Superconductivity on ScH₃ and YH₃ hydrides: Effects of applied pressure in combination with electron- and hole-doping on the electron-phonon coupling properties

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The implementation of electron- and hole-doping, in conjunction to applied pressure, is analyzed as a mechanism to induce or enhance the superconducting state on fcc YH₃ and ScH₃. In particular, the evolution of their structural, electronic, and lattice dynamical properties, as well as the electron-phonon coupling and superconducting critical temperature (T_c) is presented and discussed, as a function of the electron- and hole-doping content as well as applied pressure. The study was performed within the density functional perturbation theory, taking into account the effects of zero-point energy through the quasi-harmonic approximation, while the doping was implemented by means of the construction of the Sc₁−ₓMₓH₃ (M=Ca,Ti) and Y₁−ₓMₓH₃ (M=Sr,Zr) solid solutions modeled with the virtual crystal approximation (VCA). We found that the ScH₃ and YH₃ hydrides shown a significant improvement of their electron-phonon coupling properties under hole-doping (M=Ca,Sr) and at pressure values close to dynamical instabilities. Instead, by electron-doping (M=Ti,Zr), the systems do not improve such properties, whatever value of applied pressure is considered. Then, as a result, T_c rapidly increases as a function of x on the hole-doping region, reaching its maximum value of 92.7(67.9) K and 84.5(60.2) K at x = 0.3 for Sc₁−ₓCaₓH₃ at 10.8 GPa and Y₁−ₓSrₓH₂ at 5.8 GPa respectively, with µ∗ = 0(0.15), while for both, electron- and hole-doping, T_c decreases as a function of the applied pressure, mainly due to phonon hardening. By the thorough analysis of the electron-phonon properties as a function of doping and pressure, we can conclude that the tuning of the lattice dynamics is a promising path for improving the superconductivity on both systems.

I. INTRODUCTION

Materials with a high-superconducting critical temperature (T_c) are of great interest since at ambient conditions could have many technological applications. The theoretical breakthrough and progress for reaching high-T_c superconductivity came after the Ashcroft[1] pioneering idea, suggesting that hydrogen-rich materials could be promising candidates for high-T_c superconductivity. After that, several theoretical predictions have been proposed and performed on the crystal structure, at high pressure, of stoichiometric and hydrogen-rich materials, for which their electronic structure, lattice dynamics, and electron-phonon (el-ph) coupling properties have been calculated[2-5]. As a result of those predictions, several metal hydrides were proposed as conventional-superconductor candidates with a T_c near room-temperature[6-8]. The experimental breakthrough came with the discovery of phonon-mediated superconductivity on H₂S, with a T_c of 203 K under pressures as high as 155 GPa[9, 10]. Some years later, high-T_c superconductivity measurements were reported in other compounds, all of them at high applied pressure values, like LaH₁₀ with T_c in the range of 250-260 K[11, 12] at 170 GPa, and more recently, YH₆ with T_c = 262 K at 182 GPa[13] and YH₆ giving T_c = 220 K at 183 GPa[14], as well as a top reported T_c value of 287 K in a carbonaceous sulfur-hydride at 267 GPa[15].

As a result of the available theoretical and experimental reports, it has been determined that the tendency for superconductivity depends upon the species used to build up the metal hydride (together with hydrogen), a high density of states at the Fermi level, and that the resulting hydride compound must have a large electron-phonon coupling related to the hydrogen atoms. In particular, some of the highest T_c values have being obtained from hydrides constructed with elements that belong to the alkaline family as well as the scandium group (first group of the transition metals) [5]. Regarding this group, from calculations on YH₄, the T_c was estimated around 305-326 K at an applied pressure of 250 GPa for n = 10 [5, 7]; while for n = 6, T_c was on the range of 251-264 K at 120 GPa[5]; and for n = 4, lower T_c values (around 84-95 K) at 120 GPa were reported [16]. For this family, only the YH₉ and YH₆ have been studied experimentally, as already mentioned. For the ScH₃ family, T_c in the range of 120-169 K was predicted for different members, with n = 6, 7, 9, 10 and 12, for an applied pressure above 250 GPa[5, 17]. All the already mentioned metal hydrides can be considered as chemically precompressed phases relative to pure hydrogen, where high pressure is necessary for metallization[1].

With respect to ScH₃ and YH₃ (metal-hydrides with low hydrogen content), they have hcp structures at ambient pressure, and are driven to fcc (cubic NaCl (B1) structure) (see Fig.1) phase under applied pressure. For
YH₃, Raman [18] and infrared [19] studies found that the cubic structure can exist at approximately 10 GPa, and is clearly stabilized around 25 GPa. It has been suggested that another intermediate phase [20] or a coexisting hcp-cubic phase [21] could also appear in the 8–25 GPa pressure range. It has been shown experimentally that YH₃ can be stabilized in the fcc phase at ambient pressure by substituting Y for 10% Li (Li₀.₁Y₀.₉H₃) [22, 23]. Recently, J. Purans et al. [24] and Kong et al. [14] reported the syntheses of this metal-hydride with a pure metallic fcc phase at a broad pressure interval, 40–340 GPa. For lower applied pressure values, between 20 and 40 GPa, they found it to be a semi-metal with a distorted fcc crystal structure. Similarly, for ScH₃, Raman and infrared [25] studies observed an hcp-intermediate-cubic phase at 25 GPa. Theoretically, Kong et al. [26] reported the hcp-cubic phase transition at 25 GPa, while Pakornchote et al. [27] found the cubic phase to be energetically more stable at slightly lower pressure of 22 GPa. For these metal-hydrides, YH₃ and ScH₃, Kim et al. [5, 28] performed first principles calculations and found that the fcc structure is dynamically stable on both of them at a pressure of ≈18 GPa, with an estimated $T_c$ around 18 and 40 K, respectively, with a rapid decreased of $T_c$ as the pressure is increased, in agreement with the experimental report of Kong et al. [14] where superconductivity where not found above 5 K for metallic fcc structure.

Besides applied pressure, doping is another mechanism for metallization of metal hydrides, in order to induce or increase superconductivity by the improvement of some properties, like the electronic density of states at the Fermi level (N(0)) or the el-ph coupling. For example, the substitution of Li by Be, Mg, or Ca in LiH was studied by Zhang et al. [29]. In that work, the dopant acts as a donor which delivers electrons to the system, obtaining a n-doped material with a $T_c = 7.78$ K for an electron content as high as 2.06, calculated at ambient pressure. Another work on that direction was performed by Olean-Ameczua et al. [30]. There the authors showed the metallization of alkali-metal hydrides LiH, NaH, and KH by doping with alkaline-earth metals Be, Mg, and Ca, respectively, and analyzed the superconducting properties as a function of metal content. The maximum estimated $T_c$ values were 2.1 K for Li₀.₉₅Be₀.₀₅H, 28 K for Na₀.₈M₀.₂H, and even 49 K for K₀.₅₅Ca₀.₄₅H, without applied pressure. More recently, Villa-Cortés et al. [31] studied the structural, electronic, and lattice dynamical properties, as well as the electron-phonon coupling and superconducting critical temperature ($T_c$) of ScH₂ and YH₂ metal hydrides solid solutions, as a function of the electron- and hole-doping content, in absence of applied pressure. They found that for electron-doping content $x > 0.5$, $T_c$ increases rapidly, reaching its maximum value of the entire range at the Sc₀.₉₅Ti₀.₀₅H₂ and Y₀.₇Er₀.₃H₂ solid solutions. These results show that such scheme to induce metallization and superconductivity on metal-hydrides works as an alternative to the applied-pressure approach. So, in this paper we implement it, in addition to applied pressure, in order to study the ScH₃ and YH₃ compounds in the fcc structure (NaCl (B1) phase), which is reported to present superconductivity, as discussed previously. Under this approach we are able to trace down the evolution of the structural, electronic, and lattice dynamical properties, as well as the el-ph coupling and $T_c$, as a function of metal content, by inducing holes (p-doped) and electrons (n-doped), as well as applied pressure, of the proposed systems. Such approach is done by the construction of solid solutions with the metal atom of the hydride: Sc₁₋ₓMₓH₃ (M=Ca,Ti) and Y₁₋ₓMₓH₃ (M=Sr, Zr) within the Density Functional Theory (DFT) [32], using the virtual crystal approximation (VCA) [33], which has been successfully applied on the study of doped superconductors [30, 34–37].

The paper is organized as follows. The computational details of our method are presented in Section II. In Section III.A we present our results related to the structural properties; while in Section III.B the electronic structure analysis is shown. The lattice dynamics are discussed in Section III.C; and the electron-phonon and superconducting properties, as well as $T_c$, are shown in Section III.D. Last, our conclusions are presented in Section IV.

II. COMPUTATIONAL DETAILS

The calculations of the structural, electronic, lattice dynamics and el-ph coupling properties were carried out within the framework of Density Functional Theory (DFT) [32] and Density Functional Perturbation Theory (DFPT) [38, 39], both implemented in the QUANTUM ESPRESSO suit code [38]. The calculations were performed with a $24 \times 24 \times 24$ k-point mesh, and a 60 Ry cutoff for the plane-wave basis, while the Perdew-Burke-Ernzerhof (PBE) functional [40] was employed to take into account the exchange and correlation contributions. Fourier interpolation of dynamical matrices, calculated on a $8 \times 8 \times 8$ q-point mesh, were used to de-
FIG. 2. $PV$ equation of state of Sc$_{1-x}$M$_x$H$_3$ and Y$_{1-x}$M$_x$H$_3$, for different metal M content ($x$), studied within the ZPE scheme. $a_B$ stands for the Bohr radius.

terminate the complete phonon spectra of the studied systems. Corrections due to quantum fluctuations at zero temperature, zero-point energy (ZPE) effects, are estimated through the quasi-harmonic approximation (QHA)[30, 41]. Within this approximation, the phonon contribution to the ground-state energy is taken into account and then an equation of state for each concentration $x$ can be constructed. Thus, the electronic structure, lattice dynamics, and el-ph properties, calculated for the fcc (B1) crystal structure at different applied pressure values, incorporate the ZPE correction.

Included on the el-ph calculations, the phonon linewidths of the $q\nu$ phonon mode $\gamma_{q\nu}$ were also obtained, which are given by[42, 43]

$$\gamma_{q\nu} = 2\pi \omega_{q\nu} \sum_{k,m} g_{k+q,k}^{\nu,m} \left| g_{k+q,k}^{\nu,m} \right|^2 \delta \left( \epsilon_{k+q,m} - \epsilon_F \right) \delta \left( \epsilon_{k,n} - \epsilon_F \right),$$

(1)

where $g_{k+q,k}^{\nu,m}$ are the matrix elements of the electron-phonon interaction (calculated over a denser 48 $\times$ 48 k-point mesh), $\epsilon_{k+q,m}$ and $\epsilon_{k,n}$ are one-electron band energies, with band index $m,n$, and vectors $\vec{k} + \vec{q}, \vec{k}$, respectively, while $\omega_{q\nu}$ is the phonon frequency for mode $\nu$ at wave-vector $\vec{q}$.

With the knowledge of $\gamma_{q\nu}$ and $\omega_{q\nu}$, the isotropic Eliashberg spectral function, $\alpha^2 F(\omega)$, can be described as

$$\alpha^2 F(\omega) = \frac{1}{2\pi \hbar N(0)} \sum_{q\nu} \delta(\omega - \omega_{q\nu}) \frac{\gamma_{q\nu}}{\omega_{q\nu}},$$

(2)

where $N(0)$ is the electronic density of states (per atom and spin) at $\epsilon_F$, and a sum over a denser Fourier interpolated $q$-point mesh of 54 $\times$ 54 $\times$ 54 was required. In addition, the average electron-phonon coupling constant $\lambda$, which quantifies the coupling strength as well as the Allen-Dynes characteristic phonon frequency $\omega_m$[44], are related to the Eliashberg function as

$$\lambda = 2 \int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} = \frac{1}{2\pi \hbar N(0)} \sum_{q\nu} \frac{\gamma_{q\nu}}{\omega_{q\nu}},$$

(3)

$$\omega_m = \exp \left\{ \frac{2}{\lambda} \int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} \ln \omega \right\}.\tag{4}$$

FIG. 3. Cohesive energy of Sc$_{1-x}$M$_x$H$_3$ and Y$_{1-x}$M$_x$H$_3$ as a function of the metal M content ($x$) for the minimum pressure value in the stability range of each $x$.

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Regarding $T_c$, it was estimated for each case by solving numerically the isotropic Migdal-Eliashberg gap equations[45–47], using the respective $\alpha^2 F(\omega)$ for each content $x$ at its specific applied pressure value, and treating the Coulomb pseudopotential as an adjusted parameter.

Furthermore, we used the formalism of Rainer and Culleto for the calculation of the differential isotope effect coefficient [48, 49], $\beta(\omega)$, to gain more insight into the coupling and how a specific phonon-frequency interval contributes to $T_c$. $\beta(\omega)$ is defined as

$$\beta(\omega) = R(\omega) \alpha^2 F(\omega),$$

(5)

where $R(\omega)$ is given by

$$R(\omega) = \frac{d}{d\omega} \left[ \frac{\omega}{2T_c} \frac{\delta T_c}{\delta \alpha^2 F(\omega)} \right].$$

(6)
and the $T_c$ functional derivative respect to the Eliashberg function is expressed as [46, 47, 49, 50]

$$\frac{\delta T_c}{\delta \alpha^2 F(\omega)} = -\left(\frac{d\rho}{dT}\right)_{T_c} \frac{\delta \rho}{\delta \alpha^2 F(\omega)},$$

(7)

with $\rho$ corresponding to the breaking parameter that becomes zero at $T_c$. Finally, the isotope effect coefficient, $\alpha$, in a specific frequency interval is given by

$$\alpha = \int_{\omega_1}^{\omega_2} d\omega \beta(\omega).$$

(8)

III. RESULTS AND DISCUSSION

A. Structural properties

We performed structural optimizations of the fcc (cubic NaCl (B1)) structure ($Fm\bar{3}m$ space group) with a primitive cell of four atoms (one metal and three hydrogen) for the two $\text{Sc}_{1-x}\text{M}_x\text{H}_3$ ($\text{M}=\text{Ca, Ti}$) and $\text{Y}_{1-x}\text{M}_x\text{H}_3$ ($\text{M}=\text{Sr, Zr}$) solid solutions at different values of metal M content $x$. For both systems, the equations of state were constructed from the minimum pressure, at which each system becomes stable at the cubic structure, to 100 GPa as maximum pressure value.

For $\text{Sc}_{1-x}\text{M}_x\text{H}_3$, the equation of state was determined for concentrations up to $x = 0.5(0.4)$ of electron(hole) doping, while for $\text{Y}_{1-x}\text{M}_x\text{H}_3$, the range was for concentrations up to $x = 0.05(0.4)$ of electron(hole) doping. Electron- and hole-doping thresholds and the minimum pressures where the systems are stable were determined through dynamical instabilities, observed as imaginary frequencies in the phonon dispersion for larger $x$ contents and smaller pressure values. Phonon instabilities in metal hydrides induced by alloying have been reported previously in literature [30, 51, 52], where such dynamical behavior have been related to an increase of the heat of formation, meaning that the solid solutions become less stable.

In Fig. 2, we show the evolution of the equation of state of each metal content $x$. For both systems, $\text{Sc}_{1-x}\text{M}_x\text{H}_3$ and $\text{Y}_{1-x}\text{M}_x\text{H}_3$, increasing the electron content leads to a monotonous reduction of the volume, at a given pressure, as well as an increment in the minimum stable pressure value. For hole doping, the volume tendency is opposite, while the minimum stable pressure values are not following any specific trend. This behavior indicates a strengthening of the chemical bonding as the electron-content is increased, given by the increment of Zr- and
Ti-content, suggesting a hardening of phonon frequencies. Similarly, as the hole-content grows, by the increase of Sr- and Ca-content, the chemical bonding gets weaker, implying a softening of the phonon frequencies. A complete set of structural parameters, that is, the equilibrium volume \((V_0)\), bulk modulus \((B_0)\), and its pressure derivative \((B'_0)\) are given in Tab. I (Appendix A), for both systems, of all M content \((x)\) values studied. It is worth noting that our \(YH_3\) results are in excellent agreement with the experimental data reported by Machida et al.[53].

In Fig. 3 we show the calculated cohesive energy \((E_{coh})\) of the two systems, within their respective electron and hole stability-range at their corresponding minimum pressure threshold. This quantity is used to characterize the stability of alloys and solid solutions, and is given by the following:

\[
E_{coh} = E^{tot}_{sys} - (1 - x)E^a_N - xE^a_M - 3E^a_H, \tag{9}
\]

where \(E^{tot}_{sys}\) is the total energy of the \(N_{1-x}M_xH_3\) solid solution at content \(x\), while \(E^a_N\), \(E^a_M\), and \(E^a_H\) are the calculated total energies of the isolated atoms \(N = Y, Sc; M = Sr, Zr, Ca, Ti\), and hydrogen, respectively. In general, for the two solid solutions, the hole-doped systems are less stable than their corresponding pristine systems \((x = 0)\) (the larger the \(E_{coh}\) absolute value, the more stable the system is), nevertheless, they are still in the stability range (negative \(E_{coh}\)). For the case of electron-doped regime, while \(Y_{1-x}Zr_xH_3\) follows the same observed tendency than the hole-doped systems, we found that \(Sc_{1-x}Ti_xH_3\) is more stable than the pristine one, indicating the possibility to synthesize experimentally such solid solutions.

With the optimized lattice parameters and the corresponding equation of state for each system, at different content for their electron- and hole-doping regions, we proceeded to calculate their electronic and lattice dynamical properties for different applied pressure values at each \(x\). Furthermore, we are presenting results obtained by the ZPE scheme. While the ZPE effects on the electronic properties are hardly visible, comparing with the static scheme, on the lattice dynamical ones, there is a noticeable softening as a general effect. This tendency comes mainly from the unit cell expansion as the ZPE contribution to the energy is taken into account.

### B. Electronic properties

The evolution of the electronic band structure and the density of states at the Fermi level, \(N(0)\), is analyzed in order to evaluate the effects of electron- and hole-content and pressure on the electronic properties of the solid-solutions.

In Fig. 4 we show the band structure for \(Sc_{1-x}M_xH_3\) and \(Y_{1-x}M_xH_3\) of the pristine system and of their corresponding threshold electron- (Ti, Zr) and hole- (Ca, Sr) doping content, each of them at the minimum pressure (where the system is dynamically stable) and the maximum pressure considered (100 GPa).

It can be seen that the main pressure effect on the band structure, independent of the electron- or hole-content, is a slight increase of the bandwidth. That is, the low-energy bands are push to even lower energy, and the high-energy ones to higher values, while keeping almost unaffected the bands around the Fermi level \((E_F)\). The band structure of the pristine \(ScH_3\) shows a threefold degenerate state on the L-point (giving place to one hole-like and two electron-like bands) and a twofold degenerate state on the \(\Gamma\)-point (electron-like bands), both located at \(E_F\). In comparison, the pristine \(YH_3\) compound shows a twofold state on the L-point, also at the Fermi level, while the twofold state on the \(\Gamma\)-point is located just above \(E_F\). As the electron content is increased for \(ScH_3\) (by Ti), the degeneracy at the L-point breaks, giving place to a new twofold state that continue to move far away from \(E_F\), rising as an electron-like band and a hole-like band. Instead, at \(\Gamma\)-point the twofold state is intact, moving as a whole to lower energy values, indicating that electronic topological transitions (ETT) take place. In the case of electron-doping for \(YH_3\) (by Zr), the degenerate states at \(L\)- and \(\Gamma\)-points are maintained, while they undergo a minor shift to lower energies. Regarding the hole-content increase on both systems, \(SH_3\) by Ca and \(YH_3\) by Sr, it’s essential effect is the shift of the band structure to higher energies, without noticeable changes on the degenerate states discussed before.

Analyzing the evolution of \(N(0)\), as a function of M content \((x)\) for the minimum and maximum pressure values of both systems, \(Sc_{1-x}M_xH_3\) and \(Y_{1-x}M_xH_3\) (see Fig. 5), it can be observed that, in general, \(N(0)\) reduces at \(x = 0.1\) on the hole-doping regime, and in a more drastic way for the \(ScH_3\) case. As the hole-content increases, \(N(0)\) starts to rise slowly, getting close to its value at \(x = 0\) for the \(YH_3\) system. For the electron doping

![Figure 5](https://example.com/figure5.png)

**FIG. 5.** Evolution of the total density of states at the Fermi level, \(N(0)\), for \(Sc_{1-x}M_xH_3\) and \(Y_{1-x}M_xH_3\) as a function of the M content \(x\) spanning the range of studied applied pressure.
regime, while \( \text{YH}_3 \) undergoes a minor increase, mainly by the threshold limit on the Zr-content, \( N(0) \) of \( \text{ScH}_3 \) grows rapidly, doubling its pristine value at \( x(\text{Ti}) = 0.3 \). As \( x \) increases even more, the \( N(0) \) grow ratio slows considerably, tending to saturate. As the applied pressure raises, \( N(0) \) shows an small reduction, which is due to the expand of the bandwidth discussed previously.

C. Lattice dynamics

The phonon dispersion is presented on Fig. 6, including their respective phonon linewidth \( \gamma_{\vec{q} \nu} \) and the phonon density of states (PHDOS), for \( \text{Sc}_{1-x}\text{M}_x\text{H}_3 \) and \( \text{Y}_{1-x}\text{M}_x\text{H}_3 \) at the pristine \( x = 0 \) and the threshold electron- (Ti,Zr) and hole- (Ca,Sr) contents. In general, for both systems, the optical branches soften slightly as the hole-content increases, while they are shifted to higher frequencies as the electron-content rises. In particular for the high-frequency optical branches, while they shift almost on a rigid way above the frequencies of the pristine systems for the electron-doping case, on the hole-doping solid-solutions they show, in addition to the softening, a small renormalization in the \( T_{2g} \) and \( T_{1u} \) optical phonon branches at \( \Gamma \). While the mid-frequency region shows subtle renormalizations at \( \Gamma \)- and \( L \)-point for electron-content regime, they are stronger for the same high-symmetry points, in addition to the X-point, for hole-content systems. Regarding the acoustic branches, they remain almost unchanged for electron-doping, whereas for hole-doping they lightly harden. Interestingly, the phonon linewidths \( \gamma_{\vec{q} \nu} \) (vertical lines along the phonon branches), mainly localized around \( \Gamma \) at the \( T_{2g} \) and \( T_{1u} \) optical phonon branches for \( x = 0 \), remain almost unchanged for the hole-doping regime in both alloys, while for the electron-doping regime it slightly reduces in \( \text{Sc}_{1-x}\text{M}_x\text{H}_3 \), and increases in \( \text{Y}_{1-x}\text{M}_x\text{H}_3 \). In general, for both solid-solid-solutions, independent of doping-scheme, the observed effect of applied pressure is a rigid hardening of the phonon frequencies and a lifting of phonon anomalies, that leans to instabilities at \( K \) and \( X \)-point, for the acoustic branches.

D. Electron-phonon and superconducting properties

With the electronic and the lattice dynamics information, the electron-phonon spectral functions \( \alpha^2F(\omega) \) were calculated for the entire range of hole- and electron-content stable regimes in a broad pressure range. The \( \alpha^2F(\omega) \) for the threshold electron- and hole-content, as well as the pristine cases, at the minimum pressure where the systems are dynamically stable, can be seen in Fig.
As the electron(hole)-content increases on both systems, the high-frequency optical region of the Eliashberg function shifts to higher(lower) frequencies, while the mid-range frequency region shows an opposite behavior, and the acoustical one practically does not shift. For both systems, the weight of the spectral function is incremented as the doping goes from the electron- to the hole-content thresholds, passing through the pristine one ($x = 0$). Regarding the pressure effects, in general, for all different $x$ content cases (electron- and hole-doping), at both solid-solutions, the spectra shift to a higher frequency region as the pressure arises, going from the minimum dynamically stable value up to 100 GPa.

As the Eliashberg spectral function determines the electron-phonon coupling constant ($\lambda$) (see Eq. 3), the $\alpha^2 F(\omega)$ observed shift due to both, doping and applied pressure, has an impact on $\lambda$ as well. The evolution of the electron-phonon coupling constant as a function of frequency, $\lambda(\omega)$, is shown in Fig. 7. For the pristine ($x = 0$) and the electron-doped $\text{Sc}_{1-x}\text{Ti}_x\text{H}_3$ solid solution, it can be observed that the main contribution to $\lambda$ comes from the acoustic region. However, for the hole-doped $\text{Sc}_{1-x}\text{Ca}_x\text{H}_3$, the main contribution comes from the mid-range frequency optical phonons. The behavior of $\lambda(\omega)$ for the $\text{Y}_{1-x}\text{M}_x\text{H}_3$ solid solution is slightly different. In this case, both regions, the acoustic and the mid-range frequency optical ones, contribute almost at the same rate to $\lambda(\omega)$. It is worth noting that, for both solid-solutions, the high-frequency optical phonons have marginal contribution to $\lambda$.

In order to analyze the behavior of $\lambda$ as a function of pressure and electron- or hole-content for the solid-solutions, we present it as a color-map plot in Fig. 8. In general, it can be observed that for most of the scanned pressure values, on both doping schemes (electron and hole) $\lambda$ hardly goes beyond 1, regardless of the solid-solution. It is worth to mention that higher $\lambda$ values are obtained for pressure close to dynamical instabilities at each electron- or hole-threshold content. Interestingly, only for very specific combination of pressure and hole-content it is possible to reach higher $\lambda$ values, like 1.8 for $\text{Sc}_{0.7}\text{Ca}_0.3\text{H}_3$ at 10.8 GPa, and 2.0 for $\text{Y}_{0.7}\text{Sr}_0.3\text{H}_3$ at 5.8 GPa. In particular for the latter solid-solution, the region of pressure and hole-content that could provide $\lambda$ values close to 2 is spread between $x = 0.2$ and 0.3, and around 1 to 6 GPa on applied pressure.

In a similar fashion as $\lambda$, the evolution of the Allen-Dynes characteristic phonon frequency, $\omega_{\text{tn}}$, as a function of pressure and electron- and hole-content is shown in Fig. 9. It can be observed a hardening as the pressure increases, specially noticeable for the hole-doping regime and more subtle for the electron-doping one, while the lower $\omega_{\text{tn}}$ values are located at the pressure and hole-content regions where both solid-solutions present their maximum $\lambda$ values.

The calculated electron-phonon coupling properties were used to obtain estimates for the superconducting critical temperature, $T_c$, as a function of applied pressure and content $x$ for both solid solutions. The isotropic Migdal-Eliashberg gap equations where solved numerically with two different values of the Coulomb pseudopoten-
tential ($\mu^*$): $\mu^* = 0$ (which provides an upper limit for $T_c$) and 0.15, in order to get an idea of how strong $T_c$ could be affected by the $\mu^*$ variation. In general, we get the maximum $T_c$ at the minimum pressure values were we found dynamically stable solid solutions for each content ($x$) of both regimes, electron- and hole-doping, as can be observed in Fig. 10. Comparing doping regimes, the hole-doping one reports the highest critical temperature, with values of $T_c = 92.7(67.9)$ K and $T_c = 84.5(60.2)$ K at $x = 0.3$ for $Sc_{1-x}Ca_xH_3$ and $Y_{1-x}Zr_xH_3$ respectively, with $\mu^* = 0(0.15)$. These maximum $T_c$ values corresponds to the highest $\lambda$, the lowest $\omega_1\nu$, and a comparatively low $N(0)$ (related to its corresponding electron-doping values). Such behavior shows that the tuning of the lattice dynamics is the path to enhance superconductivity in both systems. It is worth to mention that $Y_{0.8}Sr_{0.2}H_3$, the only system that is dynamically stable at ambient pressure (0 GPa), presents $T_c = 65.4(44.3)$ K for $\mu^* = 0(0.15)$.

Regarding the pristine systems, we are fully aware that have not been experimental observation of superconductivity for fcc-phase YH$_3$ and SH$_3$ compounds. In particular, Kong et al. [14] reported no superconductivity for temperatures above 5 K for pure-fcc metallic YH$_3$, at pressures values going from 40 GPa up to 180 GPa. Then, in Fig. 11 we show our $T_c$ results for ScH$_3$ and YH$_3$, as a function of applied pressure, and from it can be seen that for pressure values above 40 GPa, $T_c$ goes below 5 K, and gets even smaller as pressure arises, in good agreement with the experimental reports. Additionally, comparing with previous results calculated by Kim et al. [28], it can be observed that the downward tendency is reproduced on both systems.

Finally, to get more insight about the contribution of the different phonon-frequency intervals to the superconductivity state, we have calculated the Rainer and Culeto differential isotope effect coefficient, $\beta(\omega)$ (Eq. 5), and the partial isotope effect $\alpha(\omega)$ (Eq. 8), which give information on how strong can $T_c$ be modified due to an infinitesimal ion-mass change in a specific phonon interval.

In Fig. 12 we present $\beta(\omega)$ and $\alpha(\omega)$ for both solid-solutions at the pressure and hole-content that presents the highest $T_c$ ($\mu^* = 0.15$): $Sc_{0.7}Ca_{0.3}H_3$ at 10.8 GPa and $Y_{0.7}Sr_{0.3}H_3$ at 5.8 GPa. We found $\alpha(\omega)$ to be $0.21(0.15)$ at the acoustic interval, and $0.27(0.33)$ for the mid-frequency region (shadow interval) for $Sc_{0.7}Ca_{0.3}H_3(Y_{0.7}Sr_{0.3}H_3)$, values that contribute to the 41(30) and 53(65), respectively, of the total isotope coefficient $\alpha = 0.49$, showing the importance of the mid-frequency region to the superconducting state.

In order to get an idea of how these different phonon regions contribute to $T_c$, we calculated the critical-temperature change, $\Delta T_c$, when a phonon region is suppressed by means of the Bergmann and Rainer

![Heatmap](image1.png)

**FIG. 9.** Allen-Dynes characteristic phonon frequency ($\omega_{\alpha\omega}$) for $Sc_{1-x}M_xH_3$ and $Y_{1-x}M_xH_3$ of the complete range of electron- and hole-content and applied pressure for each solid solution.

![Heatmap](image2.png)

**FIG. 10.** Superconducting critical temperature, $T_c$, calculated with $\mu^* = 0.15$, of $Sc_{1-x}M_xH_3$ and $Y_{1-x}M_xH_3$ at the entire range of electron- and hole-content and applied pressure for each solid-solution.
formalism\cite{46,47}:

$$\Delta T_c = \int_0^\infty d\omega \frac{\delta T_c}{\delta \alpha^2 F(\omega)} \Delta \alpha^2 F(\omega),$$

(10)

where $\Delta \alpha^2 F(\omega) = \alpha^2 F'(\omega) - \alpha^2 F(\omega)$. Here, $\alpha^2 F(\omega)$ is the total Eliashberg function and $\alpha^2 F'(\omega)$ is the one with a specific phonon region suppressed. Then, applying it to the same cases as before (the ones with the highest obtained $T_c$ for $\mu^* = 0.15$) we found $\Delta T_c$ to be $-18.7(-11.1)$ K for the acoustic region and $-52.3(-56.6)$ K for the mid-frequency region for Sc$_0.7$Ca$_0.3$H$_3$(Y$_0.7$Sr$_0.3$H$_3$), representing the later a reduction in $T_c$ of 77(94)% when the mid-frequency region is suppressed in $\alpha^2 F(\omega)$.

IV. CONCLUSIONS

We have performed a thorough analysis of the structural, electronic, lattice dynamics, electron-phonon coupling, and superconducting properties of the metal-hydride fcc solid-solutions Sc$_1-x$M$_x$H$_3$ (M=Ca,Ti) and Y$_{1-x}$M$_x$H$_3$ (M=Sr,Zr), as a function of electron- and hole-doping content $x$, as well as applied pressure. For both systems, while increasing the electron content leads to an increment of the minimum stable pressure in comparison to pristine systems, for hole-doping we found lower minimum stable pressure values for most of content $x$, even finding a particular hole-doping case, Y$_{0.8}$Sr$_{0.2}$H$_3$, that was dynamically stable at zero applied pressure. Although $N(0)$ is not improved in the whole hole-doping region for both systems, and even decreasing for Sc$_0.9$Ca$_0.1$H$_3$ in comparison with ScH$_3$, at the electron-doping regime $N(0)$ shows an important increment at $x = 0.3$ for the Sc-doped hydride, almost twice the corresponding value for the pristine system. As the pressure increases, $N(0)$ shows a reduction, which is related to the observed bandwidth expansion in both solid solutions. As for the lattice dynamics, the optical phonons soften in both systems by hole-doping, which is more pronounced for the high-frequency region than the the mid-frequency one, while the acoustic branches lightly harden. Meanwhile, for the electron-doping regime, the optical branches shift to higher values and the acoustic ones remain almost unchanged. In general, for both solid-solutions, independent of doping-scheme, the applied pressure effect is a rigid hardening of the phonon frequencies and a lifting of phonon anomalies at the acoustic branches. Regarding the electron-phonon coupling parameter, $\lambda$, the main contribution comes from the acoustic and mid-range optical phonon branches for both solid solutions, while the high-frequency optical ones have marginal participation. Interestingly, a remarkable improvement of $\lambda$ is observed in the $0.2 - 0.4$ hole-doping range and for low applied pressure values, close to dynamical instabilities, while by electron-doping, the systems do not improve such property, whatever value of applied pressure is considered. In particular, the systems can reach $\lambda$ values as high as $1.8$ for Sc$_0.7$Ca$_0.3$H$_3$ at 10.8 GPa, and $2.0$ for Y$_0.7$Sr$_0.3$H$_3$ at 5.8 GPa, which represent an improvement of 160% and 100%, respectively, in comparison with the highest $\lambda$ values at their corresponding pristine systems, under applied pressure. Then, as a consequence, the maximum superconducting critical temperature, at each system, was obtained for those particular conditions of hole-doping and pressure, with values of $T_c = 92.7(67.9)$ K.
and $T_c = 84.5(60.2) \, \text{K}$ for ScH$_3$ and YH$_3$ doped systems, respectively, with $\mu^* = 0(0.15)$, while a general reduction of $\lambda$ and $T_c$ as the applied pressure rises, independent of electron- or hole-doping content, is mainly coming from the phonon hardening. Finally, by calculating the Rainer and Culleto differential isotope effect coefficient, we found the mid-frequency region as the most crucial phonon zone to the superconducting state. Then, due to all the above, we can conclude that the tuning of the lattice dynamics is a promising path for improving the superconductivity on both systems.

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Appendix A: Equation of state parameters

In Table I we show the equation of state parameters of the third-order Birch-Murnaghan equation\cite{54} for both solid solutions, Sc$_{1-x}$M$_x$H$_3$ and Y$_{1-x}$M$_x$H$_3$, in the fcc (NaCl (B1)) structure ($Fm\overline{3}m$ space group) within the ZPE scheme.

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TABLE I. Birch-Murnaghan fit to the equation of state. $V_0$ is the reference volume at zero pressure (in $a^3_0$, where $a_0$ is the Bohr radius), $B_0$ is the bulk modulus in GPa at zero pressure, and $B'_0$ is the pressure derivative of the bulk modulus.

| $x$ | $V_0$ ($a^3_0$) | $B_0$ (GPa) | $B'_0$ |
|-----|----------------|-------------|--------|
| 0.1 | 191.10         | 100.72      | 3.66   |
| 0.2 | 197.03         | 92.94       | 3.70   |
| 0.3 | 202.76         | 86.40       | 3.70   |
| 0.4 | 207.74         | 82.47       | 3.74   |

| $x$ | $V_0$ ($a^3_0$) | $B_0$ (GPa) | $B'_0$ |
|-----|----------------|-------------|--------|
| 0.1 | 189.06         | 104.49      | 3.64   |

| $x$ | $V_0$ ($a^3_0$) | $B_0$ (GPa) | $B'_0$ |
|-----|----------------|-------------|--------|
| 0.1 | 184.52         | 106.24      | 3.69   |
| 0.2 | 180.43         | 107.47      | 3.73   |
| 0.3 | 174.96         | 116.36      | 3.68   |
| 0.4 | 170.91         | 121.80      | 3.66   |
| 0.5 | 169.66         | 116.31      | 3.77   |

| $x$ | $V_0$ ($a^3_0$) | $B_0$ (GPa) | $B'_0$ |
|-----|----------------|-------------|--------|
| 0.1 | 245.38         | 89.43       | 3.77   |
| 0.2 | 251.58         | 79.36       | 3.77   |
| 0.3 | 258.51         | 74.04       | 3.78   |
| 0.4 | 265.01         | 70.43       | 3.77   |

| $x$ | $V_0$ ($a^3_0$) | $B_0$ (GPa) | $B'_0$ |
|-----|----------------|-------------|--------|
| 0.05 | 238.20         | 89.10       | 3.79   |

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