Electron- and hole-doping on ScH2 and YH2: effects on superconductivity without applied pressure

S Villa-Cortés∗ and O De la Peña-Seaman

Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apartado Postal J-48, 72570, Puebla, México

E-mail: svilla@ifuap.buap.mx

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Abstract
We present the evolution of the structural, electronic, and lattice dynamical properties, as well as the electron–phonon (el–ph) 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. The study was performed within the density functional perturbation theory, taking into account the effect of zero-point energy through the quasi-harmonic approximation, and the solid solutions \( \text{Sc}_{1-x}M_x\text{H}_2 \) (\( M = \text{Ca, Ti} \)) and \( \text{Y}_{1-x}M_x\text{H}_2 \) (\( M = \text{Sr, Zr} \)) were modeled by the virtual crystal approximation. We have found that, under hole-doping (\( M = \text{Ca, Sr} \)), the ScH2 and YH2 hydrides do not improve their el–ph coupling properties, sensed by \( \lambda(x) \). Instead, by electron-doping (\( M = \text{Ti, Zr} \)), the systems reach a critical content \( x \approx 0.5 \) where the latent coupling is triggered, increasing \( \lambda \) as high as 70%, in comparison with its \( \lambda(x = 0) \) value. Our results show that, under hole-doping region, \( T_c \) decreases as a function of \( x \) on the hole-doping region, from \( x = 0.2 \) to \( x = 0.9 \), collapsing at the end. Alternatively, for electron-doping, \( T_c \) first decreases steadily until \( x = 0.5 \), reaching its minimum, but for \( x > 0.5 \) it increases rapidly, reaching its maximum value of the entire range at the Sc0.05Ti0.95H2 and Y0.2Zr0.8H2 solid solutions, demonstrating that electron-doping can improve the superconducting properties of pristine metal hydrides, in the absence of applied pressure.

Keywords: superconductivity, electron–phonon coupling, electron-doping, hole-doping, novel metal hydrides

(Some figures may appear in colour only in the online journal)

1. Introduction

In the last decade, several theoretical predictions have been made on the crystal structure of stoichiometric and hydrogen-rich materials at high pressures for which their electronic, dynamic and electron–phonon (el–ph) coupling properties had been calculated [1–4]. As a result from those predictions, several metal hydrides have been proposed as conventional-superconductor candidates with a superconducting critical temperature \( T_c \) near room temperature [5–7]. However, since 2015, the search for high-temperature superconductors has experienced a renewal, due to the discovery of phonon-mediated superconductivity on H3S, with a \( T_c \) of 203 K under pressures as high as 155 GPa [8, 9], as well as LaH10 with \( T_c \) in the range of 250–260 K [10, 11] at similar pressures, while, more recently, a \( T_c \) of 262 K was measured in YH9 at 182 GPa [12]. Such breakthrough was achieved by a synergy between experiments and theoretical studies, which predicted the metallization and transition to the superconducting state of H3S and LaH10 at high pressure [5, 6, 13], prior to the experimental verification.

The idea of hydrogen-rich materials metallized under pressure was first proposed by Ashcroft [14] and has become a hot topic for searching room-temperature superconductors. From
the available experimental and theoretical data, it has been suggested that the propensity for superconductivity depends upon the species used to build up the metal hydride, together with hydrogen. Some of the highest \( T_c \) values are obtained from hydrides constructed with elements that belong to the alkaline family as well as the first group of the transition metals (scandium group) [4]. Thus, several studies on the dynamical stability and superconducting state have been carried out in YH\(_n\) and ScH\(_n\) \((n \geq 3)\) stoichiometric alloys.

In particular, from calculations on YH\(_n\), the \( T_c \) was estimated around 305–326 K at an applied pressure of 250 GPa for \( n = 10 \) [4, 6]; while for \( n = 6 \) the \( T_c \) values were on the range of 251–264 K at 120 GPa [4]; and for \( n = 4 \), lower values of \( T_c \) (84–95 K) at 120 GPa were reported [15]. However, was not until recently that measurements for a sibling system, YH\(_6\), were realized, getting a \( T_c \) of 262 K at 182 GPa [4, 12]. For the case of the ScH\(_n\) family, high \( T_c \) values in the range of 120–169 K were predicted for different members, like ScH\(_2\), ScH\(_3\), ScH\(_4\), ScH\(_6\), and ScH\(_8\), all above of an applied pressure of 250 GPa [4, 16].

On both families, ScH\(_n\) and YH\(_n\), their members with lowest hydrogen content \((n = 3, 2)\) have not been so widely studied, mainly for their lack of compelling superconducting properties. For ScH\(_3\) and YH\(_3\), their highest \( T_c \) have been estimated to be 20 and 40 K, respectively, at low pressure \((\approx 20 \text{ GPa})\) [4, 17]. For YH\(_2\) there are not reports about its superconducting properties or \( T_c \), so far. Regarding ScH\(_2\), there are some theoretical studies that found that \( T_c \) rises under pressure, with a maximum value of 38 K at 30 GPa. Such behavior was attributed to the hybridization between 1s-states of H-atom and d-states of Sc-atom under pressure [4, 18].

Besides applied pressure, doping is another procedure to induce or increase superconductivity by enhancing some properties like the electronic density of states (DOS) at the Fermi level \((N(0))\) or the el–ph coupling. An example of such procedure is the one of Zhang et al [19], where the substitution of Li by Be, Mg, or Ca in LiH was studied. There, the dopant acts as a donor which delivers electrons to the system, obtaining an n-doped material with a \( T_c \approx 7.78 \text{ K} \) for an electron content as high as 2.06, calculated at ambient pressure. More recently, Olea-Amezquita et al [20] 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 concentration. The maximum estimated \( T_c \) values were 2.1 K for Li\(_{0.95}\)Be\(_{0.05}\)H, 28 K for Na\(_{0.9}\)Mg\(_{0.1}\)H, and even 49 K for K\(_{0.55}\)Ca\(_{0.45}\)H, in absence of applied pressure. Such scheme to induce metallization and superconductivity on metal-hydrides could work as an alternative to the applied-pressure approach on the ScH\(_n\) and YH\(_n\). So, in this paper we implement it on the less-studied members of the family: ScH\(_2\) and YH\(_2\), and trace down the evolution of the structural, electronic and lattice dynamics properties, as well as the el–ph coupling and \( T_c \), as a function of concentration, inducing electrons (n-doped) and holes (p-doped) into the proposed systems. Such approach is done by the construction of solid solutions with the metal atom of the hydride: Sc\(_{1-x}\)M\(_x\)H\(_2\) \((M = Ca, Ti)\) and Y\(_{1-x}\)M\(_x\)H\(_2\) \((M = Sr, Zr)\) within the density functional theory (DFT) [21], using the virtual crystal approximation (VCA) [22], which has been successfully applied on the study of doped superconductors [20, 23–26].

The paper is organized as follows. The computational details that support our method are presented in section 2. In section 3.1 we present our results related to the structural properties; while in section 3.2 the electronic structure analysis is shown. The lattice dynamics is discussed in section 3.3; and electron–phonon and superconducting properties, as well as \( T_c \), are shown in section 3.4. Last, our conclusions are presented in section 4.

2. Computational details

In order to study the superconducting state on the proposed systems, the electronic structure, the phonon dispersion and the el–ph coupling properties were obtained for the \( Fm\overline{3}m \) crystal structure, without applied pressure (figure 1). We calculated the ground state properties within the framework of DFT [21], while the lattice dynamics and coupling properties were obtained within the density functional perturbation theory (DFPT) [27, 28], both implemented in the QUANTUM ESPRESSO suit code [27]. The calculations were performed with an 80 Ry cutoff for the plane-wave basis, and a \( 24 \times 24 \times 24 \) \text{ k-point mesh}. The Perdew–Burke–Ernzerhof (PBE) functional [29] was employed to take into account the exchange and correlation contributions.

Complete phonon spectra were accessed by a Fourier interpolation of dynamical matrices calculated on an \( 8 \times 8 \times 8 \) \text{ q-point mesh}. Corrections due to quantum fluctuations at zero temperature, zero-point energy (ZPE) effects, are estimated through the quasi-harmonic approximation [20, 30] using the calculated phonon density of states (PHDOS). Within this approximation, the phonon contribution to the ground-state energy is taken into account and a new structural optimization of each concentration \( x \) can be performed. Thus, the electronic structure, lattice dynamics and electron–phonon
properties, calculated with these lattice parameters, include ZPE corrections.

To gain more insight, we also calculated the phonon linewidths of the $\tilde{q}$ phonon mode $\gamma_{\tilde{q}0}$, arising from the electron–phonon interaction given by [31, 32]

$$\gamma_{\tilde{q}0} = 2\pi\omega_{\tilde{q}0}\sum_{knm}\left|\frac{g_{k+\tilde{q},\tilde{m}}}{\omega_{\tilde{q}0}}\right|^2 \delta\left(\epsilon_{k+\tilde{q},\tilde{m}} - \epsilon_F\right) \delta\left(\epsilon_{\tilde{m}} - \epsilon_F\right),$$  

(1)

where $g_{k+\tilde{q},\tilde{m}}$ are the matrix elements of the electron–phonon interaction (calculated over a denser 48 × 48 × 48 k-point mesh), $\epsilon_{k+\tilde{q},\tilde{m}}$ and $\epsilon_{\tilde{m}}$ are one-electron band energies, and $\omega_{\tilde{q}0}$ is the phonon frequency for mode $\nu$ at wave-vector $\tilde{q}$.

The isotropic Eliashberg spectral function, $\alpha^2 F(\omega)$, is described as

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

(2)

where $N(0)$ is the electronic DOS, per atom and spin, at $\epsilon_F$. The average el–ph coupling constant $\lambda$, which quantifies the coupling strength as well as the Allen–Dynes characteristic phonon frequency $\omega_{Ho}$ [38], are related to the Eliashberg function as

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

(3)

and

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

(4)

Finally, the superconducting transition temperature $T_c$ was estimated for each case by solving numerically the isotropic Migdal–Eliashberg gap equations [39–41], using the respective $\alpha^2 F(\omega)$ for each content $x$, and treating the Coulomb pseudopotential as an adjusted parameter.

### 3. Results and discussion

#### 3.1. Structural properties

We performed structural optimizations of the cubic fluorite structure ($Fm\bar{3}m$ space group) with a primitive cell of three atoms (one metal and two hydrogens) for the two alloy systems at different values of metal content ($x$). Our volume results for the pristine metal dihydrides, ScH$_2$ and YH$_2$, under the ZPE and static schemes are in good agreement with the experimental data [34, 37], as well as the bulk modulus results respect to other calculations on literature, as we show in table 1.

Regarding the solid solutions, for Sc$_{1-x}$M$_x$H$_2$ the equilibrium volume was determined for concentrations up to $x = 0.95 (0.9)$ of electron(hole) doping, while for Y$_{1-x}$M$_x$H$_2$, the range was for contents up to $x = 0.8 (0.9)$ of electron(hole) doping. Electron-doping thresholds were determined through dynamical instabilities, observed as imaginary frequencies in the phonon dispersion for larger content $x$. For hole-doping, although dynamical stability was found for the complete range ($0 \leq x \leq 1$), the system did not behave as metallic for $x$ larger than the threshold. It is important to mention that phonon instabilities in metal hydrides induced by alloying have been observed before [20, 42, 43], where such dynamical behavior have been linked to an increase of the heat of formation (i.e., the alloys become less stable).

In figure 2, we show the evolution of the volume and the bulk modulus ($B_0$) as a function of metal M content $x$. In both alloys, Sc$_{1-x}$M$_x$H$_2$ and Y$_{1-x}$M$_x$H$_2$, increasing the electron content leads to a monotonous reduction of the volume and an increase of $B_0$, while for hole doping such tendencies are opposite. This behavior indicates a strengthening of the chemical bonding as the electron-content is increased, given by the increment of Zr and Ti content, as well as a weakening of it as the hole-content grows as a result of the increase of Sr and Ca content on the corresponding solid solutions.

In figure 3 we show our calculated cohesive energy ($E_{coh}$) for the two systems within their respective electron and hole range. This quantity is used to characterize stability of alloys and solid solutions, and is given by

$$E_{coh} = E_{tot}^{alloy} - (1 - x)E_N^{M} - xE_M^{H} - 2E_H^n,$$  

(5)

where $E_{tot}^{alloy}$ is the total energy of the $N_{1-x}M_xH_2$ alloy at content $x$, while $E_N^{M}$, $E_M^{H}$ and $E_H^n$ are the calculated total energies of the isolated atoms $N = Y, Sc; M = Sr, Zr, Ca, Ti$; and hydrogen, respectively. In general, the two solid solutions are in the stability range (negative $E_{coh}$), independent if it is hole- or electron-doping. In particular, the hole-doped systems are less stable.
stable than the pristine ones \((x = 0)\) (for \(E_{\text{coh}} < 0\), the larger the \(E_{\text{coh}}\) absolute value, the more stable the system is). For the case of electron-doped systems, although \(Y_{1-x}Y_{x}H_{2}\) follows the same observed tendency than the hole-doped systems, we found that \(Sc_{1-x}Sc_{x}H_{2}\) is more stable than the pristine one, indicating the possibility to synthesize such solid solutions experimentally.

With the optimized lattice parameter for each system at different content for their electron and hole doping regions, we proceeded to calculate their electronic and lattice dynamical properties. 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 the general effect is a noticeable softening (around 3.6\% at most). This tendency comes mainly from the unit cell expansion as the ZPE contribution to the energy is taken into account.

3.2. Electronic properties

In order to evaluate the effects of increasing the electron- and hole-content on the electronic properties of the solid solutions, we analyze the evolution of the electronic band structure and the DOS at the Fermi level, \(N(0)\).

In figure 4 we show the band structure for \(Sc_{1-x}Sc_{x}H_{2}\) and \(Y_{1-x}Y_{x}H_{2}\) at the pristine and the threshold electron (Ti, Zr) and hole (Ca, Sr) doping levels. It can be seen that a twofold degenerated state, close to the Fermi level, exists at the \(\Gamma\)-point in both pristine hydrides, which lies at 1.0 eV for ScH2 and 1.2 eV for YH2, giving place to a hole-like band at \(E_{F}\). As the electron-doping is increased, this band starts to fill up until a critical content, \(x(Ti) \approx 0.75\) and \(x(Zr) \approx 0.8\), where it is completely filled, and then changing its band character to electron-like for higher values of \(x\). This indicates that an electronic topological transition (ETT) takes place, since the Fermi surface corresponding to the hole-like band disappears and a Fermi surface with electron character emerges. At \(\Gamma\)-point there is a threefold degenerated state above the Fermi level at 0.9 eV for ScH2 and 1.1 eV for YH2, and as the electron-doping content increases on both systems, it shifts toward \(E_{F}\). For \(Sc_{1-x}Ti_{x}H_{2}\) the degeneracy of such state breaks at \(x(Ti) = 0.5\), giving place to a new twofold state that continue to move toward \(E_{F}\) as \(x\) increases, crossing it at \(x(Ti) = 0.7\), rising as an electron-like band. For \(Y_{1-x}Zr_{x}H_{2}\), instead, the shift of the threefold state toward \(E_{F}\) is monotonous, crossing \(E_{F}\) at \(x(Zr) = 0.7\), creating an electron-like band. Such behavior, like the observed at \(\Gamma\)-point, also indicates and ETT at \(\Gamma\)-point.

Analyzing the evolution of the DOS at the Fermi level, \(N(0)\), of both systems, \(Sc_{1-x}Sc_{x}H_{2}\) and \(Y_{1-x}Y_{x}H_{2}\) (see figure 5), it can be observed that \(N(0)\) presents little dispersion on the M-content range between the hole-doping of \(x = 0.6\) and electron-doping of \(x = 0.5\), for both hydrides. For higher \(x\) on the hole-doping regime, \(N(0)\) reduces drastically, giving a maximum reduction of \(\approx 60\%\) at the threshold content. At the electron doping regime, for \(x \geq 0.5\), \(N(0)\) shows an important increment of \(\approx 60\%\) and \(\approx 40\%\) for Sc- and Y-doped hydrides, respectively, indicating a steady improvement of the metallization with the increase of electron doping.

3.3. Lattice dynamics

We now discuss the lattice dynamical properties as a function of doping within the stability range of each solid-solution. The phonon dispersion is presented on figure 6 including their respective phonon linewidth \(\gamma_{q}\) and the PHDOS for \(Sc_{1-x}Sc_{x}H_{2}\) and \(Y_{1-x}Y_{x}H_{2}\) at the pristine \(x = 0\) and the threshold electron (Ti, Zr) and hole (Ca, Sr) doping contents. In general, for both systems, the optical and acoustic branches soften as the hole-doping increases, while they are shifted to higher frequencies as the electron-doping rises. In
Figure 4. Electronic band structure and DOS, for $\text{Sc}_1-x\text{M}_x\text{H}_2$ and $\text{Y}_1-x\text{M}_x\text{H}_2$ at the pristine ($x = 0$) and the threshold electron (Ti, Zr) and hole (Ca, Sr) doping levels.

Figure 5. Evolution of the total DOS at the Fermi level, $N(0)$, for $\text{Sc}_1-x\text{M}_x\text{H}_2$ and $\text{Y}_1-x\text{M}_x\text{H}_2$ as a function of the M content $x$.

3.4. Electron–phonon and superconducting properties

With the lattice dynamics information, the electron–phonon spectral functions $\alpha^2 F(\omega)$ were calculated for the entire range of hole- and electron-doping stable regimes. As can be seen from $\alpha^2 F(\omega)$ for the threshold electron- and hole-doping contents, as well as the pristine cases in figure 7, the electron(hole)-doping increases on both systems, the optical region of the Eliashberg function shifts to higher(lower) frequencies, while the acoustical one gets wider(narrower).

As the Eliashberg spectral function determines the el–ph coupling parameter $\lambda$ (see equation (3)), its evolution as a function of frequency, $\lambda(\omega)$, is shown in figure 7. It can be observed that the main contribution to $\lambda$ comes from the the acoustic region, reaching almost its complete value if only such frequency regime is taken into account. As the electron-doping content increases, the softening of the acoustic region boosts $\lambda$, leaving the optical one with a very minor effect. For the hole-doping case, the acoustic region loses weight, which reduces $\lambda$, and despite of the softening of the optical region, this is not large enough to increase its value.

In figure 8 the evolution of the average effective frequency $\omega_{\text{ln}}(x)$ (see equation (4)) and $\lambda(x)$ are presented for the studied solid solutions, as a function of M content ($x$). For both solid solutions, $\omega_{\text{ln}}(x)$ shows minor changes on the hole-doping regime. However, on the electron-doping region it starts to exhibit a decline at $x = 0.4$, reaching the minimum value on the entire range (around 10 meV) at the threshold $x$ content on each case. $\lambda(x)$, for both systems, keeps fairly constant (around...
Figure 7. Eliashberg function and the partial integrated el–ph coupling parameter $\lambda(\omega)$ for Sc$_{1-x}$M$_x$H$_2$ and Y$_{1-x}$M$_x$H$_2$ at $x = 0$ and at the threshold electron- and hole-doping content $x$ for each solid solution.

Figure 8. The Allen–Dynes characteristic phonon frequency ($\omega_{ln}$) and the el–ph coupling constant ($\lambda$) for Sc$_{1-x}$M$_x$H$_2$ and Y$_{1-x}$M$_x$H$_2$ as a function of the M content ($x$).

$\lambda(0) = 0.25$ until $x = 0.5$ on the hole-doping region, and then it starts to diminish as low as 0.14 at the limit value of hole-doping contents. For electron-doping, $\lambda(x)$ decreases slightly until 0.2 at $x = 0.5$, and then it increases rapidly, reaching a maximum value of 0.42 at the threshold content on each solid solution. Thus, we have determined that, under hole-doping, the ScH$_2$ and YH$_2$ hydrides do not improve their el–ph coupling properties, showing a reduction of 44% on $\lambda$. Instead, by electron-doping, the systems reach a critical content $x \approx 0.5$ where the latent coupling is triggered, increasing $\lambda$ as high as 70%, in comparison with its value $\lambda(0)$ at the pristine systems.

Finally, the calculated el–ph coupling properties were used to obtain estimates for the superconducting critical temperature $T_c$ as a function of content $x$ for both solid solutions. Numerically solving the isotropic Migdal–Eliashberg gap equations, three different values of the Coulomb pseudopotential ($\mu^*$) were employed: $\mu^* = 0$ (which provides an upper limit for $T_c$), 0.05 and 0.1, in order to get an idea of how strong $T_c$ can be affected by the variation of $\mu^*$. In particular for ScH$_2$, we get $T_c$ equal to 2.5, 0.5 and 0.1 K for $\mu^* = 0$, 0.05, and 0.1, respectively, in good agreement with an experimental report from Fisk and Johnston [44] which shows that no superconductivity can be found above 2 K. Regarding the evolution as a function of hole- and electron-doping, it can be seen from figure 9, for both solid solutions, that $T_c$ (calculated with $\mu^* = 0$) shows a slightly increase at $x = 0.2$ on the hole-doping region, but then $T_c$ decreases quickly until $x = 0.9$, where it collapses. As a function of the electron-doping content, $T_c$ first decreases steadily until $x = 0.5$, reaching its minimum. For $x > 0.5$, $T_c$ increases rapidly, reaching a maximum $T_c$ value of 3.7 K for Sc$_{0.05}$Ti$_{0.95}$H$_2$, and 2.4 K for Y$_{0.02}$Zr$_{0.8}$H$_2$. Such behavior is basically the same when $T_c$ is calculated using $\mu^* = 0.05(0.1)$, however, now the maximum $T_c$ values are lower: 1.9(1.1) K for the Sc-hydride solid solution, and 1.2(0.6) K for the Y-hydride one. Despite the low $T_c$ values obtained, it was demonstrated that hole- and electron-doping could improve the superconducting properties of pristine metal hydrides, in the absence of applied pressure. These results could help to design and implement novel schemes, additional to applied pressure, to increase the superconducting critical temperature in other members of the ScH$_n$ and YH$_n$ hydrides.

4. Conclusions

We have performed a detailed analysis of the structural, electronic, lattice dynamics, el–ph coupling, and
superconducting properties of the metal-hydride solid-solutions Sc₁₋ₓMₓH₂ (M = Ca, Ti) and Y₁₋ₓMₓH₂ (M = Sr, Zr) as a function of the electron- and hole-doping content x. The evolution of the electronic band-structure, under electron-doping, indicates two different ETT that take place in both solid solutions: one at the L-point for x(Ti) ≈ 0.75 and x(Zr) ≈ 0.8; and another at the Γ-point for x ≈ 0.7 in both systems. While N(0) is not improved in the whole hole-doping region, and even decreasing drastically for x ≥ 0.6, at the electron-doping regime for x ≥ 0.5, however, N(0) shows an important increment of approximately 60% and 40% for Sc- and Y-doped hydrides, respectively, indicating a steady improvement of the metallization. Simultaneously, the phonons soften by the hole-doping, whereas it harden for electron-doping. Interestingly, the linewidths reduce for the former, and increase for the latter, a behavior that indicates a suppression or increment, respectively, of the el–ph coupling, which is confirmed by the evolution of λ(x). In particular, under hole-doping, both hydrides do not improve λ, rather, its value drops approximately 44% respect to its value at the pristine systems. Instead, by electron-doping, both solid-solutions reach a critical content x ≈ 0.5 where the latent coupling is triggered, increasing λ as high as 70%, in comparison with λ(0). Then, due to all above, we found that for the hole-doping region the superconducting critical temperature shows a slightly increase at x = 0.2, but then it decreases quickly until x = 0.9, where it collapses. For the electron-doping regime, T_c reach a maximum value of 3.7(1.1) K for Sc₀.₉₅Ti₀.₀₅H₂, and 2.0(0.6) K for Y₀.₂Zr₀.₈H₂ taking μ = 0.0(0.1). Then, our results shown that, in the absence of applied pressure, the hole- and electron-doping could improve the superconducting properties of pristine metal hydrides.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

ORCID iDs

S Villa-Cortés © https://orcid.org/0000-0001-8009-645X
O De la Peña-Seaman © https://orcid.org/0000-0001-6590-3807

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