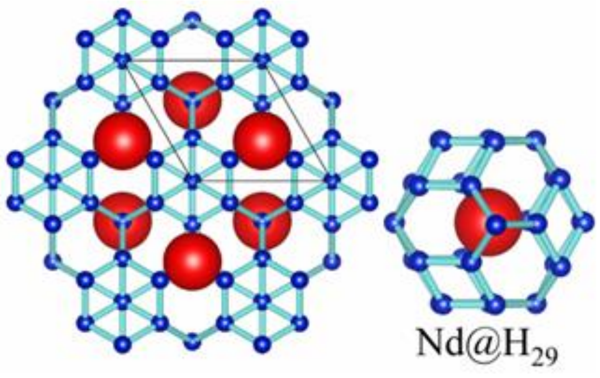
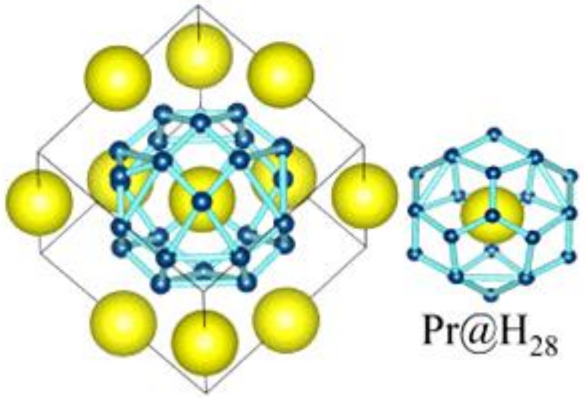
Recent advances in high-temperature superconductivity in ternary hydrides

Dmitrii Semenok

Skolkovo Institute of Science and Technology





USPEX Computational Materials Discovery

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Supported by the Russian Scientific Foundation grant No. 19072-30043 «Computational materials design laboratory»

Superconductivity surrounds us

Medicines against COVID

Nuclear magnetic resonance spectrometer

Single-photon detectors

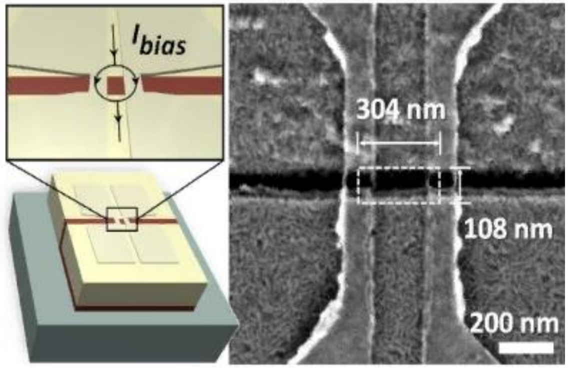
Tomography

Synchrotrons and colliders

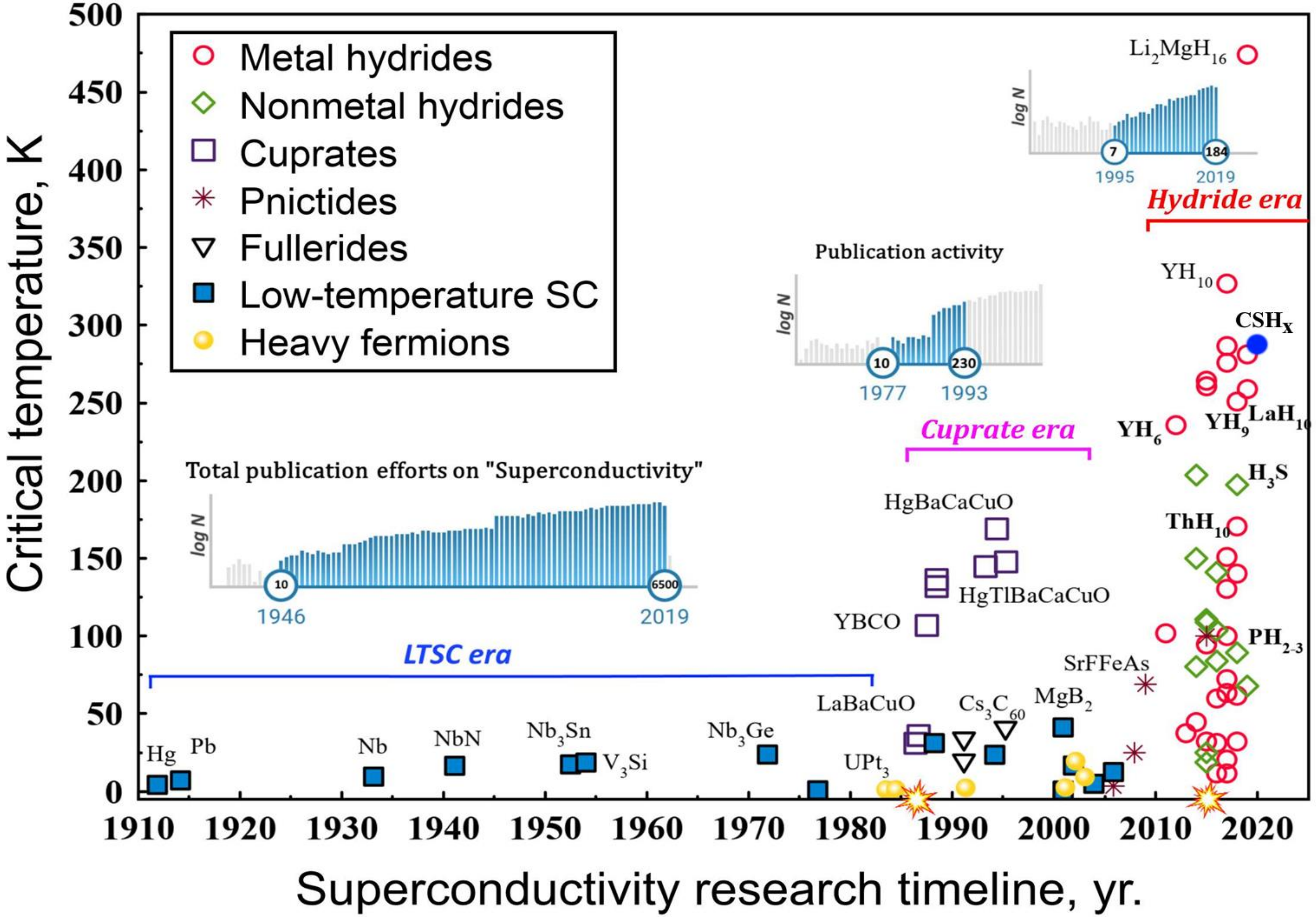
Magnetic field sensors

Quantum supercomputer

Maglev trains and SC gyroscopes in Int. Space Station

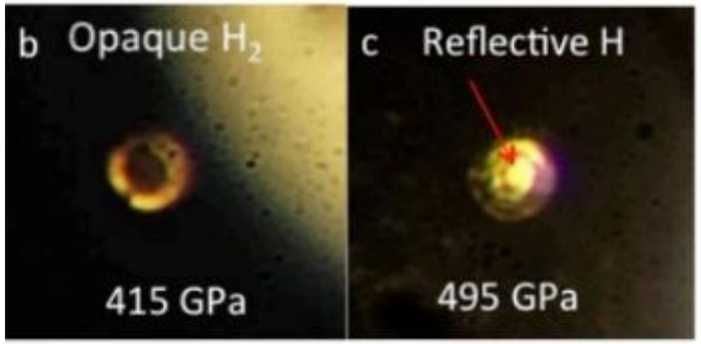


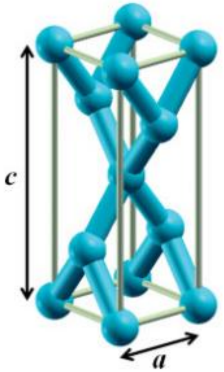
112 years of progress in superconductivity

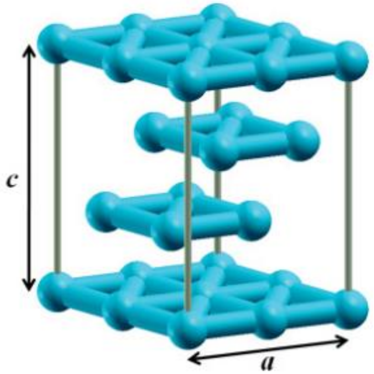


High-temperature superconductivity in hydrides under pressure

Metallic hydrogen: T_C is 217-356 К at ~500 GPa







***I*4_1/amd, 0.7 TPa** **R-3m, 2 TPa**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Observation of the Wigner-Huntington transition to metallic hydrogen

Ranga P. Dias, Isaac F. Silvera*

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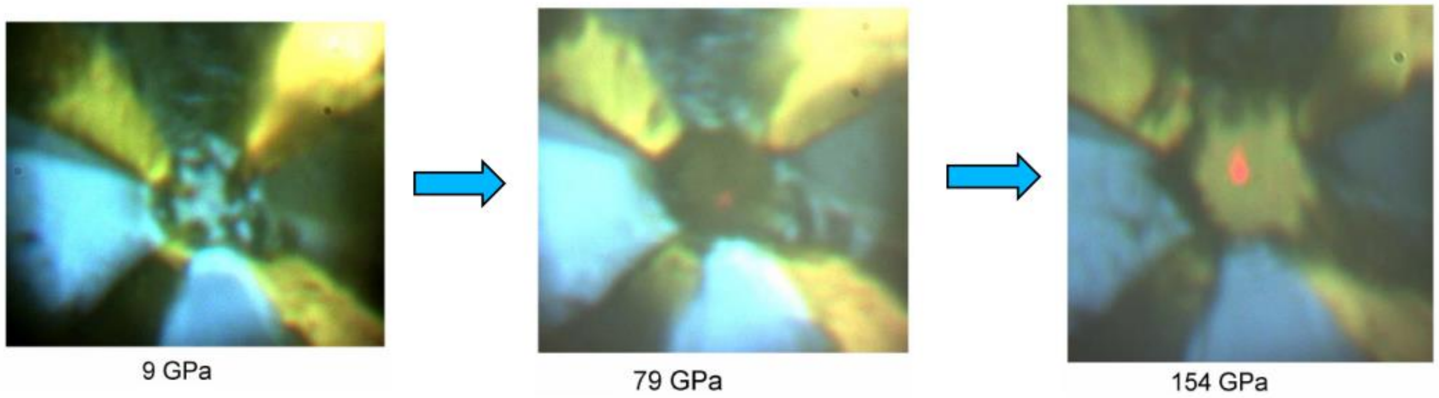
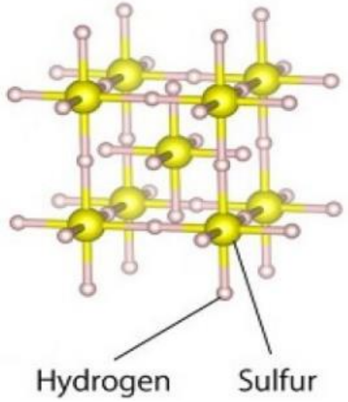
Science 17 Feb 2017:
Vol. 355, Issue 6326, pp. 715-718
DOI: 10.1126/science.aal1579

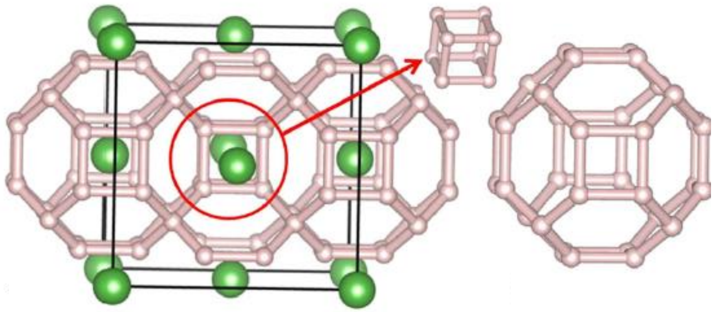
Metallic sulfur hydride: T_C is up to 203 К at 155 GPa





In addition PH_2, SiH_x and H_3Se were also synthesized (T_c < 100 K)

Another example – record high T_C in LaH_{10} (150 GPa)



The maximum T_C ~ 250-260 K

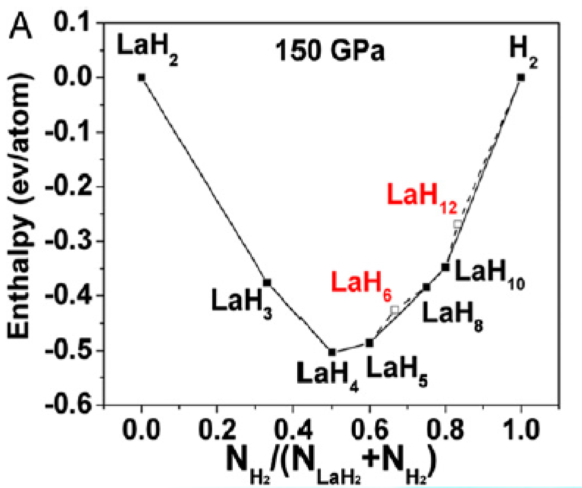
PNAS

Potential high-T_c superconducting lanthanum and yttrium hydrides at high pressure

Hanyu Liu[a], Ivan I. Naumov[a], Roald Hoffmann[b], N. W. Ashcroft[c], and Russell J. Hemley[d,e,1]

[a]Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015; [b]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853; [c]Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853; [d]Department of Civil and Environmental Engineering, The George Washington University, Washington, DC 20052; and [e]School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853

Contributed by Russell J. Hemley, May 5, 2017 (sent for review March 20, 2017; reviewed by Panchapakesan Ganesh, Jeffrey M. McMahon, and Dimitrios Papaconstantopoulos)



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Evidence for superconductivity above 260 K in lanthanum superhydride at megabar pressures

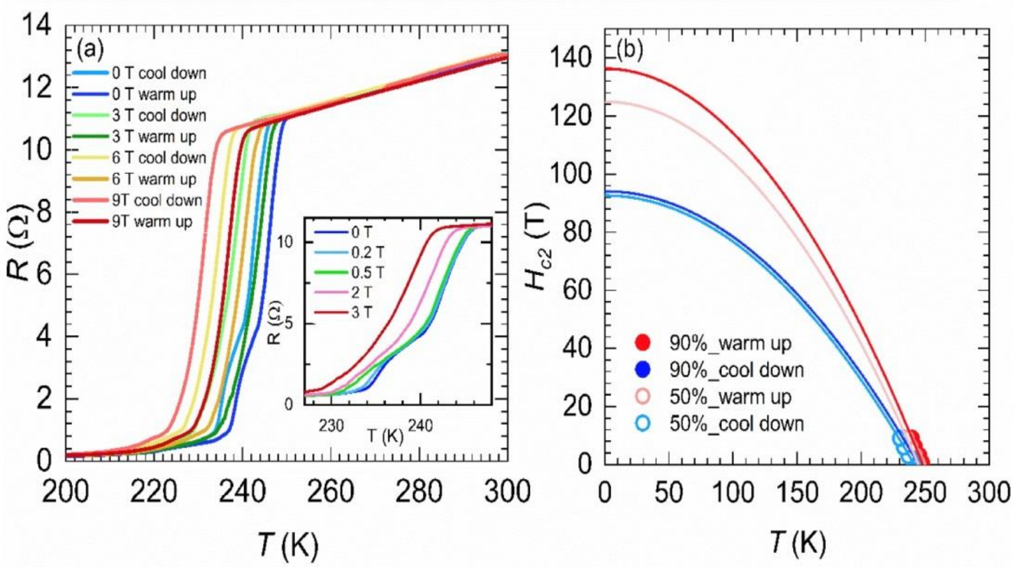
Maddury Somayazulu, Muhtar Ahart, Ajay K Mishra, Zachary M. Geballe, Maria Baldini, Yue Meng, Viktor V. Struzhkin, Russell J. Hemley

(Submitted on 23 Aug 2018 (v1), last revised 29 Aug 2018 (this version, v3))

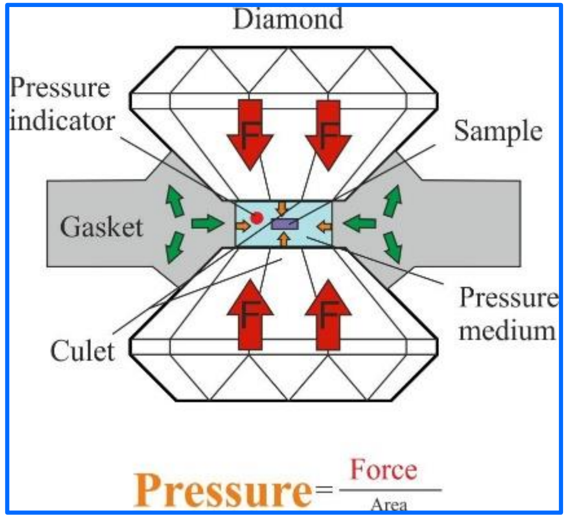
Superconductivity at 250 K in lanthanum hydride under high pressures

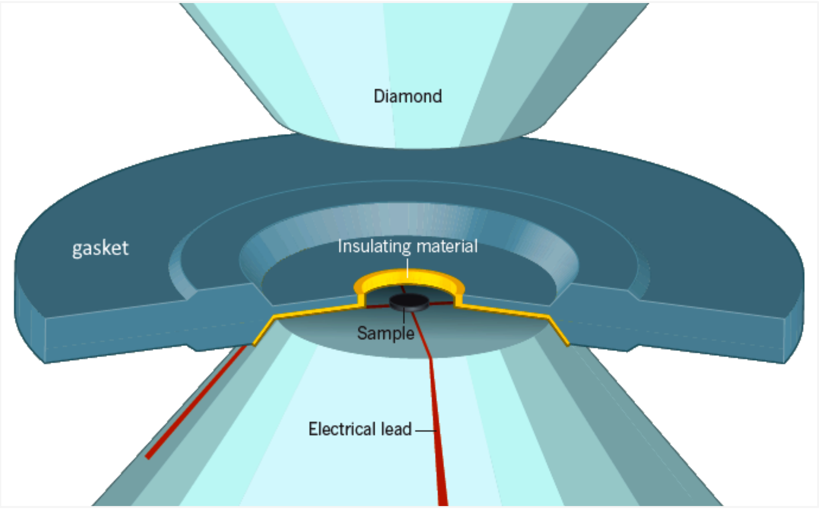
A. P. Drozdov, P. P. Kong, V. S. Minkov, S. P. Besedin, M. A. Kuzovnikov, S. Mozaffari, L. Balicas, F. Balakirev, D. Graf, V. B. Prakapenka, E. Greenberg, D. A. Knyazev, M. Tkacz, M. I. Eremets

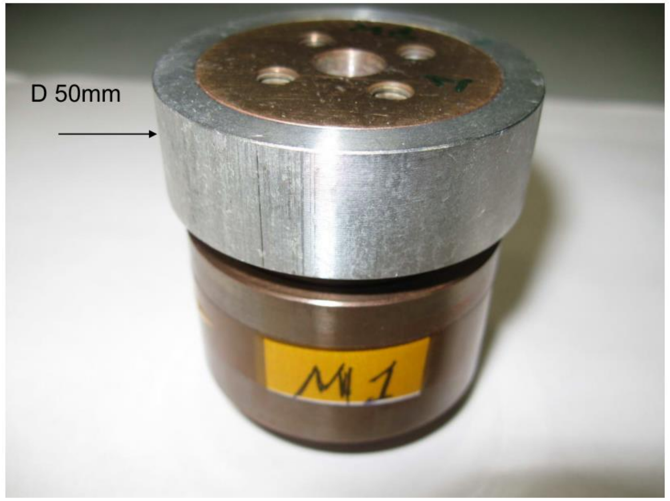
(Submitted on 4 Dec 2018)

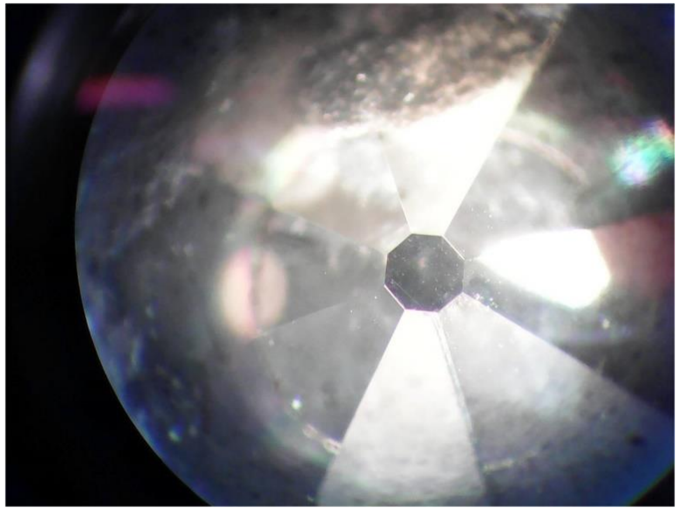


High pressure or small sample ?



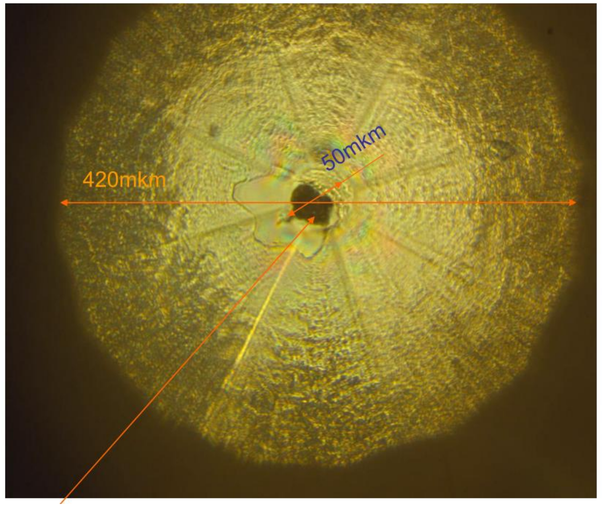






Diamond anvil

Gasket + anvils



Sample

Moscow collaboration: HTSC hydrides in diamond anvil cells

Skoltech (THEORY + Xe FIB)

PETRA, ESRF, Spring-8, SSRF
synchrotron research (X-ray diffraction)
DETERMINATION OF STRUCTURE

Crystallography Institute RAS
DIAMOND ANVIL CELLS, LASER HEATING

Lebedev’s Physical Institute (LPI)
TRANSPORT MEASUREMENTS

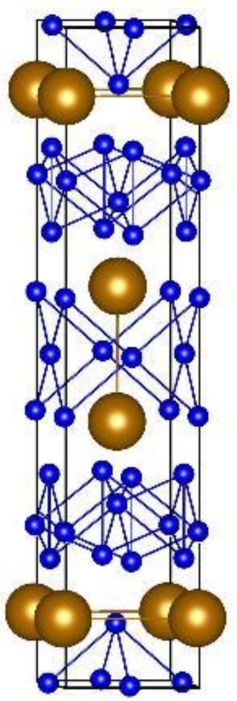
Current progress of research: 12 binary metal-hydrogen systems

LiH_6 NaH_7 FeH_5 LaH_{10} $YH_{6\text{-}9}$ $UH_{7\text{-}9}$ $ThH_{9\text{-}10}$ $CeH_{9\text{-}10}$ BaH_{12} PrH_9 NdH_9 EuH_9

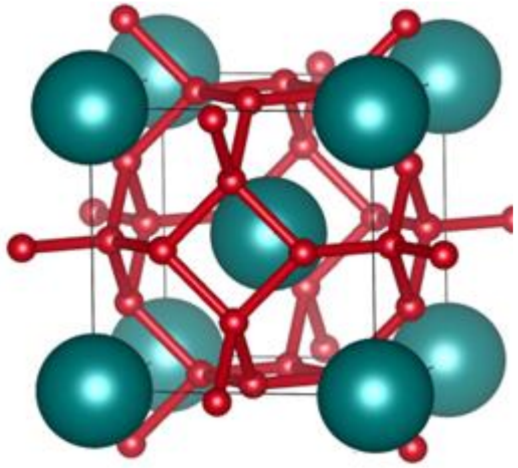
Molecular hydrides (LiH6, NaH7)

Metallic hydrides (LaH10 … BaH12)

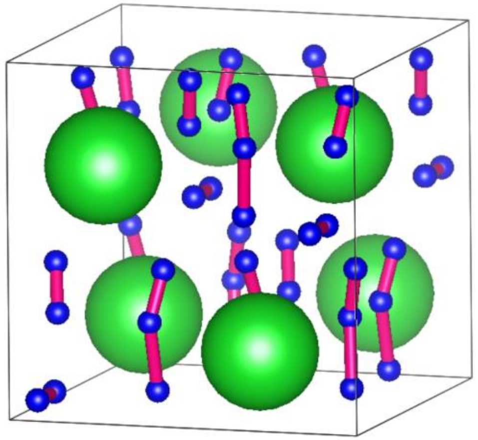
Magnetic metallic hydrides (PrH9, NdH9, EuH9)



FeH_5



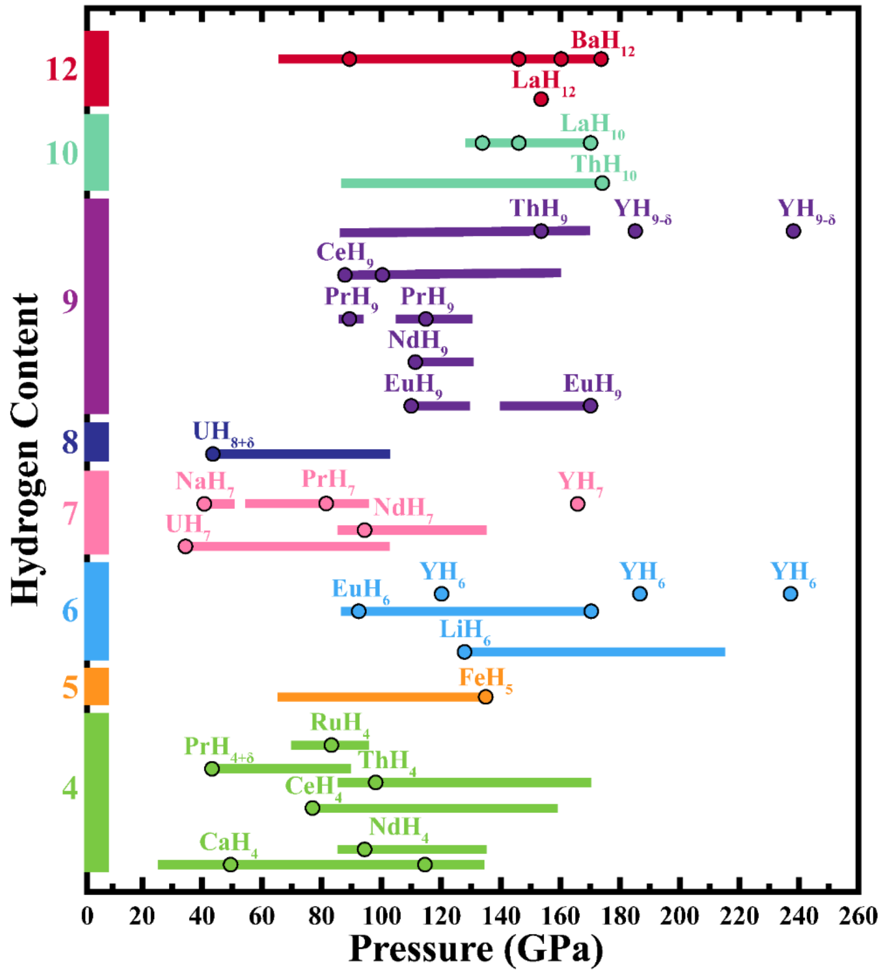
YH_6



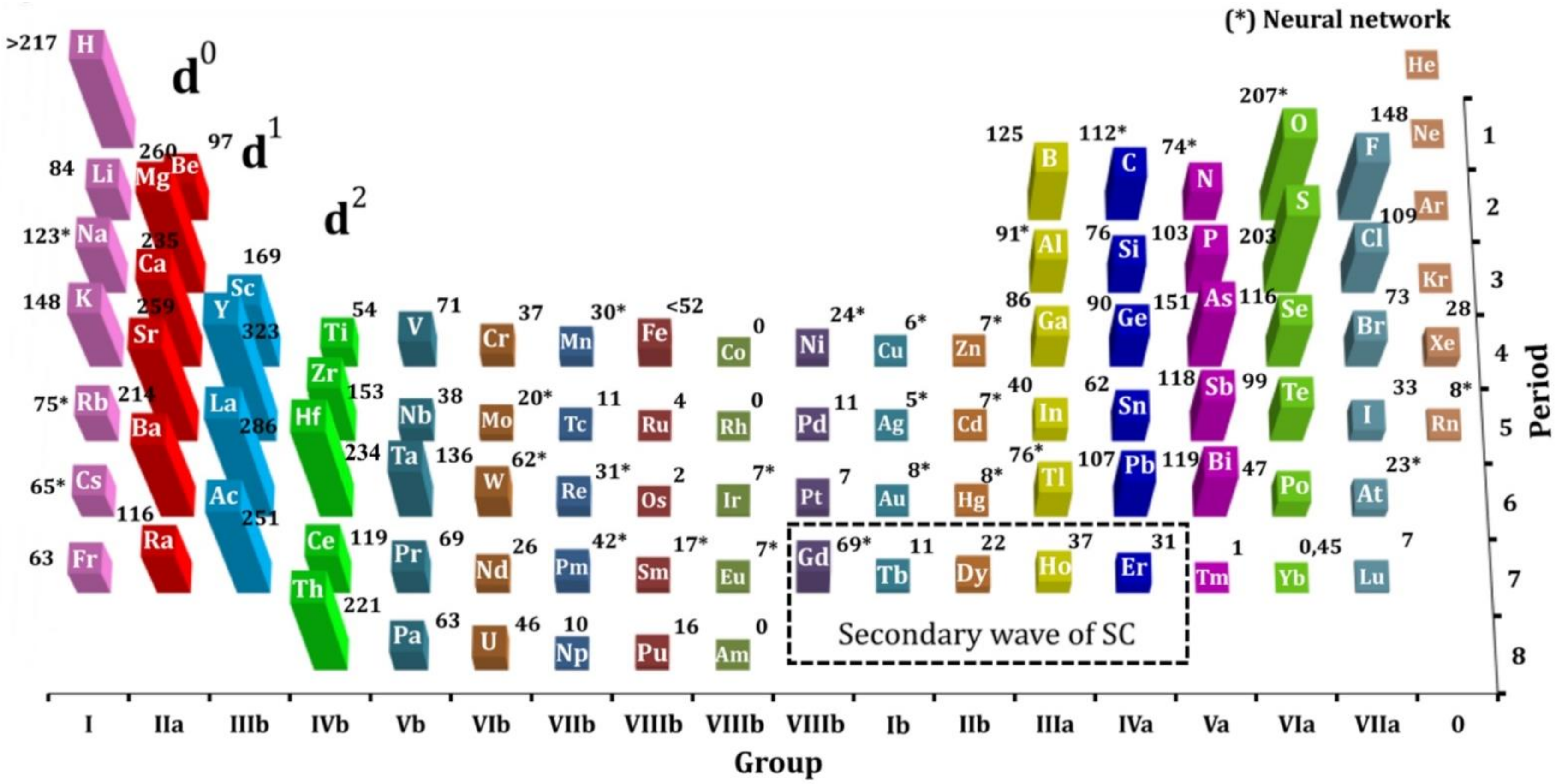
BaH_{12} (H_2, H_3^- группы)

Different hydrogen form – different physical properties

Magnetism suppresses superconductivity



Distribution of superconductivity in BINARY hydrides



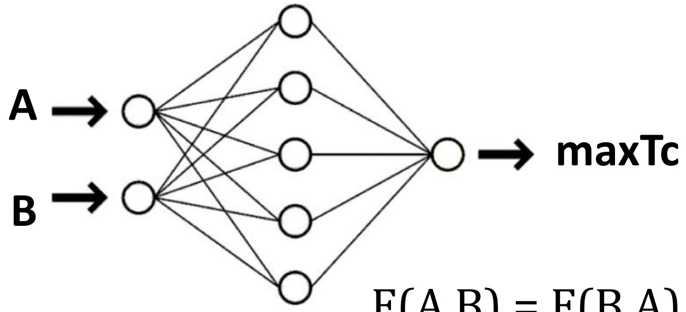
DFT calculations, statistical analysis, experiment and the use of neural networks show that the distribution of BINARY superconducting hydrides has a pronounced maximum for d^0-d^1 elements + Mg ("lability belt").

► *D. Semenok et al. "On Distribution of Superconductivity in Metal Hydrides", Current Opinion in Solid State & Materials Science*, ***2020***, *doi:10.1016/j.cossms.2020.100808.*

►*Feng Peng et al. "Hydrogen Clathrate Structures in Rare Earth Hydrides at High Pressures: Possible Route to Room-Temperature Superconductivity", 10.1103/PhysRevLett.119.107001*

Distribution of superconductivity in TERNARY hydrides (~4608 systems)

15 layers of 12 neurons in a layer

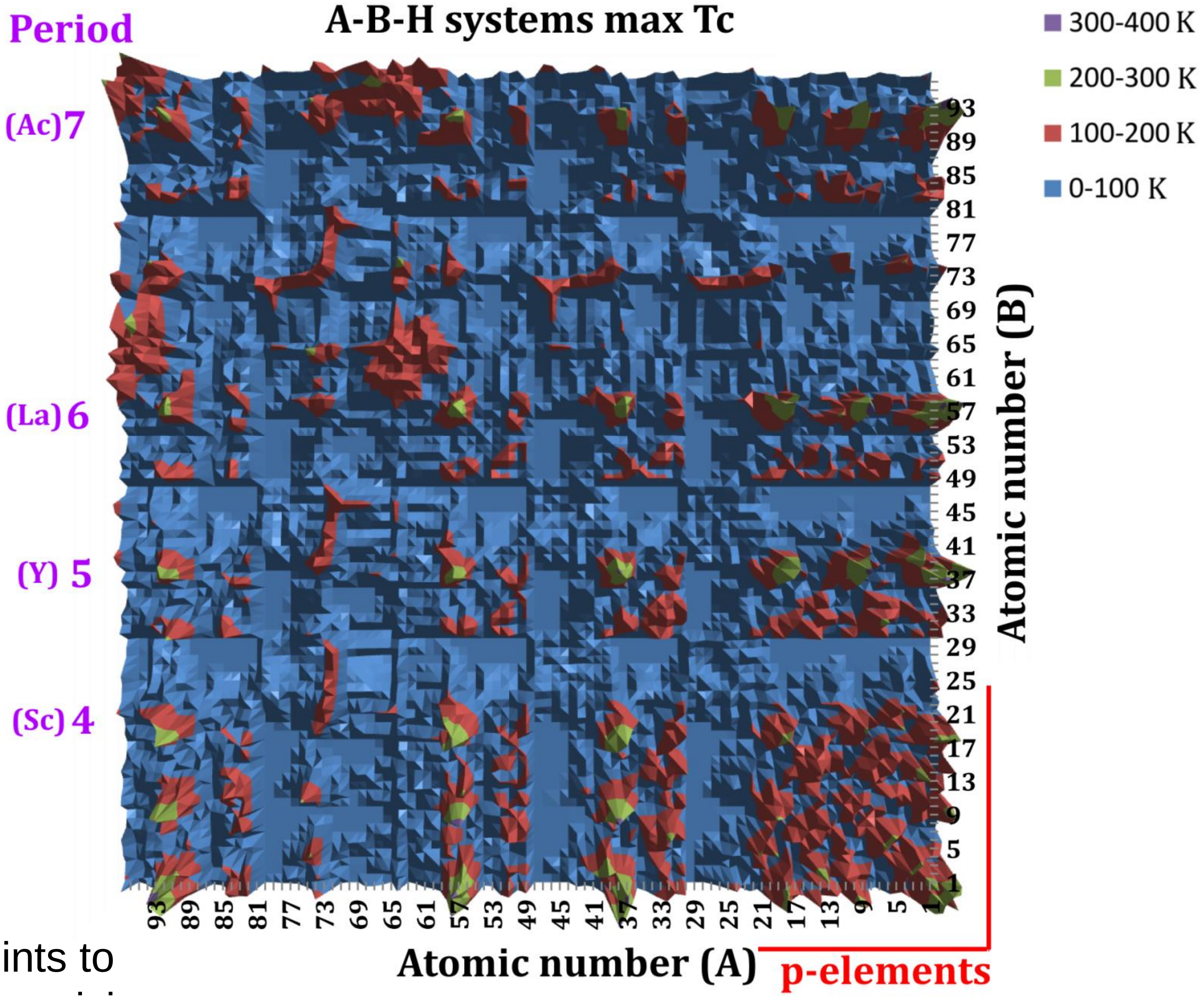


F(A,B) = F(B,A)
F(A,A) = maxT_C (A)
F(1,A)=F(A,A)

Fact 1: we do not have enough calculated ternary systems to get reliable results from the AI model.

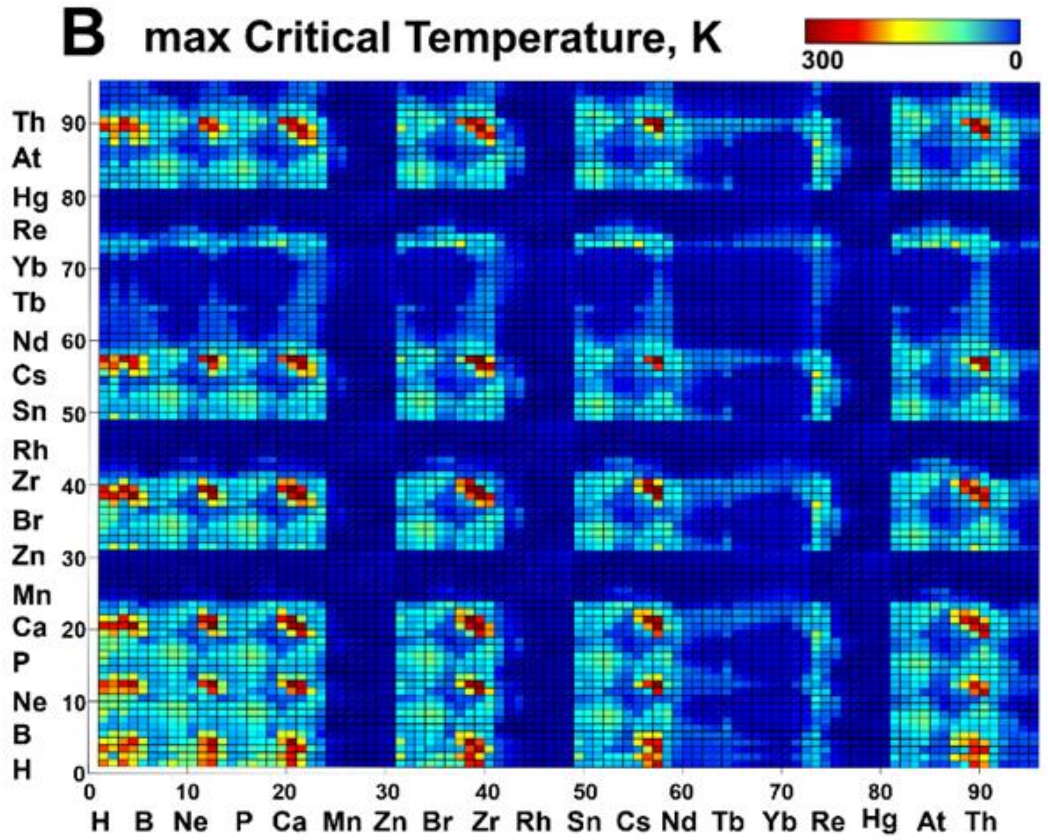
Number of studied ternary systems ~15

Fact 2: we can consider binary systems (~ 50) as degenerate ternary. In this case the model points to combination of elements from the d-belt as the promising area for research.



Distribution of superconductivity in TERNARY hydrides (~4608 systems)

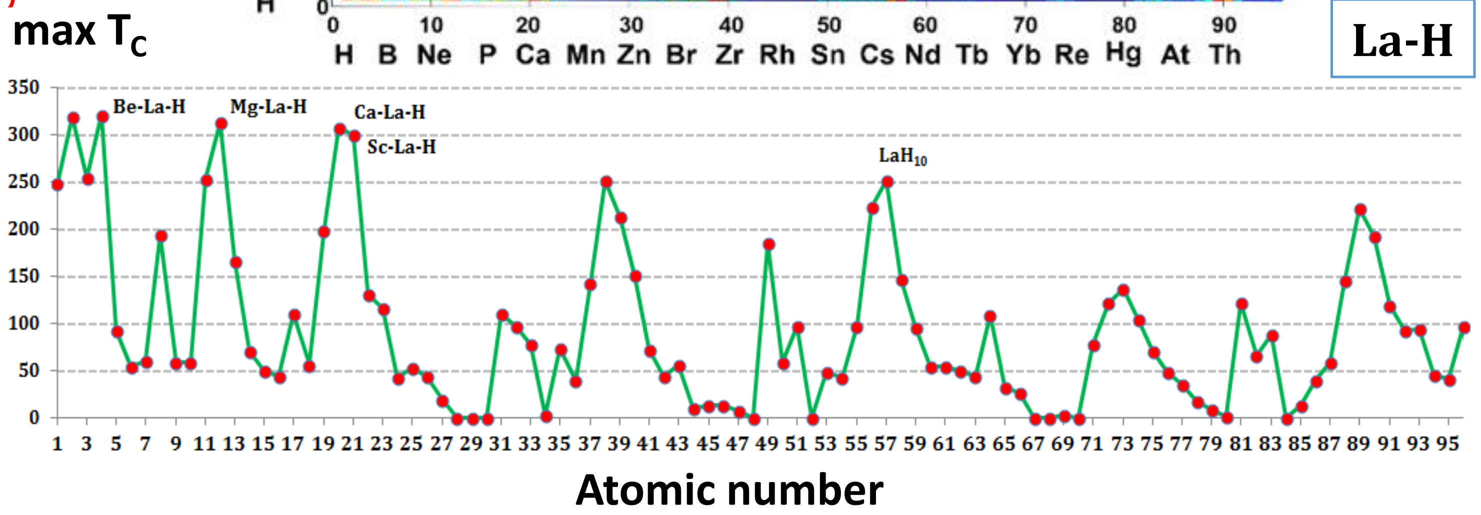
Entry No	First atom (A)	Second atom (B)	Expected T_C, K	Expected stabilization pressure, GPa	Expected H-content (per A+B)
1	Th	Li	257	195	10
2		Na	265	196	9.5
3		K	258	195	9.5
4		Ca	265	209	10.5
5		Sr	271	208	10.5
6		Y	240	214	11
7		Ba	260	206	10.5
8		La	276	213	11.5
12	La	Li	267	190	9
13		Be	250	204	9.5
14		Na	259	190	9
15		Mg	281	205	9.5
16		K	228	189	9
17		Ca	280	204	10
18		Sc	271	210	10.5
19		Sr	268	203	10
20		Y	286	209	10.5



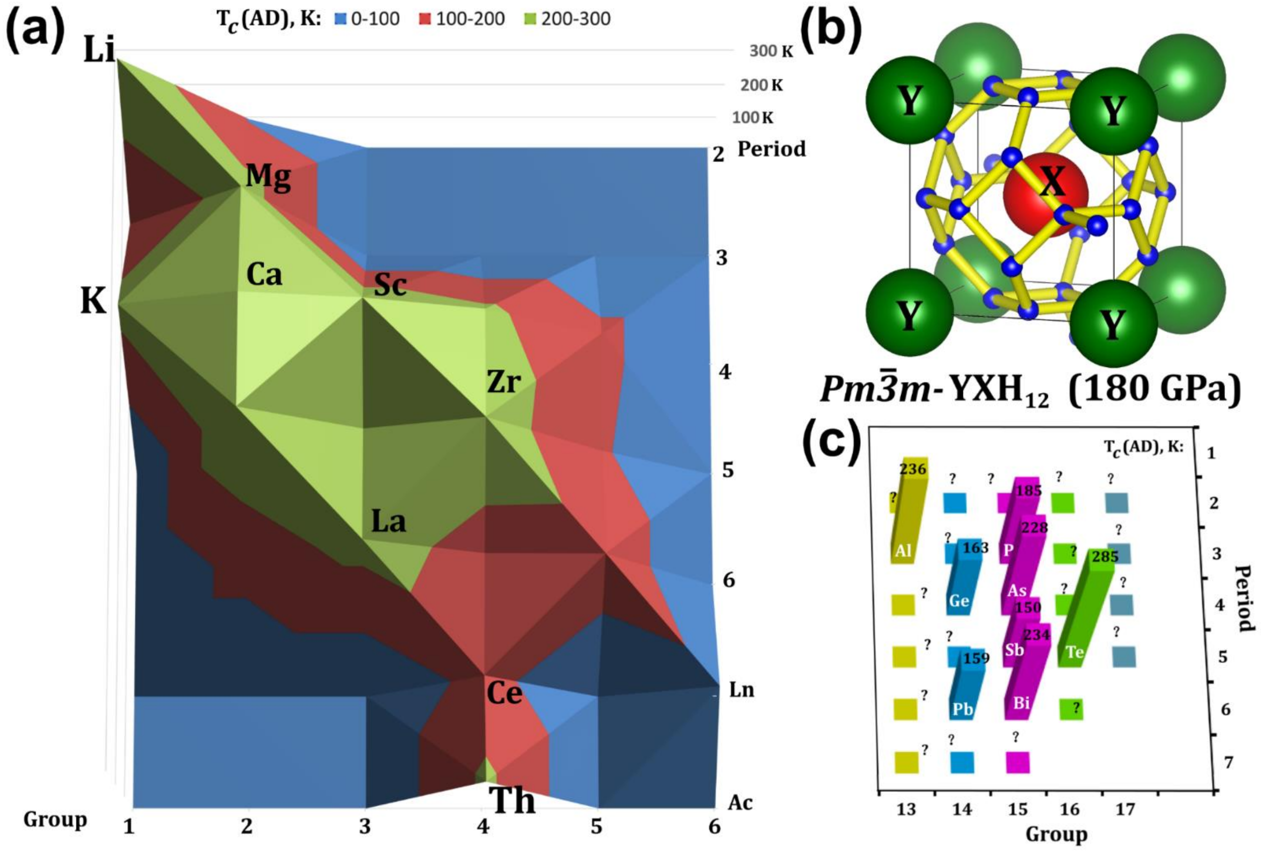
RESULT:

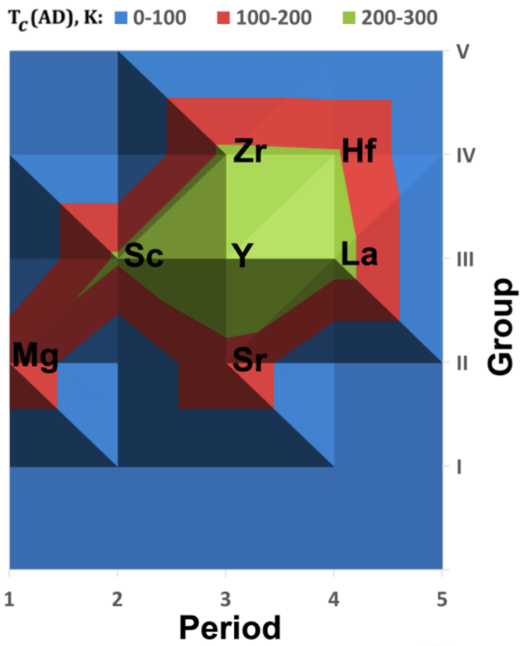
95 % of ternary systems have T_c< 150 K, and just 48 systems have T_c > 250 K

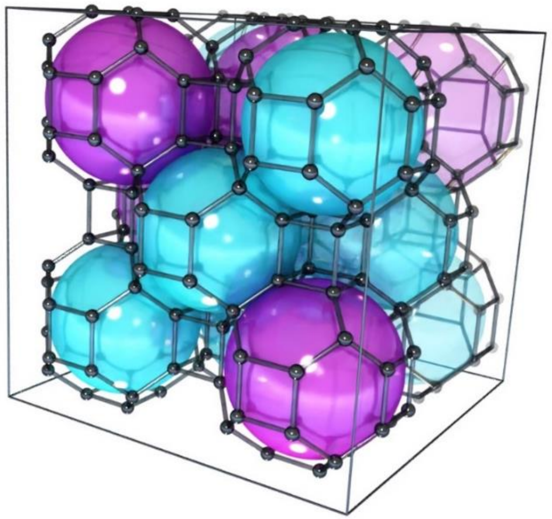
In ternary hydrides, even higher T_C can be achieved at lower pressure and hydrogen content than in binary hydrides.



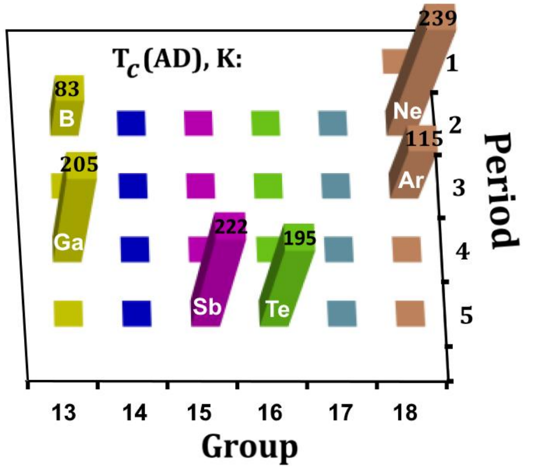
Doping of known superhydrides: YH_6 and LaH_{10}





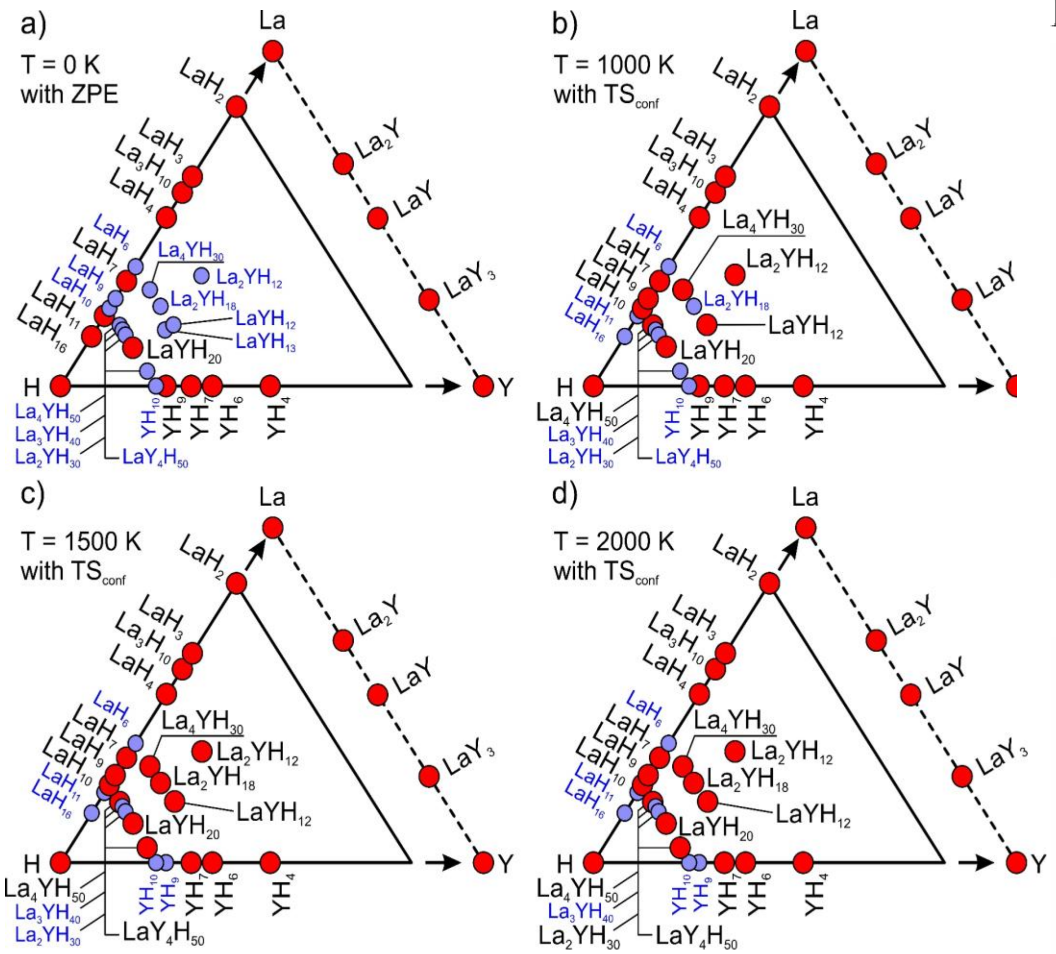


***R-3m*-LaXH$_{20}$ (180 GPa)**

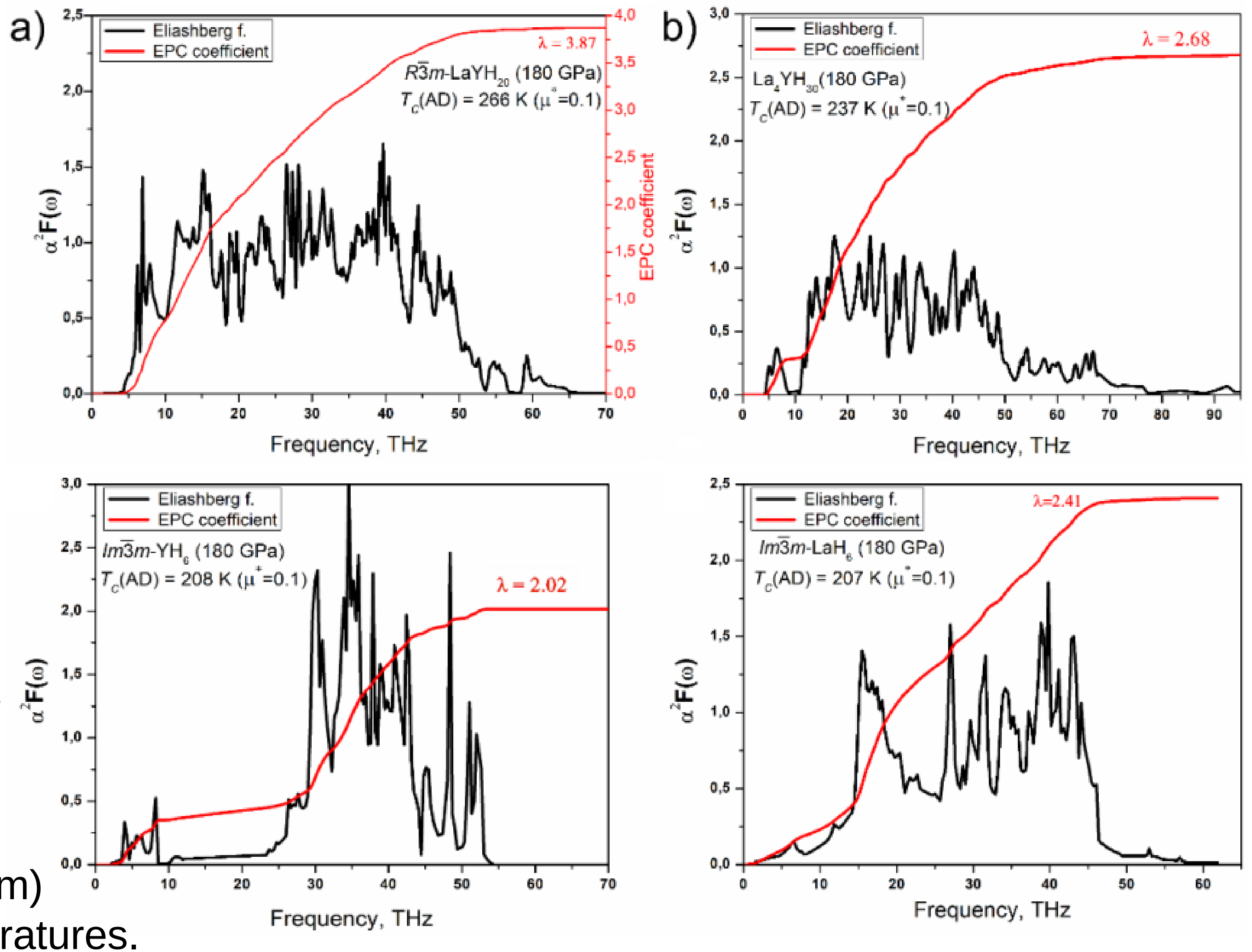


Direct calculations show that there may be the **SECOND GROUP** of HTSC ternary hydrides: a combination of metals and non-metals $(Y,Te)H_{12}$, $(La,Ne)H_{20}$

Theoretical investigation of La-Y-H ternary hydrides

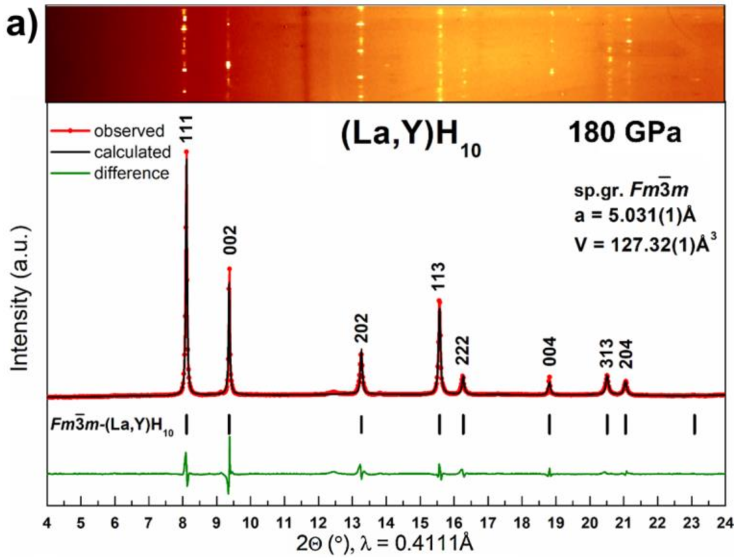


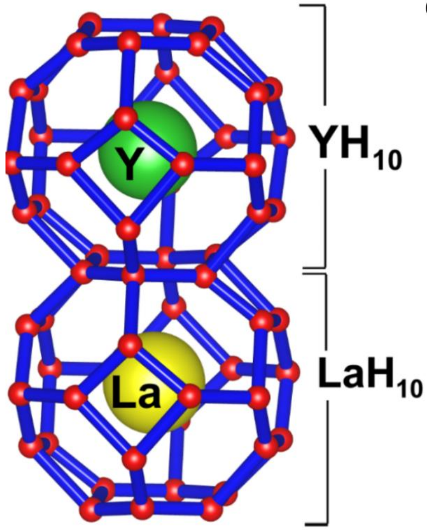
Eliashberg functions of La-Y-H phases

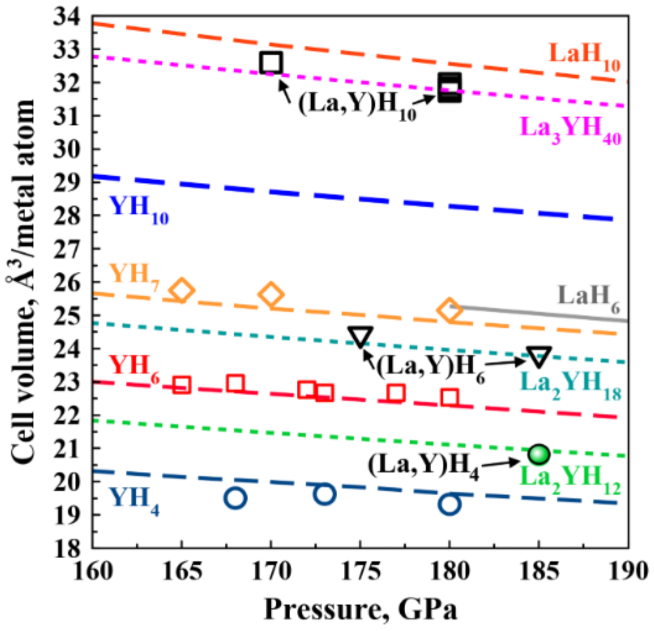


Analysis shows that (La,Y)$H_{4,6,10}$ substituted superhydrides are close to CH (in 10-30 meV/atom) and can be synthesized, especially at high temperatures.

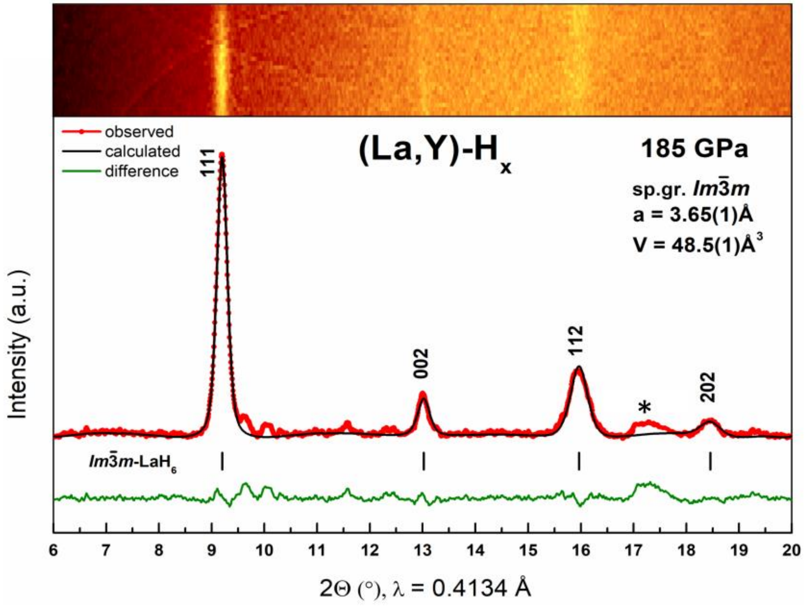
Experiment 1: La-Y-H ternary hydrides with J_C up to 3500 A/mm^2

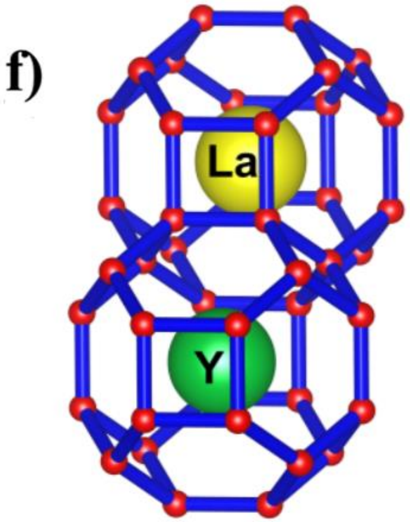




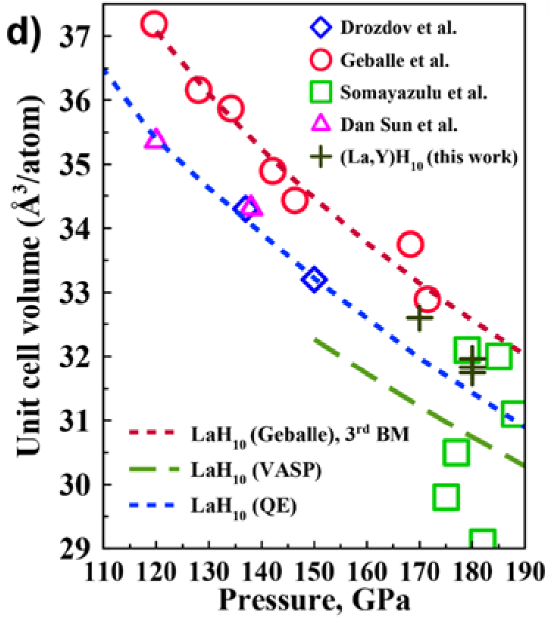


This YH_{10} should be room-temperature superconductor with T_C > 300 K



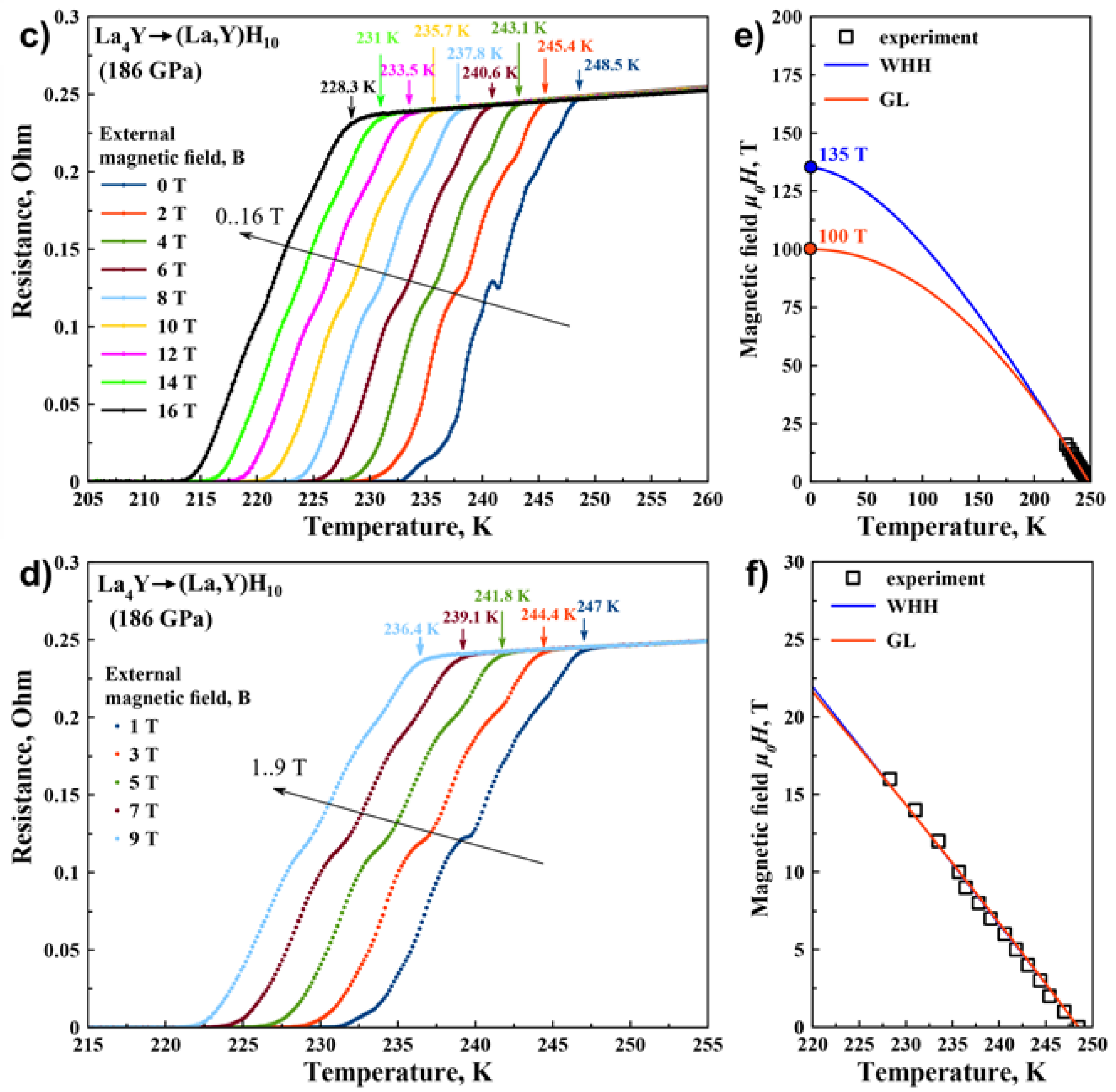


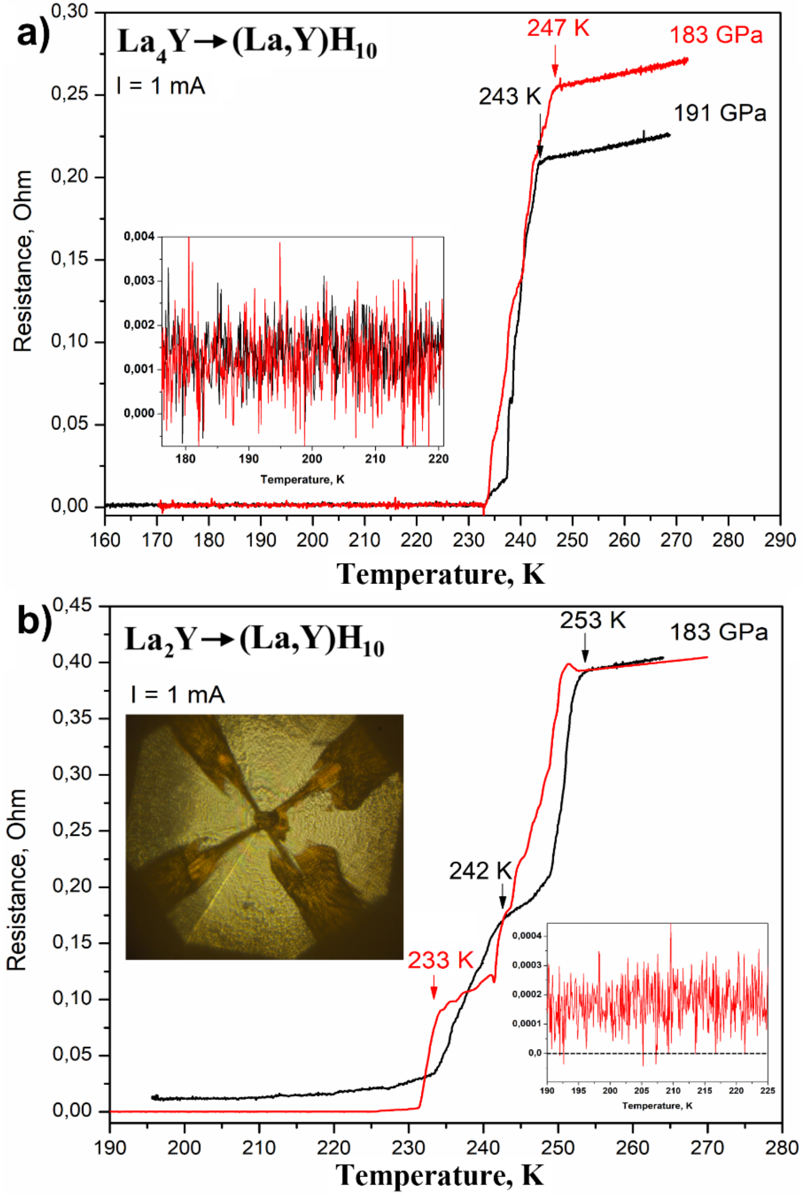
La_2YH_{18} (185 GPa)



These ternary hydrides are **SOLID SOLUTIONS** and their X-ray diffraction is similar to XRD of pure La or Y hydrides.
The main difference is the unit cell volume.

Experiment 1: La-Y-H ternary hydrides: $(La,Y)H_4$, $(La,Y)H_6$, $(La,Y)H_{10}$





LaY
La_2Y
La_4Y
LaY_4

Critical temperature depends on external magnetic field within the BCS model of superconductivity

Experiment 2: C-S-H system

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Article | Published: 14 October 2020

Room-temperature superconductivity in a carbonaceous sulfur hydride

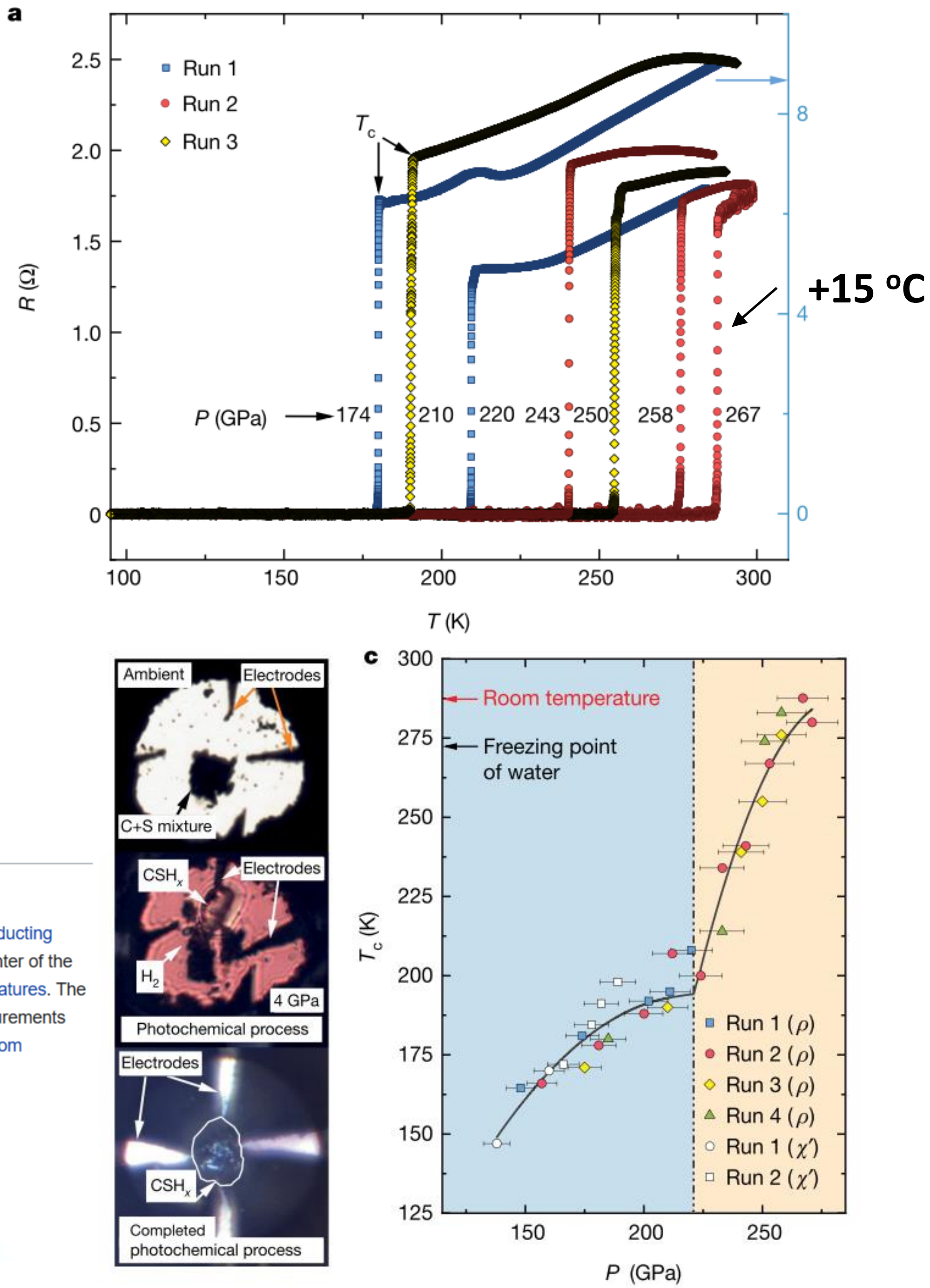
Elliot Snider, Nathan Dasenbrock-Gammon, Raymond McBride, Mathew Debessai, Hiranya Vindana, Kevin Vencatasamy, Keith V. Lawler, Ashkan Salamat & Ranga P. Dias

Nature **586**, 373–377(2020) | Cite this article

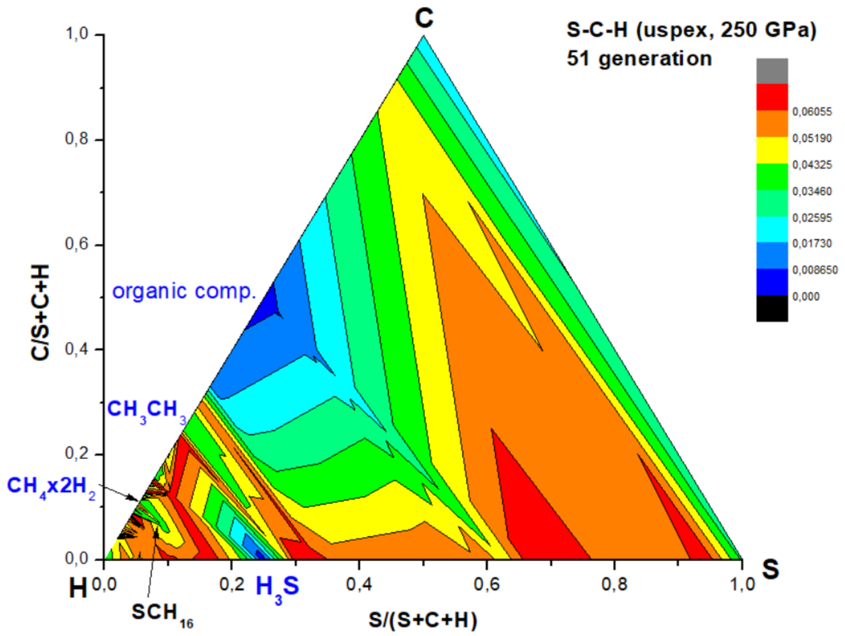
Carbonaceous sulfur hydride

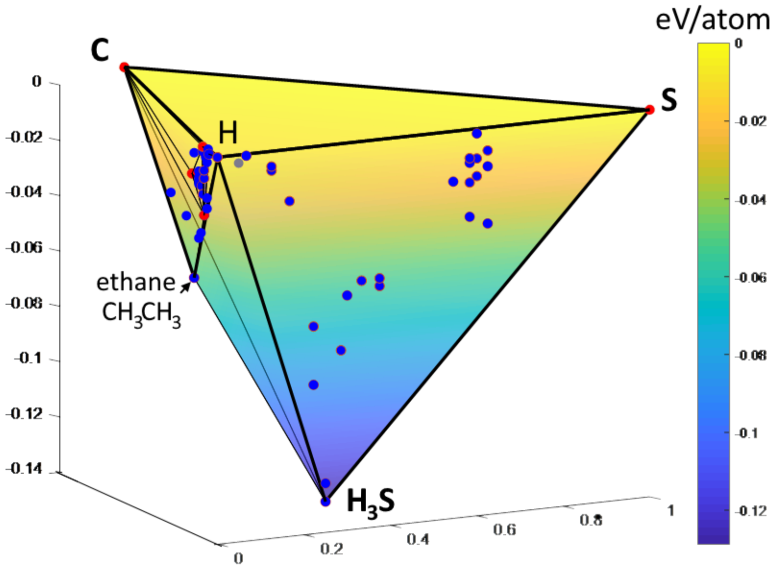
From Wikipedia, the free encyclopedia

Carbonaceous sulfur hydride is a room-temperature superconductor that was announced in October of 2020. The material has a maximum superconducting transition temperature of 15 °C (59 °F) at a pressure of 267 gigapascals (GPa). This is a pressure equivalent to three quarters of the pressure at the center of the Earth.[1] The technical term "room-temperature superconductor" means temperatures as low as the melting point of ice, rather than typical room temperatures. The material is an uncharacterized ternary polyhydride compound of carbon, sulfur and hydrogen with a chemical formula that is thought to be CSH_8. Measurements under extreme pressure are difficult, and in particular the elements are too light for an X-ray determination of crystal structure.[2] This is the closest to room temperature achieved for a superconductor, with an onset almost 30° C higher than the previous record-holder.[3]



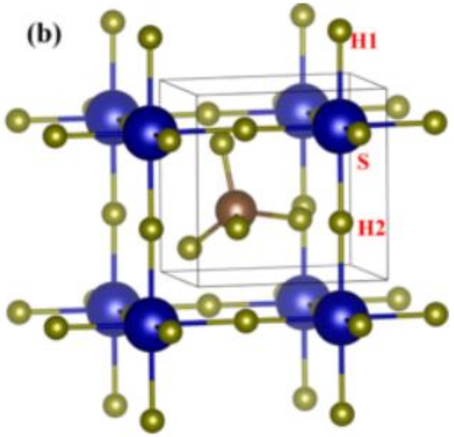
Theoretical investigation of C-S-H system, search for stable phases

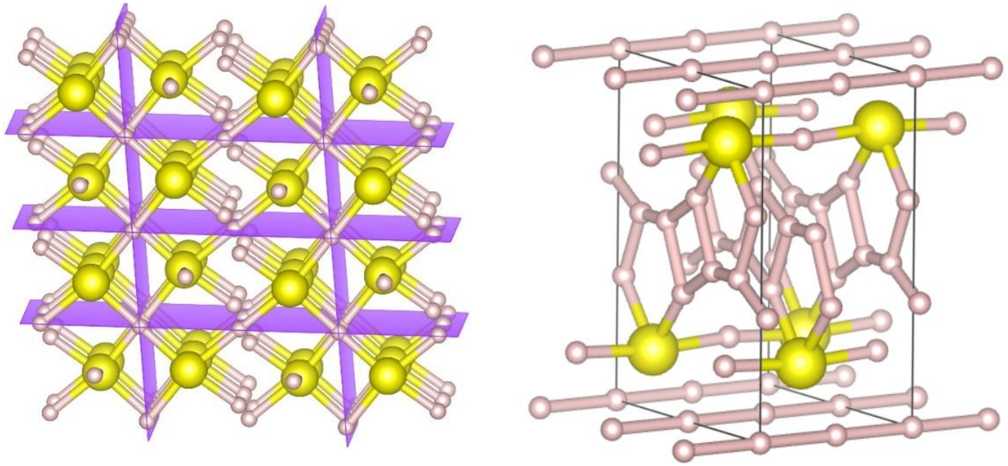


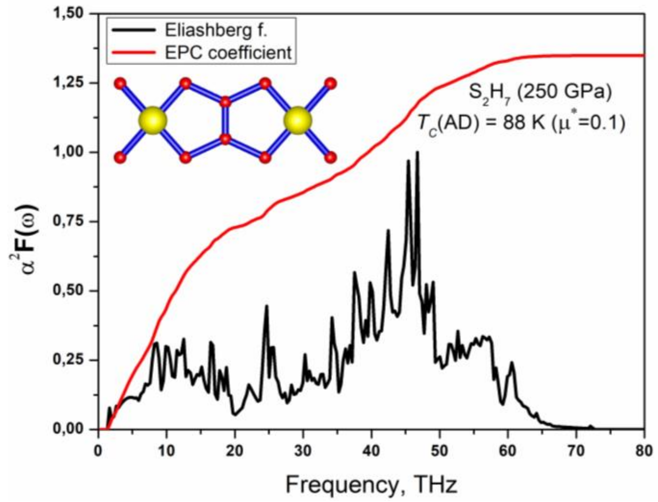


3D convex hull of C-S-H almost **do not contain stable** ternary hydrides.

Most part of ternary C-S hydrides have **positive** formation enthalpy.







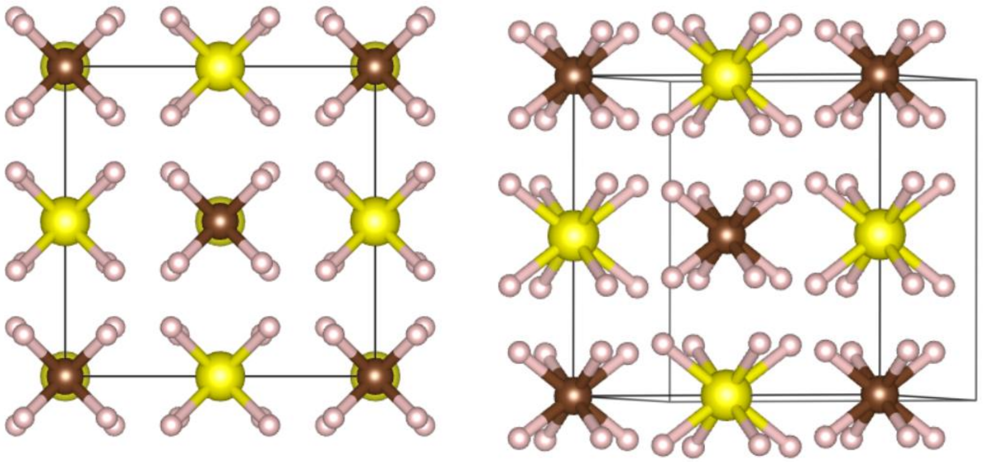
S_2H_7 (1D infinite H-H-H chains)

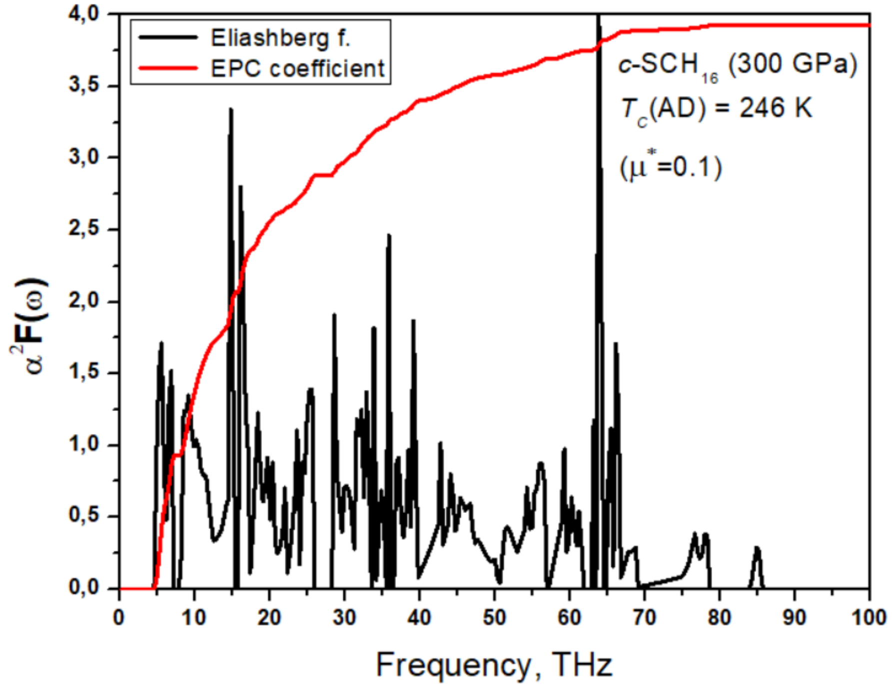
PRB 2020: CSH_7

10.1103/PhysRevB.101.134504

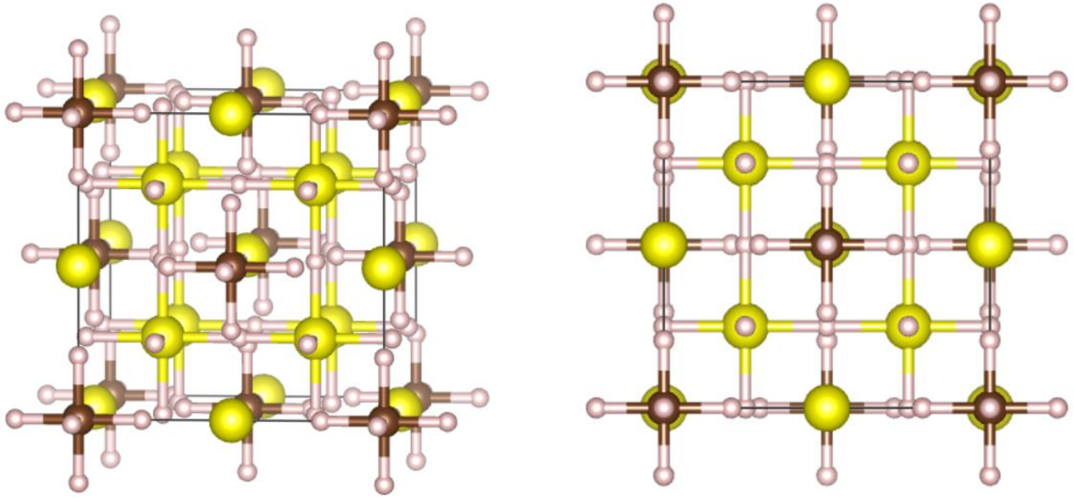
T_C values ranging from 100 K to 190 K

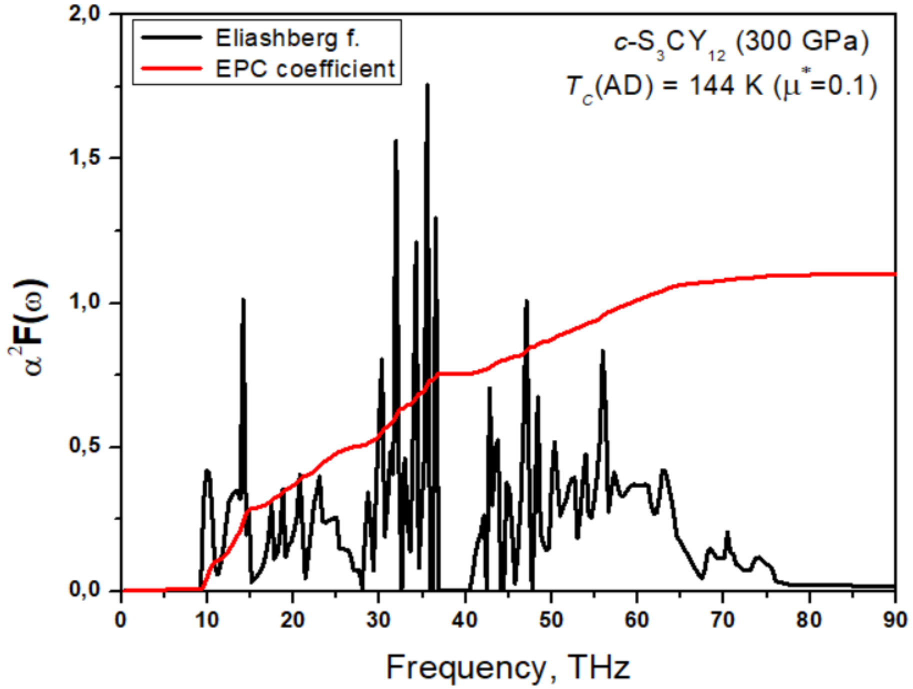
Fm-3m-SCH_{16} (300 GPa, XH_8)





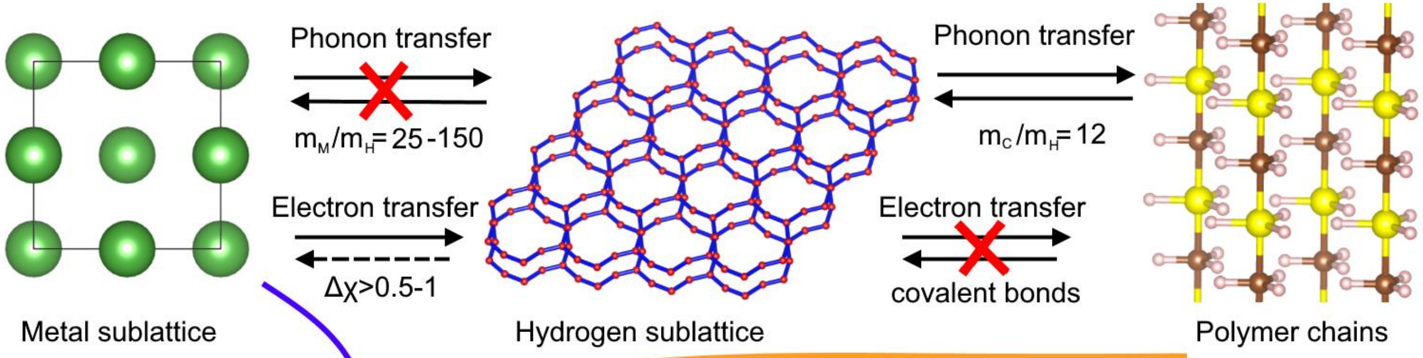
Fm-3m-S_3CH_{12} (300 GPa, XH_3)

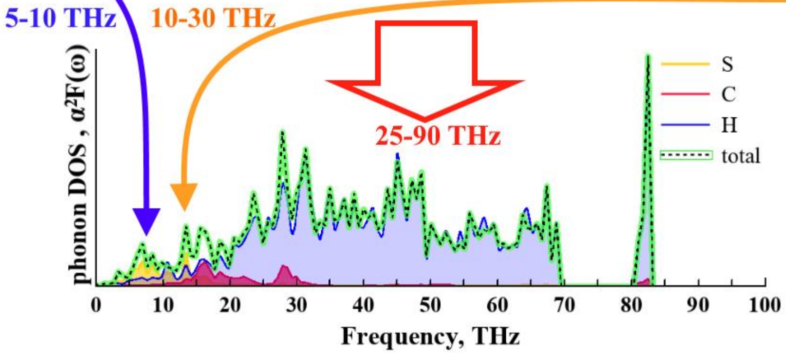


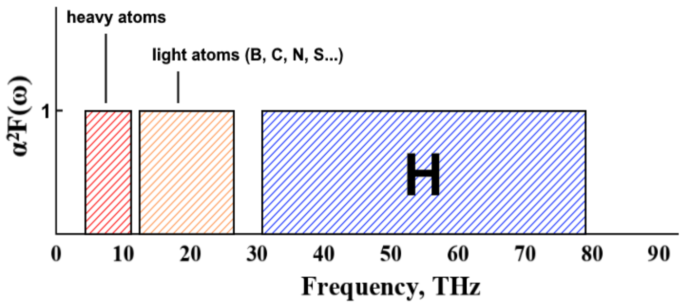


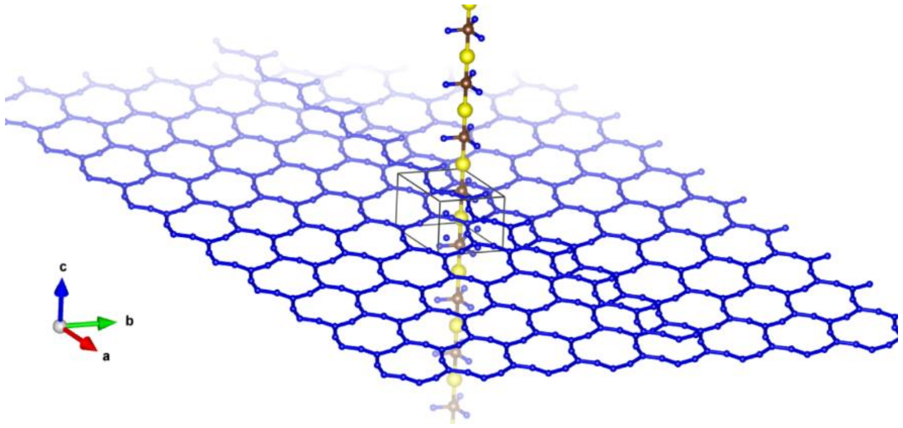
Theoretical investigation: C-S-H system, *h*-CSH_{16} as an interesting model system

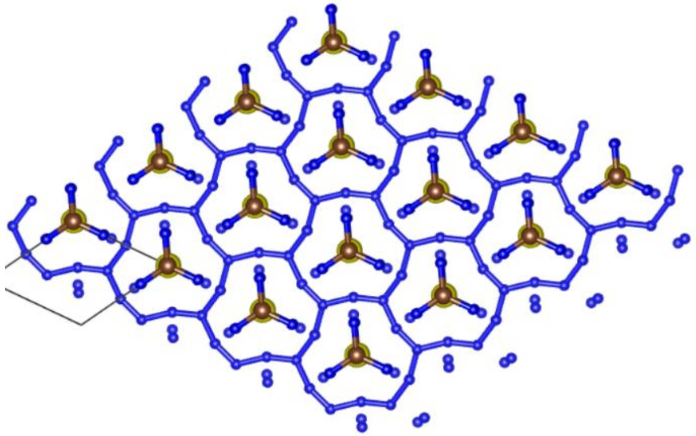
One of the found ternary structures was *P-62m*-CSH_{16} which consists of 2D layers of hydrogen stitched with polymer **[-S-CH_3-]$_n$**









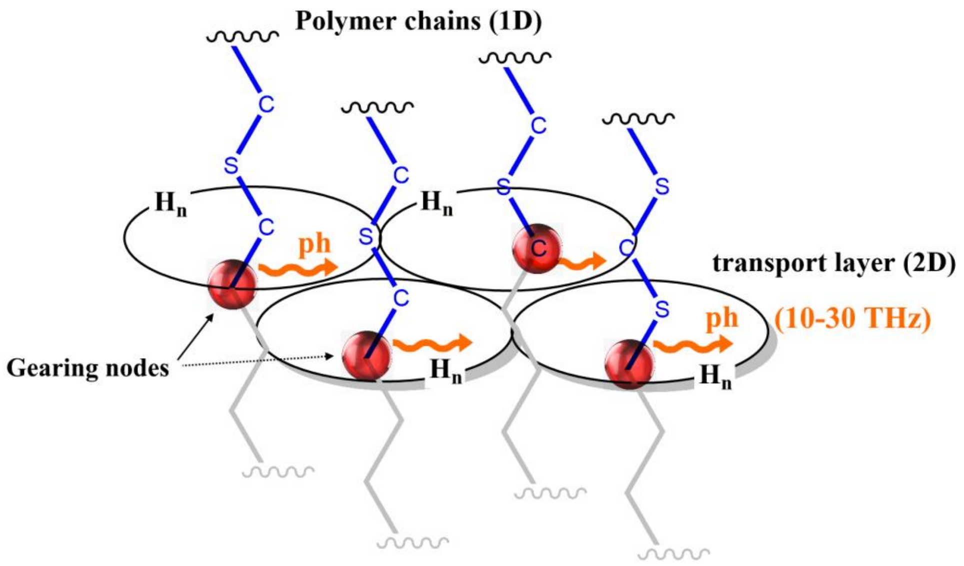


This structure was found in NPU (Xi'an, Haiyang Niu group)

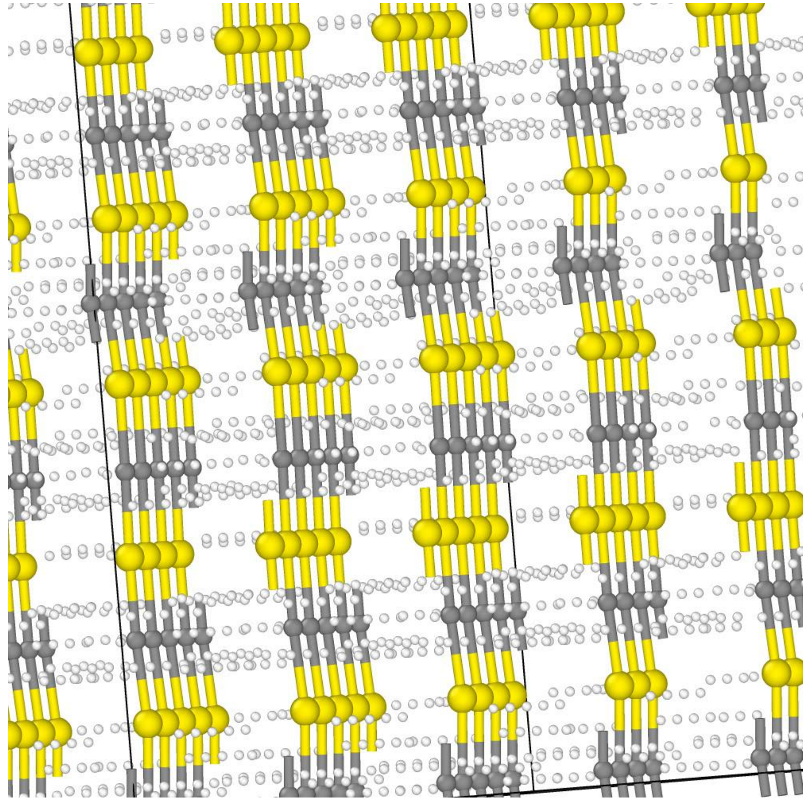
Graphene-like hydrogen stabilized by infinite polymeric chains [-S-CH_3-]$_n$ with pentacoordinate carbon may be responsible for room-temperature superconductivity in C-S hydrides

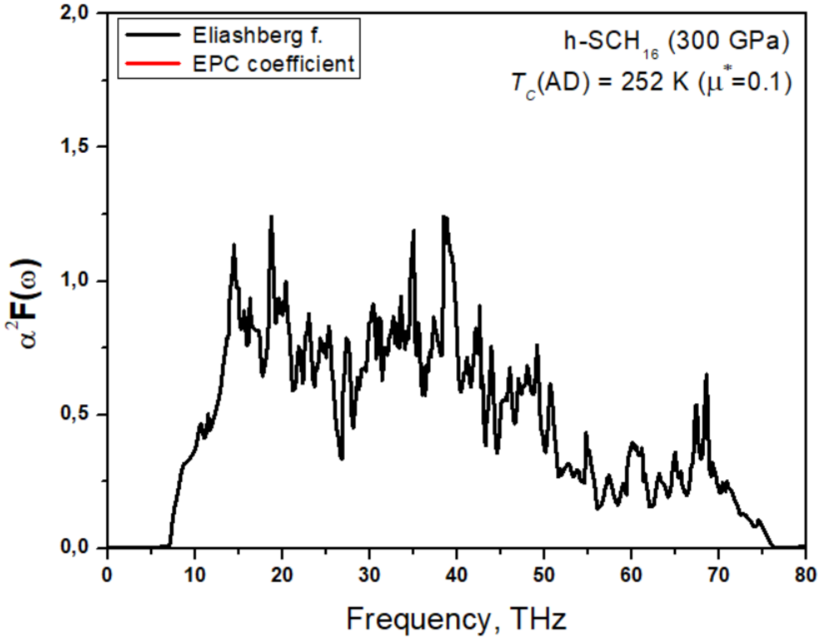
Experiment 2: C-S-H system, electron phonon interaction

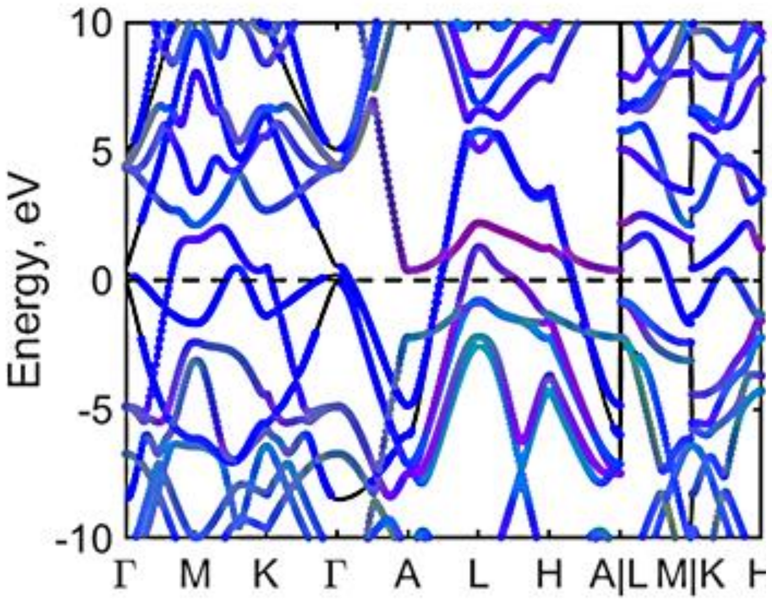
1000 K

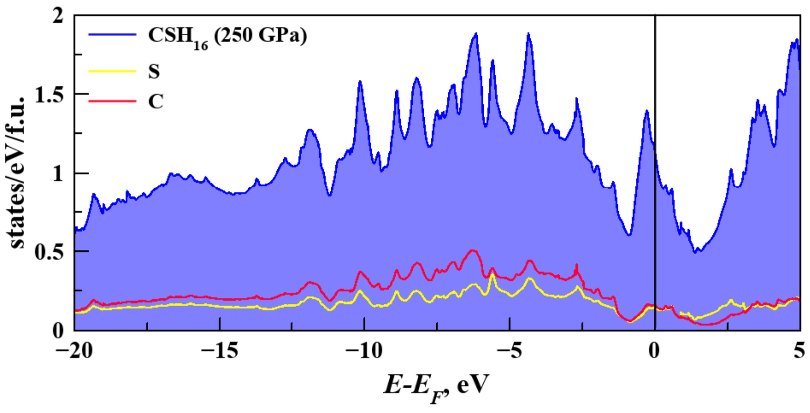


QE, VASP calculations confirm this universal idea:
T_C(300 GPa) > 250 K
and several vHs are placed close to the Fermi level









Conclusion: world of the "Avatar" becomes reality