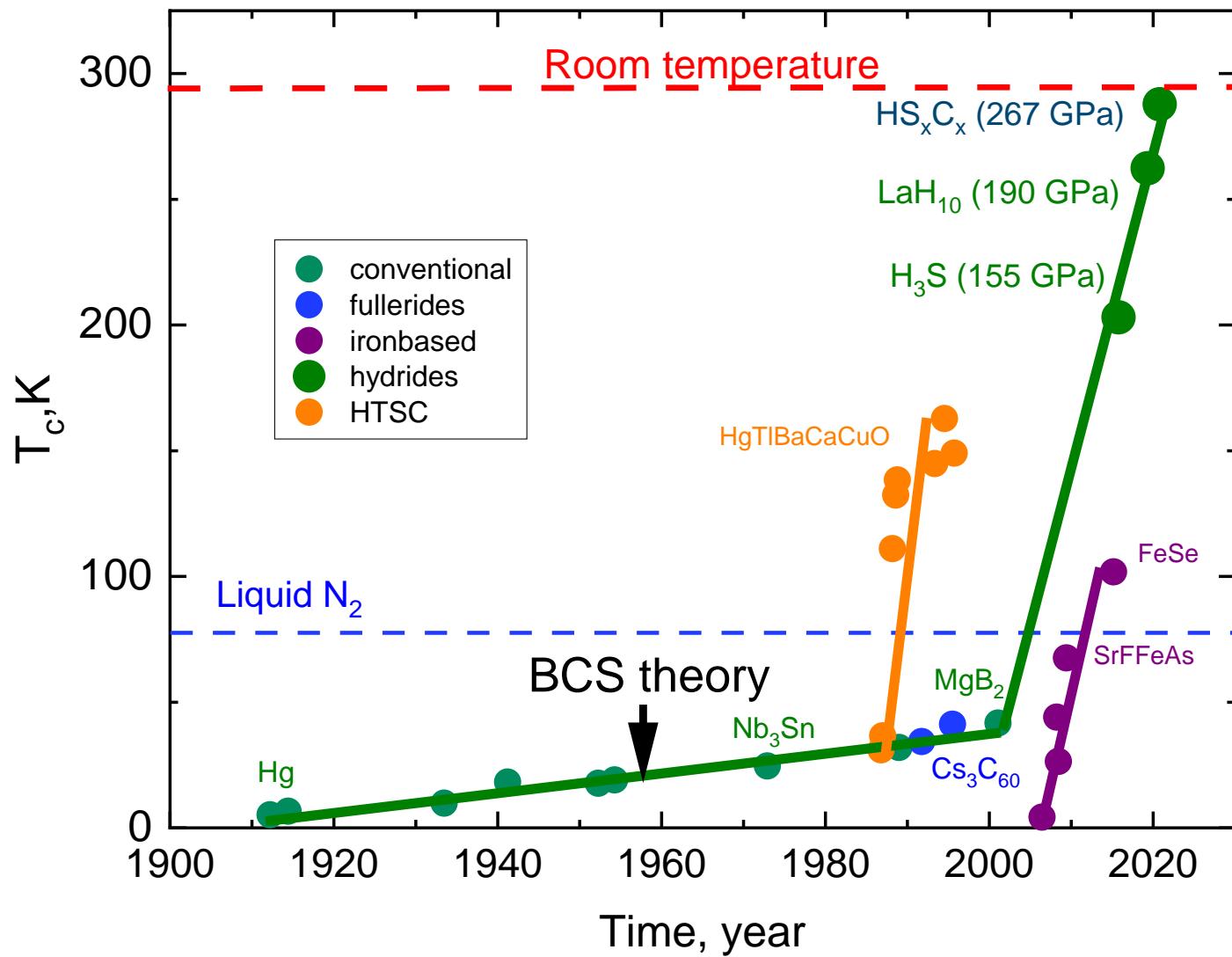


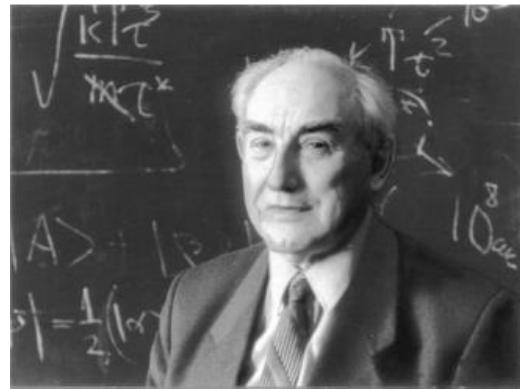
High-temperature conventional superconductivity at high pressures

M. I. Eremets

Max-Planck-Institut für Chemie, Hahn-Meitner Weg 1, 55128 Mainz, Germany

Critical temperature of superconductivity with time





V. L. Ginzburg
Nobel Prize in Physics in 2003

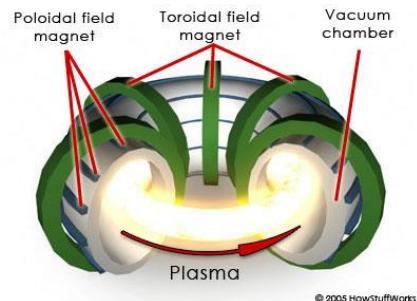
1. Controlled nuclear fusion.
2. High - temperature and room – temperature superconductivity.
3. Metallic hydrogen. Other exotic substances
4. Two-dimensional electron liquid (the anomalous Hall effect and other effects).
5. ...

The list of 'especially important and interesting problems' of 1999

the 21st century.

1. Controlled nuclear fusion.
2. High-temperature and room-temperature superconductivity.
3. Metallic hydrogen. Other exotic substances.
4. Two-dimensional electron liquid (the anomalous Hall effect and other effects).
5. Some questions of solid-state physics (heterostructures in semiconductors, quantum wells and dots, metal-dielectric transitions, charge- and spin-density waves, mesoscopics).
6. Second-order and related phase transitions. Some examples of such transitions. Cooling (in particular, laser cooling) to superlow temperatures. Bose-Einstein condensation in gases.
7. Surface physics. Clusters.
8. Liquid crystals. Ferroelectrics. Ferrotoroids.
9. Fullerenes. Nanotubes.
10. The behavior of matter in superstrong magnetic fields.
11. Nonlinear physics. Turbulence. Solitons. Chaos. Strange attractors.
12. X-ray lasers, gamma-ray lasers, superhigh-power lasers.
13. Superheavy elements. Exotic nuclei.
14. Mass spectrum. Quarks and gluons. Quantum chromodynamics. Quark-gluon plasma.
15. Unified theory of weak and electromagnetic interactions. W^\pm and Z^0 bosons. Leptons.
16. Standard Model. Grand unification. Superunification. Proton decay. Neutrino mass. Magnetic monopoles.
17. Fundamental length. Particle interaction at high and superhigh energies. Colliders.
18. Nonconservation of CP invariance.
19. Nonlinear phenomena in vacuum and in superstrong magnetic fields. Phase transitions in a vacuum.
20. Strings. M theory.
21. Experimental verification of the general theory of relativity.
22. Gravitational waves and their detection.
23. The cosmological problem. Inflation. The Λ term

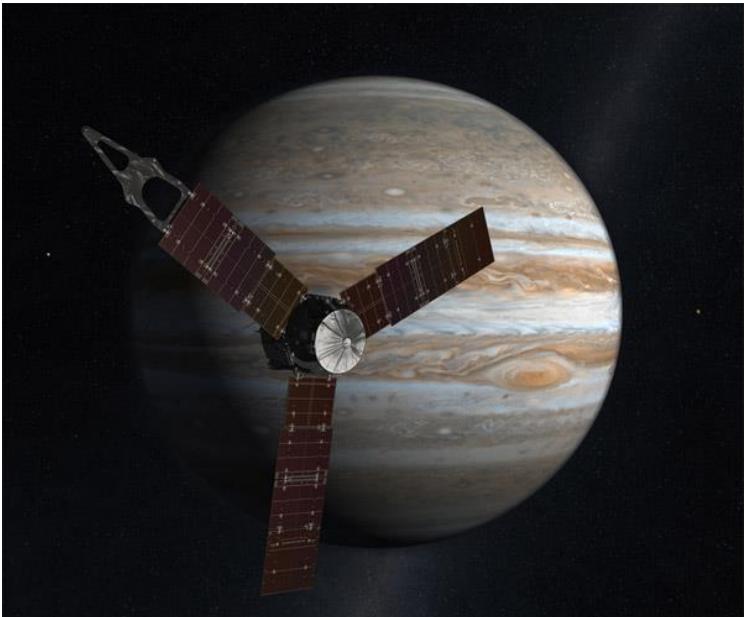
Nuclear Fusion



© 2005 HowStuffWorks

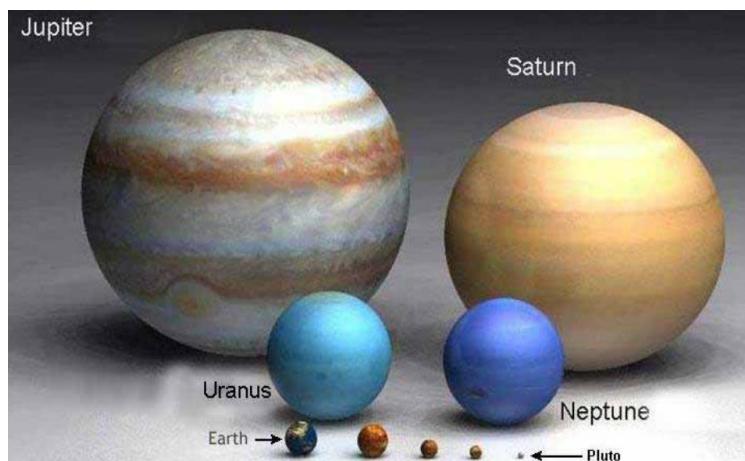
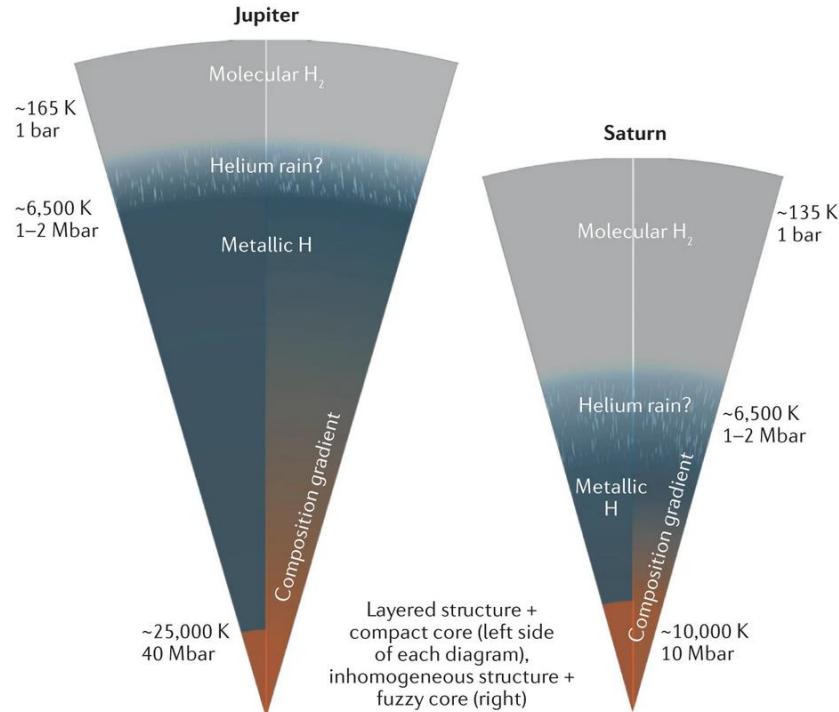
Metallic hydrogen

Hydrogen in the Solar system



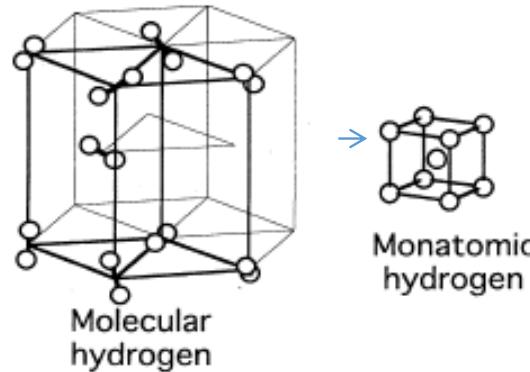
Juno mission

July 4, 2016
1.1 billion USD



Helled et al 2020

Metallic hydrogen



Wigner and Huntington
(1935)

Superconductivity and superfluidity in metallic hydrogen

Ashcroft 1968 PRL Babaev *et al* (2004)

$$T_c \sim 0.2 \sqrt{\lambda} \omega_D \quad T_c = 0.2 \sqrt{2} 2000K \rightarrow T_c \sim 500 K$$

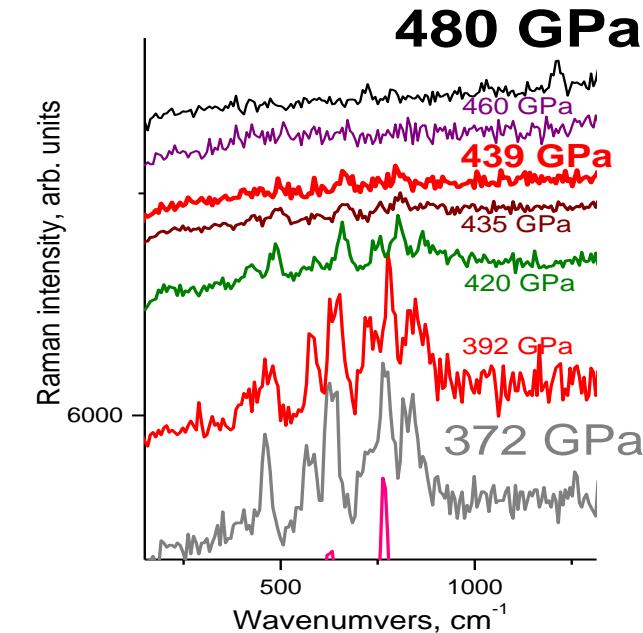
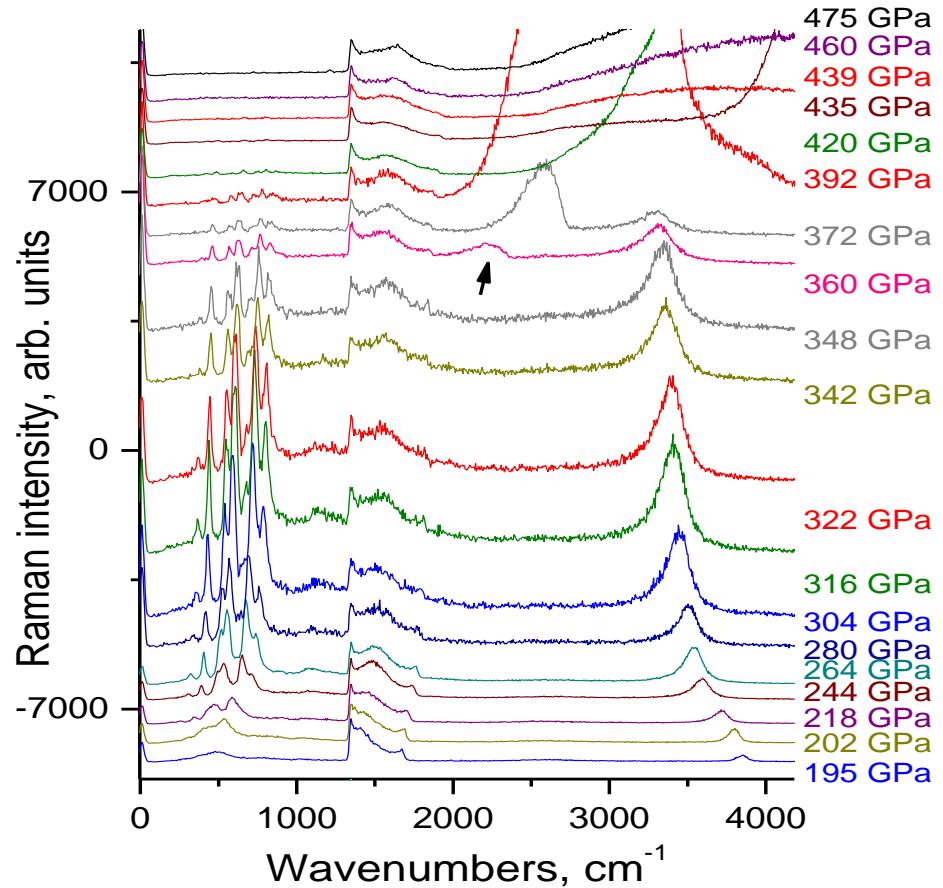
$$T_c \sim 350-700 K$$

P ~500 Gpa

McMahon and Ceperley (2012)

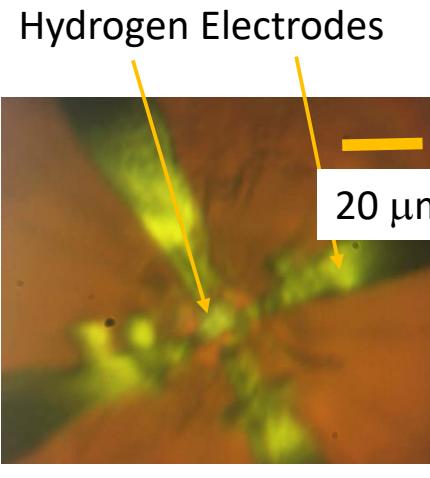
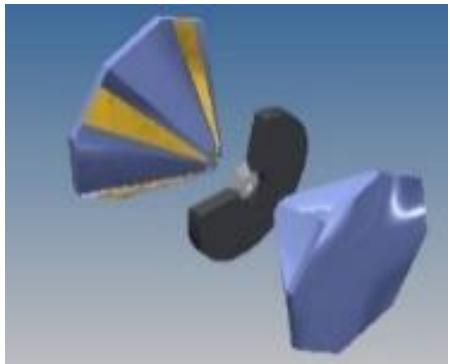
Diamond $\omega_D = 1860 K$

Raman spectra of hydrogen at 480 GPa

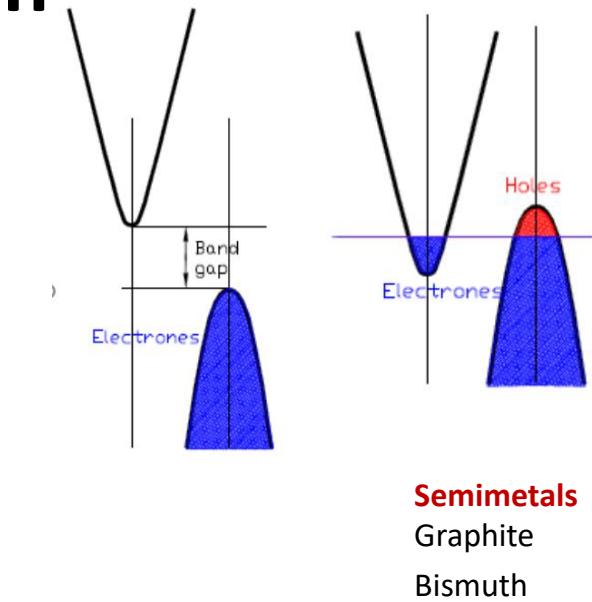
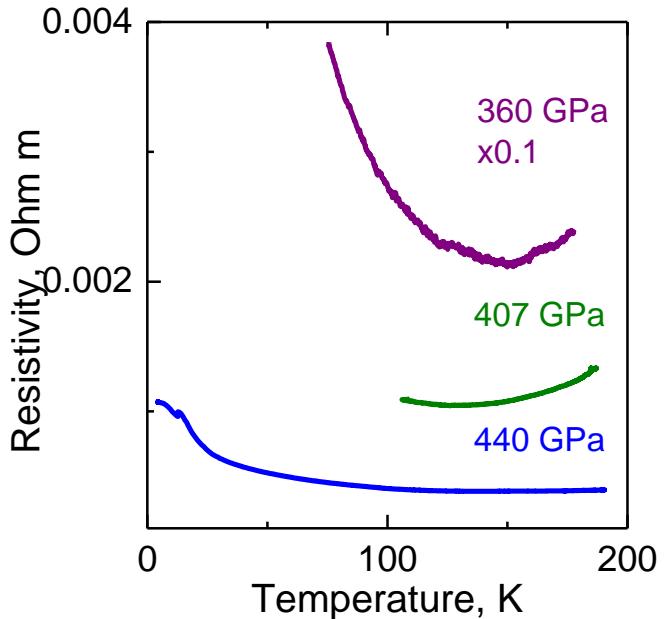


Eremets et al (2019) *Nature Physics* **15** 1246

Semimetallic hydrogen



380 GPa and 180 K



Hydrogen transforms to metal at ~ 360 GPa in molecular state.
No superconductivity

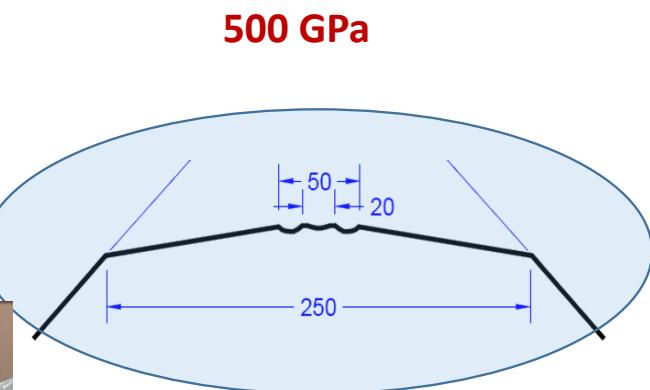
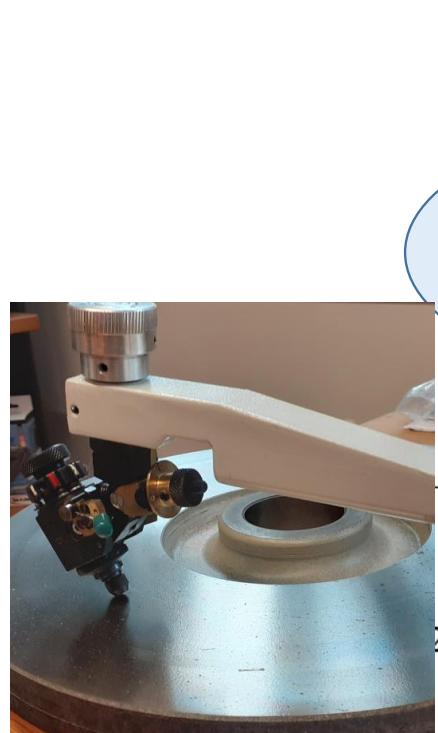
Theory

Monacelli et al (2020) *Nature Phys.*
Gorelov et al (2020) *PRL* (2020) 124, 116401

Experimental techniques

Diamond anvil cell

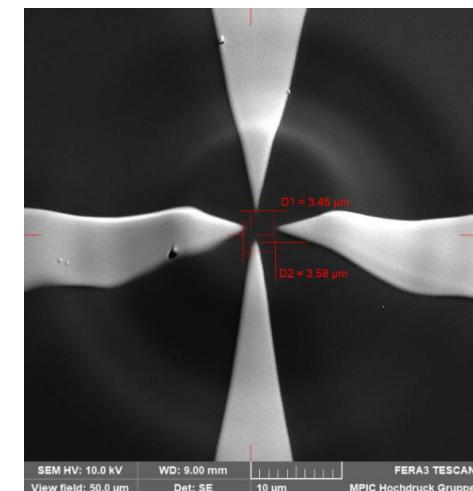
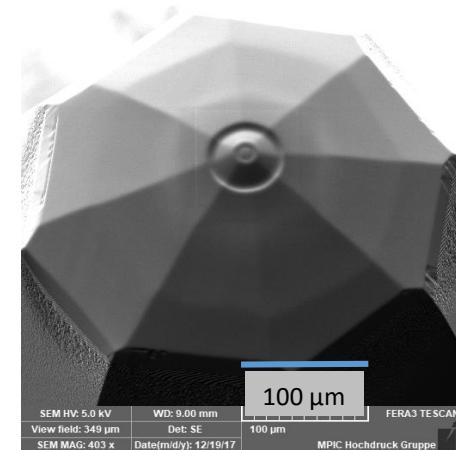
Focused ion beam



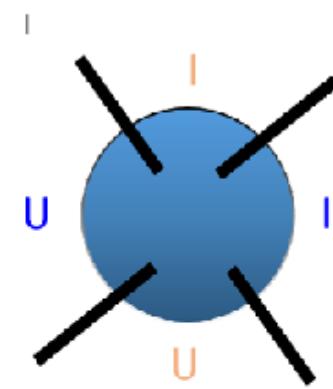
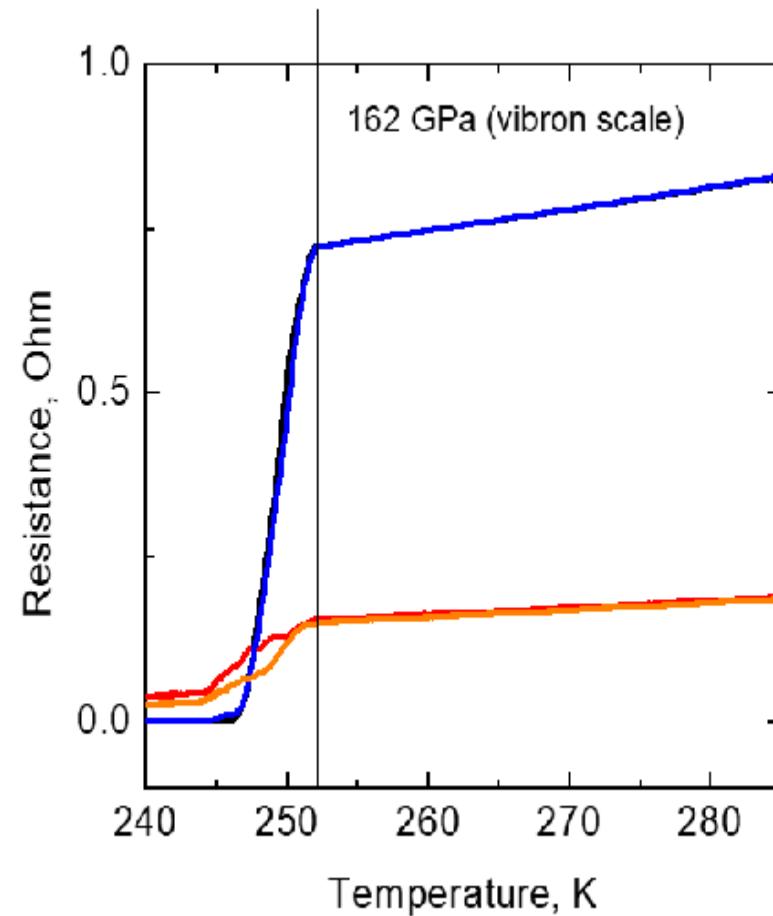
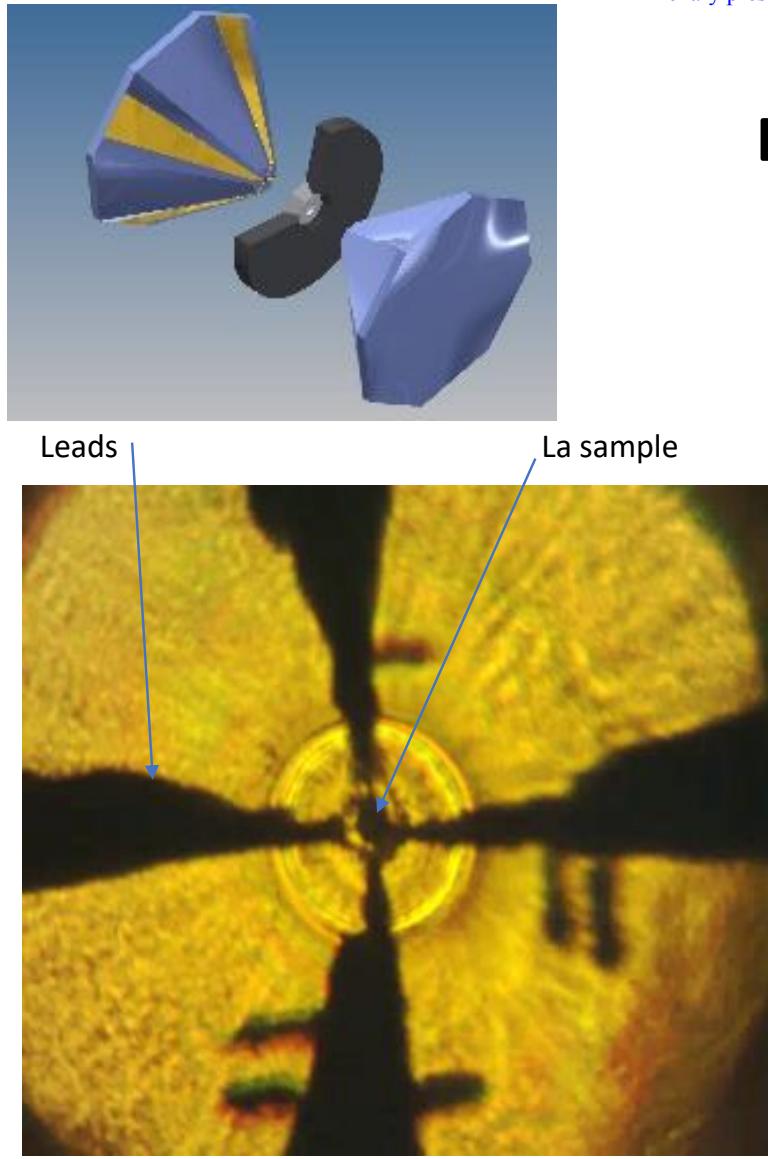
500 GPa



TESCAN



Electrical measurements



N. Ashcroft 2004:

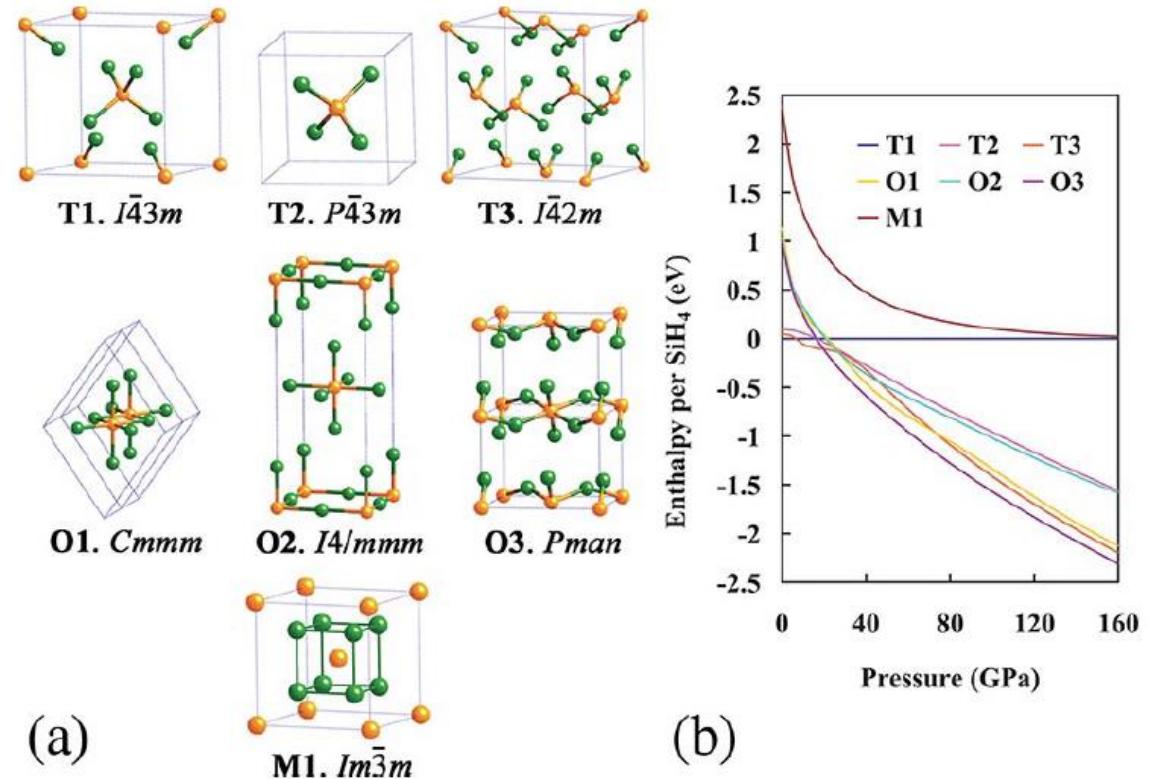
*Superconductivity in Hydrogen dominant materials:
 CH_4 , SiH_4 , GeH_4 ...*

metallic at high pressures ~100- 200 GPa

N. Ashcroft 2004:
Superconductivity in Hydrogen dominant materials: CH_4 , SiH_4 , GeH_4 ...

chemical intuition

SiH₄ at High Pressure. PRL 96, 017006 (2006)
structure **O3**, metallization onset 91 GPa
 $T_c = \textcolor{red}{166 \text{ K}}$ at 202 GPa



Superconductivity in hydrogen-rich materials

Experiment: no superconductivity

$\text{LiH} + \text{H}_2$ 150 GPa

LiBH_4 P>200 GPa

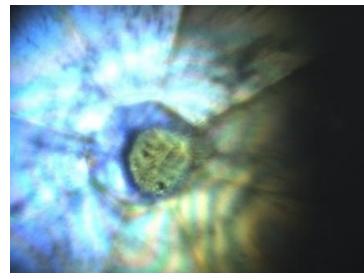
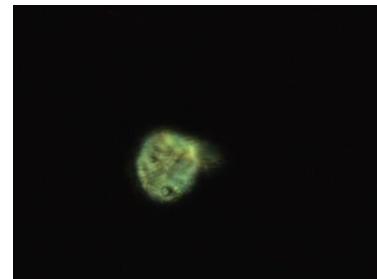
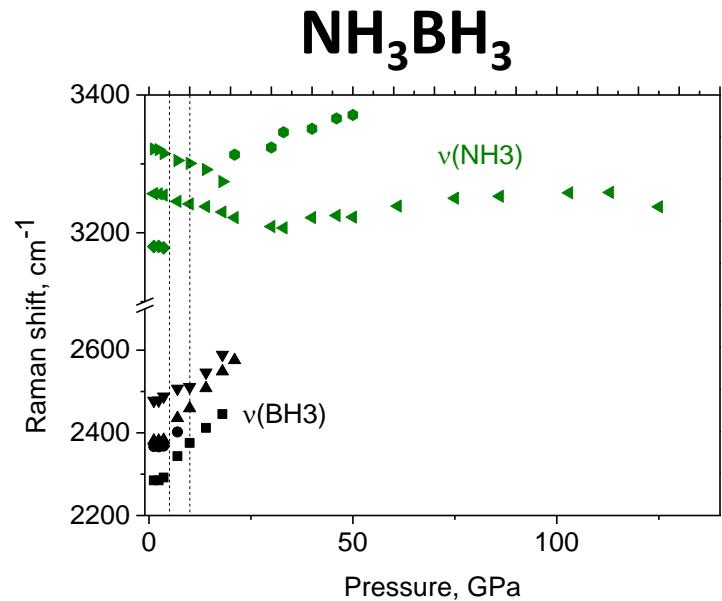
NaBH_4 at P<130 GPa

$\text{Si}(\text{CH}_3)_4$ at P<140 GPa

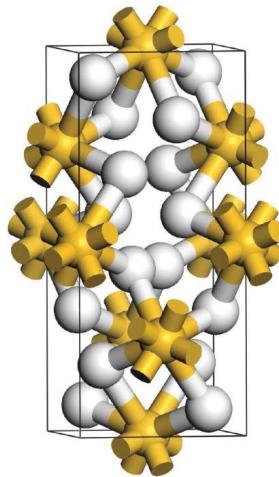
$\text{B}_{10}\text{H}_{14}$ at P<200 GPa

NH_3BH_3 at P<200 GPa

Li_2S at P<200 GPa

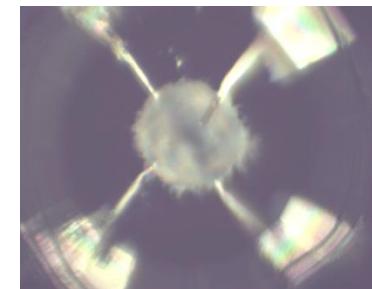
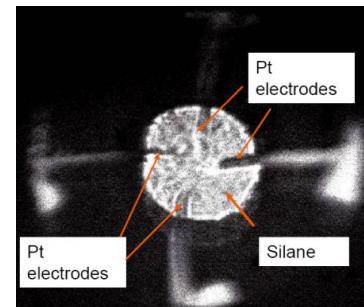


Metallization and superconductivity in silane

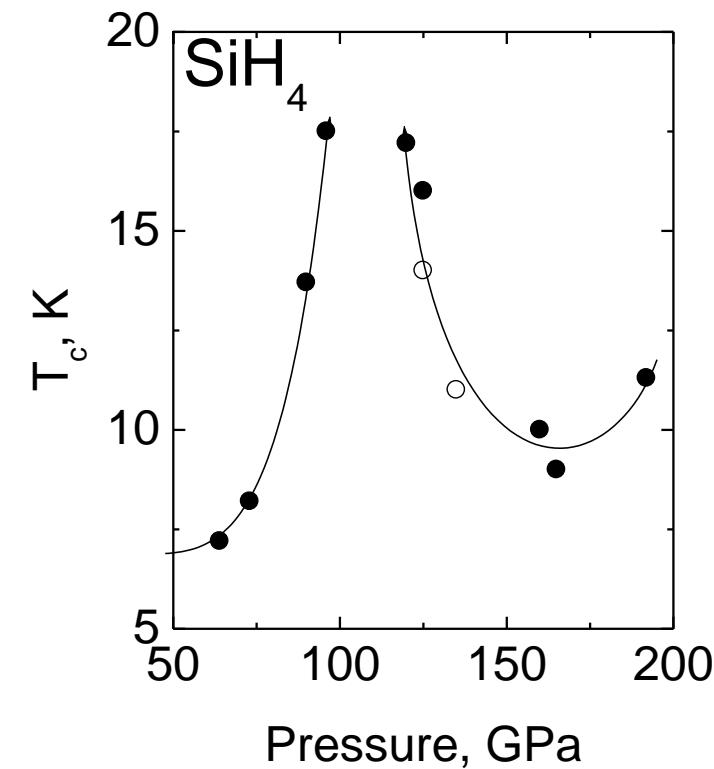


$I4_1/a$

Predictions: Pickard and Needs
Phys. Rev. Lett. **97** 045504 (2006)



$P=50-100 \text{ GPa}$



M. Eremets et al *Science* 2008

DFT theory – accurate calculation of electronic and phonon spectra

Crystal predictions

Random sampling
Evolutionary algorithms
Particle swarm optimization

Some reviews:

1. Flores-Livas, J. A. *et al.* A perspective on conventional high-temperature superconductors at high pressure: Methods and materials. *Physics Reports* **856**, 1-78 (2020).
2. Pickard, C. J., Errea, I. & Eremets, M. I. Superconducting hydrides under pressure. *Annual Review of Condensed Matter Physics* **11**, 57-76 (2020).
3. Pickett, W. & Eremets, M. I. The quest for room-temperature superconductivity in hydrides. *Physics today* **72(5)** 52-58 doi:10.1063/PT.3.4204. (2020).
4. Gor'kov, L. P. & Kresin, V. Z. High Pressure and Road to Room Temperature Superconductivity. *Rev. Modern Phys.* **90**, 011001 (2018).

CaH_6 $T_c \sim 220\text{--}235\text{ K}$ at 150 GPa (2012)

YH_6 $251\text{--}264\text{ K}$ at 120 GPa

LaH_{10} 280 K at 210 GPa

$\text{SiH}_4(\text{H}_2)_2$ – $98\text{--}107\text{ K}$ at 250 GPa

$\text{GeH}_4(\text{H}_2)_2$ – $76\text{--}90\text{ K}$ at 250 GPa

Si_2H_6 : 139 K at 275 GPa

GaH_3 $73\text{--}86\text{ K}$ at 160 GPa

GeH_3 100 K at 180 GPa

GeH_4 : 64 K at 220 GPa

SnH_4 62 K at 200 GPa

H_2S 80 K at 160 GPa

KH_6 60 K at 166 – 300 GPa

$\text{LiH}+\text{H}_2$: LiH_6 82 K at 300 GPa. LiH_8 $T_c = 31\text{ K}$ at 100 GPa

SiH_4 . Metallic phase C2/c at 262 GPa, with $T_c \sim 16\text{ K}$.

AlH_3 24 K at 110 GPa

NbH_4 38 K at 300 GPa

BeH_2 $30\text{--}40\text{ K}$ $P > 200\text{ GPa}$ 2014

LiH $P > 300\text{ GPa}$ (Zurek et al PNAS 2009)

$\text{Xe}(\text{H}_2)_8$ metallization at 250 GPa

LiBeH_3 Hu et al PRB 79, 134116 (2009) – insulating to 530 GPa

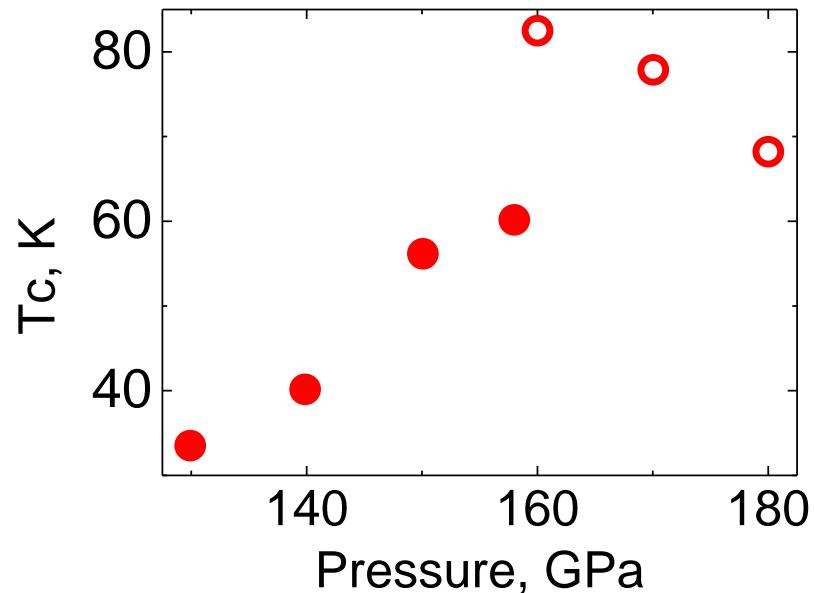
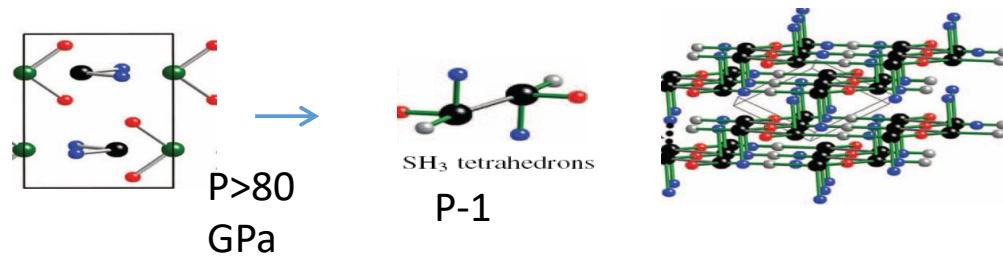
Hydrogen sulfide

THE JOURNAL OF CHEMICAL PHYSICS 140, 174712 (2014)



The metallization and superconductivity of dense hydrogen sulfide

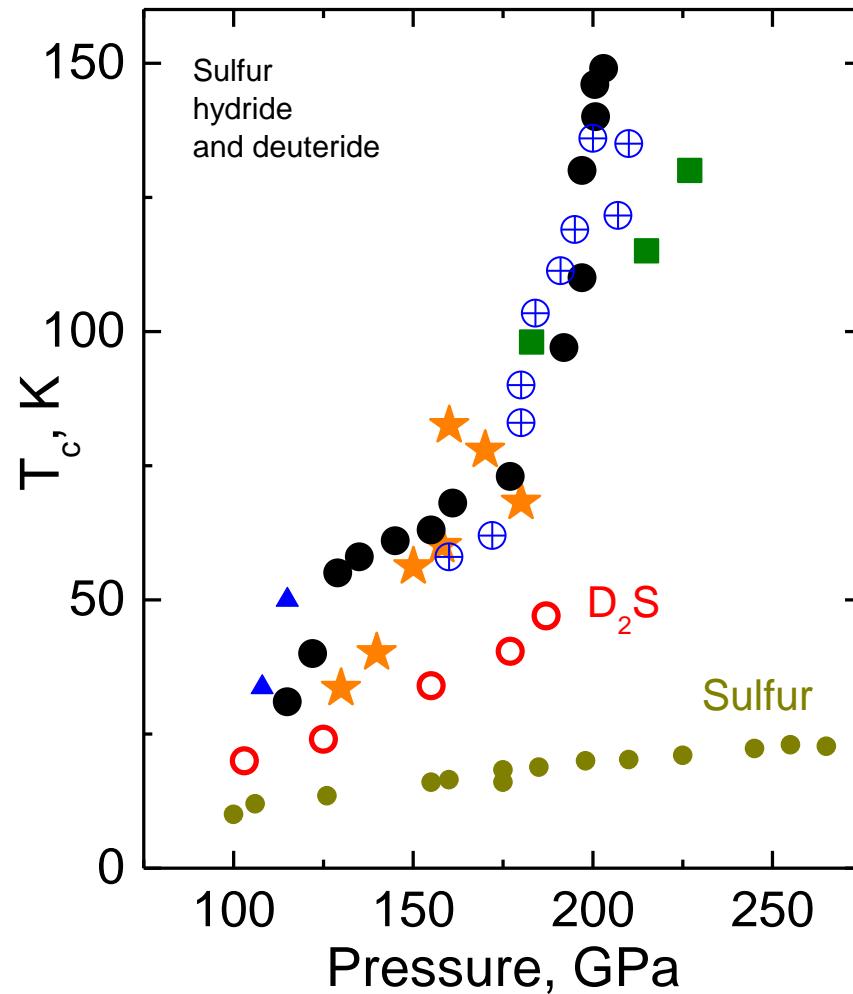
Yinwei Li,^{1,a)} Jian Hao,¹ Hanyu Liu,² Yanling Li,¹ and Yanming Ma^{3,b)}



Hydrogen sulfide

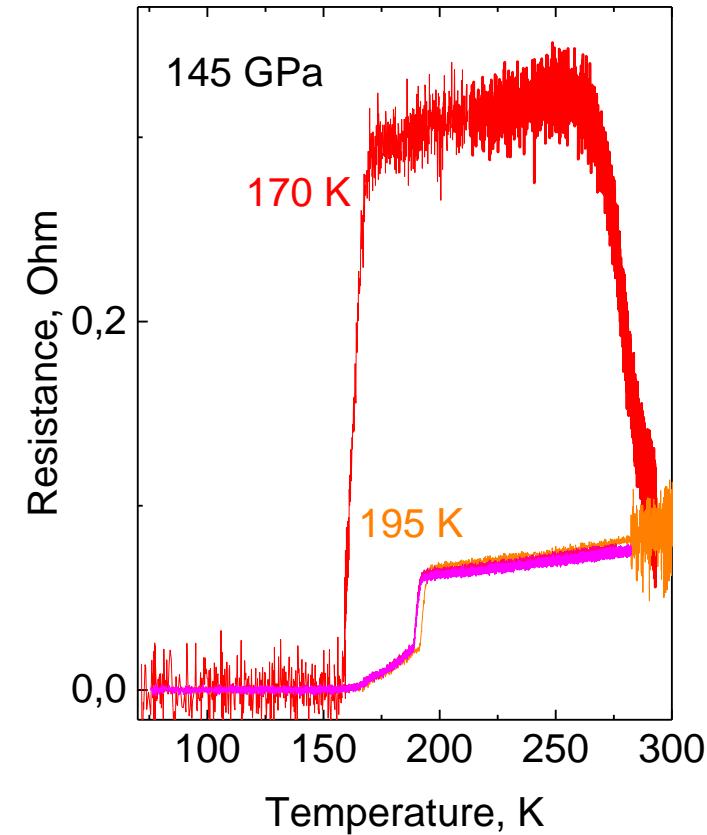
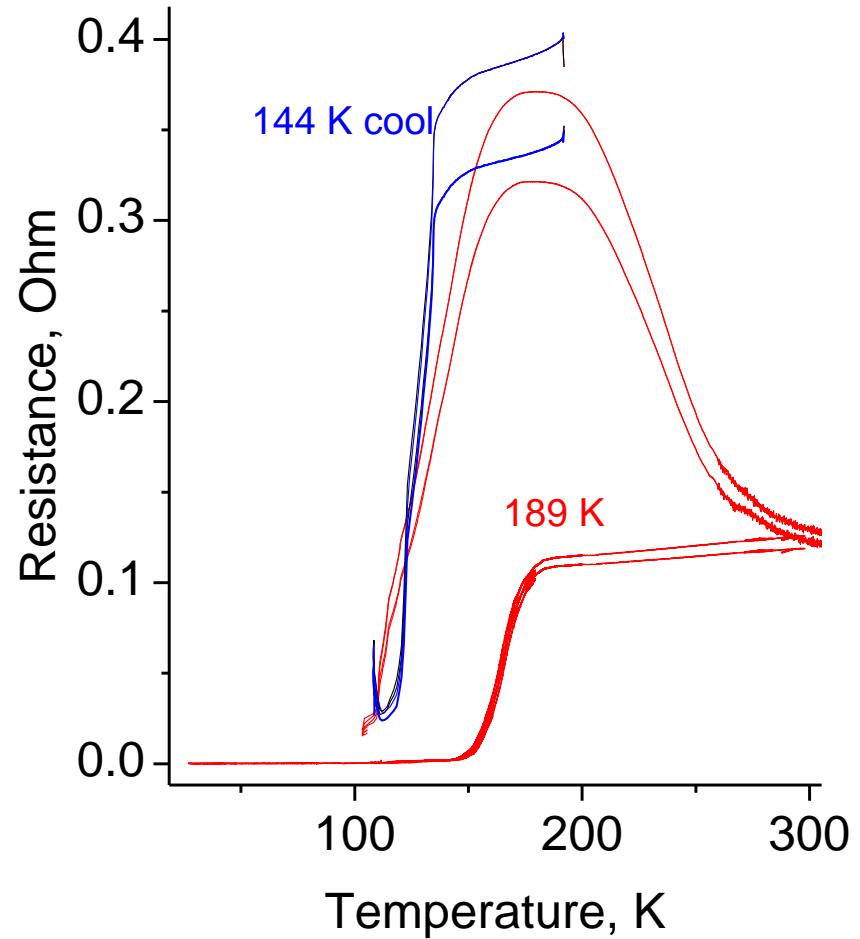


Alexander
Drozdov



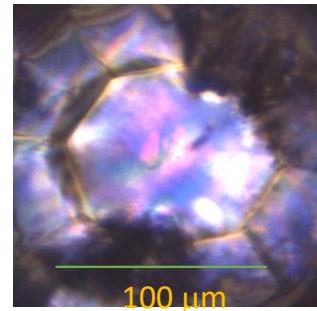
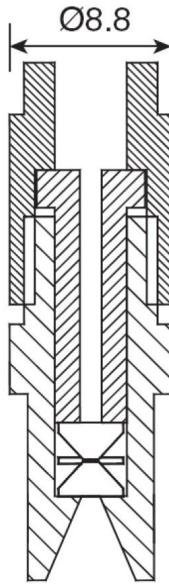
A. Drozdov, M. Eremets et al,
Nature **525**, 73 (2015)

Temperature effect on the sample



Evidence of the superconductivity in sulfur hydride

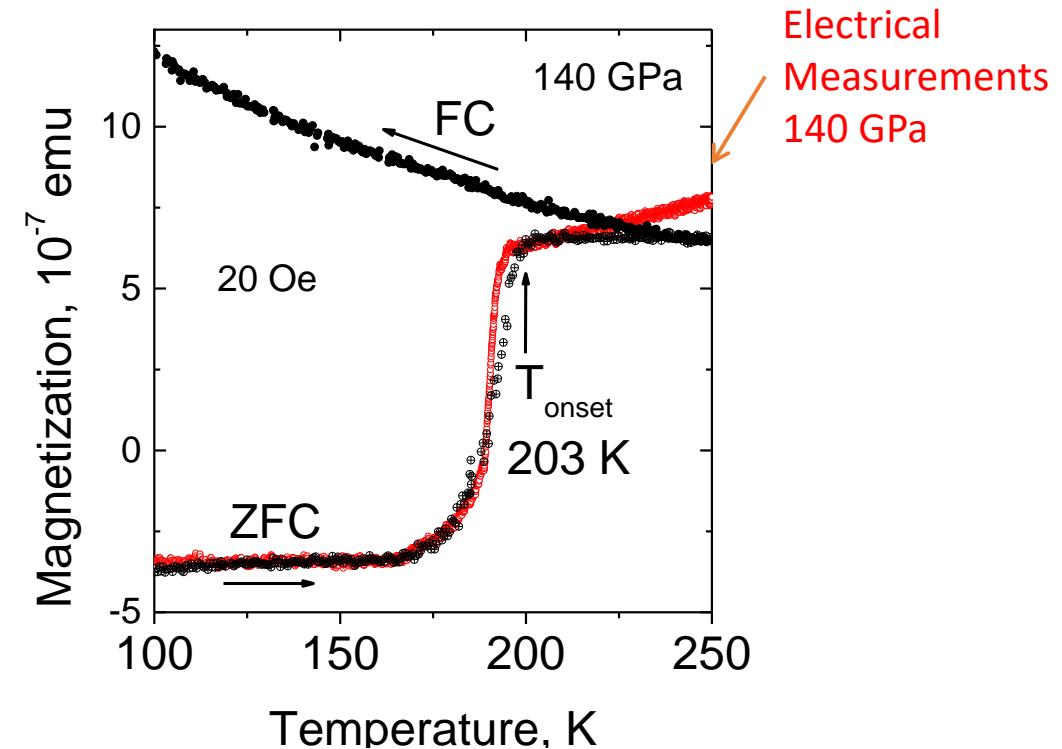
Susceptibility measurements in SQUID



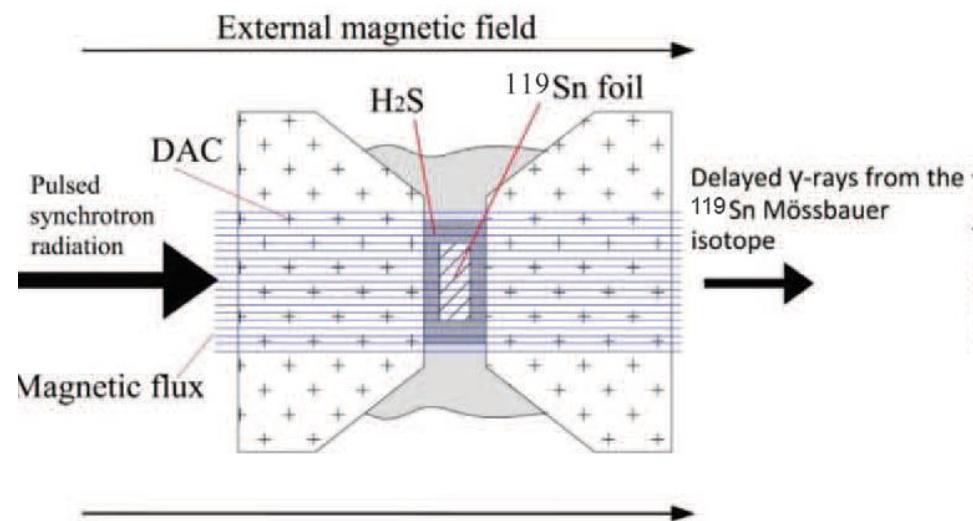
140x120x25 μm^3
Rev Sci Instr 2009

$$M(\text{disk}) \approx 0.2 r^3 H$$

R=50 μm , H=20 Oe $M=6 \cdot 10^{-7}$ emu

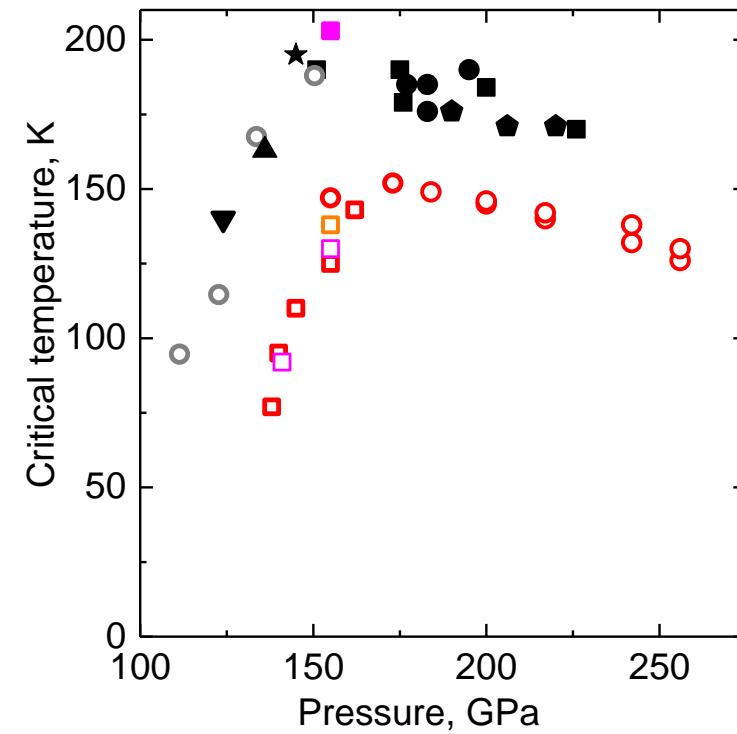
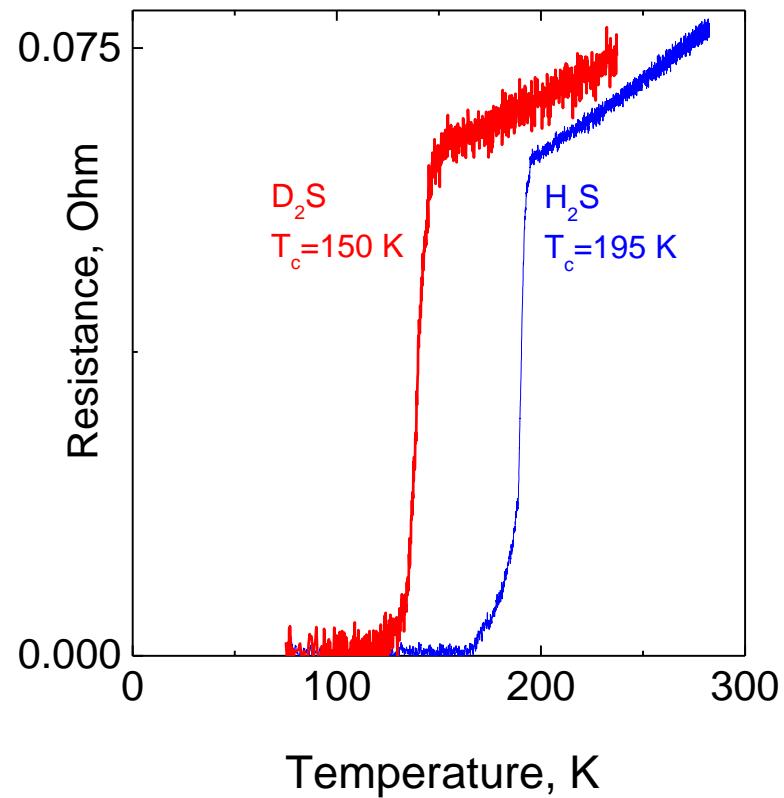


Observation of superconductivity in hydrogen sulfide from nuclear resonant scattering



I. A. Troyan *et al* (2016) Science, 351, 1303

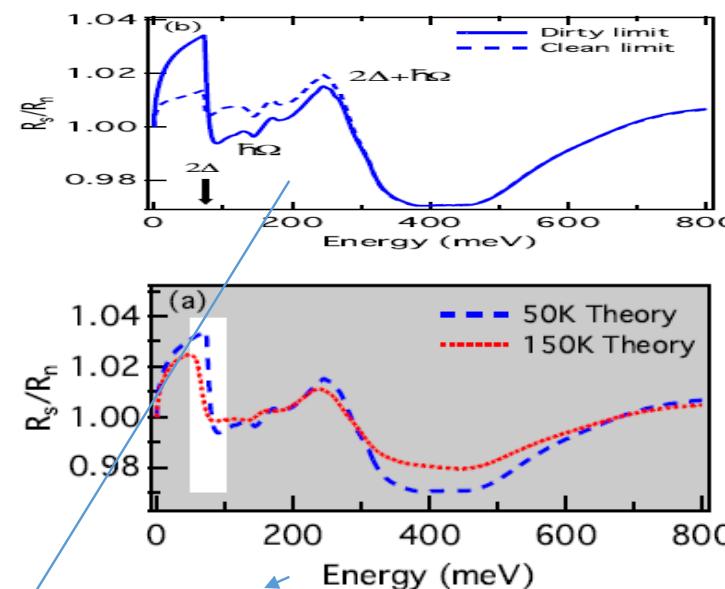
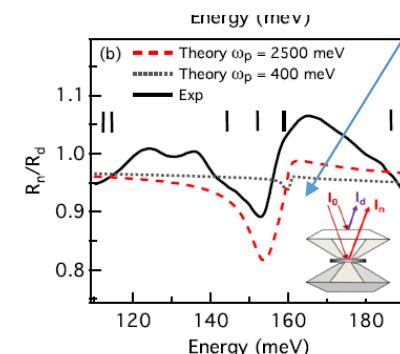
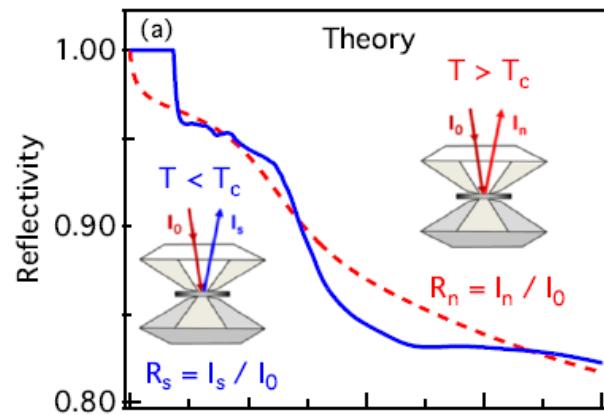
Isotope effect



$$\beta = 0.3$$

$$\beta \equiv -d \ln T_c / d \ln M$$

Infrared studies



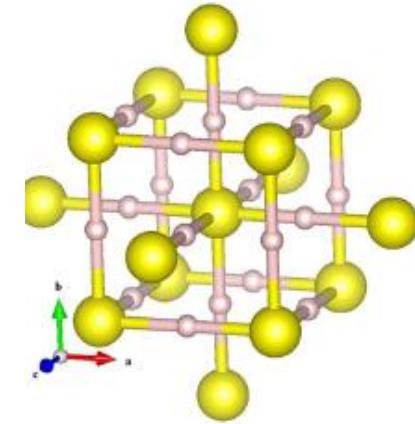
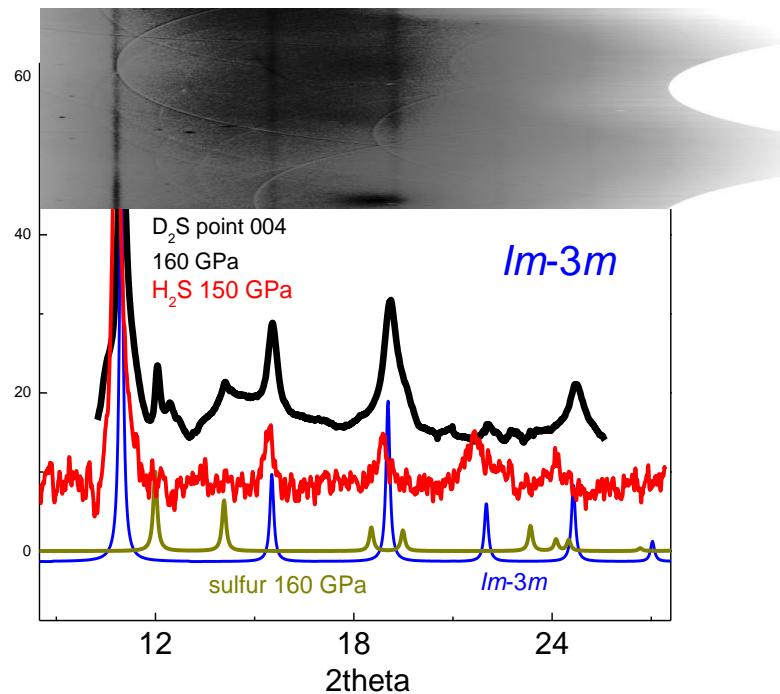
SC gap 70 meV, i.e. $\sim 550 \text{ cm}^{-1}$

$$2\Delta/T_c = 4$$

Electronic Raman

Capitani, F. et al. *Nature Phys.* **13**, 859 (2017)

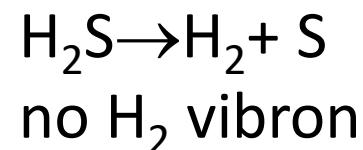
X-ray diffraction



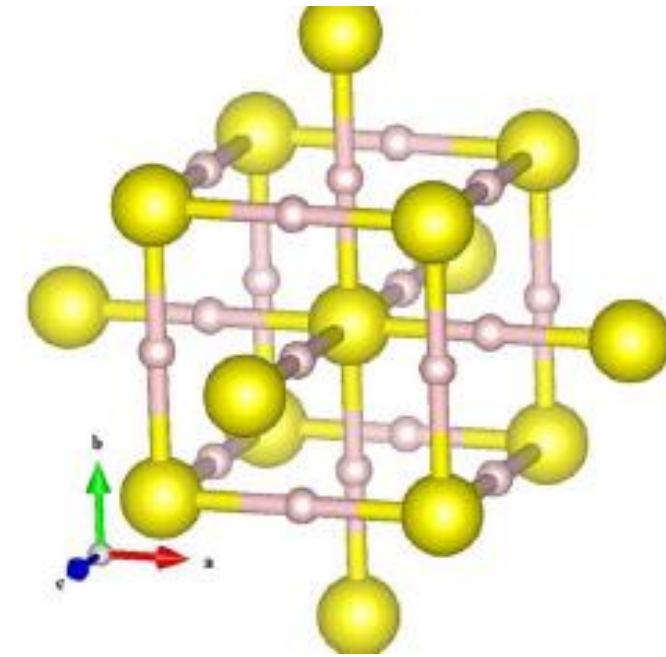
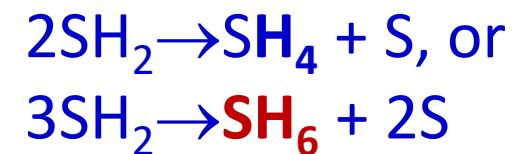
Duan, D. et al. *Sci. Reports* **4**, 6968 (2014).

SPring-8 BL10XU in collaboration with K. Shimizu

Transformation of H_2S to H_3S



Sulfur – hyper valence SF_6



Duan DF et al. Pressure-induced metallization of dense $(\text{H}_2\text{S})_2\text{H}_2$ with high- T_c superconductivity.
Sci Rep 2014; **4**: 6968.

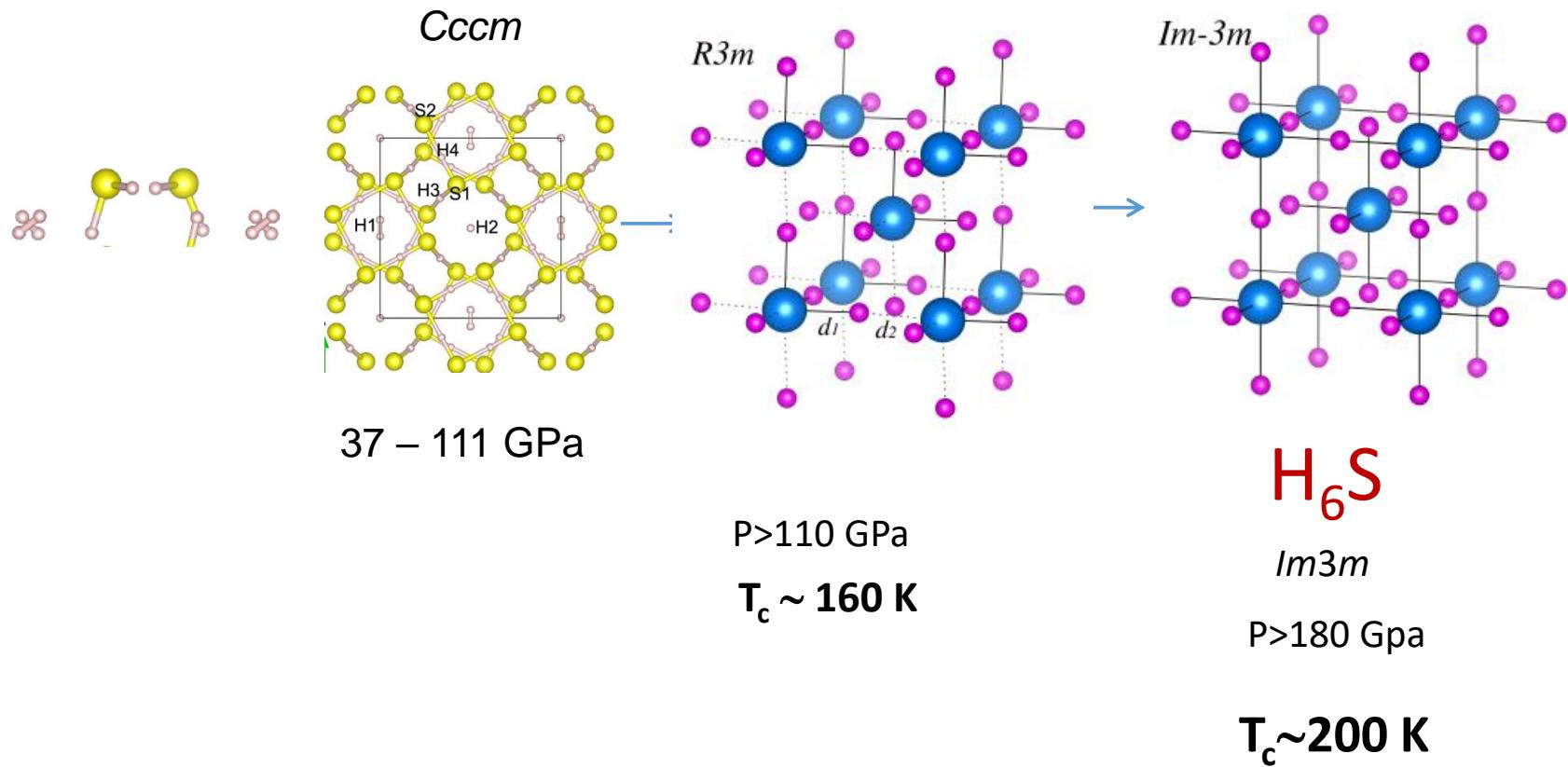
Duan, D. et al. Pressure-induced decomposition of solid hydrogen sulfide. *Phys. Rev. B* **91**, 180502(R) (2015).

Pressure-induced metallization of dense $(\text{H}_2\text{S})_2\text{H}_2$ with high- T_c superconductivity

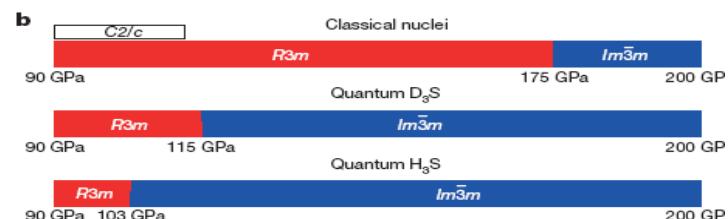
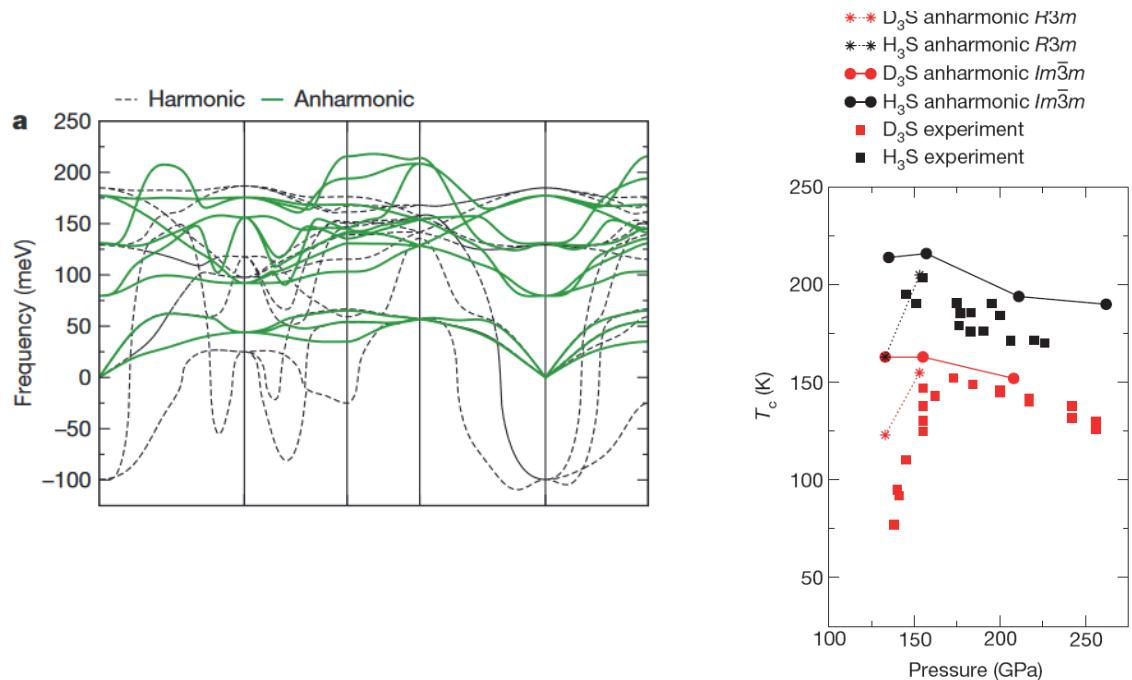
Defang Duan^{1,2}, Yunxian Liu¹, Fubo Tian¹, Da Li¹, Xiaoli Huang¹, Zhonglong Zhao¹, Hongyu Yu¹,
Bingbing Liu¹, Wenjing Tian² & Tian Cui¹

SCIENTIFIC REPORTS | 4

Strobel *et al* 2011 P> 3.5 GPa $(\text{H}_2\text{S})_2\text{H}_2 = \text{H}_6\text{S}$



Corrections to calculated T_c

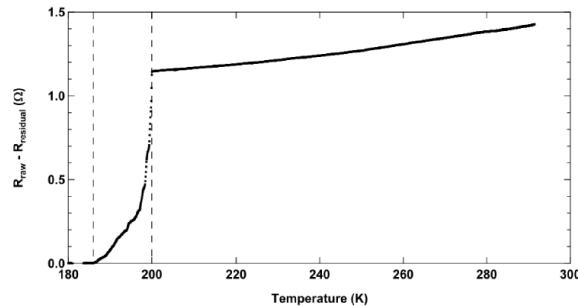
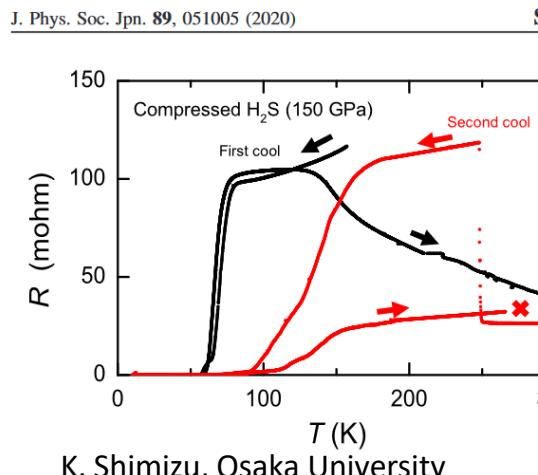


Errea, I. et al. *Nature*, 532, 81 (2016)

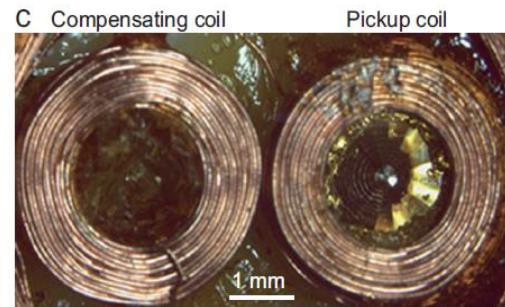
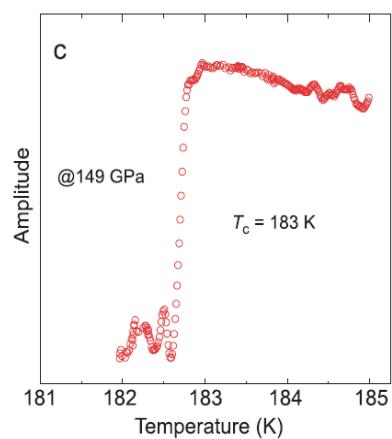
	T_c (K)	Remark
Duan <i>et al.</i> [19]	184	McMillan ($\mu^* = 0.13$)
Errea <i>et al.</i> [27]	190	const. DOS ME ($\mu^* = 0.16$) + anharmonicity
Flores-Livas <i>et al.</i> [25]	180	SCDFT ($P = 200$ GPa)
Akashi <i>et al.</i> [26]	211	SCDFT + plasmon different approximation with Ref. [25]
This work	181	
	~147	static vertex correction ~ -34 K
	~167	plasmon effect $\sim +20$ K
Experiment [15]	~160	extrapolation of Fig. 2 of Ref. [15]

W. Sano et al. *Phys. Rev. B* 93, 094525 (2016)

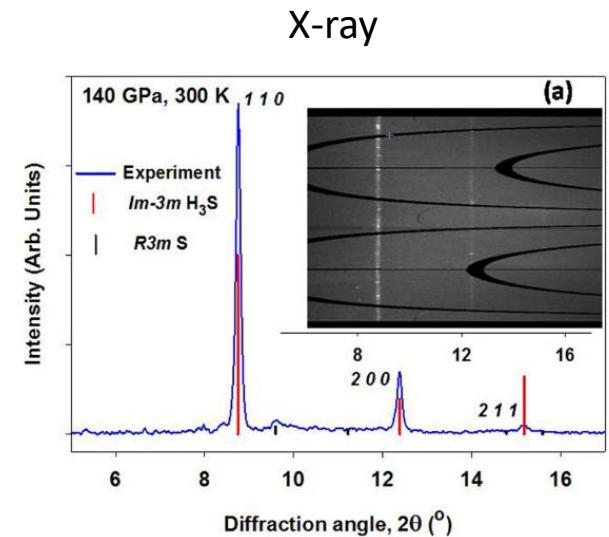
Verification in other laboratories



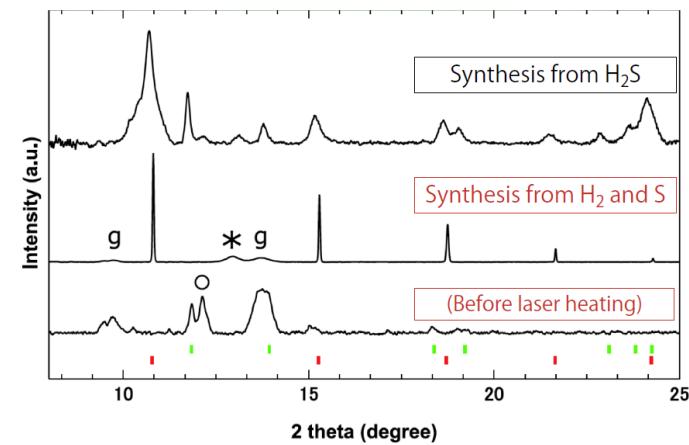
Nakao et al J. Phys. Soc. Jpn 88, 123701 (2019)



X. Huang et al, Nat. Sci. Rev. 6: 713, 2019



Goncharov et al Pys. Rev. B95, 140101(R) (2017)

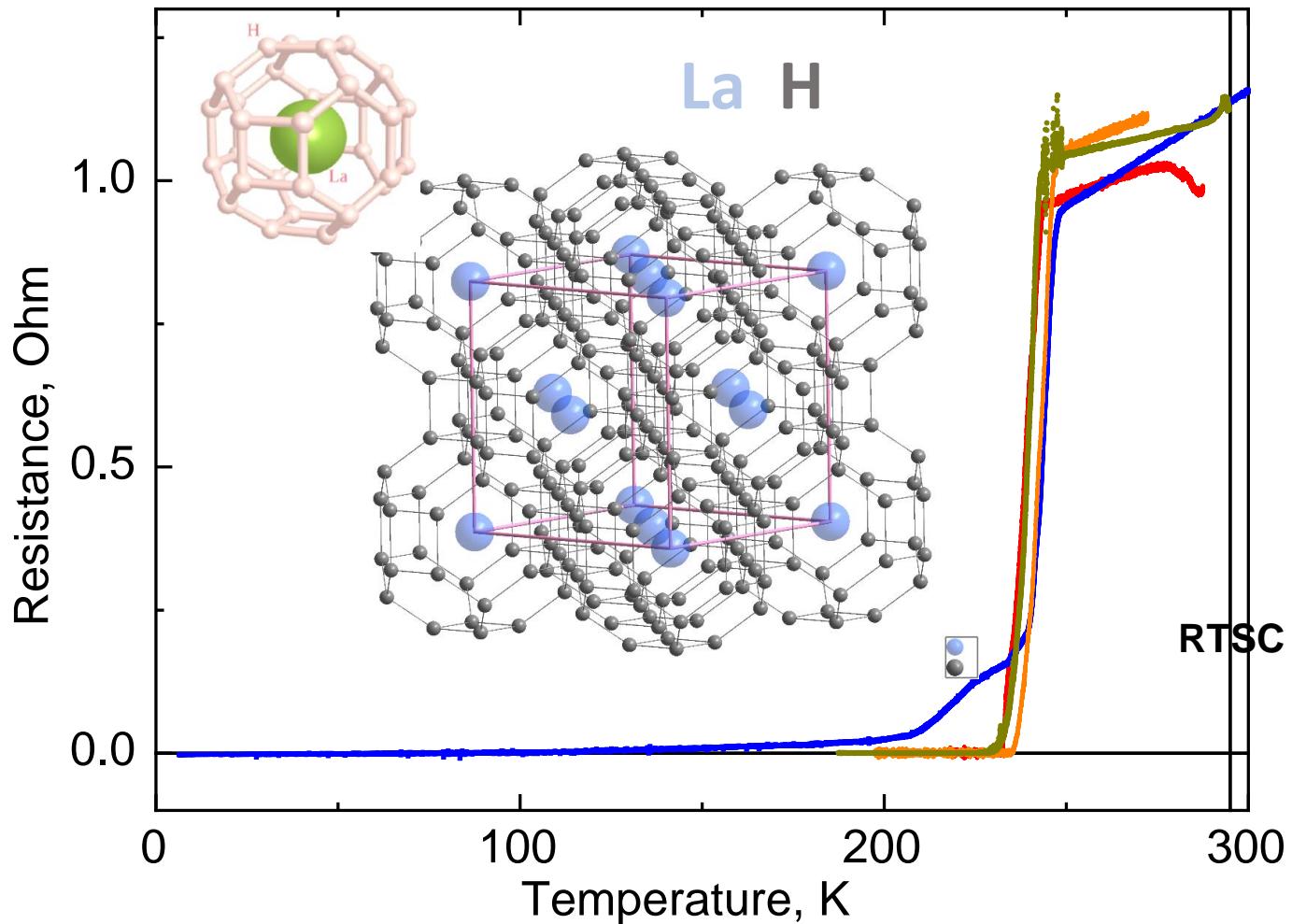


A firm basis for the study on the pressure-induced hydride superconductors is thus established

R. Akashi JPSJ News and Comments 16, 18 (2019)

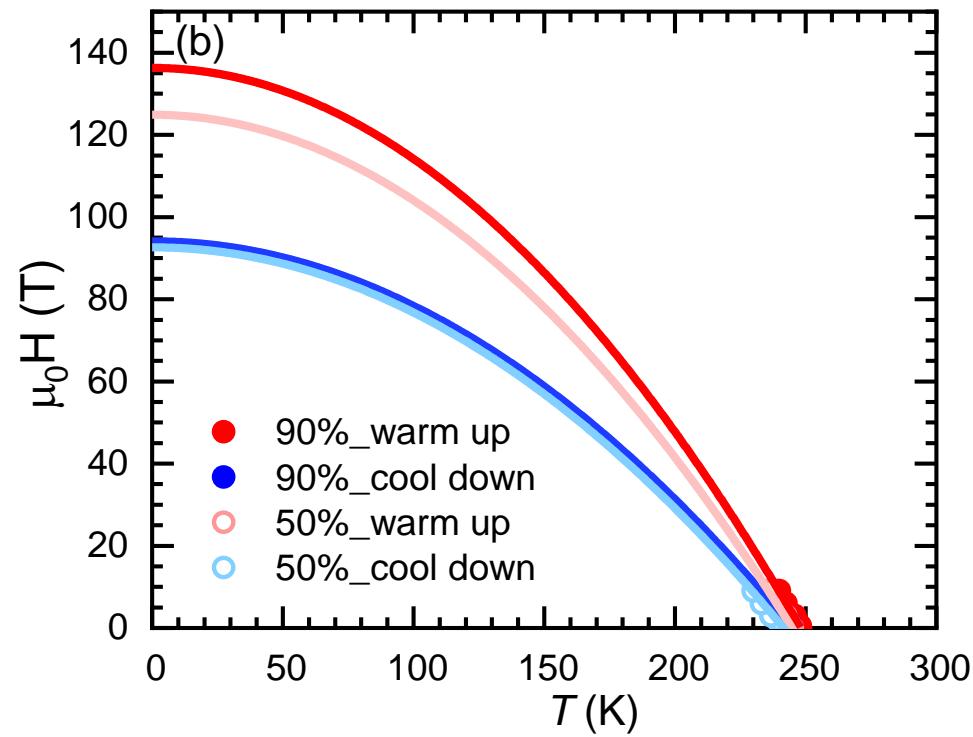
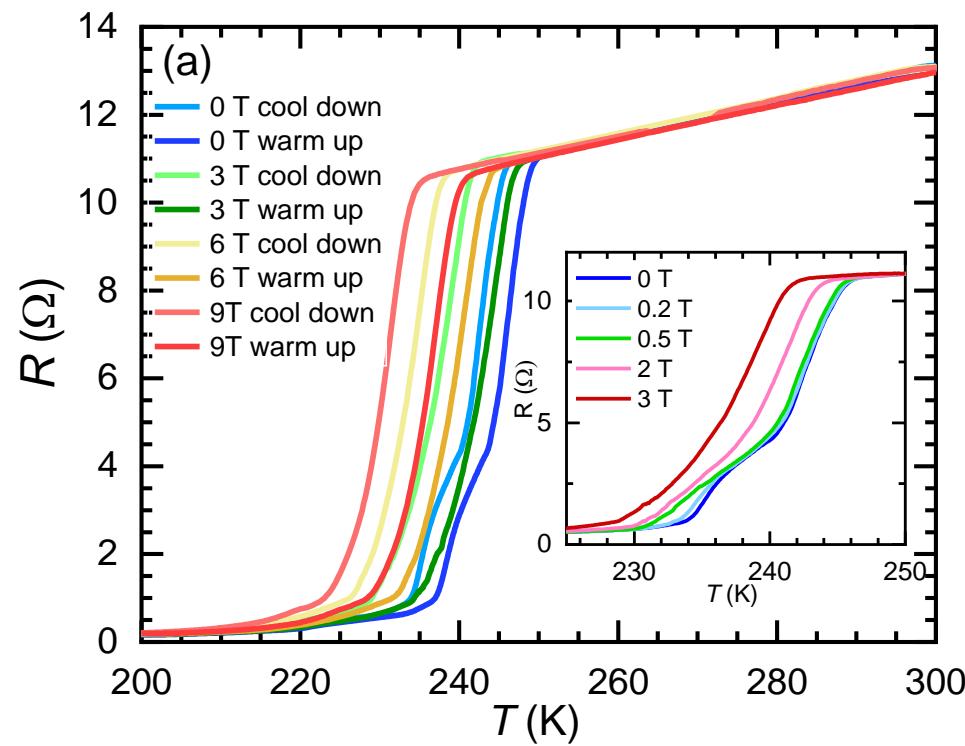
Lanthanum hydride

Superconductivity in lanthanum hydride

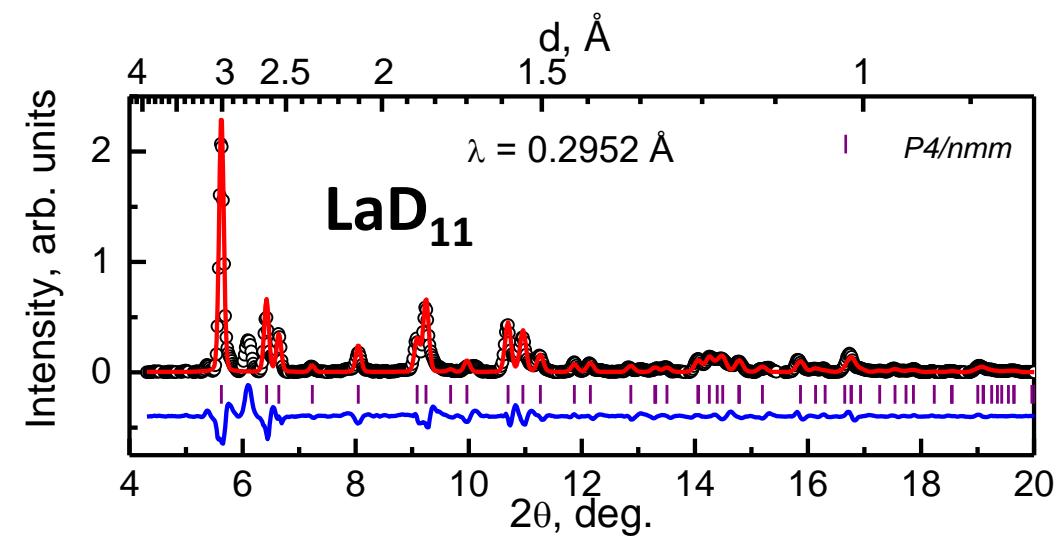
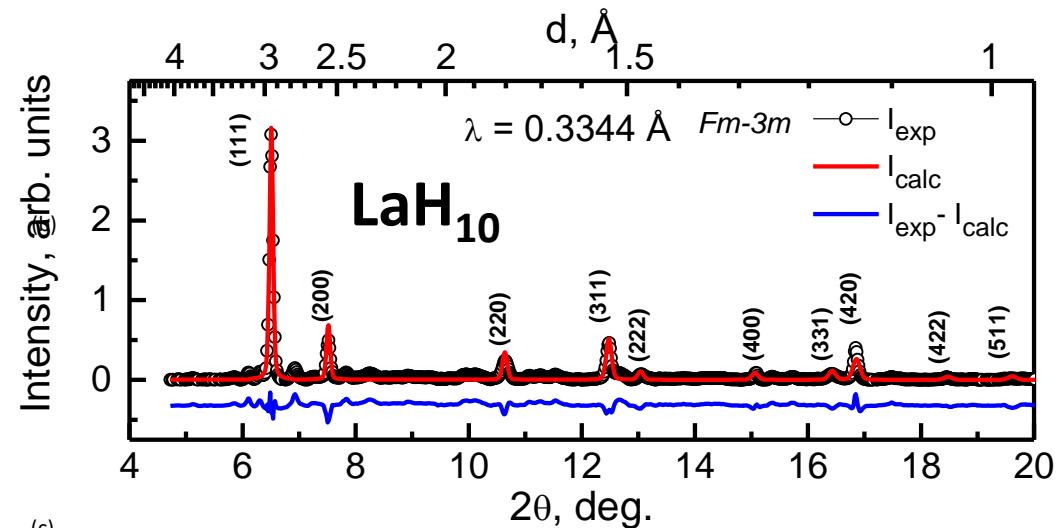
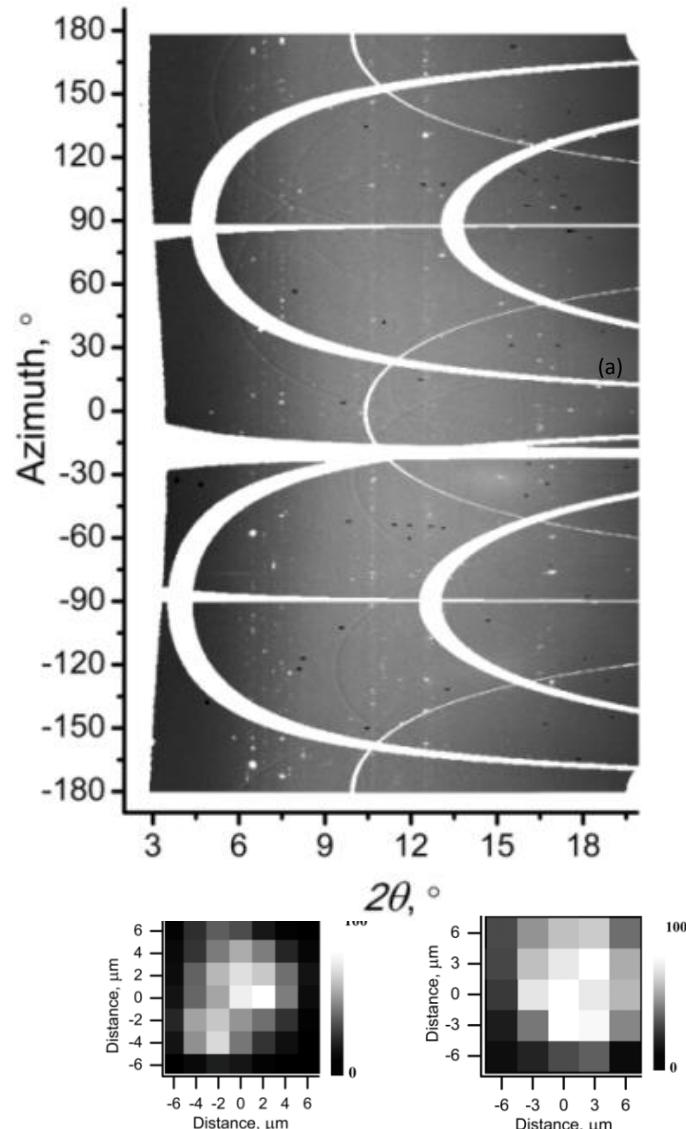


Drozdov, A. P. et al. *Nature* **569**
528 (2019)

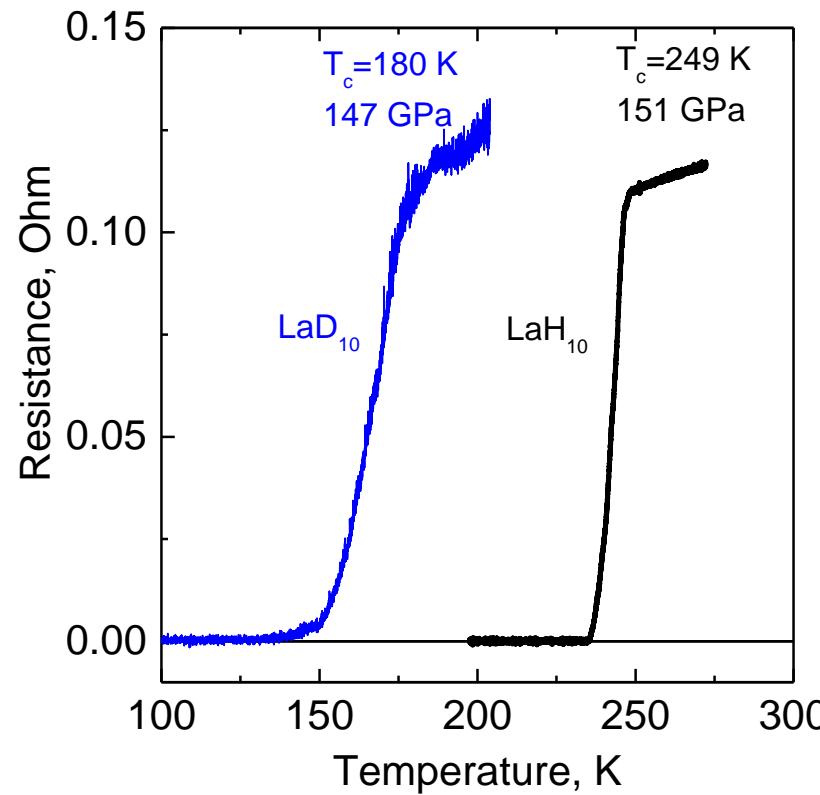
Superconducting transition in dependence on external magnetic fields



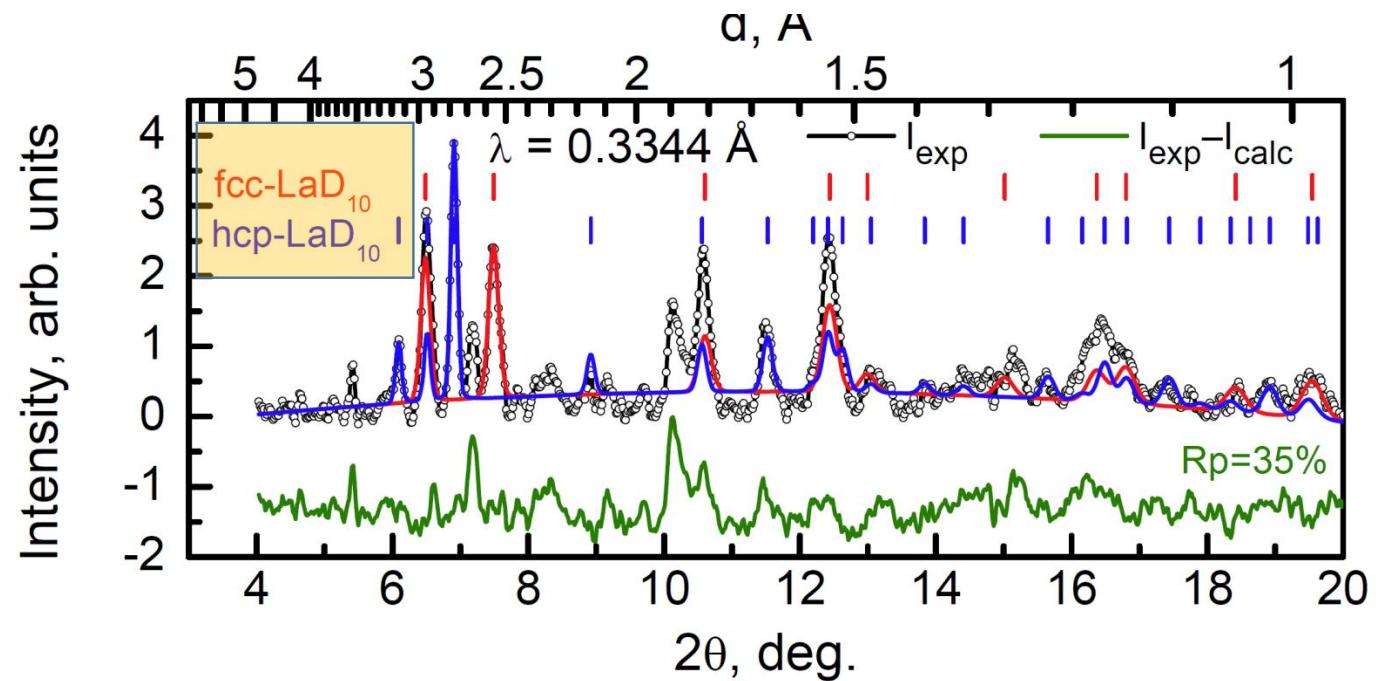
X-ray diffraction



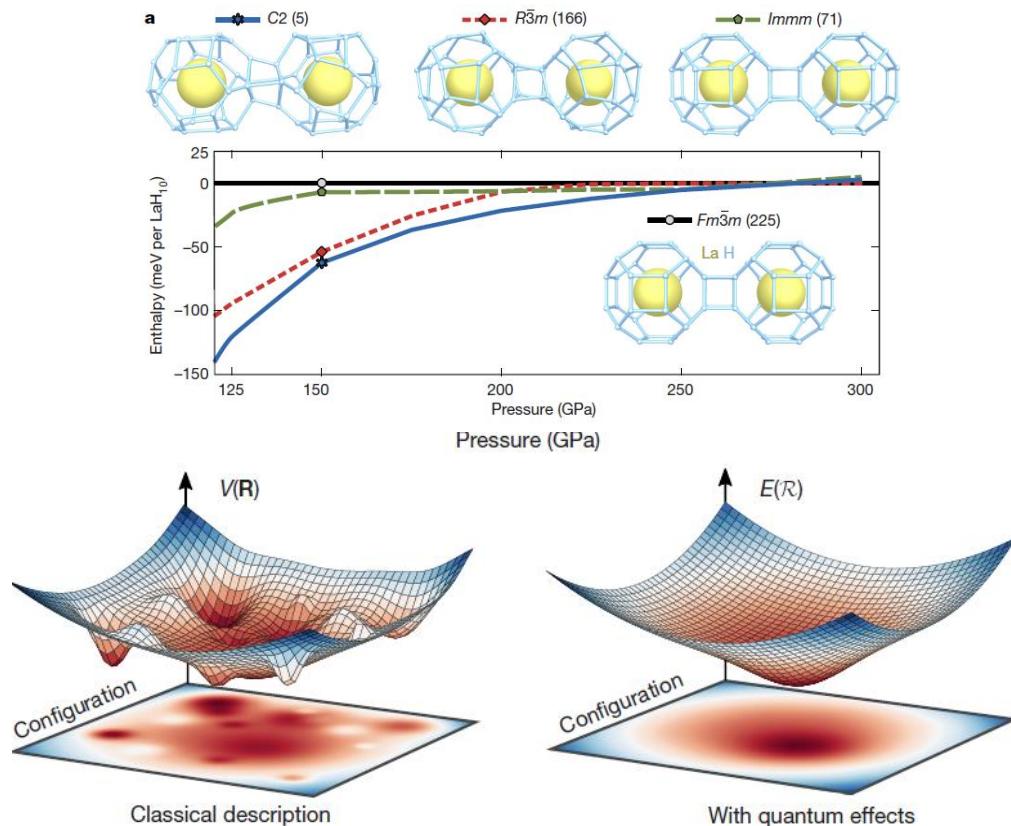
Isotope effect for LaH₁₀



$$\alpha=0.46$$



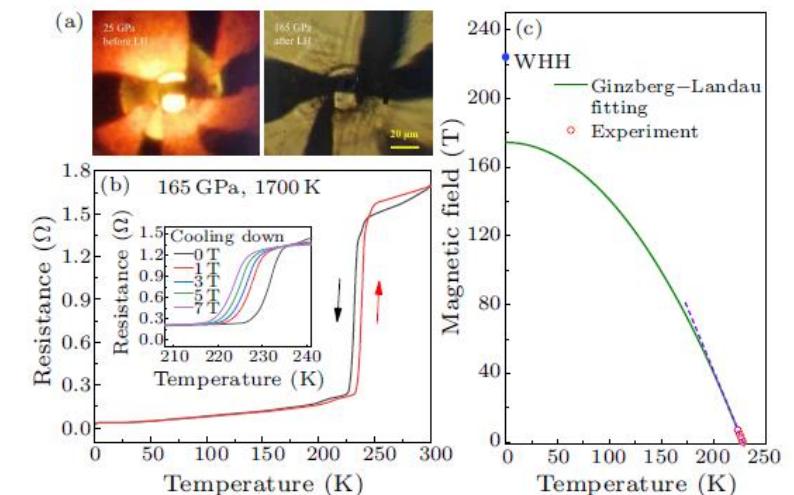
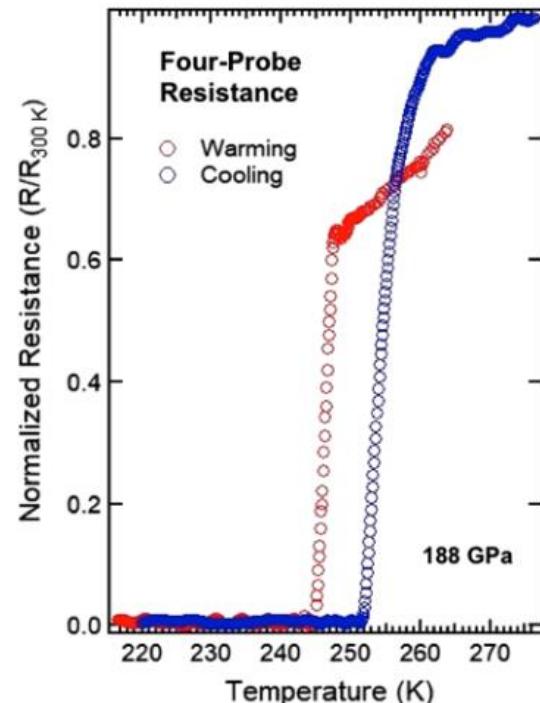
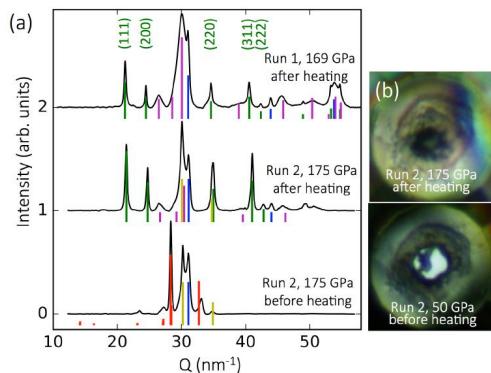
Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride



... if we consider correctly quantum fluctuations probably we will find high- T_c superconductors at much lower pressures.

Errea et al *Nature* **578** (2020).

Other laboratories



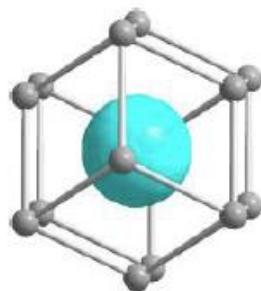
F. Hong et al Chin. Phys. Lett. 37 (2020) 107401

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,†}

Yttrium hydride

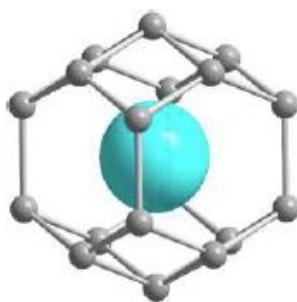
YH_3



YH_{14}

Fm-3m

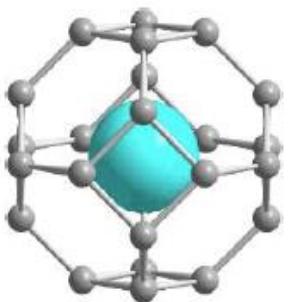
YH_4



YH_{18}

I4/mmm

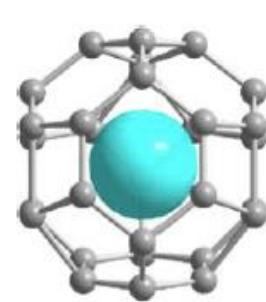
YH_6



YH_{24}

Im-3m

YH_9

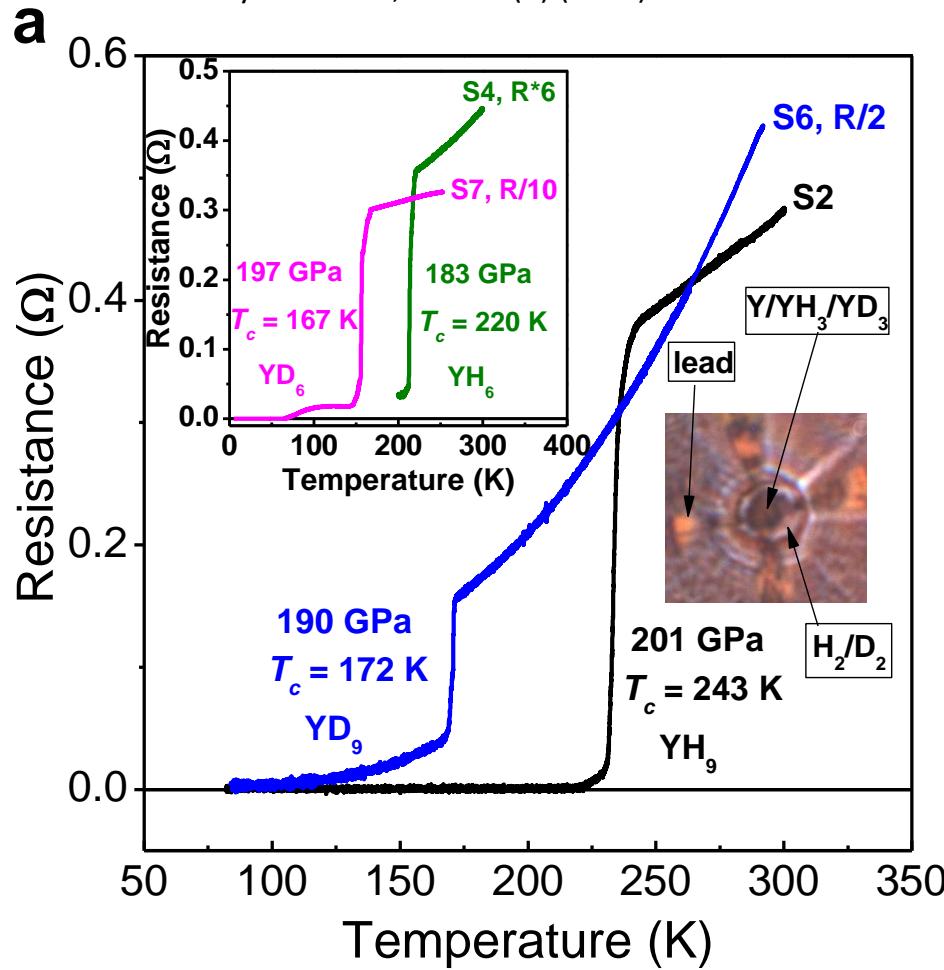


YH_{29}

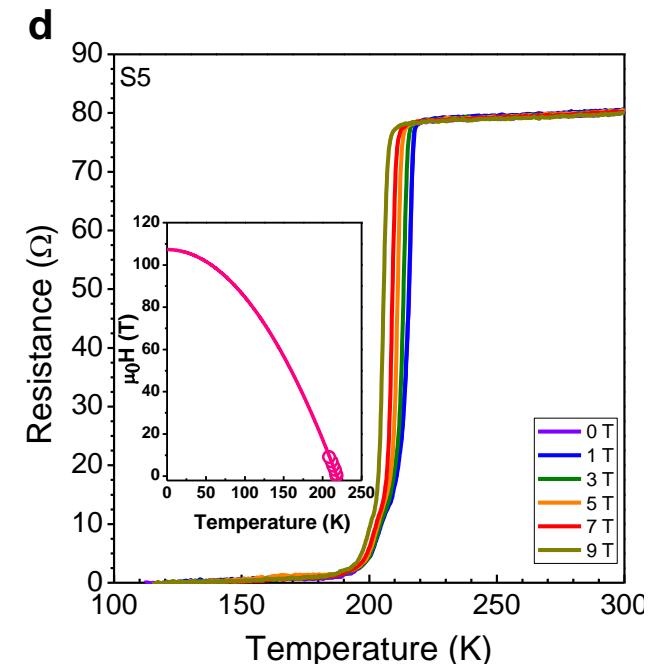
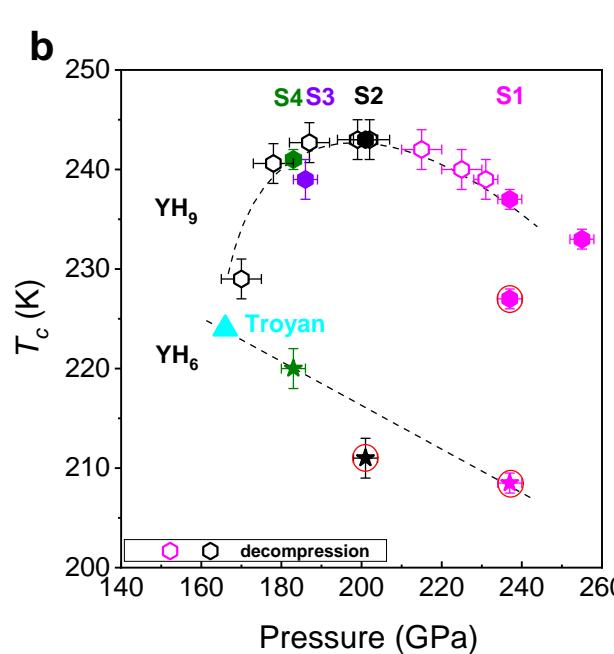
P63/mmc

YH_6 $T_c \sim 260 \text{ K}$ at 110 GPa $T_c \sim 227 \text{ K}$ at 237 GPa
 YH_9 $T_c \sim 265 \text{ K}$ at 200 GPa, $T_c \sim 243 \text{ K}$ at 200 GPa
 YH_{10} $T_c \sim 315 \text{ K}$ at 250 GPa T_c ??????

H. Liu et al *Proc. Nat. Acad. Sci.* 114, 6990 (2017)
 F. Peng et al *Phys. Rev. Lett.* 119, 107001 (2017)
 Heil et al *Phys. Rev. B* 99, 220502(R) (2019)

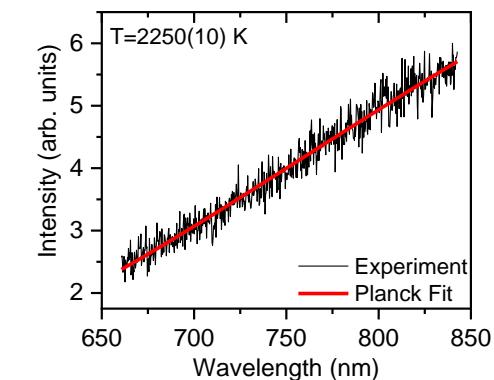
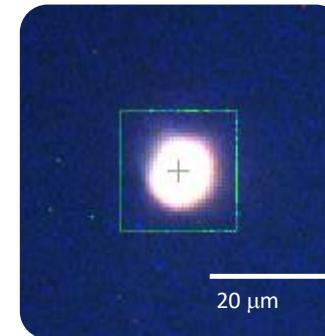
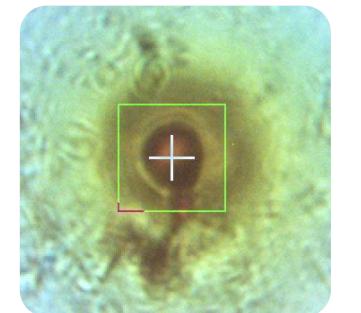
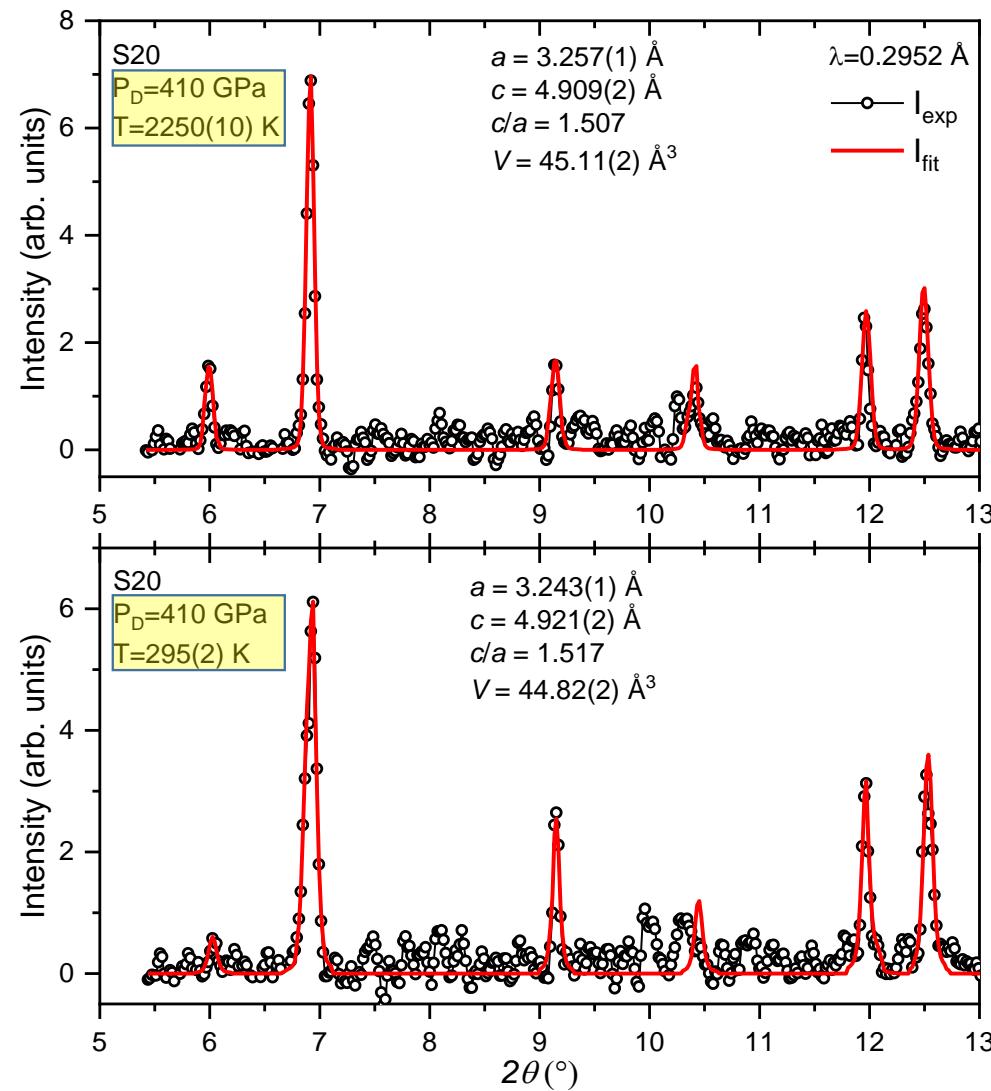


Yttrium hydride



Kong, P. P. et al. Superconductivity up to 243 K in yttrium hydrides under high pressure *arXiv:1909.10482* (2019)

X-ray diffraction from YH9 at 410 GPa and 2230 K

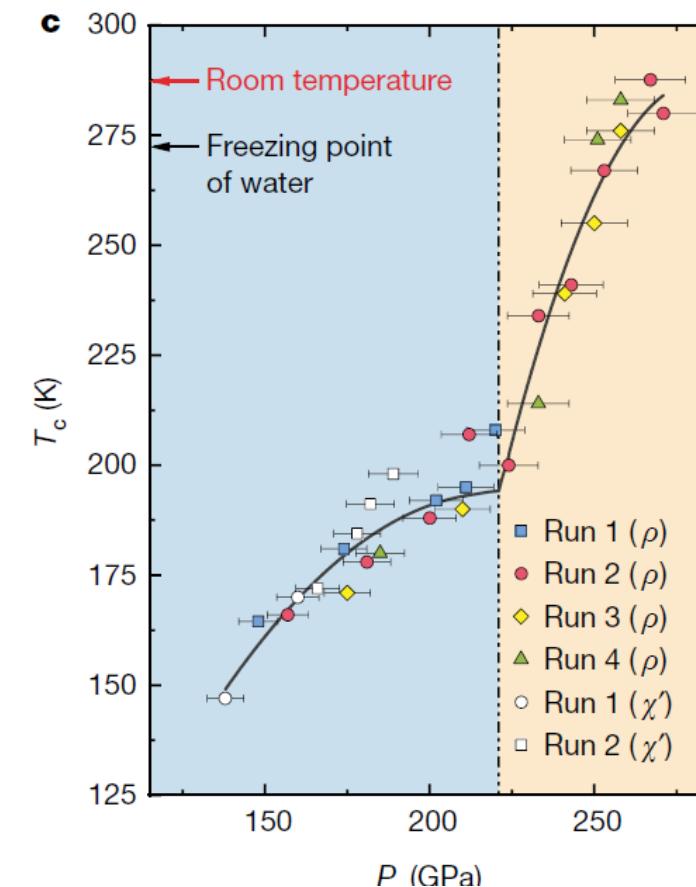
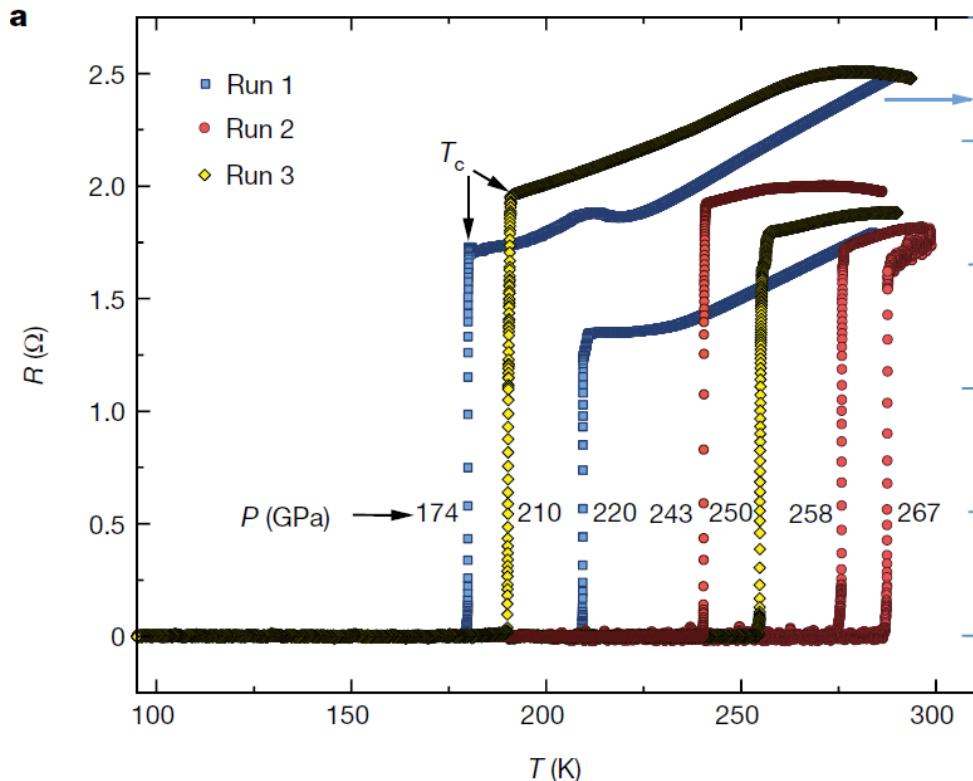


Room-temperature superconductivity in a carbonaceous sulfur hydride

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

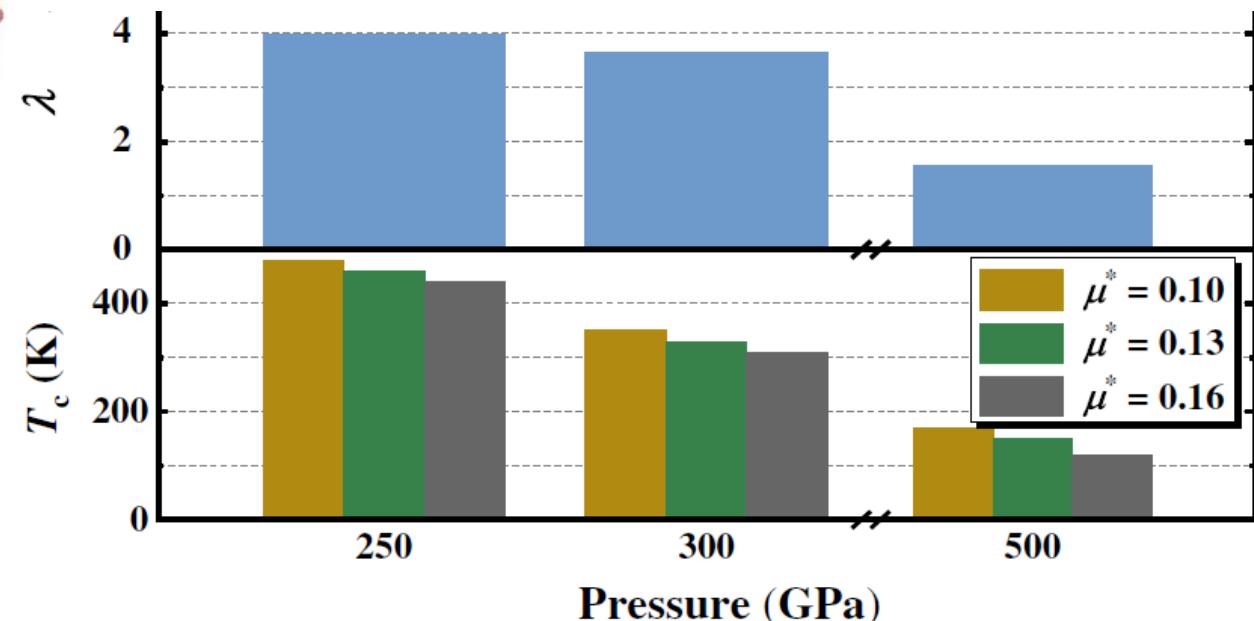
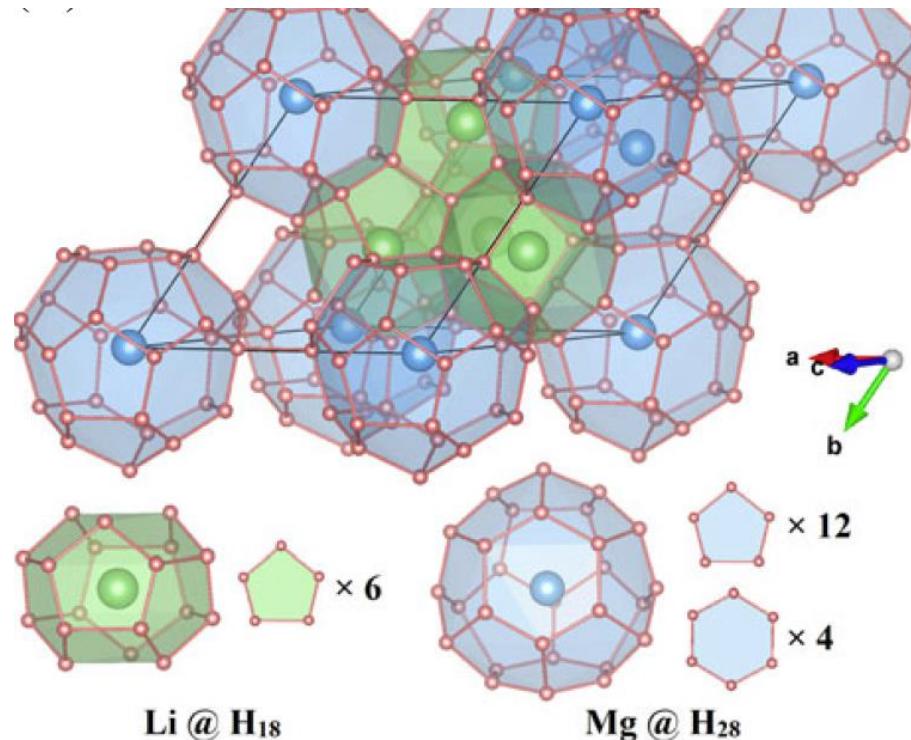
Received: 31 August 2020

Elliot Snider^{1,6}, Nathan Dasenbrock-Gammon^{2,6}, Raymond McBride^{1,6}, Mathew Debessai³,
Hiranya Vindana², Kevin Vencatasamy², Keith V. Lawler⁴, Ashkan Salamat⁵ & Ranga P. Dias^{1,2,✉}



Route to a Superconducting Phase above Room Temperature in Electron-Doped Hydride Compounds under High Pressure

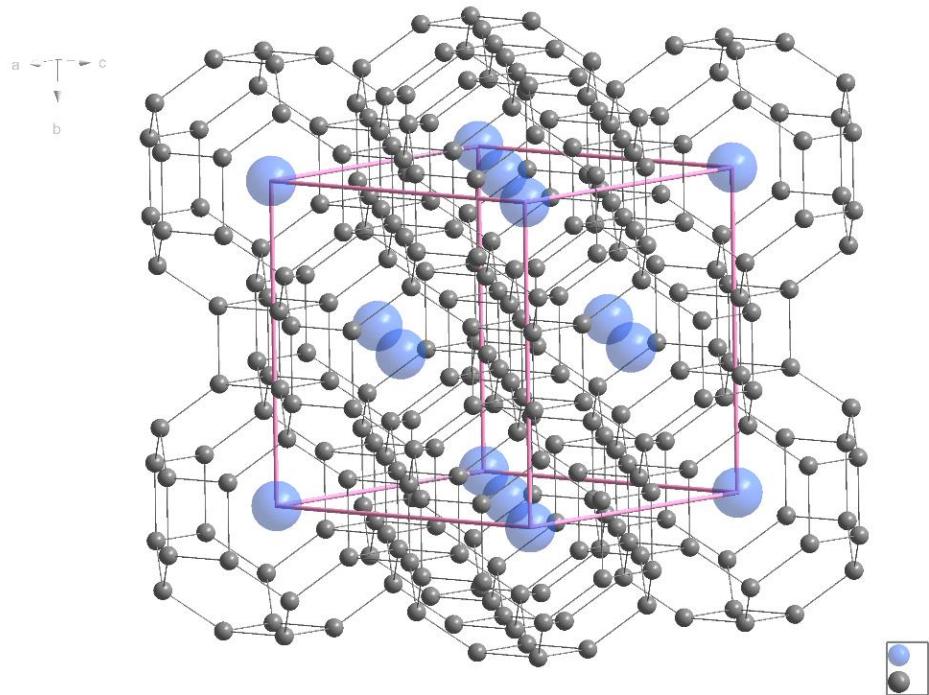
Ying Sun,¹ Jian Lv,¹ Yu Xie,¹ Hanyu Liu,^{1,*} and Yanming Ma^{1,2,†}



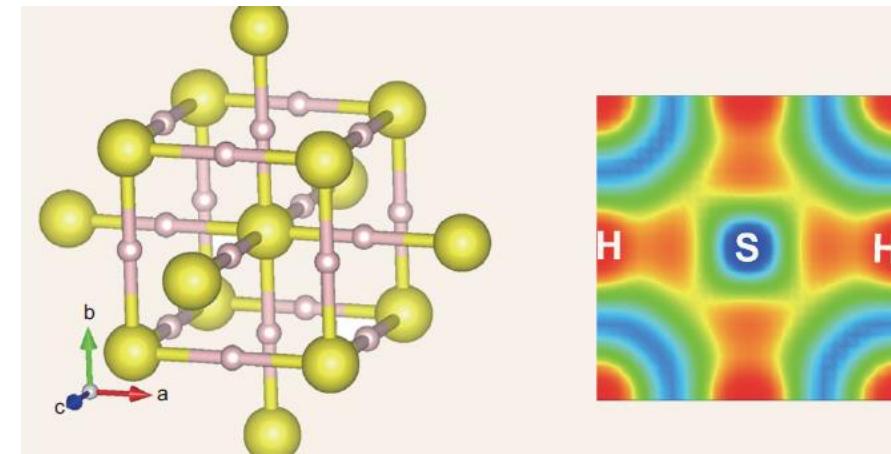
$\text{Li}_2\text{MgH}_{16}$ ($Fd\bar{3}m$)

Experimentally studied hydrides

- SiH₄ 17 K** Eremets et al , *Science* 319 68 1506 (2008)
- BaReH₉ 7 K** Muramatsu et al, *J. Phys. Chem. C* 119 18007 (2015)
- H₃S 203 K** Drozdov et al, *Nature* 525 (2015)
- PH₃ 100 K** Drozdov et al, *arXiv:1508.06224* (2015)
- LaH₁₀ 260 K** Somayazulu et al *Phys. Rev. Lett.* 122 027001 (2019)
- LaH₁₀ 250 K** Drozdov et al *Nature* (2019)
- ThH₁₀ 160 K** Semenok et al, *Materials Today* (2019)
- YH₆ 224 K** Troyan et al *arXiv 1908.01534* (2019)
- YH₆ 227 K** Kong et al *arXiv 1909.10482* (2019)
- YH₉ 243 K** Kong et al *arXiv 1909.10482* (2019)
- PrH₉ 9 K** Zhou et al, *Sci. Adv.* 2020; 6 (2020)



LaH₁₀ – model of
metallic hydrogen

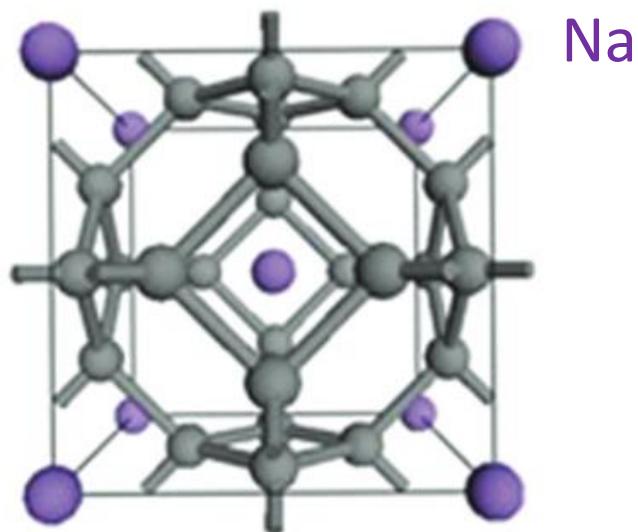


H₃S - covalent metal

Duan et al *Nation. Sci. Rev.* 4: 121–135, 2017

Ambient pressure conventional superconductivity

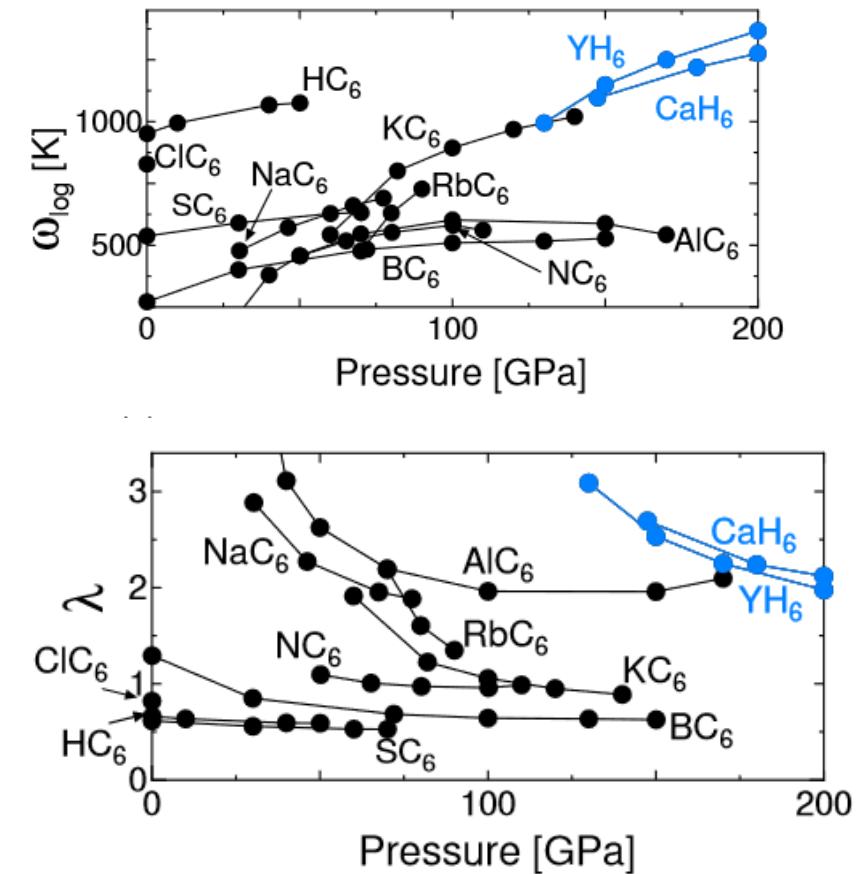
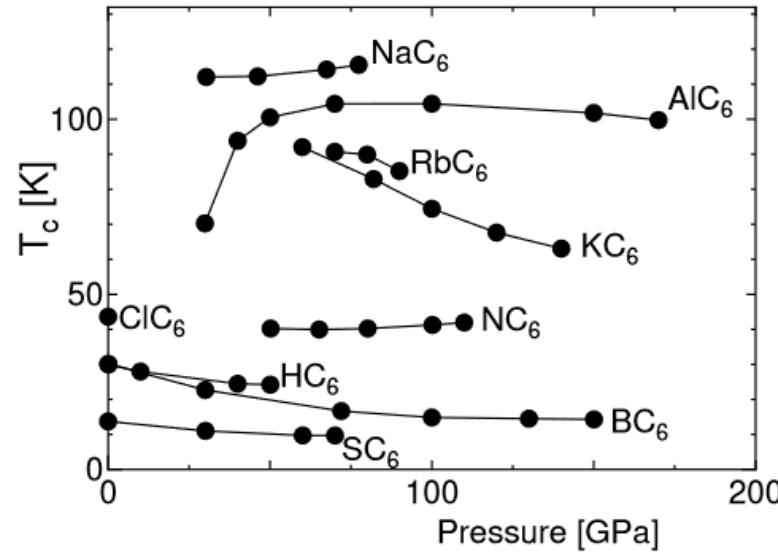
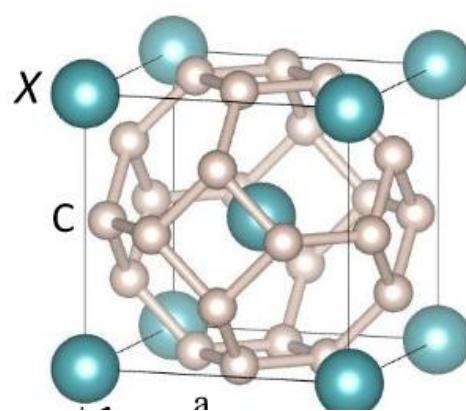
Ambient pressure superconductors



NaC_6 $T_c=116$ K

Lu *et al* Superconductivity in dense
carbon-based materials, Phys. Rev. B **93**,
104509 (2016)

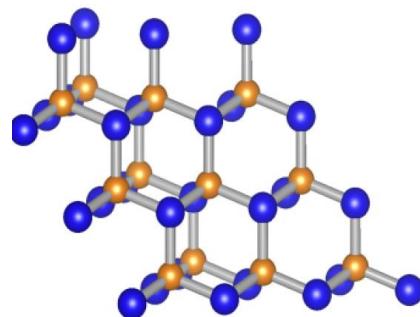
Superconductivity of carbon compounds with sodalite structure



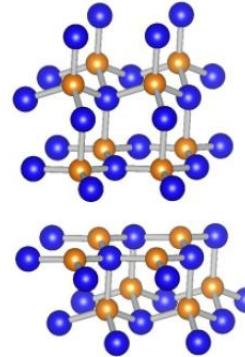
PHYSICAL REVIEW B 102, 024519 (2020)

High-temperature conventional superconductivity in the boron-carbon system: Material trends

Santanu Saha^{1,*}, Simone Di Cataldo^{1,2}, Maximilian Amsler,^{3,4} Wolfgang von der Linden,¹ and Lilia Boeri²

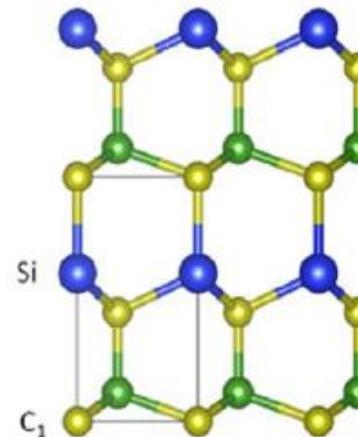


$\lambda = 2.3$ $T_c = 75$ K



$\lambda = 1.1$ $T_c = 53$ K

320 metastable structures with fixed composition B:C (50%/50%)



BSiC₂

$T_c = 74$ K

P. Chen and H.T.Jeng 2020
New J. Phys. 22 033046

Doping, alloying

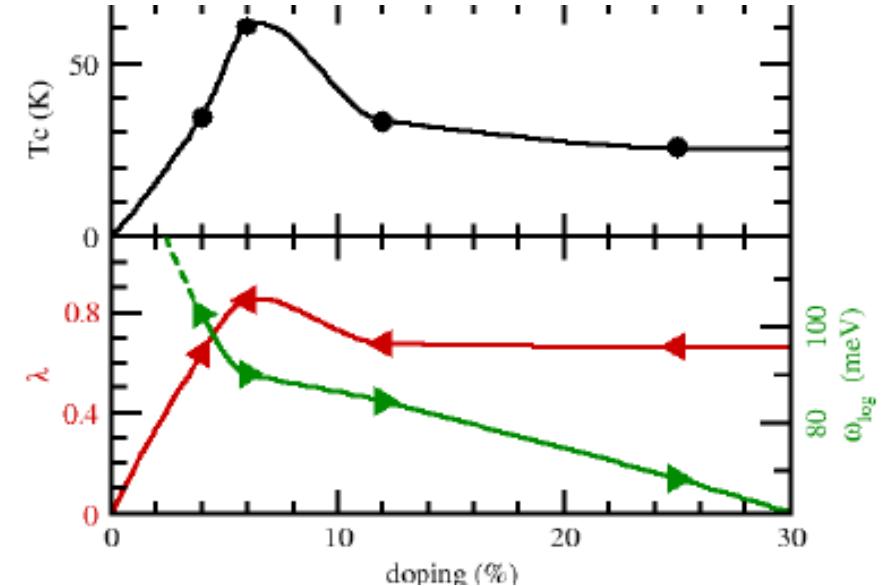
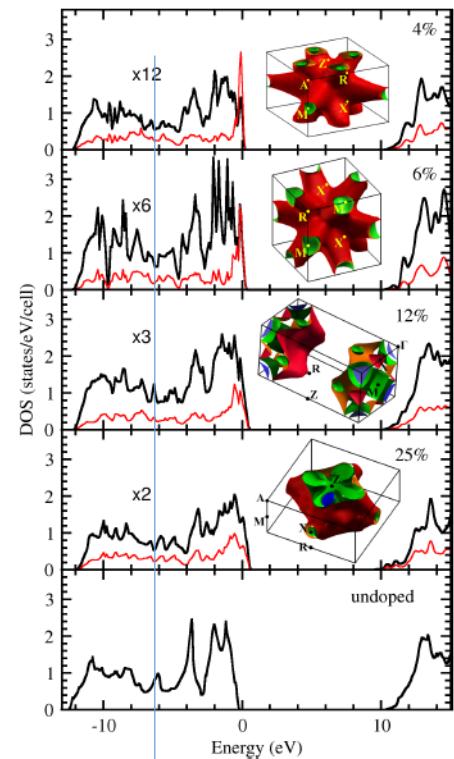
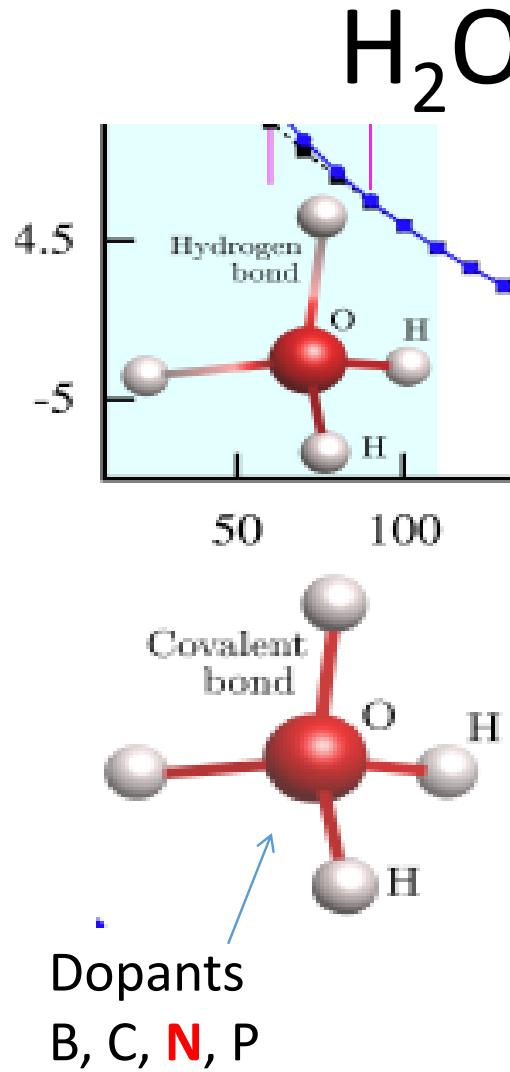
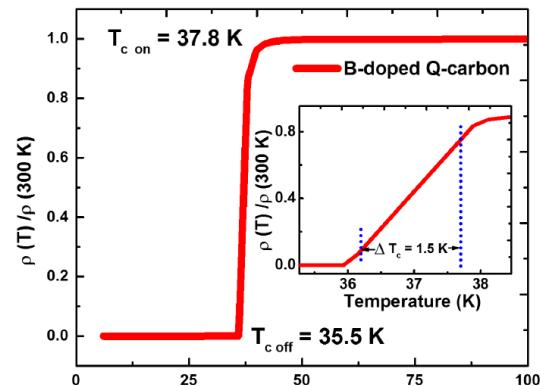


Figure 3. (Color online) Density of states (DOS) and Fermi

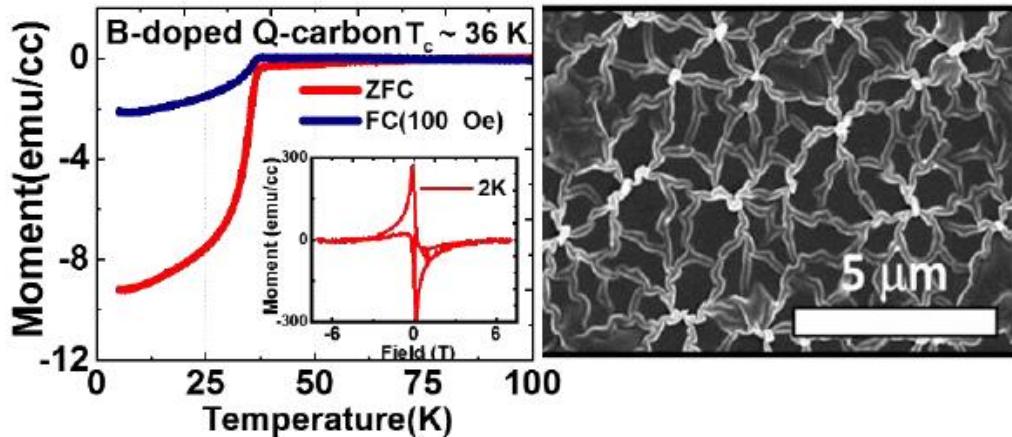
Diamond $\omega_D = 1860$ K,

$T_c > 100$ K but doping

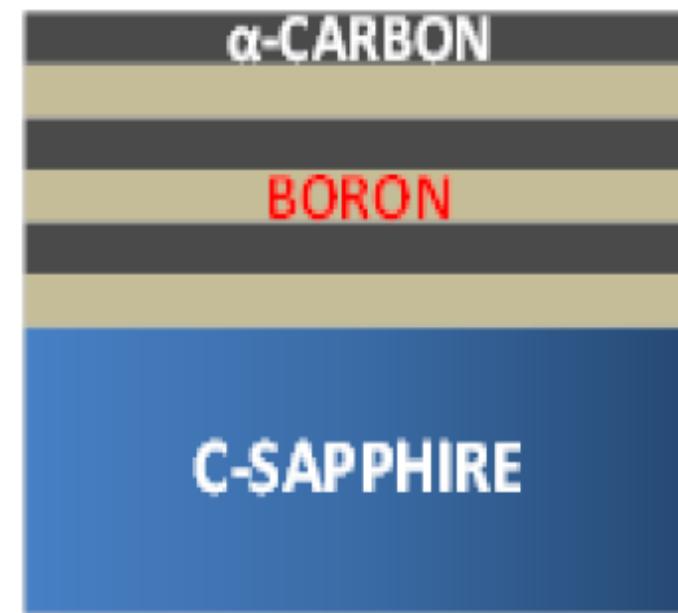
Moussa, J. E. & Cohen, M. L *Phys. Rev. B* **77**, 064518 (2008)



$T_c = 56$ K

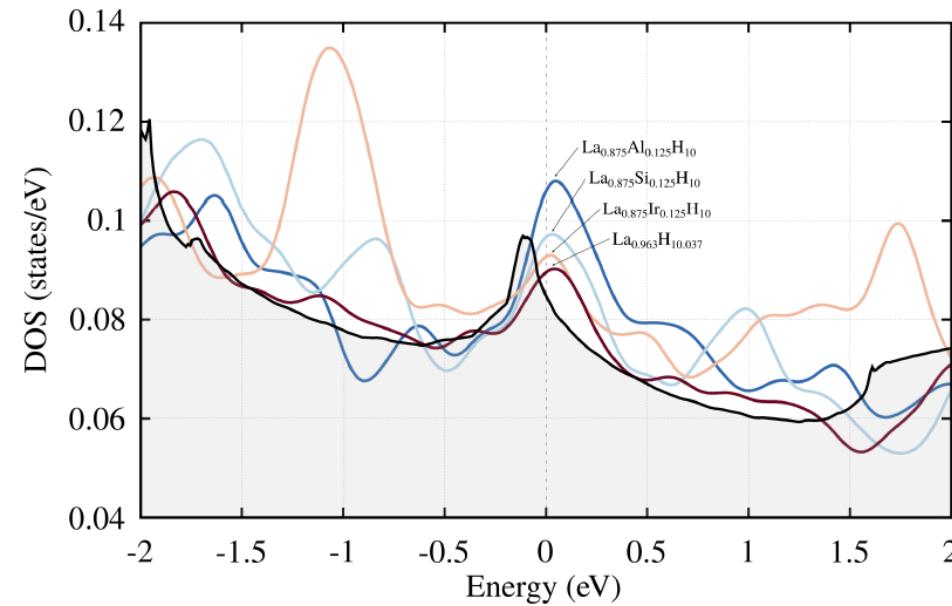
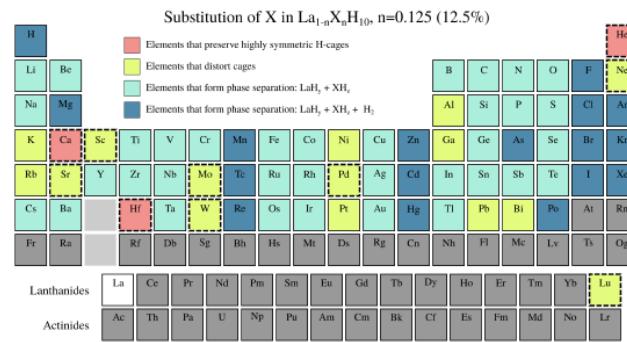


High-Temperature Superconductivity in
Boron-Doped Q-Carbon
A. Bhaumik, R. Sachan, J. Naraya
ACS Nano 2017, and Appl.Phys.



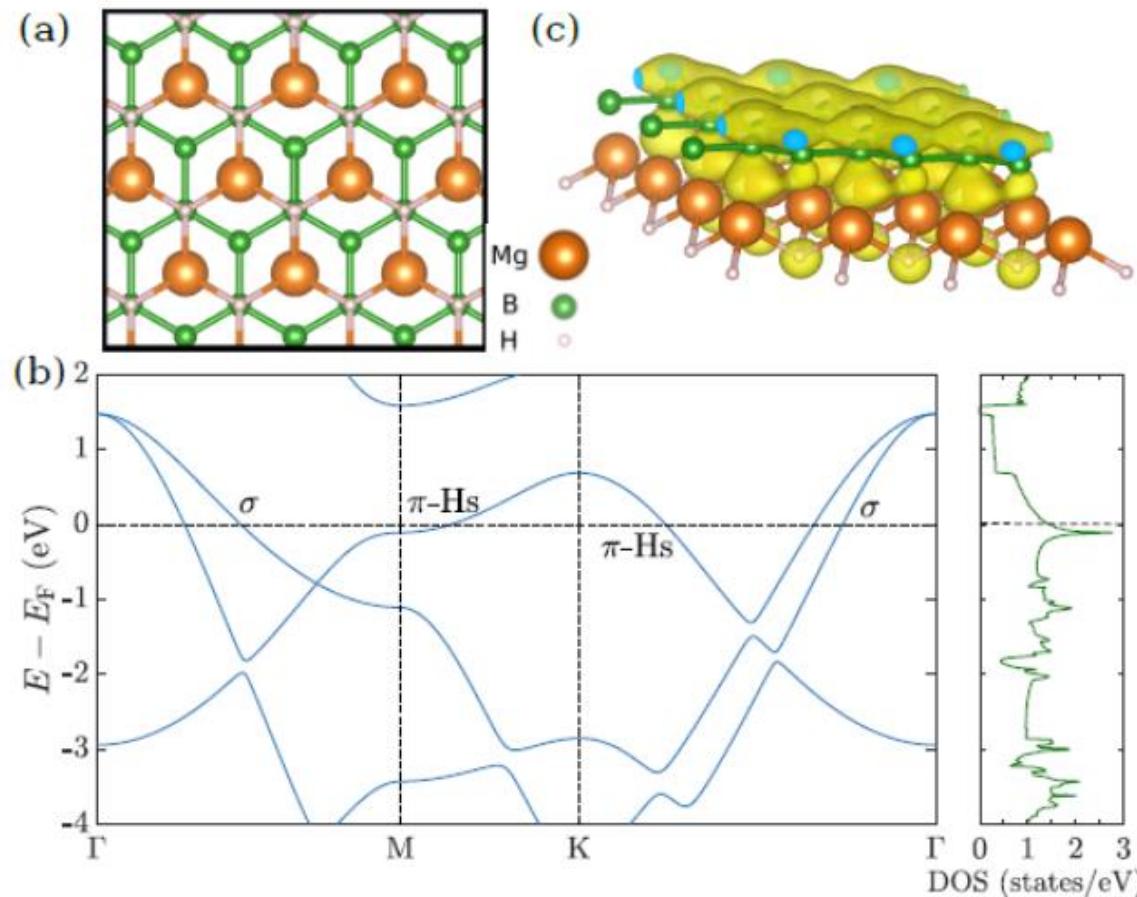
Nonequilibrium doping
nanosecond melting and recrystallization

Reaching room temperature superconductivity by optimizing doping in LaH_{10} ? José A. Flores-Livas et al 2020 arXiv:2010.06446



aluminium to increase the occupation at the Fermi level by more than 30 %
 Increase of $T_c \sim 15\%$

Hydrogen doping



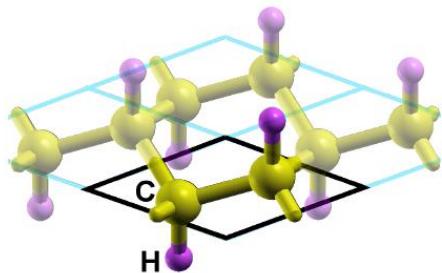
Hydrogen-induced high-temperature superconductivity in two-dimensional materials: Example of hydrogenated monolayer MgB₂

J. Bekaert,^{1,*} M. Petrov,¹ A. Aperis,² P. M. Oppeneer,² and M. V. Milošević^{1,†}

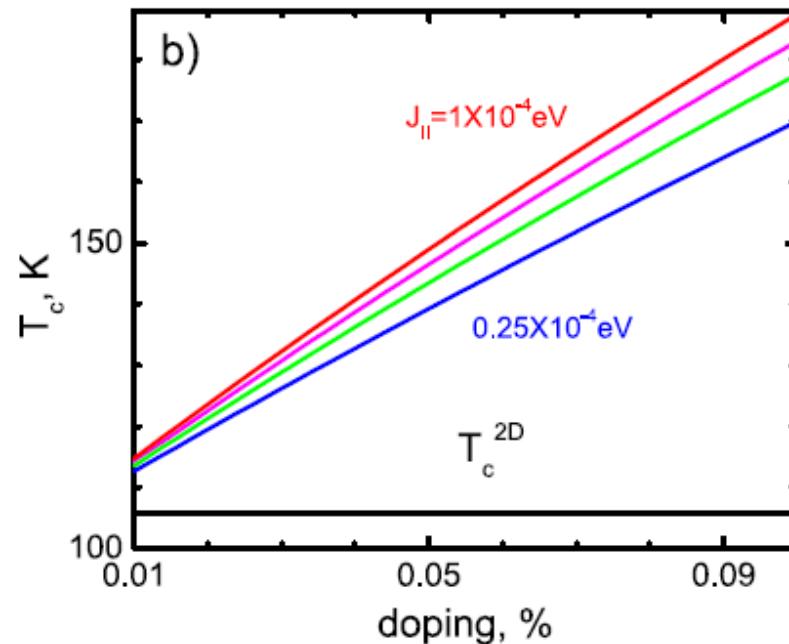
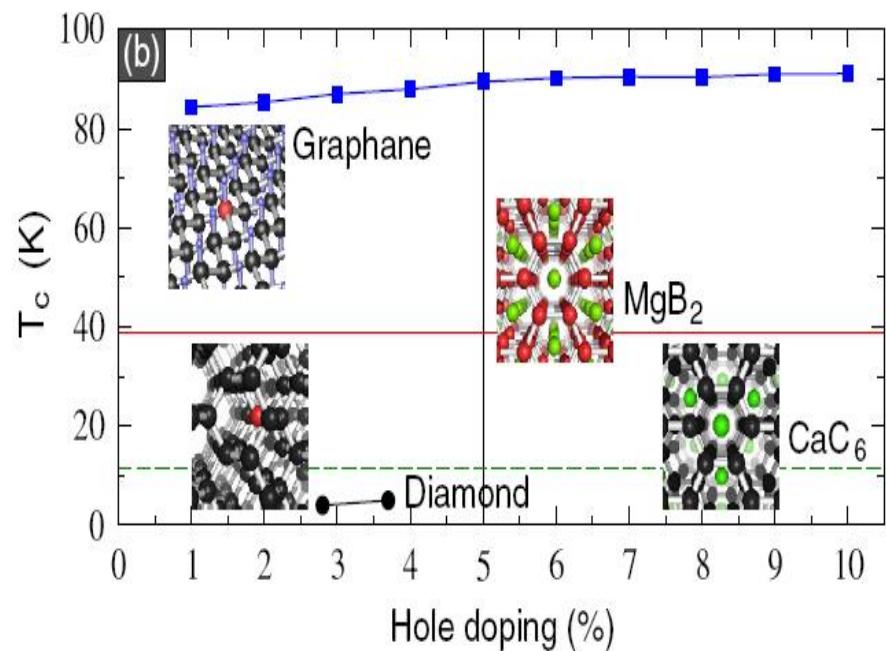
¹Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium

²Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20 Uppsala, Sweden

(Dated: February 12, 2019)

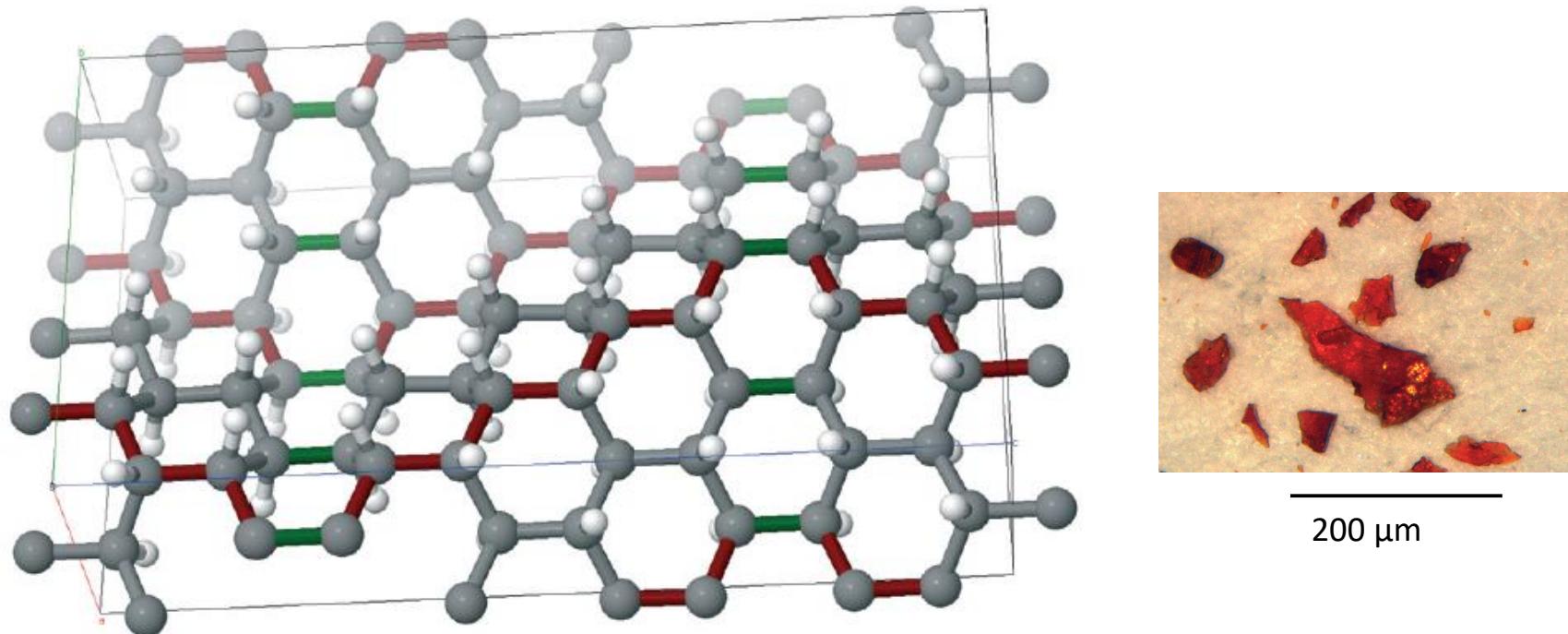


Graphane C-H ambient pressure



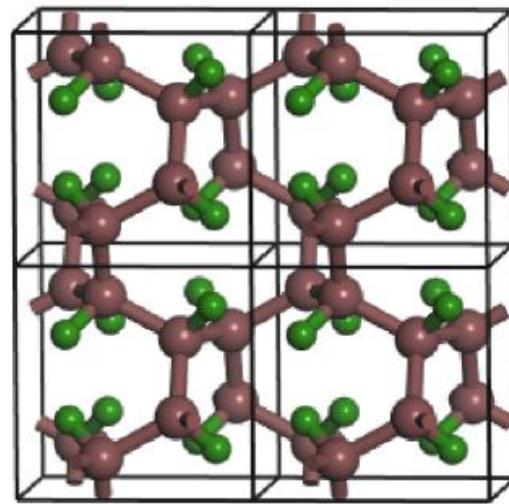
G. Savini, A. C. Ferrari, and F. Giustino, PRL, 105, 037002 (2010)

V.M. Loktev · V. Turkowski 2011



Kondrin, M. V. et al. Bulk graphanes synthesized from benzene and pyridine. *CrystEngComm* **19**, 958–966 (2017)

Increasing SC with hydrogen



diamond-like cubic hydrocarbon $K_4\text{-CH}$
Tc ~80 K

Chao-Sheng Lian et al *Sci. Reports*, 7, 1464

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Synchrotron SOLEIL

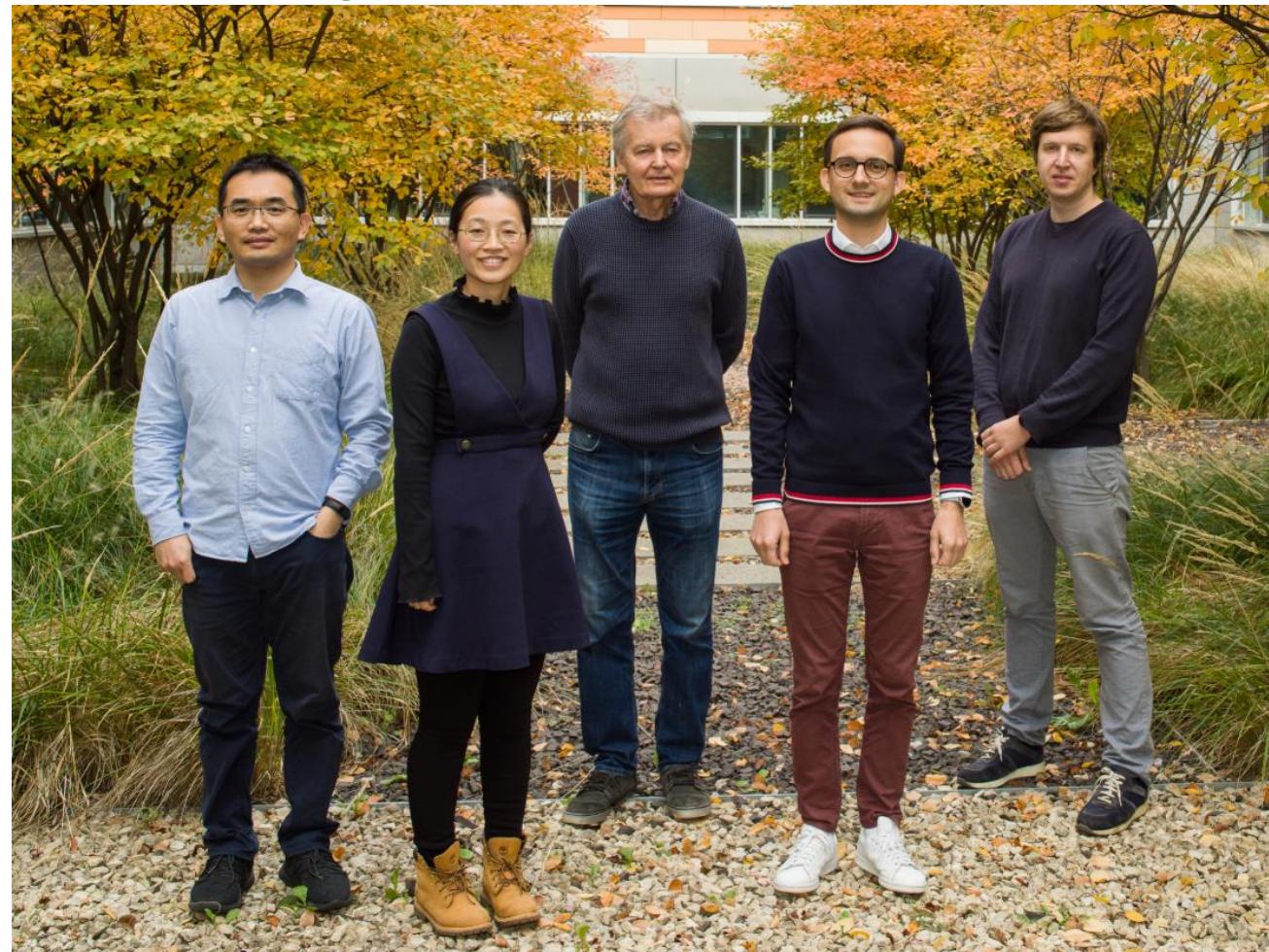
T. Timusk, P. Roy

W. Pickett,

Ch. Pickard, I. Errea, Y. Ma,

L. Boeri, J. A. Flores-Livas, A. Sanna, G. Profeta, R. Arita

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