enable systematic exploration of vast chemical and structural spaces [9,39]. This perspective is especially relevant for A15-structure hydrides, which have been highlighted as promising candidates for high-temperature superconductivity [21,22,40–45]. A15 phases are A_3B compounds adopting the cubic $Pm\bar{3}n$ space group, where A is typically a transition metal and B any other element. Previous studies have predicted several A15 hydrides with theoretically favorable superconducting properties, yet none were found thermodynamically stable at moderate pressures around 50 GPa.

In this work, we combine *ab initio* calculations with machine-learning-accelerated chemical exploration to search for high- T_c hydrides in the A15 framework. We focused our search at a moderate pressure of 50 GPa, since pressures

below one megabar are experimentally more accessible. Compared to experiments at higher pressures, a larger culet size can be used in the diamond anvil cell, producing a larger sample that is easier to characterize *post mortem*. This pressure range also facilitates the use of pure H_2 as a hydrogen source, avoiding the impurities introduced by using ammonia borane. Moreover, moderate pressure synthesis can facilitate quenching at ambient pressure, as exemplified by $Y_3Fe_4H_{20}$ where the lowest stabilization pressure was around 60 GPa [15]. Therefore, the 50 GPa pressure range is a promising region to search for potential ambient metastable superconducting hydrides.

We identify $YSbH_6$ [$H_3(Y_{0.5}Sb_{0.5})A_3B$ binary], in a cubic phase ($Pm\bar{3}$), as a promising candidate with a predicted T_c of 118 K at 50 GPa. This phase lies 26 meV/atom above the convex hull at 120 GPa, suggesting possible metastability, though it becomes less favorable at lower pressure (108 meV/atom at 50 GPa). While not on the convex hull and thus not thermodynamically stable, the compound satisfies the dynamical stability criteria and illustrates how kinetic factors may enable the experimental synthesis of metastable hydrides. Indeed, for this level of theory, this distance from the hull is low, as exemplified by the case of anatase and rutile, two polymorphs of TiO_2 . These two phases are both observed experimentally, despite rutile being calculated (using the PBE exchange correlation functional) to be around 24 meV/atom in enthalpy above the anatase phase [46].

Furthermore, we apply an approach for more accurate T_c estimations on coarse electronic $\mathbf{k}$ grids, aiming to improve the reliability of superconductivity predictions in high-throughput studies [47–49]. As illustrated by the broad range of reported T_c values for Mg_2IrH_6 (80–160 K) [9,10], conventional methods remain highly sensitive to computational parameters. Our dual focus—accurate superconducting property prediction and rigorous stability assessment—addresses one of the key challenges in the discovery by high-throughput calculations of room-temperature superconductors at moderate pressures.

II. METHODS

We performed an *ab initio* prototype search at 50 GPa on A15- ABH_6 structures, where A and B were systematically selected from a large subset of the periodic table (see Supplemental Material for details [50]). We combined this constrained structure search with a multistage high-throughput screening to find promising high- T_c candidates. Using the method introduced in a previous study [9], structures that were nonmetallic, displayed magnetic instabilities, or were found to be dynamically unstable (at Γ) were removed from the search. The superconducting transition temperature of the remaining structures was then calculated and ranked. The highest estimated T_c was for $Pm\bar{3}$ - $YSbH_6$ (>100 K in the initial search), which motivated the present study and constitutes the main focus of this work.

After confirming dynamic stability at 50 GPa on $3 \times 3 \times 3$ phonon grids in the initial screening, we evaluated the dynamic stability of $YSbH_6$ as a function of applied pressure on finer grids to check for possible charge density wave instabilities. At each pressure, the phonon dispersion and density

of states were calculated using CASTEP, with a phonon grid of density $0.06 \times 2\pi \text{ \AA}^{-1}$ and an electronic grid of twice this density.

To evaluate the superconducting transition temperature T_c , we recalculated the phonons on the same $\mathbf{k}$ and $\mathbf{q}$ grids and obtained the electron-phonon matrix elements using the QUANTUM ESPRESSO code. The matrix elements were evaluated via interpolation onto a fine electronic $\mathbf{k}$ grid with a spacing of $0.015 \times 2\pi \text{ \AA}^{-1}$. We used the pseudo-dojo PBEsol ONCVSP potentials [51,52] with a kinetic energy cutoff of 100 Ry, to ensure that the total energy was converged to within 1 meV/atom. The T_c was then evaluated using both the Allen-Dynes and the isotropic Migdal-Eliashberg equations. A Coulomb pseudopotential of $\mu_{AD}^* = 0.125$ was used in the Allen-Dynes equation. For the Eliashberg equations, the Matsubara cutoff energy was set to 7000 meV, resulting in a Migdal-Eliashberg Coulomb pseudopotential of $\mu_{ME}^* = 0.227$. The T_c was calculated using both an in-house Eliashberg solver A2TC and the ISOME code [53]. A density of states rescaling factor was applied to the Eliashberg spectral function $\alpha^2 F(\omega)$ to accelerate the convergence of T_c [47–49].

To investigate the overall thermodynamic stability of $Pm\bar{3}$ YSbH₆, extensive structure searches on the Y-Sb-H ternary system were performed using ephemeral data derived potentials (EDDPs) [54,55]. These machine-learned interatomic potentials were used to accelerate exploration of the energy landscape, and were trained on DFT energies using the same method as in previous studies of the Mg-Ir-H and Lu-N-H systems [9,39]. We trained several EDDPs tailored for searches at either 50 or 120 GPa and used these to perform both AIRSS [37] and hot-AIRSS [56] at these pressures. The anneal was set to last 50 ps with a temperature range of 1000–2000 K. In total, over 400 000 structures were sampled in our calculations.

To generate the convex hull of all the structures predicted by EDDPs, we performed DFT geometry optimizations at 0 K on two collections of around 300 lowest energy structures found at 50 and 120 GPa respectively. For these well-converged calculations, we used a 900 eV plane-wave cutoff, a $\mathbf{k}$ -point spacing of $2\pi \times 0.02 \text{ \AA}^{-1}$, CASTEP C19 pseudopotentials, and the PBEsol exchange-correlation functional. We did not take anharmonicity into account in our calculations.

Further details on the results and elements used in the initial prototype screening, the T_c calculation parameters, the EDDPs training and structure searches, and convex hulls calculated at 50 GPa are reported in the Supplemental Material [50].

III. RESULTS

We searched for the highest T_c hydride within the A15 framework at moderate pressure of 50 GPa and investigated its synthesizability. In this work, we propose a high- T_c ternary hydride, YSbH₆, found at 108 meV/atom above the convex hull at 50 GPa, with an estimated $T_c = 118 \text{ K}$, as a promising candidate. The structure consists of a cubic $Pm\bar{3}$ lattice with $a = 3.6659 \text{ \AA}$ (see Fig. 1). The Y and Sb atoms occupy the $1a$ (0, 0, 0) and $1b$ (1/2, 1/2, 1/2) Wyckoff sites, respectively, and the hydrogen atoms occupy the $6g$ (0, 0.7425, 0.5) site, form-

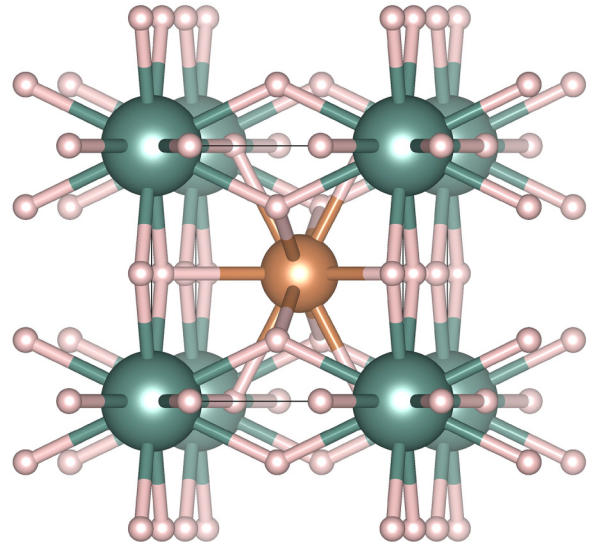


FIG. 1. The crystal structure of $Pm\bar{3}$ YSbH₆. Y, Sb, and H atoms are indicated as green, orange, and light pink spheres respectively. Y and Sb are surrounded by 12 hydrogen atoms forming a coordination system.

ing a polyhedron of 12 hydrogen atoms around Sb and Y (see Fig. 1). The metal-hydrogen distances are $d(\text{Sb-H}) = 2.07 \text{ \AA}$ and $d(\text{Y-H}) = 2.03 \text{ \AA}$ at 50 GPa. Although the phase remains above the hull at higher pressures, its formation enthalpy decreases to 26 meV/atom at 120 GPa, indicating possible metastability. We first combined *ab initio* calculations with exploration of chemical space accelerated by EDDPs to assess thermodynamic stability (Sec. III A) and to generate molecular dynamic simulations to evaluate the kinetic stability (Sec. III C) of YSbH₆. We then studied the dynamical stability of the structure with first-principles calculations and determined the lowest pressure at which the structure remains dynamically stable (Sec. III B). Elastic stability and chemical bonding are discussed in Secs. III D and III E. Finally, two possible synthesis routes are presented in Sec. III F.

A. Thermodynamic stability

We investigated the synthesizability of YSbH₆ by exploring the ternary Y-Sb-H phase diagram at pressures of 50 GPa and 120 GPa. We found that although this structure is not on the convex hull at either pressure, its enthalpy distance decreases with applied pressure. Figure 2 shows the resulting convex hull at 120 GPa, where YSbH₆ lies 26 meV/atom above the hull, upon decomposition into Sb, YH₄, and YH₇. This small enthalpy difference ($\approx 300 \text{ K}$ in thermal energy) suggests that the structure may be metastable in the megabar range. The convex hull for 50 GPa is given in the Supplemental Material [50], where the structure is found farther from the hull ($\approx 100 \text{ meV/atom}$).

Interestingly, no hydrogen-rich ternary compounds are found on the hull (see the list of structures in Supplemental Material [50]). The highest H/M ratio found in a ternary compound lying on the hull is $\text{H/M} = 4/3$ in Y₂SbH₄. Within our EDDP wide search of the Y-Sb-H system at 120 GPa, we identified 110 competing phases lying under 26 meV/atom

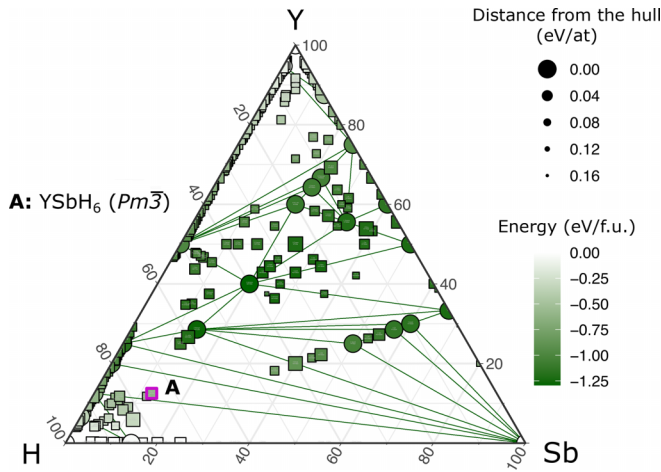


FIG. 2. Ternary convex hull at 120 GPa, calculated with the PBEsol functional. Dark green circles indicate the thermodynamically stable phases, solid lines are ridges connecting thermodynamically stable points. Metastable phases are shown as squares, their size is set according to the energy distance from the convex hull, the smaller the marker size the larger the distance from the convex hull. The convex hull displays 391 structures collected from different searches, with a total of 311 different compositions. Structures shown on the plot have been relaxed with DFT and showcase an energy distance from the hull $E_h \leq 169$ meV/at. Structures are color-coded according to their formation enthalpy (eV/f.u.) relative to Y, Sb and H elements. At 120 GPa, YSbH₆ is 26 meV/at from the hull and is indicated by a purple square. The list of all stable structures at 120 GPa is provided in the Supplemental Material (Table ST4) along with the convex hull at 50 GPa (Fig. S4 and ST5) [50].

off the convex hull. Among them, 26 are ternary phases, highlighting the complexity of the Y-Sb-H chemical space.

Our search at 50 and 120 GPa are in good agreement with previous theoretical predictions and experimental observations of binary yttrium hydrides [57–60]. Cubic YH and YH₃ were found on the convex hull at 50 GPa. Additionally, I_4/mmm YH₄ and $C2/c$ YH₇ were also found lying on the convex hull. While $Im\bar{3}m$ YH₆ was previously predicted to be on the hull by taking into account zero-point energy (ZPE) and experimentally observed above 100 GPa, the latter was found in our search only 11 meV/at above the convex hull at 120 GPa. Sb hydrides are not found on the hull at 120 GPa as predicted by Abe *et al.* study in which SbH₃ is stabilized at 150 GPa [61]. In particular SbH₃ is 18 meV/at off the hull at 120 GPa, SbH, and SbH₂ are respectively 38 and 21 meV/at from it. These results highlight the efficiency of using EDDPs to rapidly, thoroughly and reliably probe chemical spaces. Built on these results, YSbH₆ with a distance of 26 meV above the hull could potentially be synthesized if dynamic, kinetic and elastic stability are confirmed, which we assessed in the following sections.

B. Dynamic stability and T_c calculations

The phonon and electron-phonon properties of $Pm\bar{3}$ YSbH₆ were calculated for pressures from 0 to 120 GPa. The phonon dispersion relation and density of states are shown in Fig. 3. The phonon frequencies soften as the pressure

TABLE I. Table of the calculated λ and T_c using the PBEsol exchange-correlation functional. AD is the Allen-Dynes equation. Both A2TC and ISOME solve the isotropic Eliashberg equations, in either the constant density of states (cDOS) or variable density of states (vDOS) approximation [53].

Pressure (GPa)	λ	AD (K)	A2TC cDOS (K)	ISOME	
				cDOS (K)	vDOS (K)
20	3.44	86	132	130	114
30	2.21	114	136	134	120
40	1.95	108	130	130	118
45	2.07	116	143	143	119
50	1.95	110	135	134	118

is lowered, and the structure becomes dynamically unstable below approximately 20 GPa, as evidenced by the imaginary (negative) frequencies seen in the 10 GPa results. As this softening can lead to very large electron-phonon coupling strengths (λ), which can point to a charge density wave instead of superconductivity, we calculated T_c at the lowest dynamically stable pressure (20 GPa) and further from the structural transition (50 GPa). Using the PBEsol exchange-correlation functional, the calculated T_c at 50 GPa ranged from 110–135 K, depending on the exact method used. A summary of the obtained values is given in Table I. A slightly higher T_c was observed for the same pressure if instead the PBE functional was used (135–166 K). This enhancement is in part due to a slightly higher density of states at the Fermi energy and consequently a higher electron-phonon coupling strength of $\lambda = 2.34$ at 50 GPa. In this work, we have used the PBEsol exchange-correlation functional unless otherwise stated, as it was specifically revised to be more accurate than PBE for structural properties of bulk solids [62].

An accurate evaluation of T_c for this structure is complicated by the sharp features in the electronic density of states (DOS). Figure 4 shows the electronic band structure together with the total and projected DOS. The flat bands visible along part of the X-M and X-R high-symmetry paths in Fig. 4(a) are likely responsible for the van Hove singularity at the Fermi energy seen in Fig. 4(b). This peak in the density of states is partly responsible for the large electron phonon coupling strength, and consequently the high T_c of this structure. Such a sharply varying DOS near the Fermi energy presents a challenge when using the constant density of states (cDOS) Eliashberg equations. These equations assume that the DOS is constant and fixed to the value at the Fermi level, denoted N_F . Consequently, this method tends to overestimate T_c in systems with a peak at the Fermi level. In comparison, the variable density of states (vDOS) approach is able to account for the lower DOS away from the Fermi energy [53,63], resulting in a lower predicted T_c for this system. Therefore, we consider the vDOS values reported in Table I to be the most reliable estimates of T_c for this system. The T_c at 50 GPa is hence predicted to be 118 K.

Additionally, since the cDOS T_c is highly sensitive to the value of N_F , small shifts in the Fermi level can lead to large changes in the evaluated transition temperature. These shifts can be achieved by chemical doping or by changes in

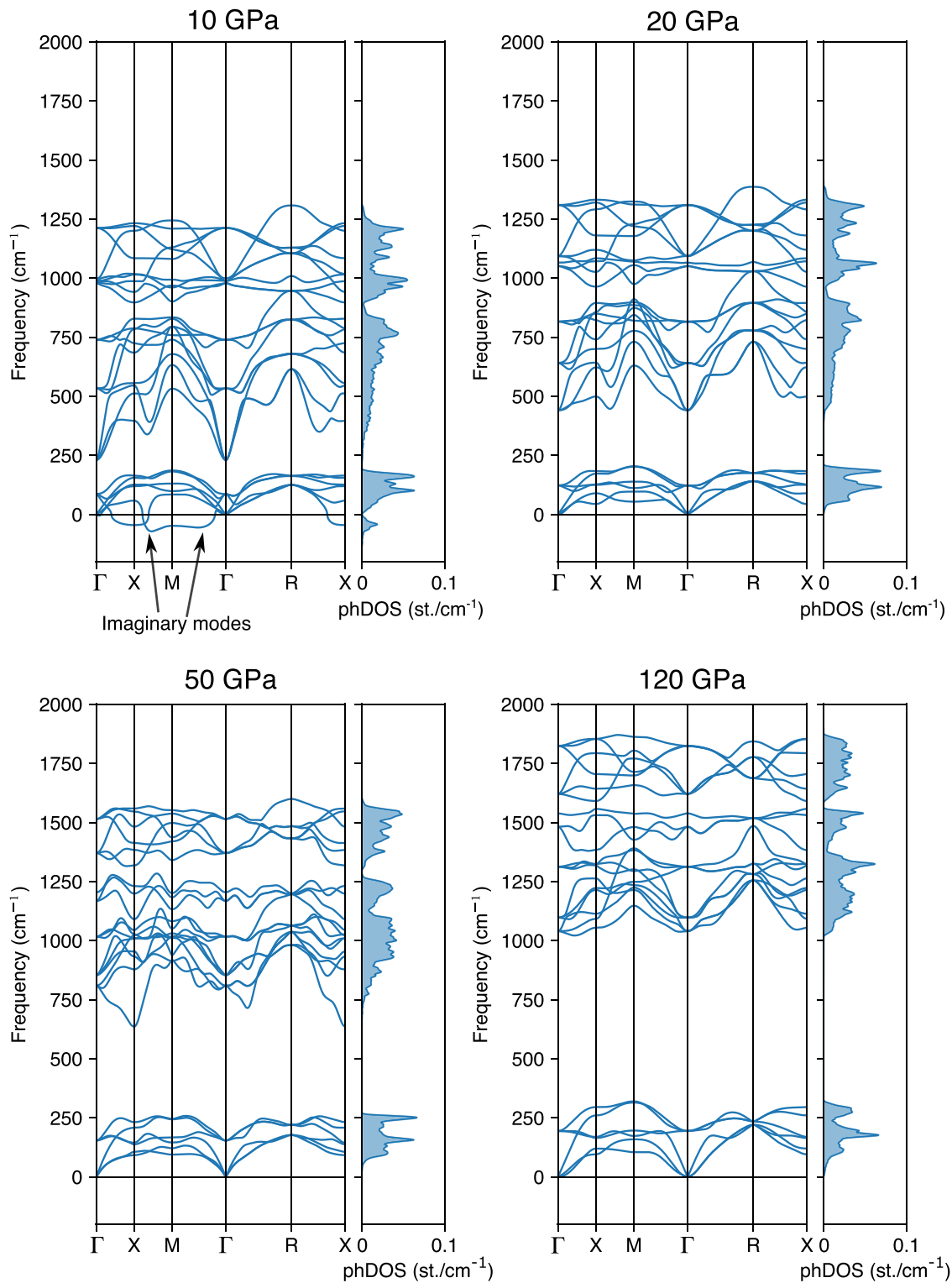


FIG. 3. The left panels show the phonon dispersion along a high symmetry path in the Brillouin zone, for different pressures from 10 to 120 GPa. The $Pm\bar{3}$ YSbH₆ structure is dynamically unstable at 10 GPa inferred by the presence of imaginary mode, but is stable above 20 GPa pressure. The right panels show the corresponding phonon density of states (phDOS).

the applied pressure. Although the Fermi energy at 50 GPa already lies close to the peak in the DOS, lowering the pressure to 45 GPa increases the N_F value to 1.90 states/eV/cell. As expected, this directly corresponds to a maximum in the cDOS T_c of 143 K. However, in comparison the vDOS esti-

mate is significantly less sensitive to the exact peak position. If the vDOS prediction is more accurate, it suggests T_c is actually largely insensitive to the pressure tuning, contrary to what might be inferred from the cDOS results alone. A plot of the density of states at different pressures, and the

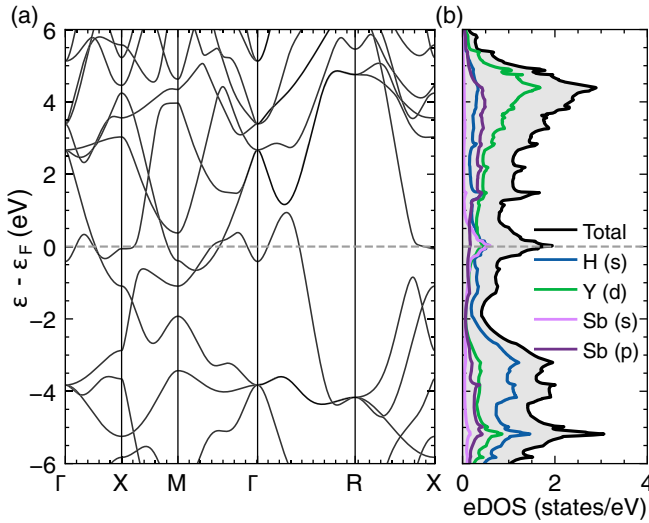


FIG. 4. (a) Electronic band structure of $Pm\bar{3}$ YSbH₆ at 50 GPa. (b) The total electron density of states (eDOS) projected onto hydrogen-1s (blue), yttrium-4d (green), and antimony-5s (pink), and antimony-5p (purple). H (s), Y (d), Sb (s), and Sb (p) orbitals all make contributions to the peak in the density of states at the Fermi energy. Black dashed line indicates the Fermi level.

superconducting gap parameter as a function of temperature are shown in Sec. 2 of the Supplemental Material [50].

Finally, a detailed inspection of the interpolated phonon frequencies around the Γ point for the 120 GPa structure appeared to show a very small imaginary mode at $\mathbf{q} = (0, 0, 0.1)$. We reevaluated this mode with DFPT using both the standard $10 \times 10 \times 10$ and a denser $20 \times 20 \times 20$ electronic grid. The coarser grid yielded only positive frequencies, but the finer grid produced a single imaginary mode of frequency 11 cm^{-1} . This mode corresponds to a slight distortion involving a shearing motion and a rotation of a hydrogen pair, which breaks the cubic symmetry. The distortion yields a monoclinic structure ($P2_1/m$ space group) with $\beta = 91.9^\circ$ and lattice parameters $a = 3.431 \text{ \AA}$, $b = 3.440 \text{ \AA}$, and $c = 3.474 \text{ \AA}$ at 120 GPa. Enthalpy calculations indicate the distorted structure is $<1 \text{ meV/atom}$ lower in enthalpy than the cubic structure. ZPE calculations using PHONOPY [64] on a $3 \times 3 \times 3$ phonon grid show the two structures have nearly identical zero-point energies (171 meV/atom for the cubic and 170 meV/atom for the distorted), again suggesting very little energetic difference between them. As the pressure is lowered, the distorted structure remains slightly energetically favorable, but the magnitude of the distortion decreases and the structure tends towards the cubic phase. The electron-phonon coupling strength in the distorted structure is lower, with $\lambda = 1.56$ at 50 GPa, but the corresponding vDOS critical temperature remains high at around 110 K (see Sec. 2 of Supplemental Material for further details [50]).

C. Kinetic stability

We performed molecular dynamic simulations using ED-DPs on a $Pm\bar{3}$ YSbH₆ compound at 120 GPa and 50 GPa at 300 K to investigate the kinetic stability, as was done in Ref. [9]. There is very little diffusion at 300 K at both

pressures on a long trajectory of 0.5 ns and the hydrogen polyhedra at both 50 GPa and 120 GPa remained intact up to at least 700 K (see Supplemental Material Sec. 6 [50]). This indicates the cubic YSbH₆ possesses a high degree of kinetic stability and could thus be metastable and potentially synthesized at high pressure. At 50 GPa there is very little diffusion, so we can expect the structure to persist after quenching from 120 to 50 GPa.

D. Elastic stability

The elasticity of a lattice is described by its matrix of second-order elastic constants:

$$C_{ij} = \frac{1}{V_0} \frac{\partial^2 E}{\partial \epsilon_i \partial \epsilon_j}, \quad (1)$$

where E is the energy of the crystal, V_0 its equilibrium volume, and ϵ_i denotes a strain in Voigt notation. C_{ij} is referred to as the stiffness constants, and is a symmetric matrix of dimensions 6×6 .

The Born elastic stability criteria [38,65] for elastic stability are satisfied if, for a cubic structure,

$$C_{11} - C_{12} > 0, \quad C_{11} + 2C_{12} > 0, \quad \& \quad C_{44} > 0. \quad (2)$$

We evaluated the elastic stability of the $Pm\bar{3}$ YSbH₆ structure by calculating the elastic constants C_{ij} at different pressures. The cubic phase has a positive C_{44} elastic constant at 20 and 50 GPa, and fulfills the first two conditions of Eq. (2), yielding the elastic stability of $Pm\bar{3}$ YSbH₆ at these moderate pressures (see Sec. 2 in the Supplemental Material [50]). However, the phase is elastically unstable at high pressure with a negative C_{44} elastic constant at 120 GPa, which is consistent with the slight phonon instability observed in Sec. III B.

E. Chemical bond analysis

To gain insight into the chemical bonding of the new A15-type YSbH₆, we computed the electron localization functions (ELF) as illustrated in Fig. S9, and performed the topological analysis of the electron density (Sec. 7.2 in the Supplemental Material [50]) [66]. Further details on the bonding analysis are reported in Sec. S7 of the Supplemental Material [50]. The ELF surrounding hydrogen appears elongated towards Sb, hinting for the presence of a Sb-H interaction as seen for AXH₆ in Ref. [21].

The shortest H-H contact measures $1.76 \text{ \AA}$ at 50 GPa and $1.65 \text{ \AA}$ at 120 GPa, corresponding to the two hydrogen atoms bridging two yttrium atoms. The remaining H-H contacts are much longer, spanning from $1.90 \text{ \AA}$ to $2.25 \text{ \AA}$ at 50 GPa. These distances exclude both the presence of molecular H₂ units, and of an extended hydrogen framework. The Bader analysis shows a mild charge transfer from Y and Sb to H (-0.35 e), and QTAIM descriptors reveal that the H-Y bonds and the H-Sb bonds are the strongest, resembling a typical metal-ligand type of interaction. The topological analysis of the electron density revealed that a very weak interaction exists only between the closest hydrogen atoms (corresponding to the $1.76 \text{ \AA}$ contact at 50 GPa). However, no other H-H connection was found. This additional aspect confirmed the absence of an extended, clathrate-like, hydrogen network. We

therefore classify YSbH_6 as a coordination system, where Y and Sb act as metal center, and H as ligand.

F. Possible synthesis routes

We now discuss the possible synthesis route to achieve $Pm\bar{3}$ YSbH_6 under megabar pressure in a diamond anvil cell. Experimentally, YSbH_6 could be synthesized via either compression of YSb powder in a hydrogen gas environment, like in Ref. [15]; or using YH_3 powder together with SbH_3 gas environment. According to our calculations, both synthesis routes have the potential to access the metastable YSbH_6 phase under pressure but requires tailored and rigorous high-pressure protocols. Further details on the proposed synthesis pathways are reported in Sec. 8 in the Supplemental Material [50]. The synthesized phase under pressure could then potentially be quenched to lower pressures, given the structure's dynamic, kinetic, and elastic stability at 20–50 GPa.

IV. DISCUSSION

Our results highlight both the promise and the challenges of stabilizing high- T_c superconductivity in ternary A15-type hydrides. Although $Pm\bar{3}$ YSbH_6 displays a high predicted T_c in the range 110–135 K at 50 GPa, its thermodynamic metastability relative to the convex hull ($E_h = 108$ meV/atom at 50 GPa and 26 meV/atom at 120 GPa) suggests that experimental synthesis may only be achievable above the megabar regime. Calculation of formation enthalpy does not take into account zero-point energy, which has been shown to impact the stability of some hydrides. These corrections could stabilize the compound in the same way as LaH_{10} and RbPH_3 [27,67].

The absence of ternary hydrides with high hydrogen content ($H/M \geq 3$) on the convex hull of the Y-Sb-H phase diagram highlights a general trend: hydrogen-rich ternaries are thermodynamically less favorable than their binary counterparts. Compared to the absent ternaries, several binary yttrium hydrides YH , YH_3 , YH_4 , and YH_7 all lie on the hull, and coincide with theoretical predictions and experimental observations at around 120 GPa [57–60]. Nevertheless, the dynamical stability of YSbH_6 down to 20 GPa, combined with molecular dynamics simulations that indicate kinetic resilience, is encouraging. A previous study explored various A and X elements in the AXH_6 structures in the pressure range of 50–400 GPa [21]. Wei *et al.* kept structures stable with respect to their decomposition into the binary hydrides and the single elements, and seems to have missed YSbH_6 as a promising compound.

The harmonic phonon calculations of the $Pm\bar{3}$ phase at 10 GPa reveal small phonon instabilities throughout X-M path on the Brillouin zone. Including ionic quantum fluctuations and anharmonicity within the stochastic self-consistent harmonic approximation (SSCHA) as shown for the perovskite RbPH_3 [27], the phase might be dynamically stabilized at 10 GPa or lower pressure.

The calculated superconducting transition temperatures show some variation between the different methods, ranging from 110 K with the Allen-Dynes up to 135 K with the constant DOS (cDOS) Eliashberg approach at 50 GPa. As

mentioned earlier, we expect the sharp peak in the DOS at the Fermi energy to cause an overestimation for the cDOS Eliashberg equations, since these instead assume the DOS is constant and fixed to the value at the Fermi level. As such, we suggest that the best estimate is instead given by the variable DOS value of 118 K, which happens to be very close to the Allen-Dynes prediction. A further source of uncertainty arises from the choice of Gaussian smearing width used in the evaluation of the spectral function $\alpha^2F(\omega)$. Although the rescaling procedure described in Ref. [47] eliminates much of this variation, a spread of about 20 K remains as the smearing is varied between 0.005 Ry–0.250 Ry. We report the T_c values obtained using a 0.025 Ry smearing, which provided the most conservative estimates of T_c . A further point of interest was the disparity between PBE and PBEsol functionals in the prediction of the critical temperature value. At 50 GPa, the superconducting temperature is predicted to be 135–166 K with PBE, about 25 K higher than the PBEsol results. We suggest that part of the difference in the predicted T_c values between the two functionals arises from the higher value of the density of states at the Fermi level (N_F). The value obtained for PBE was $N_F = 1.97$ states/eV/cell, while the PBEsol value was $N_F = 1.76$ states/eV/cell. This, combined with slightly softer phonons, resulted in a larger electron-phonon coupling of $\lambda = 2.34$ with the PBE functional. Regardless of the exact method used, all predictions of T_c remained above 100 K at 50 GPa, indicating that YSbH_6 is a promising candidate for high-temperature superconductivity at moderate pressures.

While EDDP-based molecular dynamics suggest kinetic stability, the predictive accuracy ultimately depends on the quality of the training dataset and would ideally be cross validated against direct first-principles molecular dynamics. However, thanks to the efficiency of machine-learning potentials, EDDPs enable simulations extending to hundreds of picoseconds, a timescale inaccessible to conventional *ab initio* molecular dynamics. Such cross validation, although desirable, remains prohibitively expensive computationally.

Overall, our findings emphasize the need for combined thermodynamic, dynamical, kinetic, and elastic assessments in the design of new superconductors. YSbH_6 stands as an instructive case where high- T_c coexists with thermodynamic metastability, underlining that synthesis feasibility rather than T_c alone should guide the prioritization of candidate compounds for experimental pursuit.

V. CONCLUSION

The work presented here, together with previous studies [9,39,55], demonstrate that the EDDPs allow exploration of ternary and higher-order systems by significantly accelerating structure prediction. This performance is obtained without the need for sophisticated (and computationally expensive) neural network architectures and relies solely on single-point DFT energy calculations for small simulation cells, rendering the approach both convenient and cost effective to train.

In summary, we have identified a metastable ternary hydride, YSbH_6 with A15 symmetry, as a promising high- T_c superconductor at moderate pressures. Using a recently proposed rescaling of the Eliashberg spectral function $\alpha^2F(\omega)$ to accelerate the convergence of the T_c calculation, we predict

a critical temperature of 118 K. A detailed assessment of dynamical, thermodynamic, kinetic, and elastic stability, supported by machine-learning potentials, indicates that YSbH₆ can likely be stabilized at 120 GPa and may persist as a metastable phase at lower pressures 20 and 50 GPa. These results establish YSbH₆ as a representative case that illustrates the balance between enhanced superconducting performance and limited thermodynamic stability in ternary hydrides, and they highlight the necessity of combining dynamical, thermodynamic, kinetic, and elastic stability analyses to guide experimental efforts toward metastable superconductors.

ACKNOWLEDGMENTS

We gratefully acknowledge Lewis Conway, Ryuhei Sato, and Francesco Belli for their discussions. We thank Tim Kamsma and William Galloway for their insightful comments on the manuscript. K.B. gratefully acknowledges support from the Engineering and Physical Sciences Research Council (Grant No. EP/W524633/1) through an EPSRC DTP

studentship in the Department of Materials Science and Metallurgy. This work was supported by the Advanced Institute for Materials Research at Tohoku University (M.C.), the Enterprise Science Fund, Intellectual Ventures (P.I.C.C. and C.J.P.), and Theoretical Condensed Matter Cambridge, Critical Mass Grant - Grant Ref: EP/V062654/1 (S.R.).

M.C., K.B., and C.J.P. conceptualized the work. M.C. performed the thermodynamic stability calculations, formation enthalpies, ELF and elastic constants calculations. C.J.P. performed the prototype structure search and screening. K.B. performed the dynamic stability, superconductivity, and ZPE calculations. S.R. performed the enthalpy calculations for the cubic and distorted phases, and the topological analysis of the electron density. P.I.C.C. performed the molecular dynamics and kinetic stability study. M.C. wrote the original draft, and all authors contributed to the manuscript.

DATA AVAILABILITY

The data that support the findings of this article are openly available [80].

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