A dream comes true: Room-temperature superconductivity

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Dipartimento di Scienze Fisiche e Chimiche & CNR-SPIN
Universita' degli Studi dell'Aquila

Vostok base in Antarctica

In 1983 a temperature of -89.2 ^{o}C was registered

Fontana Luminosa, L'Aquila

In January 2017 a temperature of $-12.0\ ^{o}C$ was registered

What happens to the electrical resistivity when we lower the temperature?

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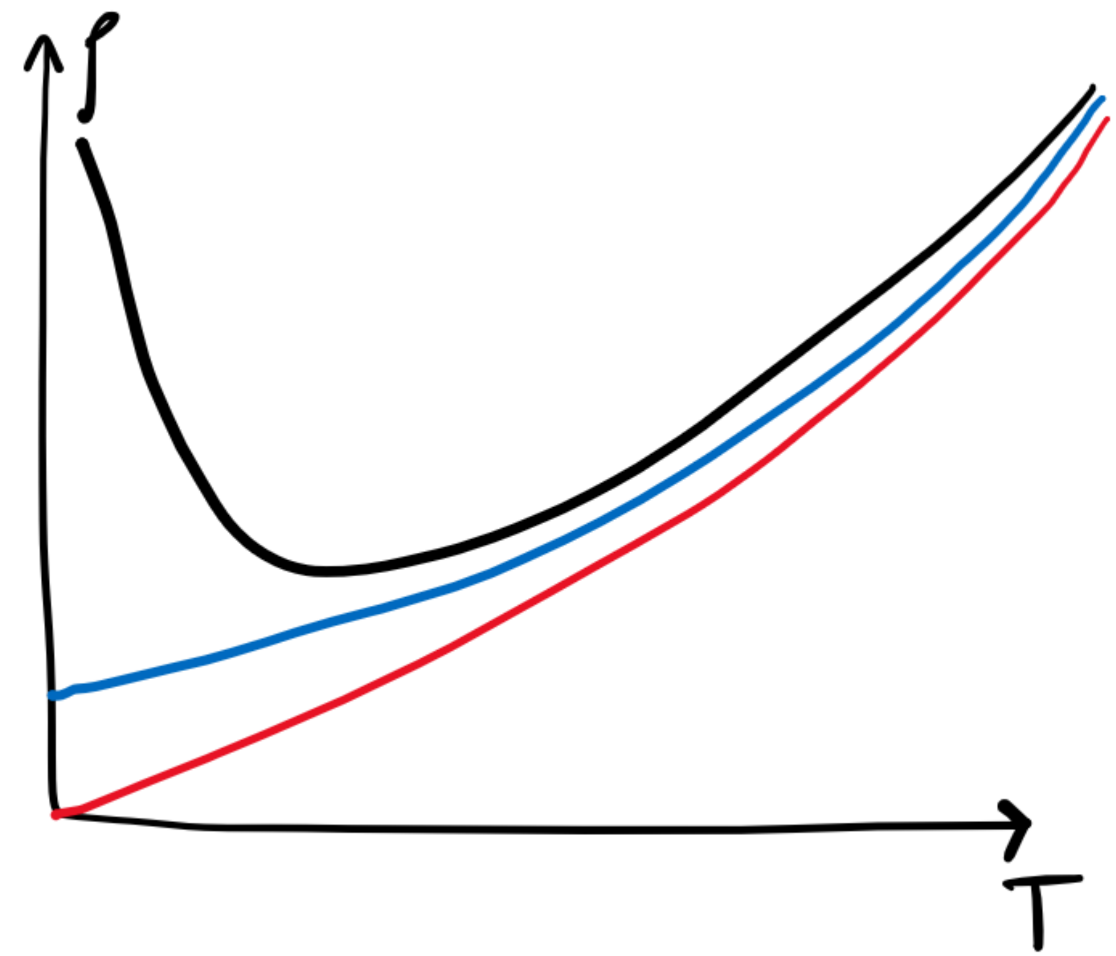
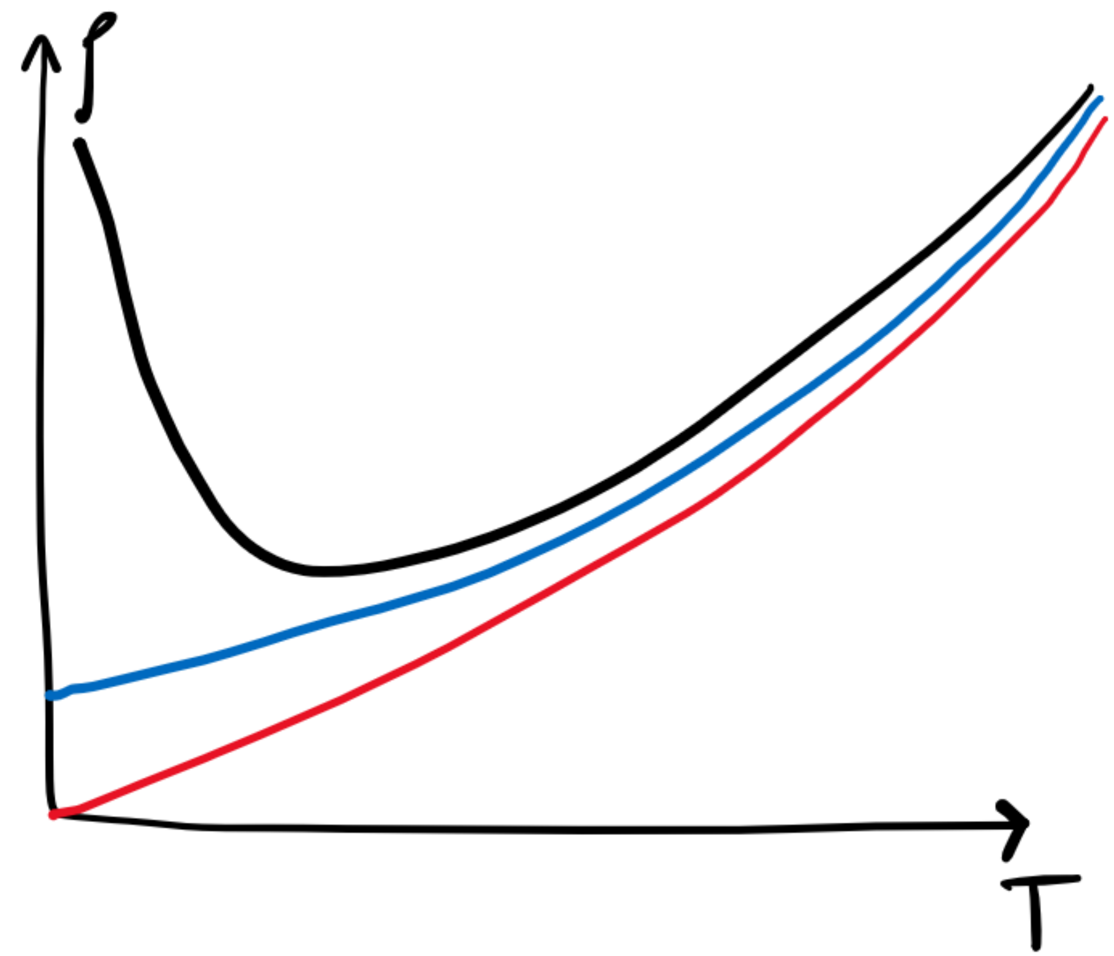


What happens to the electrical resistivity when we lower the temperature?

In 1908 liquid helium was realised by Kamerling Onnes



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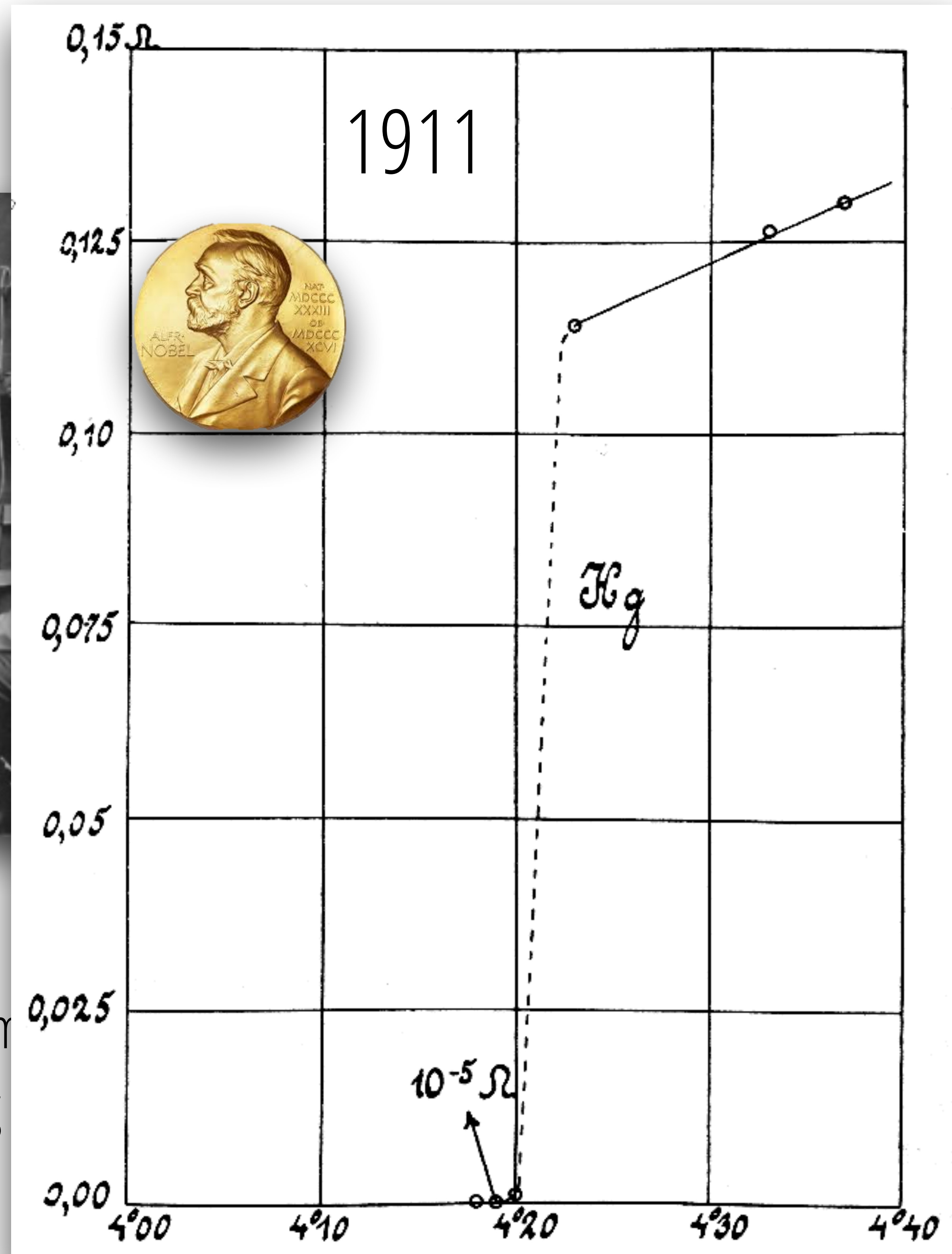

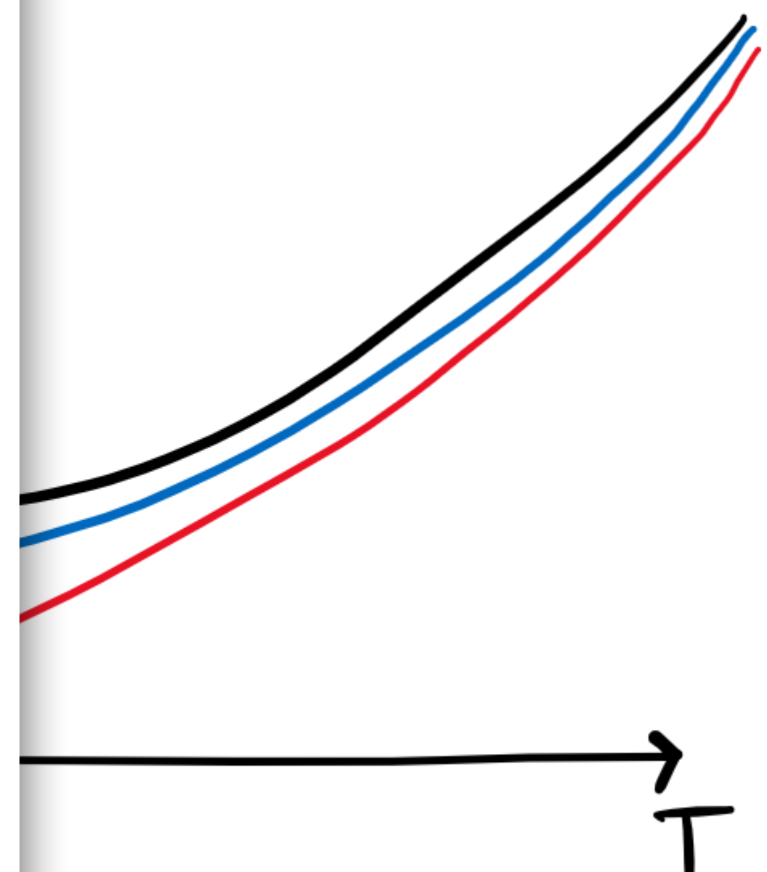

In 1908 liquid helium

Kamerling

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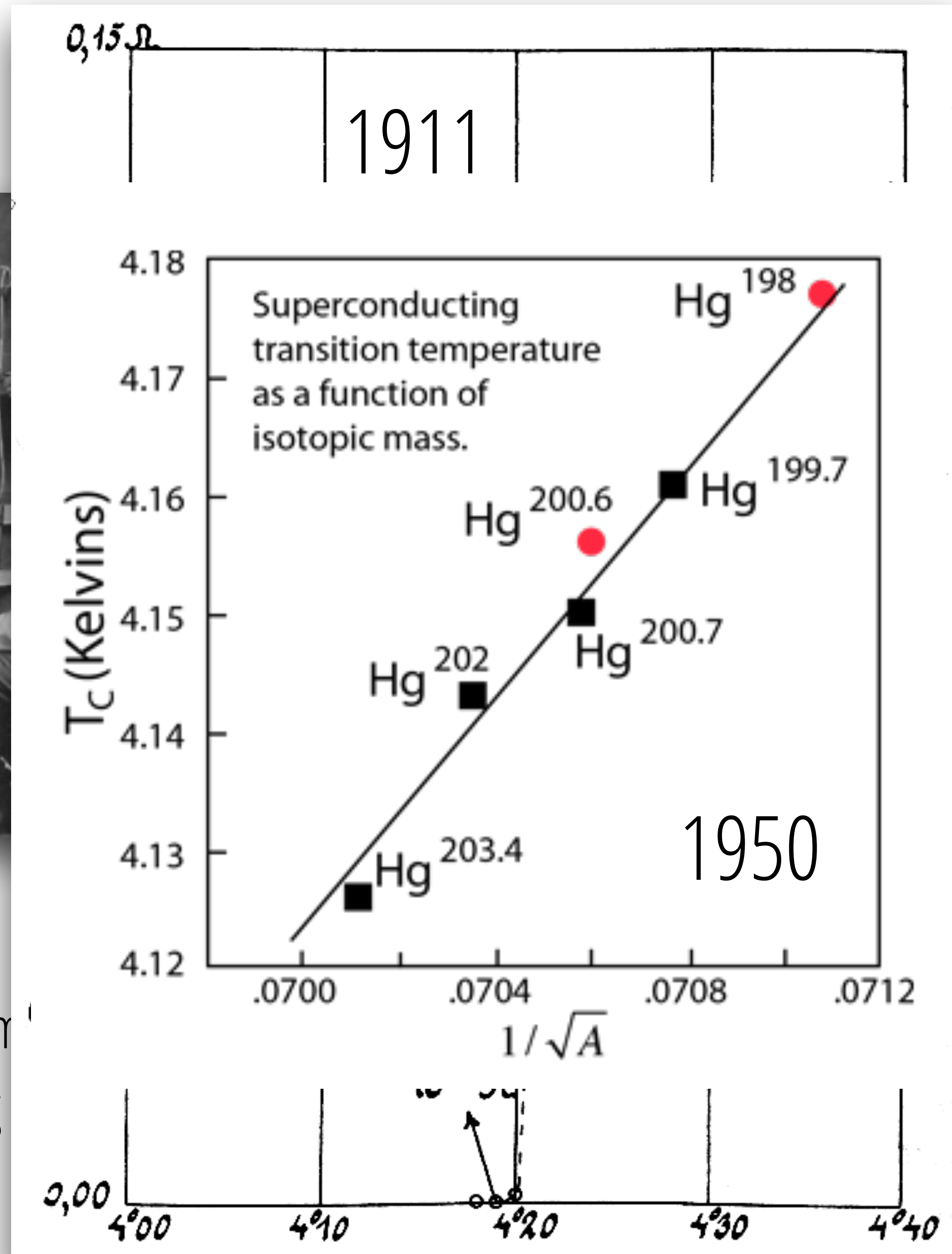
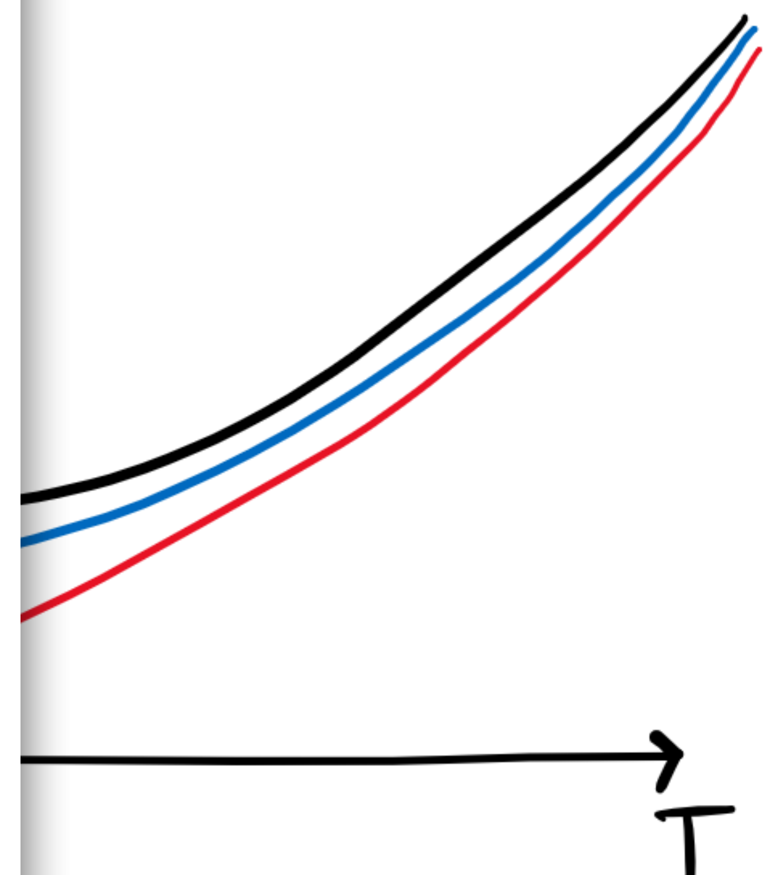
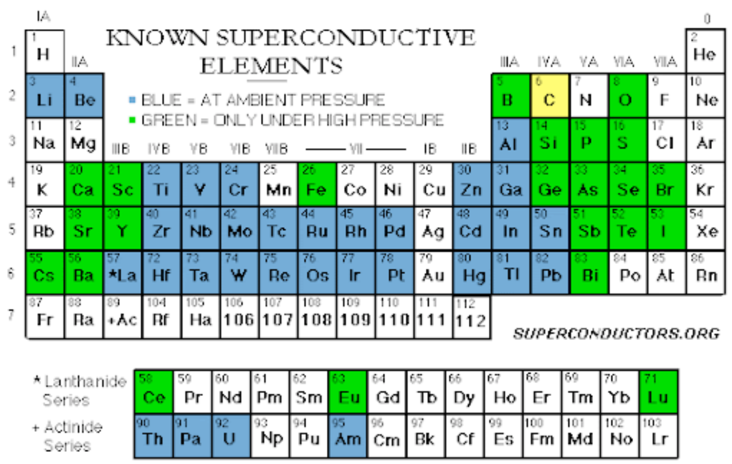




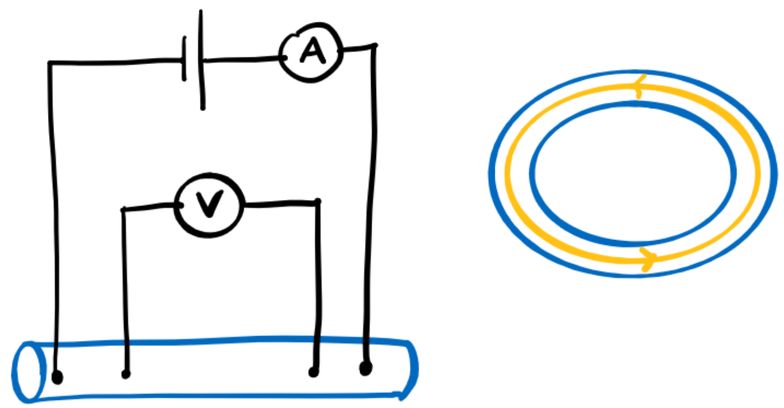
In 1908 liquid helium
Kamerling

Superconductors

It is a common phenomenon

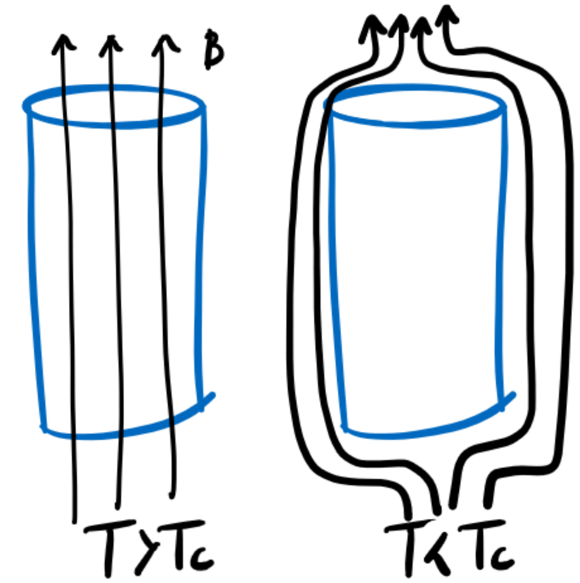


Persistent current: no Joule effect



Jc=50 kA

Meissner effect



Hc=13-18 Tesla

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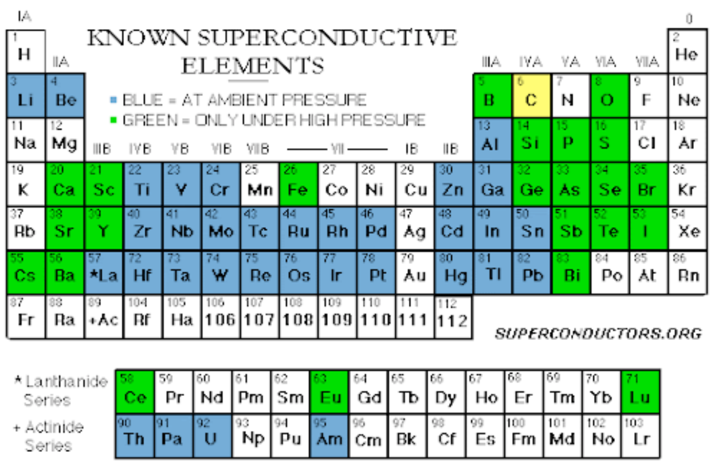

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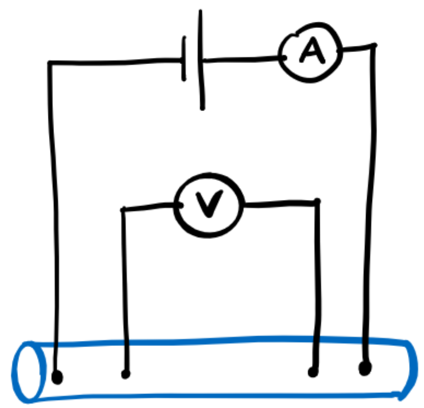

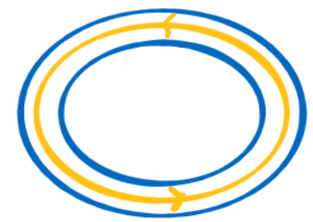

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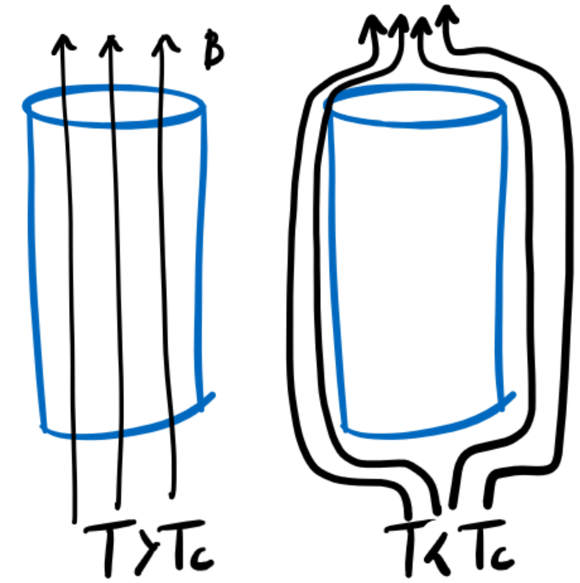


H_c=13-18 Tesla

ITER

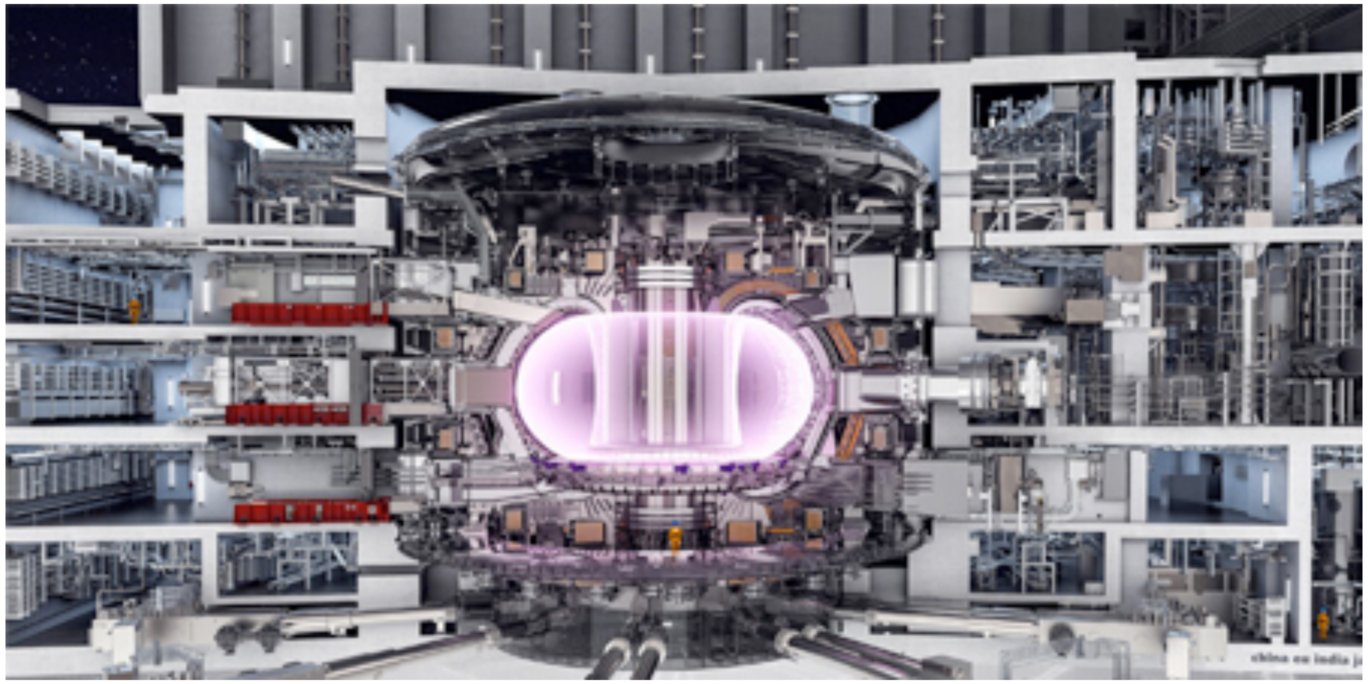
Nb3Sn@ 4K (ASG)

100.000 Km of cables

41 GJ energy

13.5 Tesla

80 kA



Input power: 620 MW

Output power: 500-700 MW

Large fraction for refrigeration

PHYSICAL REVIEW VOLUME 108, NUMBER 5 DECEMBER 1, 1957

Theory of Superconductivity*

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(Received July 8, 1957)

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Cooper instability

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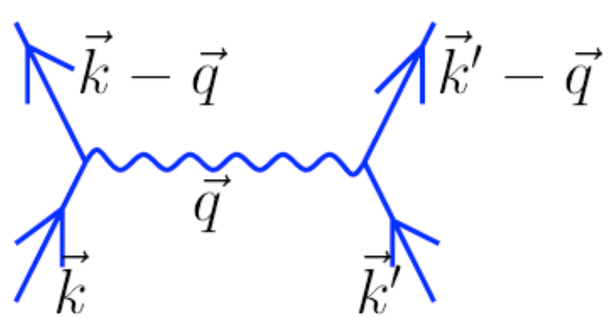

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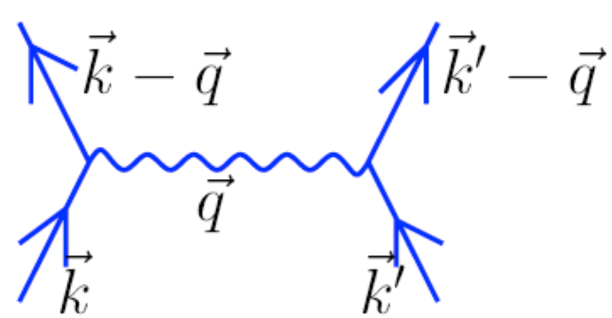
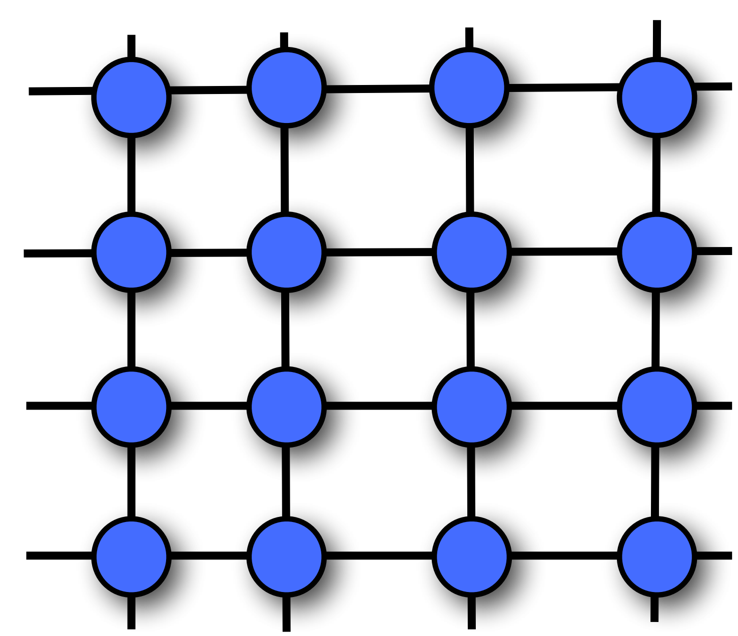


BCS ansatz



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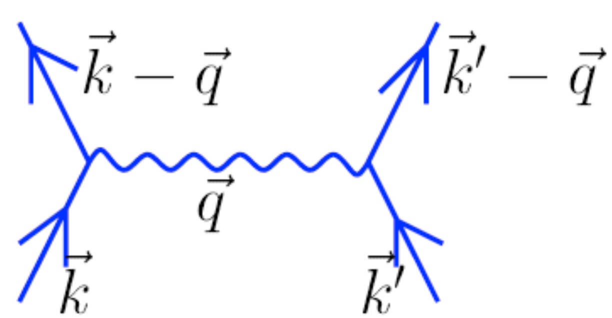

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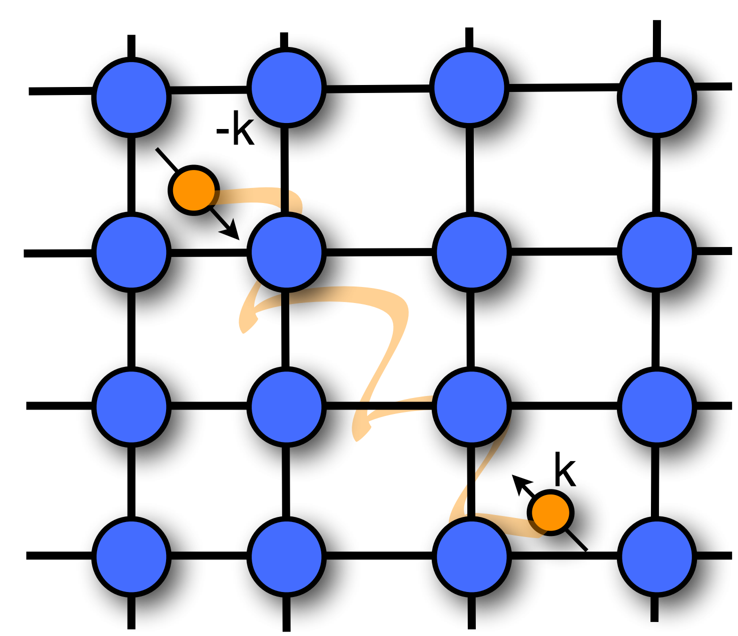

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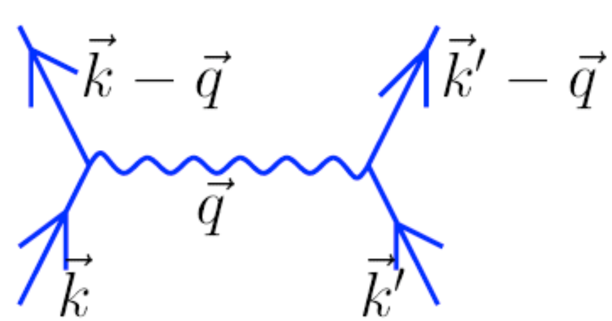

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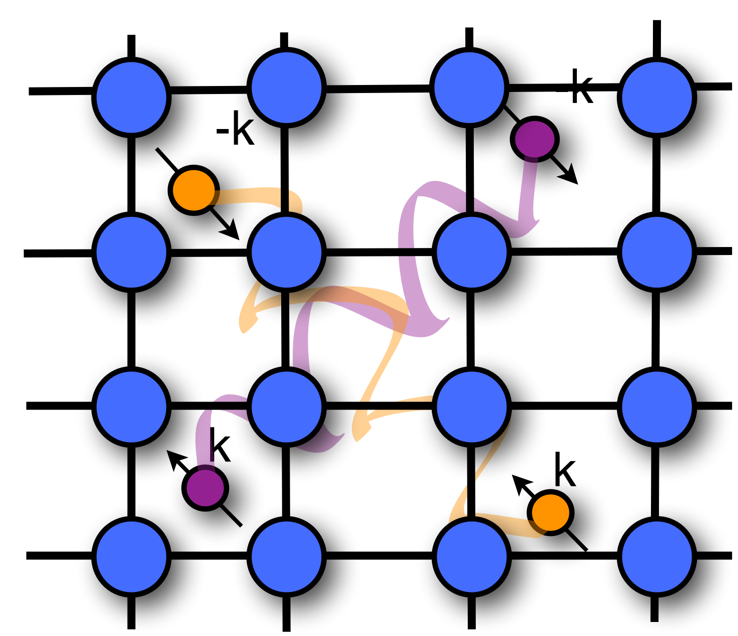

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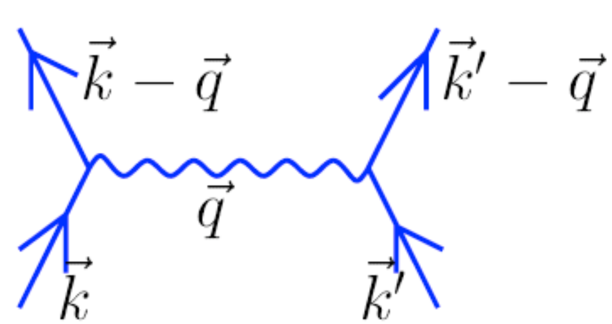

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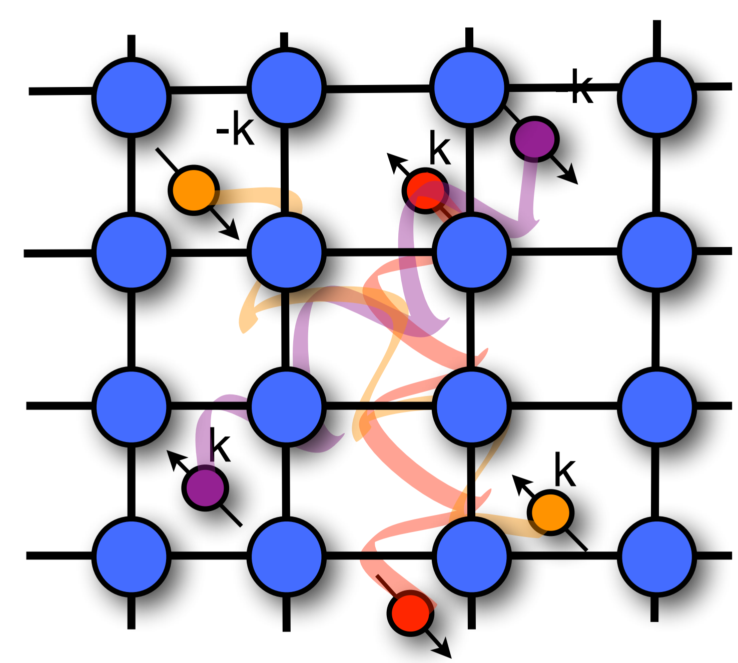

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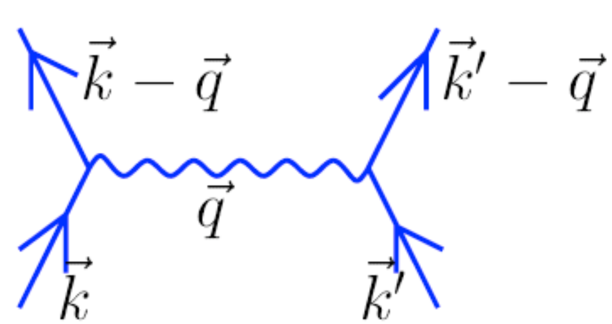

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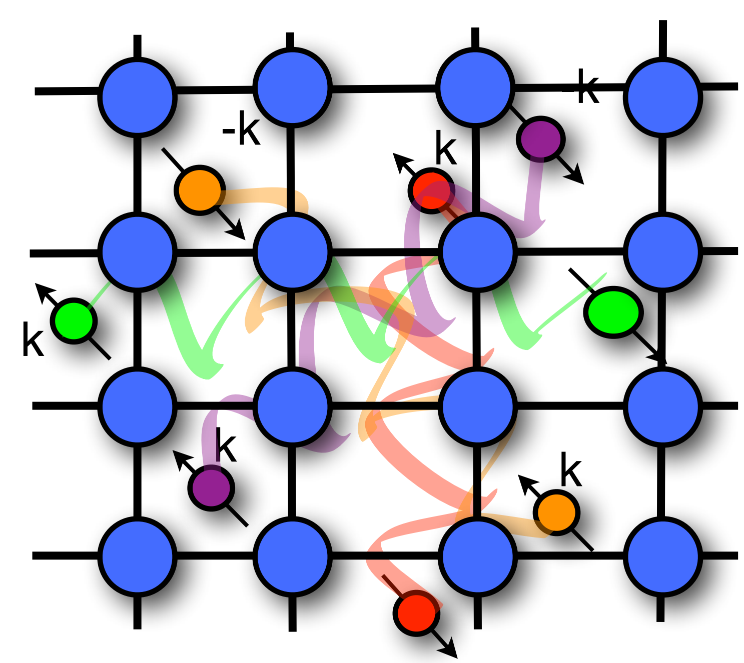
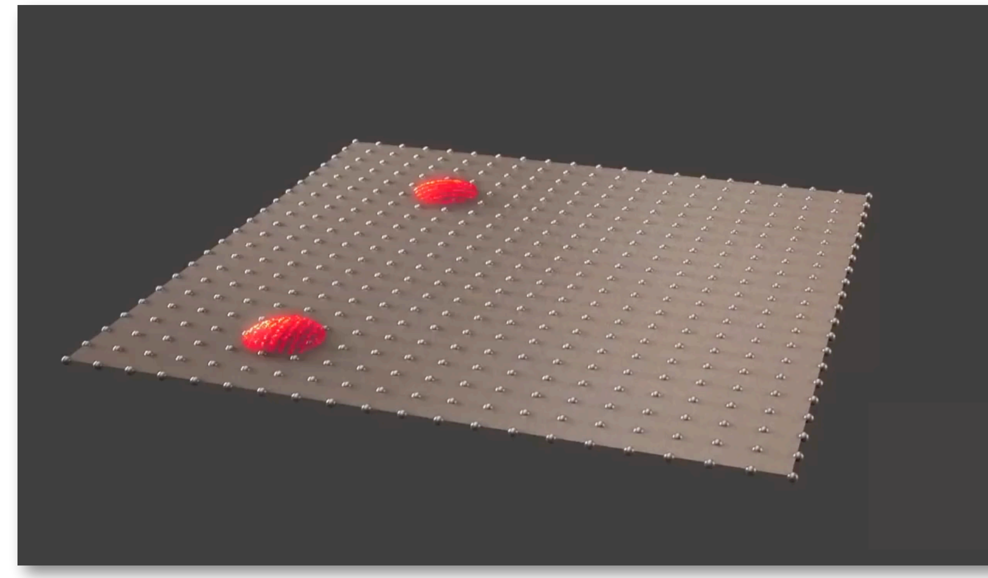


Coherent (macroscopic) state

$$\Psi_N(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) = \mathcal{A}\psi(\mathbf{r}_1, \mathbf{r}_2)\psi(\mathbf{r}_3, \mathbf{r}_4)\cdots\psi(\mathbf{r}_{N-1}, \mathbf{r}_N)(1\uparrow)(2\downarrow)(3\uparrow)(4\downarrow)\cdots(N-1\uparrow)(N\downarrow).$$

$$|\Psi_{BCS}\rangle = const.\prod_{\mathbf{k}} \exp(\alpha_{\mathbf{k}})\hat{P}^{+}_{\mathbf{k}})|0\rangle$$

$$\Psi = \prod_{\mathbf{k}=\mathbf{k}_1,\cdots,\mathbf{k}_{N/2}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow}\right)|0\rangle$$



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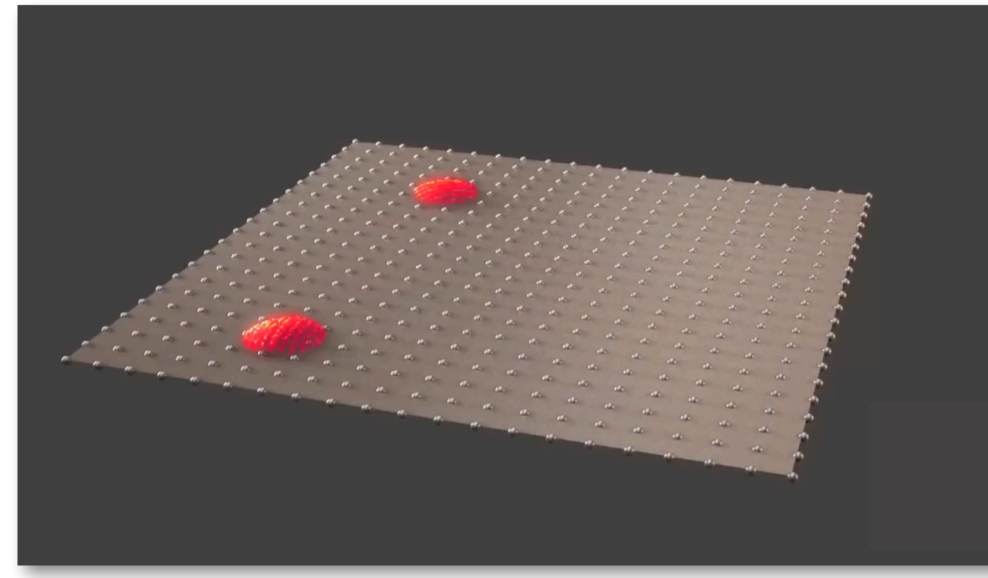


BCS predictions

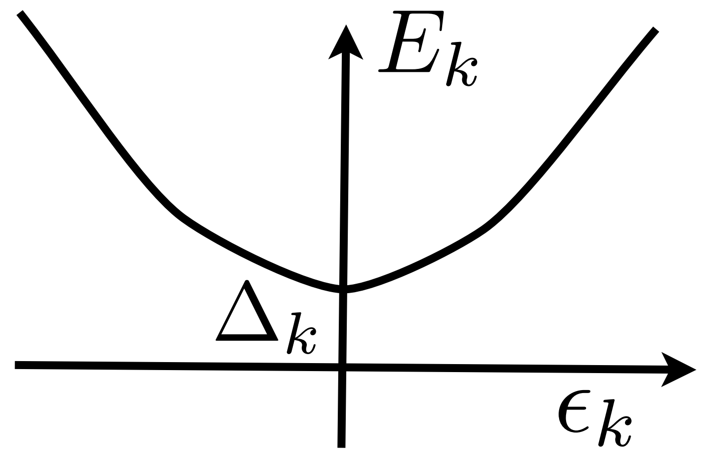
The BCS ground state has a lower energy Δ wrt the free-electron state, which depends on the temperature

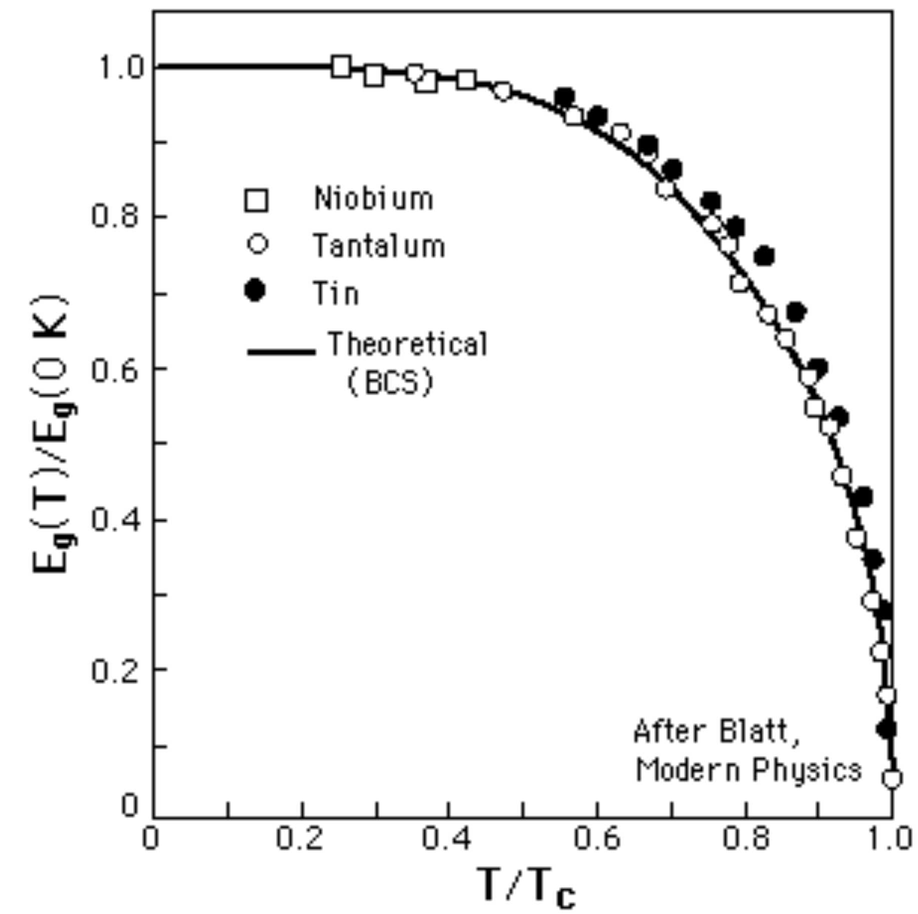
$$E_k = \sqrt{\epsilon_k^2 + |\Delta_k|^2}$$

$$\frac{\Delta(T)}{\Delta(0)} = 1.74 \ \left(1 - \frac{T}{T_c}\right)^{\frac{1}{2}}$$

$$T_c^{BCS} = \omega_D e^{-\frac{1}{\lambda}}$$

$$\lambda = N(0) \ V_{ph}$$





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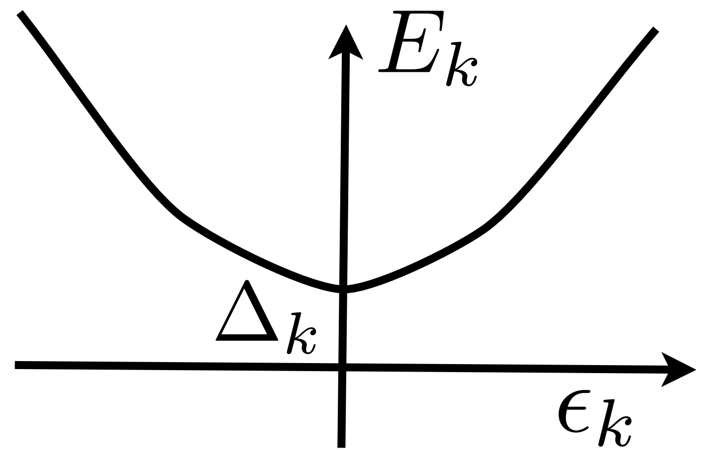

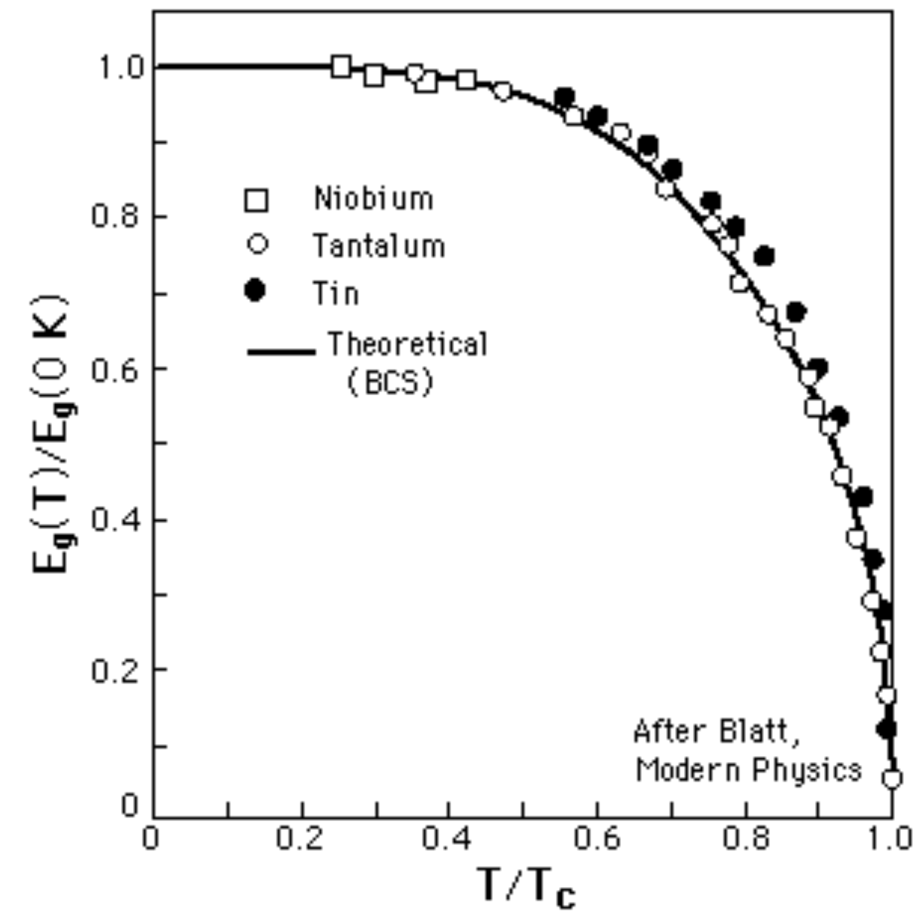

Pros

The first microscopic theory of SC

Explains many experimental evidences

The Tc formula is simple

Cons

The Tc formula is wrong

No Coulomb interaction

No retardation effects

The Migdal - Eliashberg theory ('58-'60)

The electron-electron interaction mediated by phonons is time-dependent

space-time

The Migdal - Eliashberg theory ('58-'60)

The electron-electron interaction mediated by phonons is time-dependent

The electron 1 at (x't')
causes an impulsive
force F on a ion a
$F_a = - \nabla V(x_1 - X_a)$

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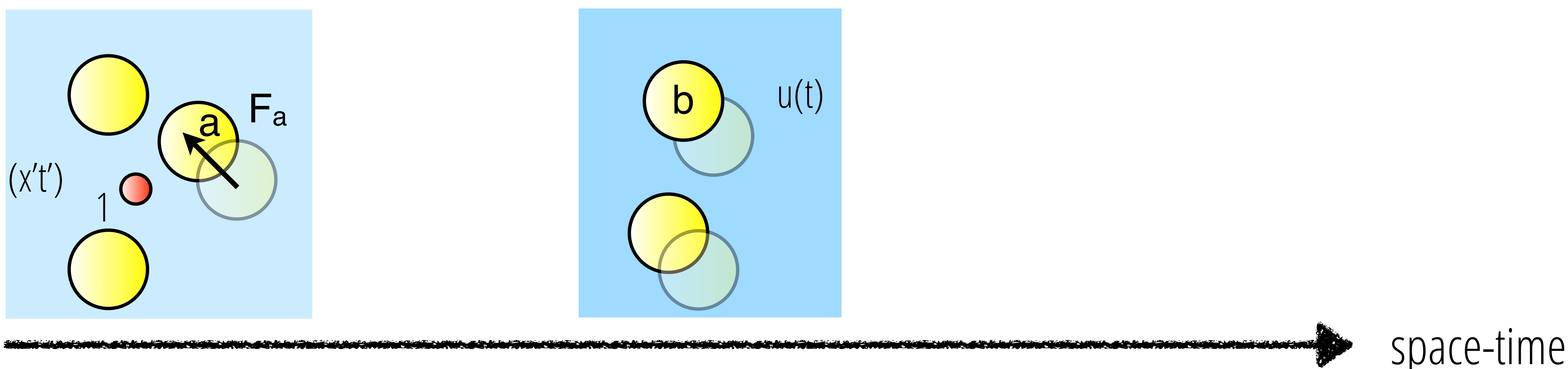

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The displacement propagates in time (t) and space (on ion b)
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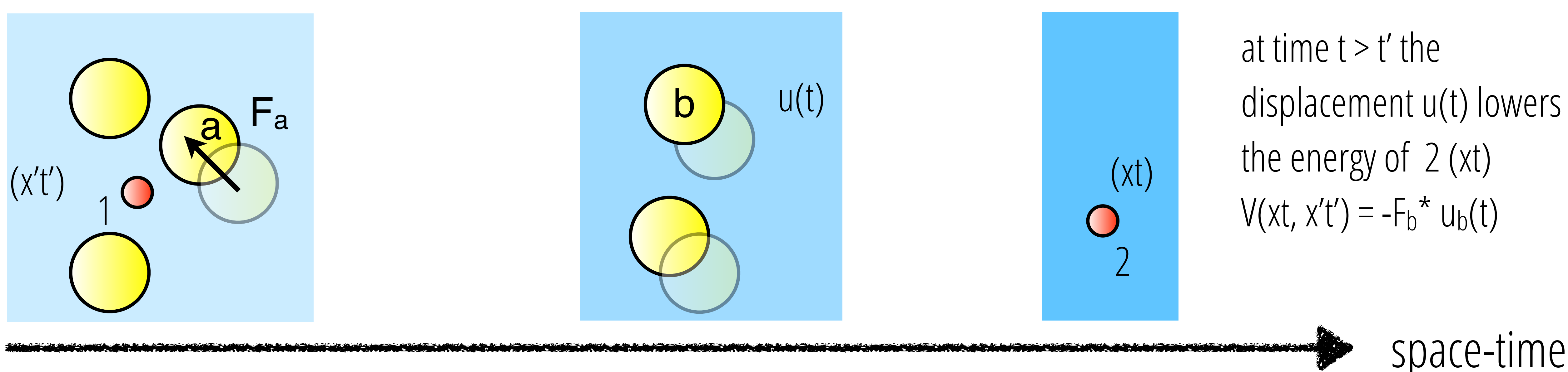

at time t > t' the displacement u(t) lowers the energy of 2 (xt)

$V(xt, x't') = -F_b{}^* u_b(t)$

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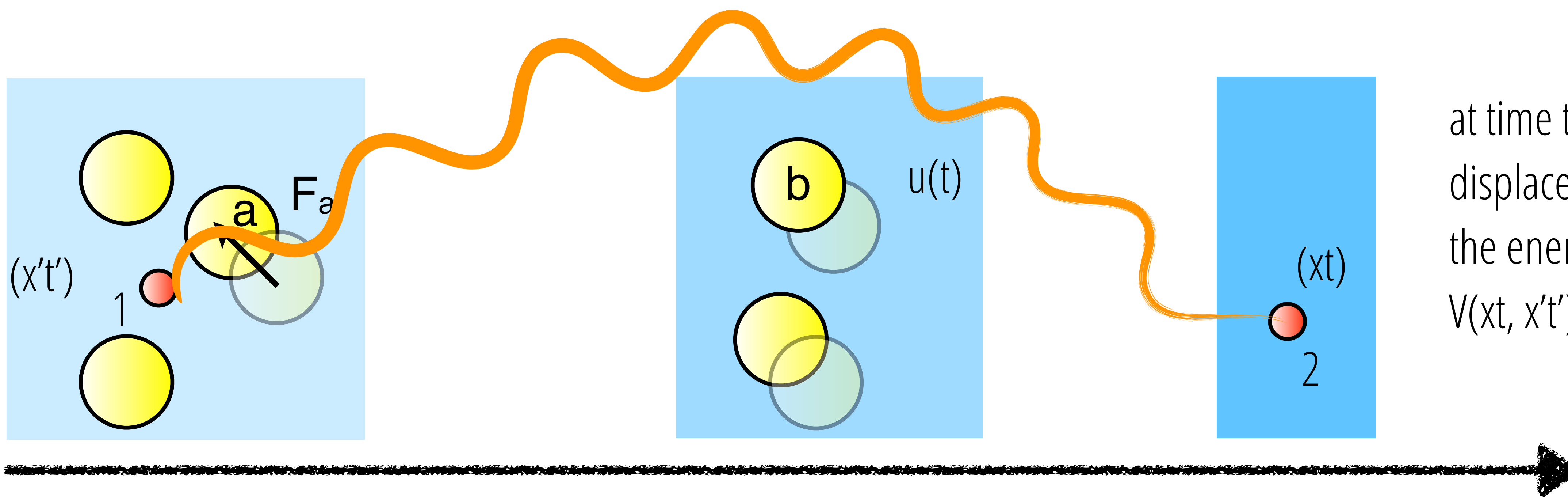

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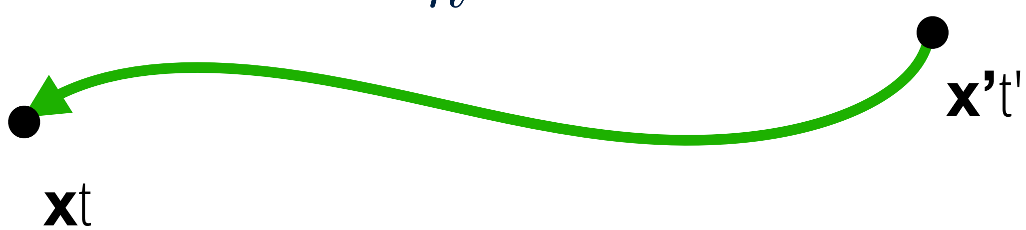
....with Green-functions

$$G(\mathbf{x}t, \mathbf{x}'t') = -\frac{i}{\hbar}\langle N|\,\hat{T}\,\hat{\psi}(\mathbf{x}t)\,\hat{\psi}^\dagger(\mathbf{x}'t')|N\rangle$$ **Electrons**

$$\mathbf{D}_{\kappa\kappa'}(tt') = -\frac{i}{\hbar}\langle\,\hat{T}\,\Delta\hat{\boldsymbol{\tau}}_\kappa(t)\,\Delta\hat{\boldsymbol{\tau}}^T_{\kappa'}(t')\,\rangle$$ **Phonons**



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Dyson equation

$$G(\mathbf{x}t, \mathbf{x}'t') = -\frac{i}{\hbar}\langle N|\,\hat{T}\,\hat{\psi}(\mathbf{x}t)\,\hat{\psi}^{\dagger}(\mathbf{x}'t')|N\rangle$$

Electrons

$$G^{-1}(\omega, k) = G_0^{-1}(\omega, k) - \Sigma(\omega, k)$$

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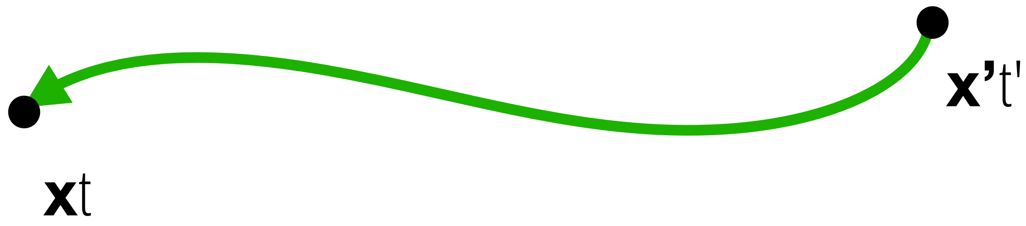

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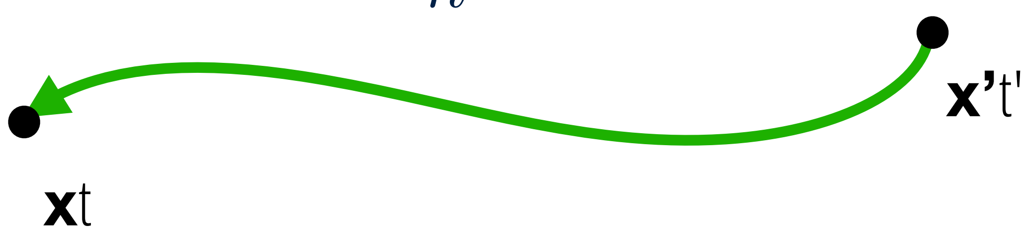

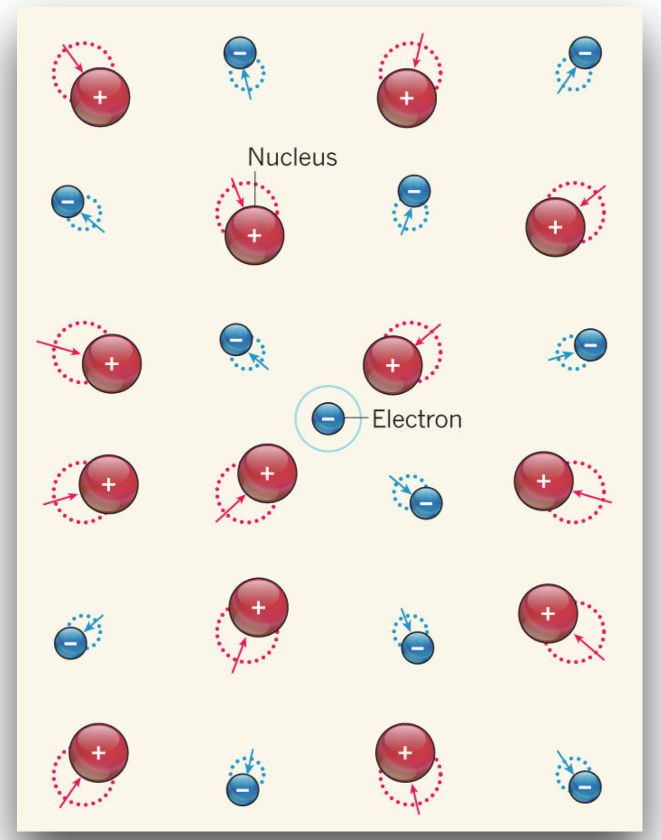

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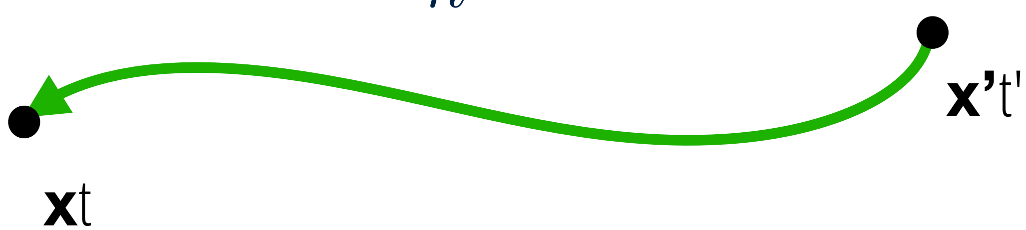

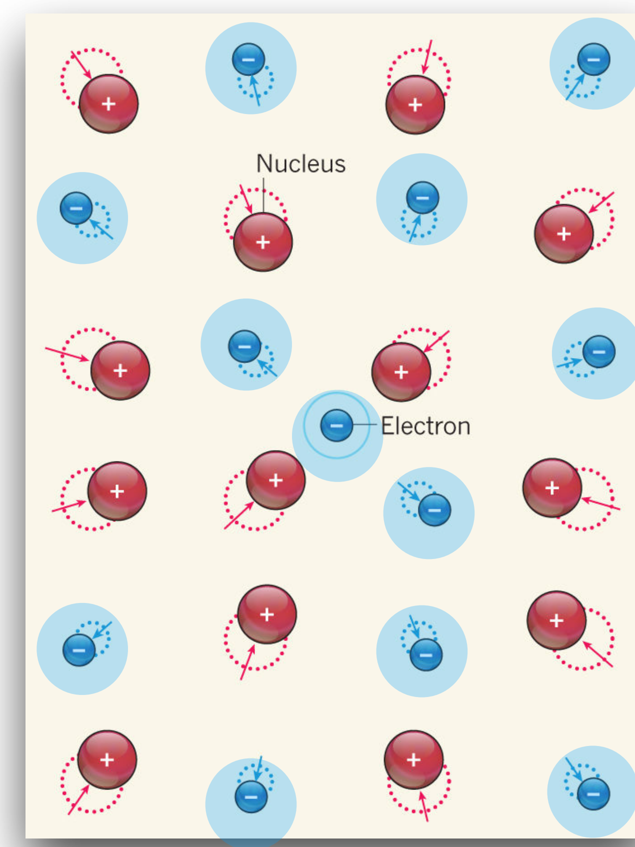

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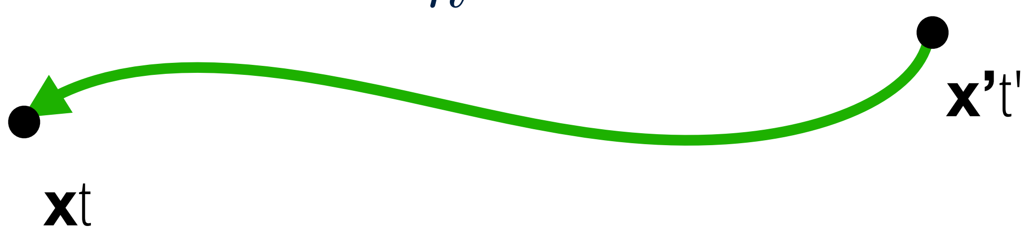

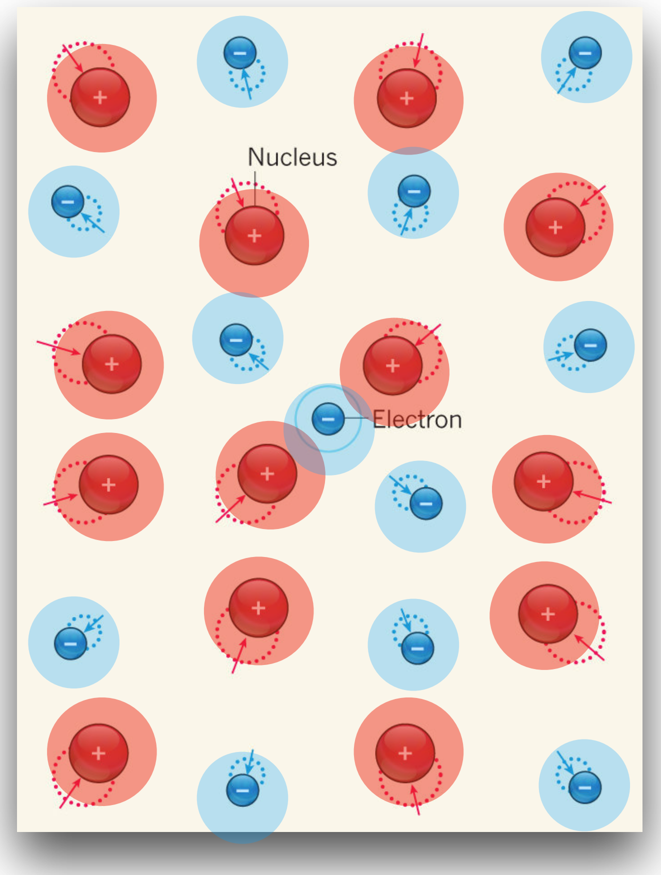

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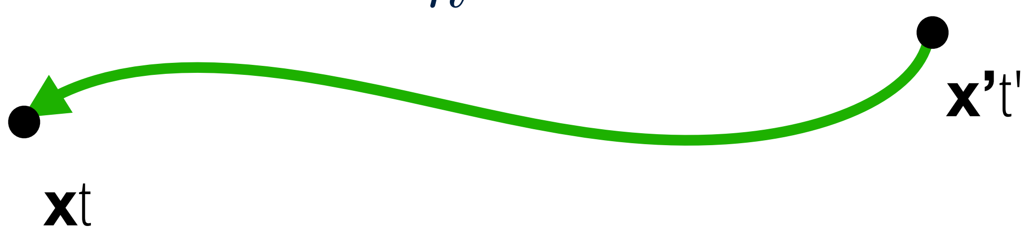

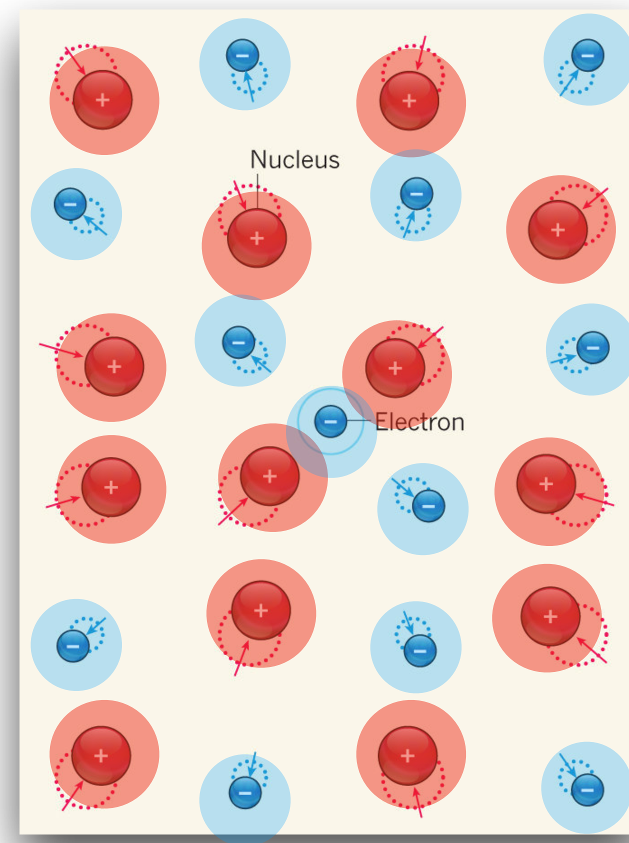

The pairing is included considering the field operator in the Nambu notation

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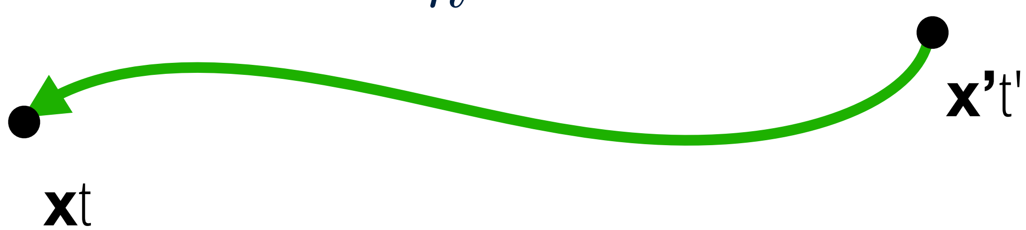

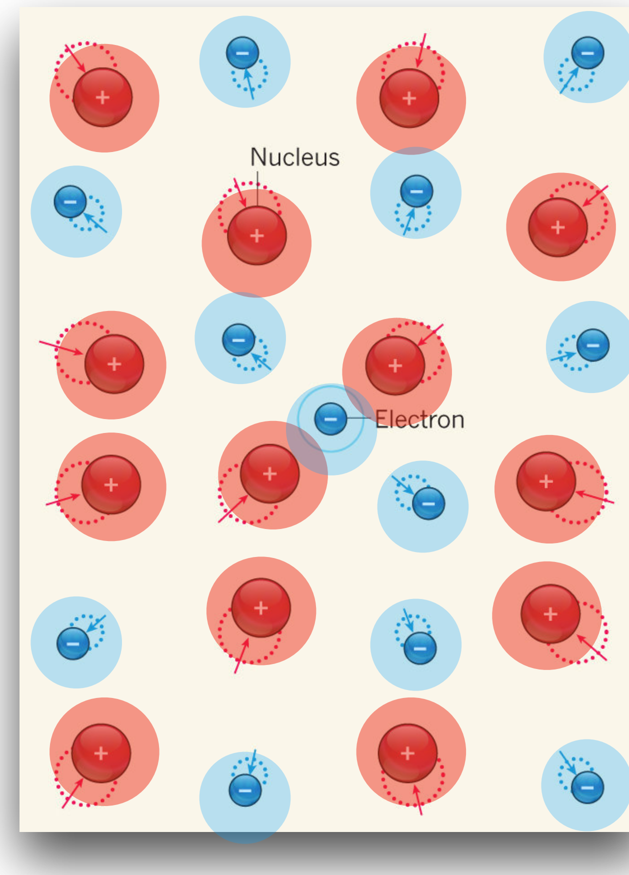

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Which is the best superconductor?

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Neil's (Ashcroft) answer

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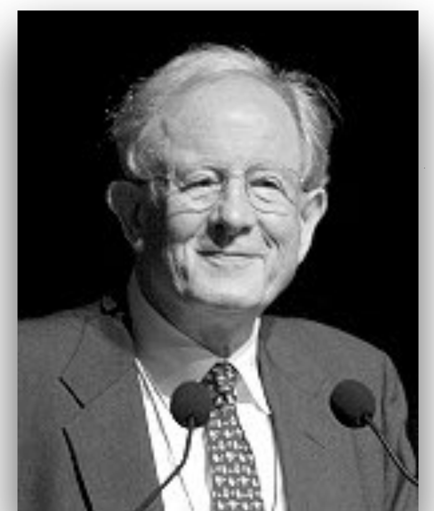
VOLUME 21, NUMBER 26 PHYSICAL REVIEW LETTERS 23 DECEMBER 1968



METALLIC HYDROGEN: A HIGH-TEMPERATURE SUPERCONDUCTOR?

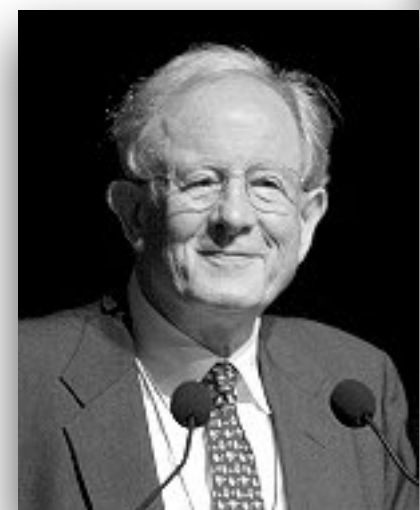
N. W. Ashcroft
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14850
(Received 3 May 1968)

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.

Which is the best superconductor?

Neil's (Ashcroft) answer

VOLUME 2 ... BER 1968



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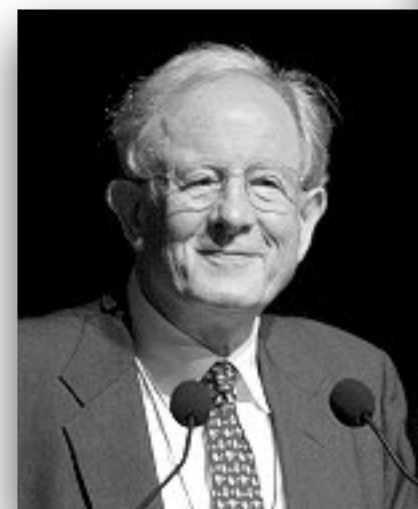
Volume 2 … ber 1968



$$T_c = \omega\, e^{-1/\lambda}$$

Which is the best superconductor?

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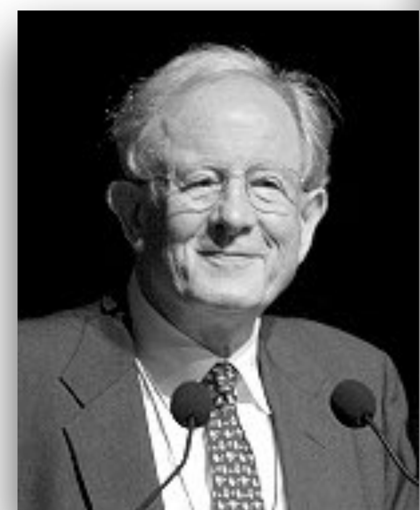
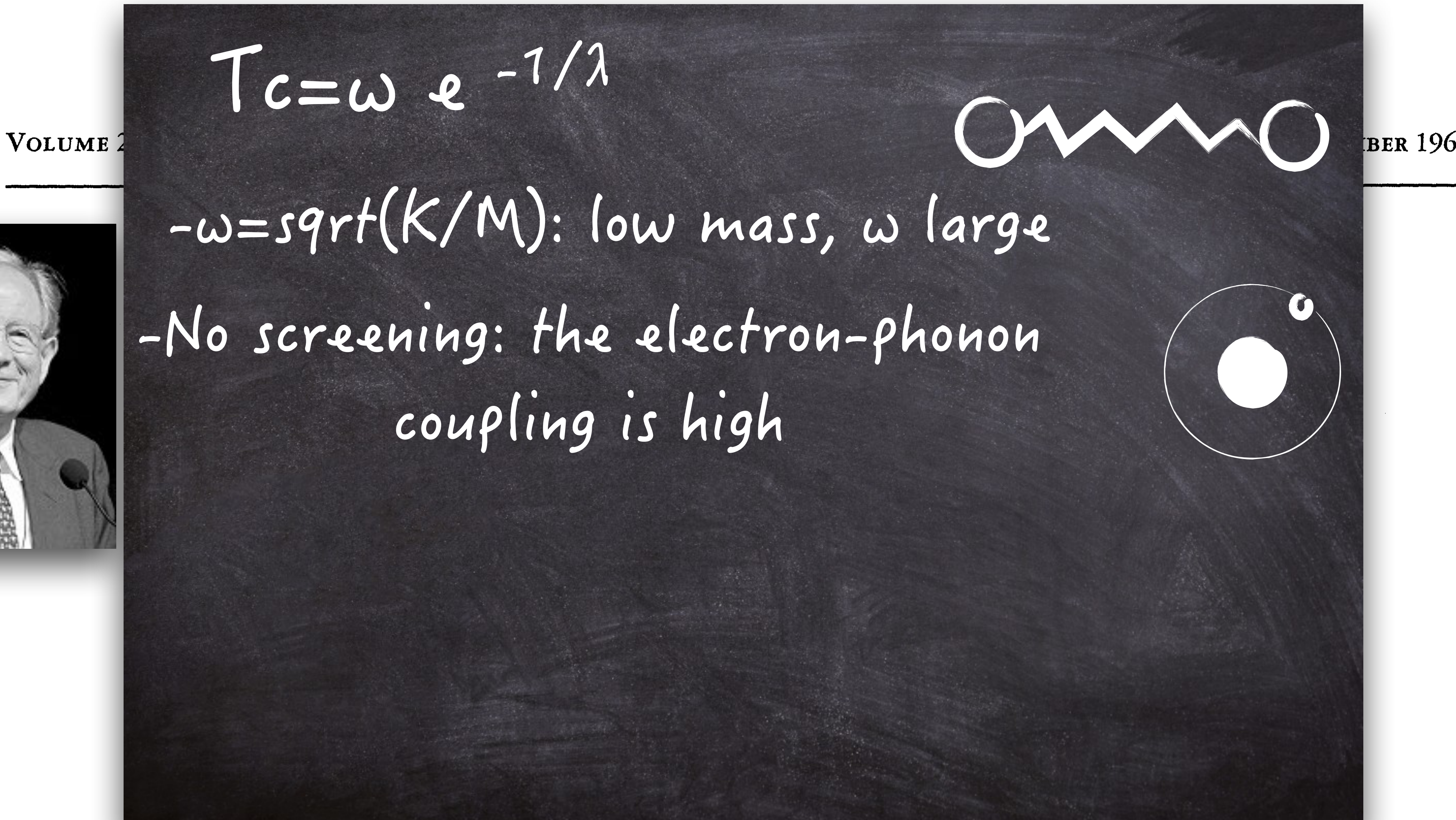


-ω=sqrt(K/M): low mass, ω large

Which is the best superconductor?

Neil's (Ashcroft) answer



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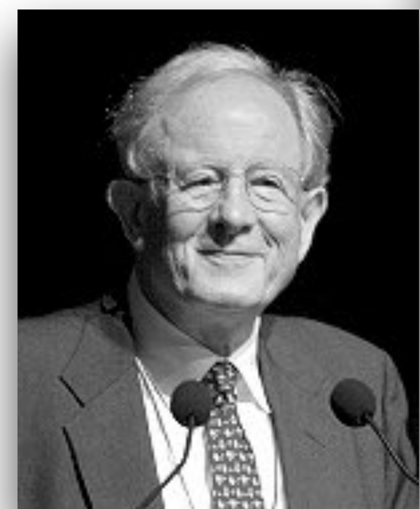

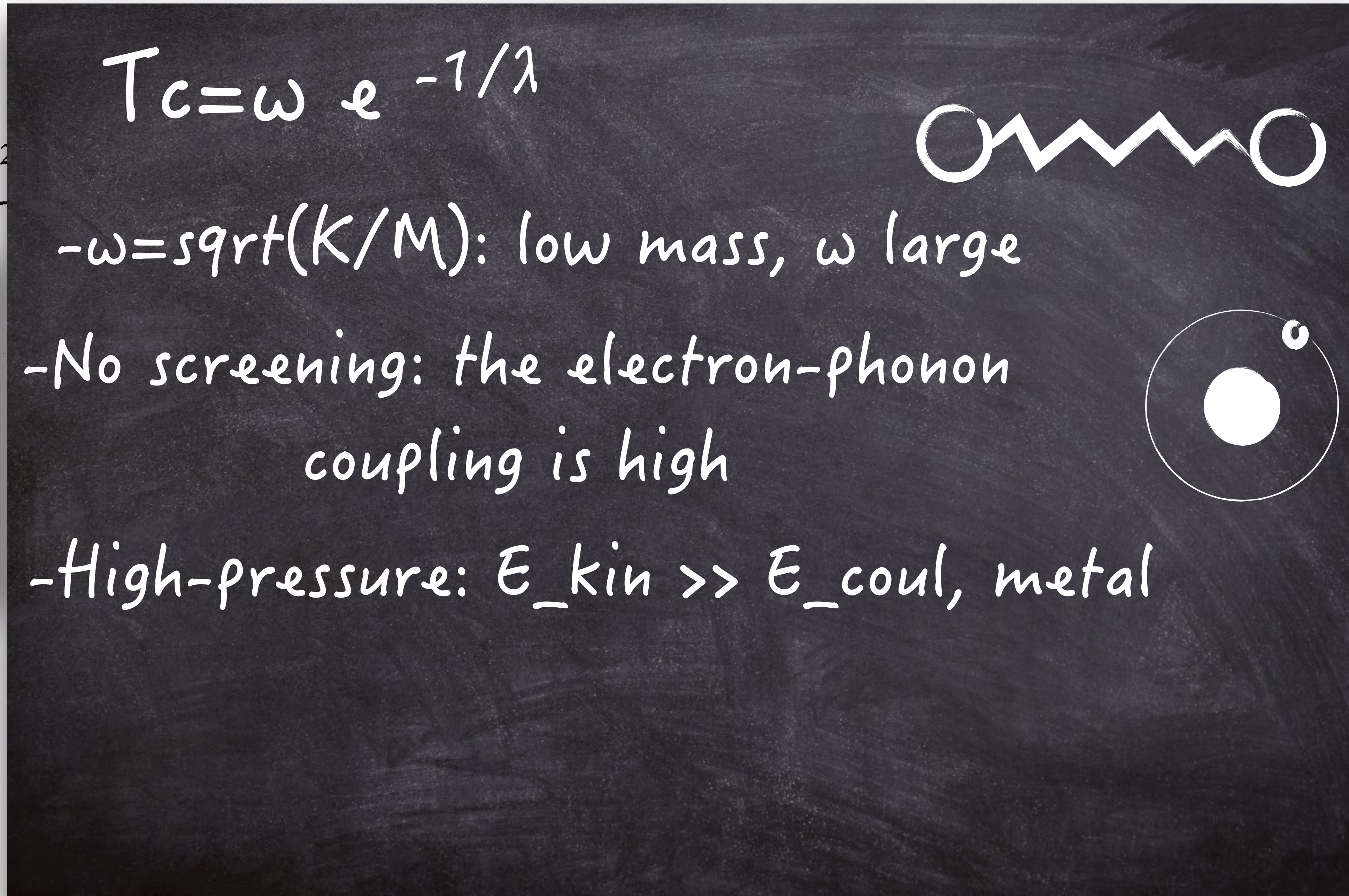

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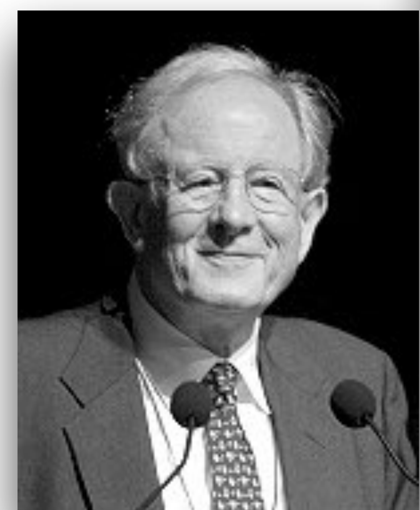
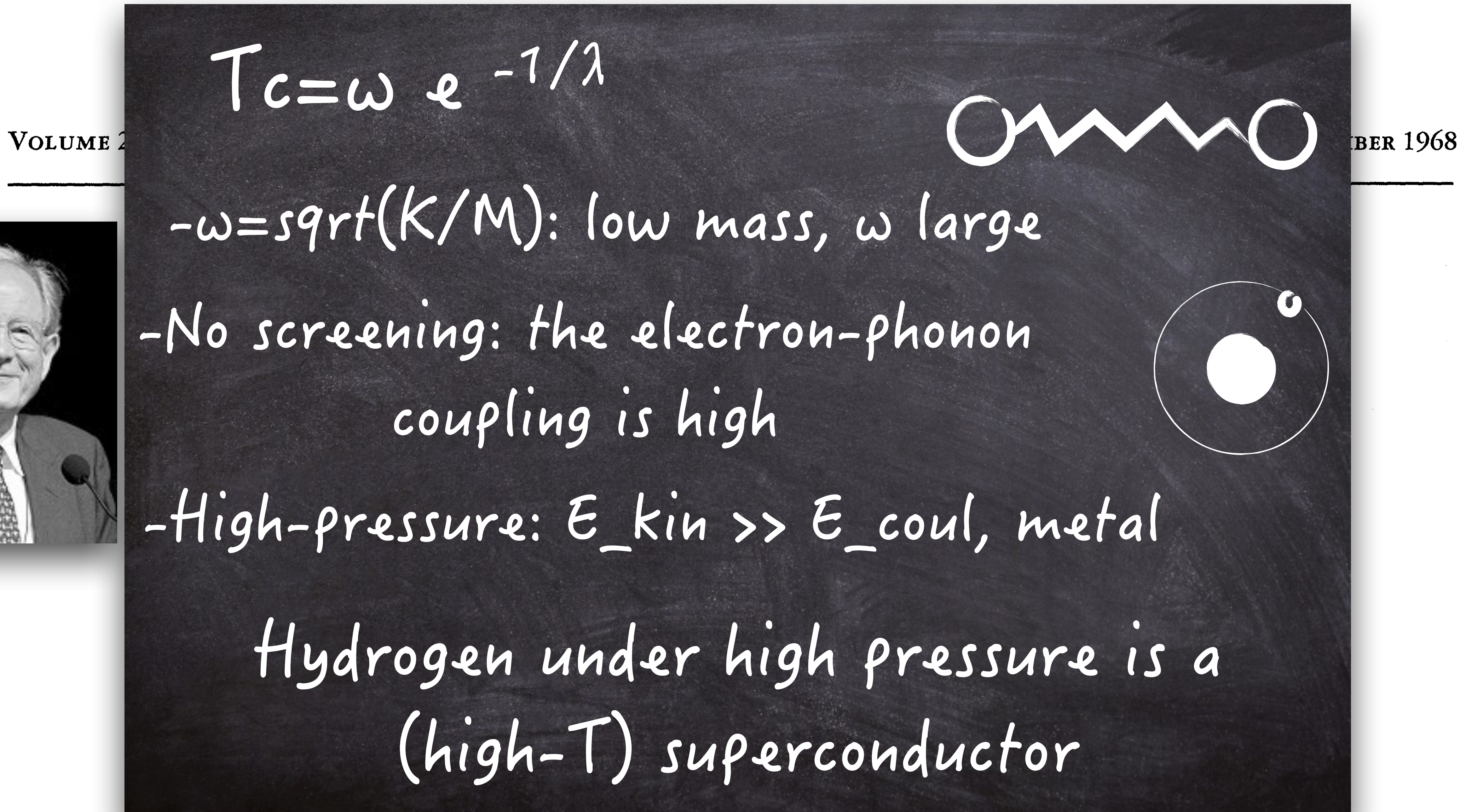
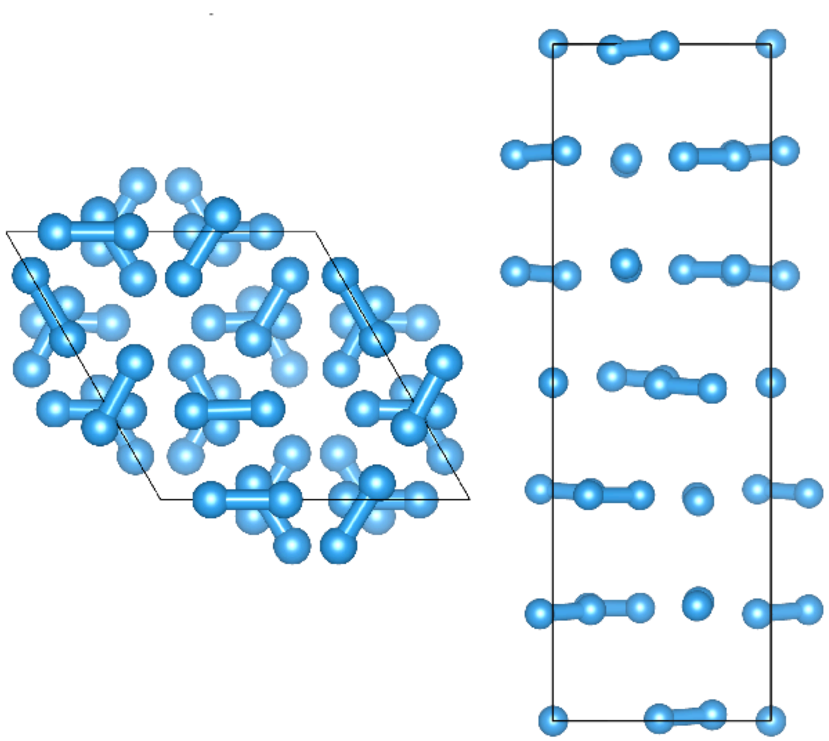




But hydrogen is (always) an insulator

where is the metal?



ON SUPERCONDUCTIVITY AND SUPERFLUIDITY

Nobel Lecture, December 8, 2003

by

Vitaly L. Ginzburg

P. N. Lebedev Physics Institute, Russian Academy of Sciences, Moscow, Russia.

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2. High-temperature and room-temperature superconductivity (HTSC and RTSC).
3. Metallic hydrogen. Other exotic substances.
4. Two-dimensional electron liquid (anomalous Hall effect and other efsfects).
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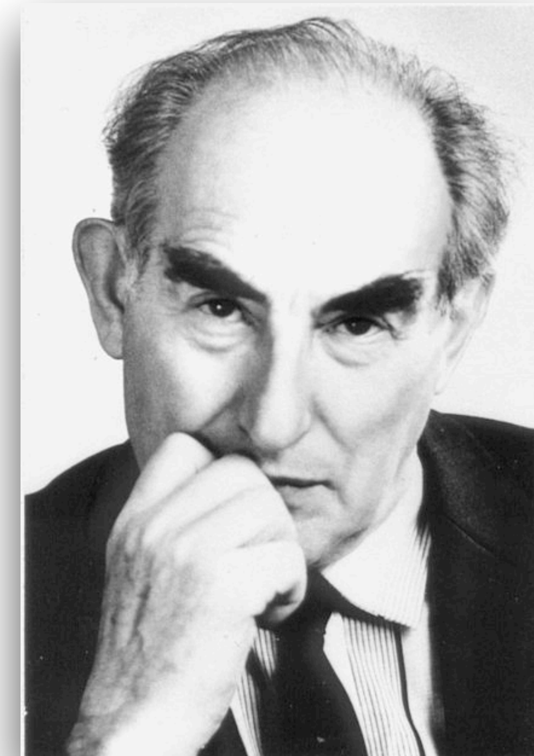

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“pioneering contributions to the theory of superconductors and superfluids”

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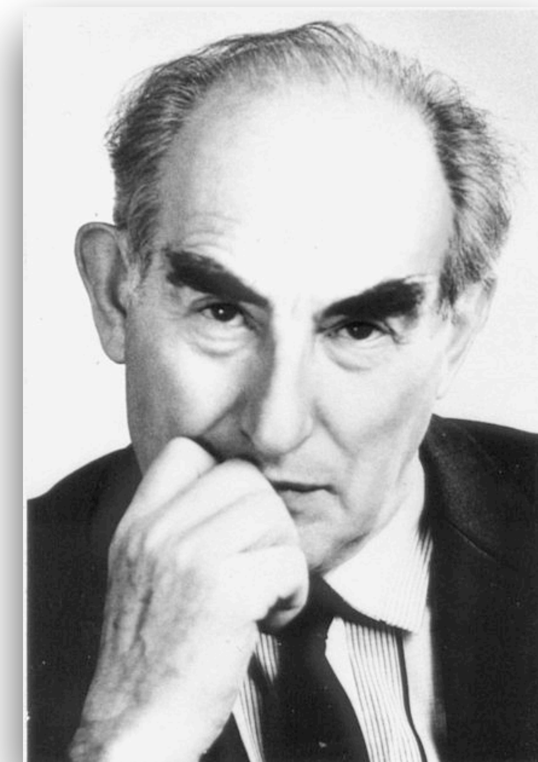

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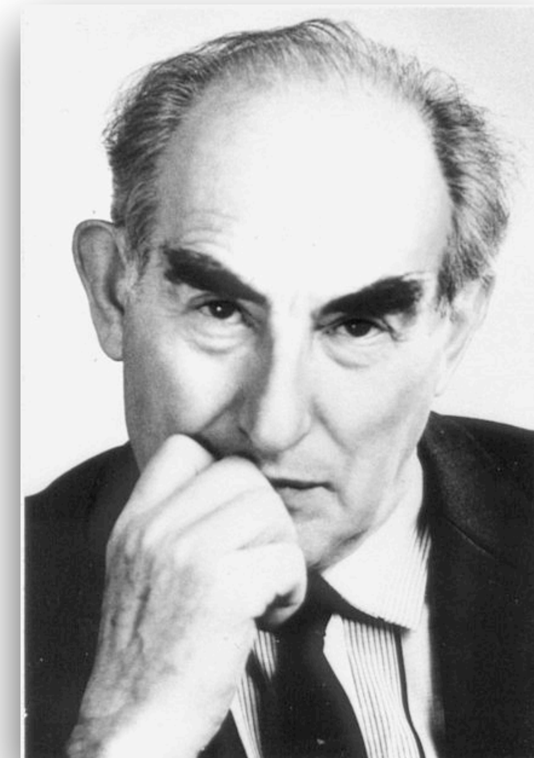

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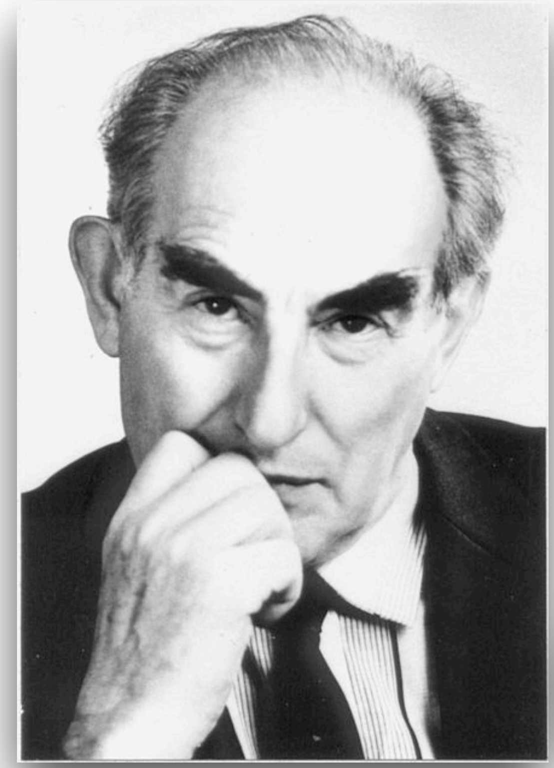

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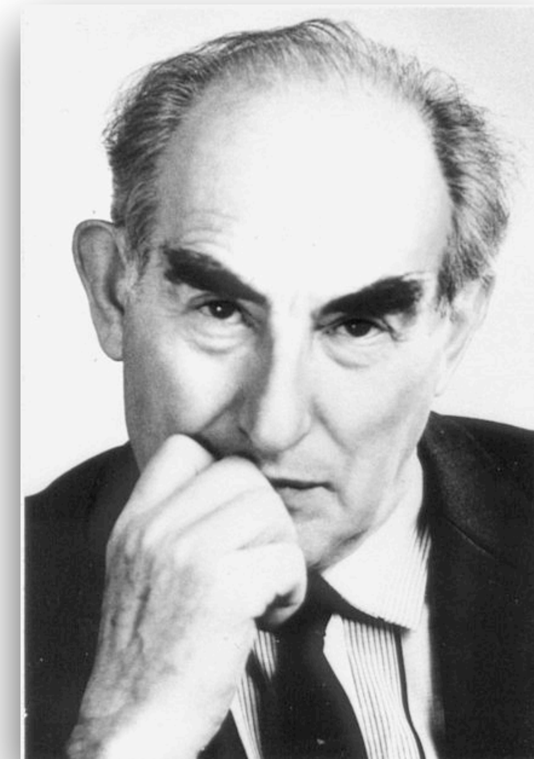

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Metallic hydrogen: The holy grail of physics

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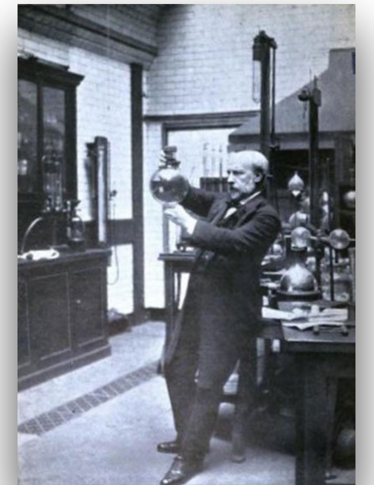
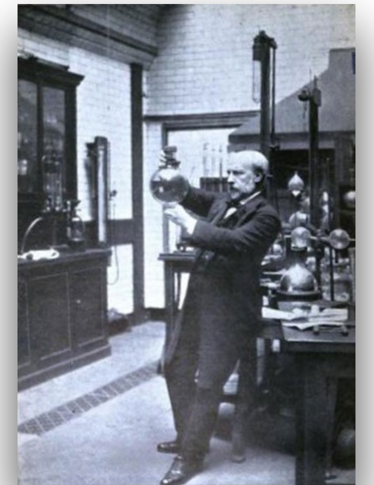


1899: Dewar produces solid hydrogen

Metallic hydrogen: The holy grail of physics



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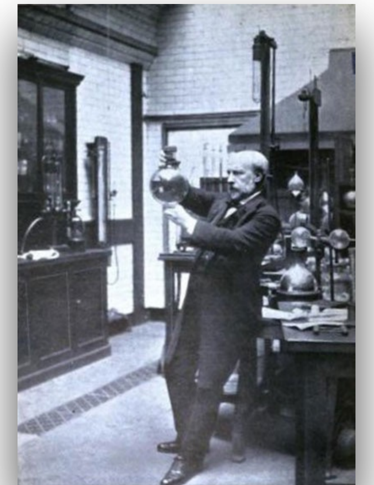

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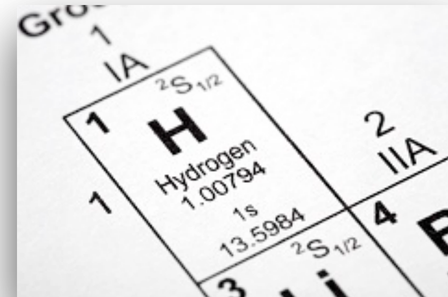

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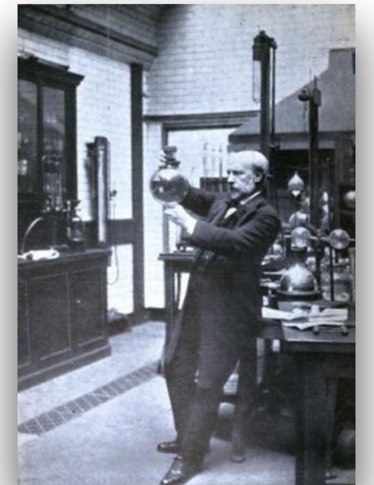

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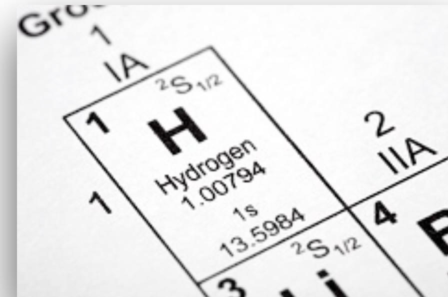
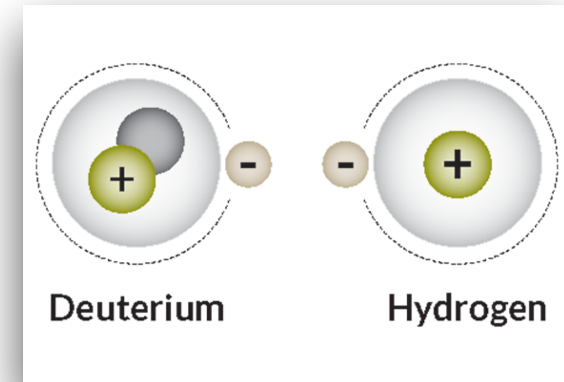
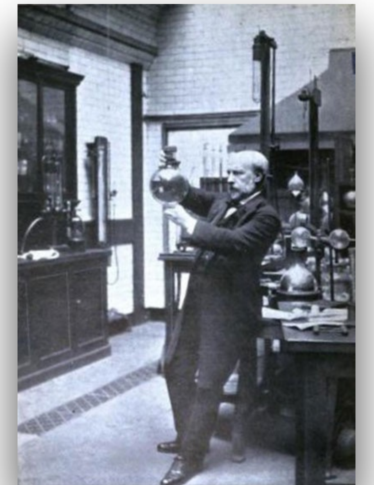


1981: Phase II discovered



Metallic hydrogen: The holy grail of physics



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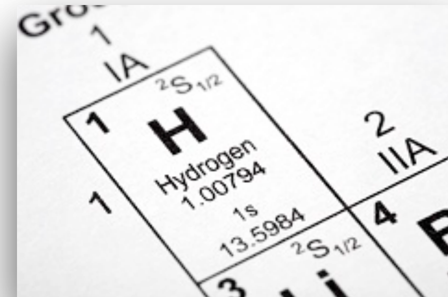

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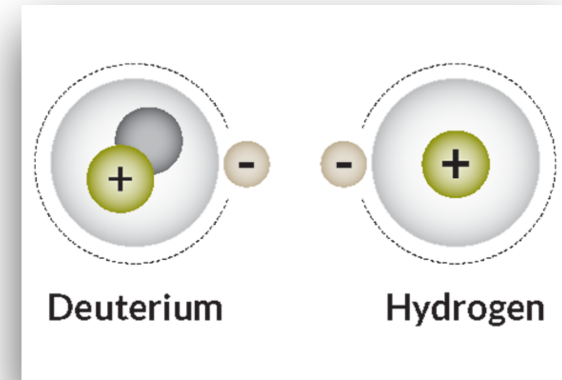

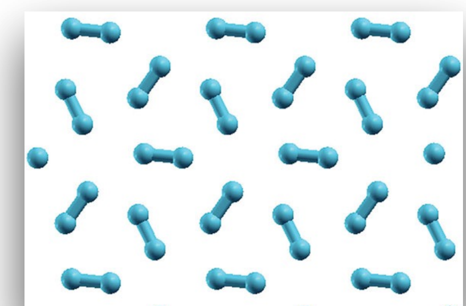

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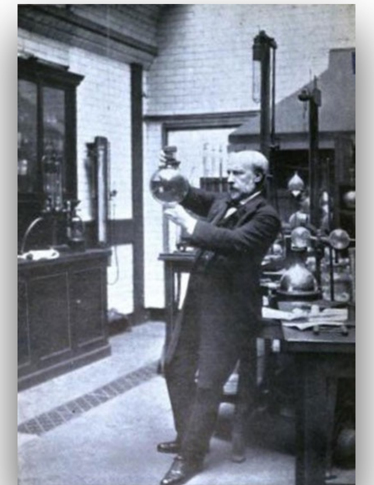

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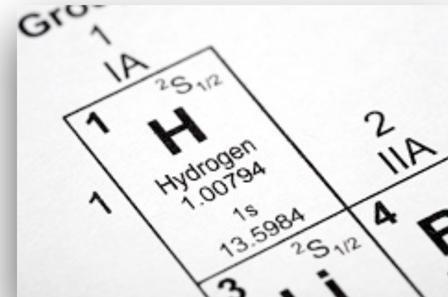

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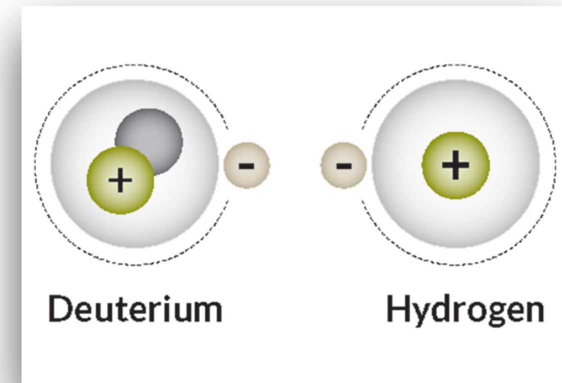

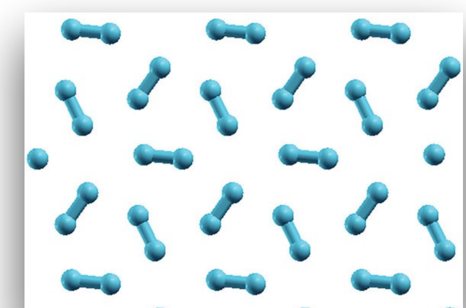

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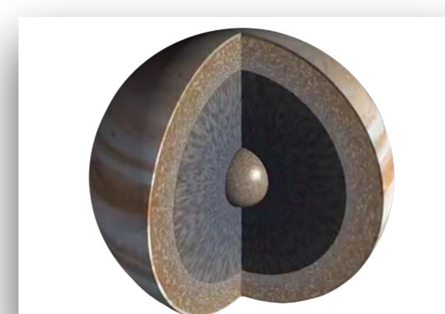

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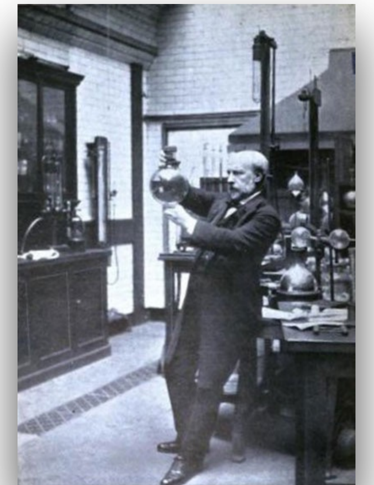

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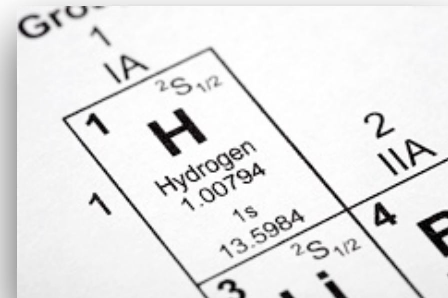

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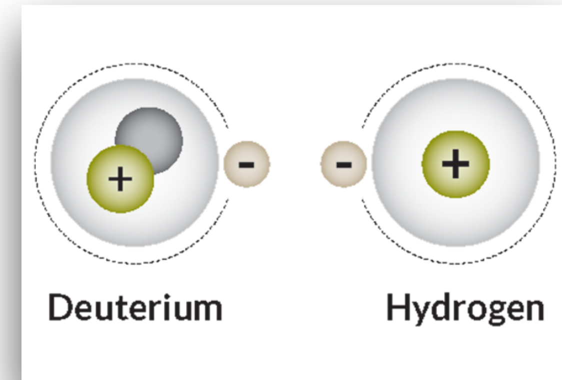

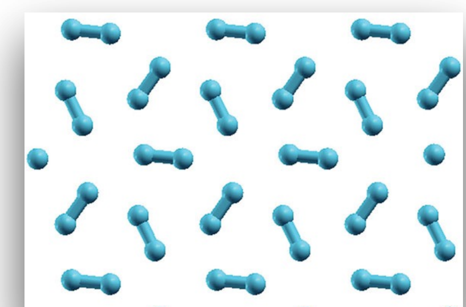

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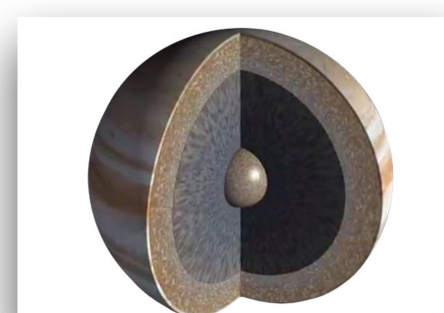
The pressure is too high, experiments too complicated, ...theoretical predictions are welcome for both normal and superconducting properties.



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The Density Functional Theory

PHYSICAL REVIEW VOLUME 136, NUMBER 3B 9 NOVEMEBR 1964

Inhomogeneous Electron Gas*

P. HOHENBERG†
École Normale Superieure, Paris, France

AND

W. KOHN‡
École Normale Superieure, Paris, France and Faculté des Sciences, Orsay, France
and
University of California at San Diego, La Jolla, California

(Received 18 June 1964)

This paper deals with the ground state of an interacting electron gas in an external potential $v(\mathbf{r})$. It is proved that there exists a universal functional of the density, $F[n(\mathbf{r})]$, independent of $v(\mathbf{r})$, such that the expression $E \equiv \int v(\mathbf{r})n(\mathbf{r})d\mathbf{r}+F[n(\mathbf{r})]$ has as its minimum value the correct ground-state energy associated with $v(\mathbf{r})$. The functional $F[n(\mathbf{r})]$ is then discussed for two situations: (1) $n(\mathbf{r})=n_0+\tilde{n}(\mathbf{r})$, $\tilde{n}/n_0<<1$, and (2) $n(\mathbf{r})=\varphi(\mathbf{r}/r_0)$ with φ arbitrary and $r_0\to\infty$. In both cases F can be expressed entirely in terms of the correlation energy and linear and higher order electronic polarizabilities of a uniform electron gas. This approach also sheds some light on generalized Thomas-Fermi methods and their limitations. Some new extensions of these methods are presented.

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$$E[n_0] \leq E[n] = T[n]+U[n]+V[n]$$

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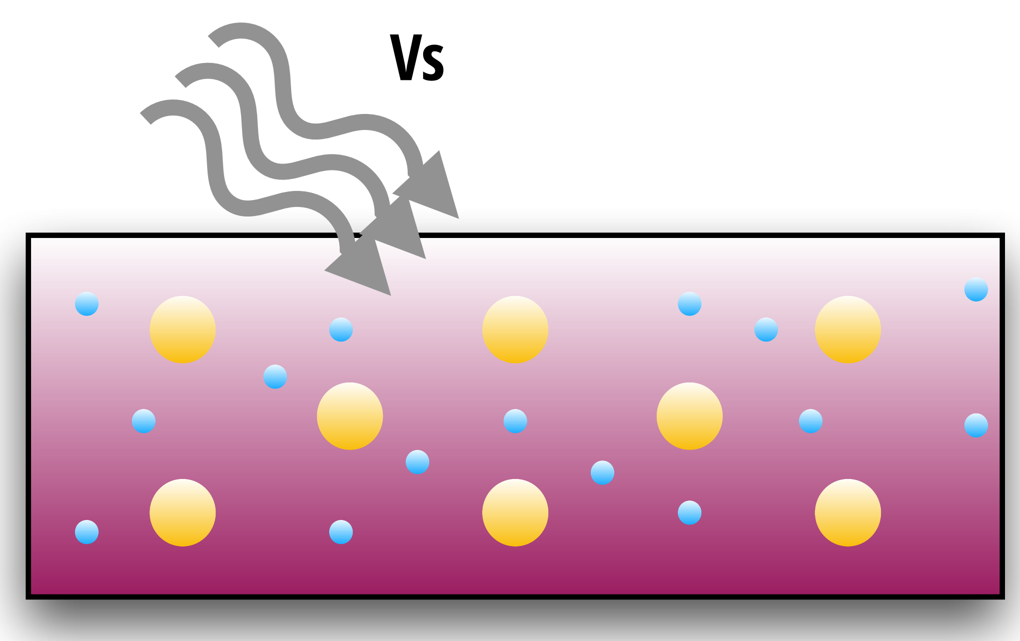

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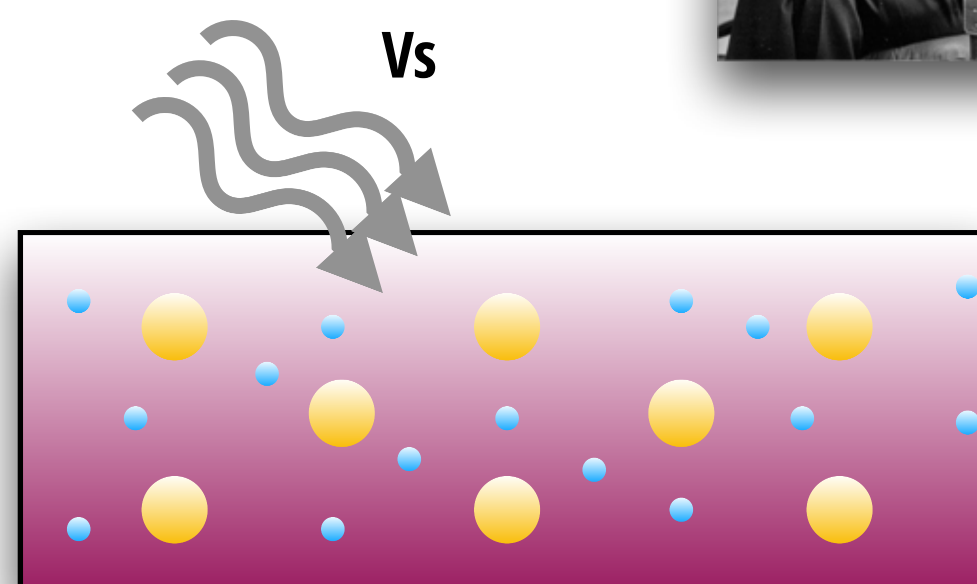

Super Conducting Density Functional Theory (2005)

Kohn-Sham system for superconductor

$$H = H_e + H_{en} + H_n + H_{ext}$$

$$\begin{aligned}
\rho(\boldsymbol{r}) &= \mathrm{Tr}\left[\varrho_0 \sum_\sigma \psi_\sigma^\dagger(\boldsymbol{r})\,\psi_\sigma(\boldsymbol{r})\right] \\
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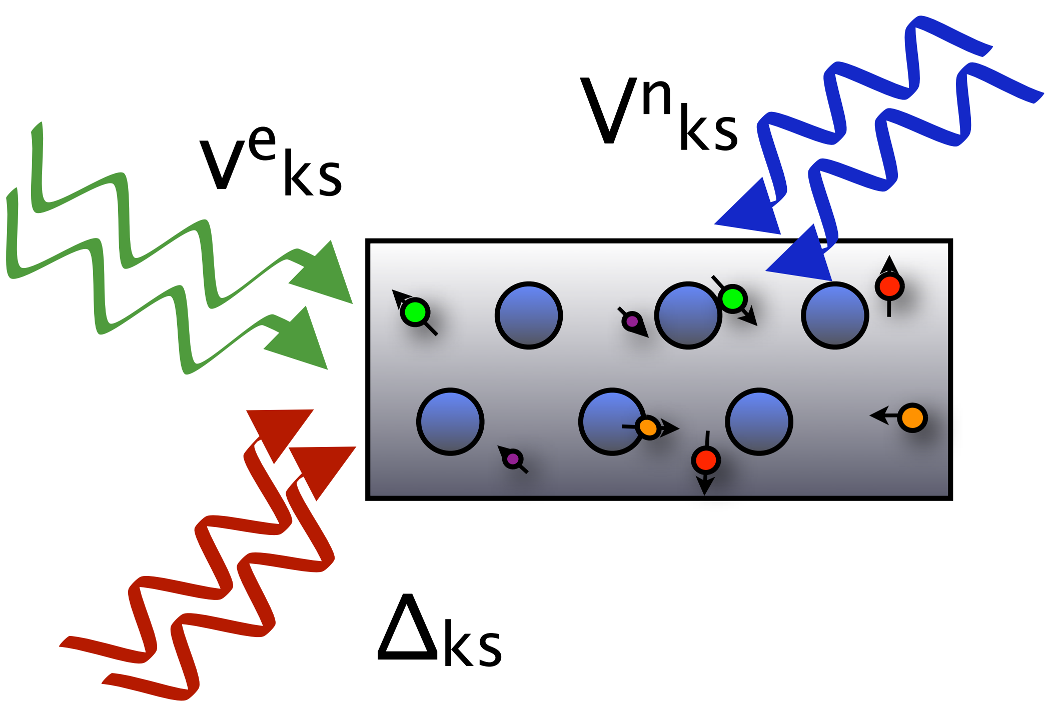


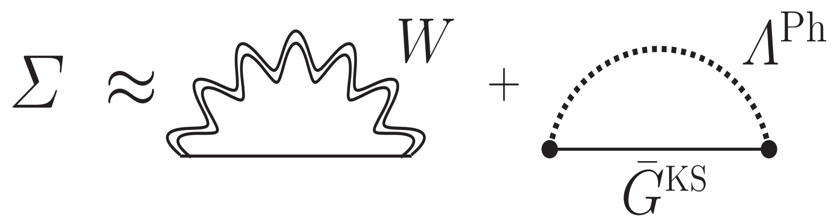
PHYSICAL REVIEW B **72**, 024545 (2005)

Ab initio **theory of superconductivity. I. Density functional formalism and approximate functionals**

M. Lüders,[1,2] M. A. L. Marques,[2,3] N. N. Lathiotakis,[2,3] A. Floris,[3,4] G. Profeta,[5] L. Fast,[2,6] A. Continenza,[5] S. Massidda,[4,*] and E. K. U. Gross[2,3]

An approach to the description of superconductors in thermal equilibrium is developed within a formally exact density functional framework. The theory is formulated in terms of three "densities:" the ordinary electron density, the superconducting order parameter, and the diagonal of the nuclear *N*-body density matrix. The electron density and the order parameter are determined by Kohn-Sham equations that resemble the Bogoliubov–de Gennes equations. The nuclear density matrix follows from a Schrödinger equation with an effective *N*-body interaction. These equations are coupled to each other via exchange-correlation potentials which are universal functionals of the three densities. Approximations of these exchange-correlation functionals are derived using the diagrammatic techniques of many-body perturbation theory. The bare Coulomb repulsion between the electrons and the electron-phonon interaction enter this perturbative treatment on the same footing. In this way, a truly *ab initio* description is achieved which does not contain any empirical parameters.

Super Conducting Density Functional Theory (2005)



$$\bar{\Sigma}_k(\omega_n) \approx \sum_m \sum_{k'} W_{kk'}(\omega_n - \omega_m)\, \bar{G}^{\mathrm{KS}}_{k'}(\omega_m) + \sum_m \sum_{k'} \Lambda^{\mathrm{Ph}}_{kk'}(\omega_n - \omega_m)\, \bar{G}^{\mathrm{KS}}_{k'}(\omega_m),$$

$$\bar{G}_k(\omega_n) = \tau^z \begin{pmatrix} G_k(\omega_n) & F_k(\omega_n) \\ F_k{}^{\dagger}(\omega_n) & G_k{}^{\dagger}(\omega_n) \end{pmatrix}$$

Interactions from first-principles

$$\Lambda^{\mathrm{Ph}}_{kk'}(\omega_n) = -\frac{1}{\pi}\int_0^{\infty} \mathrm{d}\omega \frac{2\omega}{\omega_n^2 + \omega^2} \mathfrak{Im}\left[\Lambda^{\mathrm{Ph}}_{kk'}(\omega)\right]$$

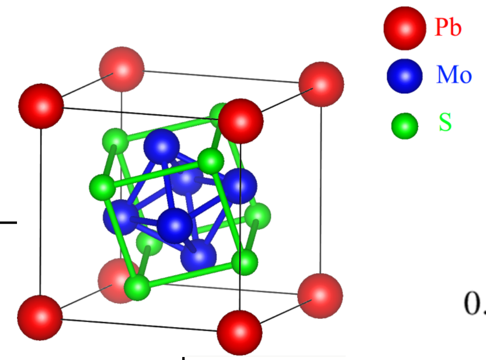
$$\mathfrak{Im}\left[\Lambda^{\mathrm{Ph}}_{kk'}(\omega)\right] = -\pi \sum_{\lambda \boldsymbol{q}} \left| g^{kk'}_{\lambda \boldsymbol{q}} \right|^2 \delta\left(\omega - \Omega_{\lambda \boldsymbol{q}}\right).$$

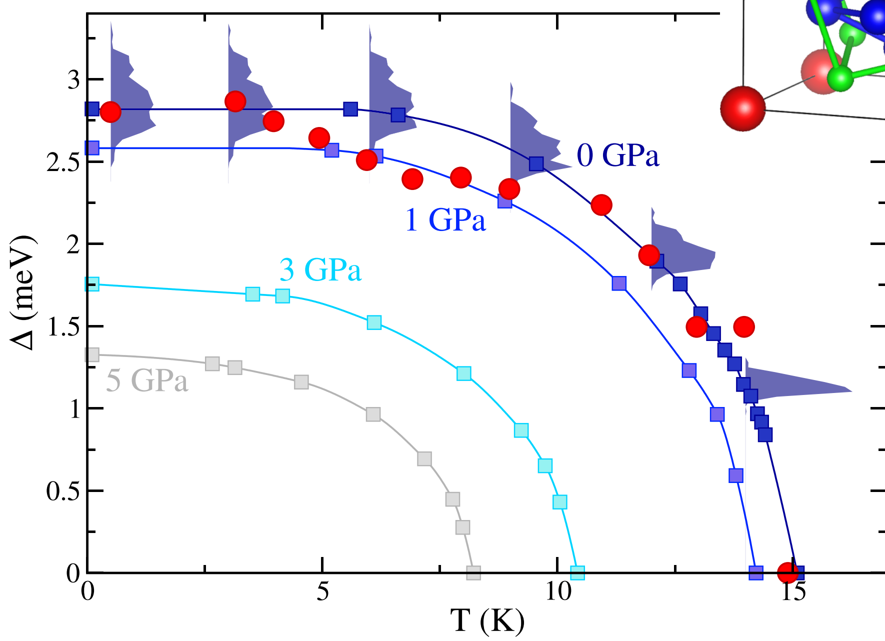
$$W_{k_1 k_2}(\omega_n) = \sum_{k'} \epsilon^{-1}_{k_1 k'}(\omega_n)\, v_{k' k_2}$$

$$\Delta^{\mathrm{xc}}_k = -\Delta^{\mathrm{xc}}_k \mathcal{Z}^{\mathrm{D}}_k - \sum_{k'} \mathcal{K}^{\mathrm{C}}_{kk'} \frac{\tanh\left(\frac{\beta E_{k'}}{2}\right)}{2E_{k'}} \Delta^{\mathrm{xc}}_{k'}$$

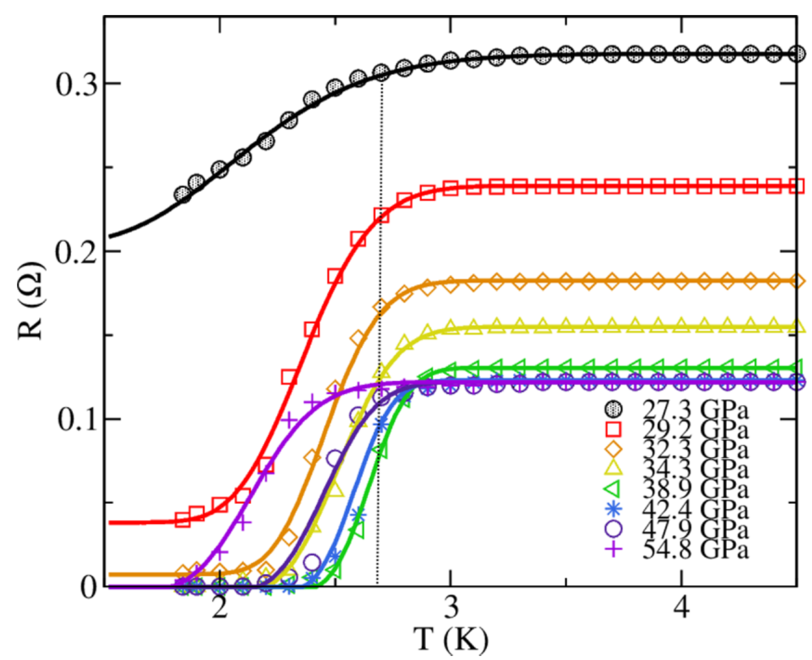
It works

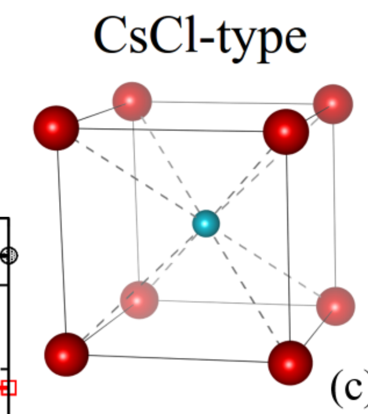
Chevrel phases, $PbMo_6S_8$

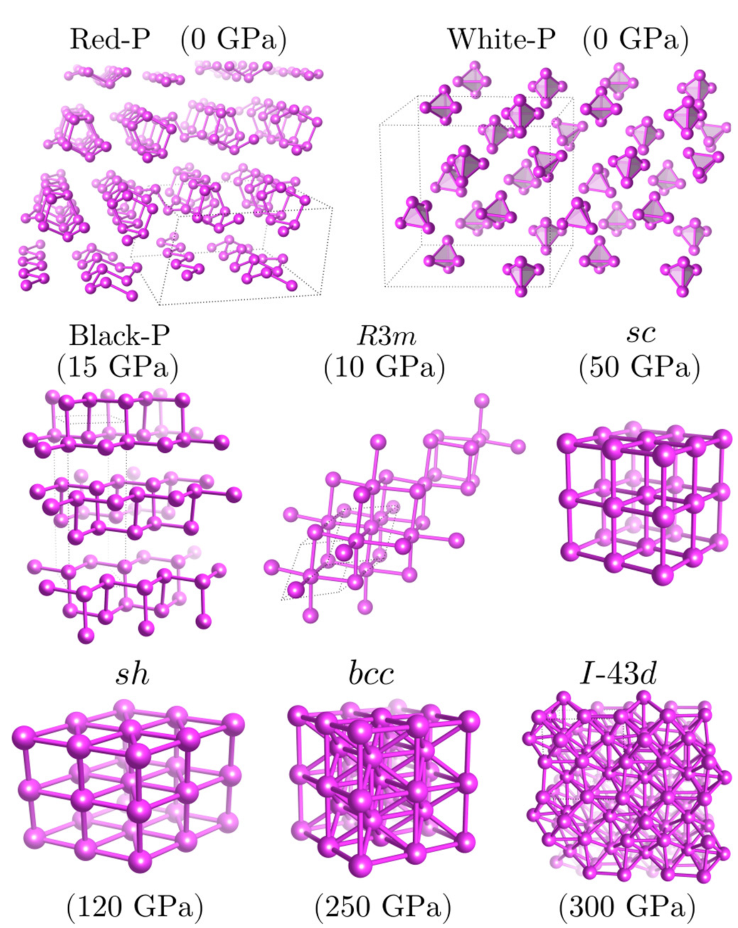




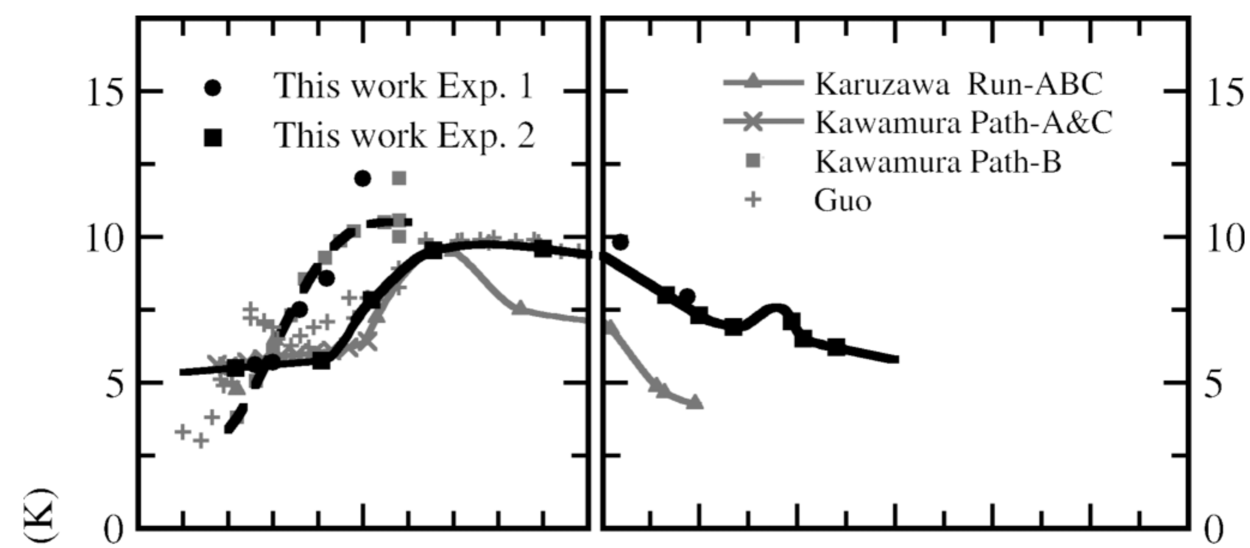
Tin-selenide, SnSe







The many phases of phosphorus under pressure



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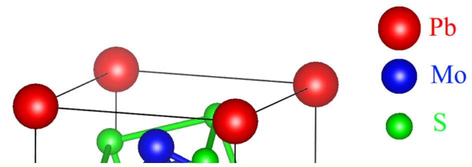
Chevrel phases, PbMo6S8



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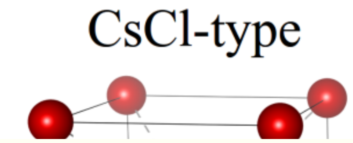

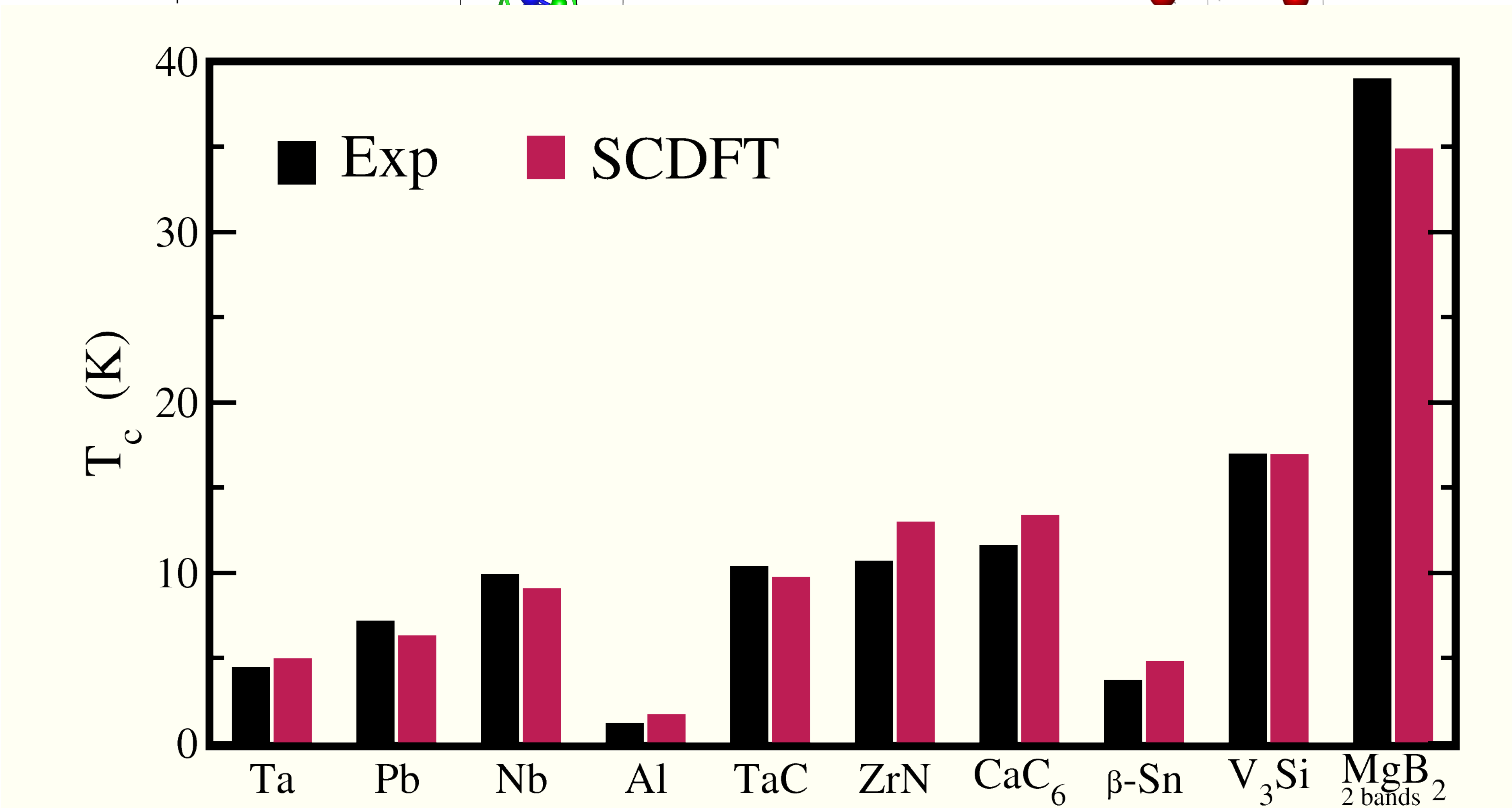

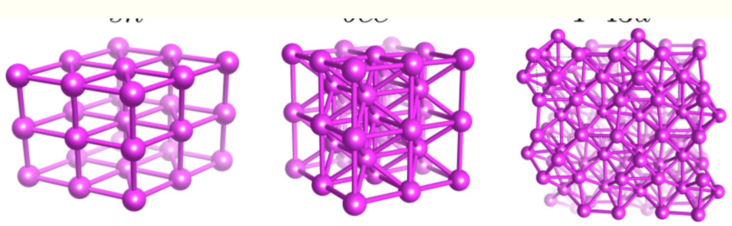

High-temperature superconducting phase in hydrogen phase III (2008)

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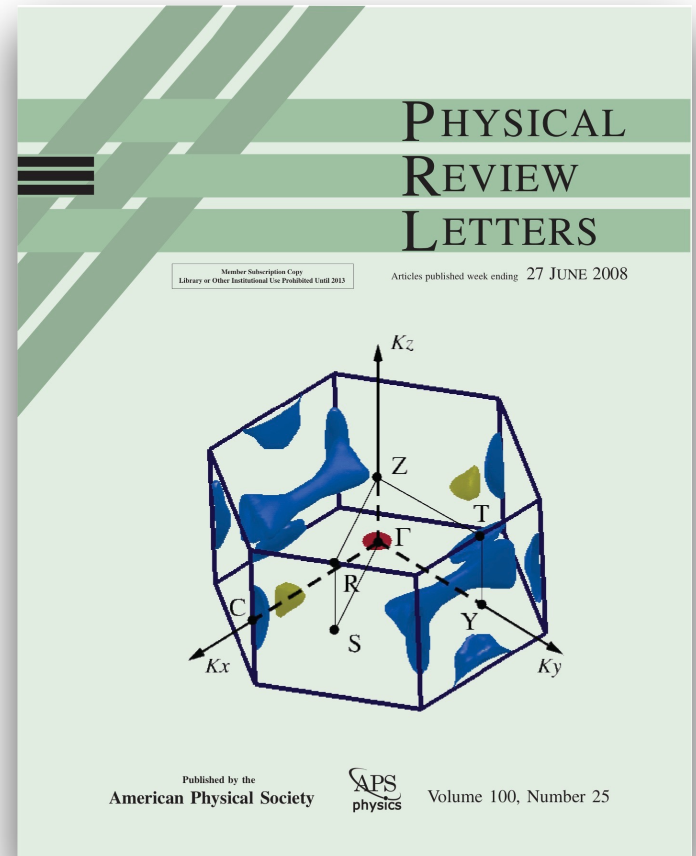

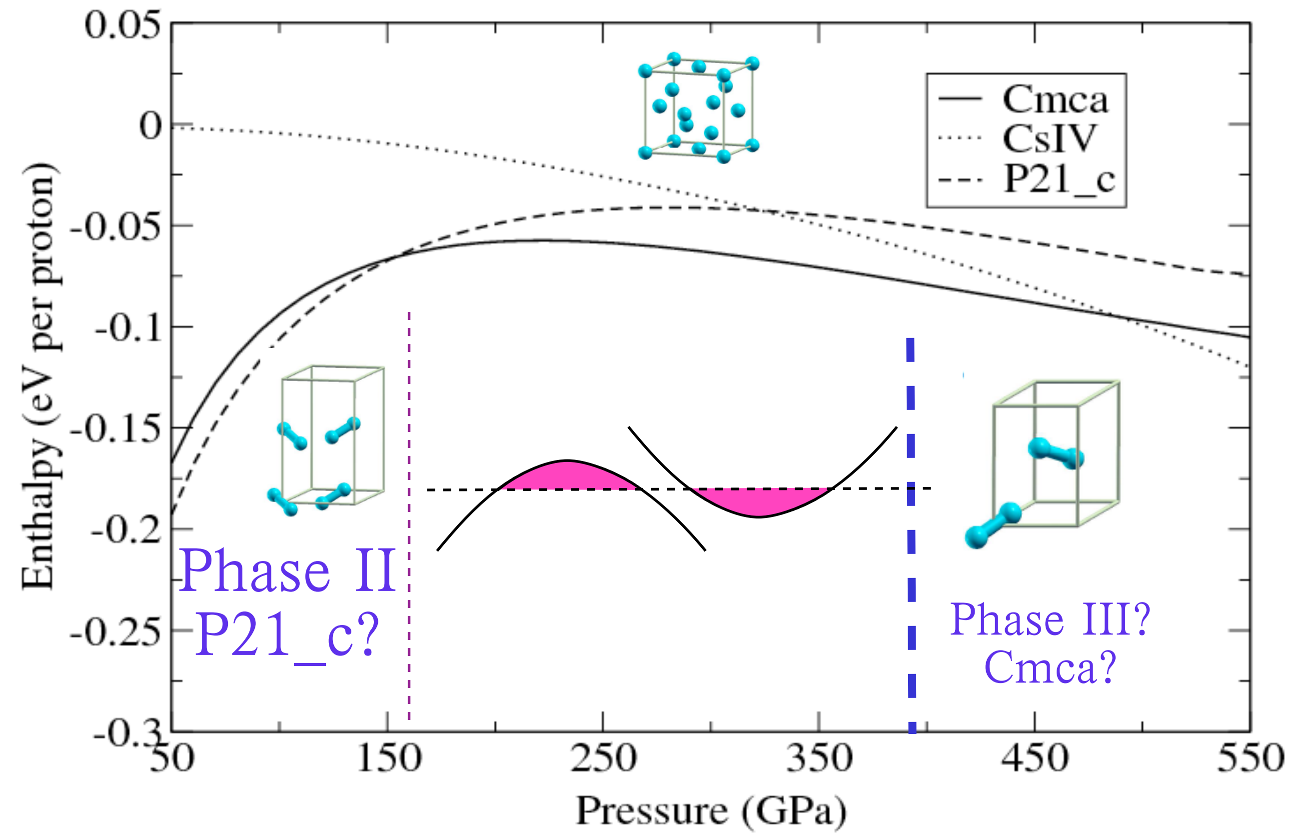

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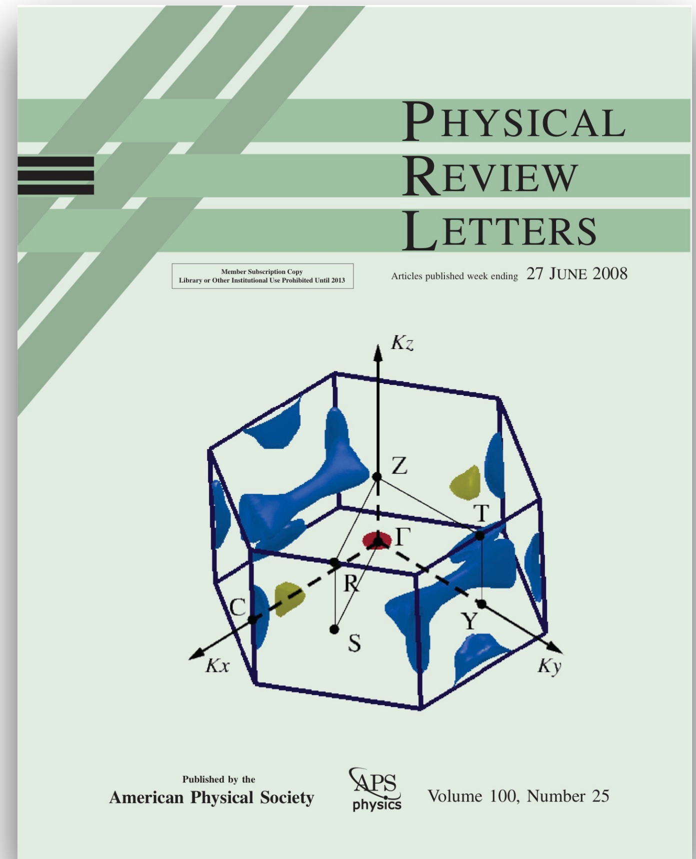

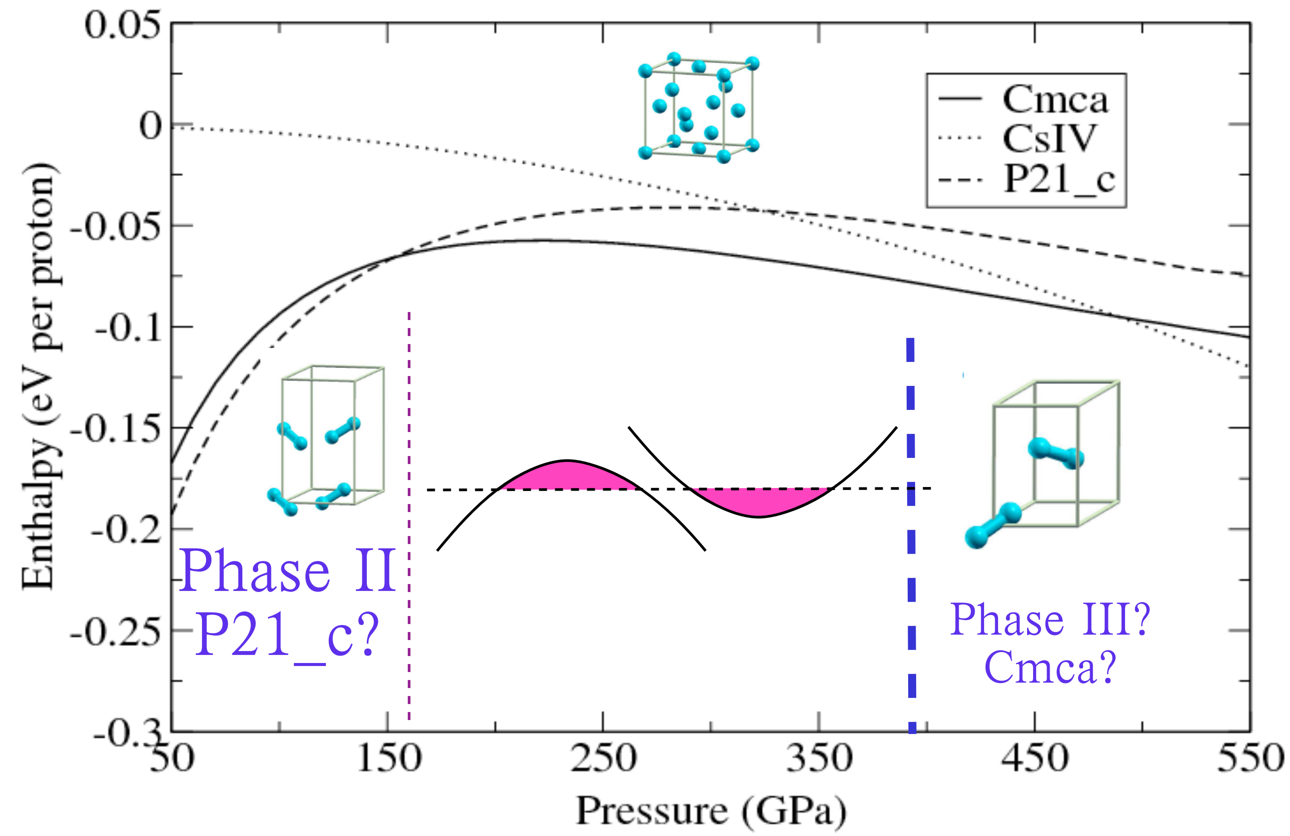

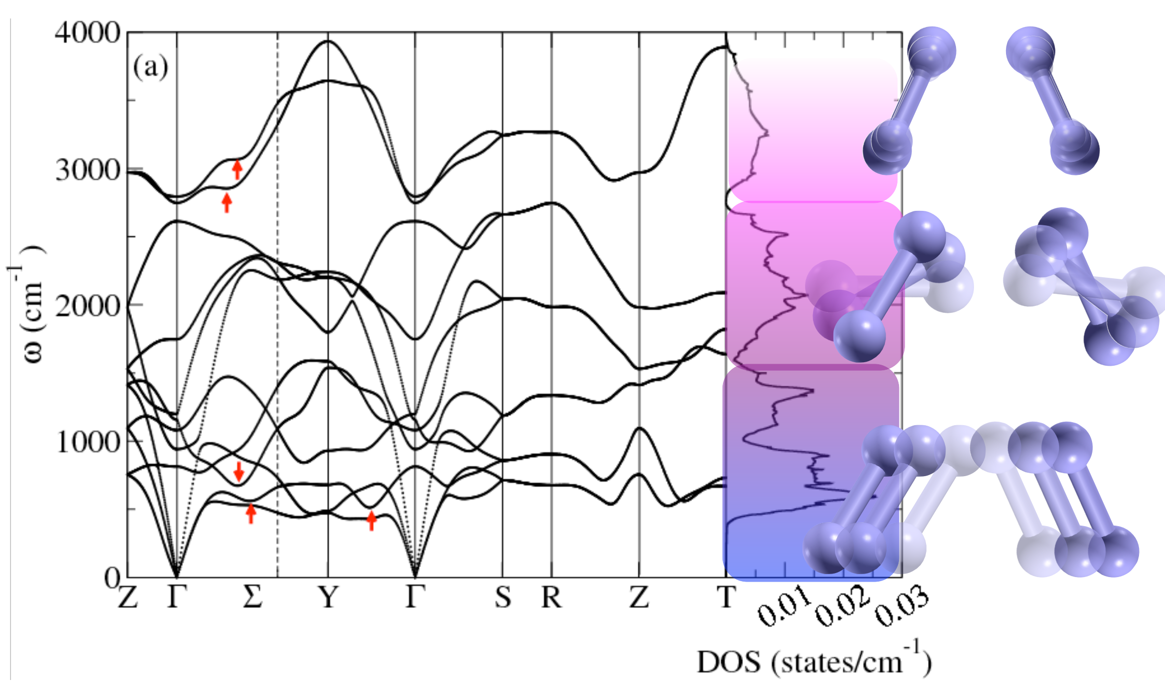

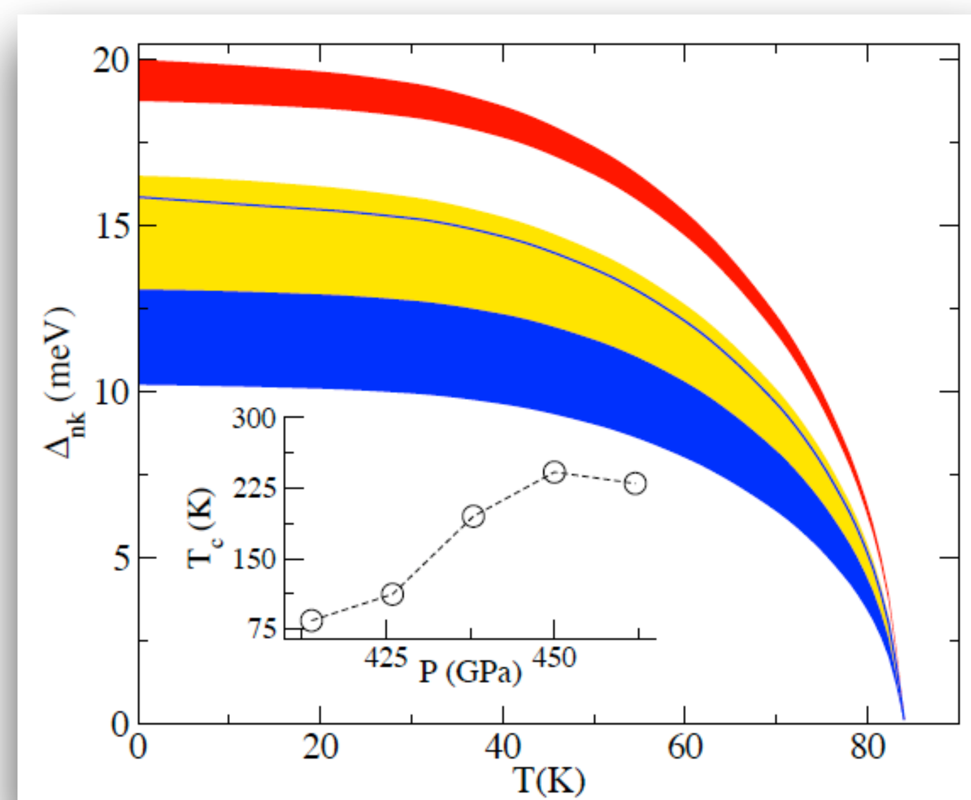

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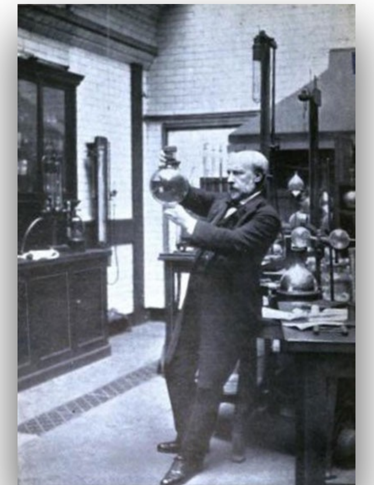

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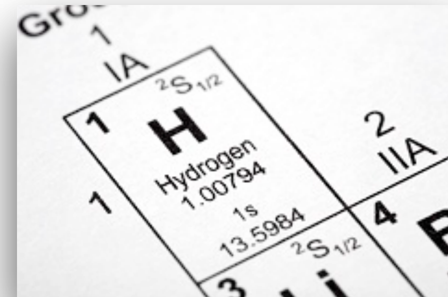

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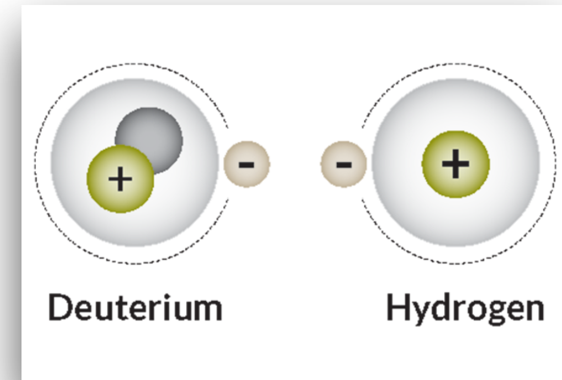

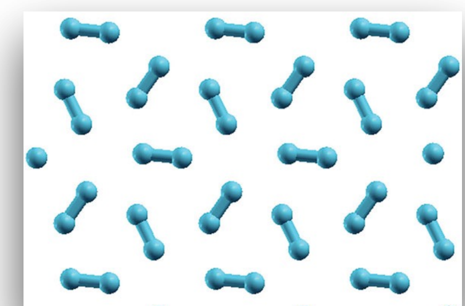

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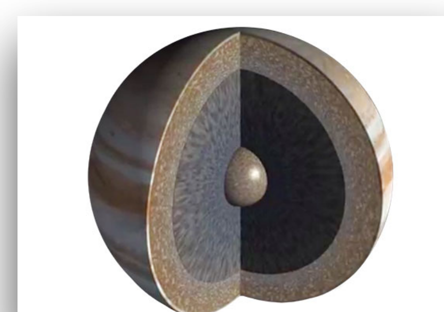

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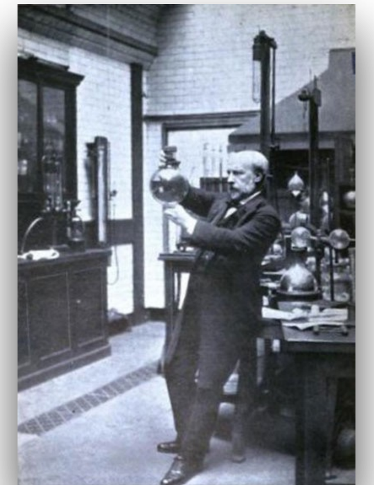

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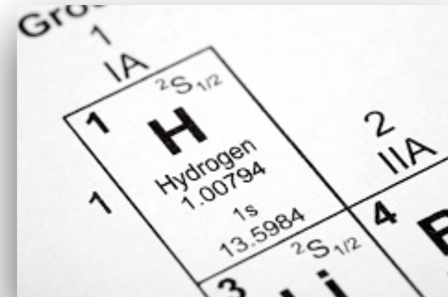

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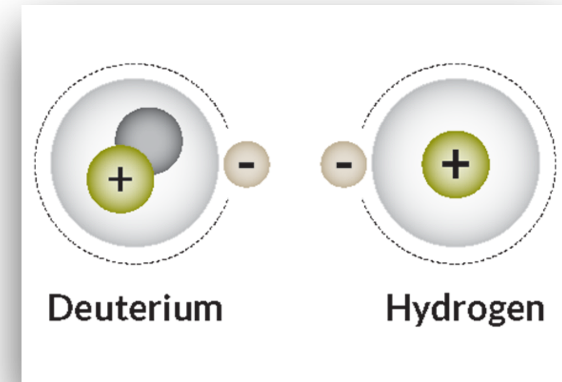

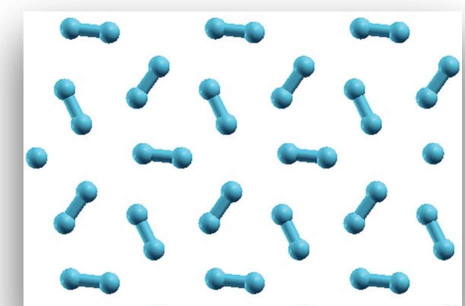

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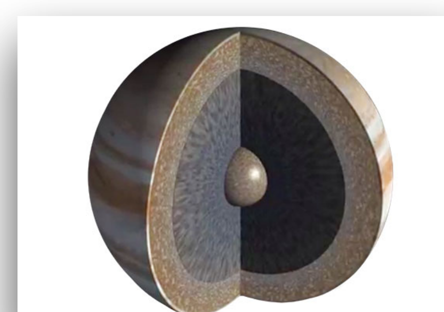

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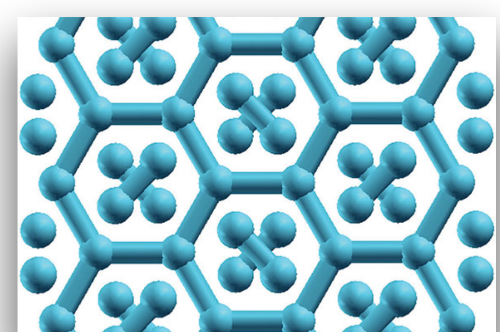
2011: Eremets discovers solid Phase IV (220 GPa)



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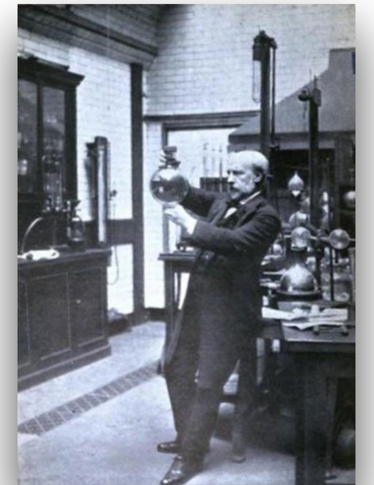

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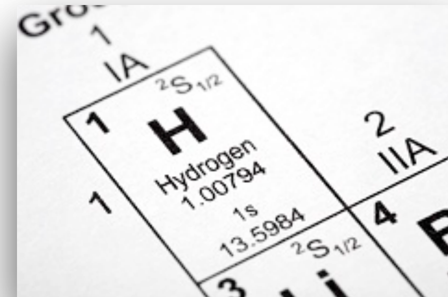

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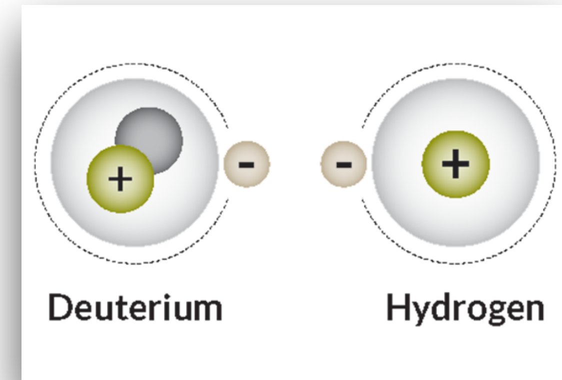

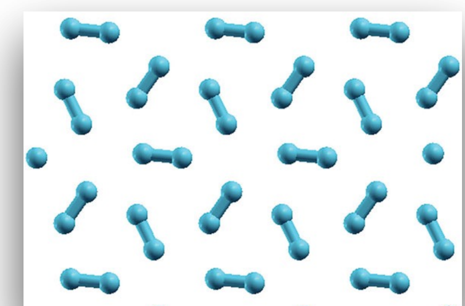

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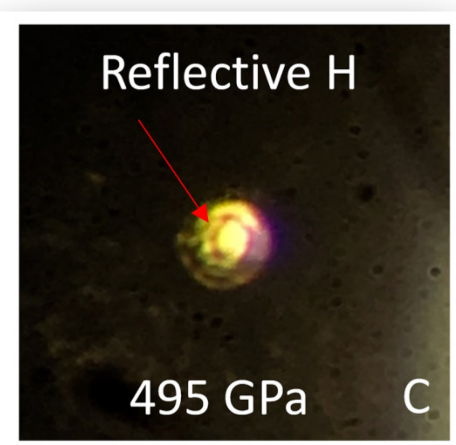
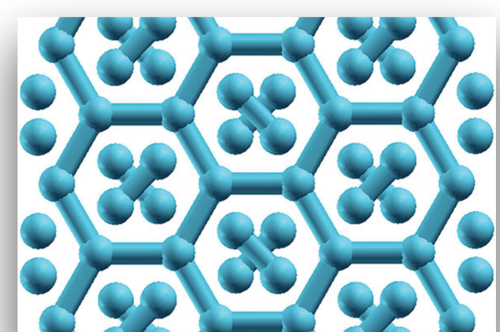
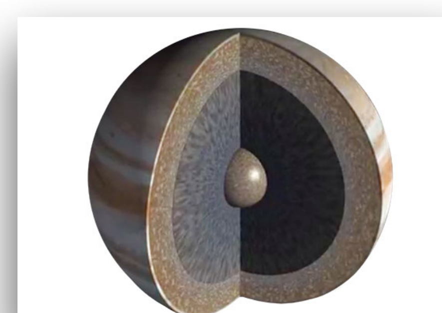


2017: Metallic hydrogen discovered by Silveira at 500 GPa (?)

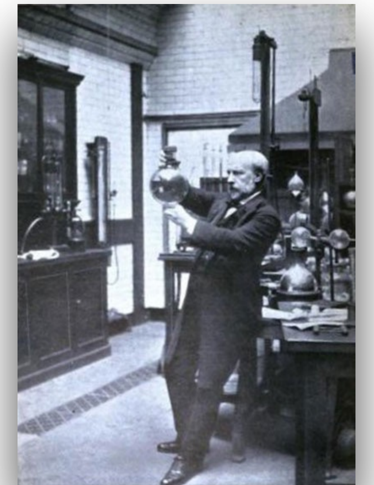
2011: Eremets discovers solid Phase IV (220 GPa)





1996: Nellis produces liquid metallic hydrogen (140 GPa and 3000K)

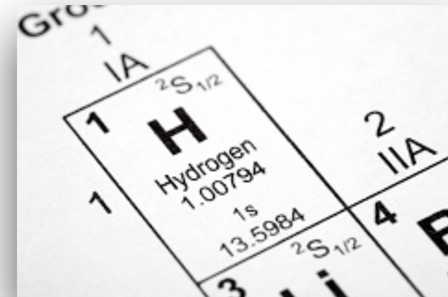
Metallic hydrogen: The holy grail of physics



1899: Dewar produces solid hydrogen

1935: Wigner predicted metallic hydrogen at 25 GPa

1968: Ashcroft's proposal



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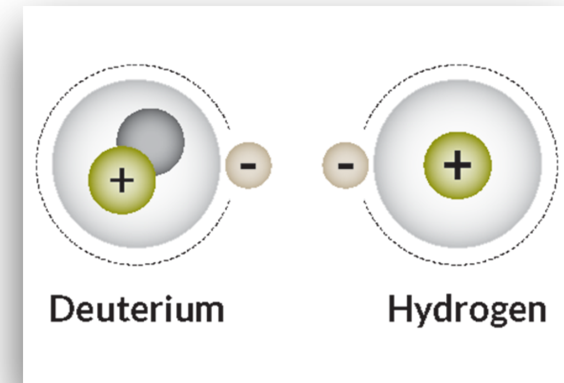
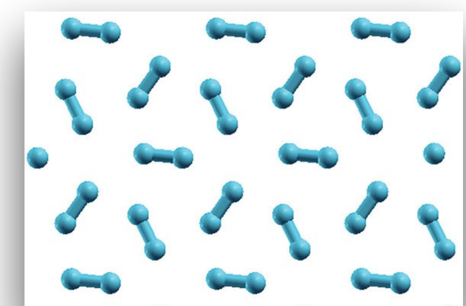


2020: Loubeyre: (Probable) Metallic hydrogen



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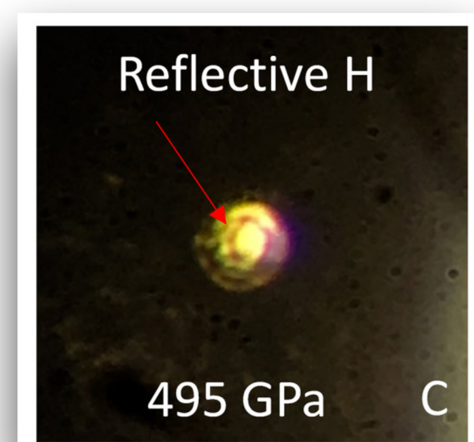

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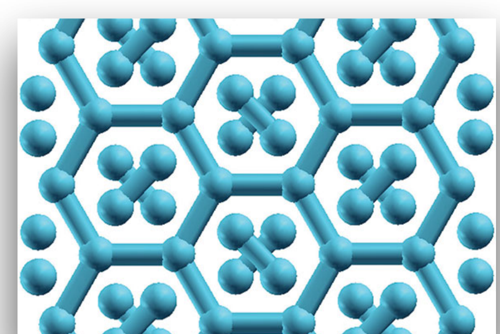

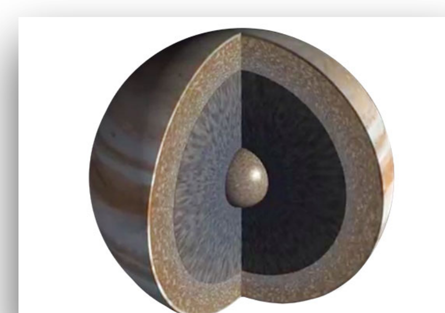

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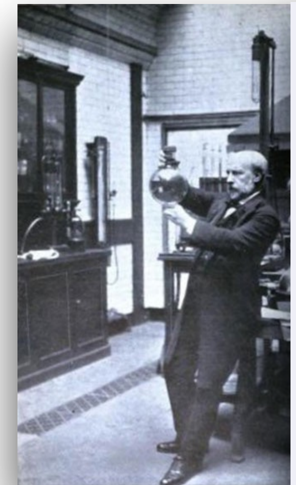

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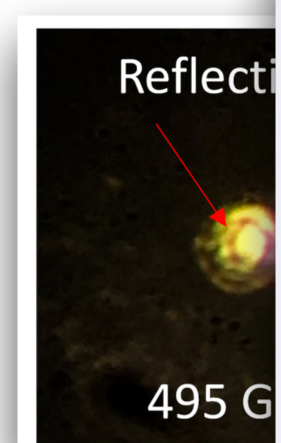

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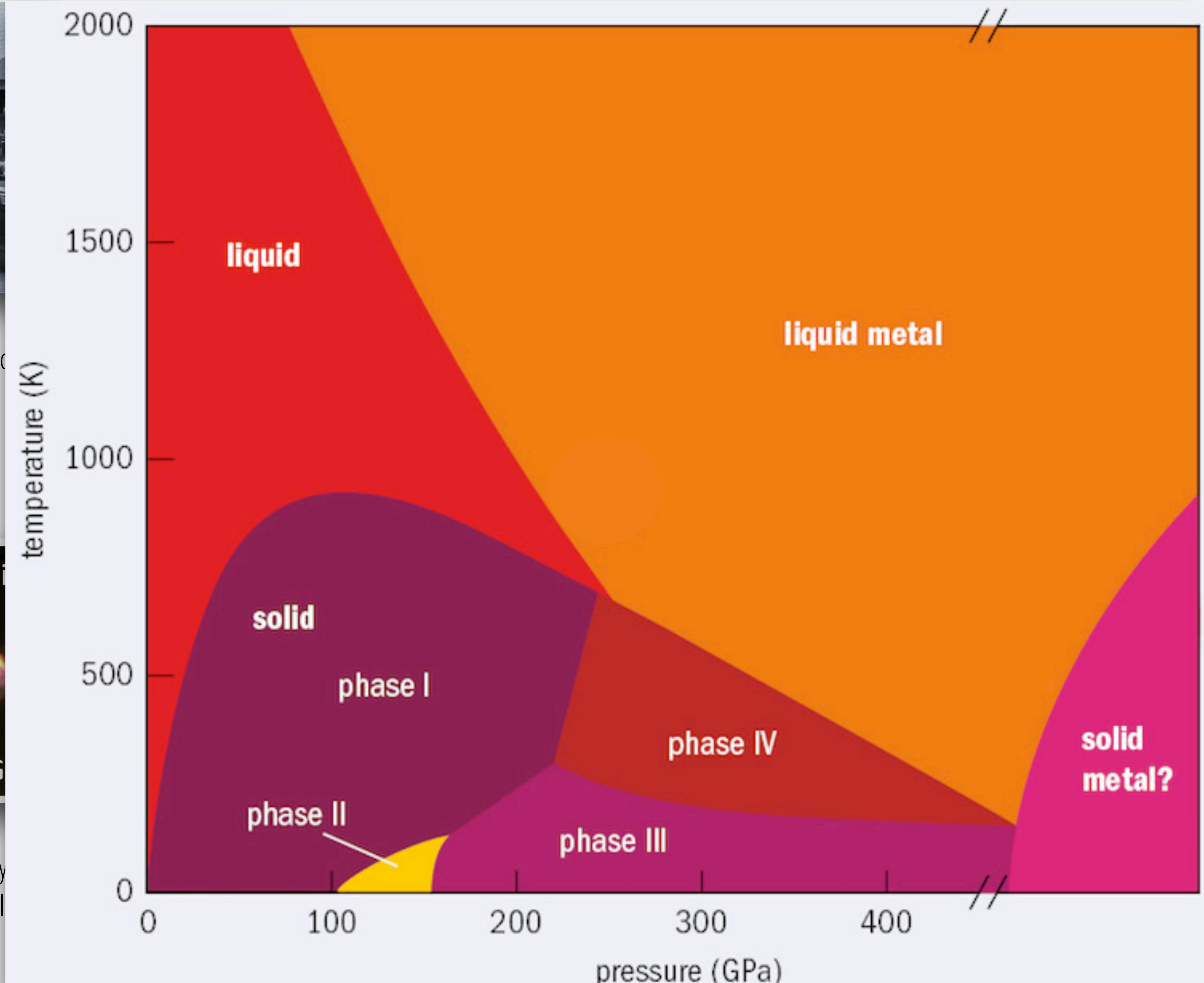
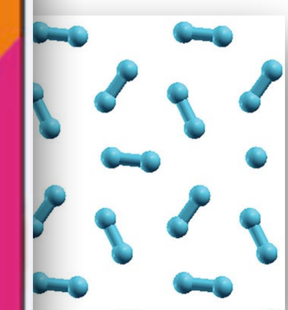


red



ase III

1996: Nellis produces liquid metallic
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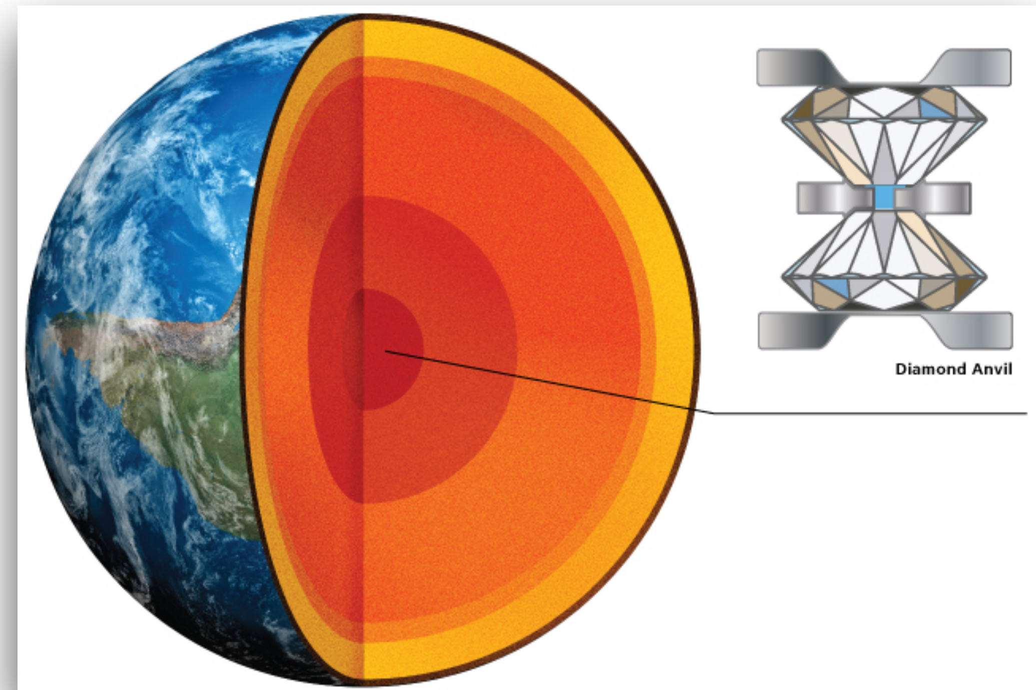
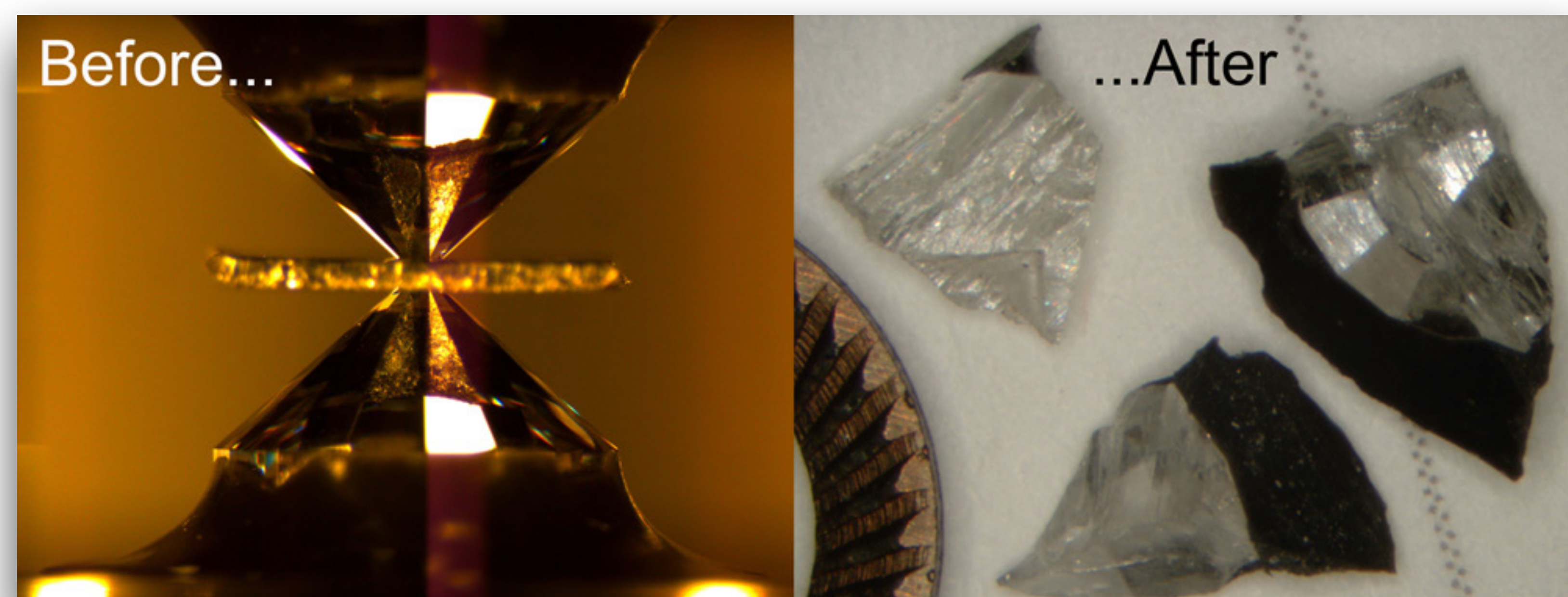
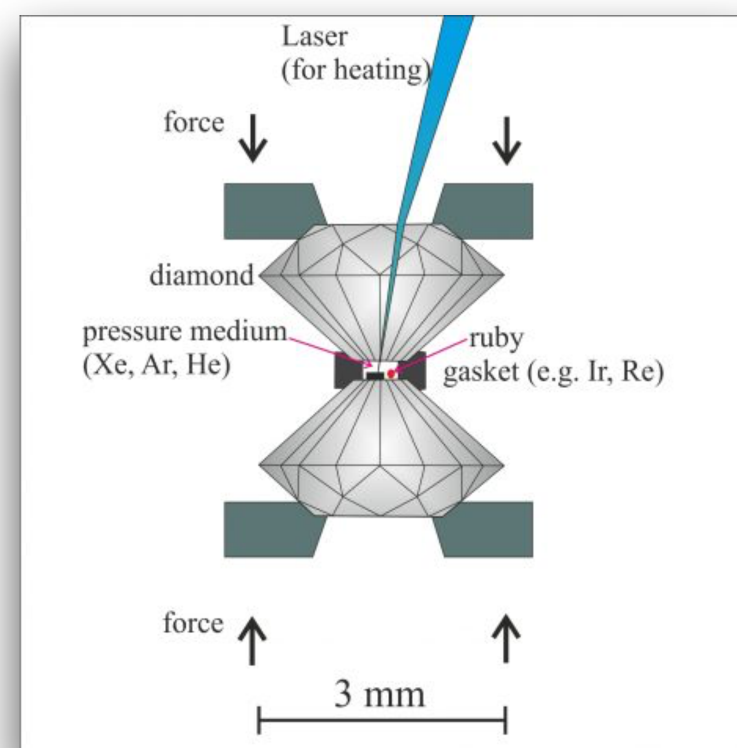
Hydrogen metallization: P > 450 GPa



Modern anvil cell reaches 350 GPa

Pressure in the inner core of earth is about 330 GPa!





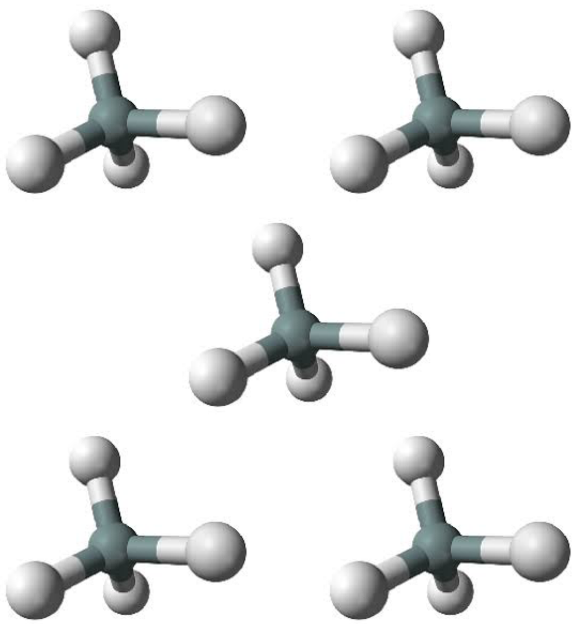
Better call Ashcroft

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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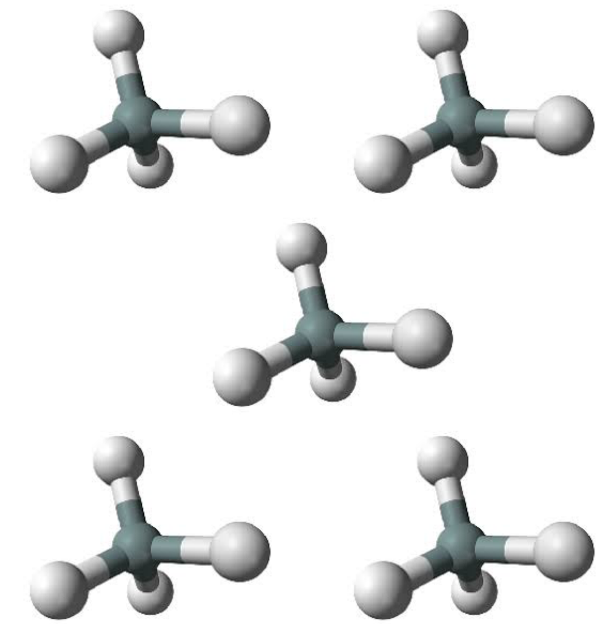
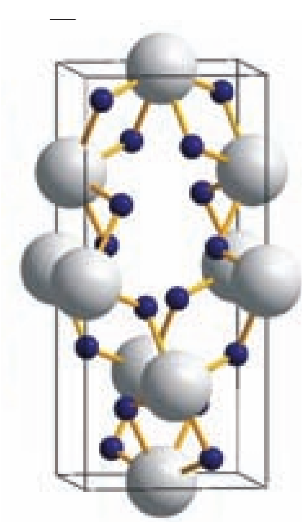


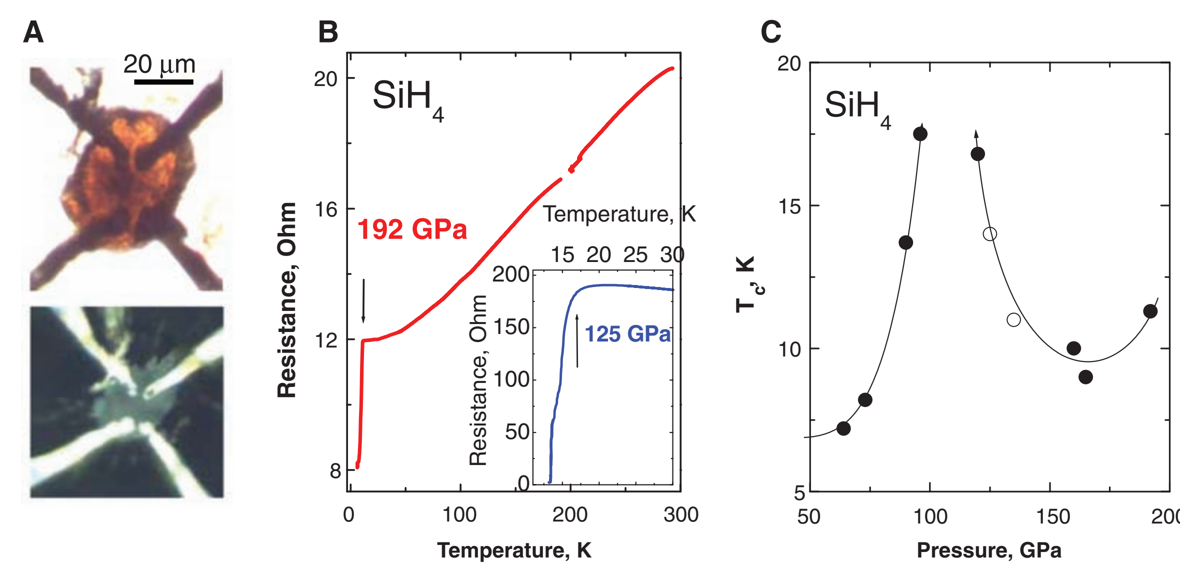


2008

Superconductivity in Hydrogen Dominant Materials: Silane

M. I. Eremets,[1]* I. A. Trojan,[1]† S. A. Medvedev,[1] J. S. Tse,[2] Y. Yao[2]

The metallization of hydrogen directly would require pressure in excess of 400 gigapascals (GPa), out of the reach of present experimental techniques. The dense group IVa hydrides attract considerable attention because hydrogen in these compounds is chemically precompressed and a metallic state is expected to be achievable at experimentally accessible pressures. We report the transformation of insulating molecular silane to a metal at 50 GPa, becoming superconducting at a transition temperature of T_c = 17 kelvin at 96 and 120 GPa. The metallic phase has a hexagonal close-packed structure with a high density of atomic hydrogen, creating a three-dimensional conducting network. These experimental findings support the idea of modeling metallic hydrogen with hydrogen-rich alloy.



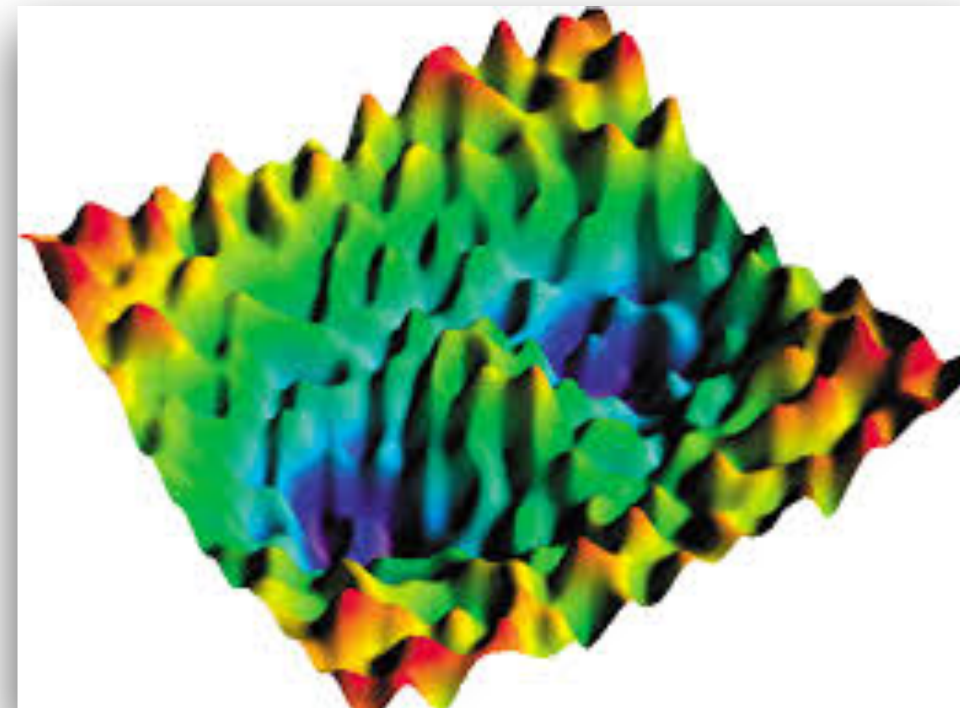
17 K is much lower than the predicted Tc

Hydrides at high pressure: search by computers

NATURE VOL. 335 15 SEPTEMBER 1988 NEWS AND VIEWS 201

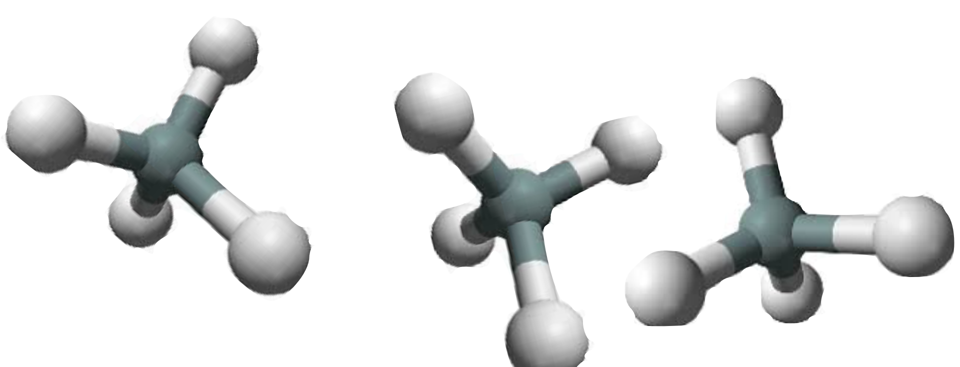
Crystals from first principles

by J. Maddox

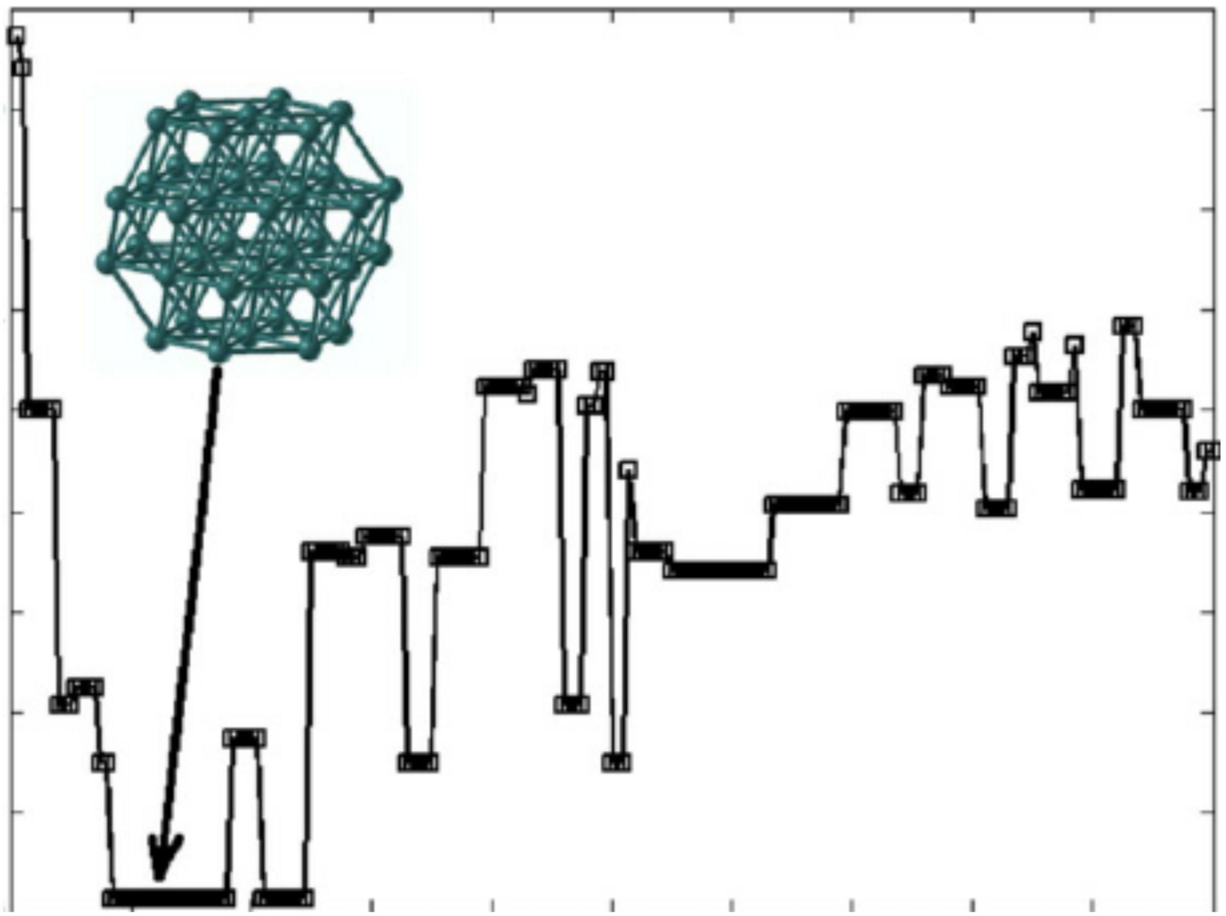


ONE of the continuing scandals in the physical sciences is that it remains in general impossible to predict the structure of even the simplest crystalline solids from a knowledge of their chemical composition. Who, for example, would guess that graphite, not diamond, is the thermodynamically stable allotrope of carbon at ordinary temperature and pressure? Solids such as crystalline water (ice) are still thought to lie beyond mortals' ken.

Yet one would have thought that, by now, it should be possible to equip a sufficiently large computer with a sufficiently large program, type in the formula of the chemical and obtain, as output, the atomic coordinates of the atoms in a unit cell.



Ab-initio random structure searching
(The Columbus egg)



Genetic Algorithms

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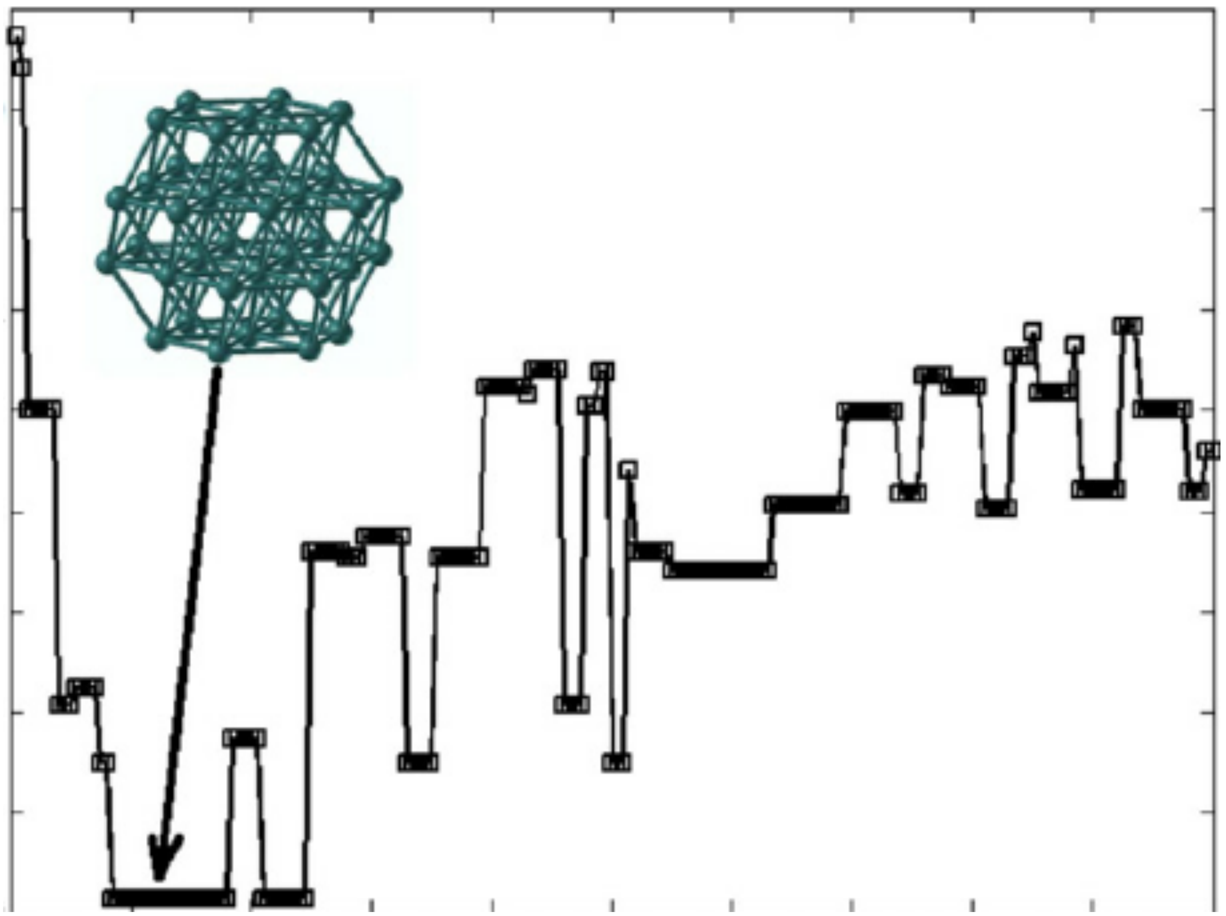

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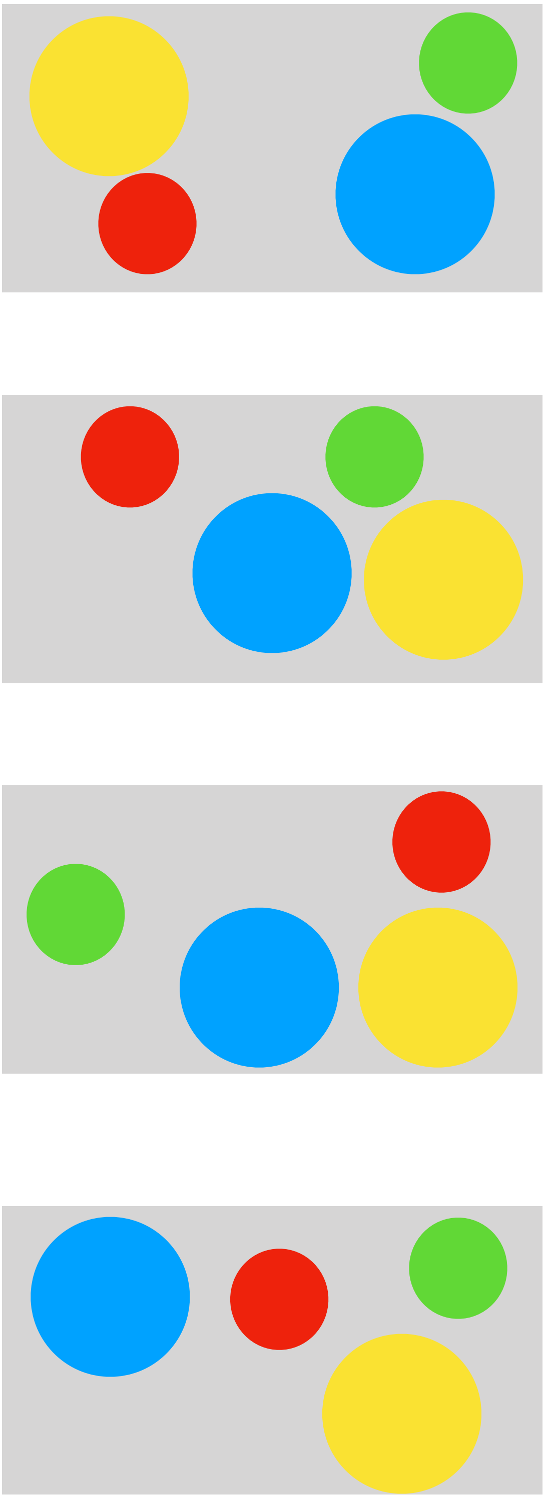

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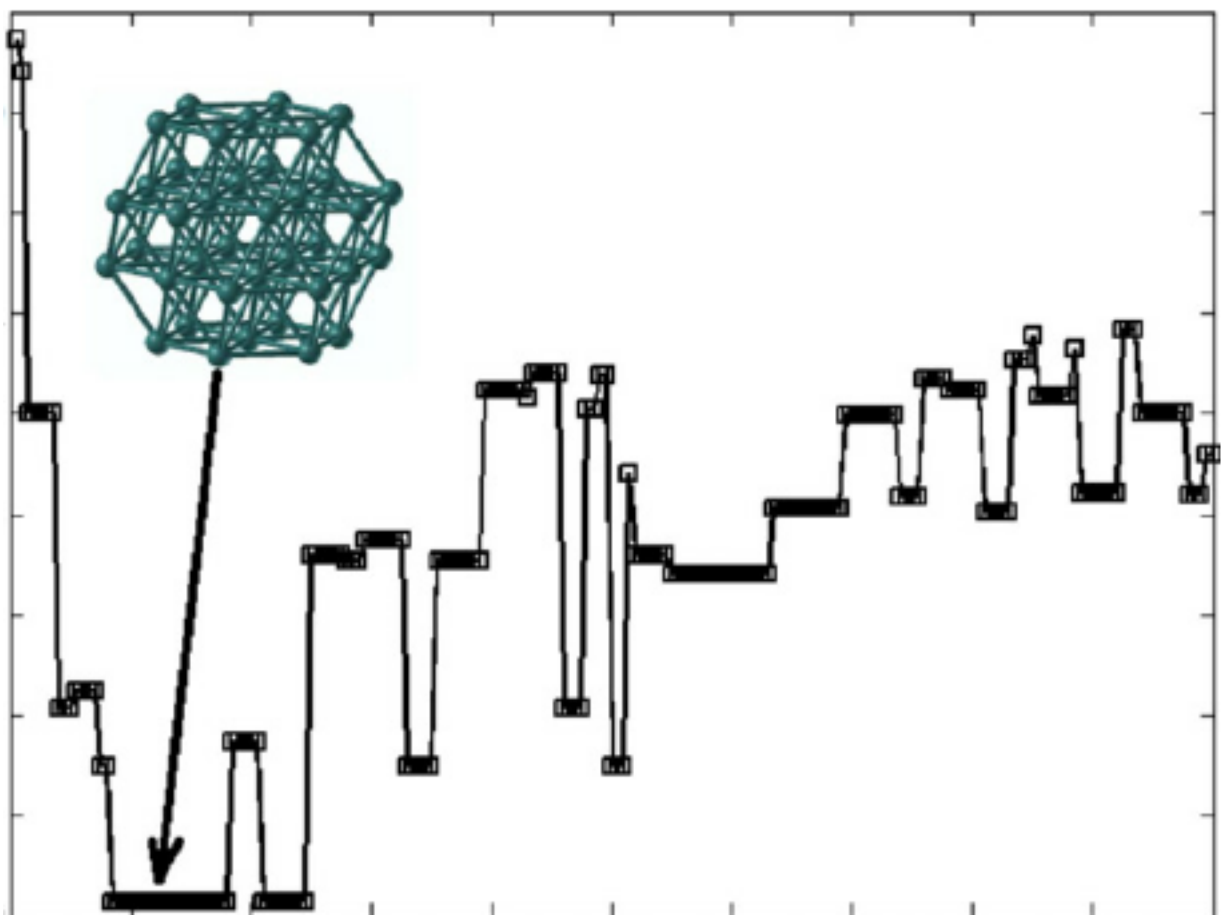

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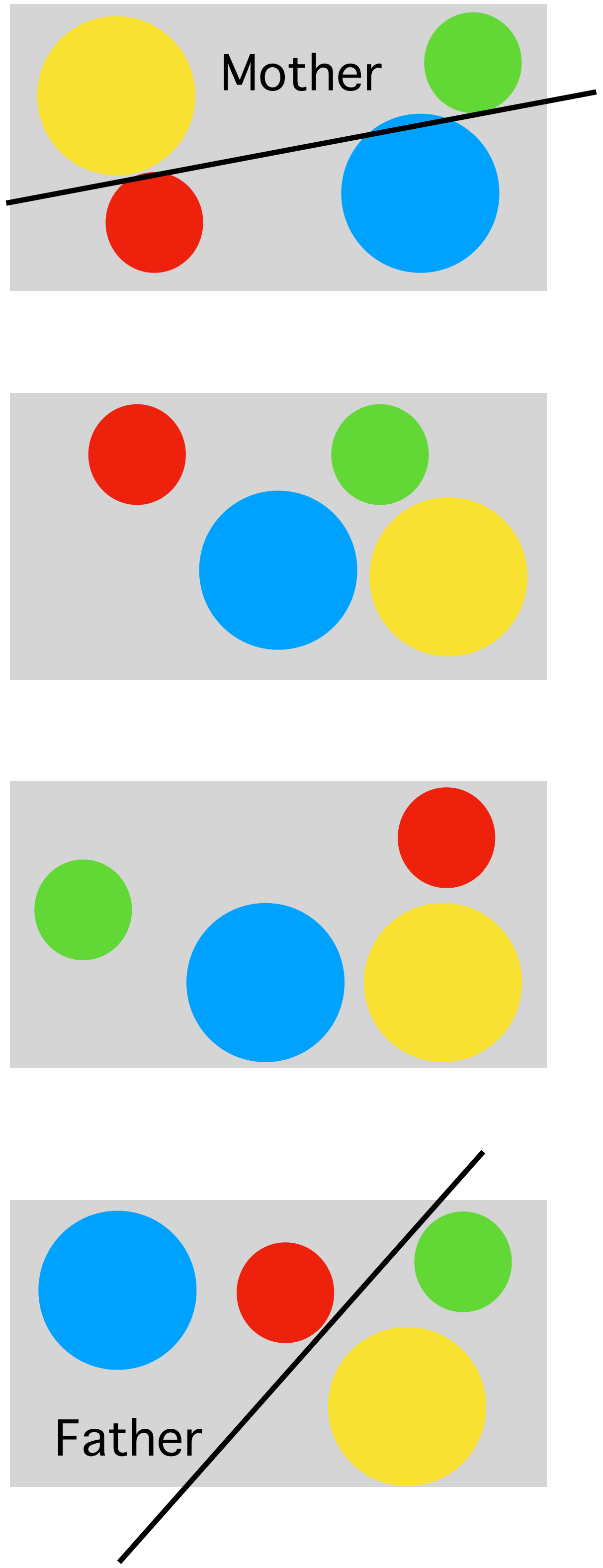

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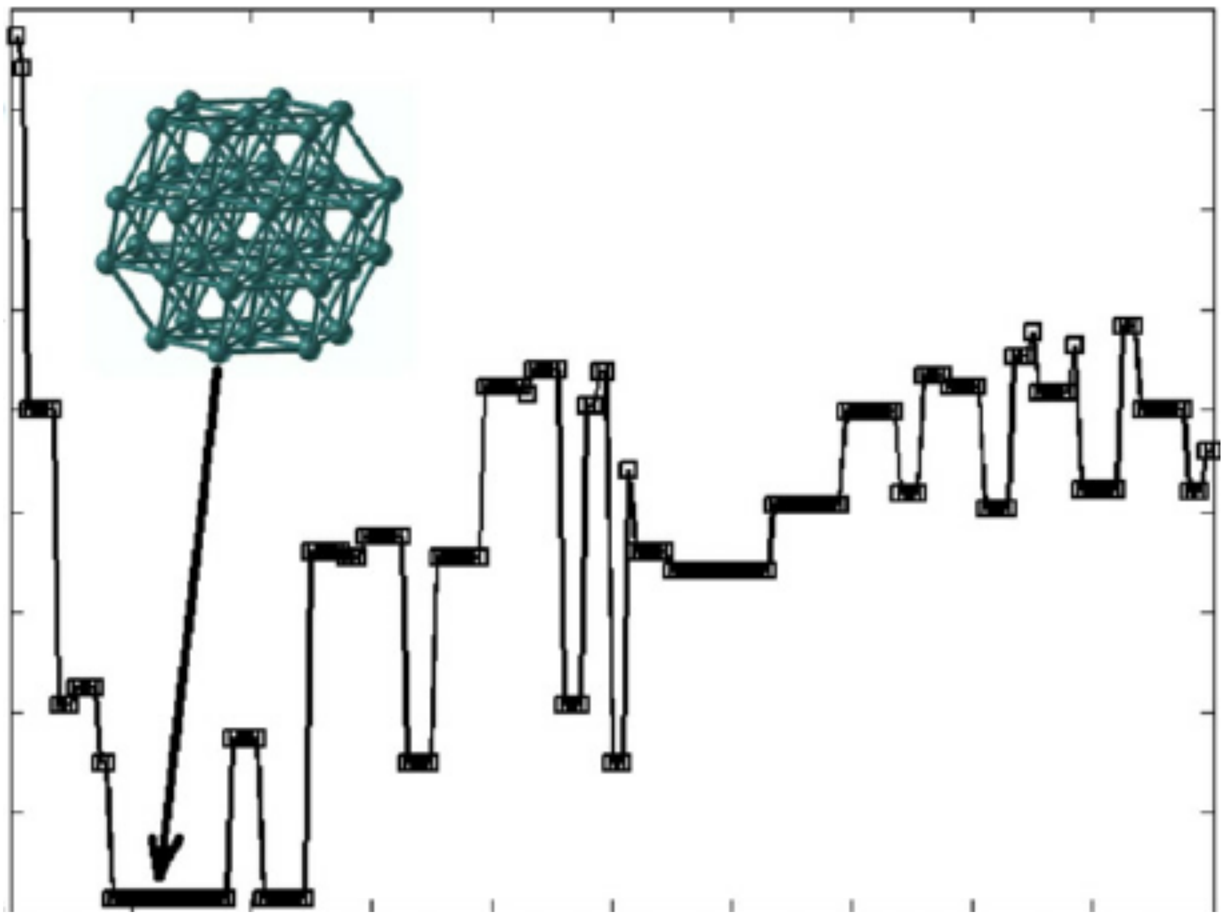

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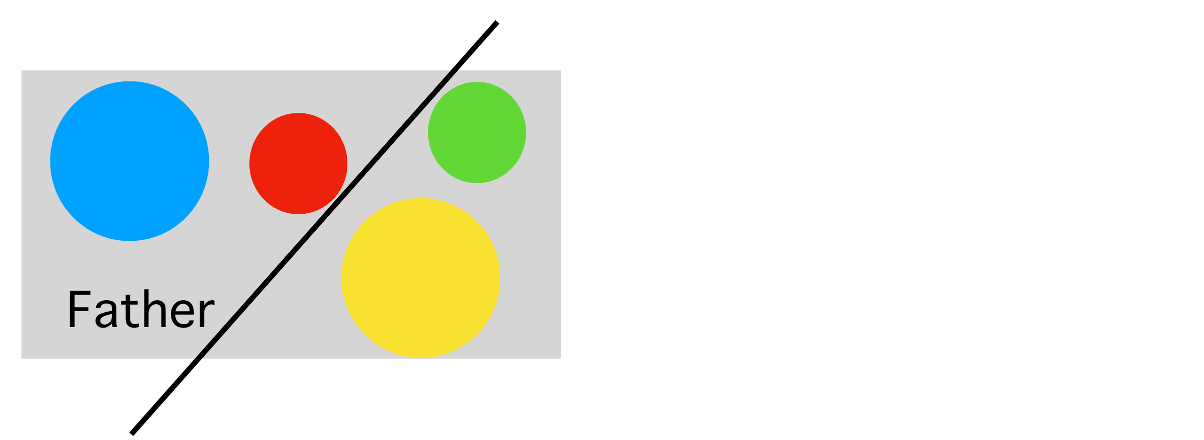

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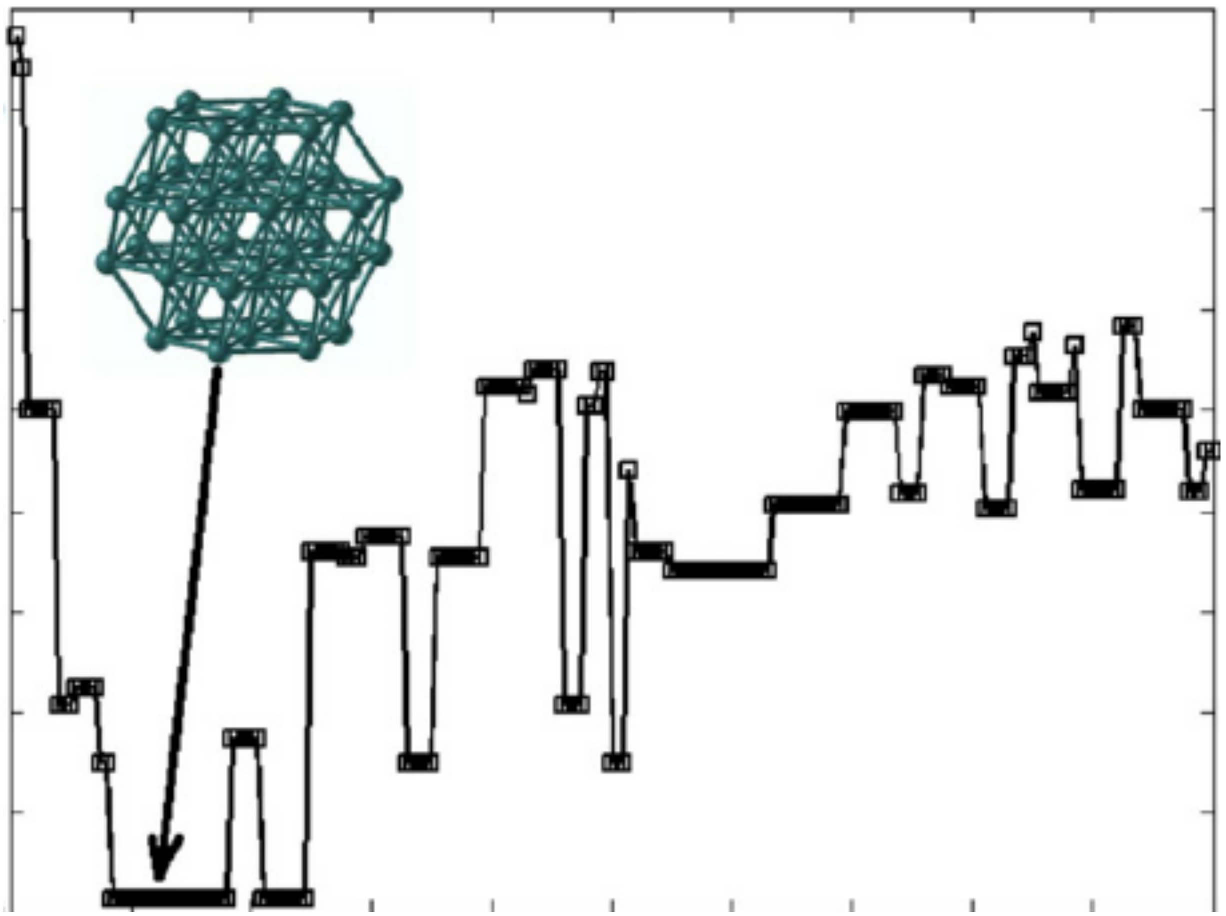

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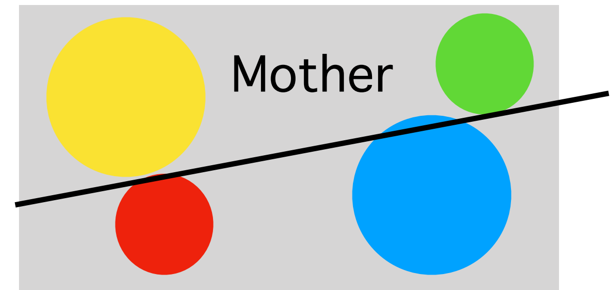

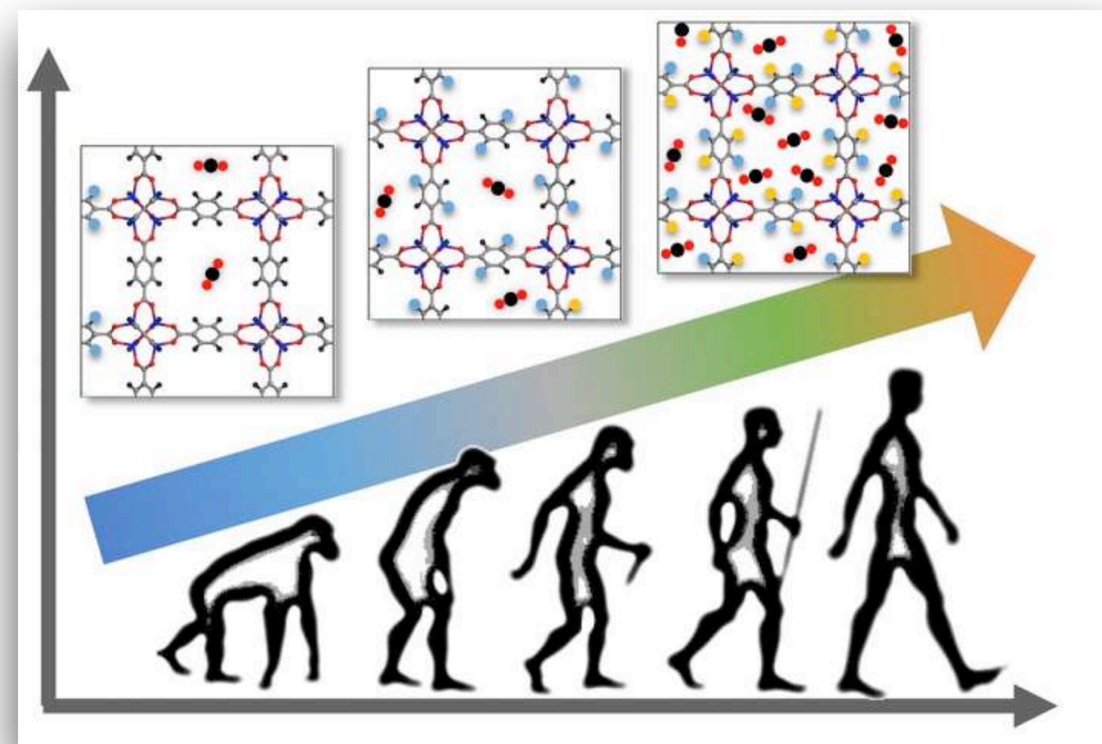

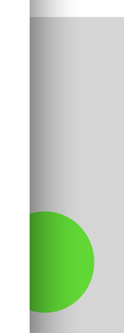

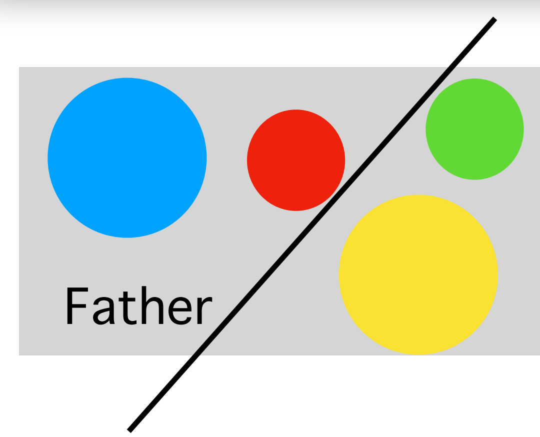

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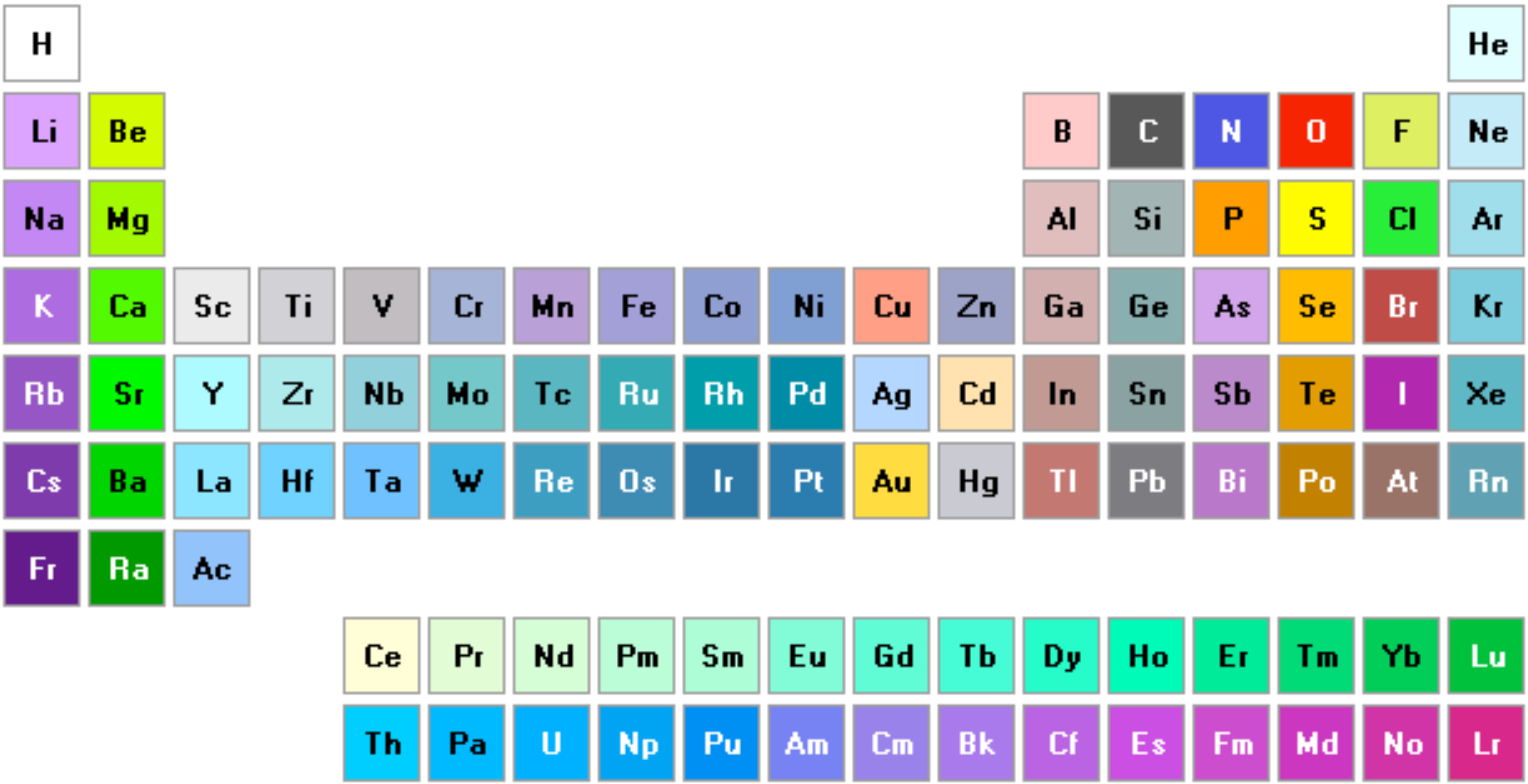
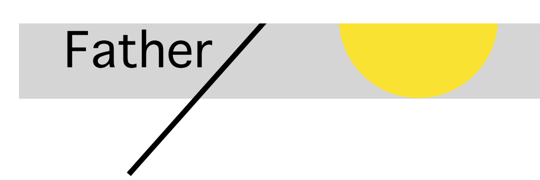
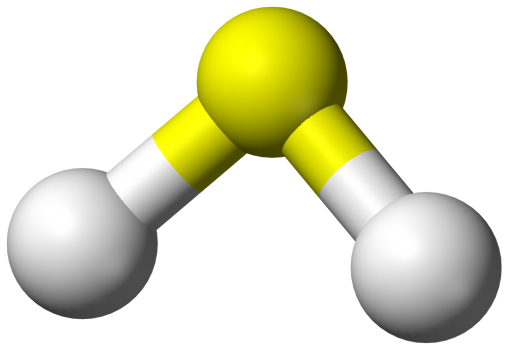




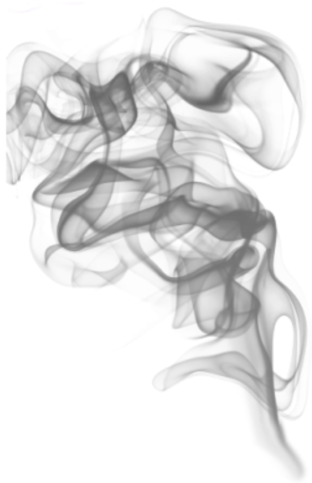
Hydrogen sulfide: the chemistry changes



Discovered in 1777

It is a colorless gas with the characteristic foul odor of rotten eggs.

It is very poisonous, corrosive, and flammable, explosive



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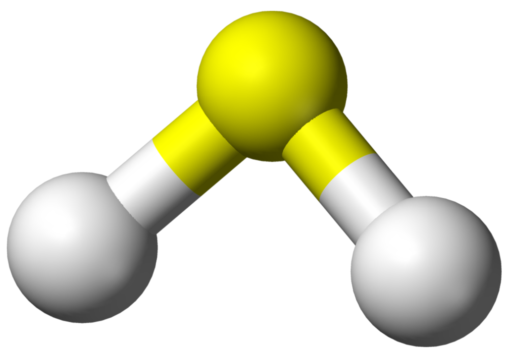

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THE JOURNAL OF CHEMICAL PHYSICS **140**, 174712 (2014)

The metallization and superconductivity of dense hydrogen sulfide

Yinwei Li,[1,a)] Jian Hao,[1] Hanyu Liu,[2] Yanling Li,[1] and Yanming Ma[3,b)]
[1]*School of Physics and Electronic Engineering, Jiangsu Normal University, Xuzhou 221116, People's Republic of China*
[2]*Department of Physics and Engineering Physics, University of Saskatchewan, Saskatchewan S7N 5E2, Canada*
[3]*State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, People's Republic of China*

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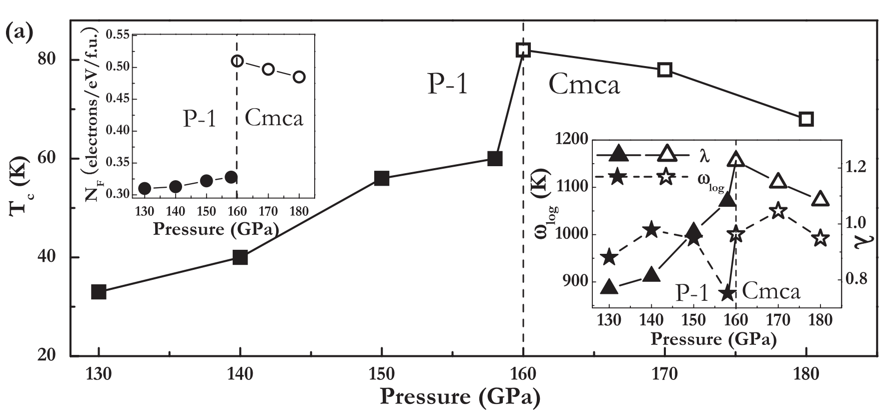

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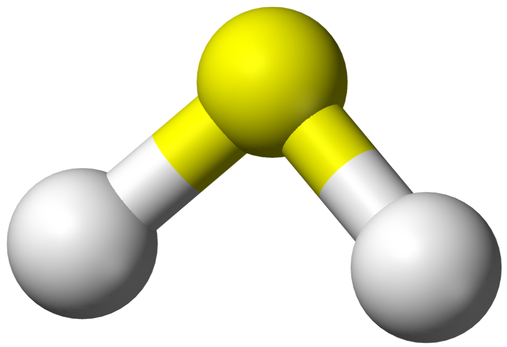

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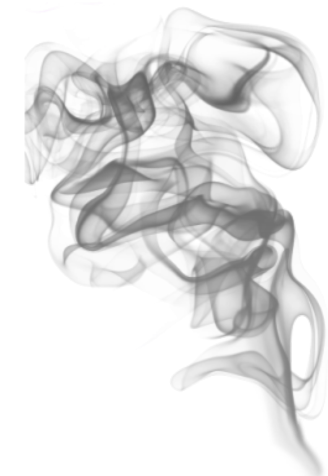

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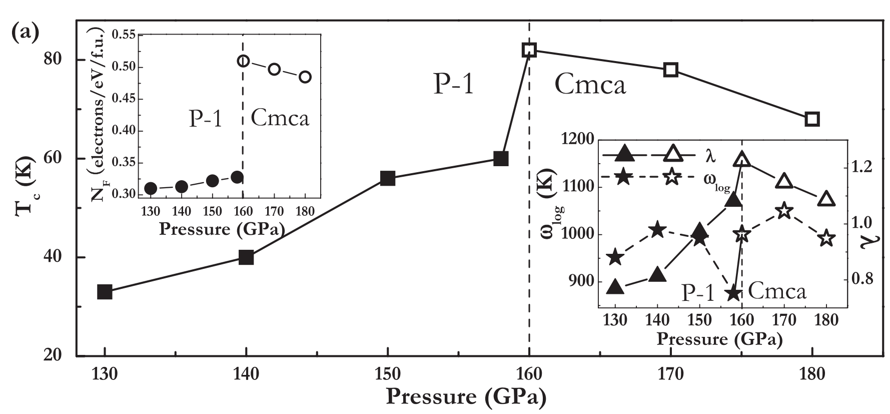

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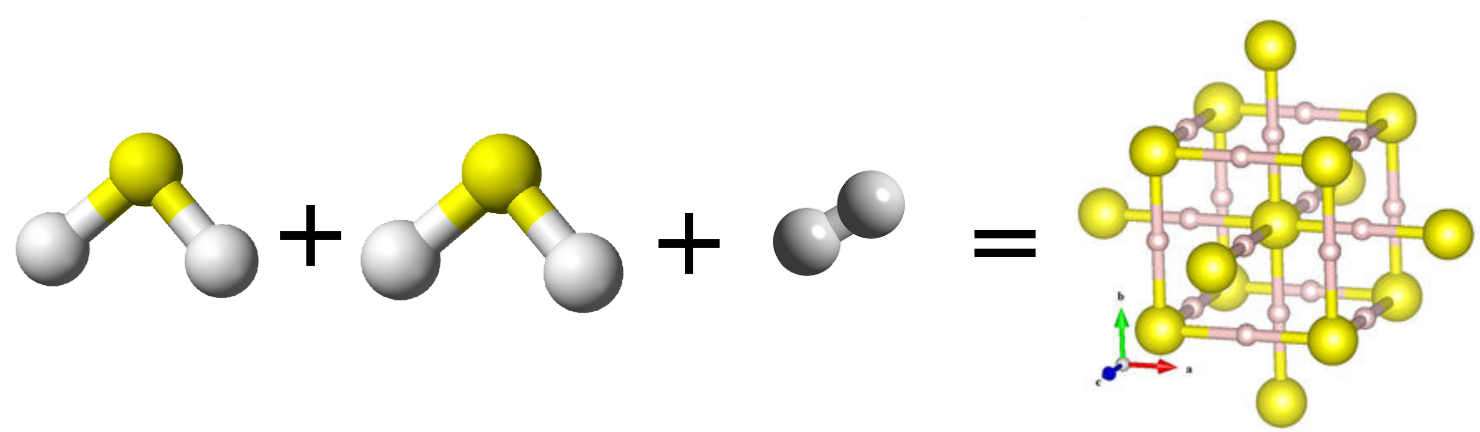
Pressure-induced metallization of dense $(H_2S)_2H_2$ with high-T_c superconductivity

Defang Duan[1,2], Yunxian Liu[1], Fubo Tian[1], Da Li[1], Xiaoli Huang[1], Zhonglong Zhao[1], Hongyu Yu[1], Bingbing Liu[1], Wenjing Tian[2] & Tian Cui[1]

[1]State Key Laboratory of Superhard Materials, College of physics, Jilin University, Changchun, 130012, P. R. China, [2]State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, 130012, P. R. China.



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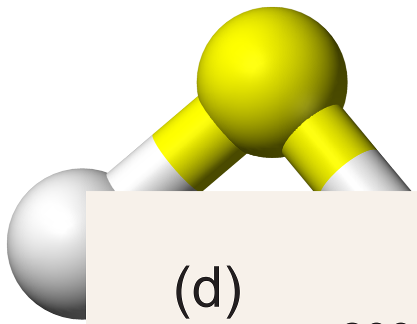

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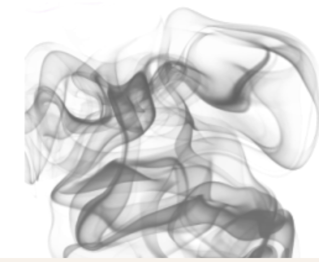
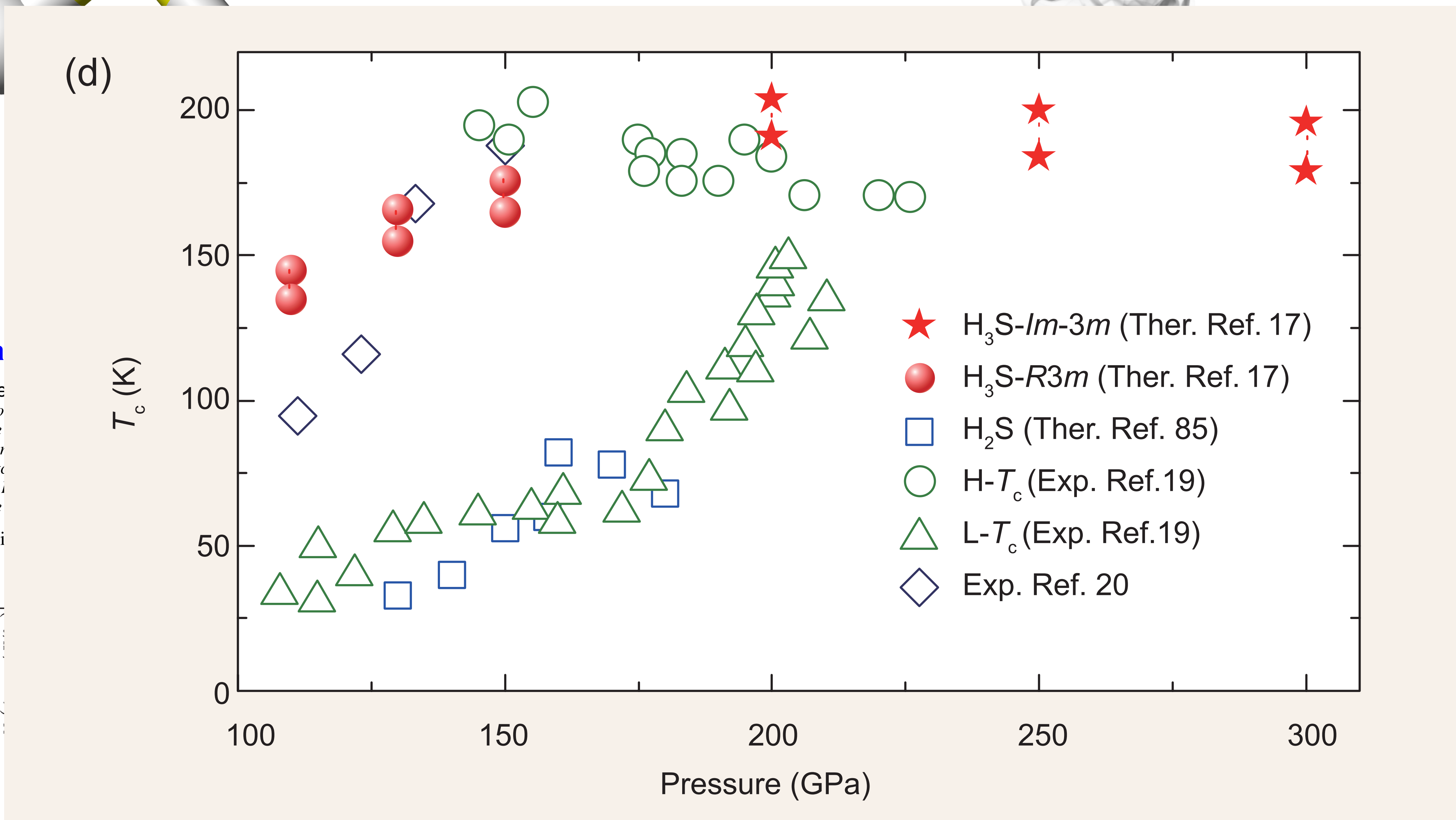
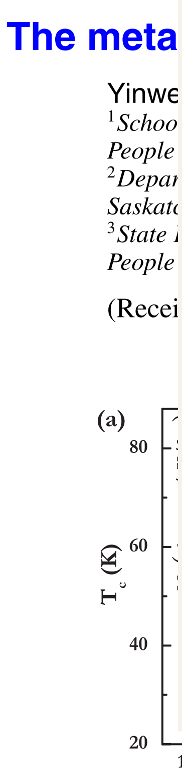
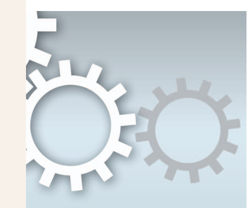




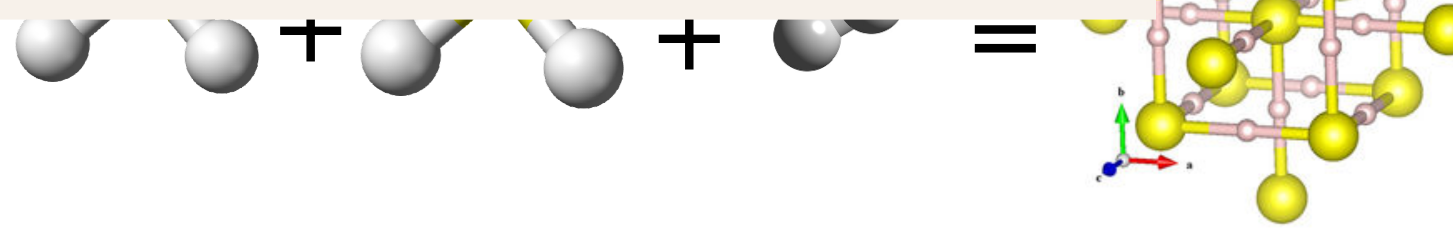




dense
uctivity

Hongyu Yu[1],

P. R. China, [2]State Key



Eremets's experiment

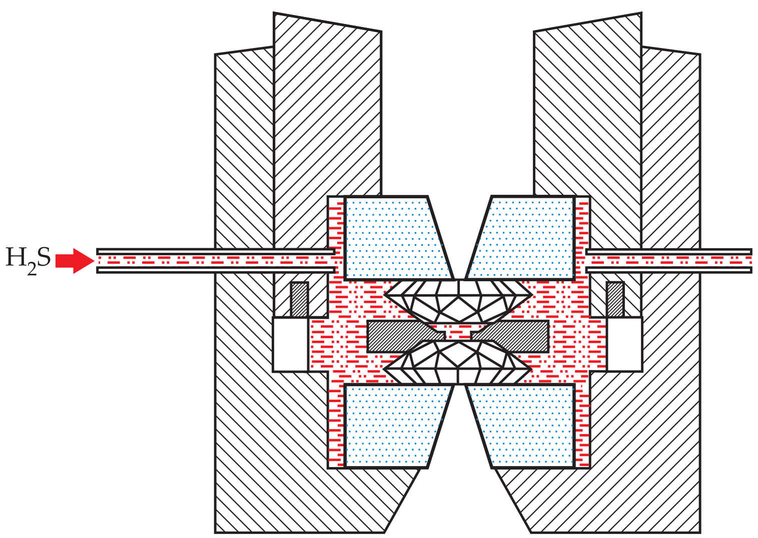
Max-Planck-Institut fur Chemie (Mainz), Germany

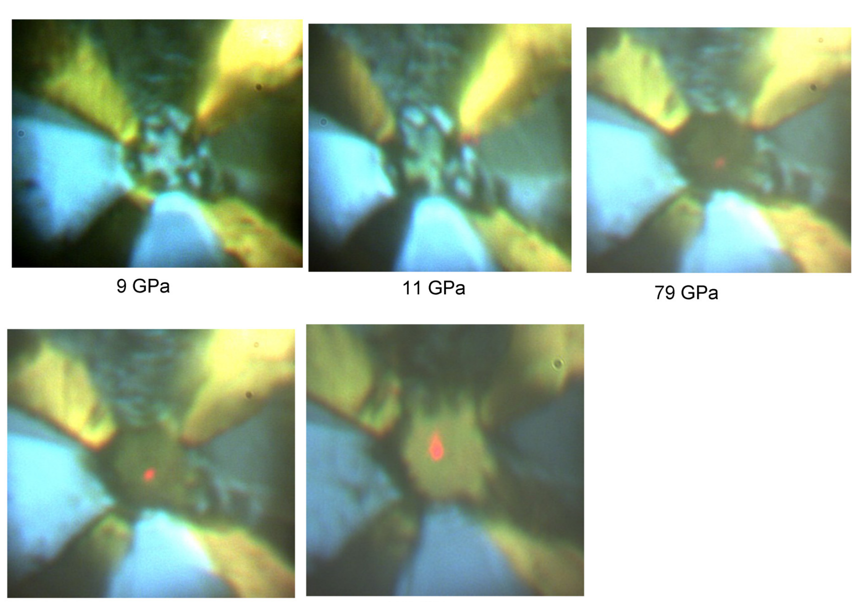
LETTER

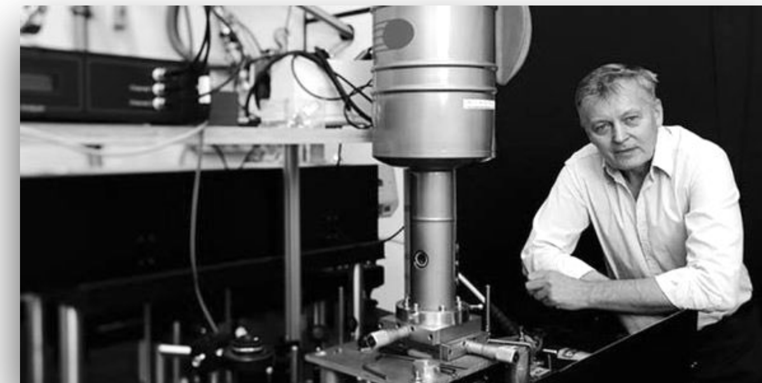
doi:10.1038/nature14964

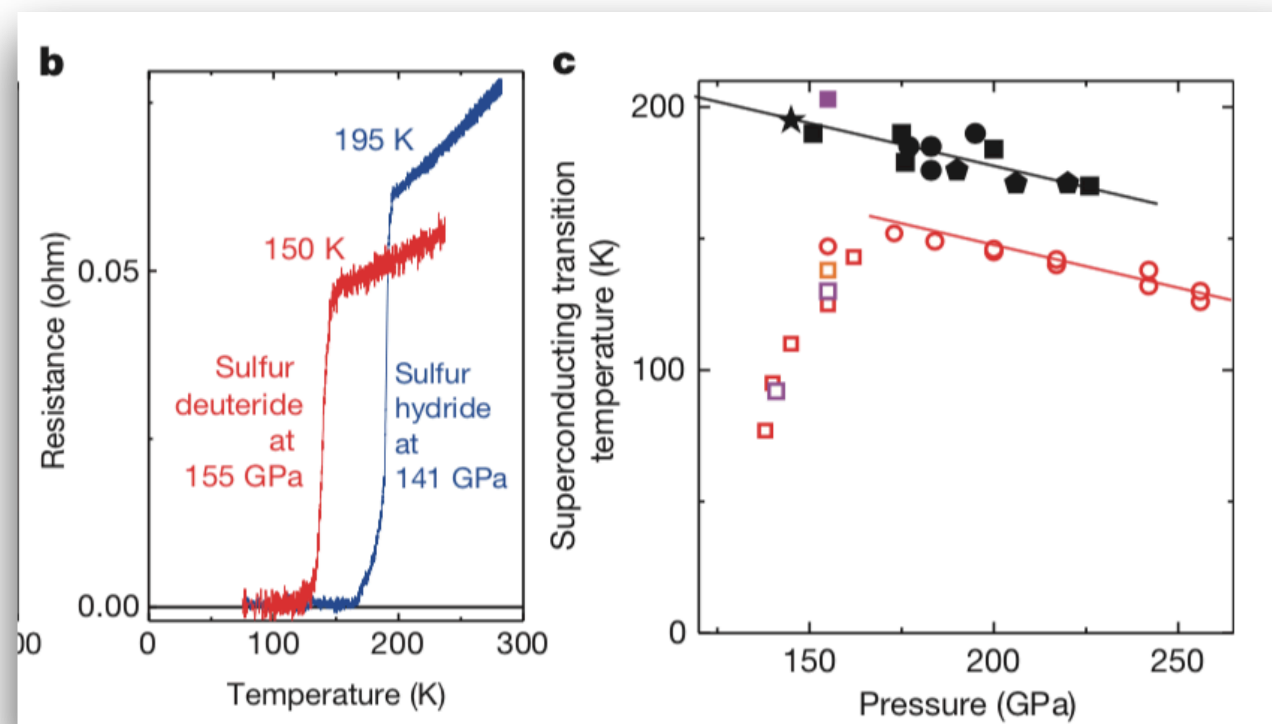
Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov[1]*, M. I. Eremets[1]*, I. A. Troyan[1], V. Ksenofontov[2] & S. I. Shylin[2]







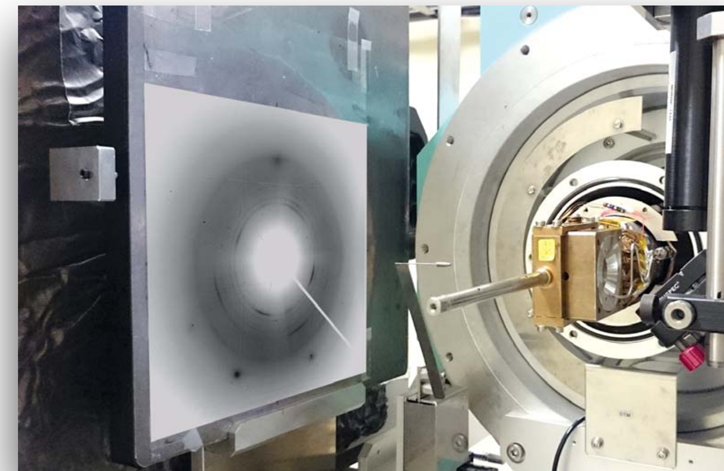


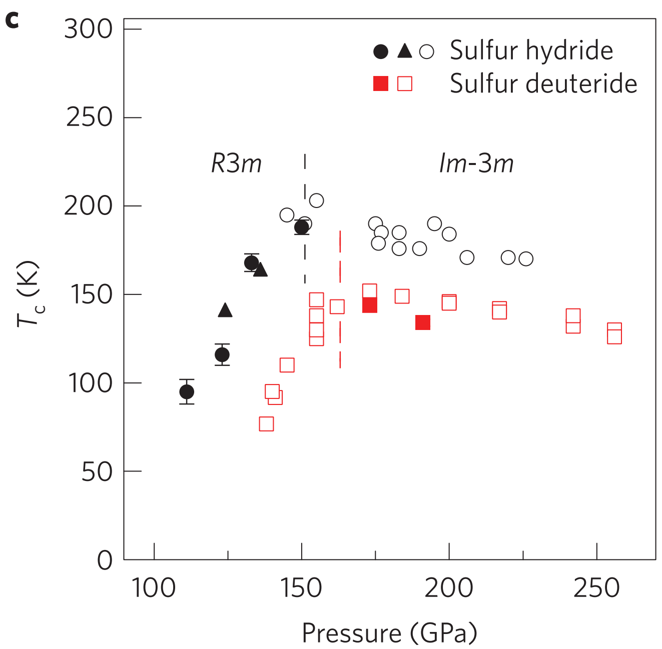
It is true

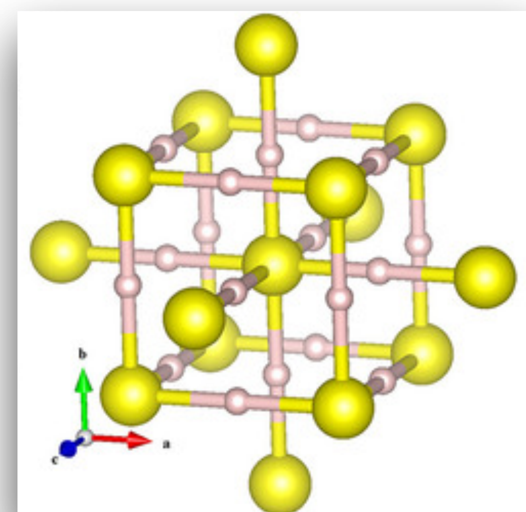
nature physics
LETTERS
PUBLISHED ONLINE: 9 MAY 2016 | DOI: 10.1038/NPHYS3760

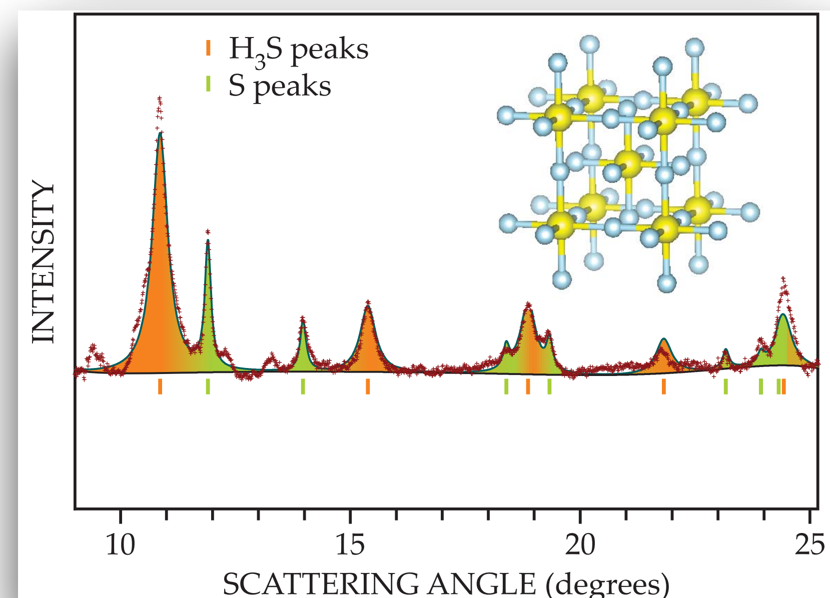
Crystal structure of the superconducting phase of sulfur hydride

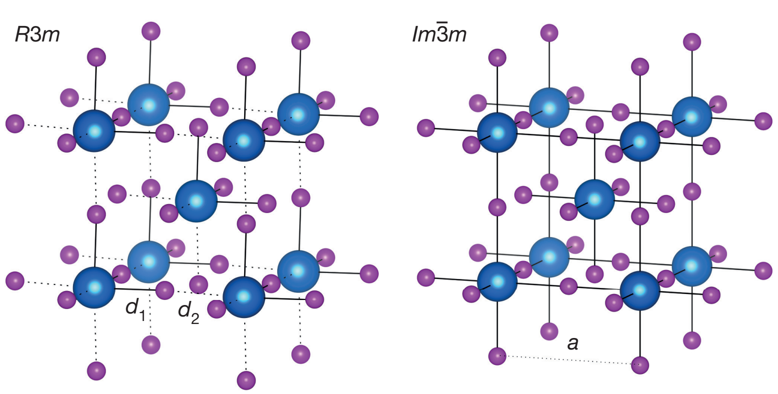
Mari Einaga[1*†], Masafumi Sakata[1], Takahiro Ishikawa[1], Katsuya Shimizu[1†], Mikhail I. Eremets[2†], Alexander P. Drozdov[2], Ivan A. Troyan[2], Naohisa Hirao[3] and Yasuo Ohishi[3]











It is true

nature physics | LETTERS
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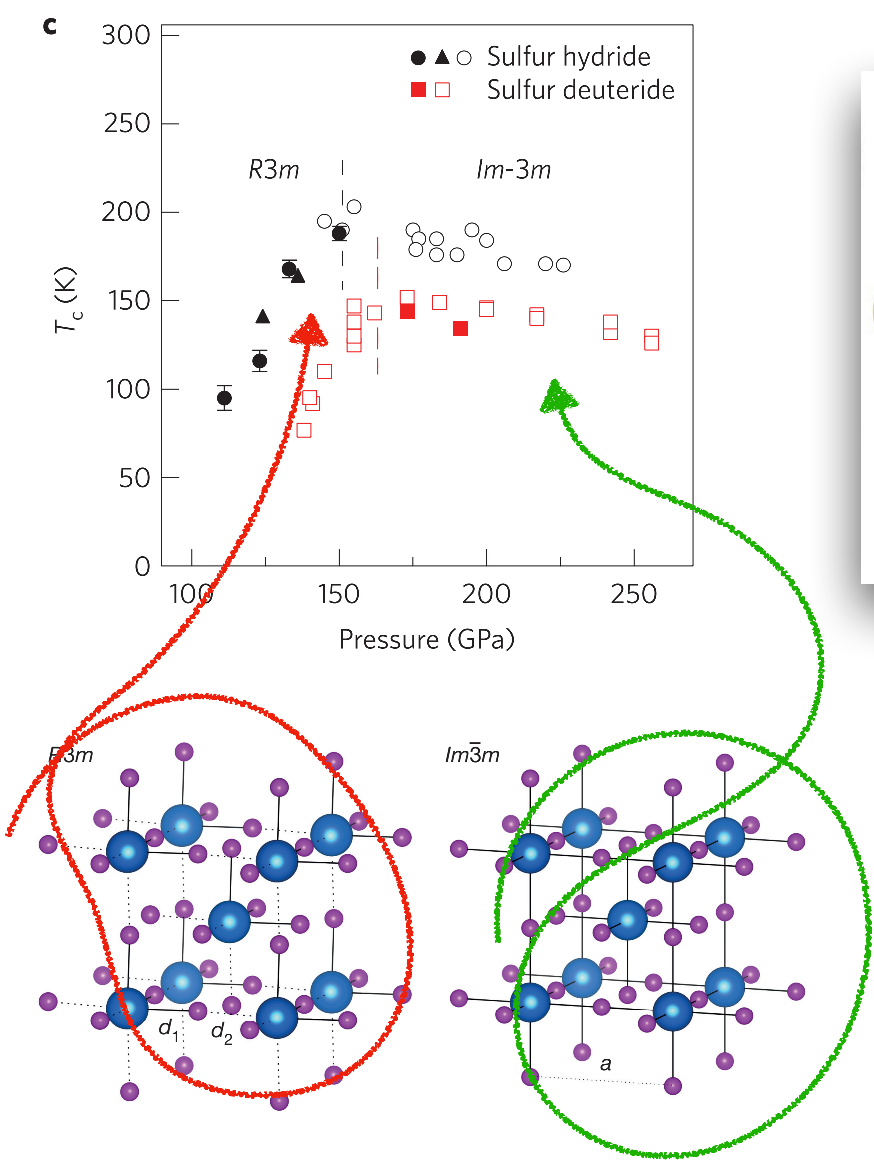

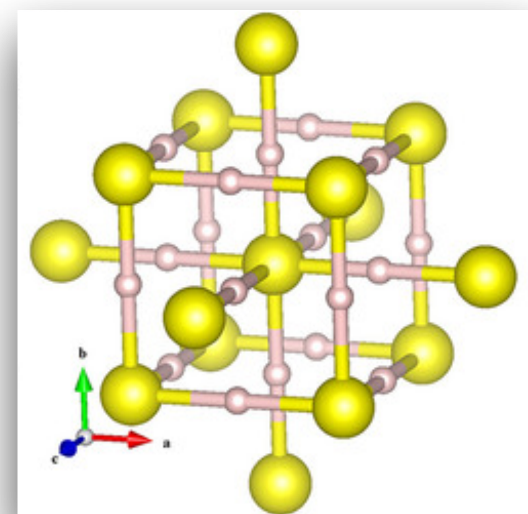

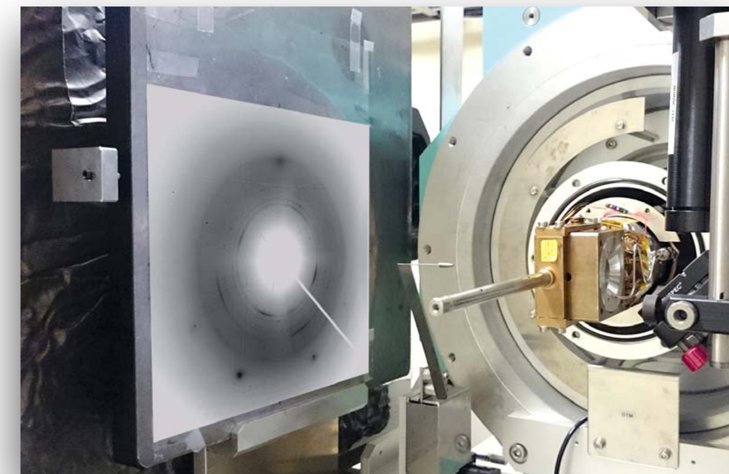

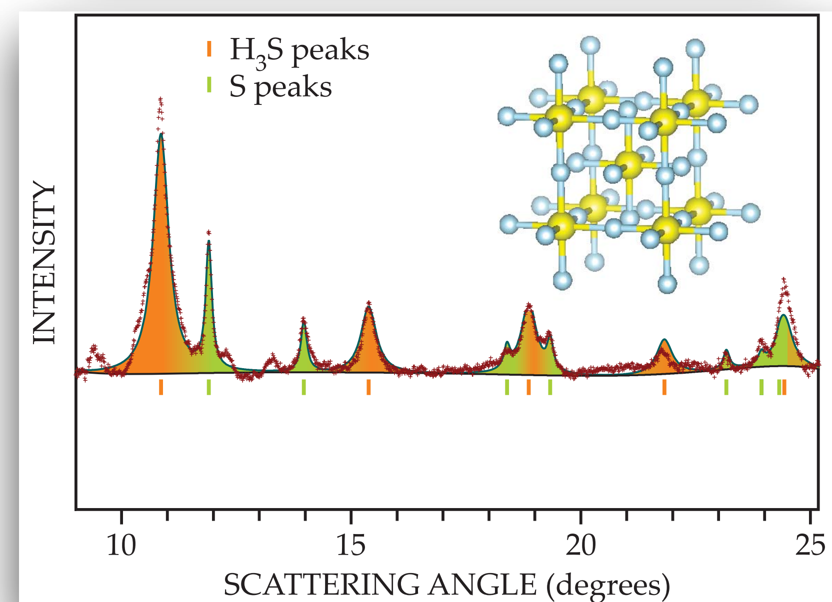

First-principles theories predict the **crystal structure** and

superconducting critical temperature as a function of the pressure

Room temperature superconductivity? It depends on where the room is.

Vostok base in Antarctica

In 1983 a temperature of -89.2 ^{0}C was registered

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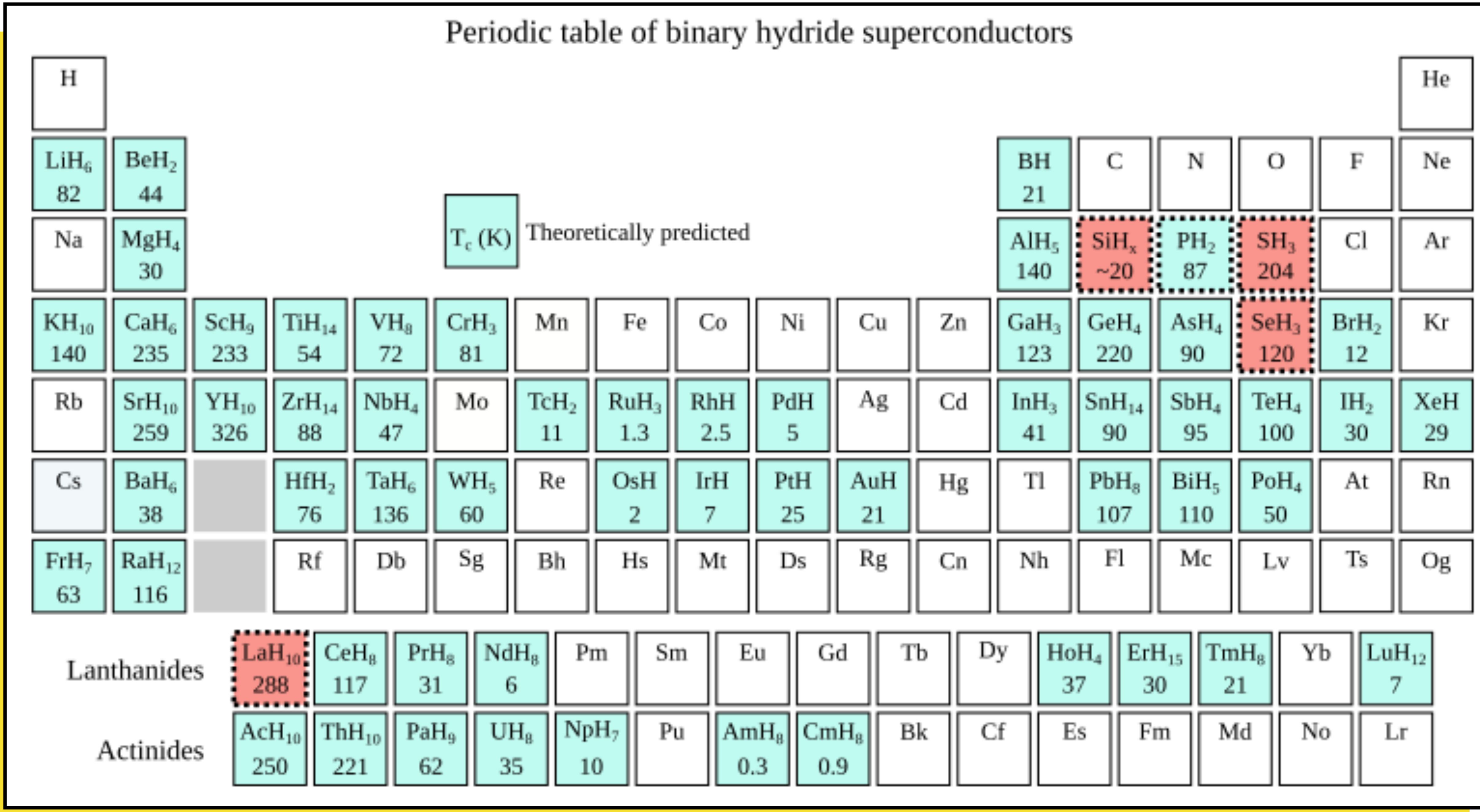
Flury of predictions

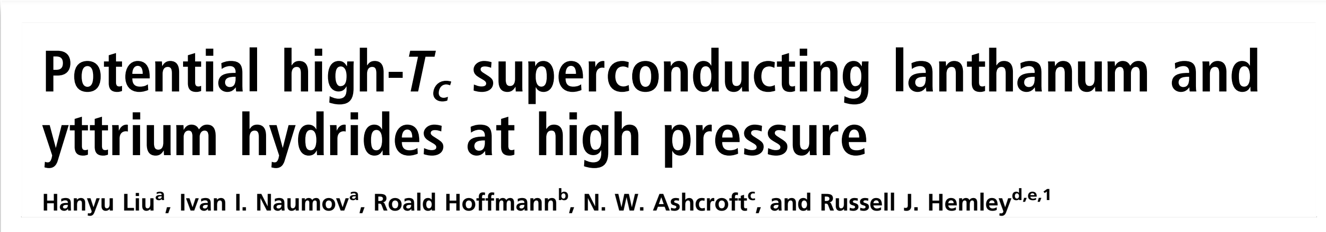


Periodic table of binary hydride superconductors

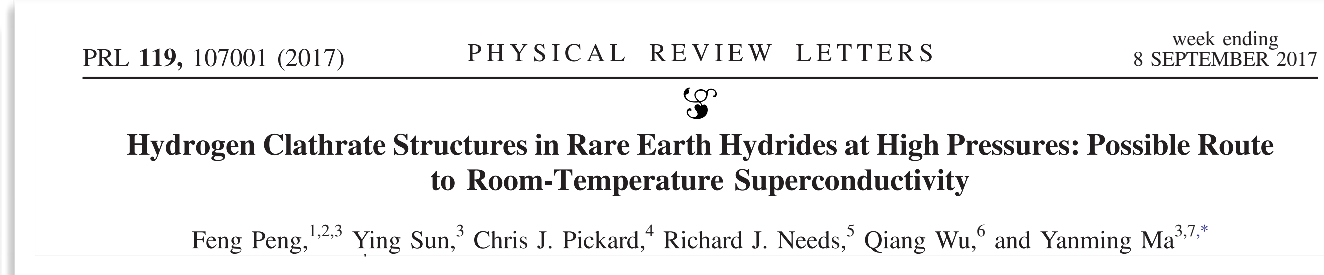
T_c (K) Theoretically predicted

H																	He
LiH_6 82	BeH_2 44											BH 21	C	N	O	F	Ne
Na	MgH_4 30											AlH_5 140	SiH_x ~20	PH_2 87	SH_3 204	Cl	Ar
KH_{10} 140	CaH_6 235	ScH_9 233	TiH_{14} 54	VH_8 72	CrH_3 81	Mn	Fe	Co	Ni	Cu	Zn	GaH_3 123	GeH_4 220	AsH_4 90	SeH_3 120	BrH_2 12	Kr
Rb	SrH_{10} 259	YH_{10} 326	ZrH_{14} 88	NbH_4 47	Mo	TcH_2 11	RuH_3 1.3	RhH 2.5	PdH 5	Ag	Cd	InH_3 41	SnH_{14} 90	SbH_4 95	TeH_4 100	IH_2 30	XeH 29
Cs	BaH_6 38		HfH_2 76	TaH_6 136	WH_5 60	Re	OsH 2	IrH 7	PtH 25	AuH 21	Hg	Tl	PbH_8 107	BiH_5 110	PoH_4 50	At	Rn
FrH_7 63	RaH_{12} 116		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og

Lanthanides	LaH_{10} 288	CeH_8 117	PrH_8 31	NdH_8 6	Pm	Sm	Eu	Gd	Tb	Dy	HoH_4 37	ErH_{15} 30	TmH_8 21	Yb	LuH_{12} 7
Actinides	AcH_{10} 250	ThH_{10} 221	PaH_9 62	UH_8 35	NpH_7 10	Pu	AmH_8 0.3	CmH_8 0.9	Bk	Cf	Es	Fm	Md	No	Lr


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

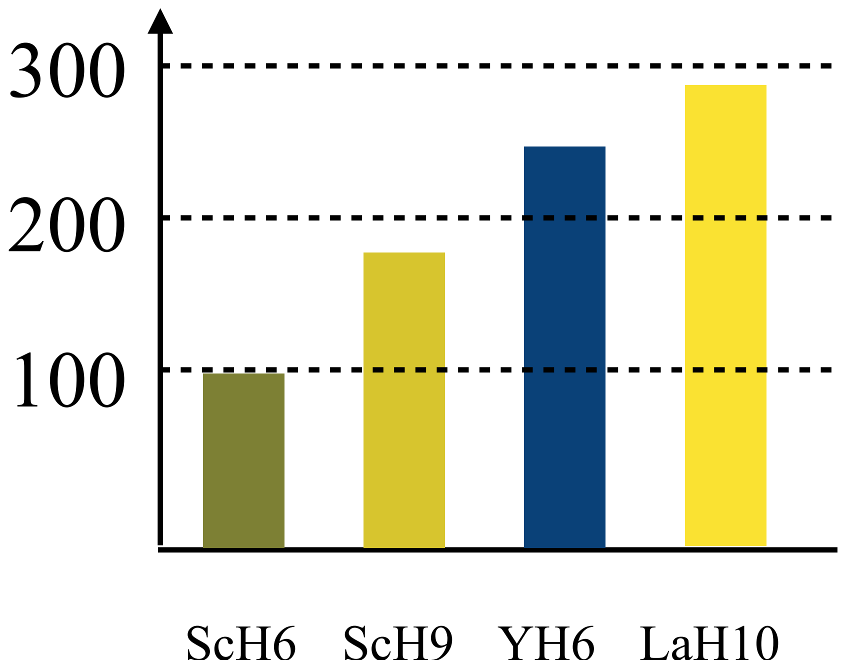
Hanyu Liu[a], Ivan I. Naumov[a], Roald Hoffmann[b], N. W. Ashcroft[c], and Russell J. Hemley[d,e,1]


PRL **119,** 107001 (2017) PHYSICAL REVIEW LETTERS week ending 8 SEPTEMBER 2017

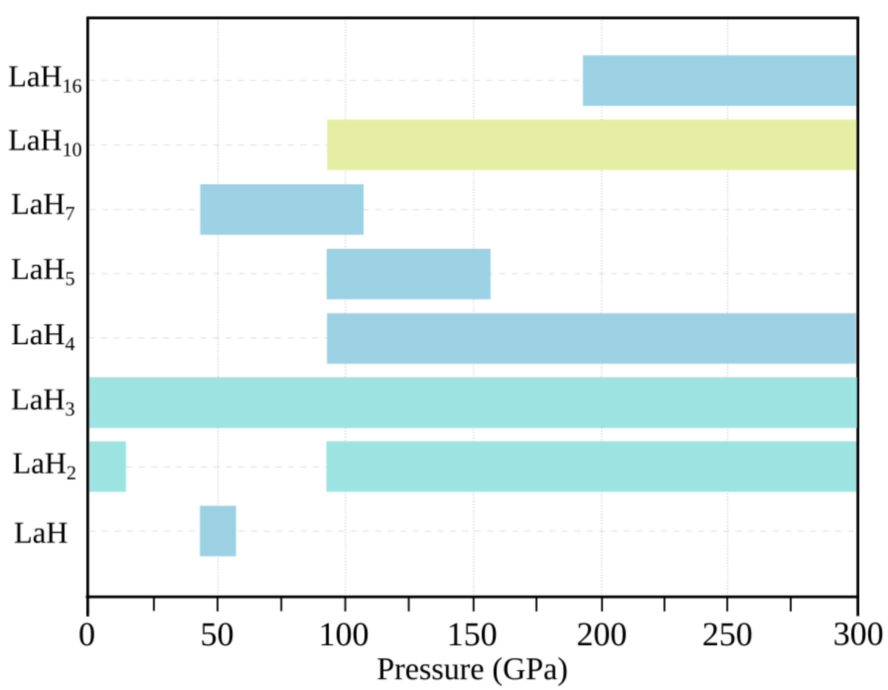
Hydrogen Clathrate Structures in Rare Earth Hydrides at High Pressures: Possible Route to Room-Temperature Superconductivity

Feng Peng,[1,2,3] Ying Sun,[3] Chris J. Pickard,[4] Richard J. Needs,[5] Qiang Wu,[6] and Yanming Ma[3,7,*]

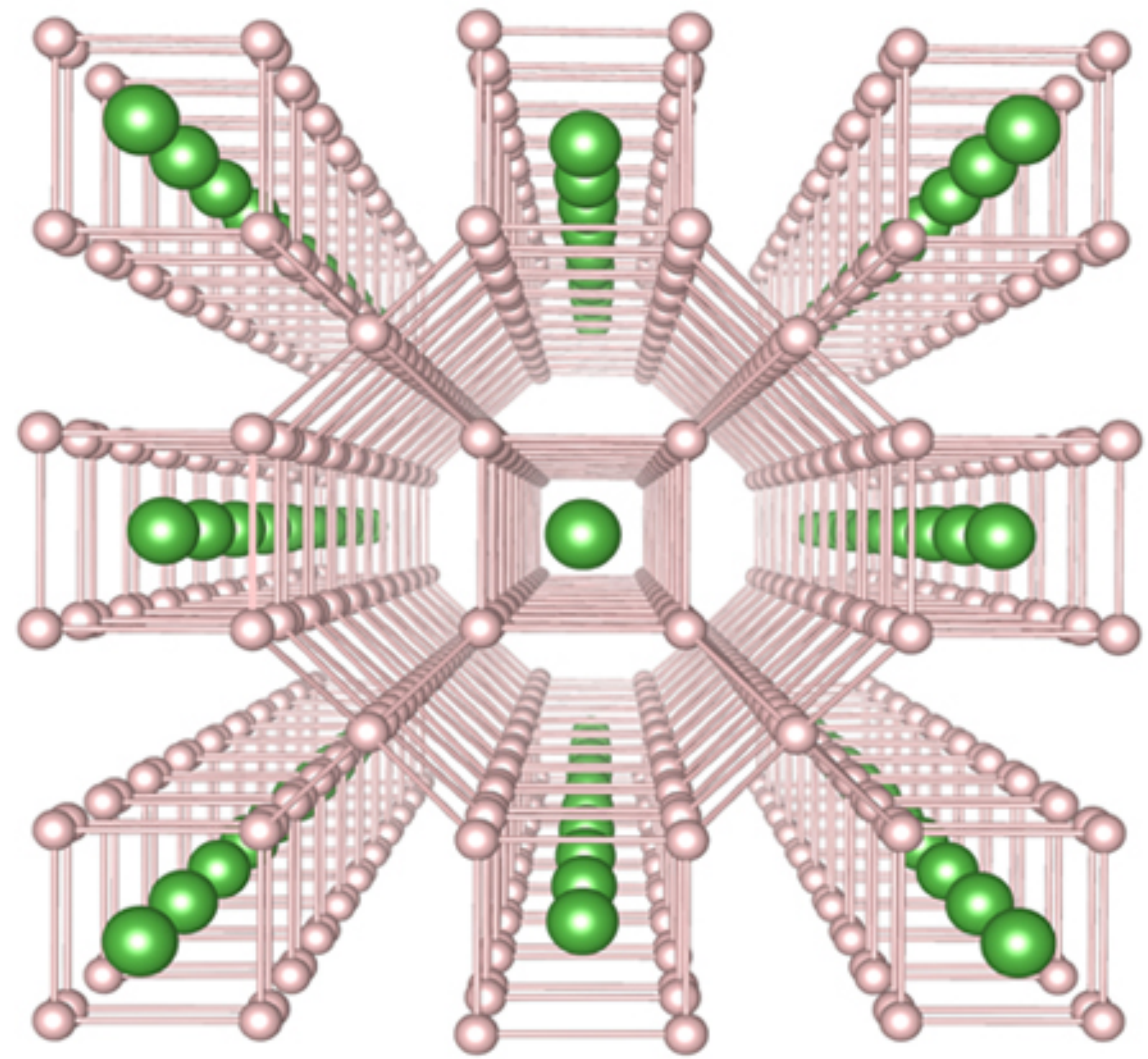
Tc=260 K



Stability range



LaH_{10}



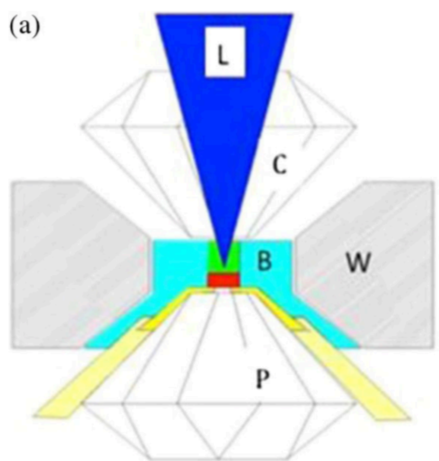
PHYSICAL REVIEW LETTERS **122,** 027001 (2019)

Editors' Suggestion Featured in Physics

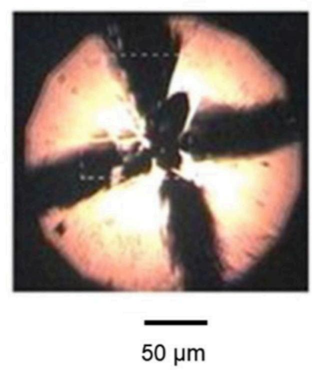
Evidence for Superconductivity above 260 K in Lanthanum Superhydride at Megabar Pressures

Maddury Somayazulu,[1,*] Muhtar Ahart,[1] Ajay K. Mishra,[2,‡] Zachary M. Geballe,[2] Maria Baldini,[2,§] Yue Meng,[3] Viktor V. Struzhkin,[2] and Russell J. Hemley[1,†]

(a)



(b)



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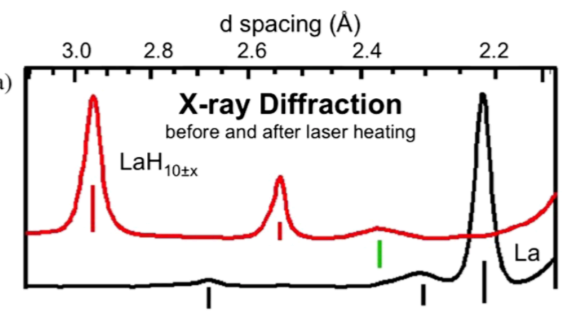

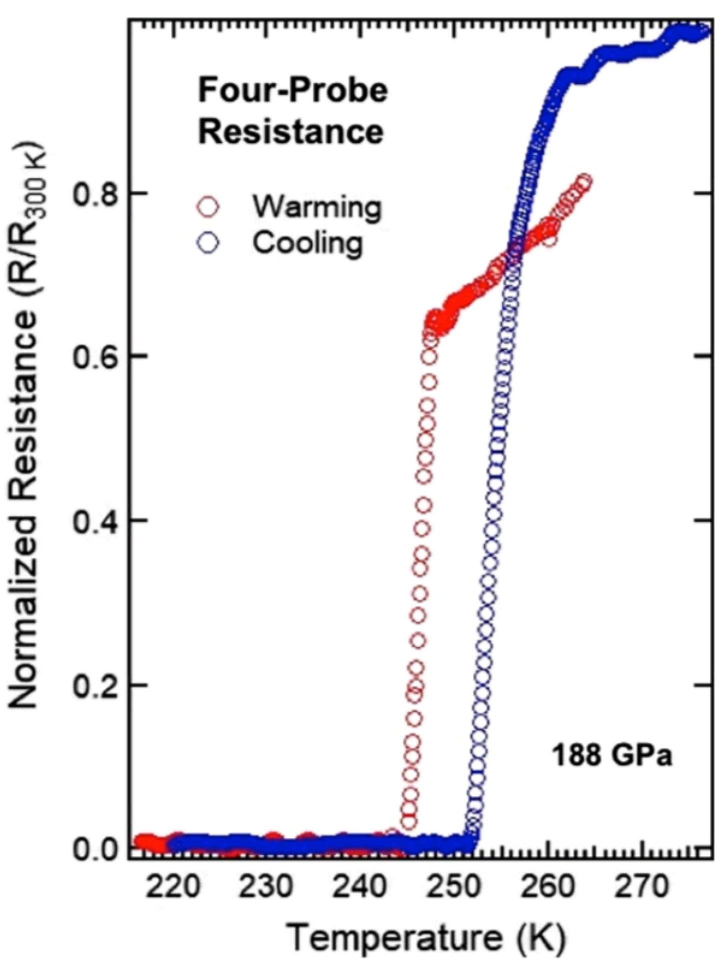

PHYSICAL REVIEW LETTERS **122,** 027001 (2019)

Editors' Suggestion   Featured in Physics

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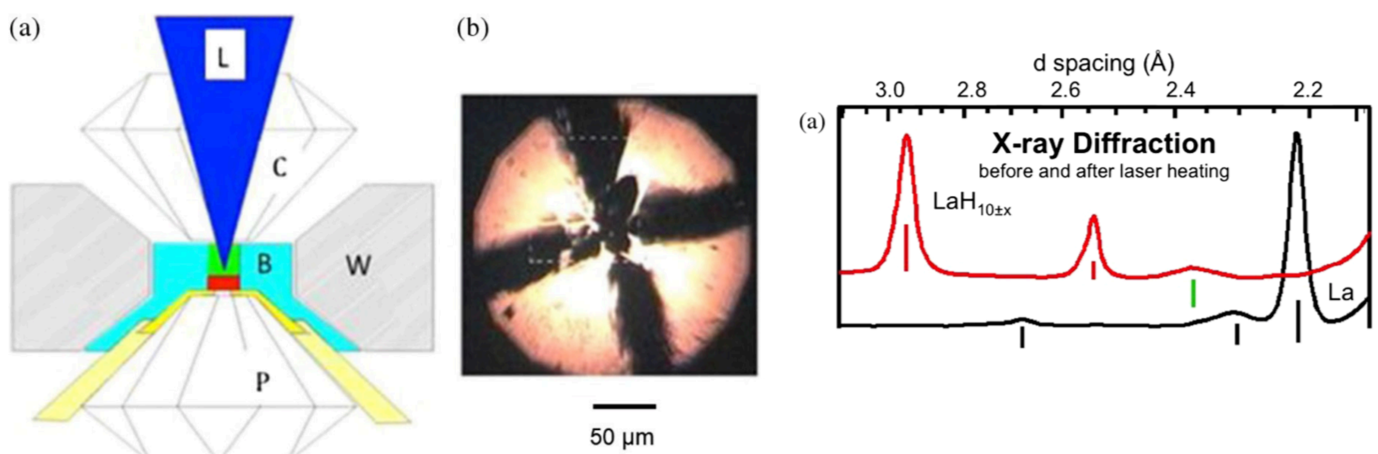
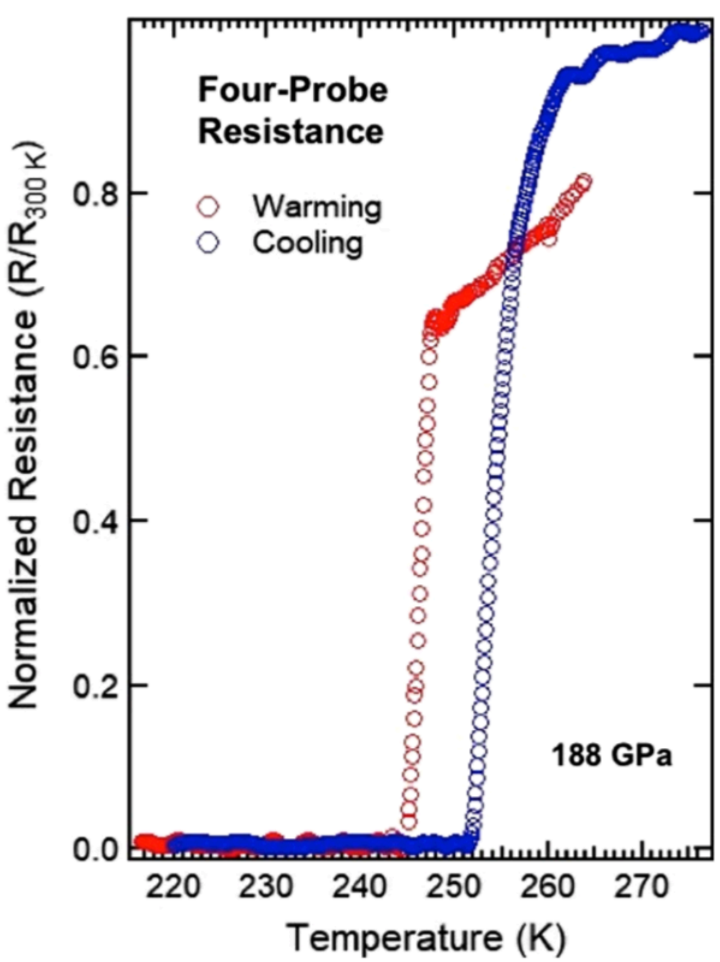
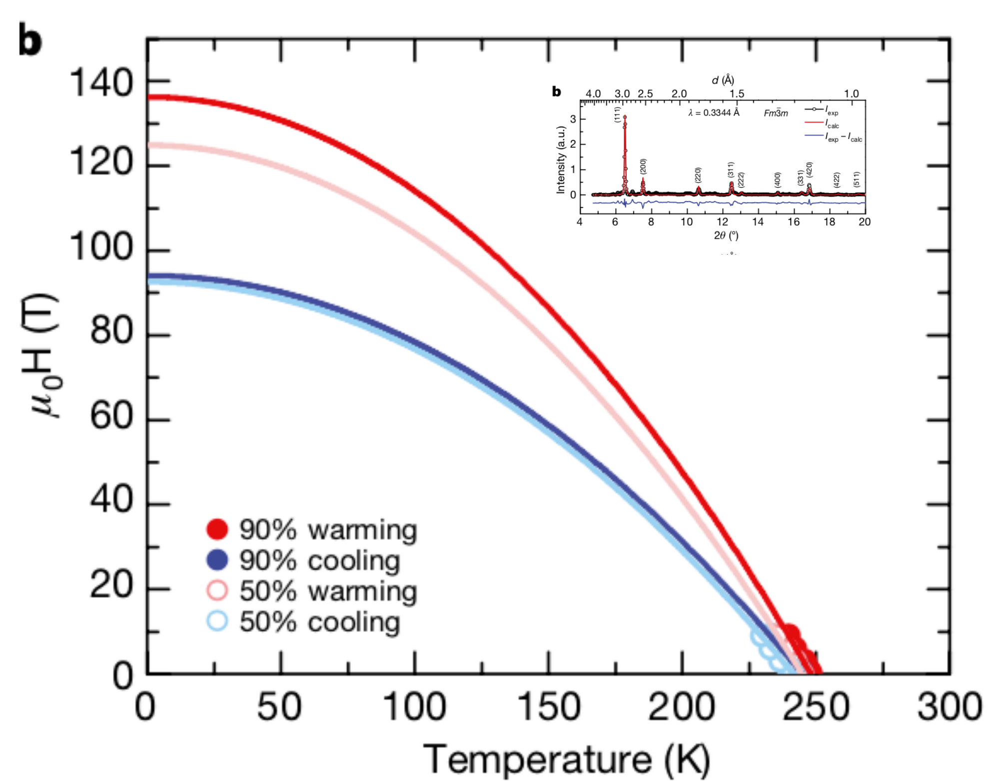




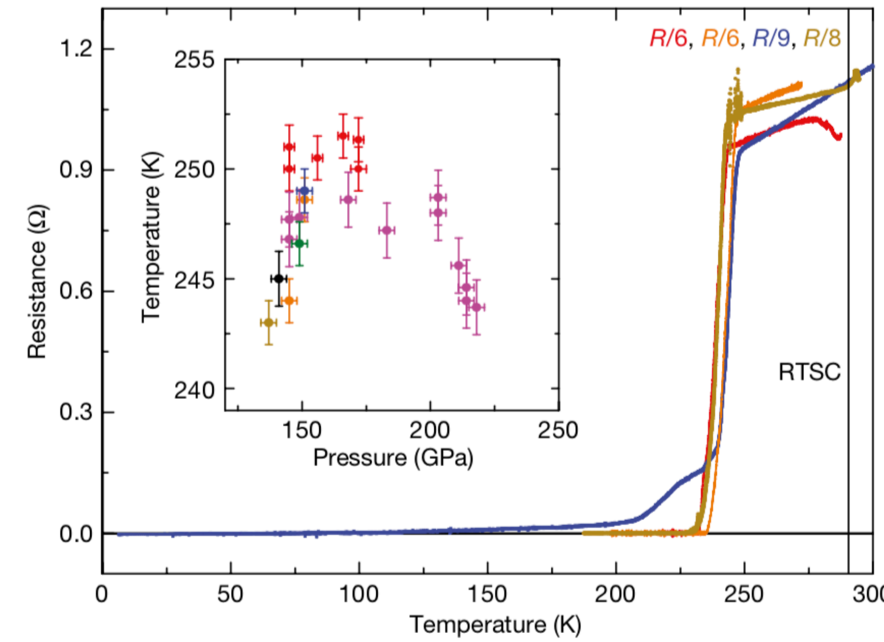


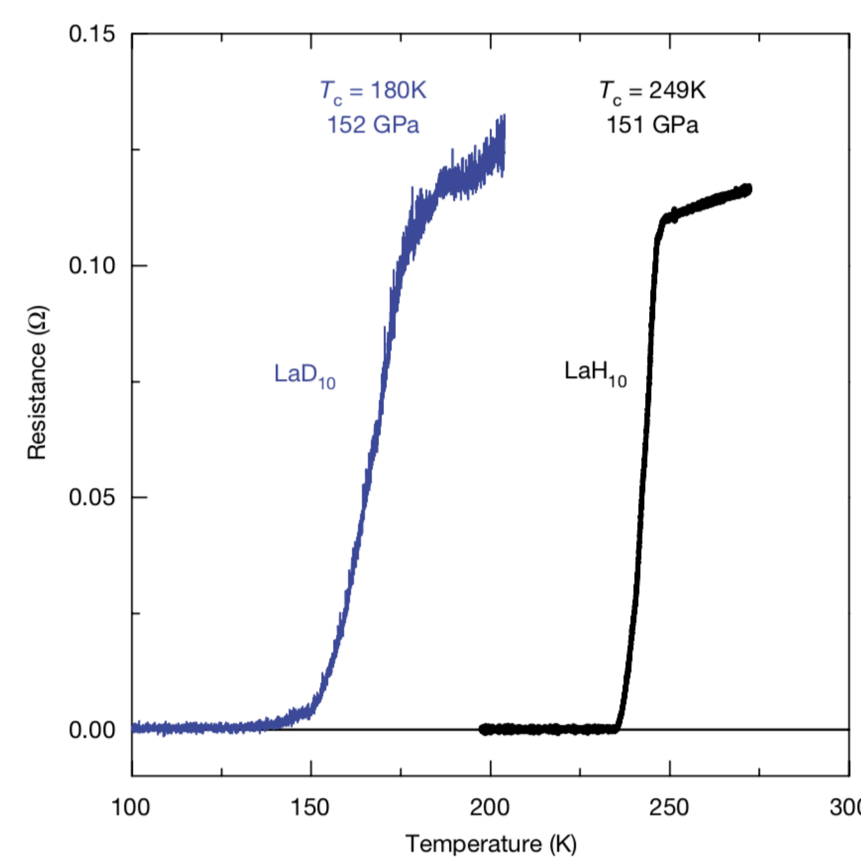
LETTER

https://doi.org/10.1038/s41586-019-1201-8

Superconductivity at 250 K in lanthanum hydride under high pressures

A. P. Drozdov[1,7], P. P. Kong[1,7], V. S. Minkov[1,7], S. P. Besedin[1,7], M. A. Kuzovnikov[1,6,7], S. Mozaffari[2], L. Balicas[2], F. F. Balakirev[3], D. E. Graf[2], V. B. Prakapenka[4], E. Greenberg[4], D. A. Knyazev[1], M. Tkacz[5] & M. I. Eremets[1]*





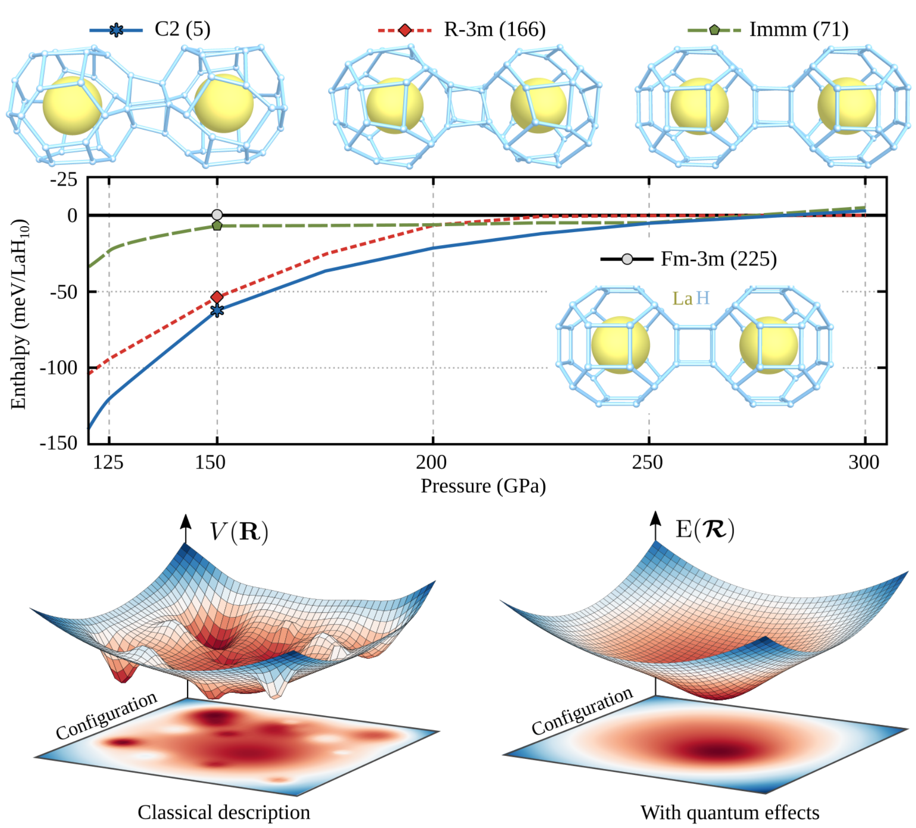
Article

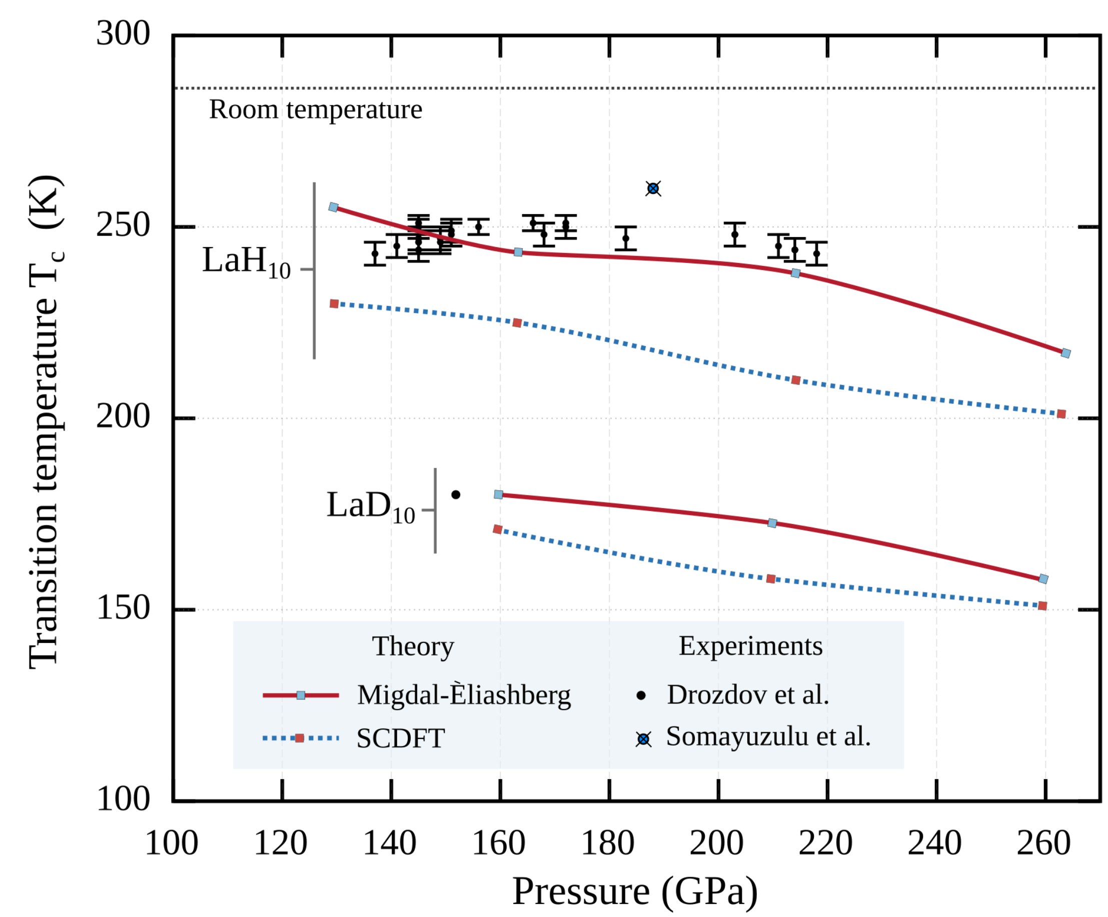
Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride

https://doi.org/10.1038/s41586-020-1955-z
Received: 24 July 2019
Accepted: 14 November 2019
Published online: 5 February 2020

Ion Errea[1,2,3], Francesco Belli[1,2], Lorenzo Monacelli[4], Antonio Sanna[5], Takashi Koretsune[6], Terumasa Tadano[7], Raffaello Bianco[2], Matteo Calandra[8], Ryotaro Arita[9,10], Francesco Mauri[4,11] & José A. Flores-Livas[4]*

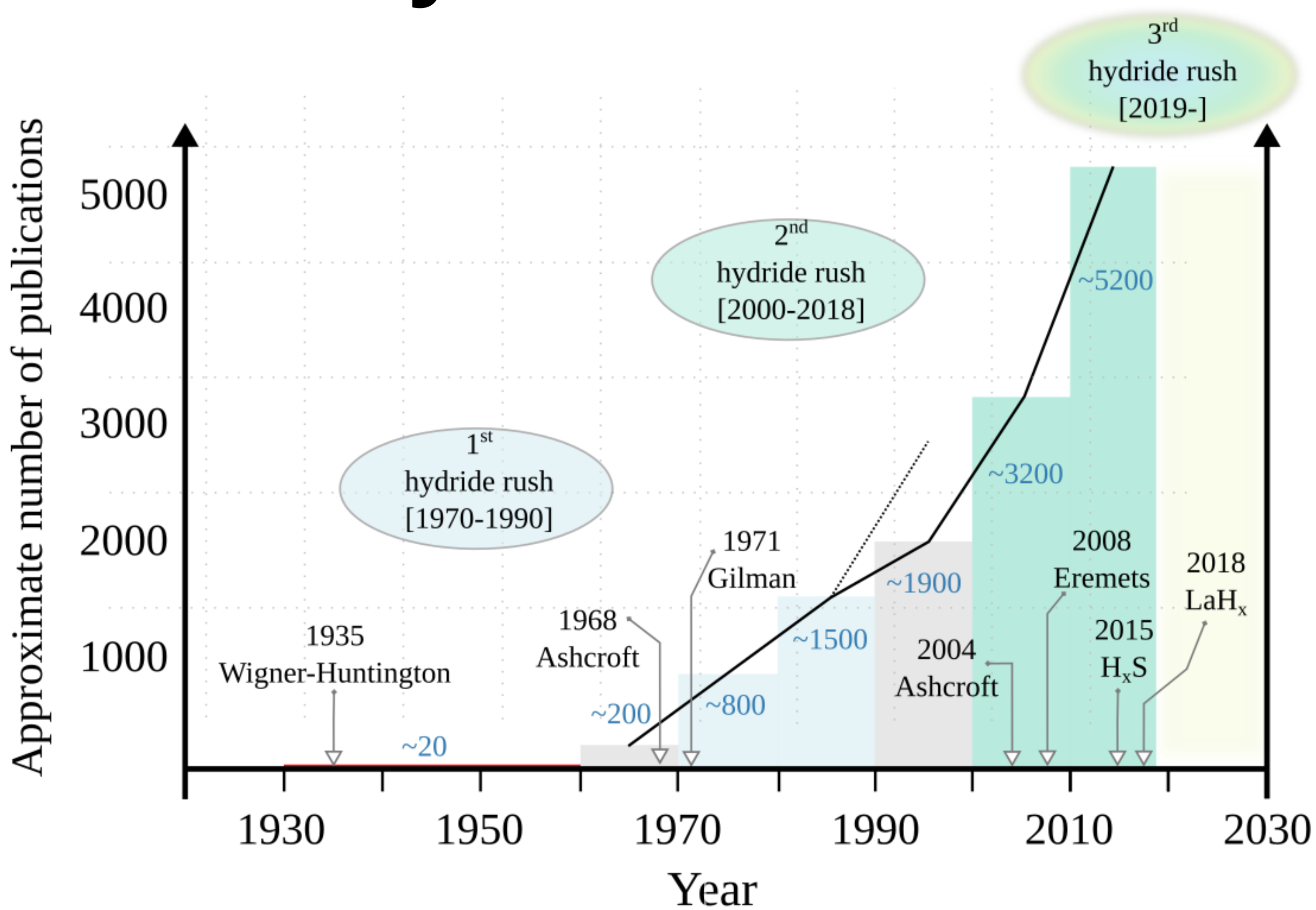
The discovery of superconductivity at 200 kelvin in the hydrogen sulfide system at high pressures[1] demonstrated the potential of hydrogen-rich materials as high-temperature superconductors. Recent theoretical predictions of rare-earth hydrides with hydrogen cages[2,3] and the subsequent synthesis of LaH_{10} with a superconducting critical temperature (T_c) of 250 kelvin[4,5] have placed these materials on the verge of achieving the long-standing goal of room-temperature superconductivity. Electrical and X-ray diffraction measurements have revealed a weakly pressure-dependent T_c for LaH_{10} between 137 and 218 gigapascals in a structure that has a face-centred cubic arrangement of lanthanum atoms[5]. Here we show that quantum atomic fluctuations stabilize a highly symmetrical $Fm\bar{3}m$ crystal structure over this pressure range. The

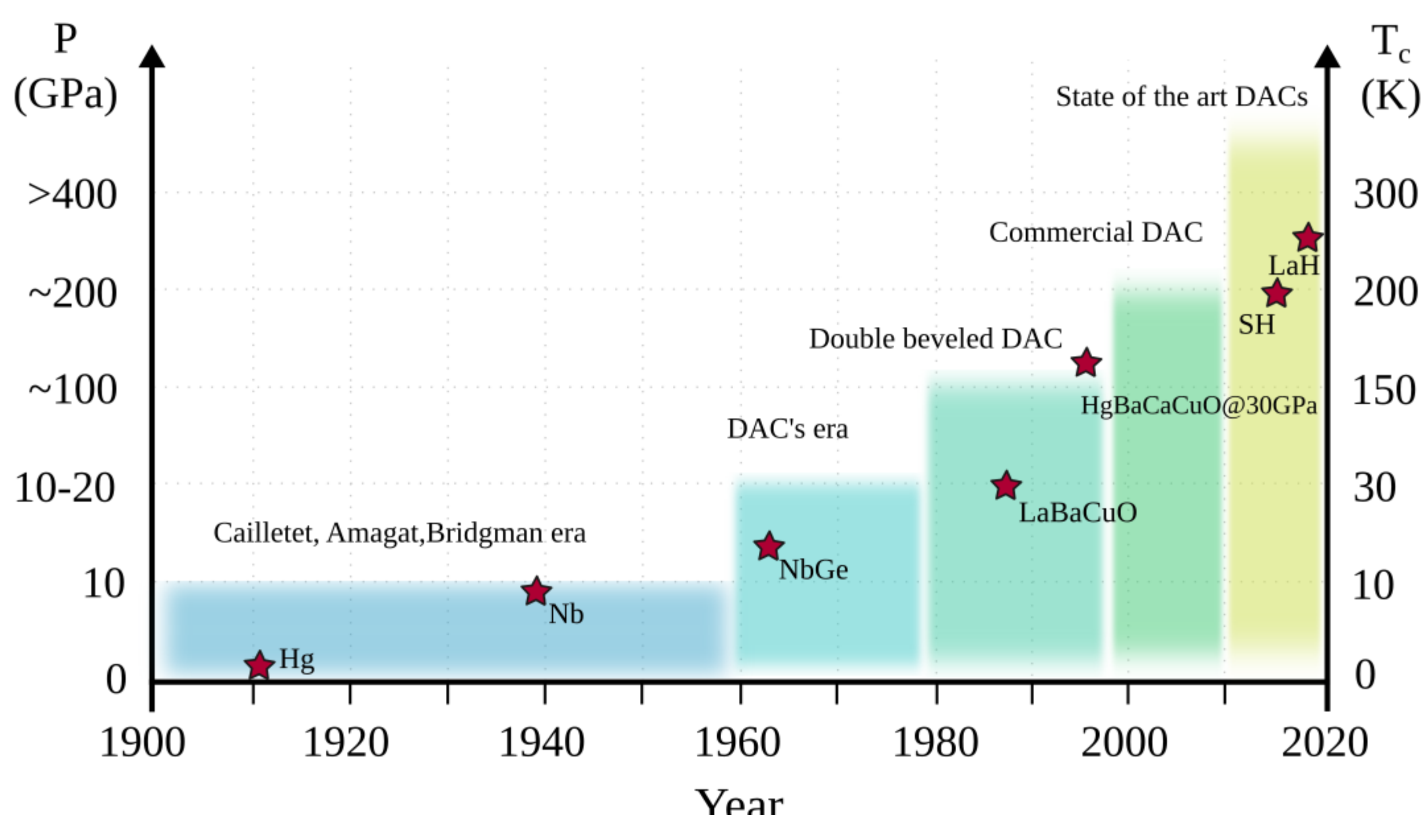




Room temperature superconductivity

Hydride revolution





Better call….

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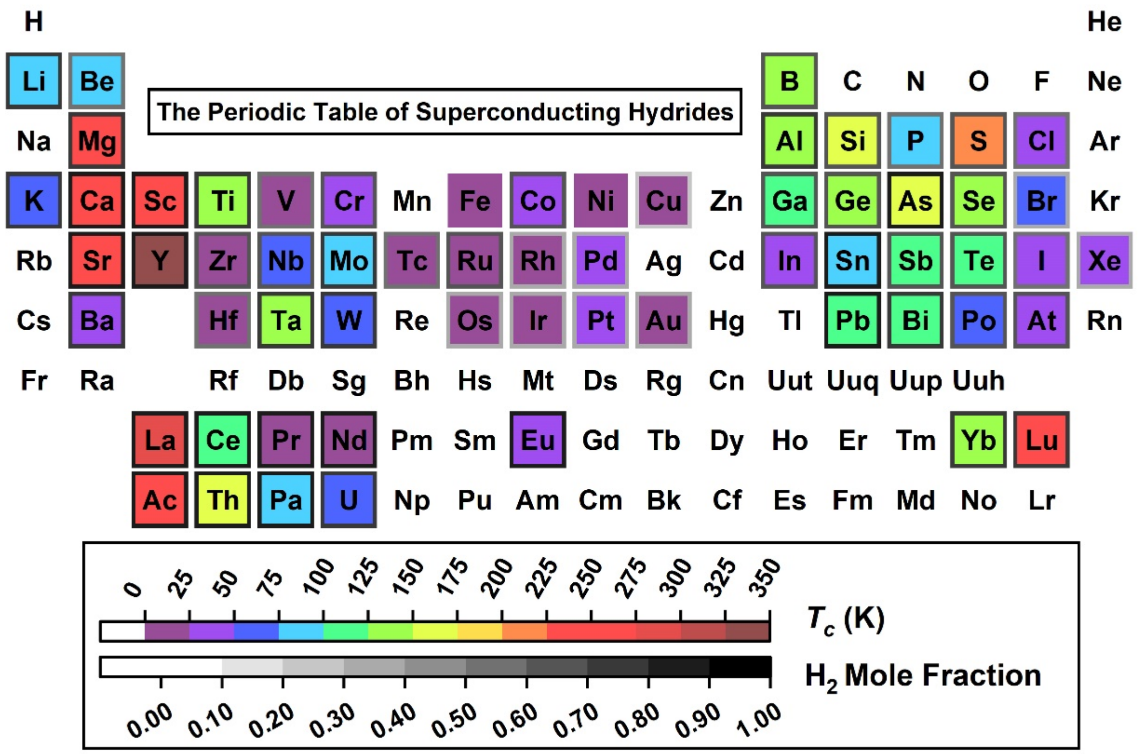
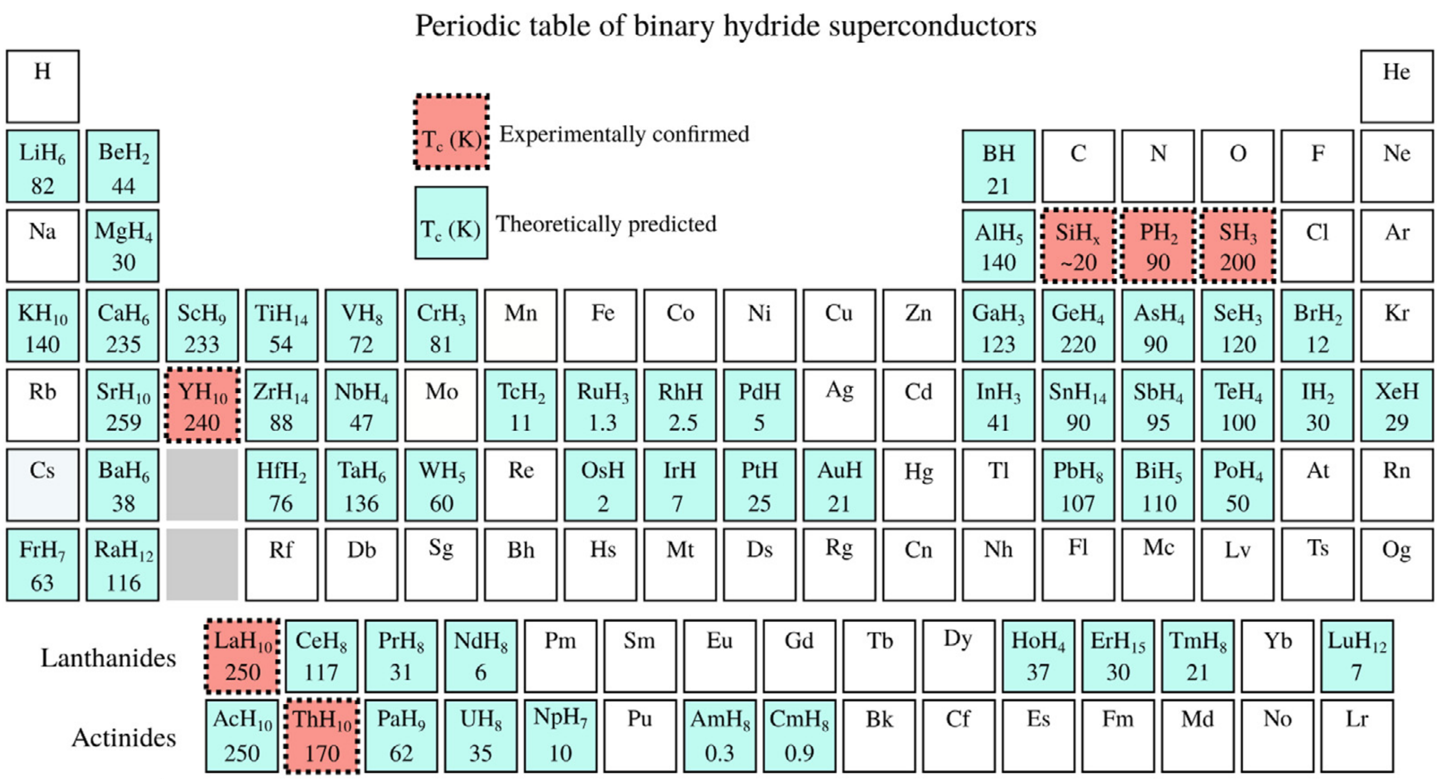
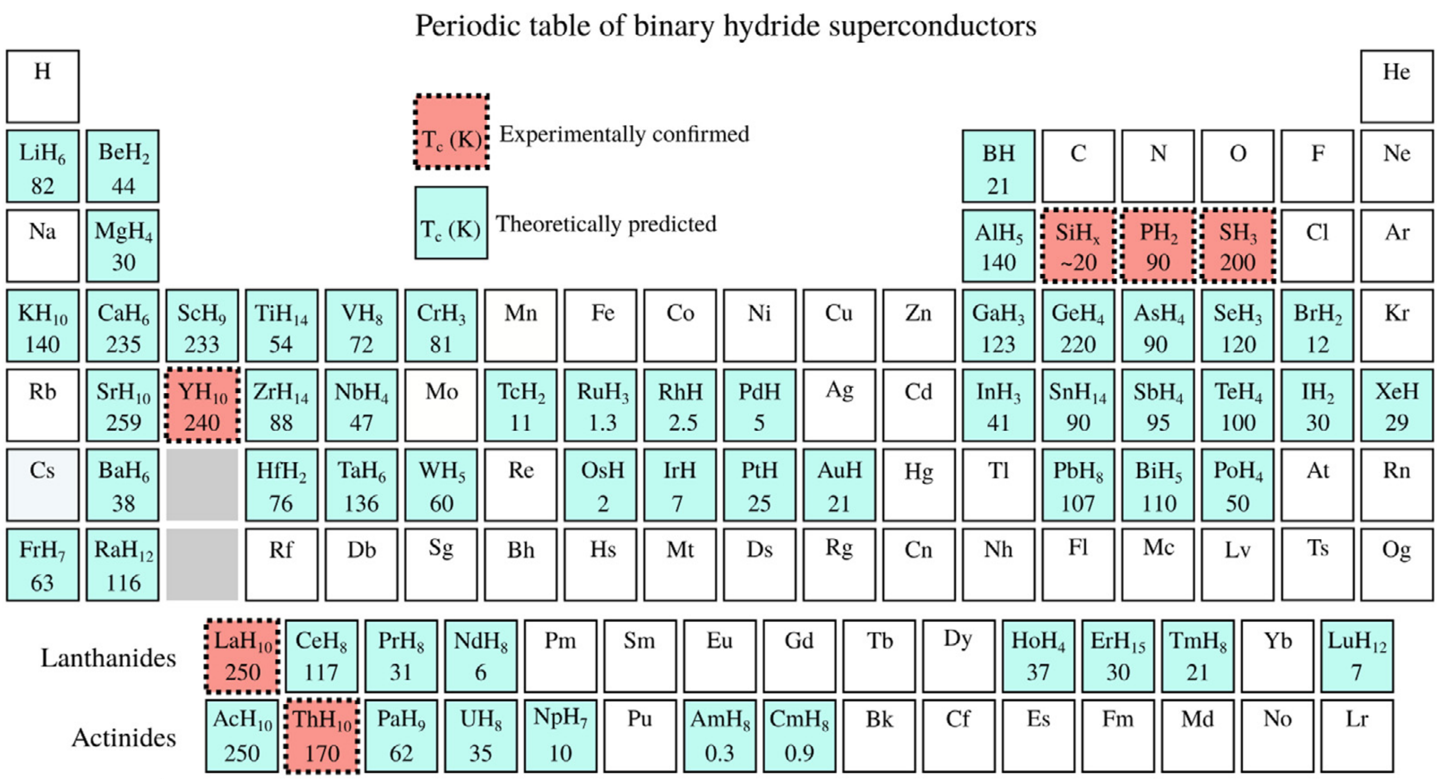

The Periodic Table of Superconducting Hydrides
H He
Li Be B C N O F Ne
Na Mg Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra Rf Db Sg Bh Hs Mt Ds Rg Cn Uut Uuq Uup Uuh
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr
0 25 50 75 100 125 150 175 200 225 250 275 300 325 350
T_c (K)
H_2 Mole Fraction
0.00 0.10 0.20 0.30 0.40 0.50 0.60 0.70 0.80 0.90 1.00

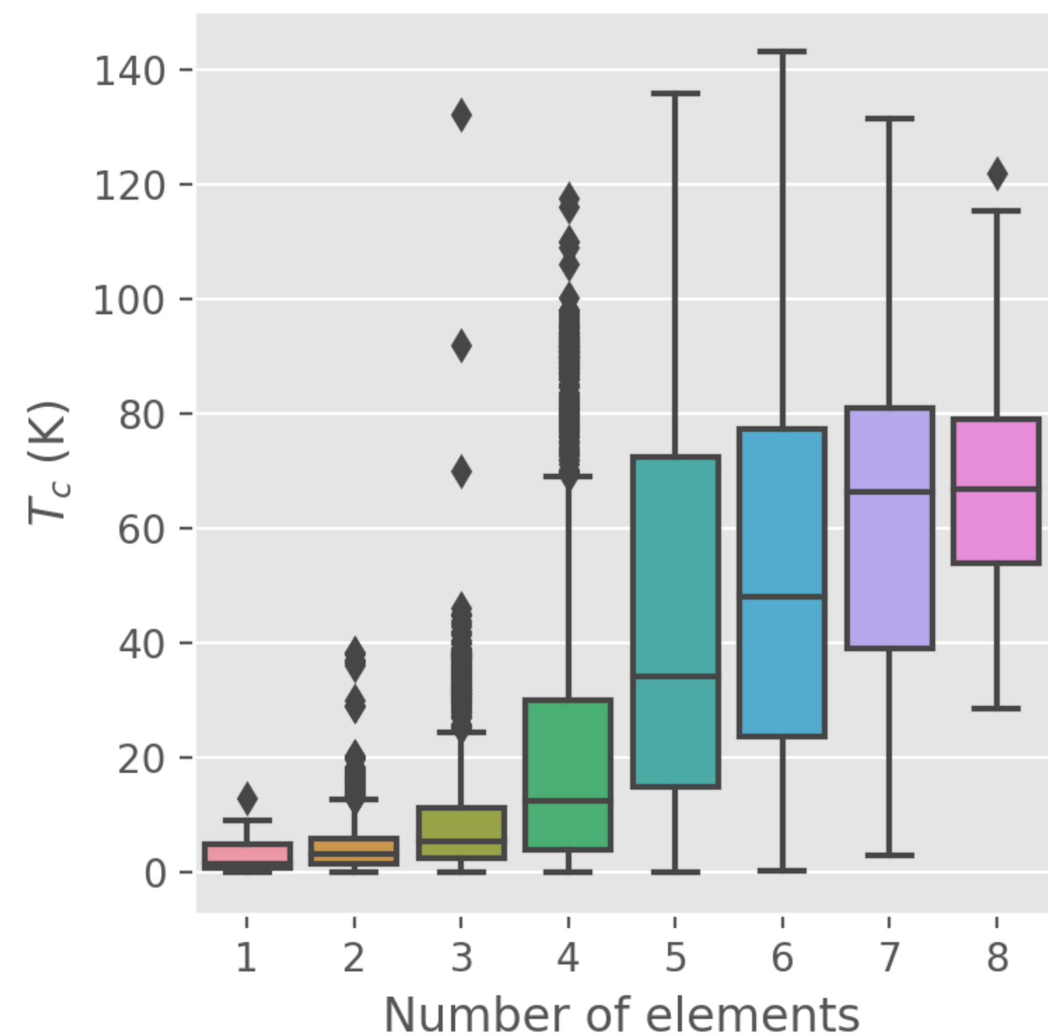
Better call....


Periodic table of binary hydride superconductors
T_c (K) Experimentally confirmed
T_c (K) Theoretically predicted
H
He
LiH_6 82
BeH_2 44
BH 21
C
N
O
F
Ne
Na
MgH_4 30
AlH_5 140
SiH_x ~20
PH_2 90
SH_3 200
Cl
Ar
KH_{10} 140
CaH_6 235
ScH_9 233
TiH_{14} 54
VH_8 72
CrH_3 81
Mn
Fe
Co
Ni
Cu
Zn
GaH_3 123
GeH_4 220
AsH_4 90
SeH_3 120
BrH_2 12
Kr
Rb
SrH_{10} 259
YH_{10} 240
ZrH_{14} 88
NbH_4 47
Mo
TcH_2 11
RuH_3 1.3
RhH 2.5
PdH 5
Ag
Cd
InH_3 41
SnH_{14} 90
SbH_4 95
TeH_4 100
IH_2 30
XeH 29
Cs
BaH_6 38
HfH_2 76
TaH_6 136
WH_5 60
Re
OsH 2
IrH 7
PtH 25
AuH 21
Hg
Tl
PbH_8 107
BiH_5 110
PoH_4 50
At
Rn
FrH_7 63
RaH_{12} 116
Rf
Db
Sg
Bh
Hs
Mt
Ds
Rg
Cn
Nh
Fl
Mc
Lv
Ts
Og
Lanthanides
LaH_{10} 250
CeH_8 117
PrH_8 31
NdH_8 6
Pm
Sm
Eu
Gd
Tb
Dy
HoH_4 37
ErH_{15} 30
TmH_8 21
Yb
LuH_{12} 7
Actinides
AcH_{10} 250
ThH_{10} 170
PaH_9 62
UH_8 35
NpH_7 10
Pu
AmH_8 0.3
CmH_8 0.9
Bk
Cf
Es
Fm
Md
No
Lr

Better call....



Another actor: AI



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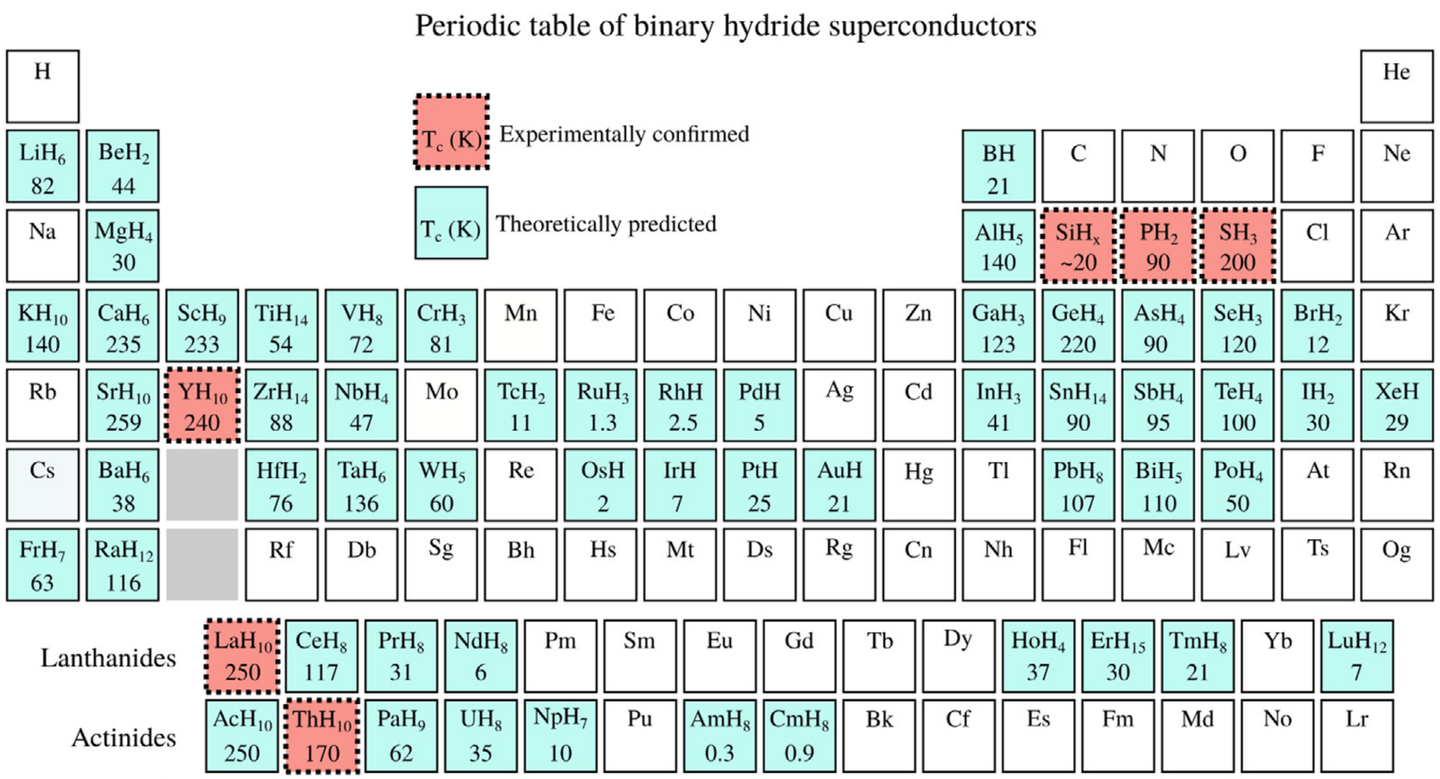

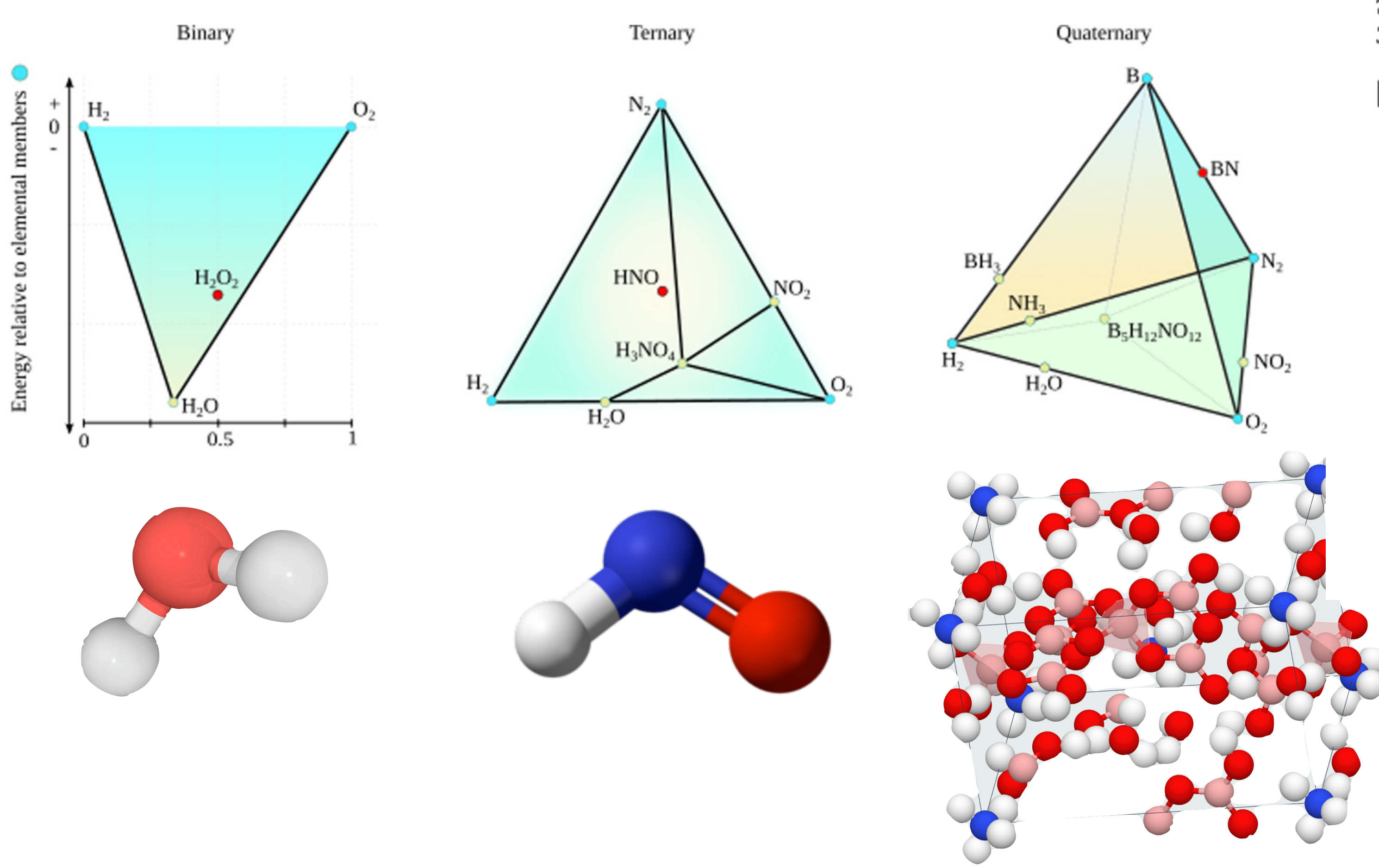

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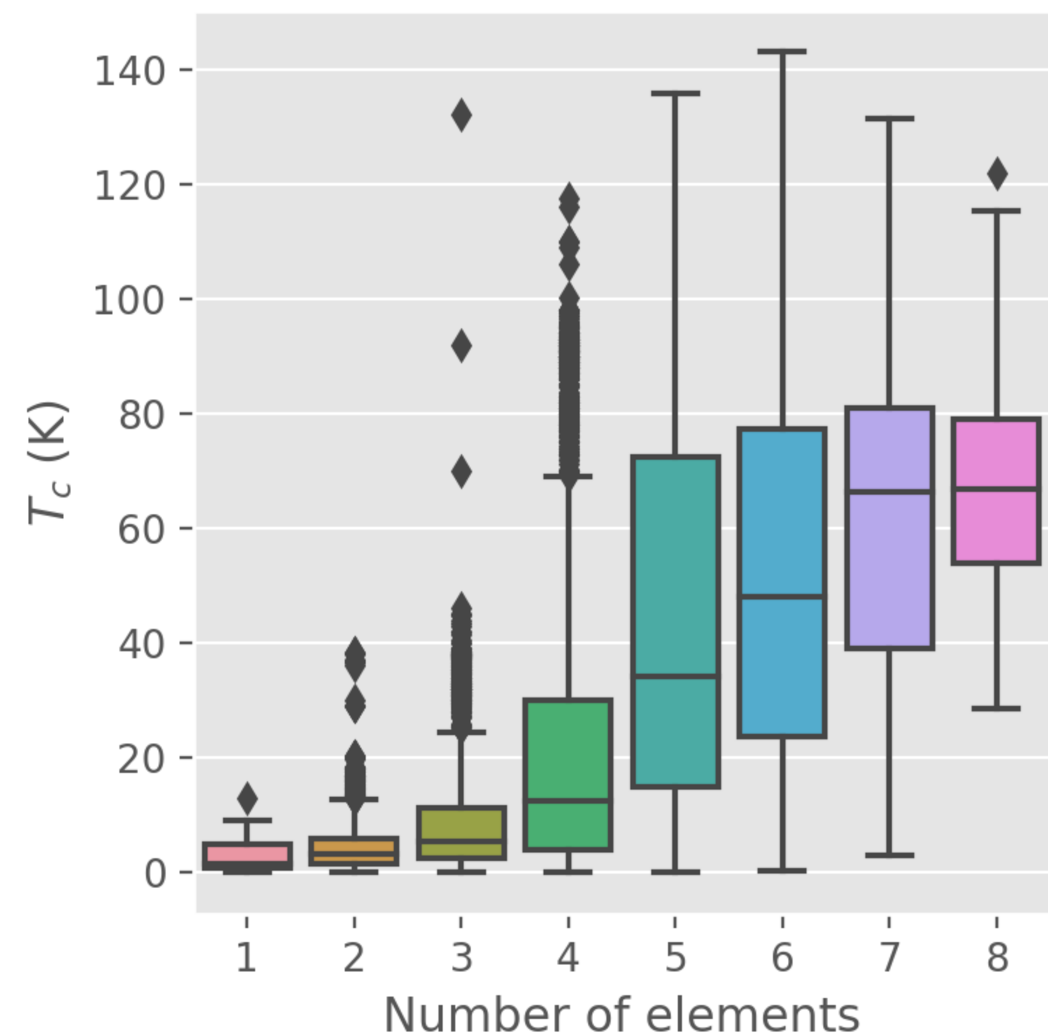


Article

Room-temperature superconductivity in a carbonaceous sulfur hydride

https://doi.org/10.1038/s41586-020-2801-z

Received: 21 July 2020

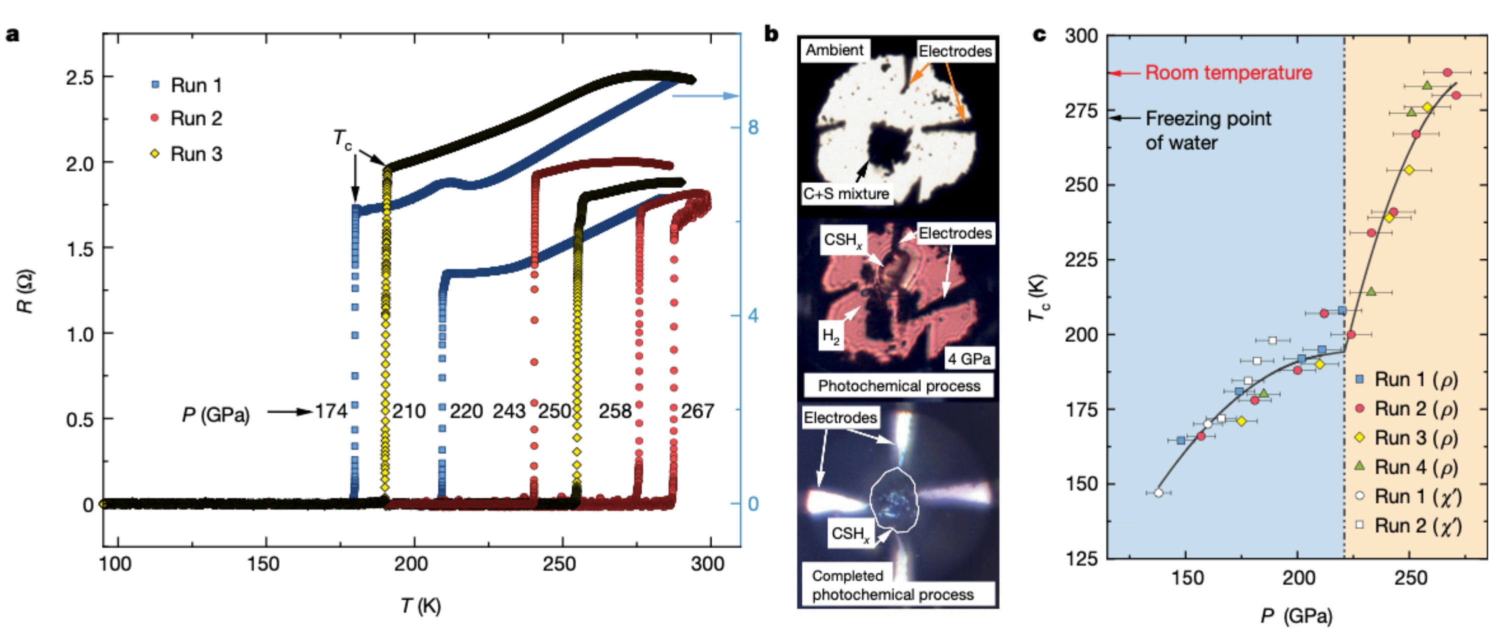
Accepted: 8 September 2020

Published online: 14 October 2020

Check for updates

Elliot Snider[1,6], Nathan Dasenbrock-Gammon[2,6], Raymond McBride[1,6], Mathew Debessai[3], Hiranya Vindana[2], Kevin Vencatasamy[2], Keith V. Lawler[4], Ashkan Salamat[5] & Ranga P. Dias[1,2]✉

One of the long-standing challenges in experimental physics is the observation of room-temperature superconductivity[1,2]. Recently, high-temperature conventional superconductivity in hydrogen-rich materials has been reported in several systems under high pressure[3–5]. An important discovery leading to room-temperature superconductivity is the pressure-driven disproportionation of hydrogen sulfide (H_2S) to H_3S, with a confirmed transition temperature of 203 kelvin at 155 gigapascals[3,6]. Both H_2S and CH_4 readily mix with hydrogen to form guest–host structures at lower pressures[7], and are of comparable size at 4 gigapascals. By introducing methane at low pressures into the $H_2S + H_2$ precursor mixture for H_3S, molecular exchange is allowed within a large assemblage of van der Waals solids that are hydrogen-rich with H_2 inclusions; these guest–host structures become the building blocks of superconducting compounds at extreme conditions. Here we report superconductivity in a photochemically transformed carbonaceous sulfur hydride system, starting from elemental precursors, with a maximum superconducting transition temperature of 287.7 ± 1.2 kelvin (about 15 degrees Celsius) achieved at 267 ± 10 gigapascals. The superconducting state is observed over a broad pressure range in the diamond anvil cell, from 140 to 275 gigapascals, with a sharp upturn in transition temperature above 220 gigapascals. Superconductivity is established by the observation of zero resistance, a magnetic susceptibility of up to 190 gigapascals, and reduction of the transition temperature under an external magnetic field of up to 9 tesla, with an upper critical magnetic field of about 62 tesla according to the Ginzburg–Landau model at zero temperature. The light, quantum nature of hydrogen limits the structural and stoichiometric determination of the system by X-ray scattering techniques, but Raman spectroscopy is used to probe the chemical and structural transformations before metallization. The introduction of chemical tuning within our ternary system could enable the preservation of the properties of room-temperature superconductivity at lower pressures.



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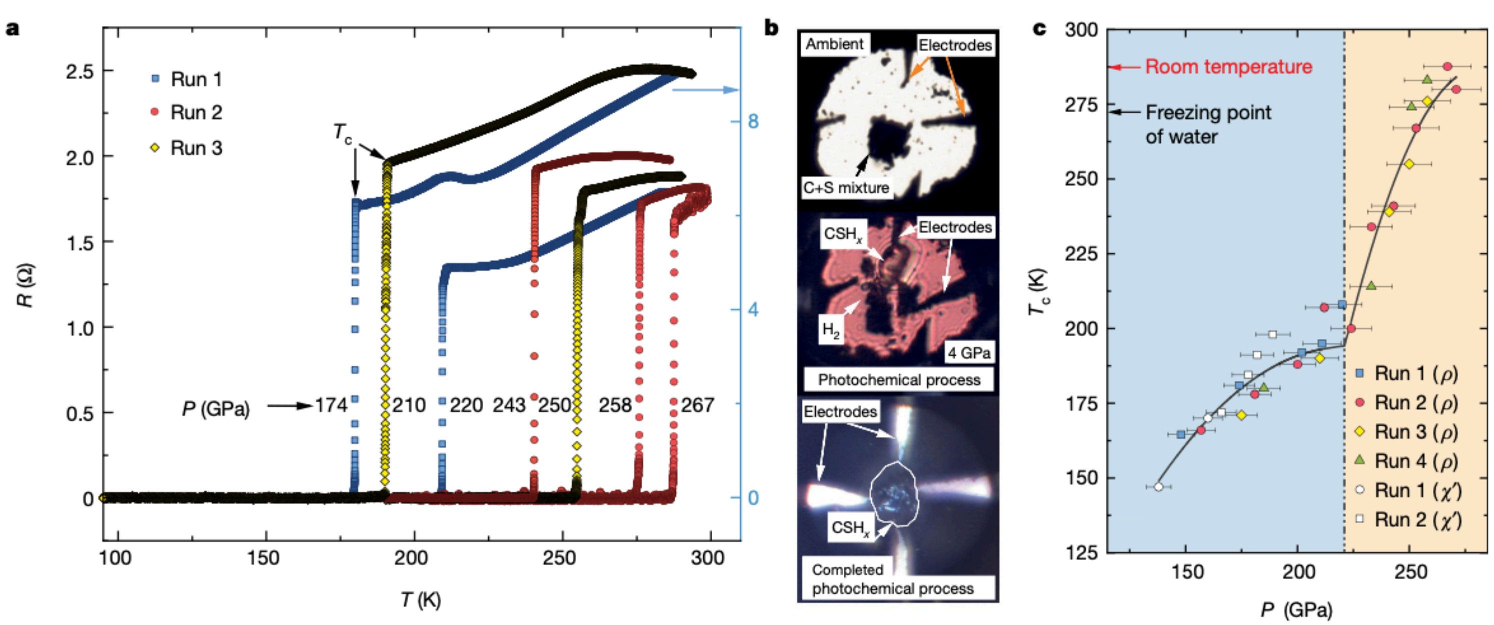

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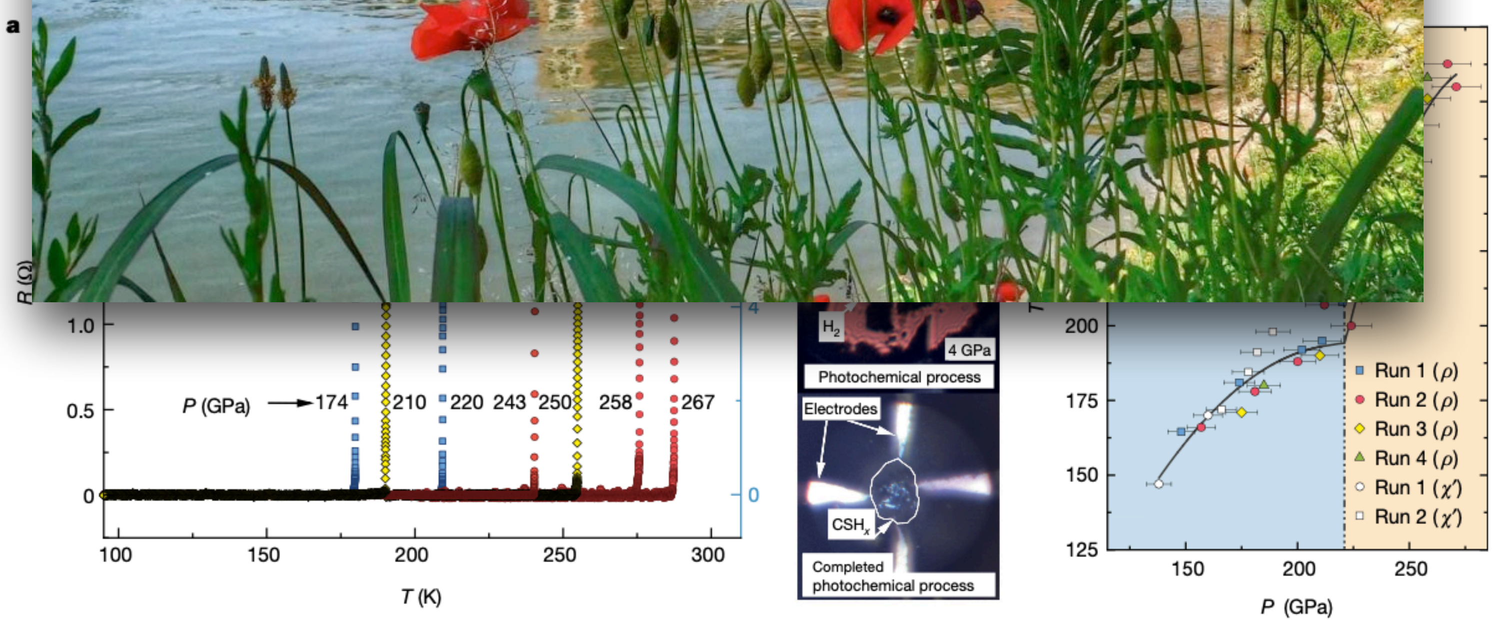
One of the long-standing challenges in experimental physics is the observation of room-temperature superconductivity[1,2]. Recently, high-temperature conventional superconductivity in hydrogen-rich materials has been reported in several systems under high pressure[3–5]. An important discovery leading to room-temperature superconductivity is the pressure-driven disproportionation of hydrogen sulfide (H_2S) to H_3S, with a confirmed transition temperature of 203 kelvin at 155



Article

Room-temperature superconductivity in a carbonaceous sulfur hydride

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Check for updates

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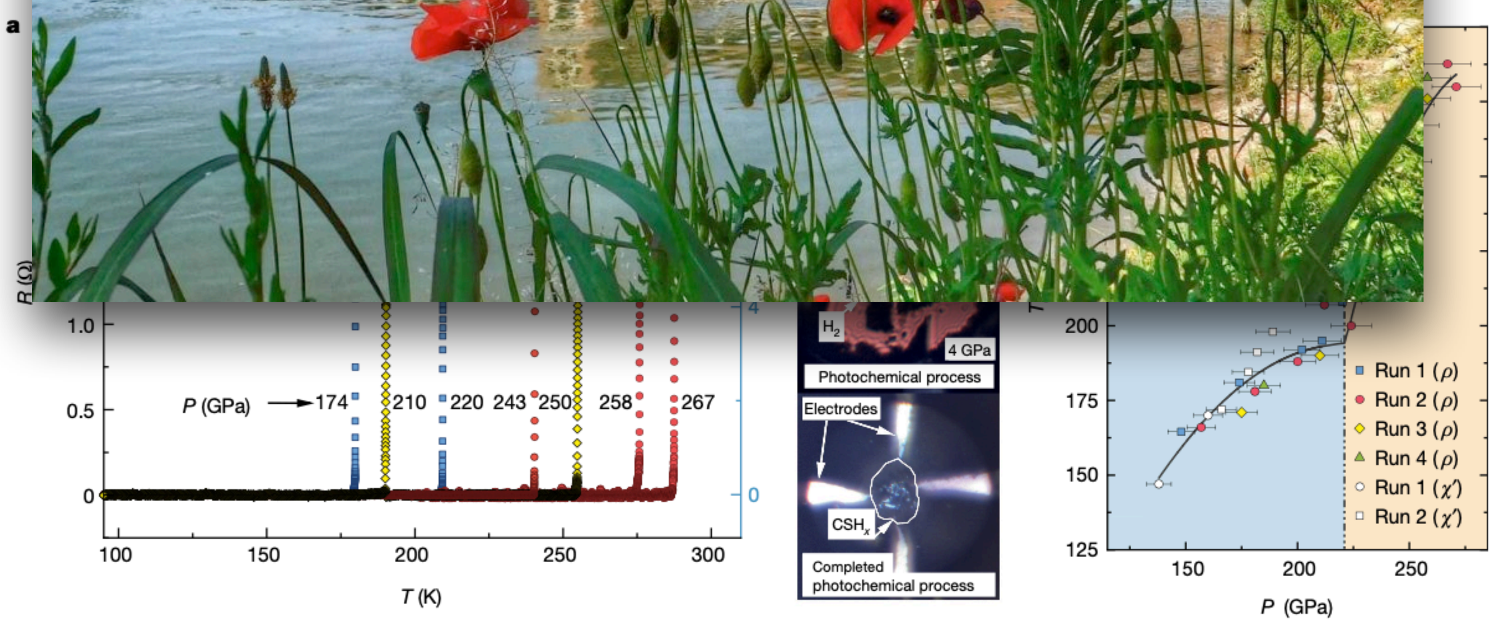
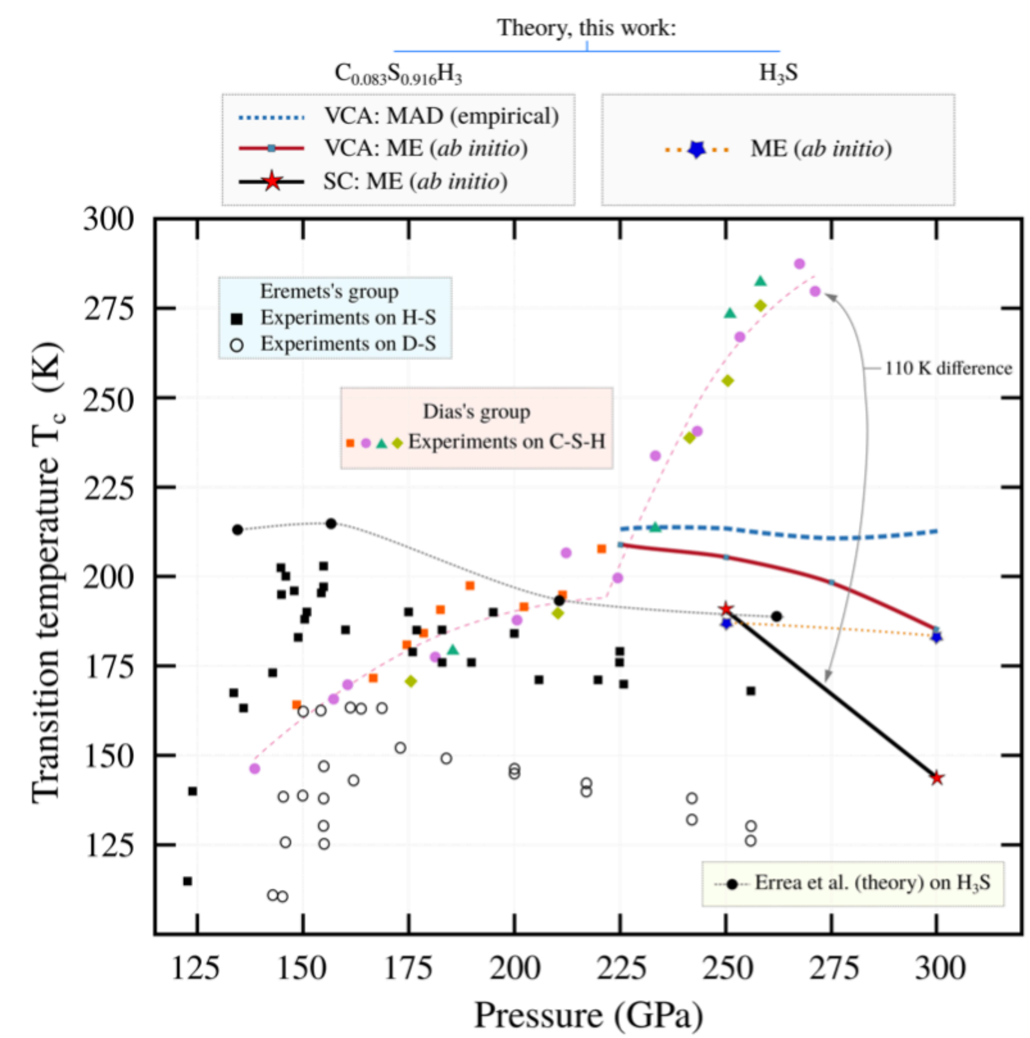


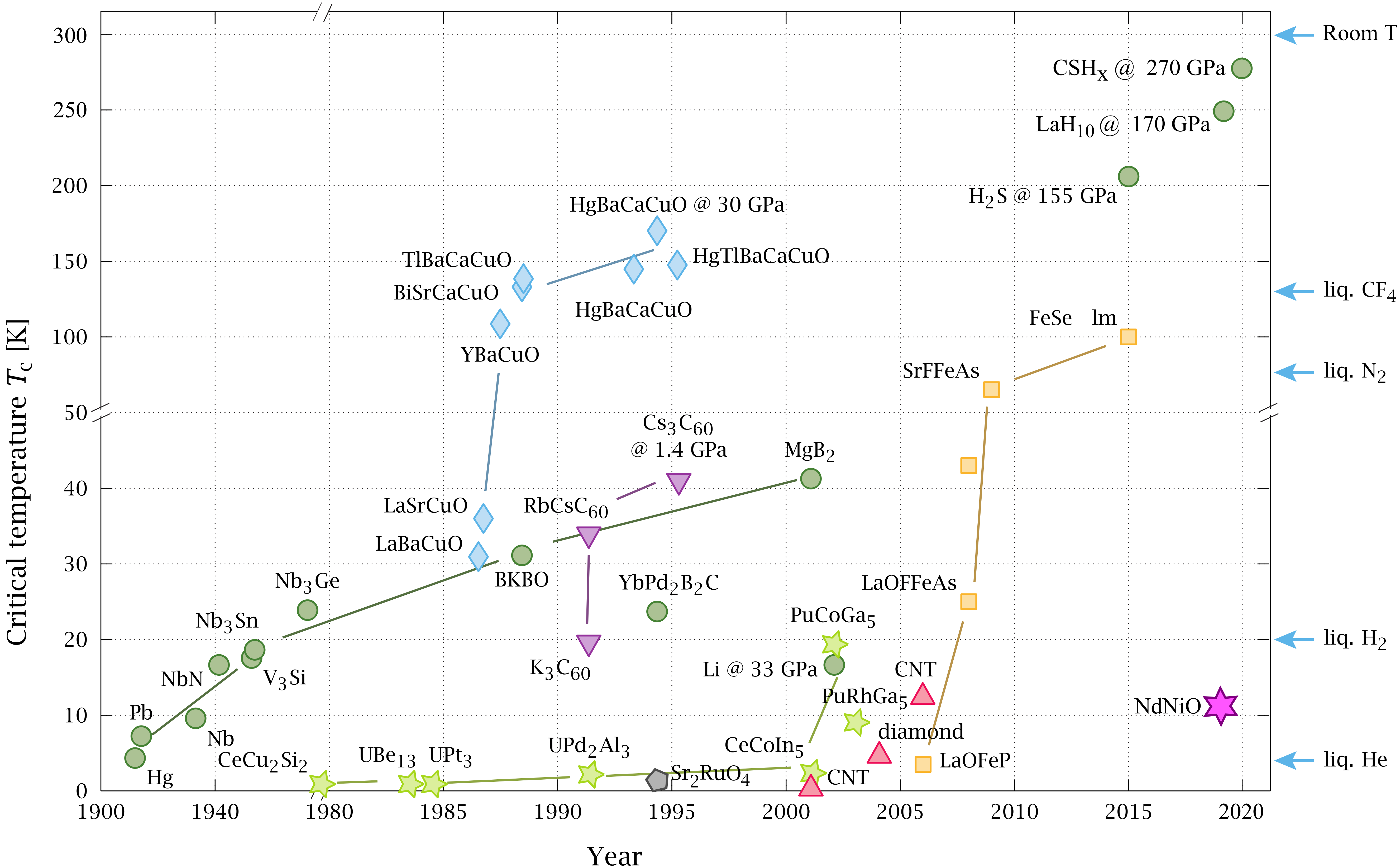
PHYSICAL REVIEW B
covering condensed matter and materials physics

Absence of conventional room-temperature superconductivity at high pressure in carbon-doped H_3S

Tianchun Wang, Motoaki Hirayama, Takuya Nomoto, Takashi Koretsune, Ryotaro Arita, and José A. Flores-Livas
Phys. Rev. B **104**, 064510 – Published 25 August 2021



But theory fails (?)

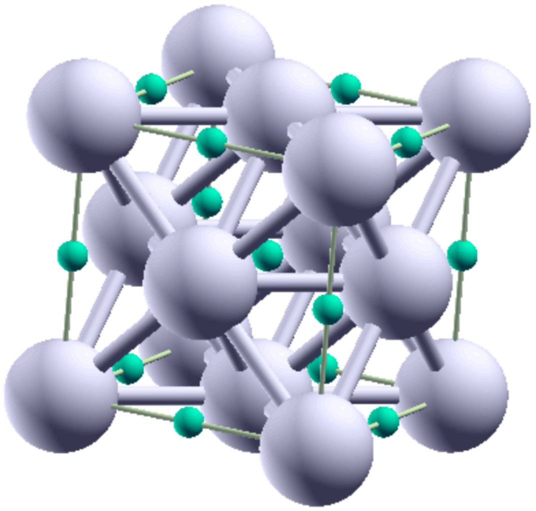


Critical temperature T_c [K]
Year
Room T
liq. CF_4
liq. N_2
liq. H_2
liq. He
CSH_x @ 270 GPa
LaH_{10} @ 170 GPa
H_2S @ 155 GPa
HgBaCaCuO @ 30 GPa
TlBaCaCuO
HgTlBaCaCuO
BiSrCaCuO
HgBaCaCuO
YBaCuO
FeSe lm
SrFFeAs
Cs_3C_{60} @ 1.4 GPa
MgB_2
LaSrCuO
$RbCsC_{60}$
LaBaCuO
BKBO
Nb_3Ge
$YbPd_2B_2C$
LaOFFeAs
$PuCoGa_5$
Nb_3Sn
NbN
V_3Si
K_3C_{60}
Li @ 33 GPa
CNT
$PuRhGa_5$
NdNiO
Pb
Nb
diamond
$CeCu_2Si_2$
UBe_{13}
UPt_3
UPd_2Al_3
$CeCoIn_5$
LaOFeP
Hg
Sr_2RuO_4
CNT

From room temperature to ambient pressure: follow the hydrogen route

From room temperature to ambient pressure: follow the hydrogen route

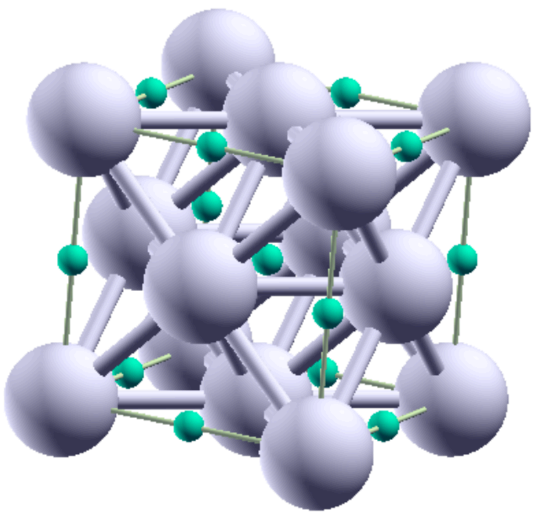
Palladium hydride



Tc=9 K

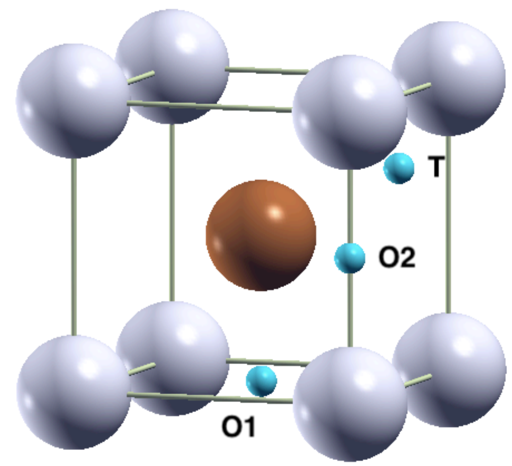
From room temperature to ambient pressure: follow the hydrogen route

Palladium hydride

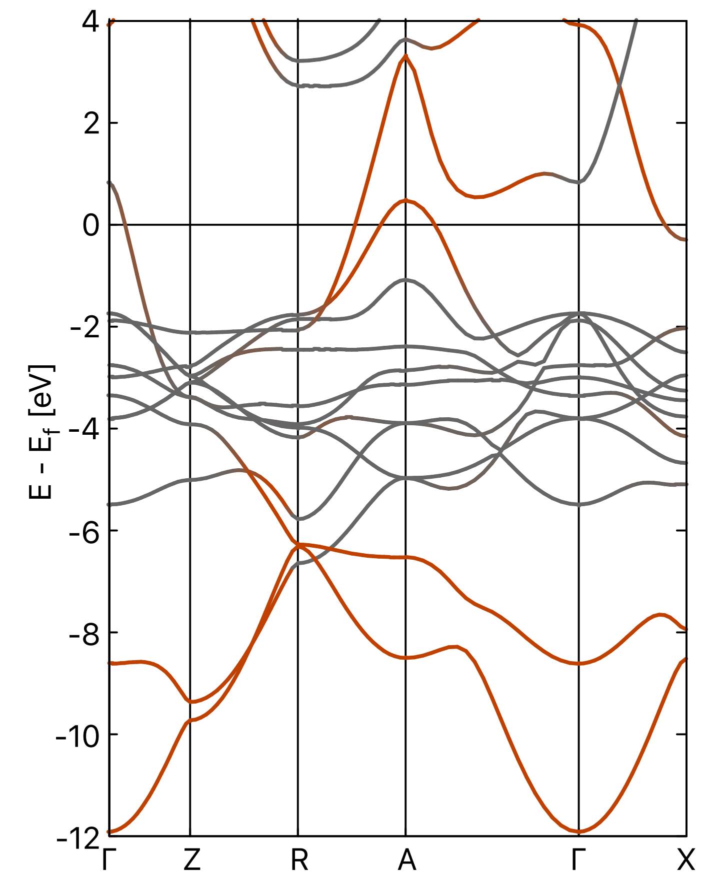


Tc=9 K

Palladium - Copper hydride

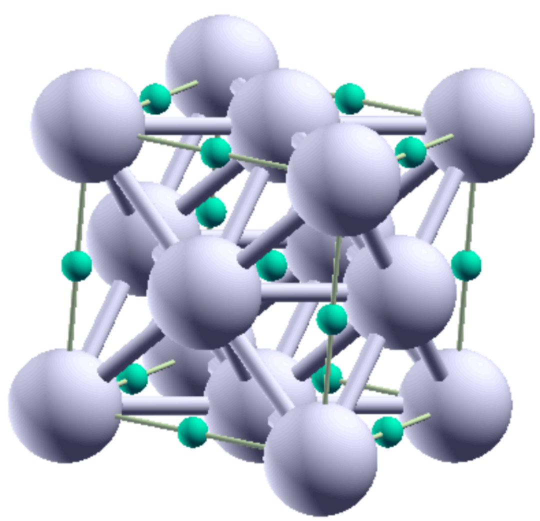


Tc=20 K



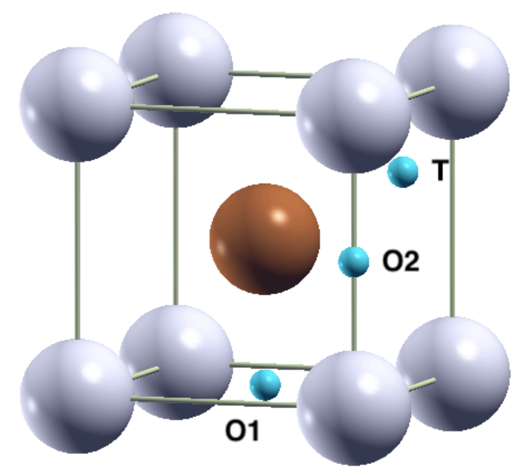
From room temperature to ambient pressure: follow the hydrogen route

Palladium hydride

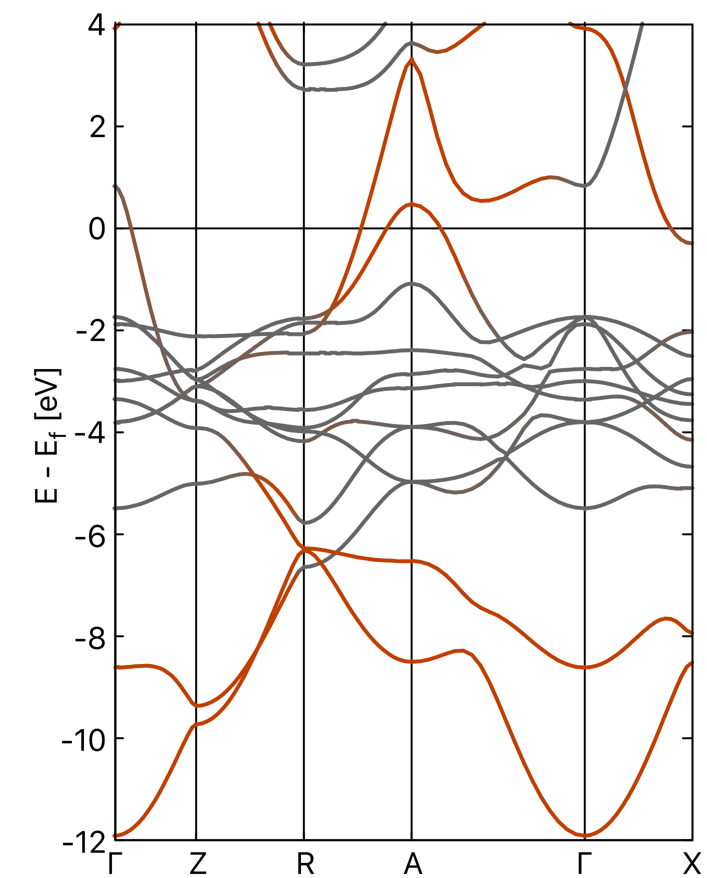


Tc=9 K

Palladium - Copper hydride

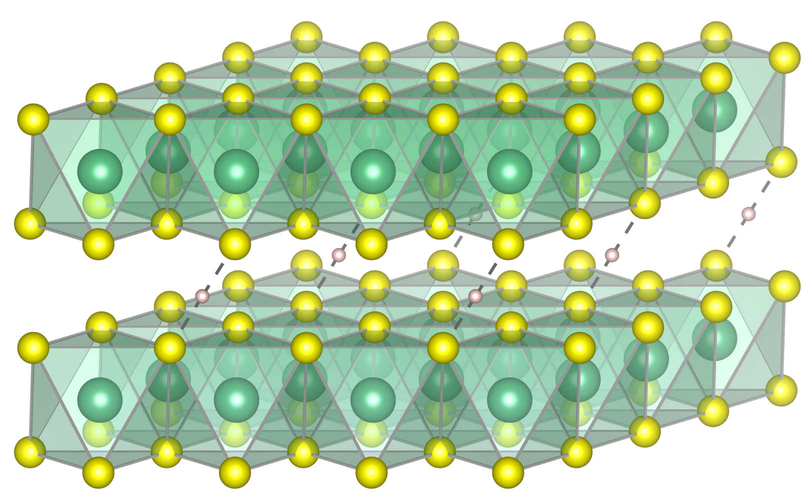


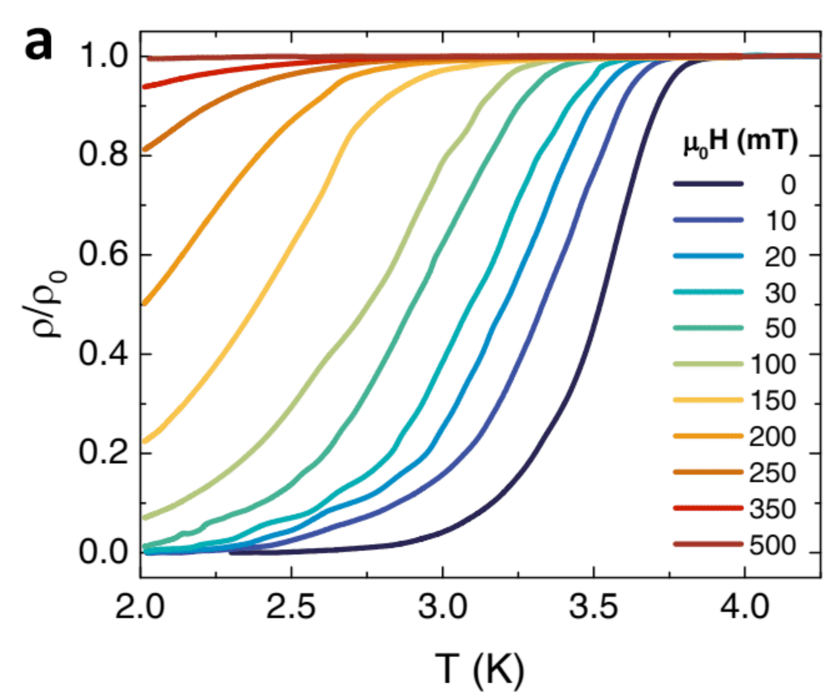
Tc=20 K



Hydrogenated TMD

Titanium diselenide, TiSe2

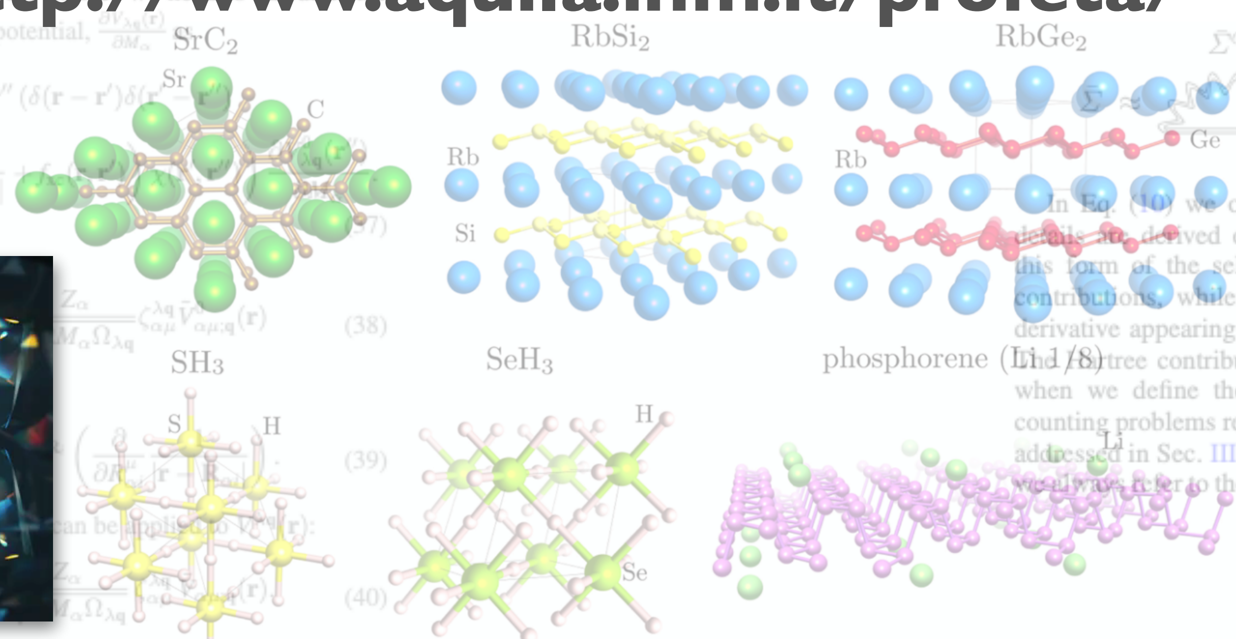


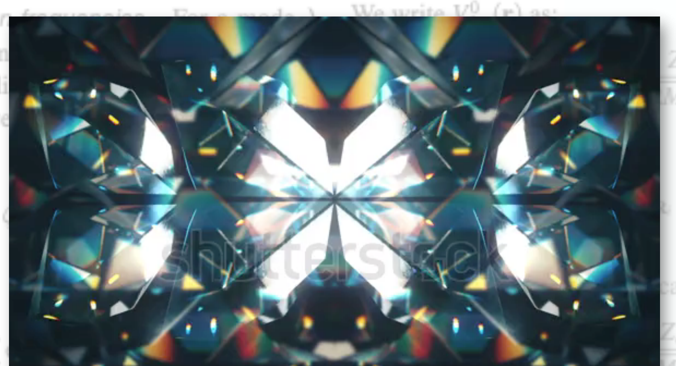


Any suggestions?

THANK YOU FOR YOUR ATTENTION

see more @ http://www.aquila.infn.it/profeta/





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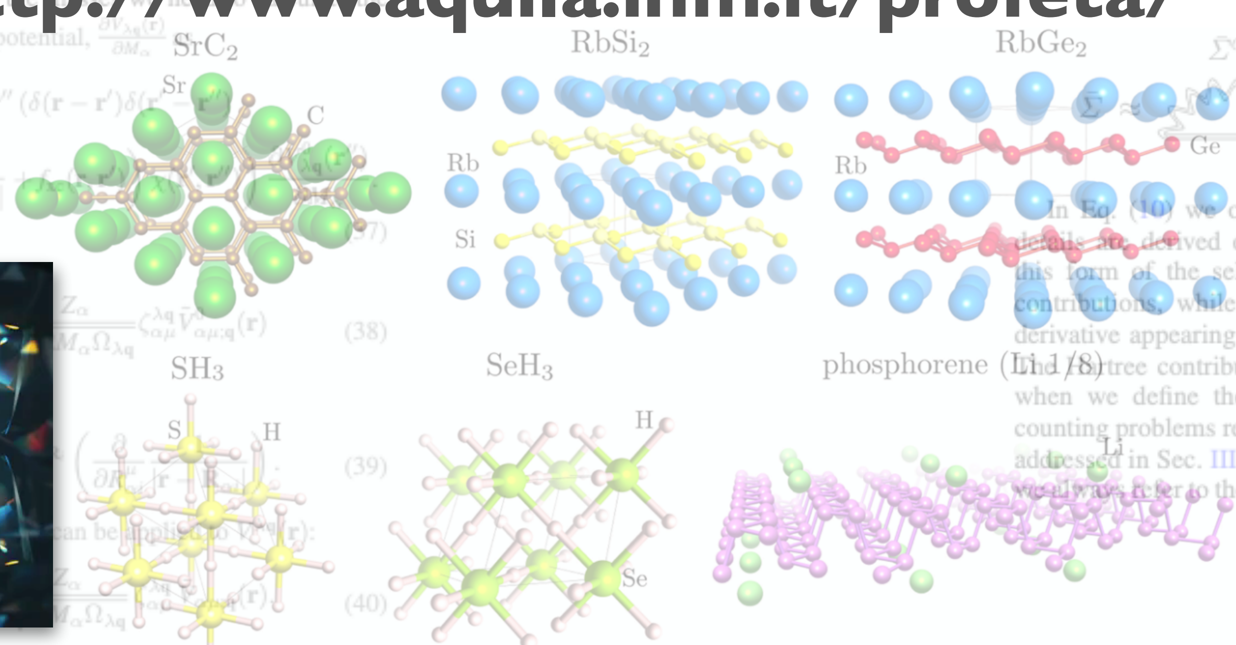

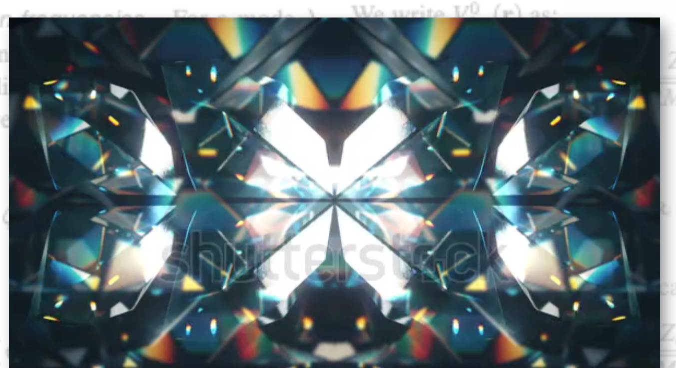

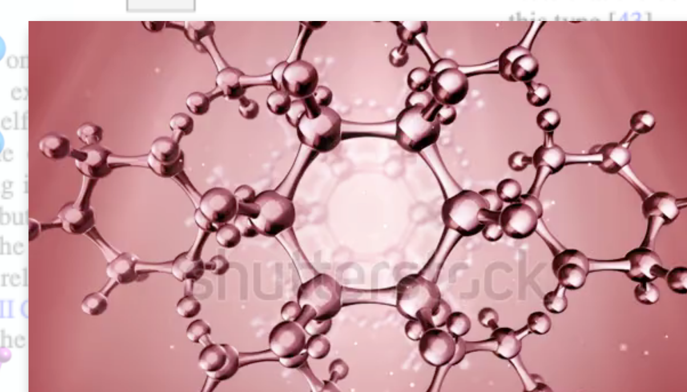

Why and how does it happen?

Frohlich (1952)

$$H_F = H_e + H_p + H_{ep}$$

$$H_e = \sum_{k,\sigma} \epsilon_k \; c^\dagger_{k,\sigma} \; c_{k,\sigma}$$

$$H_p = \sum_{q,\lambda} \hbar\omega_{q,\lambda}[b^\dagger_{q\lambda} b_{q\lambda} + \frac{1}{2}]$$

$$H_{ep} = \sum_{k\sigma} \sum_{q,G\lambda} \; g^{q+G}_{k,\lambda} \; c^\dagger_{k+q+G,\sigma} \; c_{k\sigma} \; [b_{q\lambda} + b^\dagger_{-q\lambda}]$$

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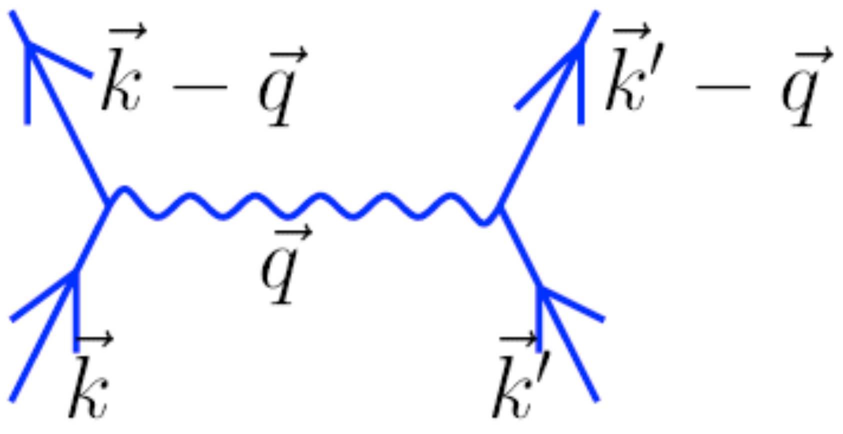
Define an effective hamiltonian (not terms which couple e and ph)

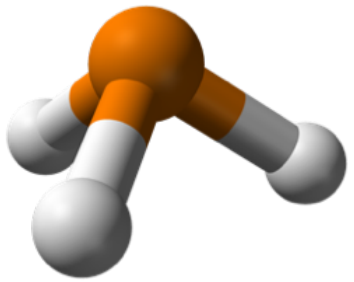
$$\tilde{H}_F = \sum_{k\sigma} \epsilon_k \; c^\dagger_{k\sigma} c_{k\sigma} + \frac{1}{2} \sum_{\substack{kk'qG \\ \sigma\sigma'}} V_{ph} \; c^\dagger_{k+q+G\sigma} \; c^\dagger_{k'-q-G\sigma'} \; c_{k'\sigma'} \; c_{k\sigma}$$

$$V_{ph} = \sum_{\lambda} \frac{\hbar\omega_{q\lambda} \; |g(q+G;\lambda)|^2}{[\epsilon_k - \epsilon_{k+q+G}]^2 - [\hbar\omega_{q\lambda}]^2}$$

if < 0 attraction !!



Isolated example? Superconducting phosphines (PH_3)



RAPID COMMUNICATIONS

PHYSICAL REVIEW B **93**, 020508(R) (2016)

Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure

José A. Flores-Livas,[1] Maximilian Amsler,[2] Christoph Heil,[3] Antonio Sanna,[4] Lilia Boeri,[3] Gianni Profeta,[5] Chris Wolverton,[2] Stefan Goedecker,[1] and E. K. U. Gross[4]

[1]*Department of Physics, Universität Basel, Klingelbergstr. 82, 4056 Basel, Switzerland*

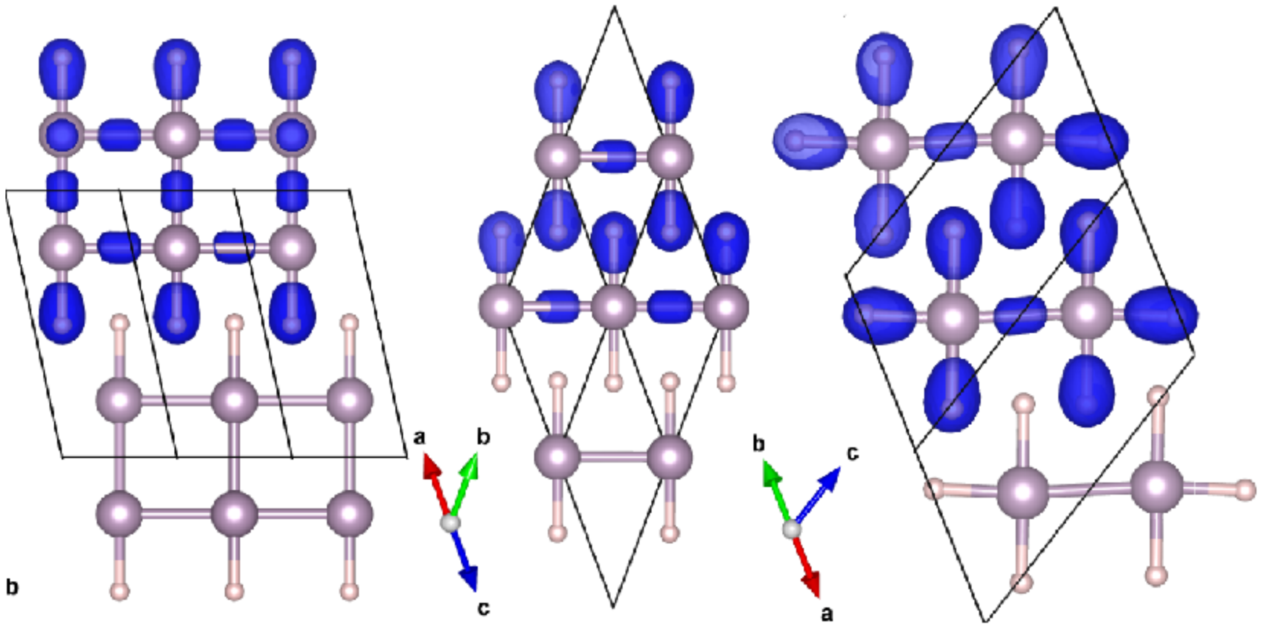
[2]*Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, United States*

[3]*Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz, 8010 Graz, Austria*

[4]*Max-Planck Institut für Microstrukture Physics, Weinberg 2, 06120 Halle, Germany*

[5]*Dipartimento di Fisica Università degli Studi di L'Aquila and SPIN-CNR, I-67100 L'Aquila, Italy*

(Received 7 December 2015; published 26 January 2016)



(a) PH_1 (b) PH_2 (c) PH_3

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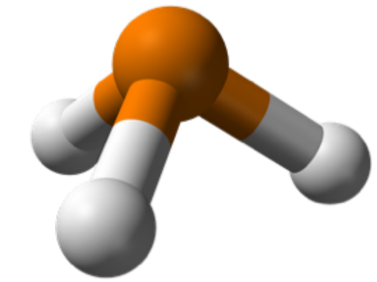

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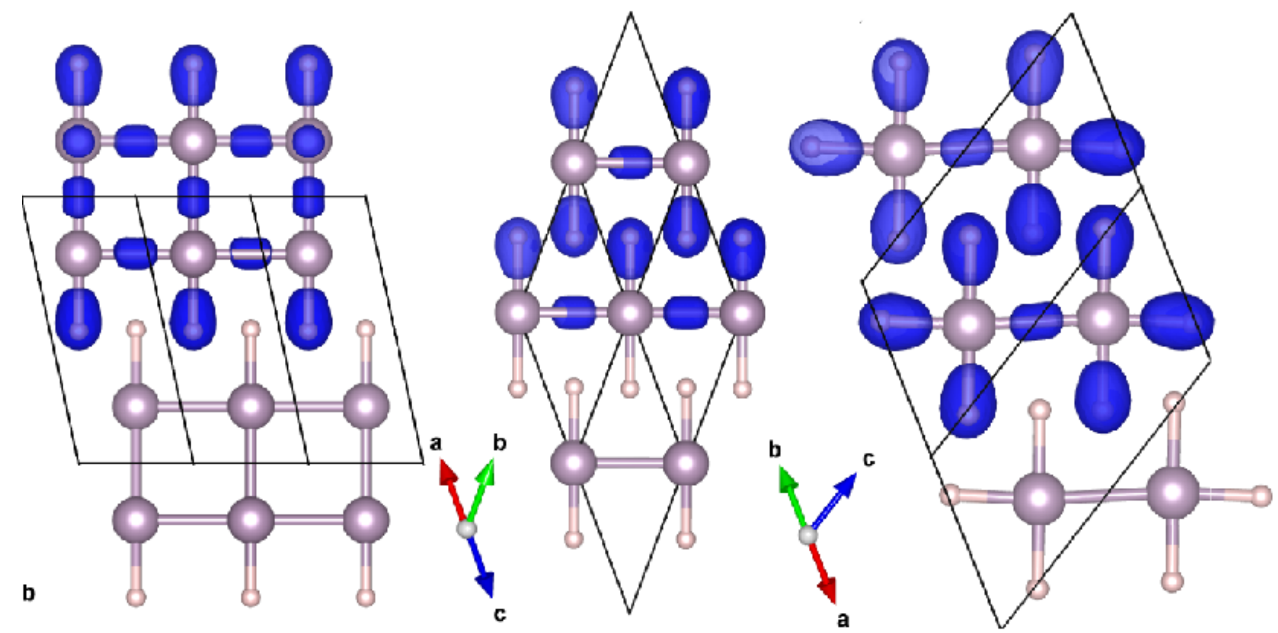

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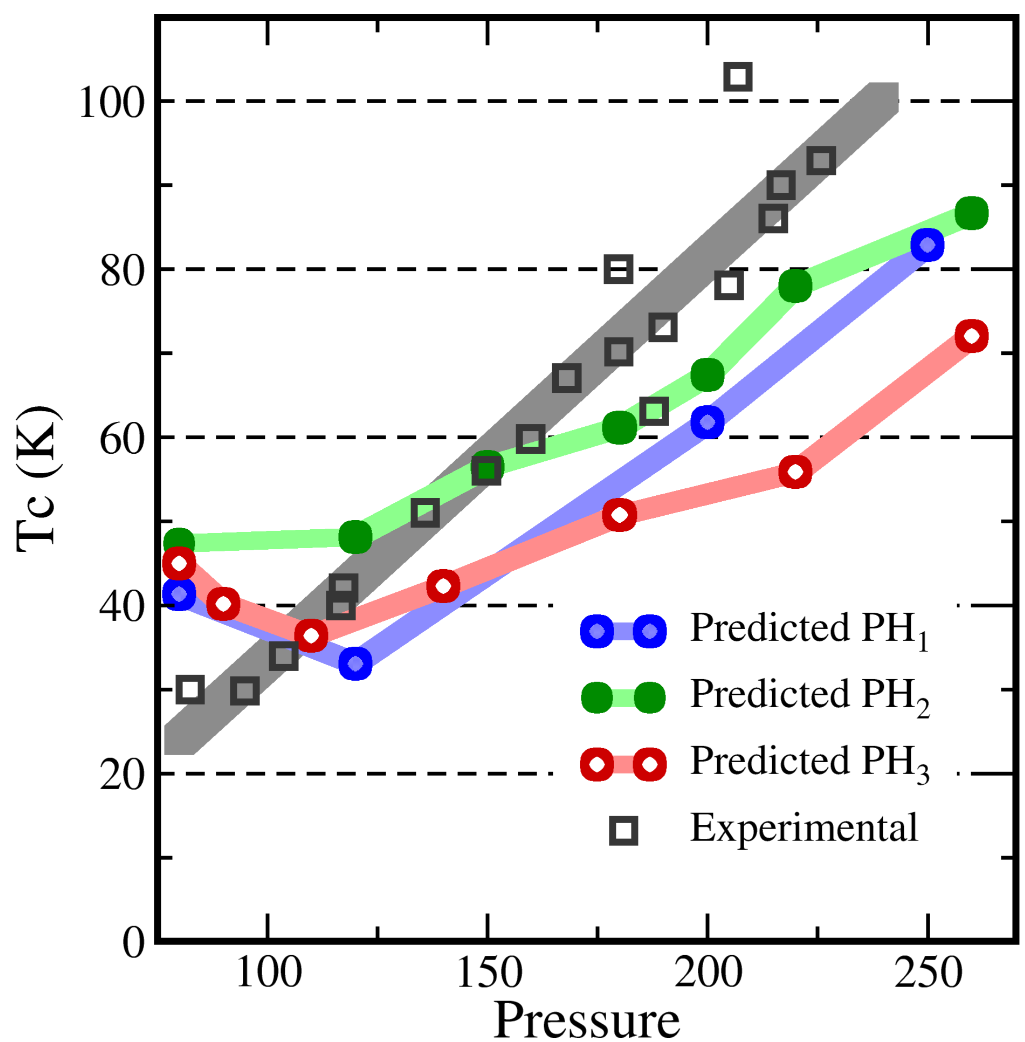

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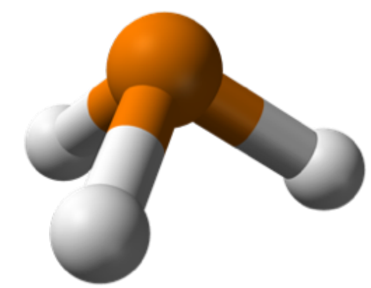

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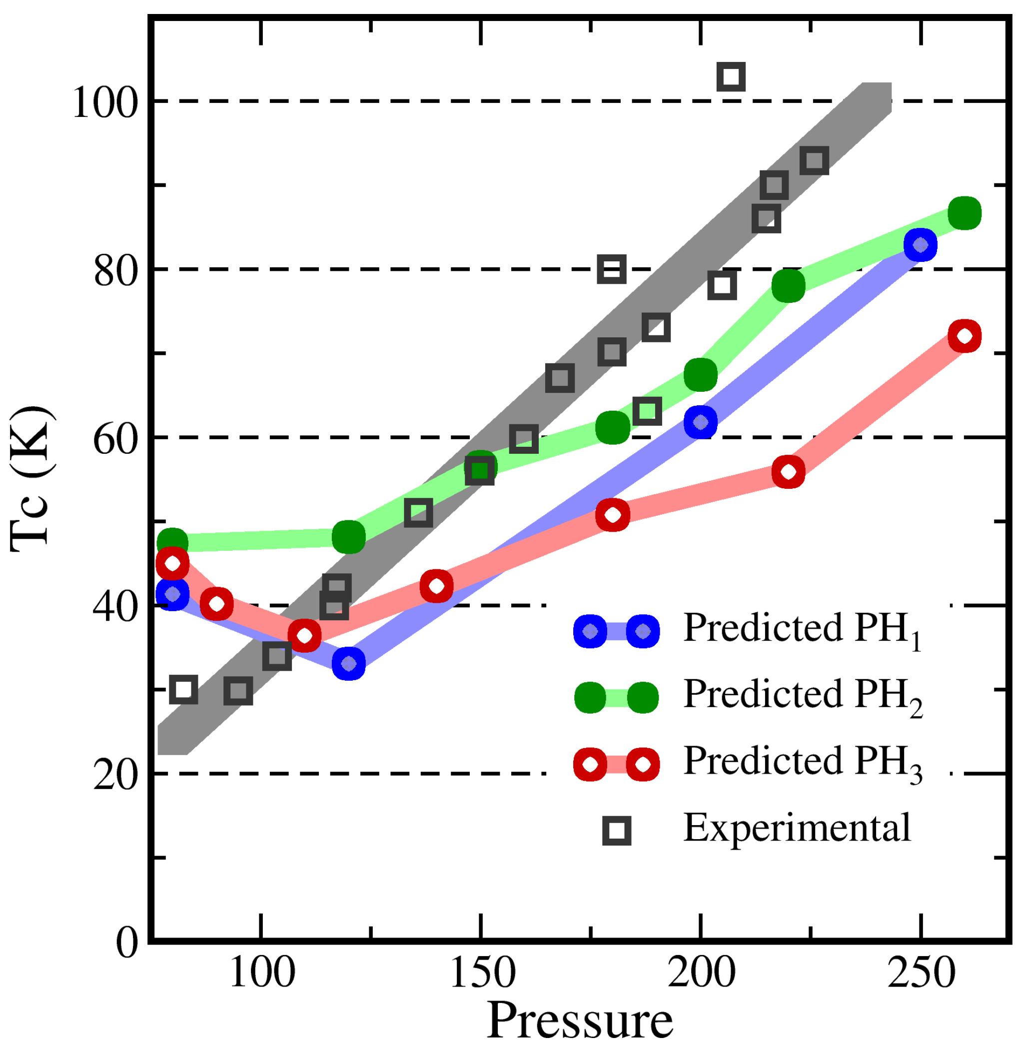

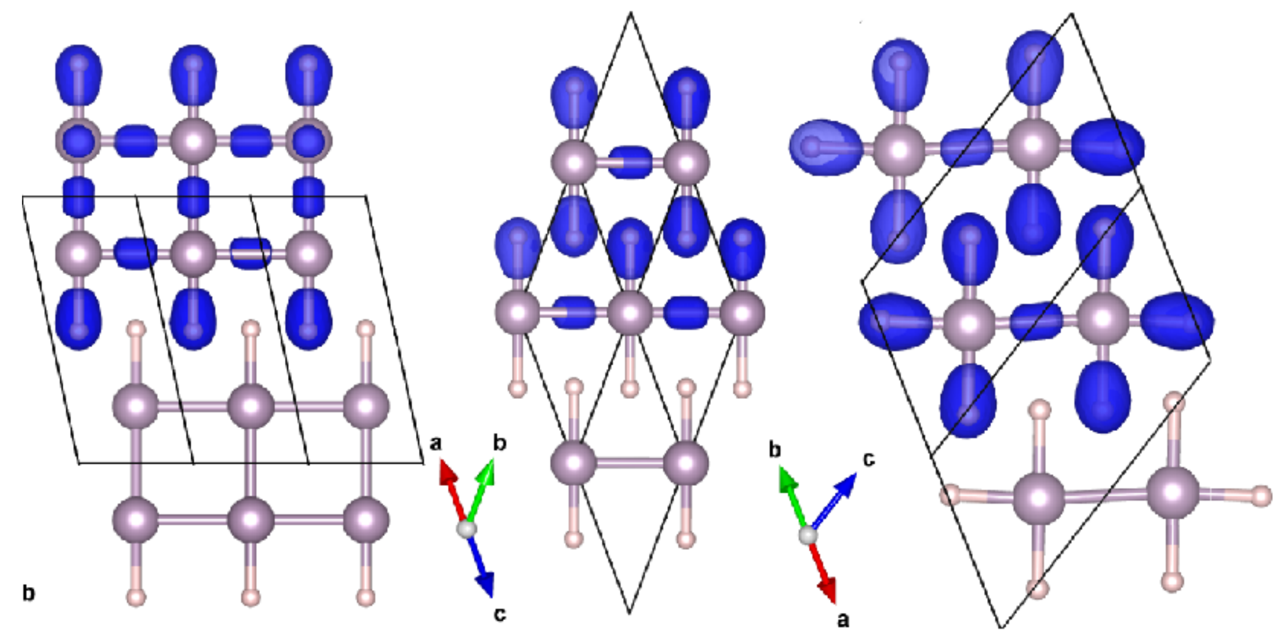

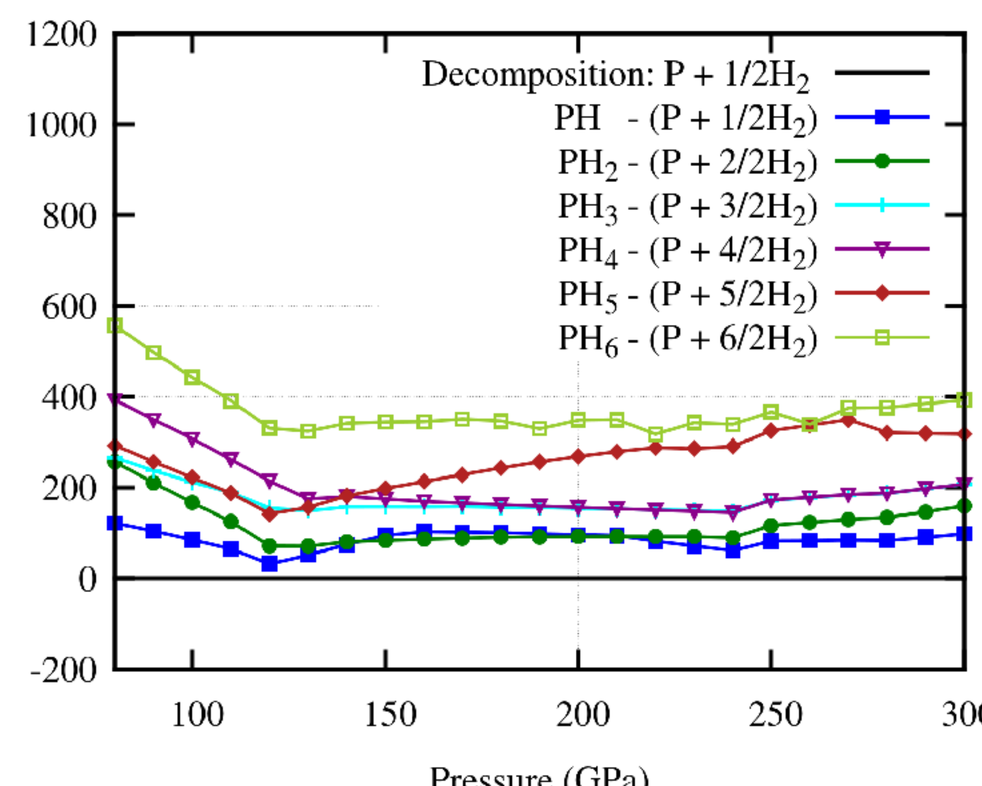

nature COMMUNICATIONS

ARTICLE

https://doi.org/10.1038/s41467-021-25372-2 OPEN

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Superconductivity up to 243 K in the yttrium-hydrogen system under high pressure

Panpan Kong [1,7], Vasily S. Minkov [1,7], Mikhail A. Kuzovnikov [2,7], Alexander P. Drozdov [1], Stanislav P. Besedin [1], Shirin Mozaffari [3], Luis Balicas [3], Fedor Fedorovich Balakirev [4], Vitali B. Prakapenka [5], Stella Chariton [5], Dmitry A. Knyazev [6], Eran Greenberg [5] & Mikhail I. Eremets [1]✉