

# Fundamental Limits on the Electron-Phonon Coupling and Superconducting $T_c$

Dmitrii V. Semenov,\* Boris L. Altshuler, and Emil A. Yuzbashyan\*

**Fundamental upper bounds on the electron-phonon interaction strength and superconducting transition temperature  $T_c$  in metals are established based on the intrinsic instability of the equilibrium between electrons and the crystal lattice under strong interaction. This instability explains why observed electron-phonon coupling constants are limited to  $\lambda \lesssim 4$ . The theory also accounts for the mechanism of metastable superconductivity with enhanced  $T_c$ , which emerges near the instability threshold. Based on theoretical analysis and comparison with experimental data, room-temperature phonon-mediated superconductivity is found to be feasible exclusively in hydrogen compounds.**

## 1. Introduction

The interaction of electrons with lattice vibrations (phonons) is at the heart of the theory of metals. It determines superconducting  $T_c$ , electrical and thermal conductivities, and many other physical properties.<sup>[1,2]</sup> Existing theoretical frameworks, such as the Bardeen-Cooper-Schiffer (BCS),<sup>[3]</sup> Migdal,<sup>[4]</sup> and Eliashberg<sup>[5]</sup> theories, provide no limits on the electron-phonon interaction and, as a result, on  $T_c$ . In this paper, we show that there are in fact intrinsic upper bounds on both these quantities dictated by the stability of the metal with respect to the electron-lattice interaction. We compare our results with experimental data and argue that room-temperature phonon-mediated superconductivity is entirely realistic but only in hydrogen-rich compounds.

The question, “What is the maximum possible superconducting  $T_c$ ?” has remained unanswered since the discovery of superconductivity by Onnes in 1911,<sup>[6]</sup> despite remarkable progress in this area.<sup>[7–14]</sup> At the same time, the  $T_c$  of real materials

never exceeded 133 K at atmospheric pressure and 160 K at elevated pressures ( $\sim 30$  GPa) in more than a hundred years (1911–2011) of experimental experience. It is believed that metallic hydrogen is a superconductor with one of the highest critical temperatures.<sup>[15,16]</sup> This is because  $T_c$  is proportional to lattice vibration frequencies, which are highest in this material since hydrogen is the lightest element. Unfortunately, producing metallic hydrogen requires pressures in excess of 450 GPa,<sup>[17,18]</sup> at the limit of reach of current experimental techniques for transport measurements.

There is, however, an ingenious solution – alloying hydrogen with other elements.<sup>[19]</sup> This provides an effective chemical pressure thus reducing the external pressure necessary to produce a stable metal.

And indeed, compressed polyhydrides became the leaders in the quest for the highest  $T_c$  since the discovery of record superconductivity in 2014 and 2018 in the cubic hydrides of sulfur ( $\text{H}_3\text{S}$ , max  $T_c = 200$  K) and lanthanum ( $\text{LaH}_{10}$ , max  $T_c = 250$  K). This “hydride revolution” gave rise to justified hopes of room-temperature superconductivity in the near future, see **Figure 1**. Moreover, several incorrect reports of  $T_c$  exceeding room temperature in the ternary systems C-S-H,<sup>[20,21]</sup> Y-Pd-H,<sup>[21]</sup> and Lu-N-H<sup>[22]</sup> emerged but were quickly refuted. At the present moment, the maximum well reproduced critical temperature is about  $T_c = 250$  K in  $\text{LaH}_{10}$ ,  $(\text{La}, \text{Y})\text{H}_{10}$ ,<sup>[23–25]</sup>  $(\text{La}, \text{Sc})\text{H}_{10}$ ,<sup>[26]</sup> and other ternary compounds containing lanthanum. At the same time, the question whether room-temperature superconductivity is attainable remains open.

Here we will approach this problem from a different perspective. Our recent studies within the Migdal-Eliashberg (ME) theory revealed that the metallic and superconducting states are unstable with respect to strong electron-phonon interaction.<sup>[27,28]</sup> A traditional measure of the strength of this interaction is the electron-phonon coupling constant  $\lambda$  defined as the sum of the couplings  $\lambda_k$  to the individual lattice vibration modes. This characterization of the interaction strength with a single number is not unique, and we introduce below another metric  $\xi$  – the *stability parameter* of the metal. It corresponds to the contribution of the electron-phonon interaction to the electronic specific heat and is also a sum of  $\lambda_k$  but with unequal weights.

Indeed, we will see that the dynamical stability of a metal requires  $\xi < \xi_* = 1$ . The metallic state ceases to be the global minimum of the free energy at a smaller value  $\xi_c < \xi_*$  via a first order phase transition and is no longer even a local minimum when  $\xi > \xi_*$ . For a fixed phonon spectrum,  $\lambda$  and  $\xi$  are directly

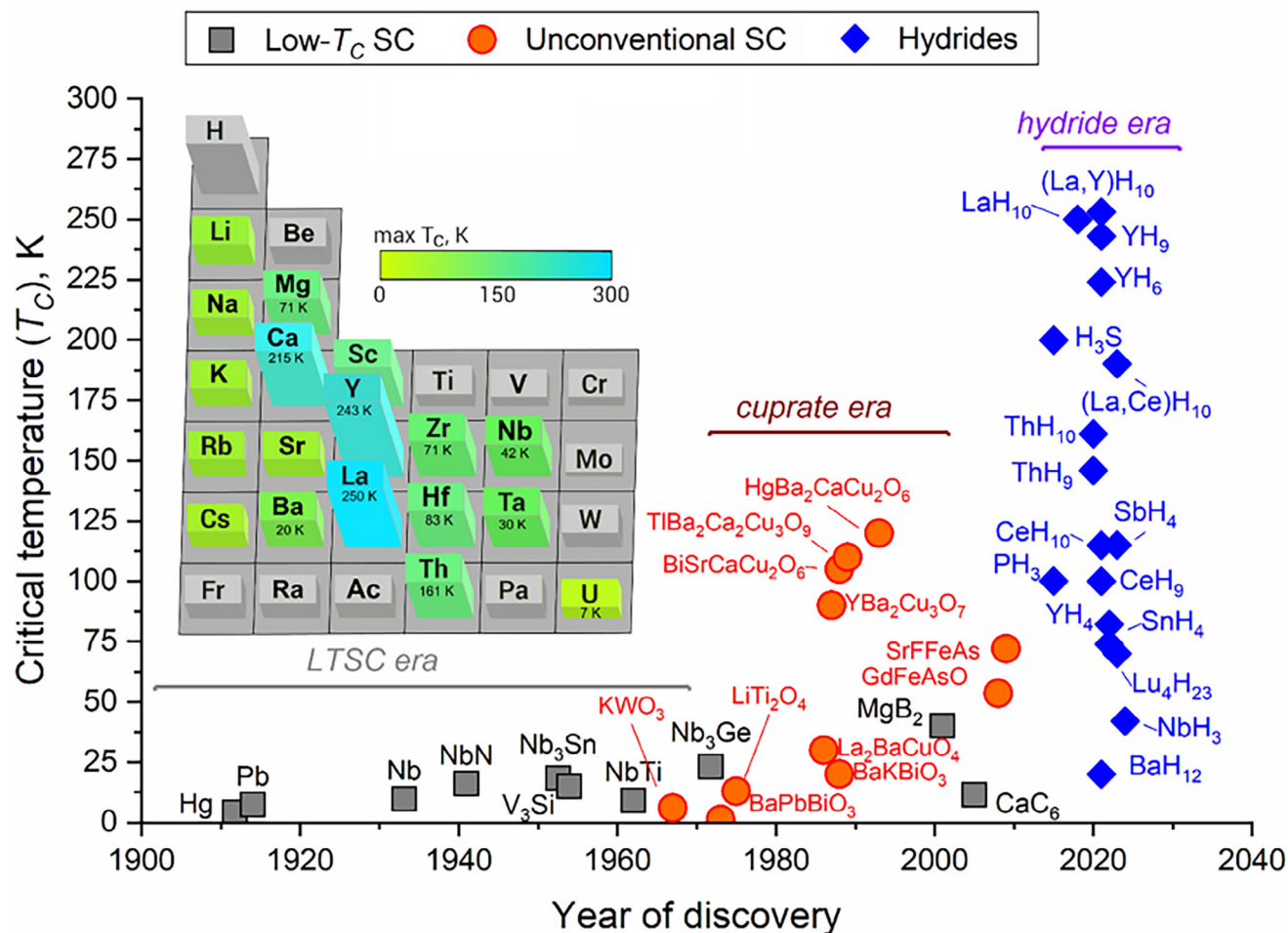
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**Figure 1.** The evolution of superconducting materials in 20th and 21st centuries as exemplified by metals, intermetallic alloys, and non-oxide ceramics (grey squares), which are well described by the BCS theory, unconventional superconductors (orange circles) and hydrides (blue rhombi). The inset shows the distribution of superconducting transition temperatures for the hydrides of various metals. Shown in grey are the metals whose polyhydrides have not been investigated for superconductivity.

proportional to each other, so that this condition translates into  $\lambda < \lambda_c < \lambda_*$ . The value of  $\lambda_*$  is smallest,  $\lambda_* = 3.69$ , for dispersionless (Einstein) phonons. When  $\lambda$  exceeds  $\lambda_c$  ( $\xi$  exceeds  $\xi_c < 1$ ), the crystal structure of the metal becomes unstable and is either destroyed or undergoes a reconstruction lowering the value of  $\lambda$  below  $\lambda_c$ . This result provides an effective tool to investigate the maximum transition temperature of electron-phonon superconductors thanks to an upper bound on  $T_c$  within the ME theory in terms of  $\lambda$  and the average square phonon frequency.<sup>[8,29]</sup>

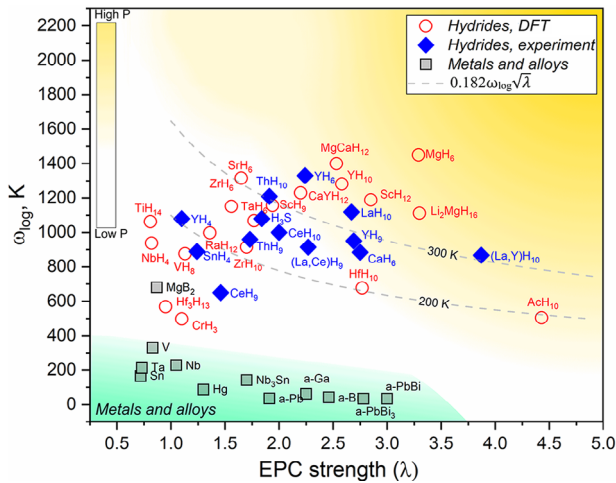
While our study explicitly addresses phonon-mediated superconductivity, the stability constraints we identified hinge fundamentally on the retarded nature of boson-mediated interactions. Retardation, quantified by the ratio of the characteristic bosonic frequency to the Fermi energy is crucial. Specifically, our theoretical results are most robust when this ratio is small, indicating substantial retardation. Our arguments remain valid even if the mediating bosonic field is effectively an order parameter constructed from fermions themselves. With this consideration, the conceptual approach presented should, in principle, be adaptable to cuprates and other unconventional super-

conductors, provided a well-defined model of boson-mediated pairing exists for these systems. However, significant modifications to our theoretical framework are necessary when characteristic bosonic frequencies become comparable to the fermionic bandwidth.

## 2. Analysis of Experimental Data

Presently, superconductors with highest critical temperatures are the polyhydrides. They also have some of the highest values of the electron-phonon interaction constant  $\lambda \sim 2 - 3$  and of the stability parameter  $\xi \sim 0.2 - 0.5$  (Table S1, Supporting Information). Interestingly, the values of  $\lambda$  for hydrides lie approximately within the same range as for soft superconducting metals Pb and Bi and their alloys, even though the critical temperatures are tens of times larger. This begs the question: Can the electron-phonon interaction be arbitrarily large or is it inherently bounded from above?

Hydride superconductors or superhydrides (Figures 2 and 3) can be synthesized only at high pressure  $P$ , about 100–200 GPa,



**Figure 2.** Distribution of superconducting materials in the  $\lambda - \omega_{\log}$  plane. a) Open red circles and filled blue rhombi show DFT (Density Functional Theory) predicted and experimentally synthesized hydrides, respectively. Filled grey squares correspond to simple metals, alloys, and  $\text{MgB}_2$ . Dashed grey lines are defined by the equation  $T_c^{\text{emp}} \equiv 0.182\omega_{\log}\sqrt{\lambda} = \text{const}$ , where  $T_c^{\text{emp}}$  is the empirical strong coupling estimate for  $T_c$ .<sup>[29]</sup>

in special diamond anvil cells. Subsequent lowering of the pressure leads to a domelike dependence of  $T_c$  on  $P$  characteristic of hydrides.<sup>[23,24,30–32]</sup> Increasing  $P$  does not lead to the destruction of the polyhydrides but is accompanied by an increase of phonon frequencies, decrease of the electron-phonon interaction strength, and, most importantly, decrease of  $T_c$ . An appropriate measure of the magnitude of phonon frequencies at these  $\lambda$ <sup>[29]</sup> is the average logarithmic frequency  $\omega_{\log}$  defined as  $\ln \omega_{\log} = \frac{1}{\lambda} \sum_k \lambda_k \ln \omega_k$ .

The situation seen when decreasing the pressure is almost the opposite – phonons soften, while  $\lambda$  and  $\xi$  grow (Figure 3b). It may seem that decreasing the pressure further and thus increasing  $\lambda$ , we can make  $T_c$  arbitrarily large, since  $T_c \propto \sqrt{\lambda}$  at large  $\lambda$  according to the ME theory.<sup>[29,33]</sup> In reality, this turns out to be impossible, since the growth of the electron-phonon interaction in hydrides inevitably leads to the distortion of the crystal structure, lowering of its symmetry, diffusion and partial loss of hydrogen, and, as a result, to an abrupt lowering of the superconducting  $T_c$  (Figure 3a). Good examples of this process are the decompression of  $\text{D}_3\text{S}$ ,<sup>[32,34]</sup>  $\text{LaH}_{10}$ ,<sup>[23]</sup>  $\text{YH}_9$ ,<sup>[30]</sup> and  $\text{CeH}_9$ <sup>[31]</sup> as well as recent studies of ternary lanthanum-cerium superhydrides  $(\text{La,Ce})\text{H}_{9-10}$ .<sup>[35,36]</sup>

### 3. Fundamental Limit on the Electron-Phonon Interaction Strength in Metals

When does a metal stop being a metal as the pull between conduction electrons and phonons increases? In a new study,<sup>[27]</sup> we discovered that the specific heat of conduction electrons ( $C_{\text{el}}$ ) turns negative when the electron-phonon coupling constant exceeds a certain threshold  $\lambda_*$ . The precise value of  $\lambda_*$  depends on the phonon spectrum and, in particular,  $\lambda_* = 3.69$  for Einstein phonons. Stability analysis of the kinetic equations<sup>[28]</sup> (Supporting Information) shows that when  $C_{\text{el}} < 0$ , the metal is unstable

with respect to an infinitesimal difference between the electron and phonon temperatures,  $T_{\text{el}}$  and  $T_{\text{ph}}$ , respectively. Specifically, if initially  $T_{\text{el}} > T_{\text{ph}}$ ,  $T_{\text{el}}$  will grow exponentially and the system will never equilibrate. This indicates that metals with  $\lambda > \lambda_*$  cannot exist in nature even in a metastable state.

This result does not rely on effective electron-phonon models, such as Holstein or Fröhlich Hamiltonians. Such simplified models inherently exhibit artificial phonon softening at a bare electron-phonon coupling  $\lambda_0 \approx 0.5$ ,<sup>[4,5,37]</sup> resulting from double counting of the static electronic contribution (overscreening).<sup>[38–40]</sup> Most importantly, this spurious lattice instability does not define a meaningful upper limit on the physical electron-phonon coupling  $\lambda$ , since  $\lambda \rightarrow \infty$  as  $\lambda_0 \rightarrow 0.5$ . In contrast, our approach provides a rigorous upper bound valid for any phonon spectrum without requiring phonon softening. In particular, this upper bound cannot be circumvented by invoking multiple phonon modes with comparable coupling strengths,<sup>[11]</sup> as this does not alter the ME expression for  $C_{\text{el}}$ .

As noted above, the stability requirement  $C_{\text{el}} > 0$  is equivalent to a certain upper limit on the electron-phonon interaction. To see this, consider a well-known expression for the electronic specific heat at temperature  $T$ <sup>[41–43]</sup> (in units  $\hbar = k_B = 1$ ),

$$C_{\text{el}} = \frac{2}{3} \pi^2 v_0 T \left[ 1 - \int_0^\infty g\left(\frac{\omega}{2\pi T}\right) \frac{2\alpha^2 F(\omega)}{\omega} d\omega \right], \quad (1)$$

where  $v_0$  is the density of states at the Fermi energy,  $g(x) = 6x^2 + 12x^3 \text{Im}\psi'(ix) + 6x^4 \text{Re}\psi''(ix)$ , and  $\psi(x)$  is the digamma function. The combination  $\alpha^2 F(\omega)$  is the Eliashberg function defined as

$$\alpha^2 F(\omega) = \sum_k \frac{\lambda_k \omega_k}{2} \delta(\omega - \omega_k), \quad (2)$$

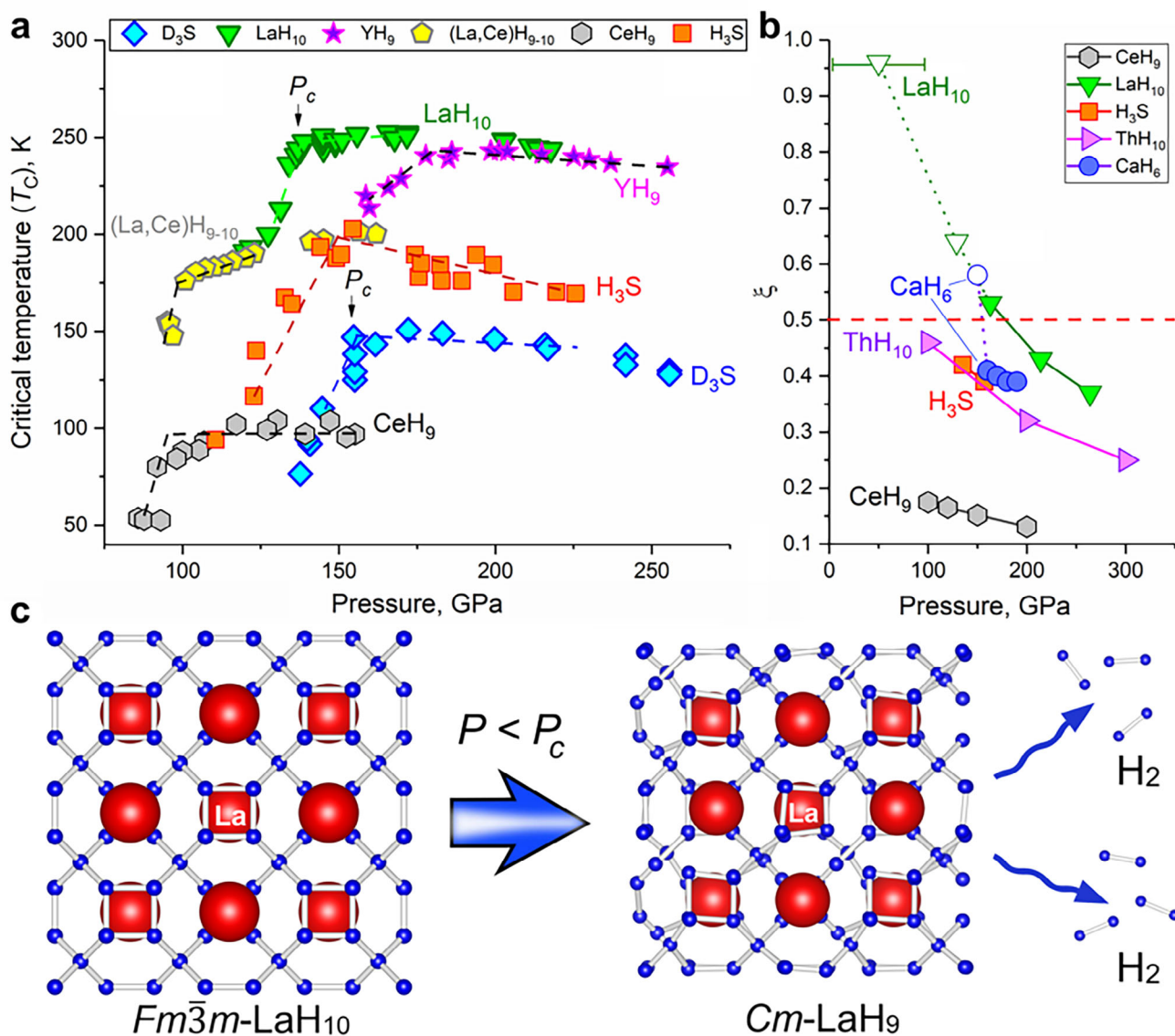
where  $\omega_k$  are the frequencies of lattice vibration modes.

With the help of Equation (1), the stability condition  $C_{\text{el}} > 0$  for all  $T > T_c$  takes the form

$$\xi \equiv \max_T \left\{ \int_0^\infty g\left(\frac{\omega}{2\pi T}\right) \frac{2\alpha^2 F(\omega)}{\omega} d\omega \right\} < 1. \quad (3)$$

The maximum is with respect to the temperature  $T$ . The stability parameter  $\xi$  is another measure of the electron-phonon interaction strength. Just as  $\lambda$ , it grows linearly with the overall scale of the Eliashberg function but is proportional to a weighted average of  $\lambda_k$ ,  $\xi = \sum_{k=1}^N \lambda_k G_k$ , where  $G_k = g\left(\frac{\omega_k}{2\pi T_{\text{max}}}\right)$ .

The phase transition from the metal (superconductor below  $T_c$ ) to a new state as we increase the electron-phonon coupling is of the first order.<sup>[27]</sup>  $C_{\text{el}} = 0$  marks the point where the metal becomes unstable with respect to small deviations from the thermal equilibrium, i.e., ceases to be a local minimum of the free energy. In first order phase transitions, such a local (absolute) instability is preceded by a metastable region  $\xi_c < \xi < \xi_* = 1$ . The metal is no longer the global minimum of the free energy past the phase-transition point  $\xi_c$ . Therefore,  $\xi_* = 1$  provides a fundamental upper bound on  $\xi$  in metals and superconductors. This implies  $\xi_c < 1$ , but the exact value of  $\xi_c$  is nonuniversal and can depend on, for example, the lattice and electronic band structures, number of carries per lattice site etc.



**Figure 3.** Instability and decomposition of polyhydrides with decreasing pressure. a) Experimentally observed dependence of the critical temperature  $T_c$  on pressure for certain polyhydrides and deuterium sulfide (D<sub>3</sub>S). As the pressure is lowered below its critical value  $P_c$ ,  $T_c$  abruptly decreases. This is accompanied by a distortion of the crystal structure and partial loss of hydrogen. b) Dependence of the stability parameter  $\xi$  on pressure for several experimentally synthesized hydrides. The  $\xi = 0.5$  line marks the supposed first order phase transition, i.e., upon crossing this line, the destruction of the structure is merely a function of time and the height of the kinetic barrier. Filled symbols correspond to experimental data, empty ones are DFT calculations. The point  $\xi = 0.96$  (LaH<sub>10</sub>) is an extrapolation obtained by multiplying the Eliashberg function  $\alpha^2F(\omega)$  for LaH<sub>10</sub> at 129 GPa by a factor of 1.5. c) Decomposition of LaH<sub>10</sub> upon lowering the pressure below  $P_c = 138$  GPa accompanied by a distortion of its cubic structure, partial loss of hydrogen (H<sub>2</sub>) and formation of lower hydrides, such as LaH<sub>9</sub>.

We analyzed data for numerous metals and superhydrides for which the Eliashberg functions are known and found<sup>[44]</sup> that all of them conform to our upper bound  $\xi < 1$ . Hydrides loose stability at  $\xi \leq 0.5$ , while  $\xi$  for other metals (Figure 4 and Table S1, Supporting Information) is significantly lower, suggesting that  $\xi_c = 0.5$  for hydrides and  $\xi_c < 0.5$  for conventional metals. We attribute  $\xi = 0.58$  in CaH<sub>6</sub> and MgH<sub>6</sub> to the fact that these are not actually existing hydrides at these pressures. Moreover, if our conjecture that  $\xi_c \leq 0.5$  holds, these two materials can only exist in a metastable state.

The condition  $\xi < \xi_* = 1$  implies also an upper bound  $\lambda < \lambda_*$  on the standard interaction parameter  $\lambda$  defined as

$$\lambda = \int_0^\infty d\omega \frac{2\alpha^2F(\omega)}{\omega} = \sum_{k=1}^N \lambda_k. \quad (4)$$

The value of  $\lambda_*$  varies with the shape of the Eliashberg function with a minimum  $\lambda_* = 3.69$  attained for Einstein phonons (Supporting Information). For Debye phonons ( $\alpha^2F \propto \omega^2$  for  $\omega \leq \omega_D$ )

and zero otherwise),  $\lambda_* = 4.72$ . For the Eliashberg function of the same shape as that for a material with given  $\xi$  and  $\lambda$  (i.e., differing from it only by an overall scale), we have

$$\lambda_* = \frac{\lambda}{\xi}, \quad \lambda_c = \frac{\lambda \xi_c}{\xi} = \lambda_* \xi_c. \quad (5)$$

In particular, we obtain  $\lambda_* = 7.39$  and (assuming  $\xi_c = 0.5$ )  $\lambda_c = 3.69$  for  $\text{YH}_9$  at 205 GPa (see Table S1, Supporting Information) and  $\lambda_c = 2.36$  for Debye phonons. The values of  $\lambda_c$  for all experimentally realized hydrides are in the range from 2.19 for  $\text{YH}_6$  to 4.12 for  $(\text{La}, \text{Y})\text{H}_{10}$ . This indicates that stability must be the reason why  $\lambda$  in actually existing metals is limited to  $\lambda < 4$ .

We argued previously that in the new state the system lowers its energy by either opening a gap or, at least, lowering the density of states at the Fermi energy.<sup>[27]</sup> We also saw that the superconducting state is more resilient against perturbations than the normal state as it already has a gap. Therefore, we expect robust metastable superconductivity when  $\lambda$  is quenched from  $\lambda < \lambda_c$  to  $\lambda > \lambda_c$  while the system is superconducting. This creates an opportunity of attaining *metastable* superconductivity with substantially higher  $T_c$  in polyhydrides at lower pressures than usual, since  $\lambda$  generally increases with decreasing  $P$ , see Figure 2. Moreover, metastable superconductivity of this type has likely been observed in pressure-quenched  $\text{FeSe}$ ,<sup>[45]</sup> but a more thorough analysis of these experiments is necessary to establish this with certainty.

#### 4. Fundamental Limit on $T_c$ in Phonon-Mediated Superconductors

In the formal limit  $\lambda \rightarrow \infty$  of the ME theory,  $T_c$  asymptotically approaches  $0.18\sqrt{\lambda\langle\omega^2\rangle}$ , while at finite  $\lambda$  it falls below this asymptote,<sup>[8,29,53]</sup> i.e.,

$$T_c < 0.18\sqrt{\lambda\langle\omega^2\rangle}. \quad (6)$$

This provides an upper bound on  $T_c$  in terms of  $\lambda$  and the average square frequency  $\langle\omega^2\rangle = \frac{2}{\lambda} \int_0^\infty \alpha^2 F(\omega)\omega d\omega$ .<sup>[54]</sup> The requirement  $C_{\text{el}} > 0$  imposes a constraint  $\lambda < \lambda_*$  on  $\lambda$ . Let  $\omega_{\text{max}}$  be the maximum available phonon frequency. Spreading out the phonon spectral function to frequencies below  $\omega_{\text{max}}$  increases  $\lambda_*$ , while decreasing  $\langle\omega^2\rangle$  and results in an overall decrease of  $T_c$  (Supporting Information). Therefore, the critical temperature for Einstein phonons ( $T_c^E$ ) with maximal  $\lambda = \lambda_* = 3.69$  and frequency  $\omega_{\text{max}}$  provides a *rigorous* upper bound on  $T_c$  for stable and metastable superconducting metals,

$$T_c < 0.32\omega_{\text{max}}, \quad (7)$$

where we used a standard algorithm<sup>[29,46]</sup> to numerically compute  $T_c^E = 0.3175\omega_{\text{max}}$ . We define a metal as a good conductor with a Fermi energy  $E_F$  much larger than typical phonon frequencies. This is the only essential assumption that goes into the Eliashberg theory from which we derived Equation (7).

Recall that metals are stable for  $\lambda < \lambda_c$  and metastable for  $\lambda_c < \lambda < \lambda_*$ . Assuming  $\xi_c = 1/2$  (see above), Equation (5) obtains  $\lambda_c = \lambda_*/2$ . Similarly calculating  $T_c^E = 0.1995\omega_{\text{max}}$  for Einstein

phonons with  $\lambda = 3.69/2$ , we determine an upper bound on  $T_c$  for stable metals,

$$T_c < 0.20\omega_{\text{max}}. \quad (8)$$

Metals with  $0.20\omega_{\text{max}} < T_c < 0.32\omega_{\text{max}}$  can therefore only exist in a metastable state.

In the Debye model  $\omega_{\text{max}}$  is equal to the Debye frequency  $\omega_D$ . However, since real solids do not conform to the Debye model,  $\omega_D$  is not uniquely defined. In particular, its value depends on the quantity used to extract it (e.g., the phonon specific heat vs. resistivity). We therefore prefer to use the edge of the phonon spectrum (Eliashberg function) as  $\omega_{\text{max}}$  whenever possible (Table S1, Supporting Information). Note that both our upper bounds (7) and (8) are significantly more generous than the heuristic bound of  $0.1\omega_D$  proposed in ref. [10]. However, observe that, for example,  $(\text{La}, \text{Ce})\text{H}_{9-10}$  at 123 GPa with  $T_c = 190$  K and  $\omega_D = 1107$  K, extracted from the temperature dependence of the electrical resistance, violates the latter bound, so it apparently does not hold for compressed hydrides. Indeed, to fall below the  $0.1\omega_D$  bound,  $(\text{La}, \text{Ce})\text{H}_{9-10}$  must have a Debye frequency of about 2000 K, which exceeds all calculated and experimental values of  $\omega_D$  ever obtained for synthesized superhydrides (Table S5, Supporting Information).

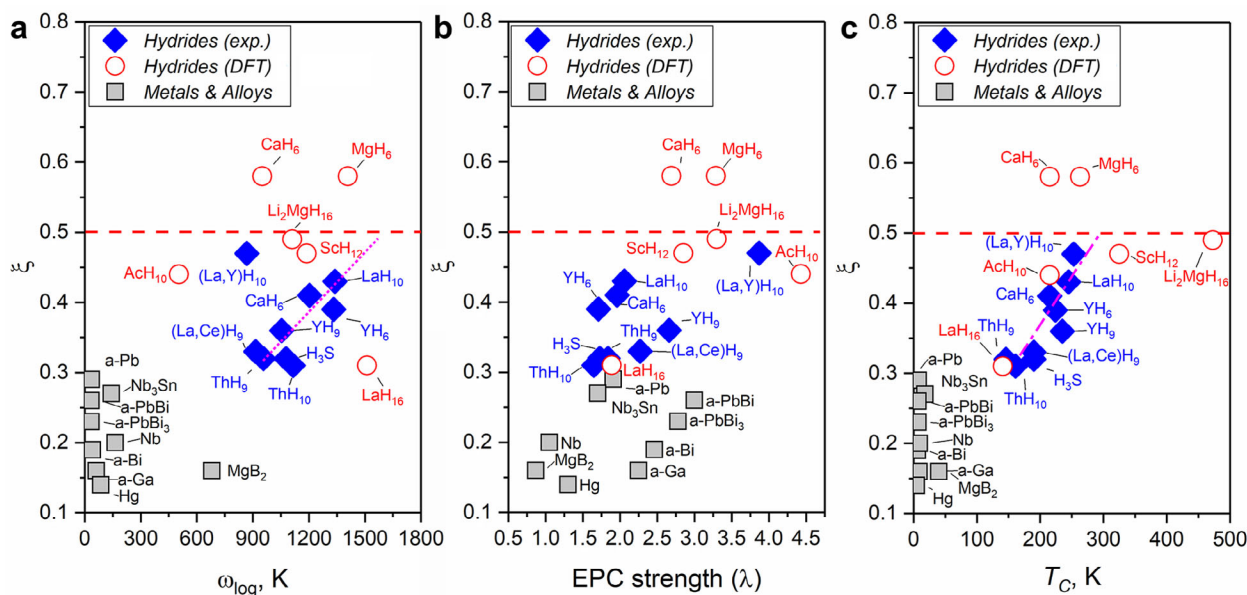
Our results suggest that room-temperature superconductivity is achievable in metals with  $\omega_{\text{max}} > 1500$  K and  $\lambda \geq 2$ , which up until now has only been observed in hydrides at high pressure. Moreover, since we have condensed the entire phonon weight to  $\omega = \omega_{\text{max}}$  to maximize  $T_c$ , the maximum of the Eliashberg function cannot be far below  $\omega = 1500$  K in a room-temperature superconductor.

We can obtain an absolute numerical upper bound on  $T_c$  by observing that the maximum phonon frequency cannot exceed the ionic plasma frequency and that interactions will only renormalize  $\omega_{\text{max}}$  down.<sup>[47]</sup> The ionic plasma frequency is inversely proportional to the square root of the ionic mass, and we therefore expect it to be the highest in the metallic hydrogen. According to recent ab-initio calculations of the Eliashberg function for solid atomic hydrogen at 500 GPa,<sup>[48]</sup>  $\omega_{\text{max}} = 3000 \text{ cm}^{-1} = 4320$  K for harmonic phonons (as the ones in the Eliashberg theory), see also.<sup>[12]</sup> However, this Eliashberg function has a sharp maximum below  $\omega_0 = 3000$  K dropping very quickly from the maximum to zero at  $\omega_{\text{max}}$ . In addition, theoretical estimates of the Debye frequency for the metallic hydrogen are in the range 3000–3500 K.<sup>[16,49]</sup> It is therefore safe to replace  $\omega_{\text{max}}$  in Equations (7) and (8) with  $\omega_0 = 3000$  K, and we obtain the following absolute upper bounds on  $T_c$  in stable and metastable metals:

$$T_c^{\text{stable}} < \frac{600 \text{ K}}{\sqrt{A}}, \quad T_c^{\text{metastable}} < \frac{950 \text{ K}}{\sqrt{A}}, \quad (9)$$

where  $A$  is the atomic mass (in atomic units) of the lightest element in the material.

It is important to note that  $\omega_{\text{max}}$  grows (roughly linearly) with pressure, see, e.g.,<sup>[12]</sup> and Figure S1a, Supporting Information. For the above bounds, we used  $\omega_{\text{max}}$  at 500 GPa – the current upper limit for transport measurements. However, there is a negative correlation between  $\omega_{\text{max}}$  and other



**Figure 4.** Values of the stability parameter  $\xi$  for various hydrides as a function of a) average logarithmic frequency  $\omega_{\log}$ , b) electron-phonon coupling constant  $\lambda$ , and c) superconducting  $T_c$ . Filled and empty symbols correspond to experiment and DFT calculations, respectively. Dashed violet lines indicate the trend apparent among the best hydride superconductors.

characteristic phonon frequencies and the electron-phonon interaction strength (Figure 2 and Figure S1b, Supporting Information), which we did not take into account in our analysis, such that increasing the pressure beyond 500 GPa will likely result in an overall decrease rather than increase of  $T_c$ .

## 5. Conclusion

We established intrinsic upper bounds on the electron-phonon interaction strength and superconducting  $T_c$  in metals. Materials where this interaction exceeds a certain threshold cannot exist in nature in a metallic state, similar to the states of the Van der Waals gas with negative compressibility. Just as in the case of the Van der Waals gas, there is an absolute instability (negative electronic specific heat) that signals a first order phase transition without immediately telling us what the new phase is. However, based on additional considerations<sup>[27]</sup> and experiment, we believe that the tendency is toward a lattice reconstruction.

It is generally known that superconducting  $T_c = \kappa \omega_{\max}$ , where  $\omega_{\max}$  is the maximum or some other characteristic phonon frequency and the coefficient  $\kappa$  is a monotonically increasing function of the strength of the electron-phonon interaction (overall height of the Eliashberg function). As a result, a fundamental bound on  $T_c$  is impossible without a limit on the interaction strength. Prior work suggested that  $\kappa$  might be somehow limited by stability, but was unsuccessful in furnishing definitive evidence of an instability as well as in determining its character and criteria for it. Our work fills this crucial gap and provides the precise stability limit.

It is clear from the bounds (9) that stable room-temperature phonon-mediated superconductivity can only be achieved in hydrogen ( $A = 1$ ) and deuterium ( $A = 2$ ) compounds. Substitution of hydrogen with deuterium typically decreases  $T_c$  by a factor of roughly 1.4<sup>[23,30–32,50,51]</sup> (isotope effect) consistent with Equa-

tion (9). Helium-3 and 4 are extremely unlikely candidates,<sup>[52]</sup> and, in addition,  $T_c < 300$  K already for  $A = 4$ .

At the same time, there are no fundamental reasons why  $T_c$  cannot exceed room temperature in hydrides, at least under sufficiently high pressure. All that is required to engineer such superconductors is an electron-phonon coupling constant  $\lambda = 2 - 3$ , arising primarily from phonons with frequencies near or above 1500 K. Moreover, we showed that the upper bound on  $T_c$  increases by a factor of 1.59 for metastable metals, and that further enhancement is possible if the pressure (and hence the electron-phonon coupling) is quenched while the material is in the superconducting state, as observed in recent FeSe experiments.<sup>[45]</sup>

Our results provide a theoretical foundation for the pursuit of room-temperature superconductivity in polyhydrides, demonstrating that such temperatures are not precluded by any fundamental limits. This conclusion is supported by recent first-principles predictions of high- $T_c$  superconductivity in binary and ternary hydride compounds such as  $\text{ScH}_{12}$ ,<sup>[55]</sup>  $\text{LaSc}_2\text{H}_{24}$ ,<sup>[56]</sup> and related systems. On the experimental side, although progress is more gradual, mounting evidence points to the emergence of new superconducting phases such as  $\text{LaH}_{12}$ <sup>[57]</sup> within the extensively studied La-H<sup>[58–60]</sup> and ternary La-Sc-H<sup>[61]</sup> systems. These materials occasionally exhibit partial transitions in the range of 265–280 K, already approaching room temperature. While experimental challenges persist—including the synthesis of pure phases, precise control of stoichiometry, and stabilization under lower pressures—these advances highlight a promising route toward room-temperature superconductivity in hydrides.

## Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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## Conflict of Interest

The authors declare no conflict of interest.

## Author Contributions

D.V.S. collected statistical data, prepared figures and tables, and performed numerical calculations. E.A.Y. and B.L.A. contributed theoretical analysis. E.A.Y. carried out analytical and related numerical calculations. E.A.Y. and D.V.S. wrote the text. All authors discussed the results and made helpful inputs to all parts of the manuscript.

## Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request. The code for computing the stability parameter  $\xi$  from the Eliashberg function is available at <https://doi.org/10.5281/zenodo.15550102>.

## Keywords

electron-phonon interaction, high-pressure, hydrides, metals, superconductivity

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