Recent advances in high-temperature superconductivity in ternary hydrides

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Superconductivity surrounds us

Medicines against COVID

Single-photon detectors
Tomography
Synchrotrons and colliders
Magnetic field sensors
Quantum supercomputer

Maglev trains and SC gyroscopes in Int. Space Station

Nuclear magnetic resonance spectrometer
112 years of progress in superconductivity

Critical temperature, K

Total publication efforts on "Superconductivity"

Log N

Publication activity

Hydride era

Cuprate era

LTSC era

Superconductivity research timeline, yr.

Metal hydrides
Nonmetal hydrides
Cuprates
Pnictides
Fullerides
Low-temperature SC
Heavy fermions

Li$_2$MgH$_{16}$

YH$_{10}$

CSH$_x$

YH$_9$LaH$_6$

YH$_6$

H$_2$S

HgBaCaCuO

HgTlBaCaCuO

YBCO

SrFeAs

UT$_3$
High-temperature superconductivity in hydrides under pressure

Metallic hydrogen: \( T_c \) is 217-356 K at ~500 GPa

Metallic sulfur hydride: \( T_c \) is up to 203 K at 155 GPa

In addition \( \text{PH}_2, \text{SiH}_x \) and \( \text{H}_3\text{Se} \) were also synthesized \((T_c < 100 \text{ K})\)
Another example – record high $T_C$ in LaH$_{10}$ (150 GPa)

The maximum $T_C \sim 250$-260 K

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

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\textsuperscript{*}Contributed by Russell J. Hemley, May 5, 2017; revised by Parachuleeporn Garreth, Jeffrey M. McMahon, and Dimitrios Vaitis (Corresponding Author)
High pressure or small sample?

Diamond anvil

Gasket + anvils

Sample
Moscow collaboration: HTSC hydrides in diamond anvil cells

Skoltech (THEORY + Xe FIB)

Crystallography Institute RAS
DIAMOND ANVIL CELLS, LASER HEATING

Lebedev’s Physical Institute (LPI)
TRANSPORT MEASUREMENTS

PETRA, ESRF, Spring-8, SSRF
synchrotron research (X-ray diffraction)
DETERMINATION OF STRUCTURE
Current progress of research: 12 binary metal-hydrogen systems

Molecular hydrides

Metallic hydrides

Magnetic metallic hydrides

Different hydrogen form – different physical properties
Magnetism suppresses superconductivity
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”).


► 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

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.
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$_{10}$

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

Analysis shows that \((\text{La},\text{Y})\text{H}_{4.6,10}\) 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

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$_{10}$

Critical temperature depends on external magnetic field within the BCS model of superconductivity
Experiment 2: C-S-H system

Room-temperature superconductivity in a carbonaceous sulfur hydride

Elliott Snider, Nathan Dassenbrock-Gammon, Raymond McBride, Matthew Debesai, Hiranya Vindana, Kevin Vencatasamy, Keith V. Lawler, Ashkan Salamat & Ranga P. Dias

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Carbonaceous sulfur hydride

Carbonaceous sulfur hydride is a room-temperature superconductor that was announced in October 2020. The material has a maximum superconducting transition temperature of 165 K (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. 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 polyhydrite compound of carbon, sulfur and hydrogen with a chemical formula that is thought to be CSHx. Measurements under extreme pressure are difficult, and in particular the elements are too light for an X-ray determination of crystal structure. This is the closest to room temperature achieved for a superconductor, with an onset almost 30°C higher than the previous record holder.
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.

PRB 2020: CSH$_7$

10.1103/PhysRevB.101.134504

$T_C$ values ranging from 100 K to 190 K

S$_2$H$_7$ (1D infinite H-H-H chains)
$Fm\text{-}3m\text{-}SCH_{16}$ (300 GPa, XH$_8$) $Fm\text{-}3m\text{-}S_3CH_{12}$ (300 GPa, XH$_3$)
Theoretical investigation: C-S-H system, \( h\)-CSH\textsubscript{16} as an interesting model system

One of the found ternary structures was \( P-62m\)-CSH\textsubscript{16} which consists of 2D layers of hydrogen stitched with polymer \([\text{-S-CH}_3\text{-}]_n\).

Graphene-like hydrogen stabilized by infinite polymeric chains \([\text{-S-CH}_3\text{-}]_n\) with pentacoordinate carbon may be responsible for room-temperature superconductivity in C-S hydrides.

This structure was found in NPU (Xi’an, Haiyang Niu group)
Experiment 2: C-S-H system, electron phonon interaction

QE, VASP calculations confirm this universal idea: $T_c(300 \text{ GPa}) > 250 \text{ K}$ and several $\nu$Hs are placed close to the Fermi level at $1000 \text{ K}$. 

[Graph showing energy states and frequency distribution]
Conclusion: world of the “Avatar” becomes reality