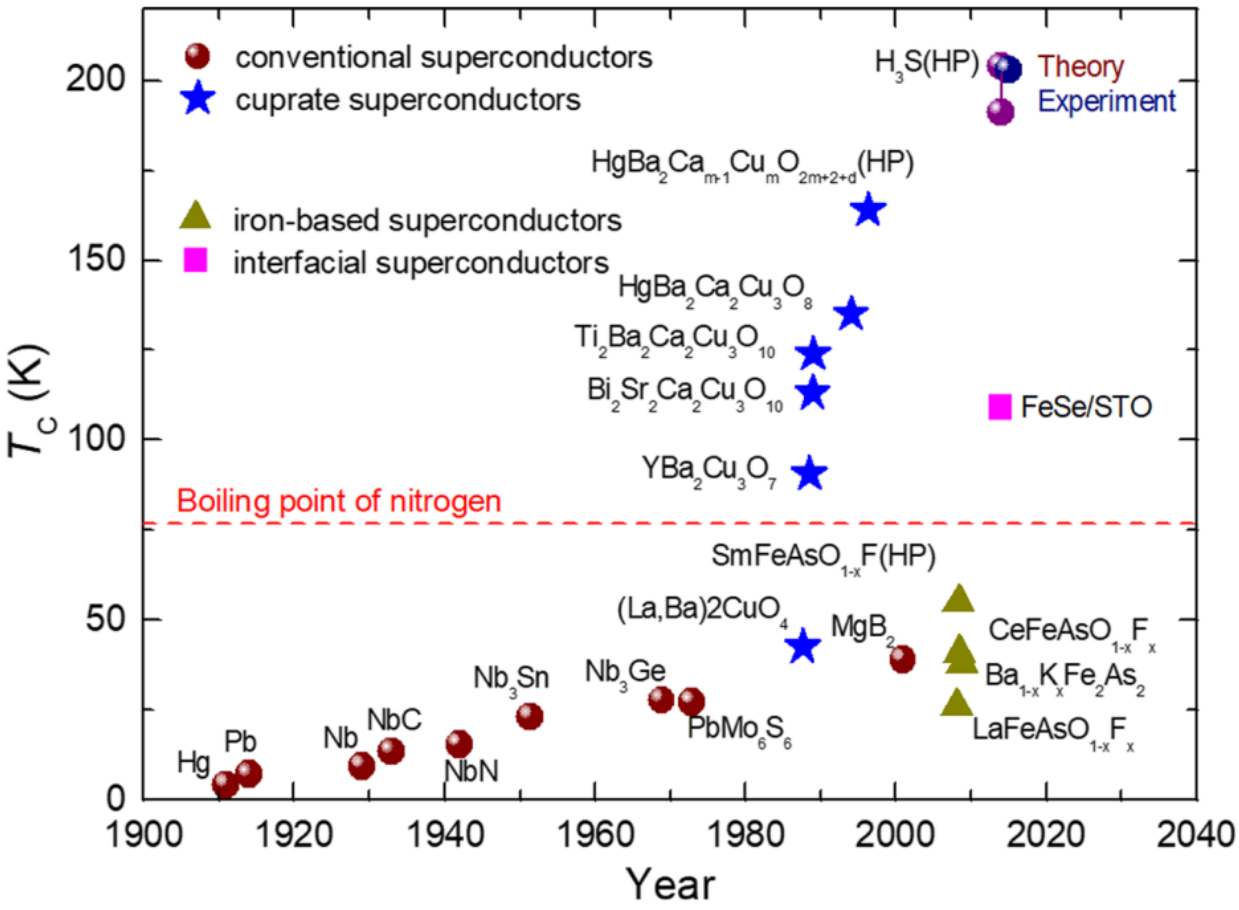
# Superconductivity on Metal Hydrides

**Sergio Villa Cortés**

Instituto de Física - BUAP

$5^{th}$ School of Superconductivity - México

# The early days of room-temperature superconductivity




*Defang Duan, Hongyu Yu, Hui Xie and Tian Cui. Journal of Superconductivity and Novel Magnetism (2019) 32:53–60*

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LETTER

doi:10.1038/nature14964

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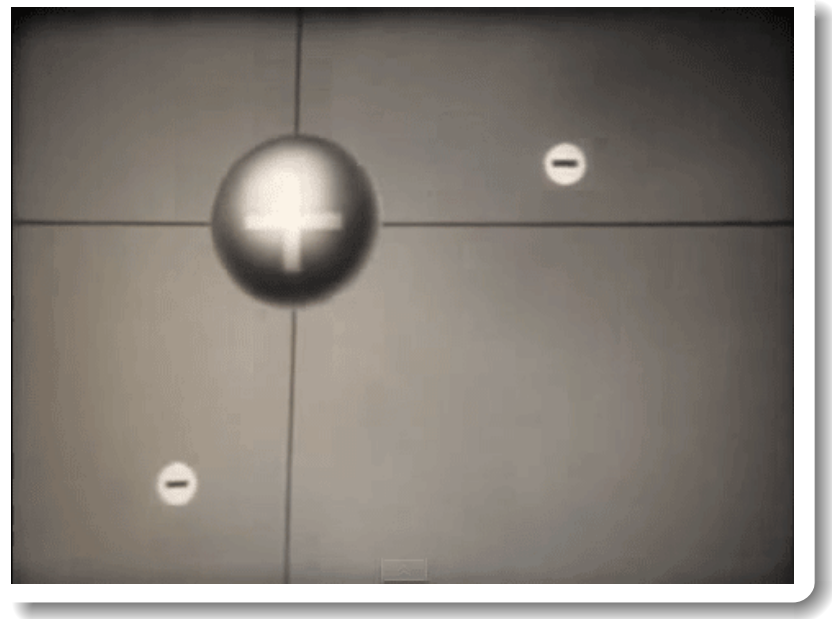
# First, the Cooper Pairs

**Paired electrons moving freely (without resistance) through a crystal lattice**



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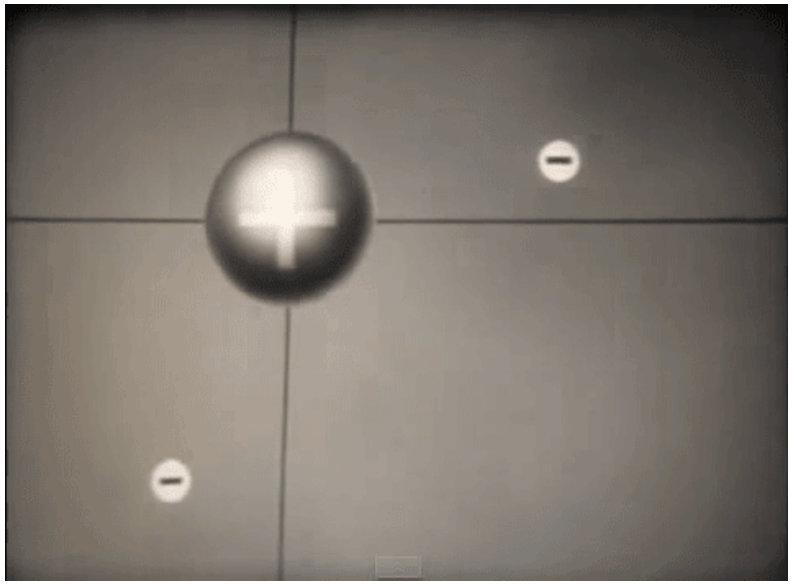
LEON N. COOPER

*Physics Department, University of Illinois, Urbana, Illinois*

(Received September 21, 1956)

IT has been proposed that a metal would display superconducting properties at low temperatures if the one-electron energy spectrum had a volume-independent energy gap of order $\Delta \simeq kT_c$, between the ground state and the first excited state.[1,2] We should like to point out how, primarily as a result of the exclusion principle, such a situation could arise.



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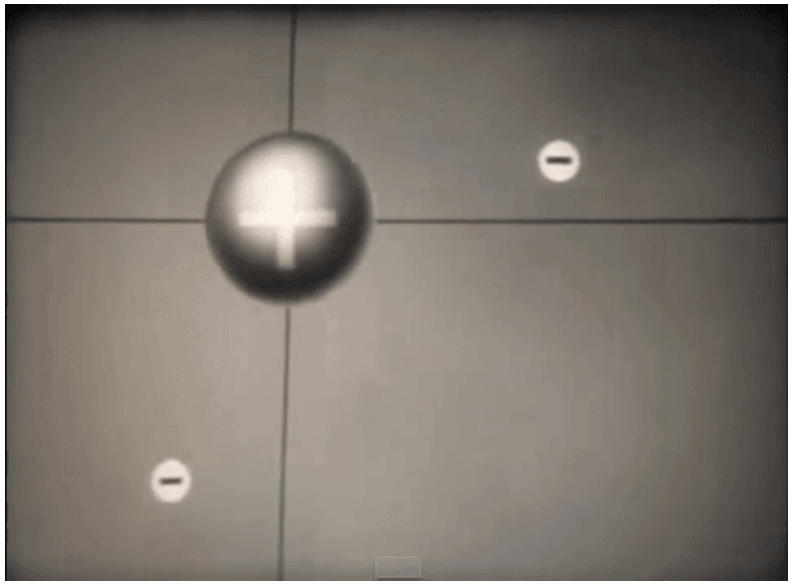

.. an attractive interaction between two fermions near the Fermi surface leads to the appearance of a bound pair. The noninteracting ground state lowers its energy by an amount $\Delta$, becoming unstable.

# The BCS Theory: The First Microscopic Theory ....

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# Migdal Formalism: Electrons in an electron-ion system

SOVIET PHYSICS JETP VOLUME 34 (7), NUMBER 1 JULY, 1958

*APPLICATION OF QUANTUM FIELD THEORY METHODS TO THE MANY BODY PROBLEM*

V. M. GALITSKII and A. B. MIGDAL

Moscow Engineering-Physics Institute

Submitted to JETP editor July 12, 1957; resubmitted October 24, 1957.

J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 139-150 (January, 1958).

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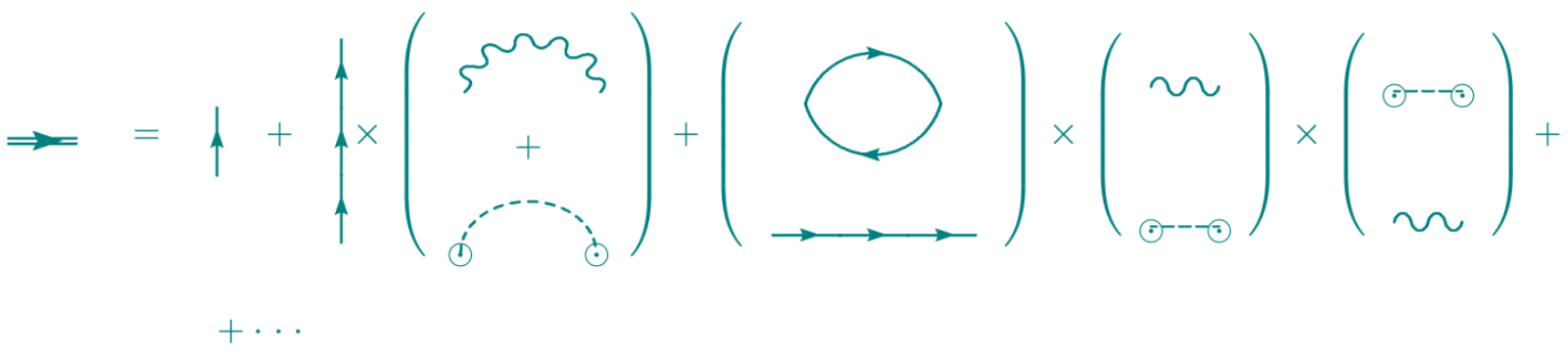

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SOVIET PHYSICS JETP VOLUME 34 (7), NUMBER 6 DECEMBER, 1958

*INTERACTION BETWEEN ELECTRONS AND LATTICE VIBRATIONS IN A NORMAL METAL*

A. B. MIGDAL

Moscow Institute of Engineering Physics

Submitted to JETP editor July 12, 1957; resubmitted March 20, 1958

J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 1438-1446 (June, 1958)

A method is developed which enables one to obtain the electron-energy spectrum and dispersion of the lattice vibrations without assuming that the interaction between electrons and phonons is small.

# The Normal State Self Energy: Electrons in an electron-ion system

*The phonons and the electrons are mutually interacting and affecting each other's properties.*

$$\Sigma\left(\boldsymbol{k}, i\omega_n\right) = \frac{1}{\beta}\sum_{\boldsymbol{k}'m}\left[\frac{\lambda_{\boldsymbol{k}\boldsymbol{k}'}\left(i\omega_n - i\omega_m\right)}{N\left(\mu\right)} - V^{eff}_{\boldsymbol{k}\boldsymbol{k}'}\right] G\left(\boldsymbol{k}', i\omega_m\right)$$

*This means that we have an effective electron-electron interaction due to the emission and absortion of phonons*

$$V^{eff}_{\boldsymbol{k}\boldsymbol{k}'} = \frac{V_{\boldsymbol{k}\boldsymbol{k}'}}{\epsilon}, \qquad g^{eff}_{\boldsymbol{k}\boldsymbol{k}'} = \frac{g_{\boldsymbol{k}\boldsymbol{k}'}}{\epsilon},$$

*and a dressed electron-phonon interaction with a phonon frequency renormalized by the accompanying electron cloud .*

# Eliashberg Generalization: Electrons in an electron-ion system

SOVIET PHYSICS JETP VOLUME 11, NUMBER 3 SEPTEMBER, 1960

*INTERACTIONS BETWEEN ELECTRONS AND LATTICE VIBRATIONS IN A SUPERCONDUCTOR*

G. M. ÉLIASHBERG

Leningrad Physico-Technical Institute, Academy of Sciences, U.S.S.R.

Submitted to JETP editor October 18, 1959

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A perturbation theory is developed for the Green's function in which the Green's function calculated for the superconducting ground state is used as the zero approximation. Dyson equations are written down from which the electron Green's function can be determined. Interaction between electrons and phonons is not assumed to be small. The spectrum and the damping of the excitations are calculated.

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SOVIET PHYSICS JETP VOLUME 12, NUMBER 5 MAY, 1961

*TEMPERATURE GREEN'S FUNCTION FOR ELECTRONS IN A SUPERCONDUCTOR*

G. M. ÉLIASHBERG

Leningrad Physico-Technical Institute, Academy of Sciences, U.S.S.R.

Submitted to JETP editor July 4, 1960

J. Exptl. Theoret. Phys. (U.S.S.R.) **39**, 1437-1441 (November, 1960)

The temperature Green's function for electrons in a superconductor are computed by the diagram technique for $T \neq 0$. An estimate is made of the region near the critical temperature for which the usual analysis, which makes use of a temperature-dependent gap in the excitation spectrum, is no longer valid. The magnitude of this temperature range is of the order of $(2\Delta(0)/\omega_0)^4 T_c$.

# The Superconducting State Green Function

It is defined as:

$$\hat{G}\left(\boldsymbol{k}, \tau-\tau'\right) \equiv -\left\langle T_{\tau}\left[\hat{\Psi}_{\boldsymbol{k}}(\tau)\, \hat{\Psi}_{\boldsymbol{k}}^{\dagger}\left(\tau'\right)\right]\right\rangle,$$

where the field operators are given by

$$\hat{\Psi}_{\boldsymbol{k}}=\begin{bmatrix} \hat{\psi}_{\boldsymbol{k}\uparrow} \\ \hat{\psi}_{-\boldsymbol{k}\downarrow}^{\dagger} \end{bmatrix}, \qquad \hat{\Psi}_{\boldsymbol{k}}^{\dagger}=\left[\hat{\psi}_{\boldsymbol{k}\uparrow}^{\dagger}, \hat{\psi}_{-\boldsymbol{k}\downarrow}\right].$$

This give us the Green function:

$$\hat{G}\left(\boldsymbol{k}, i\omega_n\right)=\begin{pmatrix} G\left(\boldsymbol{k}, i\omega_n\right) & \mathcal{F}\left(\boldsymbol{k}, i\omega_n\right) \\ \mathcal{F}^{\dagger}\left(\boldsymbol{k}, i\omega_n\right) & -G\left(-\boldsymbol{k}, i\omega_n\right) \end{pmatrix}.$$

# The Superconducting State Self Energy

Using diagrammatic perturbation techniques (Feynman diagrams) it is found that the Green function satisfies the Dyson equation:

$$\hat{G}^{-1}\left(\boldsymbol{k}, i\omega_n\right) = \hat{G}_0^{-1}\left(\boldsymbol{k}, i\omega_n\right) - \hat{\Sigma}\left(\boldsymbol{k}, i\omega_n\right),$$

where the single particle Green function is given by:

$$\hat{G}_0^{-1}\left(\boldsymbol{k}, i\omega_n\right) = \begin{pmatrix} i\omega_n - \varepsilon_k & 0 \\ 0 & i\omega_n + \varepsilon_k \end{pmatrix},$$

$$\hat{\Sigma}\left(\boldsymbol{k}, i\omega_n\right) = \frac{1}{\beta}\sum_{\boldsymbol{k}' m}\left[\frac{\lambda_{\boldsymbol{k}\boldsymbol{k}'}\left(i\omega_n - i\omega_m\right)}{N\left(\mu\right)} - V_{\boldsymbol{k}\boldsymbol{k}'}^{eff}\right]\hat{\tau}_3\hat{G}\left(\boldsymbol{k}', i\omega_m\right)\hat{\tau}_3$$

# The Linearized Migdal-Eliashberg Equations (LMEE) with constant DOS are

$$\rho\bar{\Delta}_n = \pi T \sum_m \left[\lambda_{nm} - \mu^* - \delta_{nm}\frac{|\tilde{\omega}_n|}{\pi T}\right]\bar{\Delta}_m,$$

here $\rho$ is the breaking parameter that becomes zero at $T_c$. The frequency $\tilde{\omega}_n$ is

$$\tilde{\omega}_n = \omega_n + \pi T \sum_m \lambda_{nm} sign\left(\omega_m\right),$$

and $i\omega_n$ are the Matsubara frecuencies, $i\omega_n = i\pi T\left(2n+1\right)$. The coupling parameter $\lambda_{nm}$ is defined as

$$\lambda_{nm} = 2\int_0^\infty \frac{d\omega\omega\alpha^2 F\left(\omega\right)}{\omega^2 + \left(\omega_n - \omega_m\right)^2}.$$

# The Linearized Migdal-Eliashberg Equations (LMEE) with energy dependent DOS are

$$\rho\bar{\Delta}_n = \pi T \sum_m \left[ (\lambda_{nm} - \mu^*)\, \tilde{N}(|\tilde{\omega}_m|) - \delta_{nm}\, |\tilde{\omega}_m| \right] \bar{\Delta}_m,$$

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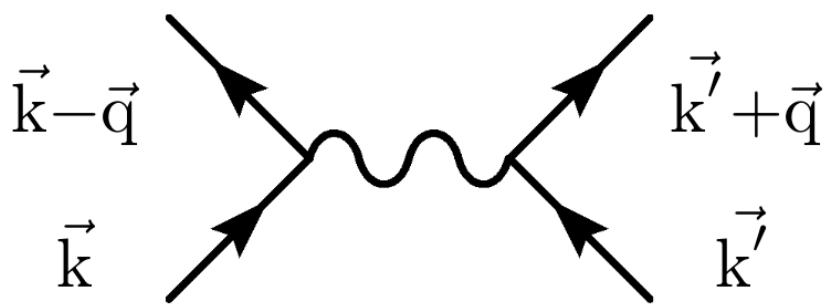
and $i\omega_n$ are the Matsubara frecuencies, $i\omega_n = i\pi T\,(2n+1)$. The function $\tilde{N}(|\tilde{\omega}_m|)$ is defined as

$$\tilde{N}(|\tilde{\omega}_n|) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\varepsilon \frac{N(\varepsilon)}{N(\mu)} \frac{|\tilde{\omega}_n|}{|\tilde{\omega}_n|^2 + \varepsilon^2}.$$

# 1960, in conventional superconductors we need:



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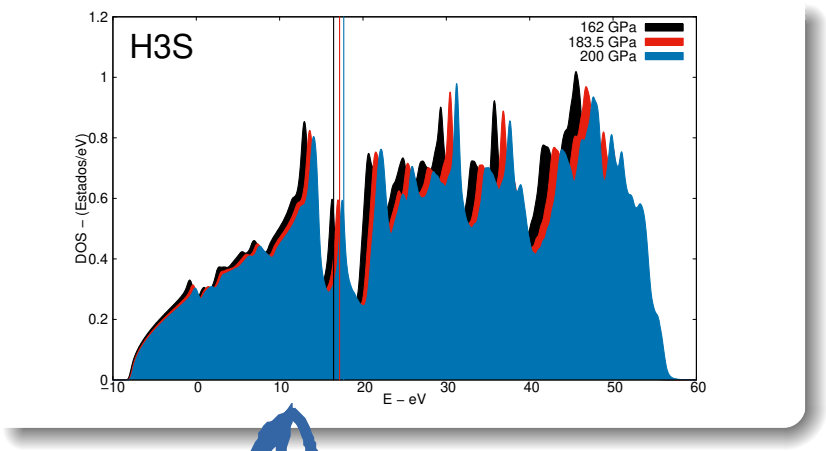


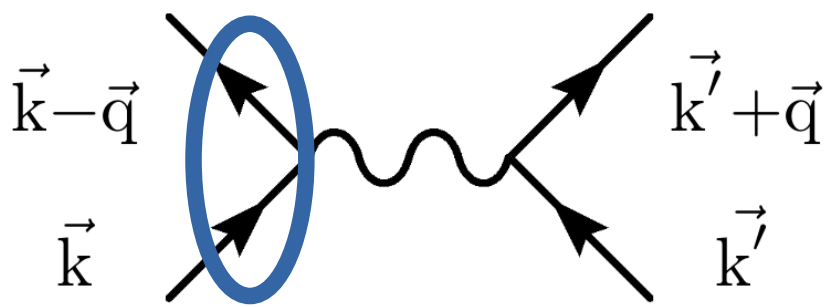

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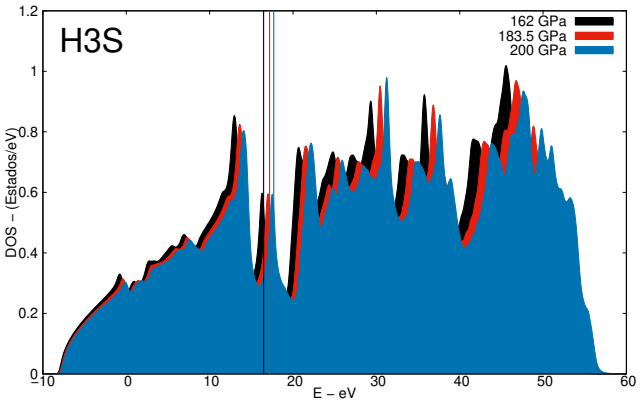


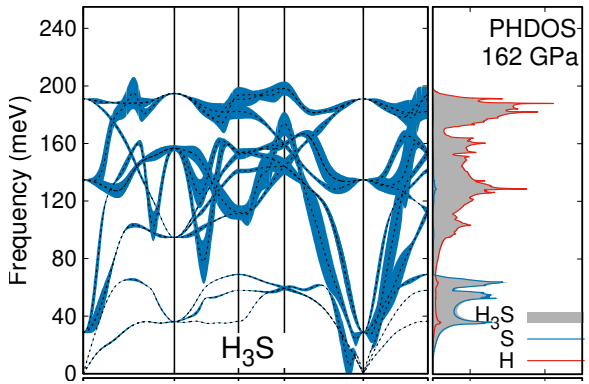


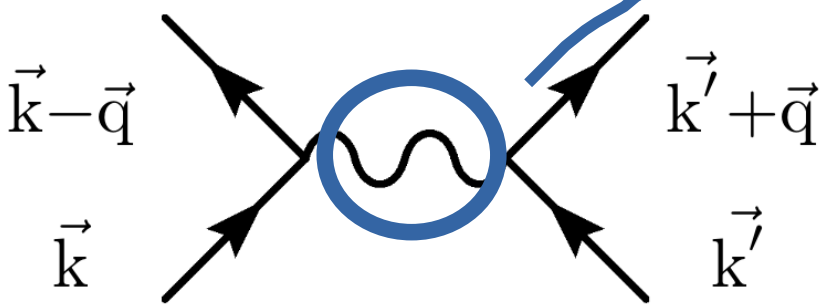

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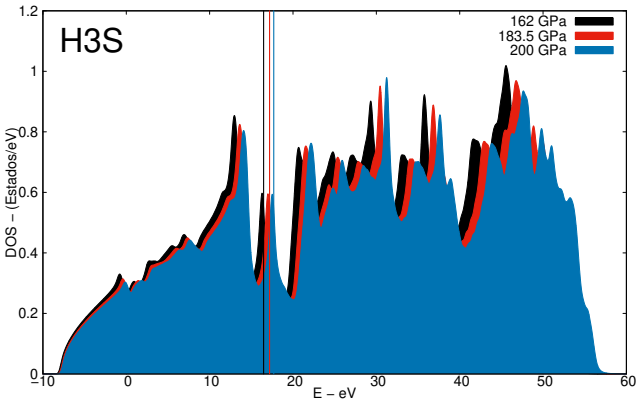


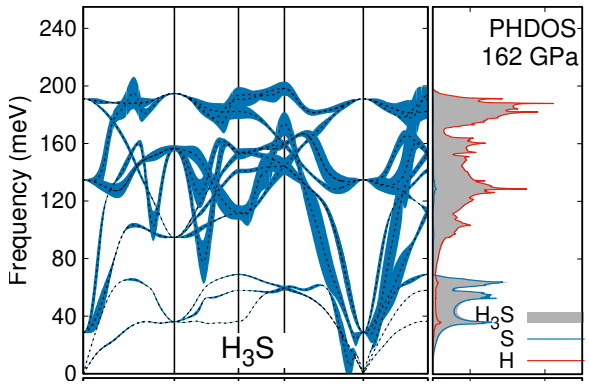


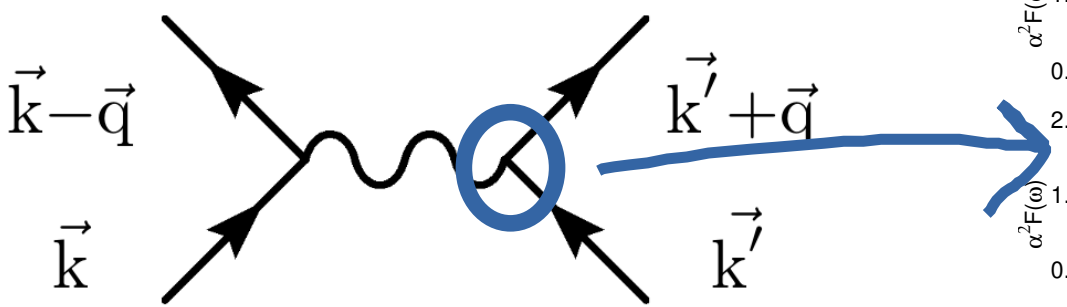


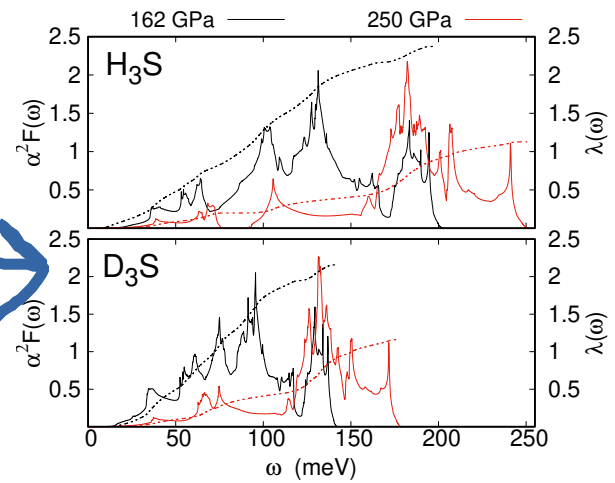

# The early days of room-temperature superconductivity

VOLUME 21, NUMBER 26 PHYSICAL REVIEW LETTERS 23 DECEMBER 1968

## METALLIC HYDROGEN: A HIGH-TEMPERATURE SUPERCONDUCTOR?

N. W. Ashcroft
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14850
(Received 3 May 1968)

Application of the BCS theory to the proposed metallic modification of hydrogen suggests that it will be a high-temperature superconductor. This prediction has interesting astrophysical consequences, as well as implications for the possible development of a superconductor for use at elevated temperatures.

VOLUME 92, NUMBER 18 PHYSICAL REVIEW LETTERS week ending 7 MAY 2004

## Hydrogen Dominant Metallic Alloys: High Temperature Superconductors?

N.W. Ashcroft
*Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853-2501, USA*
*Donostia International Physics Center, San Sebastian, Spain*
(Received 29 December 2003; published 6 May 2004)

The arguments suggesting that metallic hydrogen, either as a monatomic or paired metal, should be a candidate for high temperature superconductivity are shown to apply with comparable weight to alloys of metallic hydrogen where hydrogen is a dominant constituent, for example, in the dense group IVa hydrides. The attainment of metallic states should be well within current capabilities of diamond anvil cells, but at pressures considerably lower than may be necessary for hydrogen.

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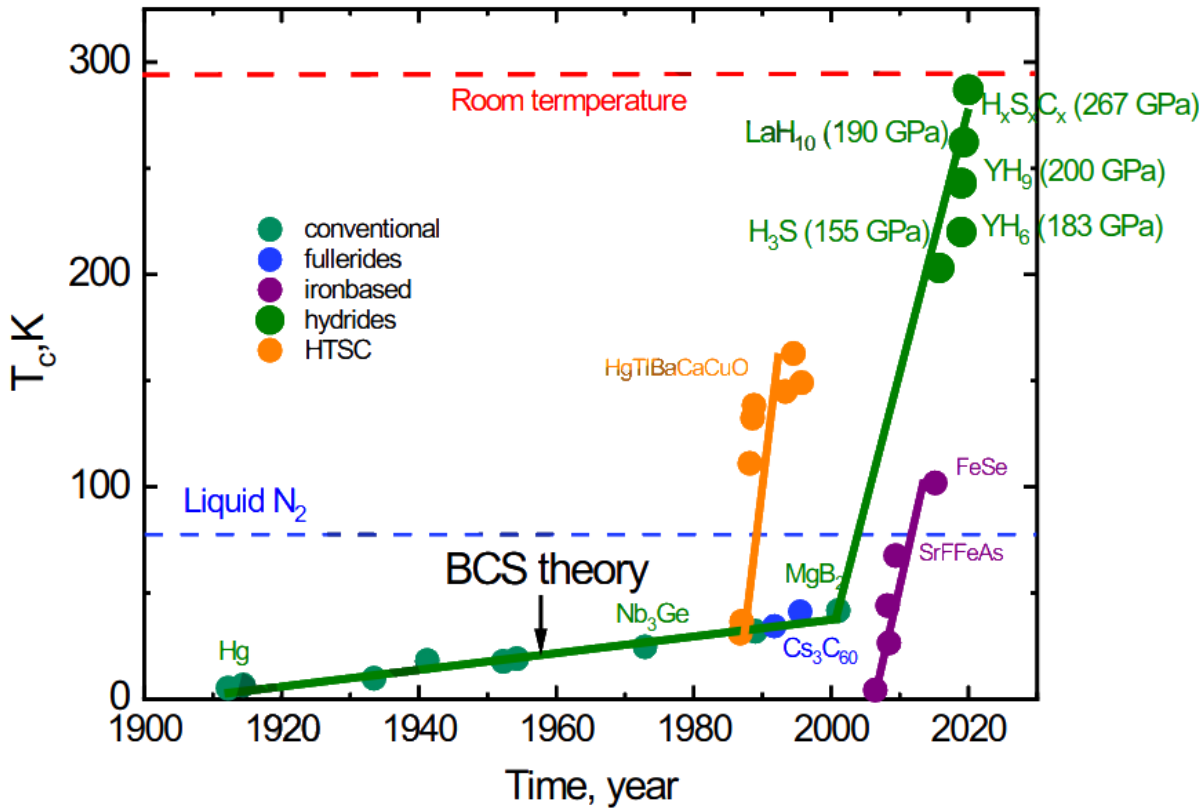


*The 2021 Room-Temperature Superconductivity Roadmap, Lilia Boeri et al 2021 J. Phys.: Condens. Matter in press https://doi.org/10.1088/1361-648X/ac2864*

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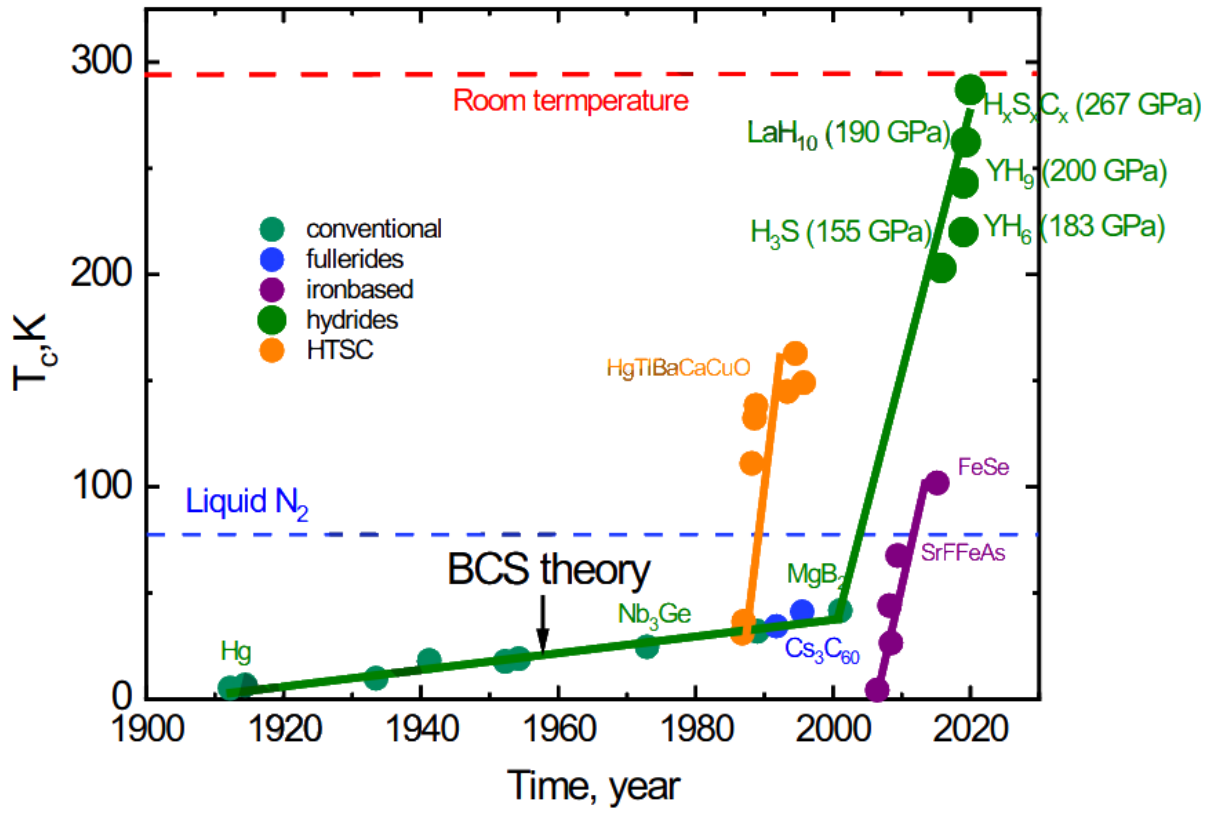


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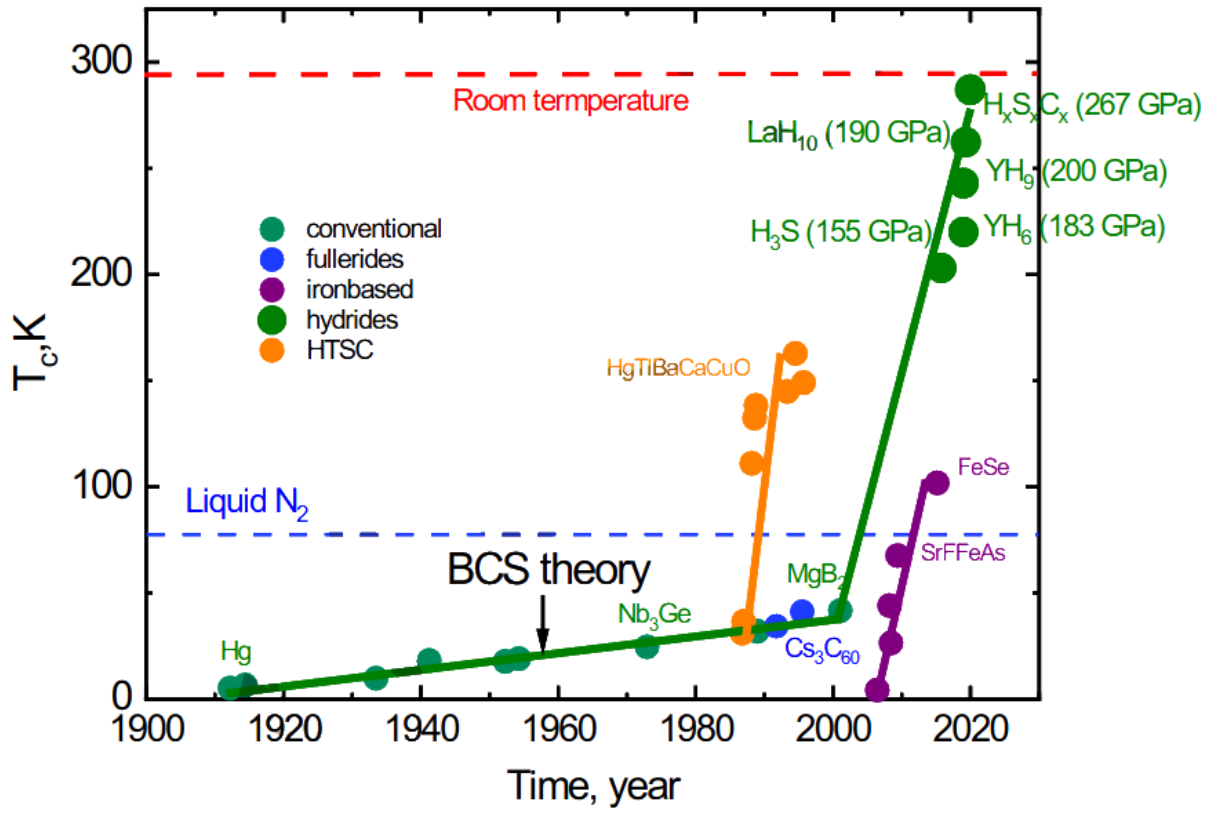


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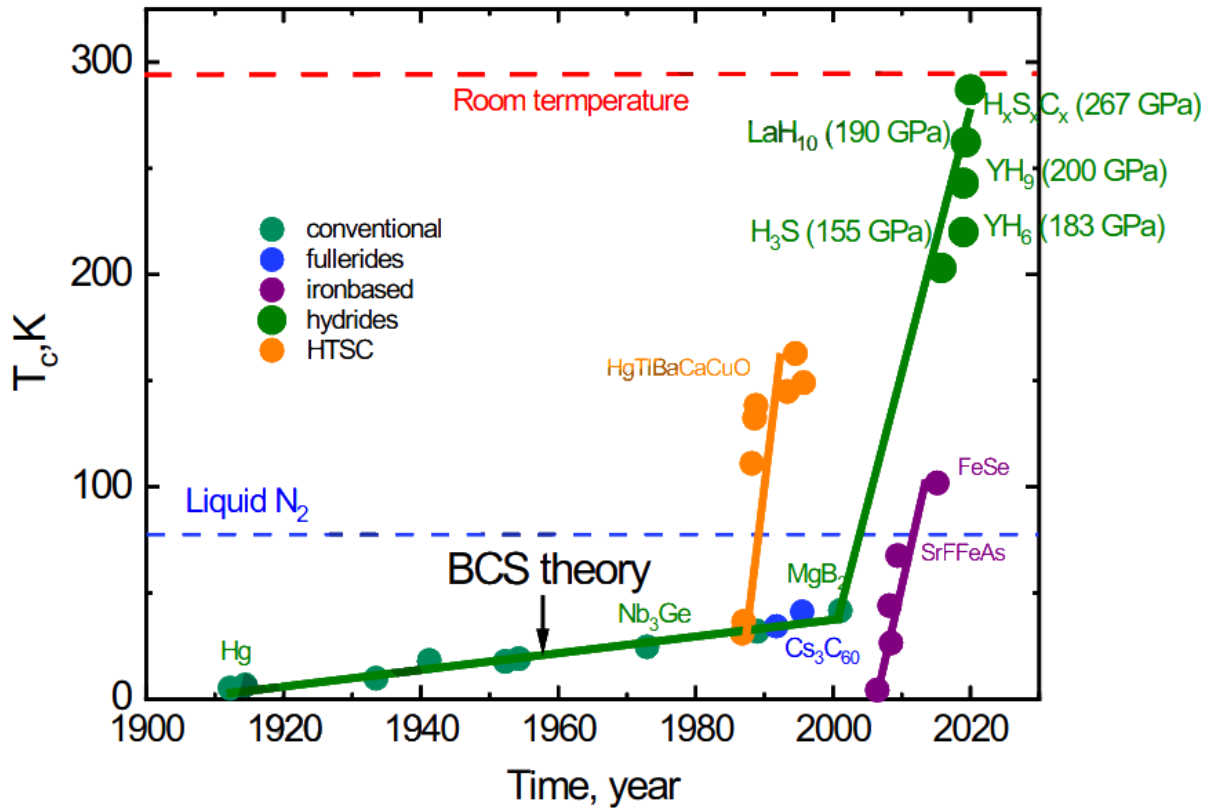


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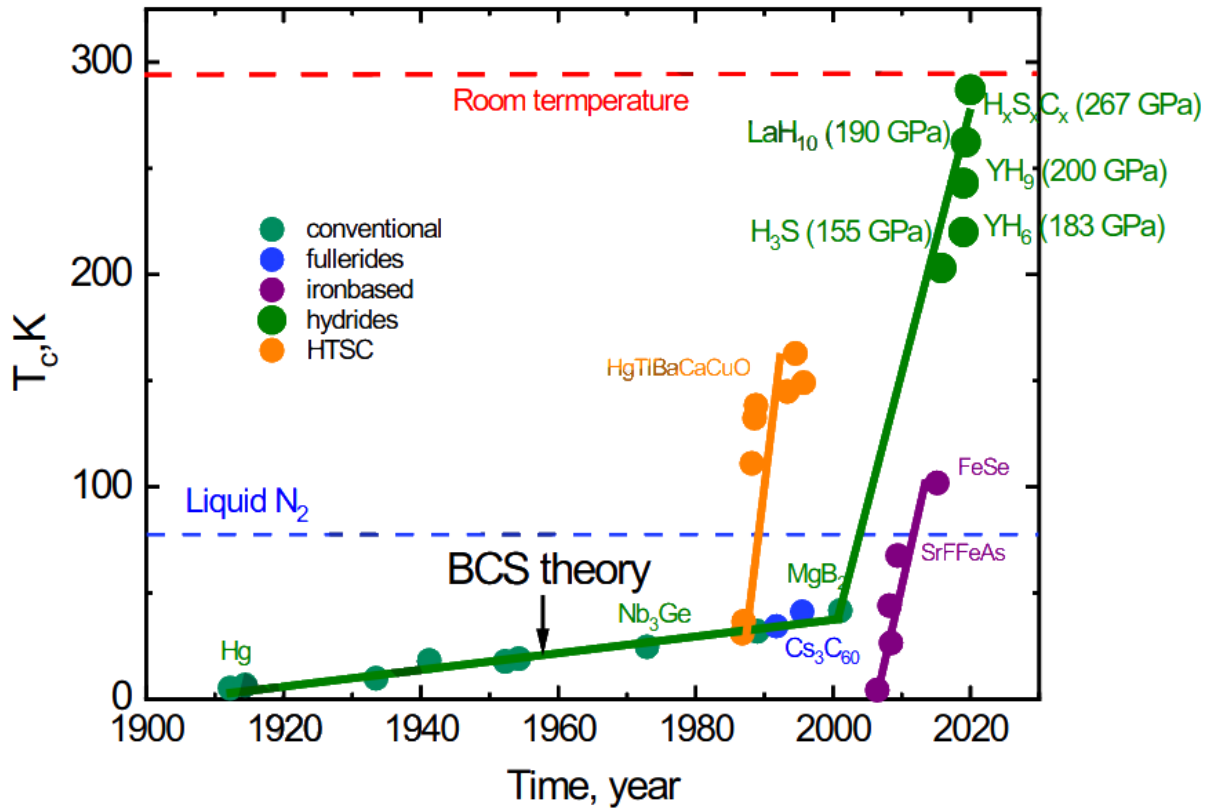


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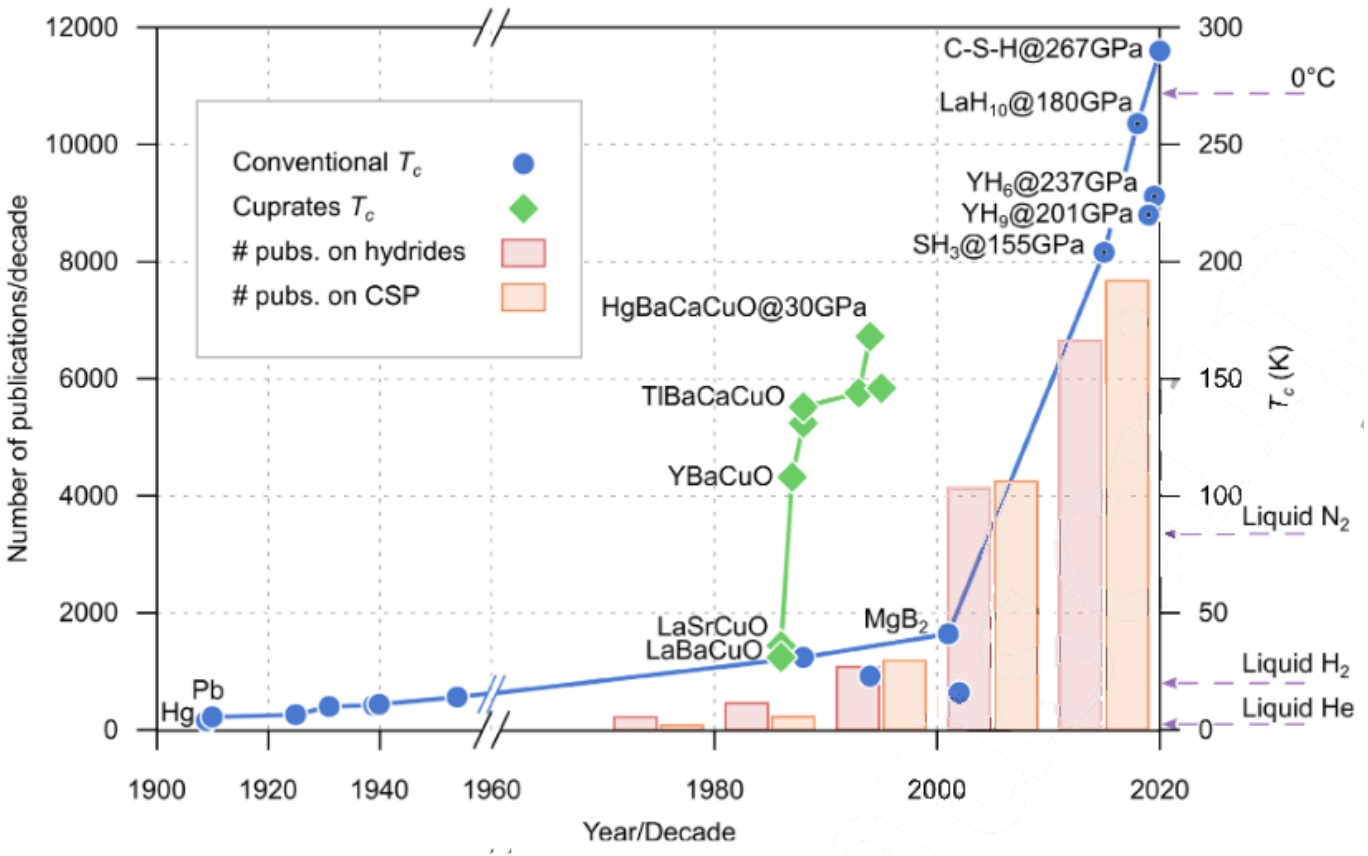
2015- $H_3S$, 2019 - $LaH_{10}$, 2020 - Carbonaceous Sulfur Hydride, 2021 - $YH_9$ - $YH_6$

# The early days of room-temperature superconductivity at high pressure conditions




*The 2021 Room-Temperature Superconductivity Roadmap, Lilia Boeri et al 2021 J. Phys.: Condens. Matter in press https://doi.org/10.1088/1361-648X/ac2864*

# The early days of room-temperature superconductivity at ambient pressure

Besides applied pressure, doping is another procedure for metallization, thus to induce or increase superconductivity by enhancing some properties like the electronic density of states at the Fermi level (N (0)) or the electron-phonon coupling.

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**LiH, NaH, and KH**

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**RbH**

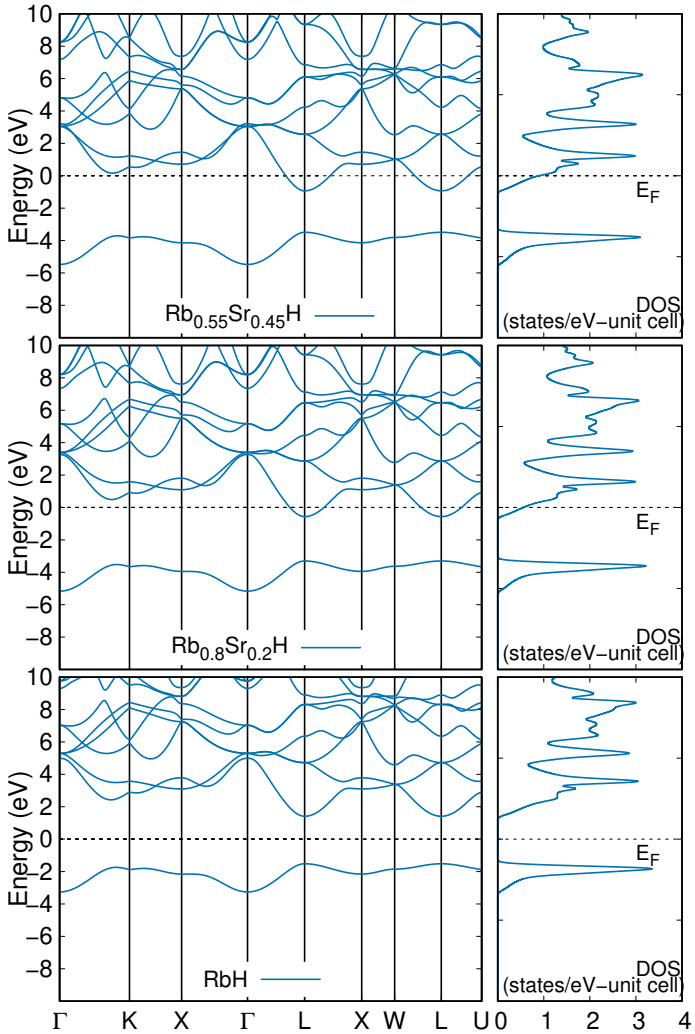
## *Enhancement*

*Dr. Sergio Villa* and Prof. Omar de la Peña

**$ScH_2$, $YH_2$**

**$ScH_3$, $YH_3$**

# Metallization: From semiconductor to superconductor




*Electronic band structure and density of states (DOS), for $Rb_{x-1}Sr_xH$ at the pristine ($x = 0$) and the threshold electron (Sr) doping levels.*

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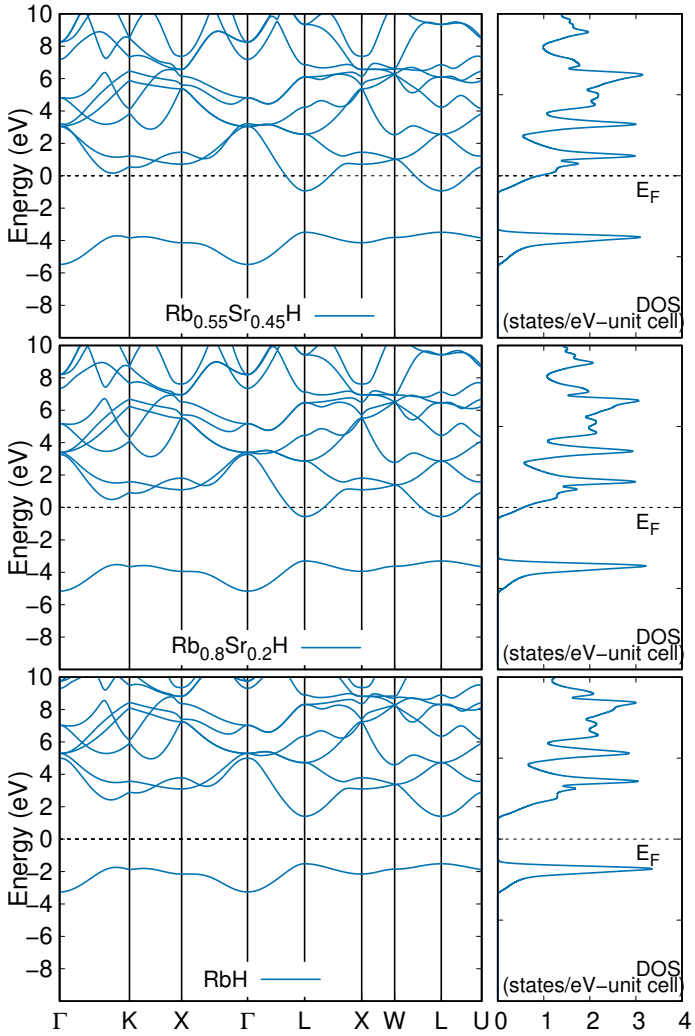


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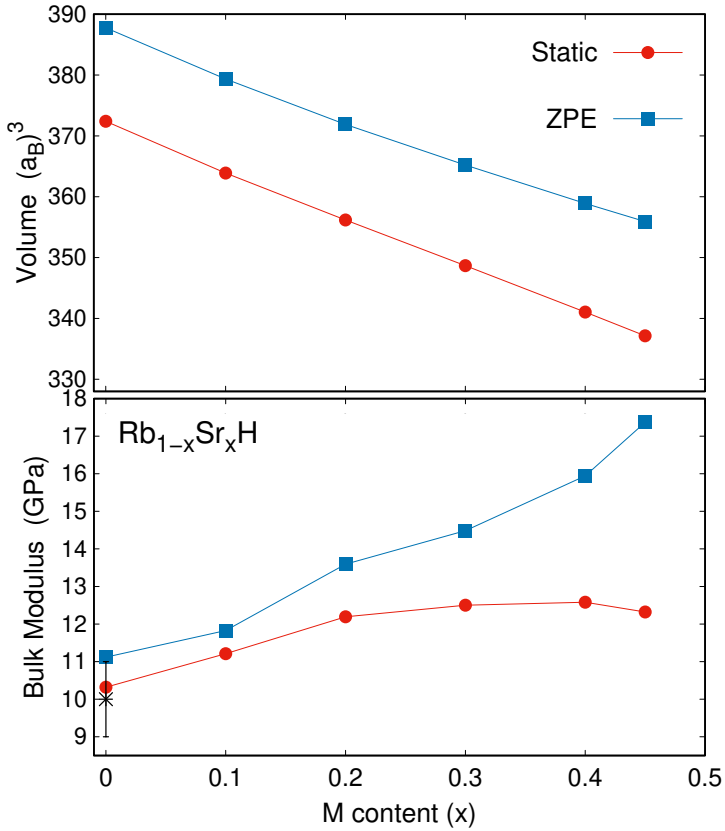


*Volume and bulk modulus ($B_0$) for $Rb_{x-1}Sr_xH$ as a function of Sr content ($x$).*

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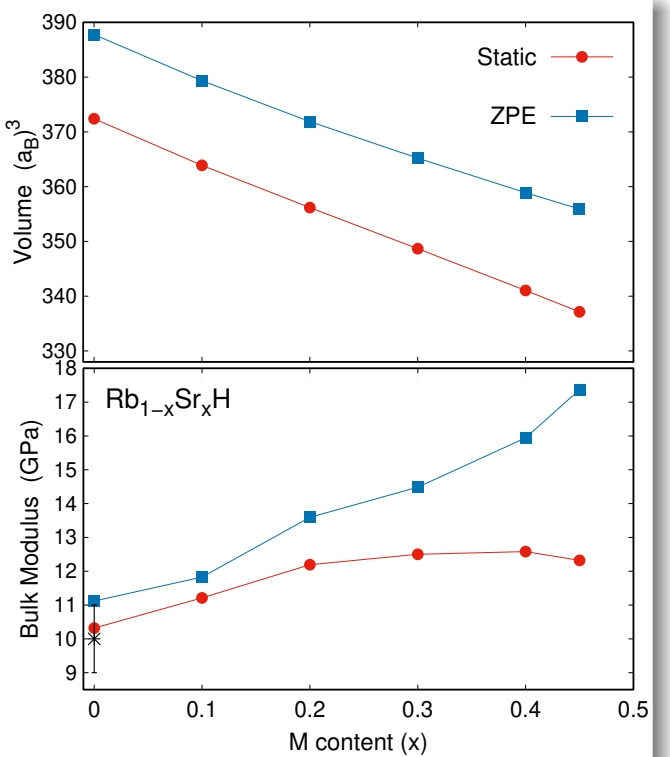


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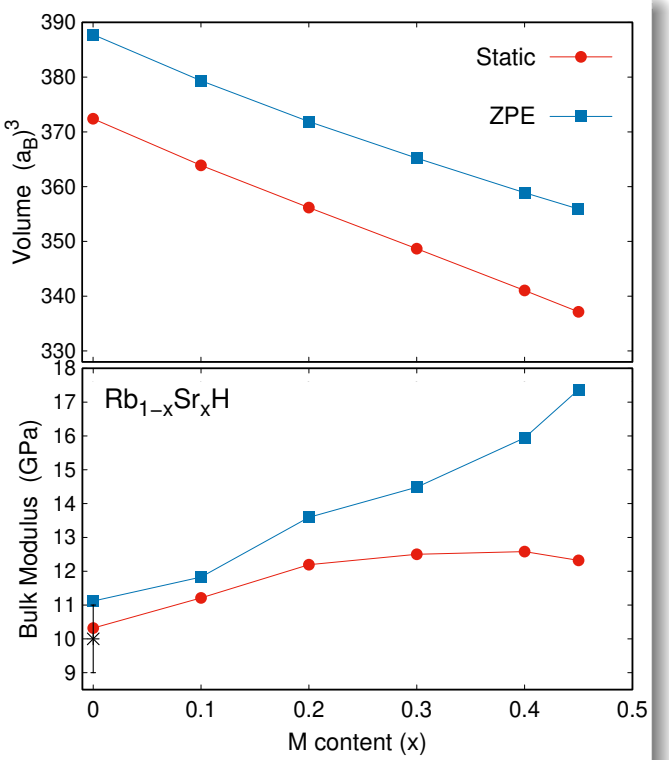


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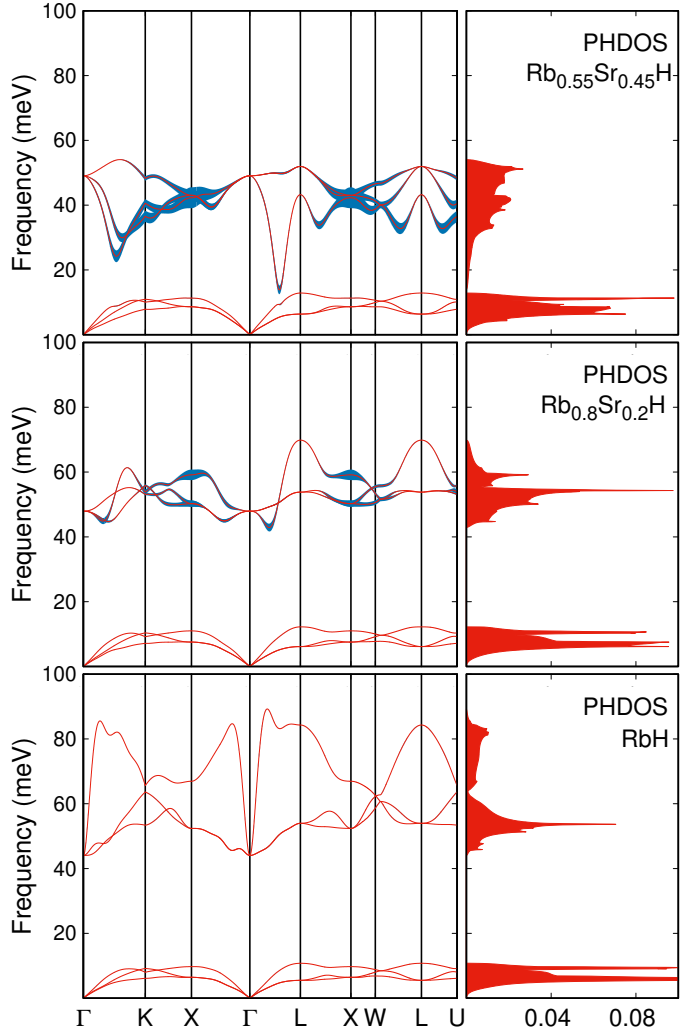


*Phonon dispersion, linewidths (as vertical lines along the phonon branches) and PHDOS for $Rb_{x-1}Sr_xH$ at the pristine and the threshold electron (Sr) doping contents.*

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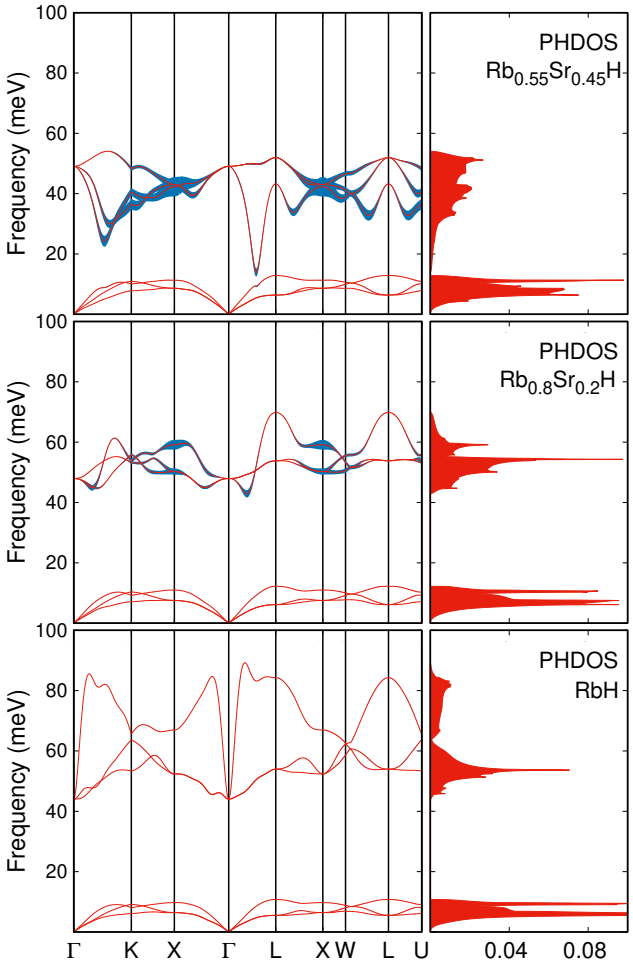


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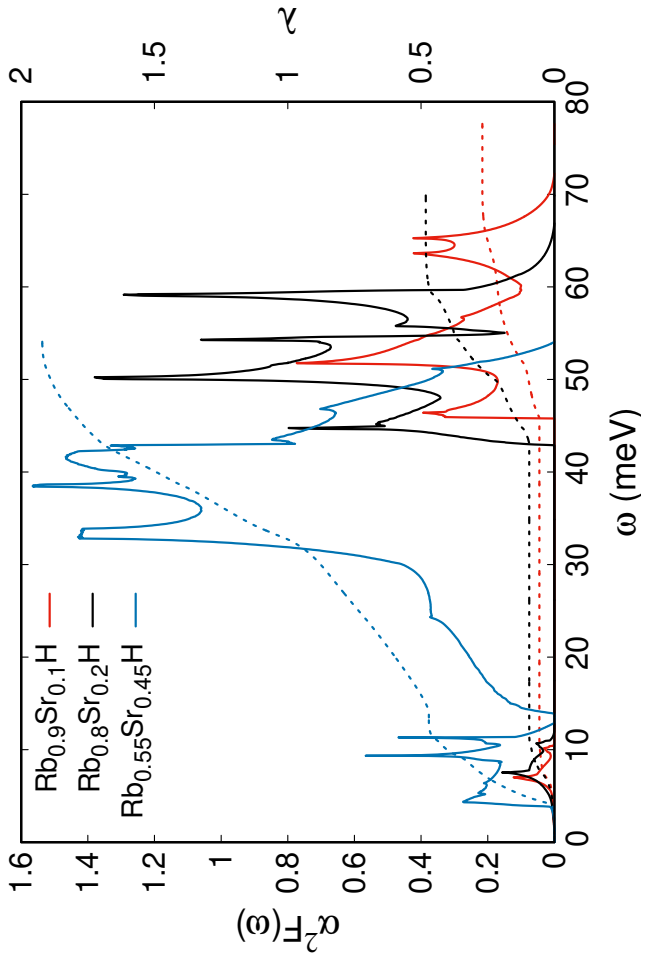
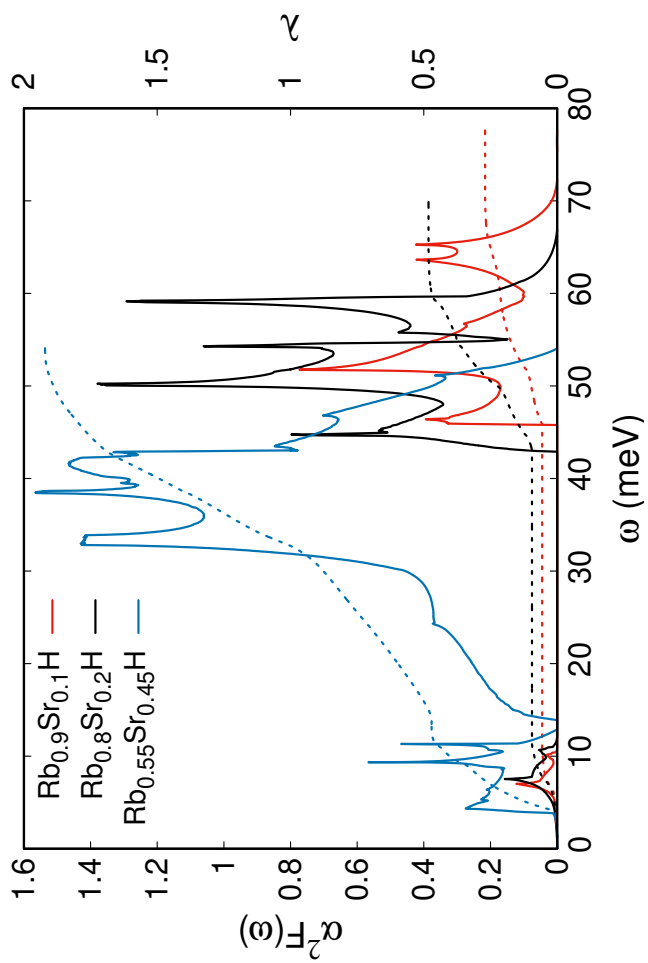



*Eliashberg function and the partial integrated electron-phonon coupling parameter $\lambda(\omega)$ for $Rb_{x-1}Sr_xH$ at $x = 0$ and at the threshold electron-doping content $x$ for each solid solution.*

# Metallization: From semiconductor to superconductor

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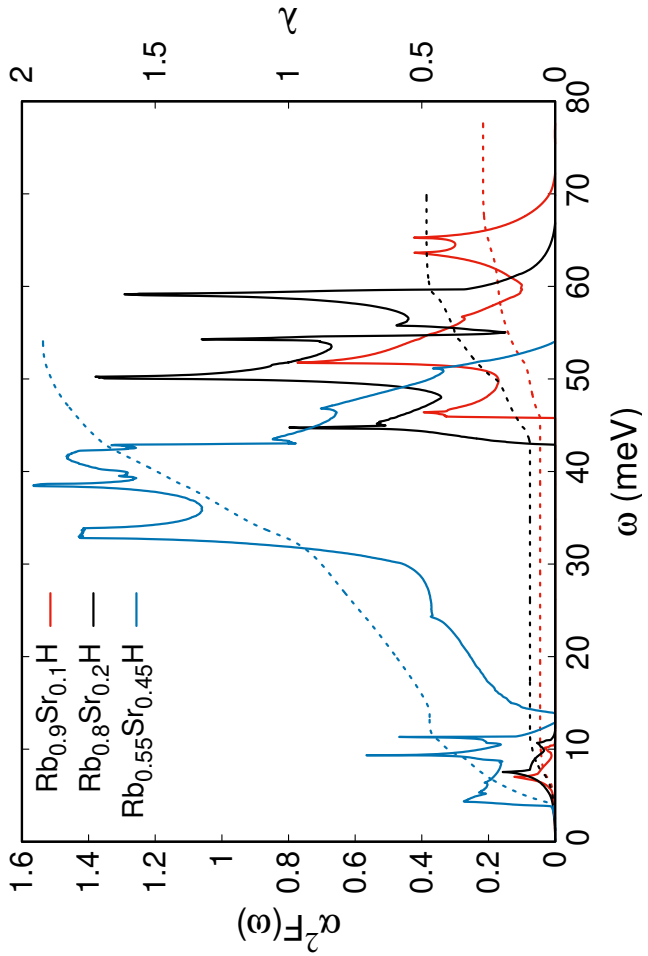


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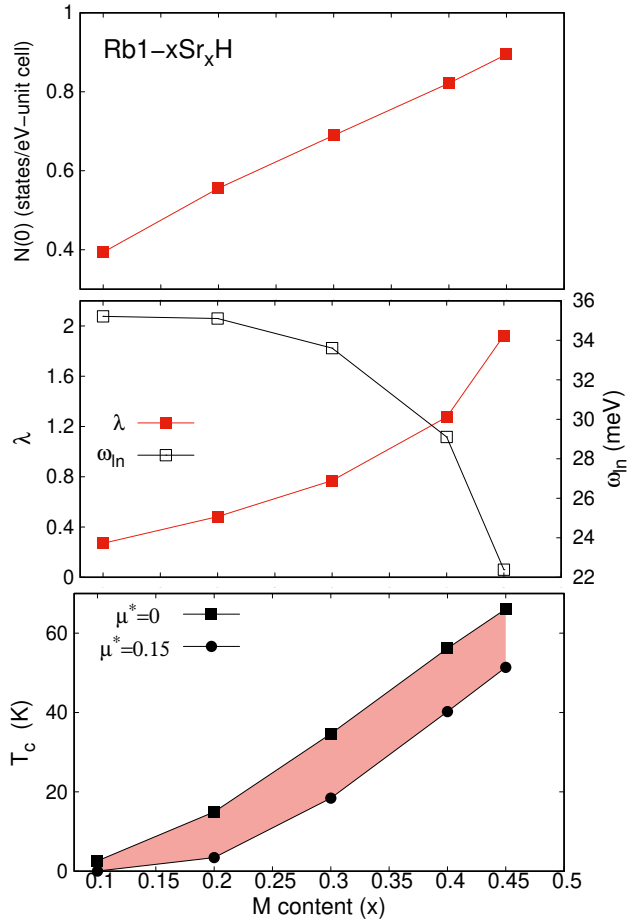


*Evolution of the total density of states at the Fermi level (N (0)), the Allen-Dynes characteristic phonon frequency ($\omega_{ln}$ ), the electron–phonon coupling constant ($\lambda$), and the superconducting critical temperature, $T_c$, calculated with $\mu^* = 0.15$ and 0, of $Rb_{x-1}Sr_xH$ at the entire range of electron-content for each solid-solution.*

# Enhancement: Holes and Electrons .....

$$CaH_x \longleftarrow ScH_x \longrightarrow TiH_x$$

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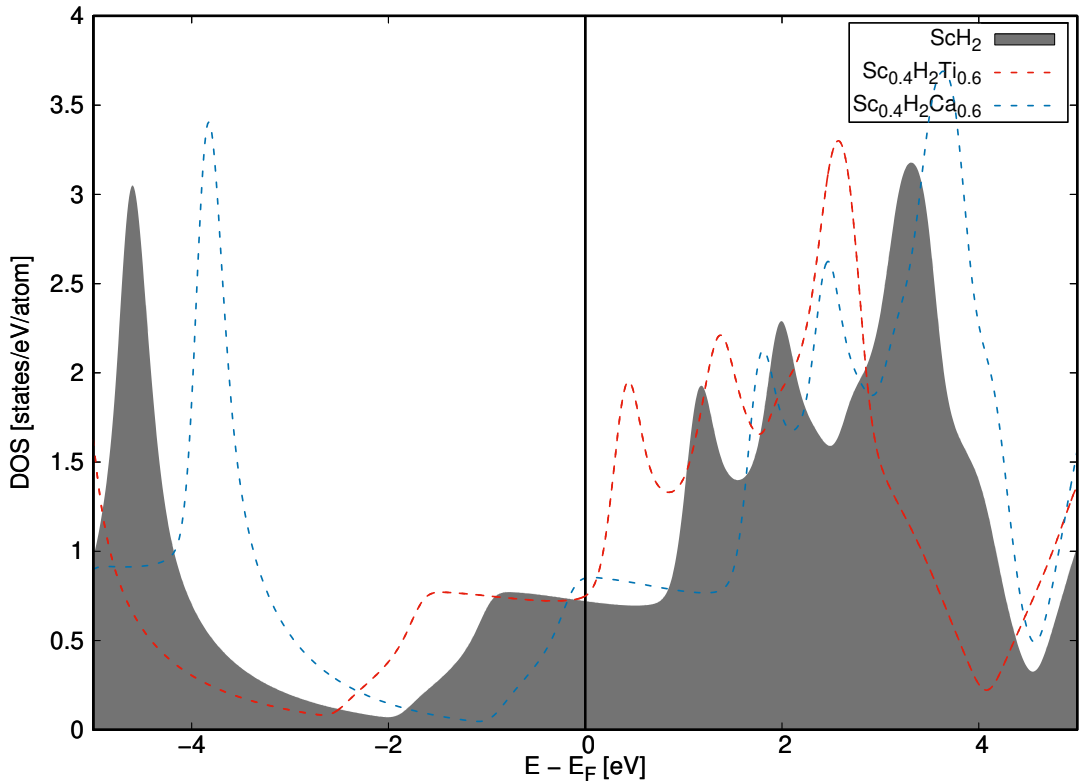
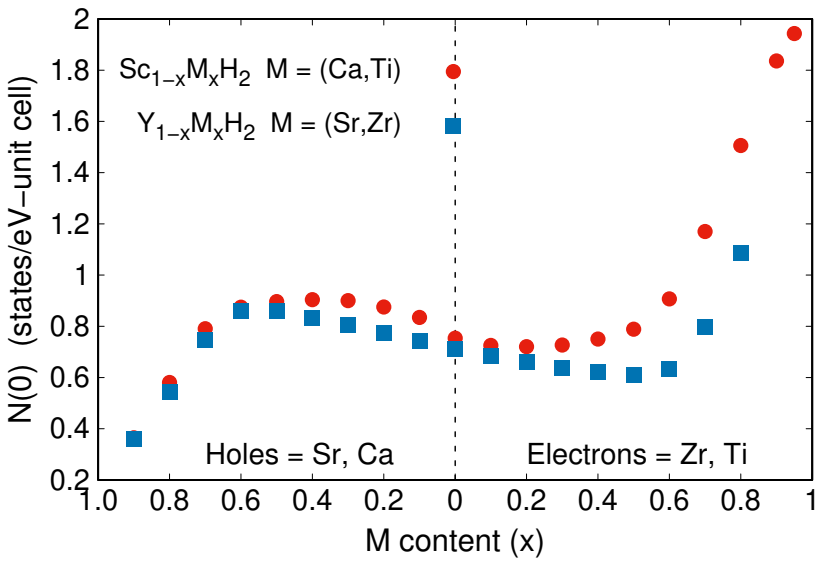


# Enhancement: Becoming a superconductor due to doping




*Evolution of the total density of states at the Fermi level, N(0), for $Sc_{x-1}M_xH_2$ and $Y_{x-1}M_xH_2$ as a function of the M content x.*

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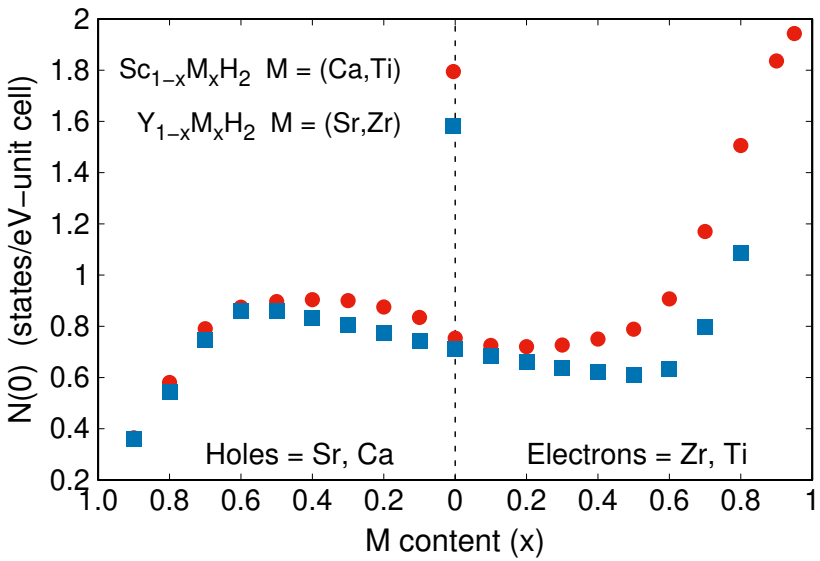


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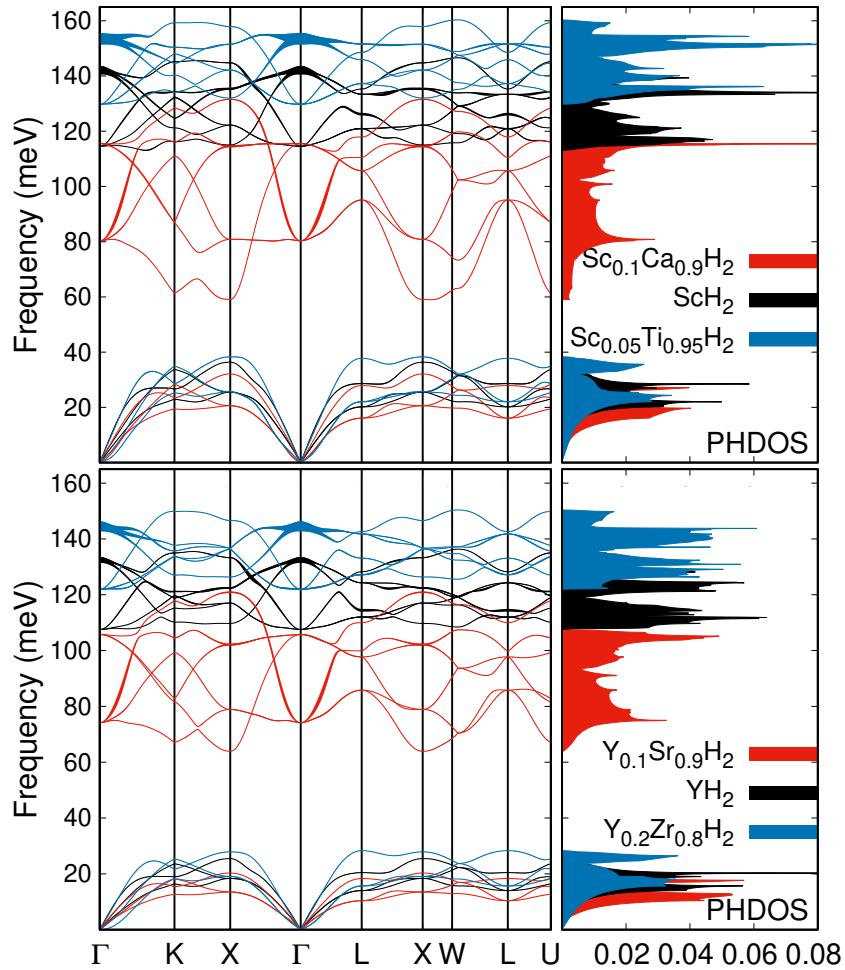


*Phonon dispersion, linewidths (as vertical lines along the phonon branches) and PHDOS for $Sc_{x-1}M_xH_2$ and $Y_{x-1}M_xH_2$ at the pristine and the threshold electron (Ti,Zr) and hole (Ca,Sr) doping contents.*

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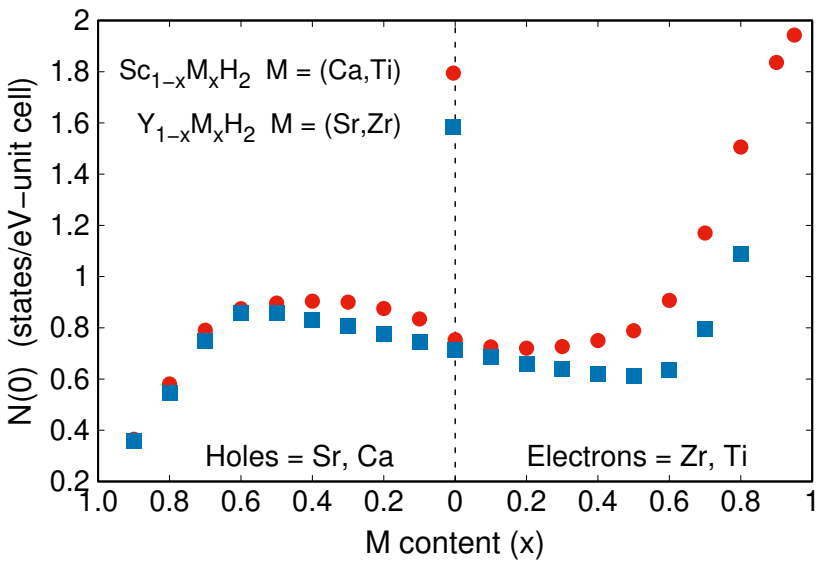


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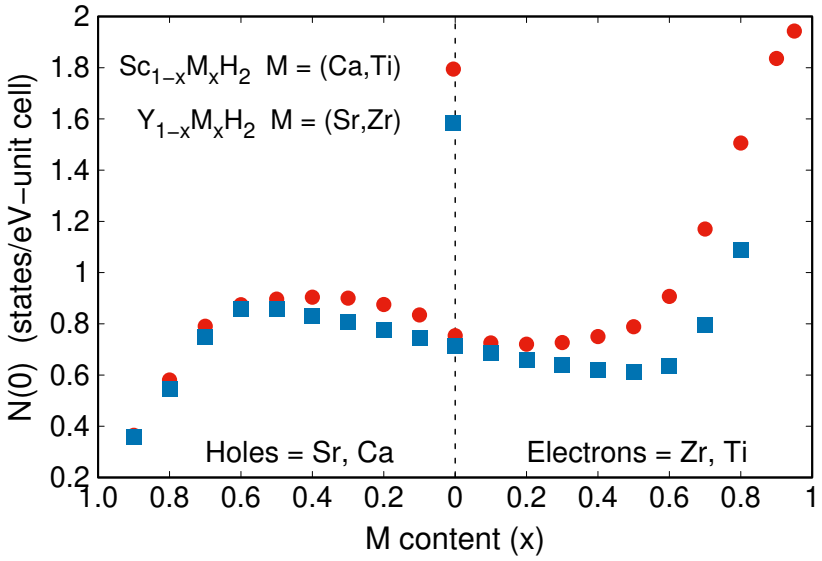


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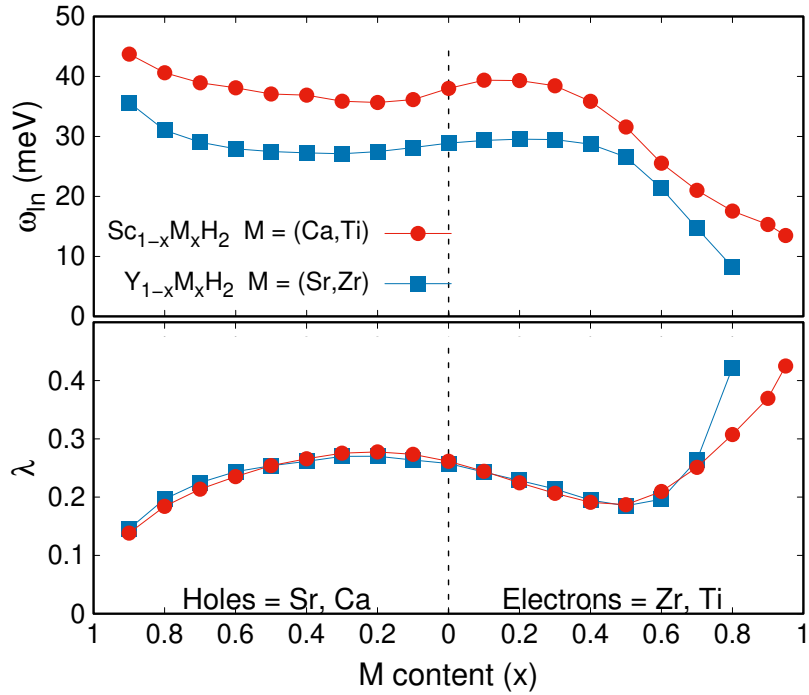


*The Allen-Dynes characteristic phonon frequency ($\omega_{ln}$) and the electron–phonon coupling constant ($\lambda$) for $Sc_{x-1}M_xH_2$ and $Y_{x-1}M_xH_2$ as a function of the M content (x).*

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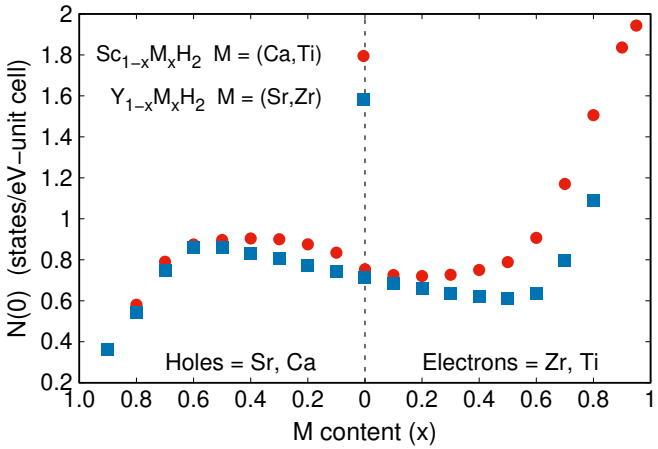


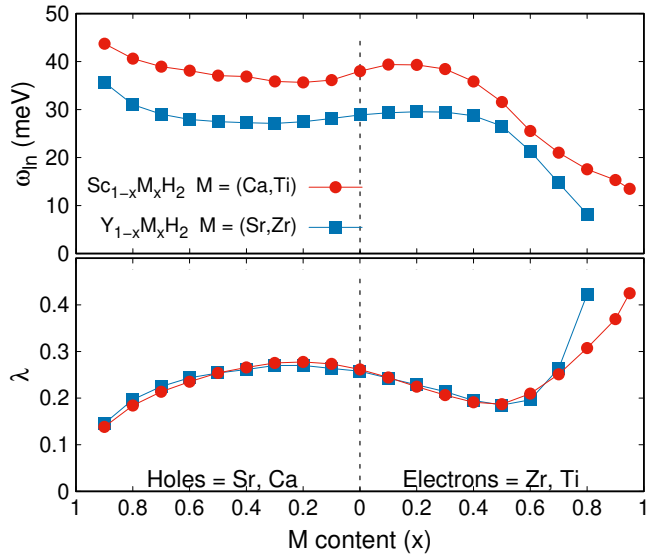

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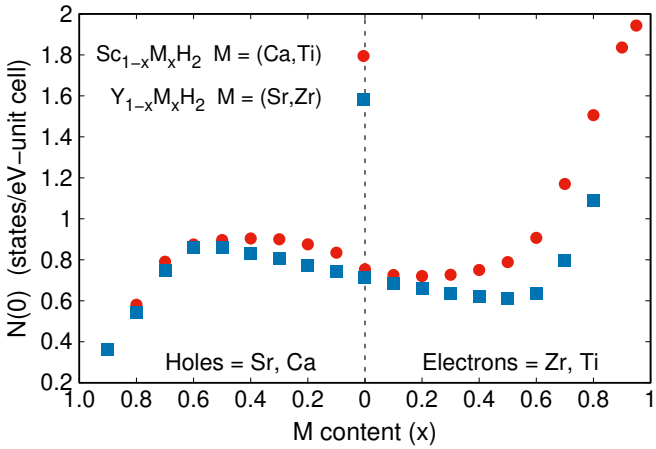
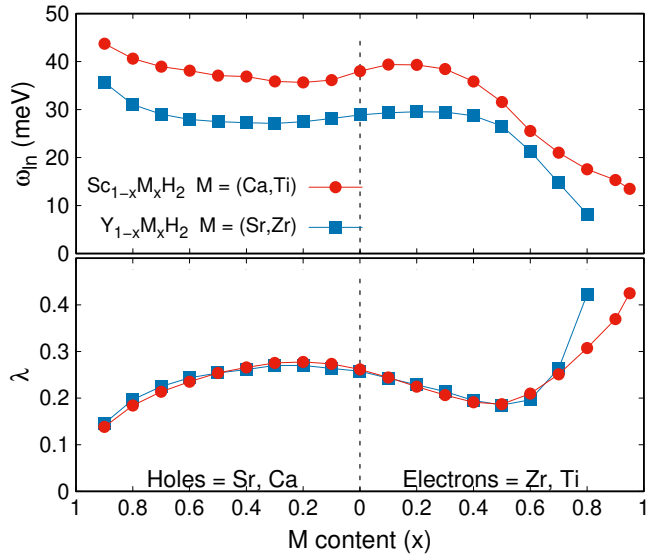
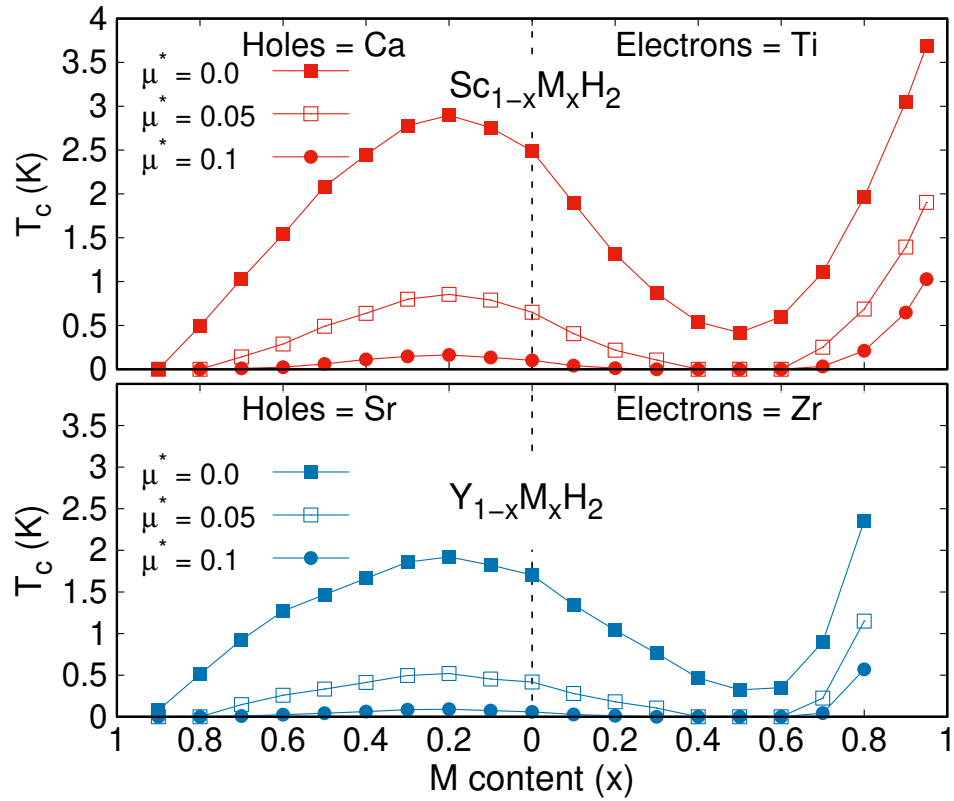
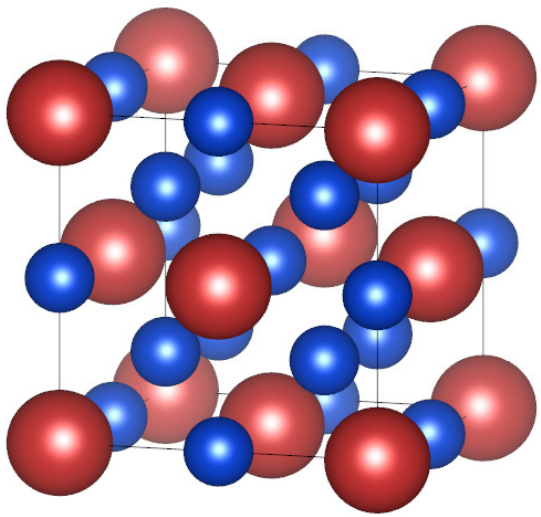


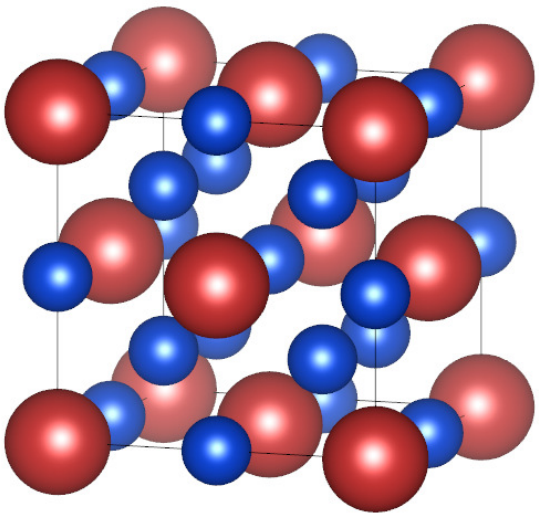

*Calculated superconducting critical temperature $T_c$ as a function of metal M content (x) for $Sc_{x-1}M_xH_2$ and $Y_{x-1}M_xH_2$ at different values of the Coulomb pseudopotential ($\mu^* = 0$, 0.05, 0.1).*

# Improvement: Boosting the superconducting $T_c$ due to doping



*Cubic NaCl (B1) structure (space group $Fm\bar{3}m$) of the $Sc_{x-1}M_xH_3$ and $Y_{x-1}M_xH_3$ solid solutions. The Scandium(Ytrium) and Hydrogen atoms are represented by large red and small blue spheres, respectively.*

# Improvement: Boosting the superconducting $T_c$ due to doping



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- $ScH_3$, 18 K
- $YH_3$, 40 K

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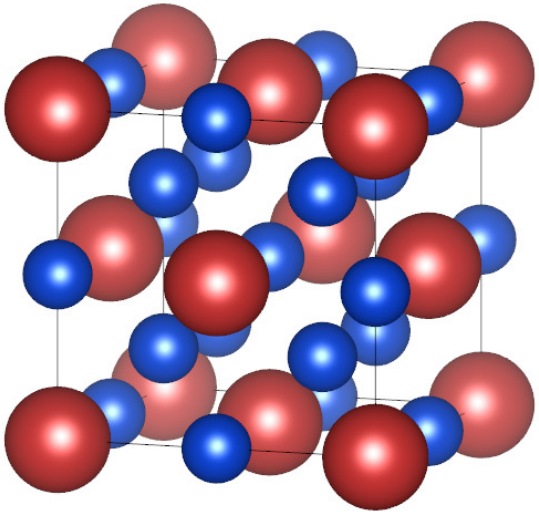

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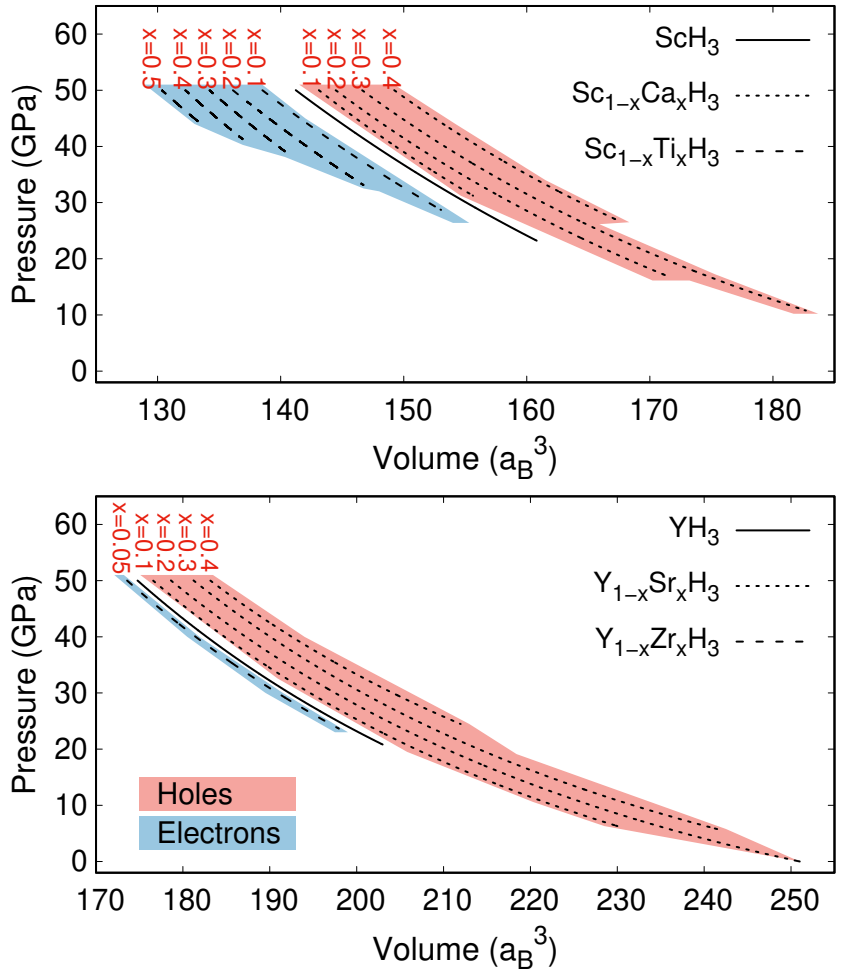
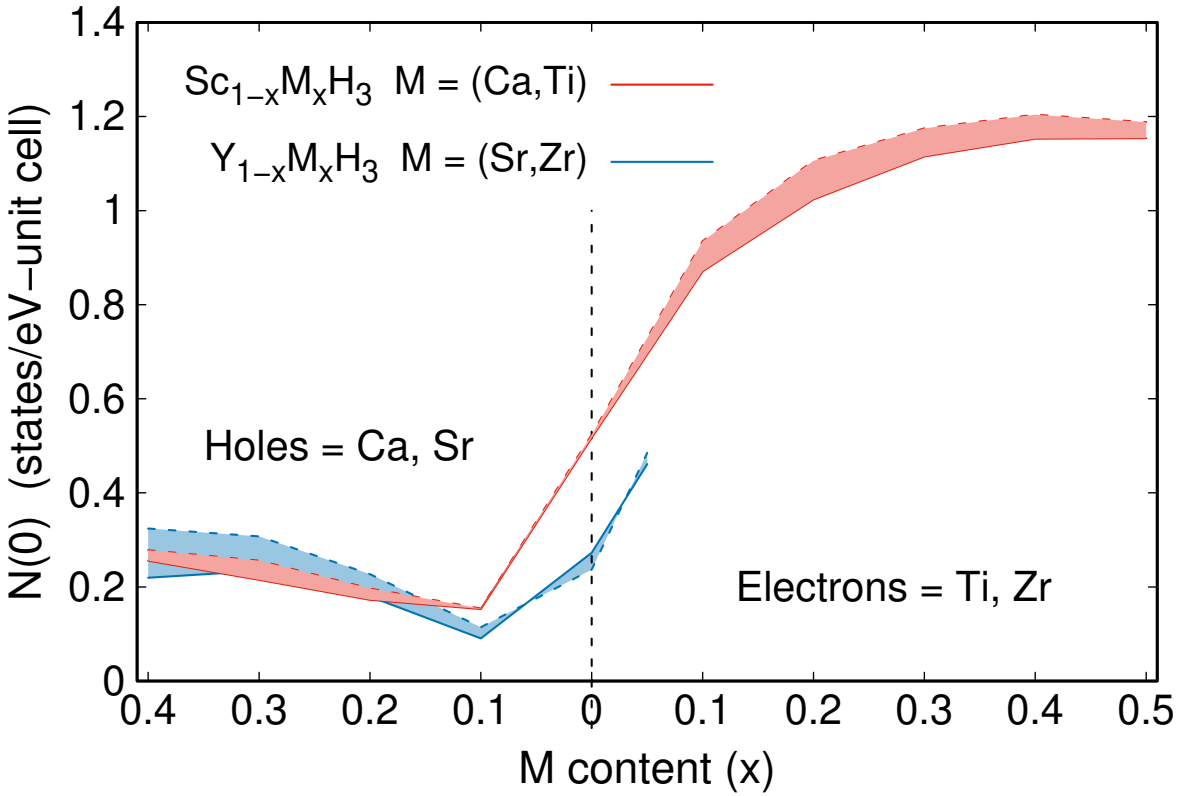



*Equation of state of $Sc_{x-1}M_xH_3$ and $Y_{x-1}M_xH_3$, for different metal M content (x), studied within the ZPE scheme.*

# Improvement: Boosting the superconducting $T_c$ due to doping




*Evolution of the total density of states at the Fermi level, N(0), for* $Sc_{x-1}M_xH_3$ *and* $Y_{x-1}M_xH_3$ *as a function of the M content x spanning the range of studied applied pressure.*

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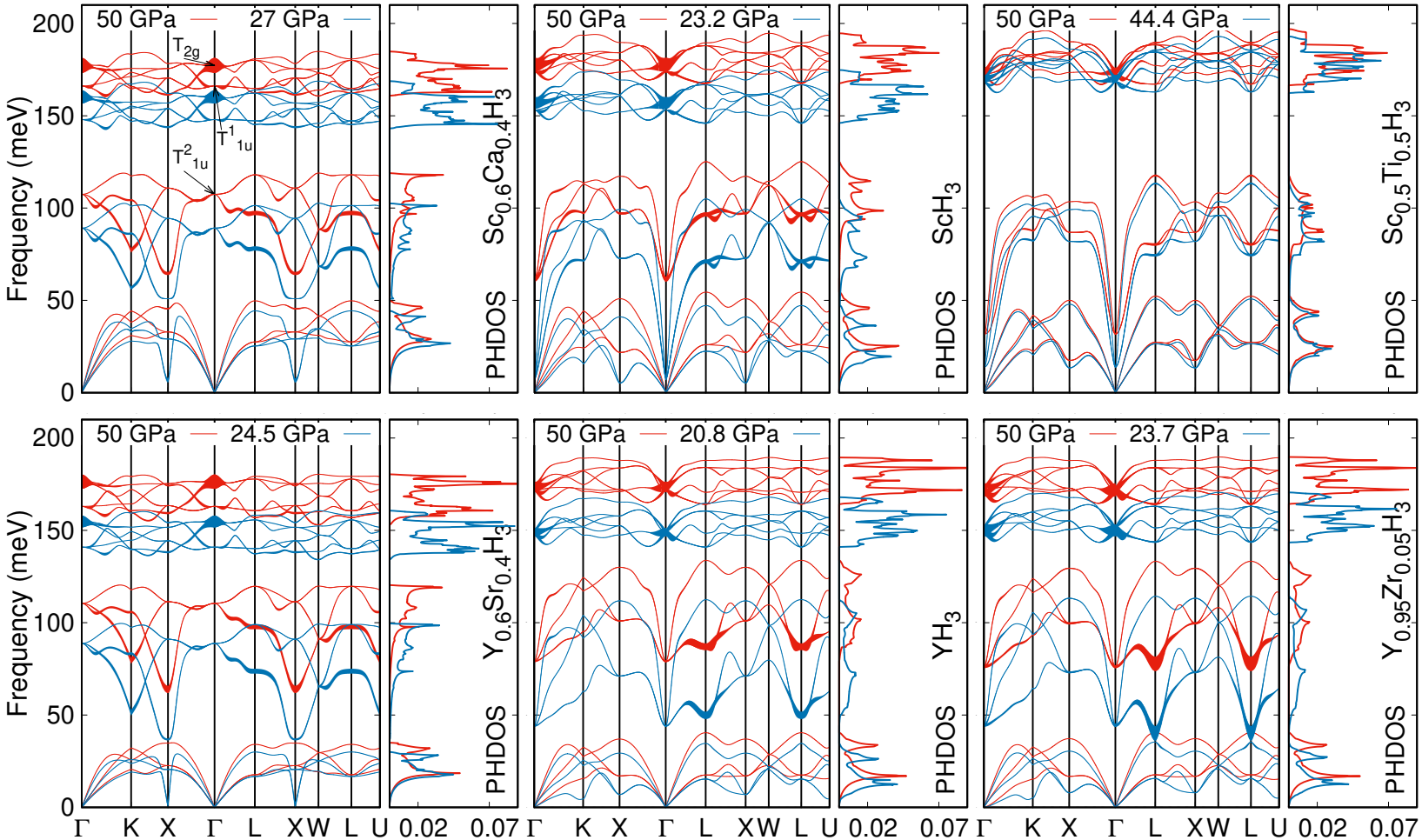


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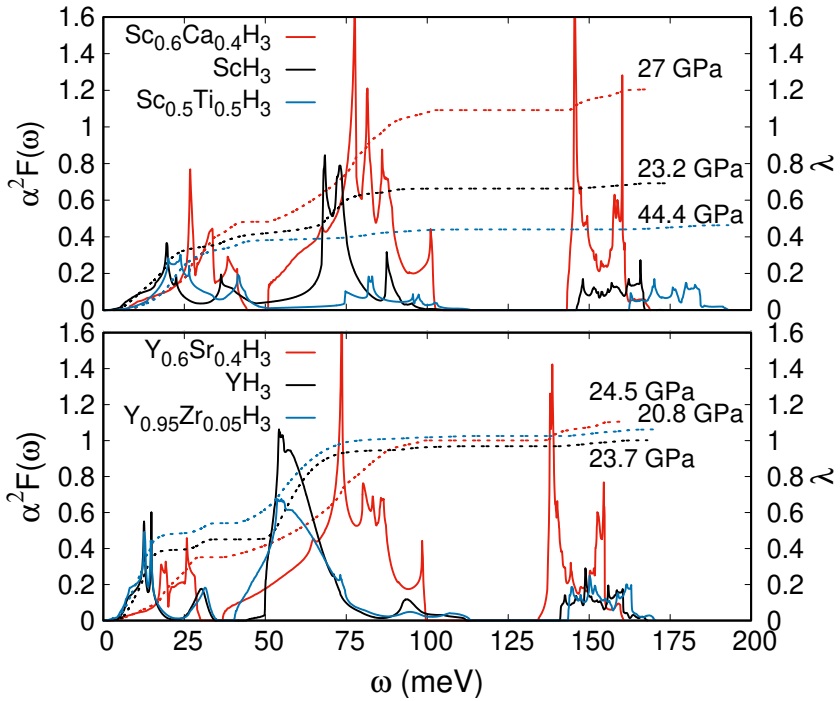
# Improvement: Boosting the superconducting $T_c$ due to doping




*Eliashberg function and partial integrated electron- phonon coupling parameter $\lambda(\omega)$ for $Sc_{x-1}M_xH_3$ and $Y_{x-1}M_xH_3$ at $x = 0$ and at the threshold electron- and hole- content for each solid-solution at the minimum pressure where the systems are dynamically stable.*

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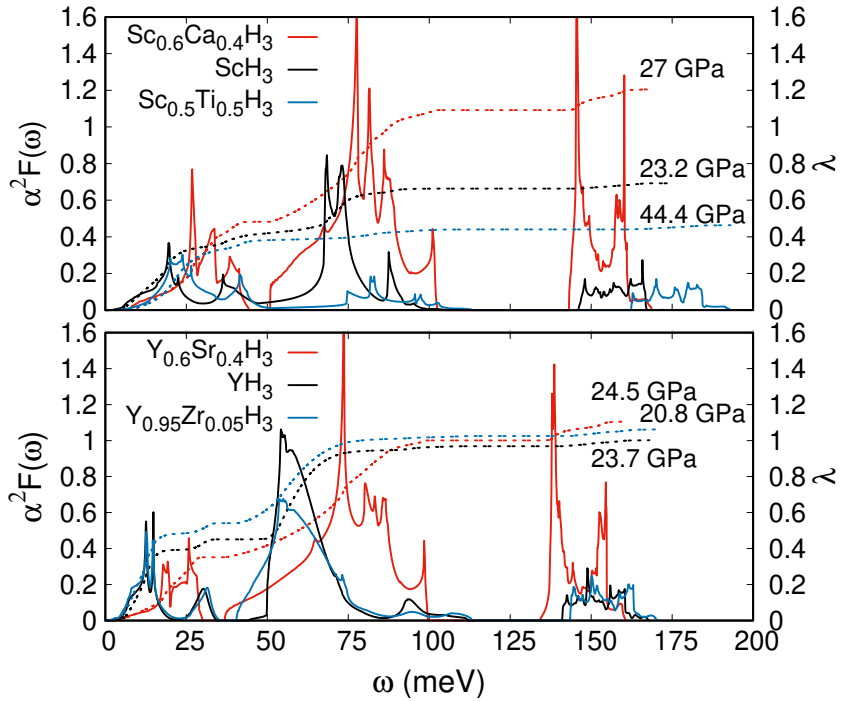


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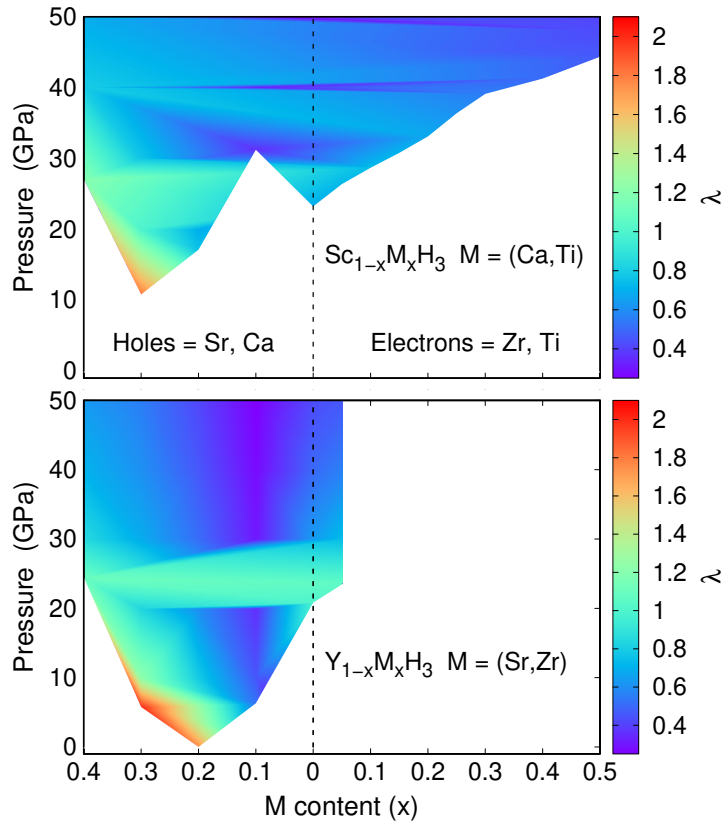
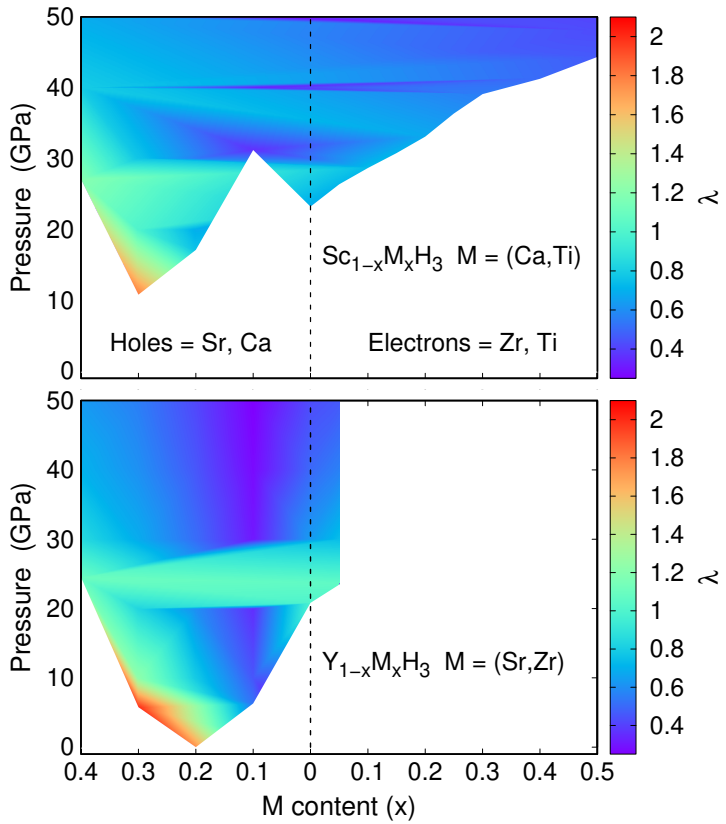



*Electron-phonon coupling constant ($\lambda$) of $Sc_{x-1}M_xH_3$ and $Y_{x-1}M_xH_3$ for the entire studied range of electron- and hole-content and applied pressure for each solid-solution.*

# Improvement: Boosting the superconducting $T_c$ due to doping

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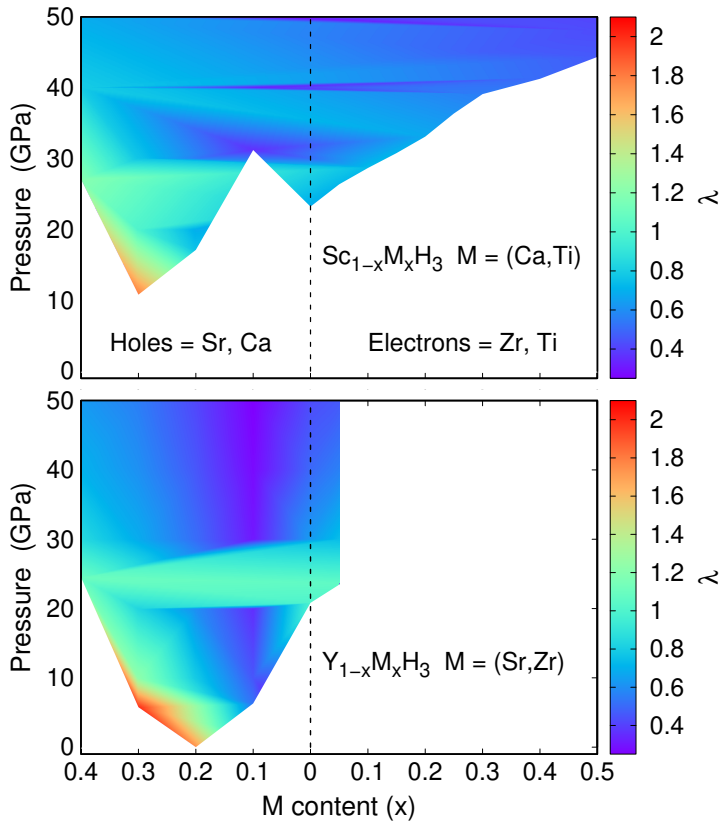


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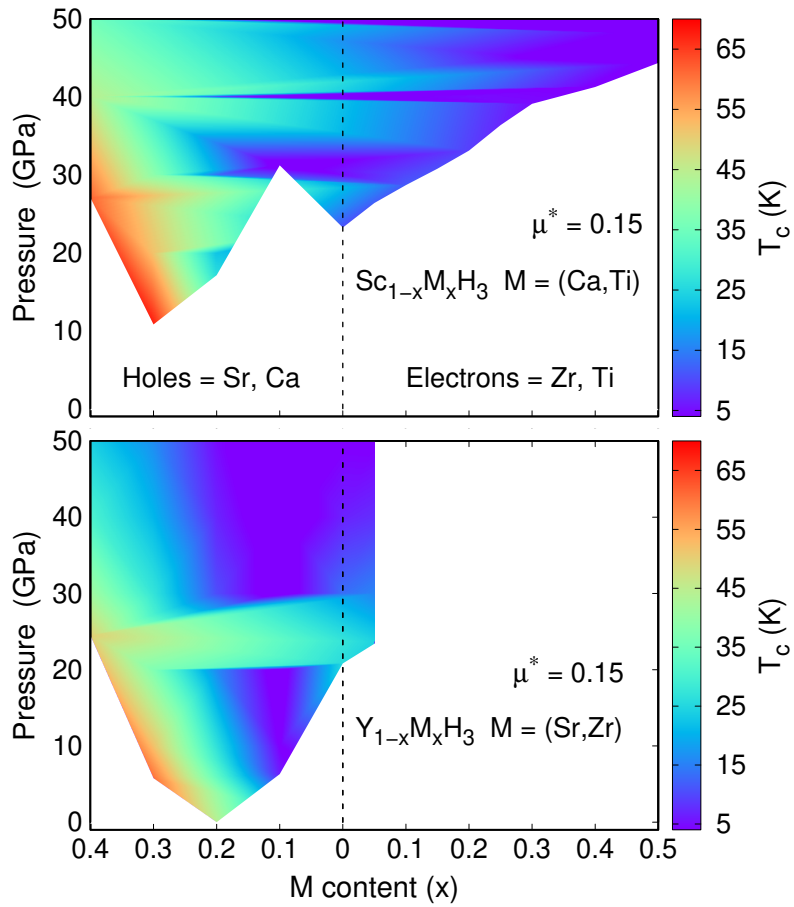
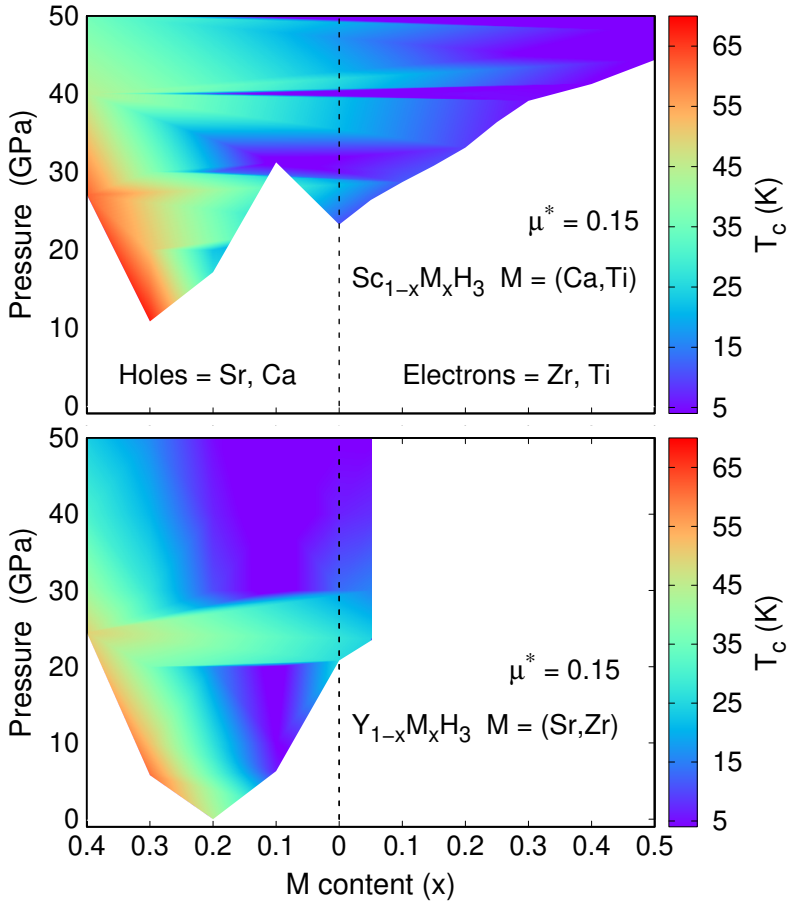



*Superconducting critical temperature, $T_c$, calculated with $\mu^* = 0.15$, of $Sc_{x-1}M_xH_3$ and $Y_{x-1}M_xH_3$ at the entire range of electron- and hole-content and applied pressure for each solid-solution.*

# Improvement: Boosting the superconducting $T_c$ due to doping

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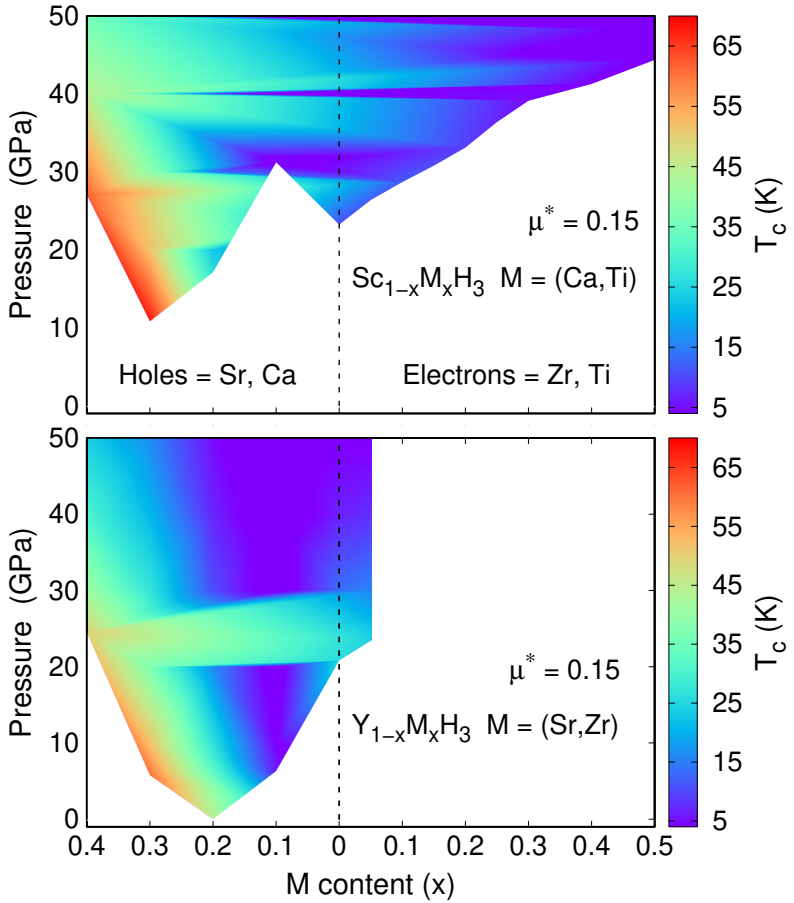
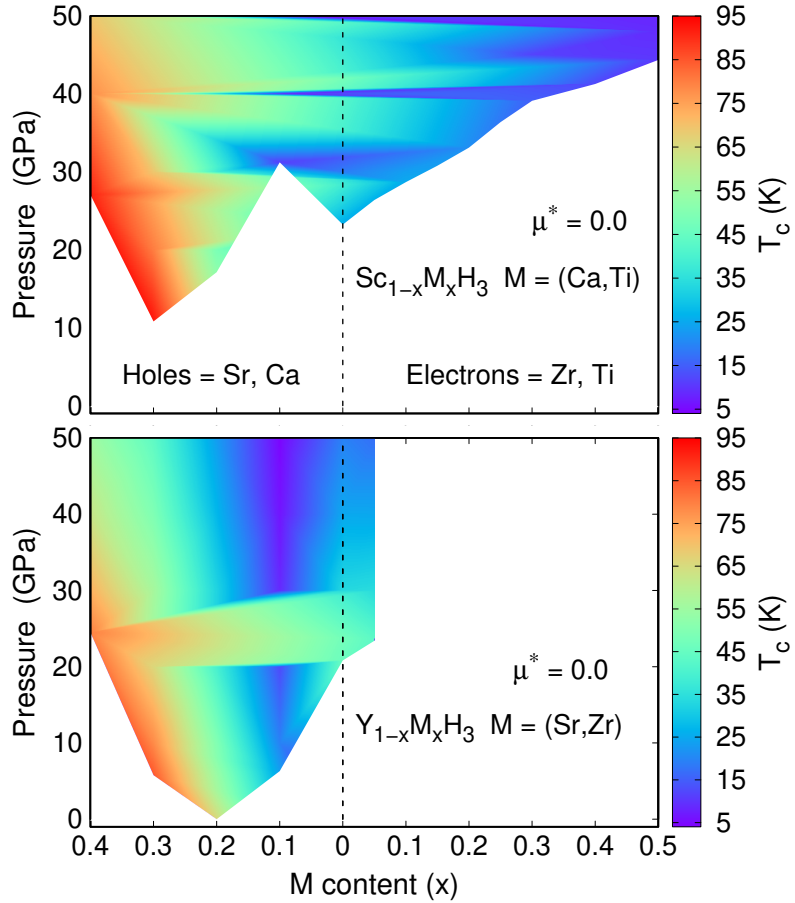
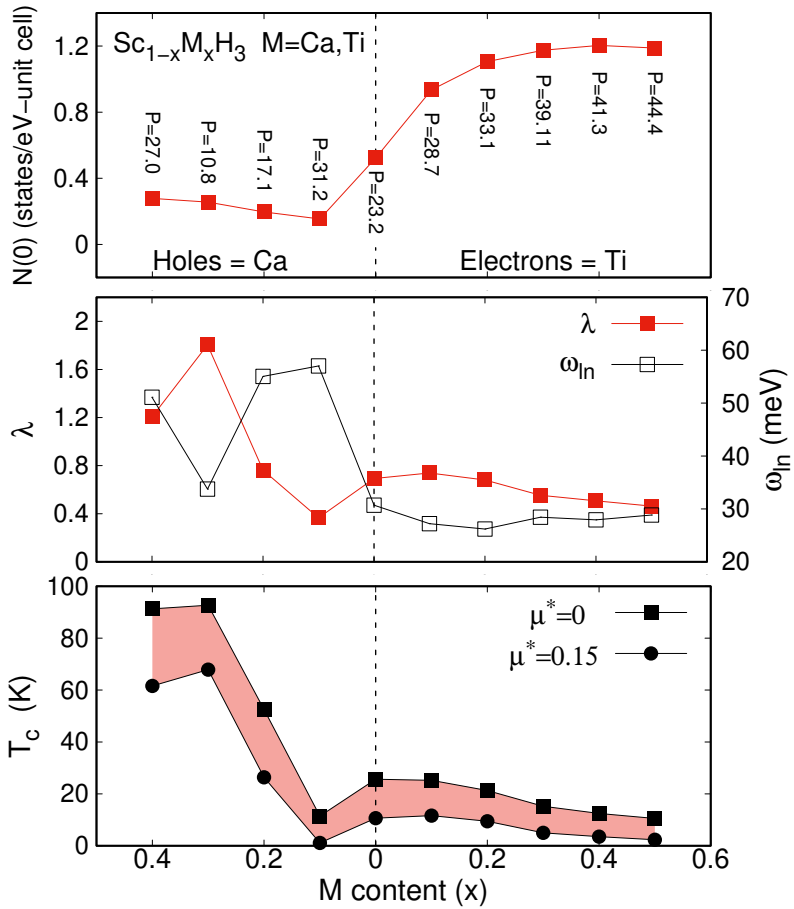



*Superconducting critical temperature, $T_c$, calculated with $\mu^* = 0.15$, of $Sc_{x-1}M_xH_3$ and $Y_{x-1}M_xH_3$ at the entire range of electron- and hole-content and applied pressure for each solid-solution.*



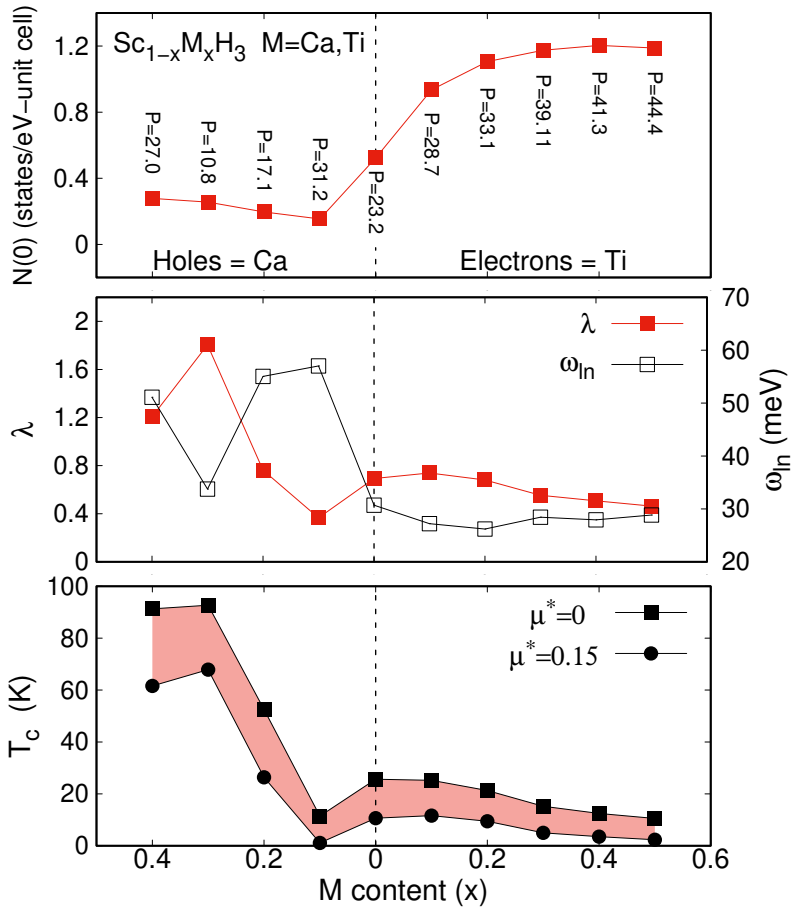

*Superconducting critical temperature, $T_c$, calculated with $\mu^* = 0$, of $Sc_{x-1}M_xH_3$ and $Y_{x-1}M_xH_3$ at the entire range of electron- and hole-content and applied pressure for each solid-solution.*

# Improvement: Boosting the superconducting $T_c$ due to doping

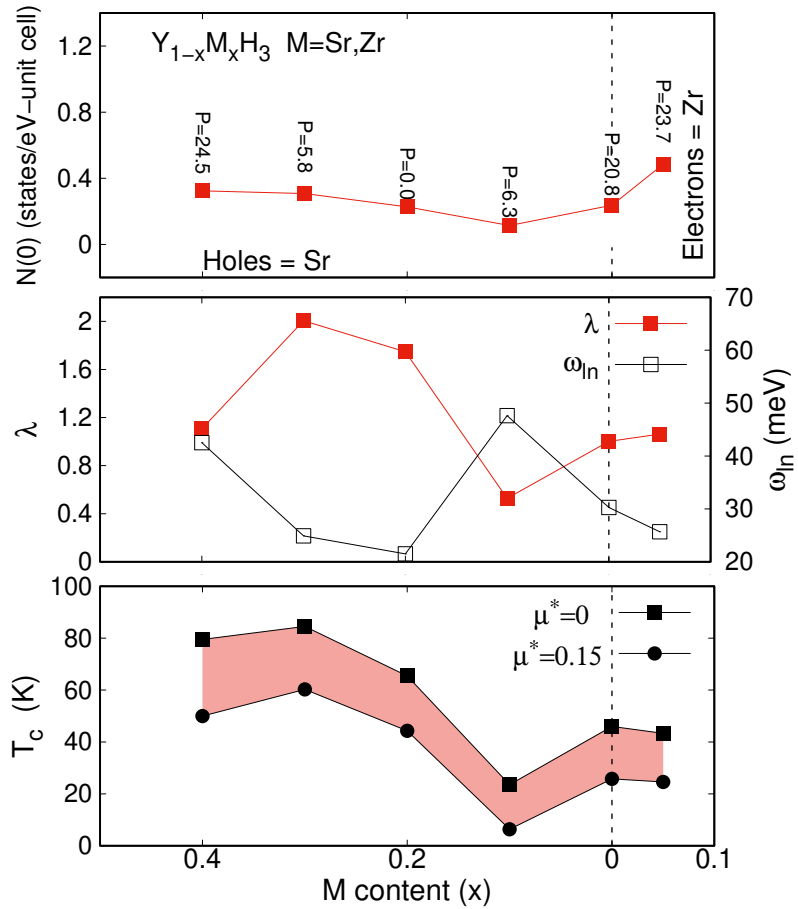



*Maximum superconducting critical temperature, $T_c$, calculated with $\mu^* = 0.15$ and 0, of $Sc_{x-1}M_xH_3$ at the entire range of electron- and hole-content for each solid-solution.*

# Improvement: Boosting the superconducting $T_c$ due to doping



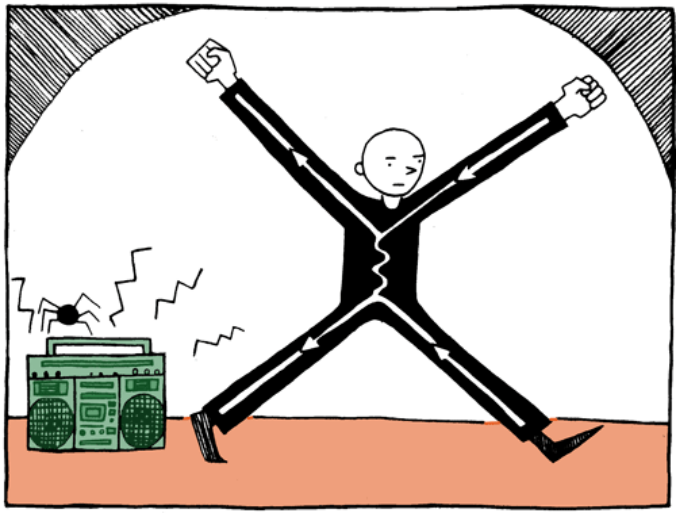

*Maximum superconducting critical temperature, $T_c$, calculated with $\mu^* = 0.15$ and 0, of $Sc_{x-1}M_xH_3$ at the entire range of electron- and hole-content for each solid-solution.*




*Maximum superconducting critical temperature, $T_c$, calculated with $\mu^* = 0.15$ and 0, of $Y_{x-1}M_xH_3$ at the entire range of electron- and hole-content for each solid-solution.*

# Next:

- *$Sc_{x-1}M_xH_3$ and $Y_{x-1}M_xH_3$ in the HPC structures at ambient pressure.*
- *$La_{x-1}M_xH_2$ and $La_{x-1}M_xH_3$.*



*See You Space Cowgirl,*
*Someday, Somewhere....*