

Chemistry Under Pressure

Eva Zurek
SUNY Buffalo



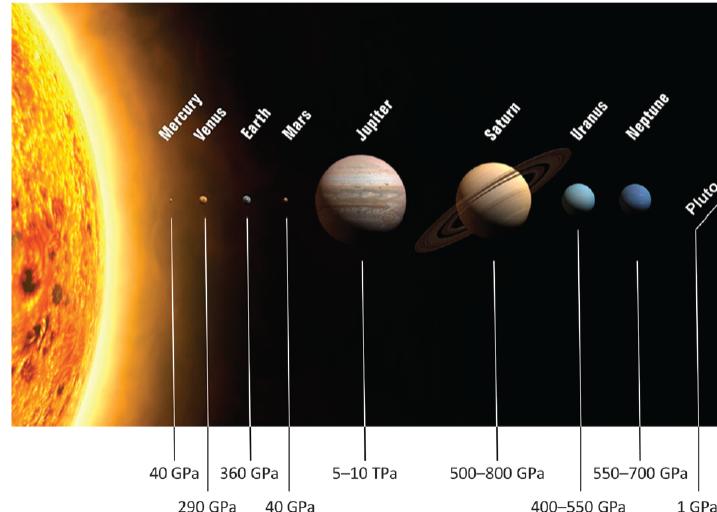
Under Pressure

1 atmosphere

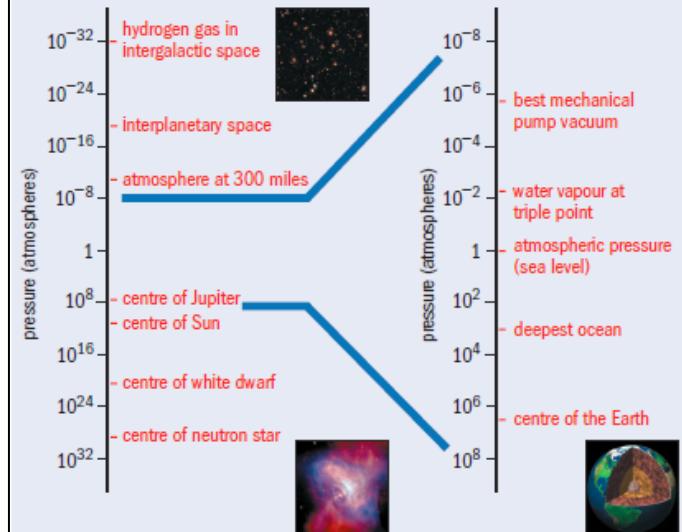


350 GPa ~ 3.5 million atmospheres
Volume contraction of about 5!
Under pressure $H = E + PV$ is important!

- geosciences
- planetary sciences
- nuclear weapons
- basic science
- high pressure chemical synthesis
- superhard materials
- metallic hydrogen (the holy grail of high pressure research)
- superconductors



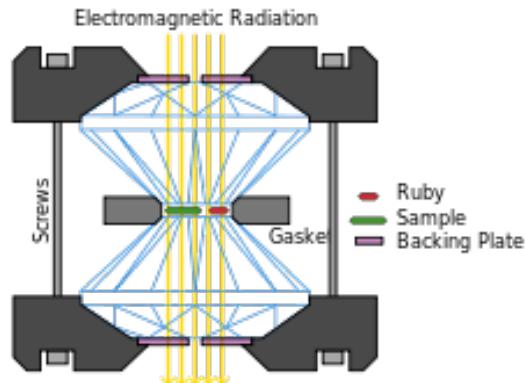
1 Orders of magnitude



Naturally occurring pressures span an astonishing 60 orders of magnitude. At the low end is the non-equilibrium pressure of hydrogen in intergalactic space, while at the other extreme lie the pressures encountered inside neutron stars. At the Earth's surface we occupy a small niche near the centre of the range. High-pressure experiments can now recreate the pressures at the centre of the Earth, and recent technological advances will extend this to the conditions found in other planets and even stars.

Achieving High Pressure

Static Pressure: Diamond Anvil Cells

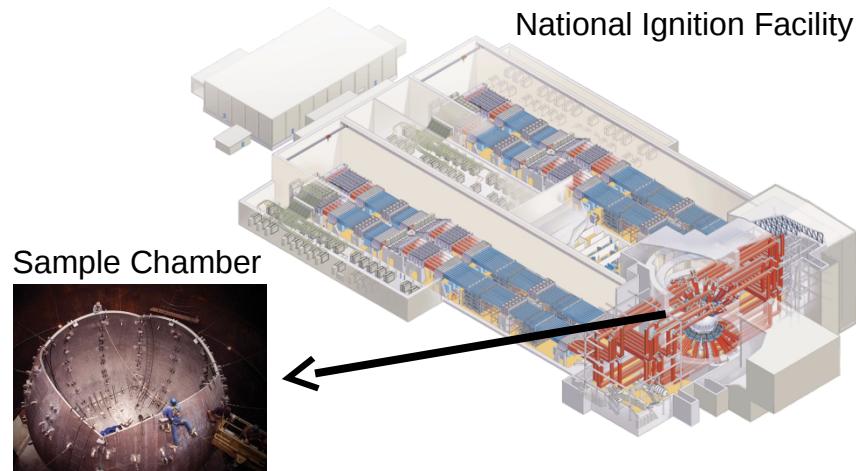


$$\text{Pressure} = \frac{\text{Force}}{\text{Area}}$$

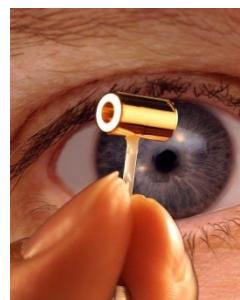
Computations: Changing the Volume!

$$P = -\left(\frac{dU}{dV}\right)_S$$

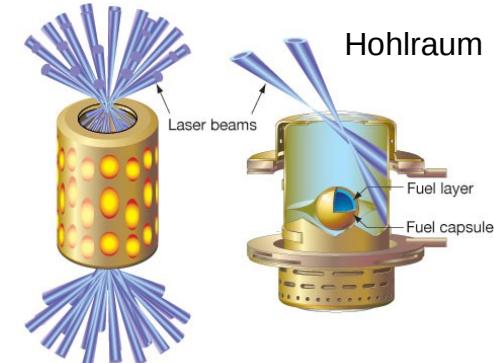
Dynamic Pressure: Shock Compression



Lasers & Sample

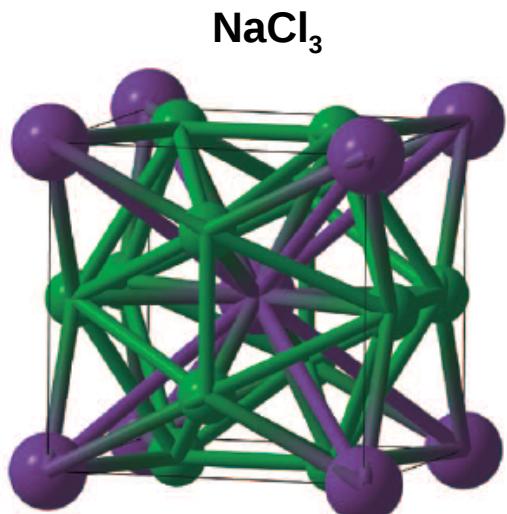


Hohlraum

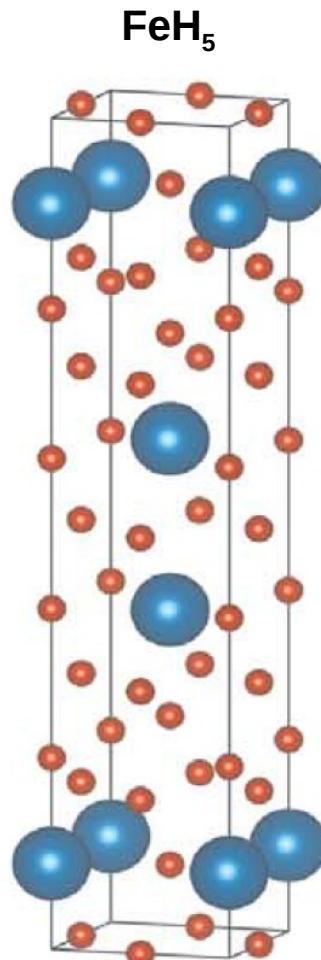


ICF Fusion Microcapsule

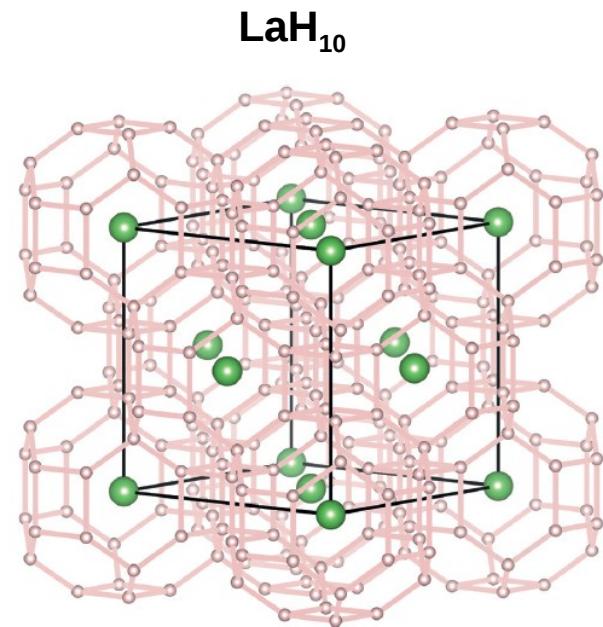
Chemical Reactivity Under Pressure



Science, 342, 1502 (2013).

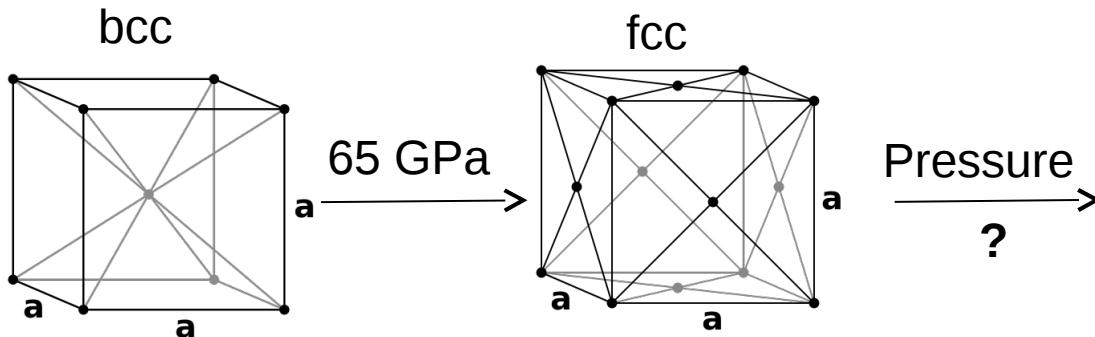


Science, 357, 382-385 (2017).



Angew. Chem. Int. Ed., 57, 688-692 (2018).

But Not Everything Becomes Metallic!



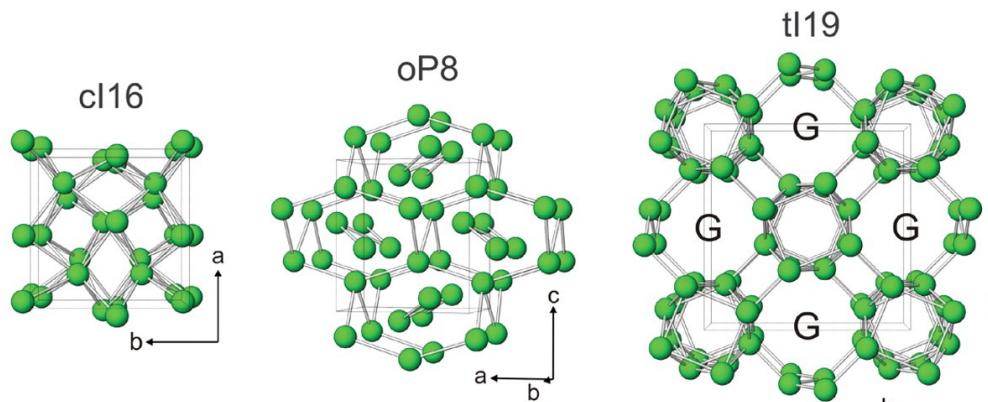
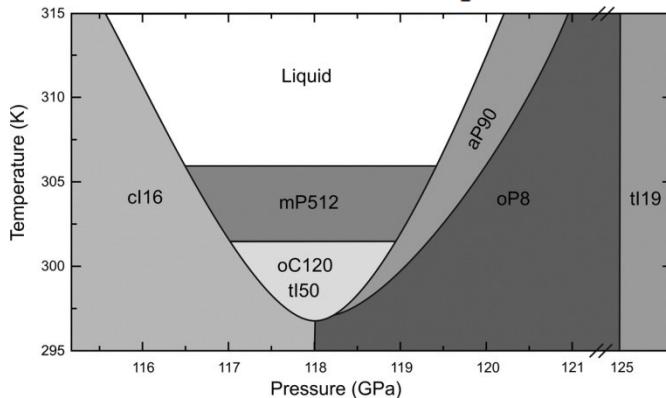
PHYSICAL REVIEW LETTERS

On the Constitution of Sodium at Higher Densities

J. B. Neaton* and N. W. Ashcroft

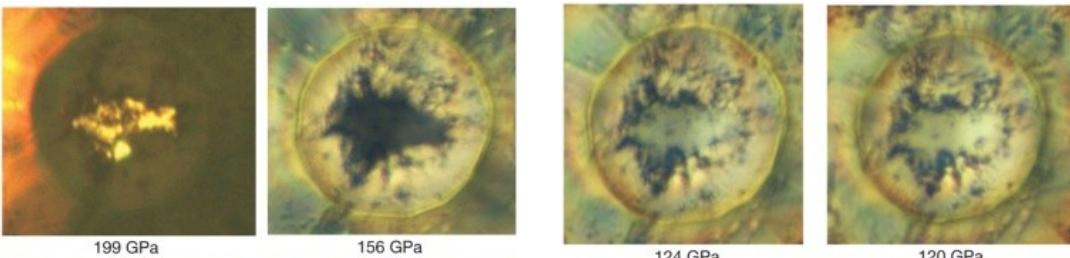
2001, 86, 2830.

Structural Diversity of Sodium

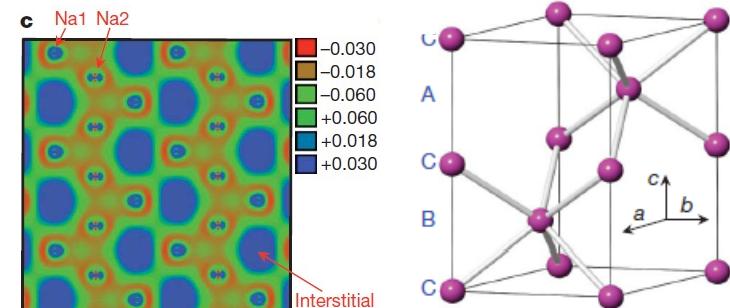


Gregoryanz et al, *Science*. 2008, 320, 1054.

Transparent dense sodium

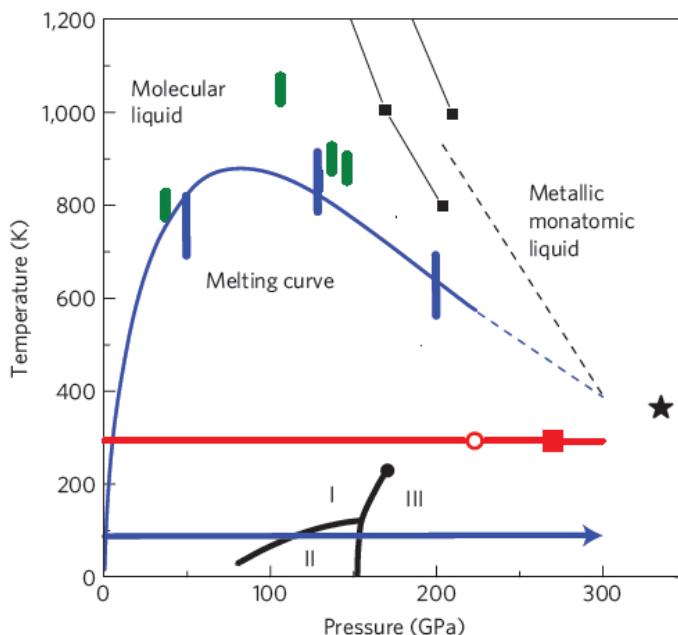
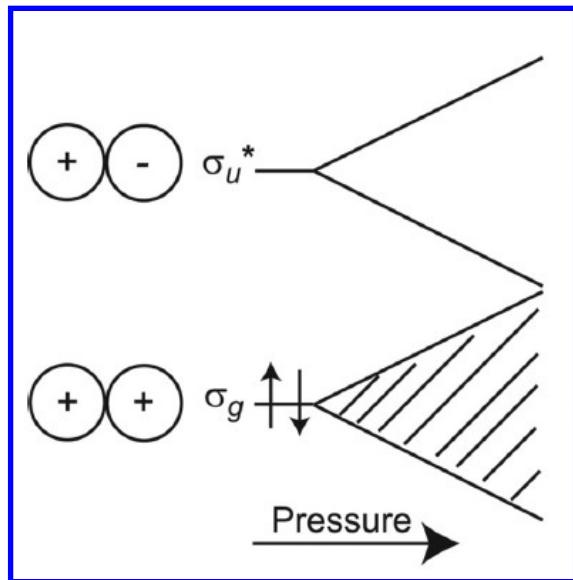


Ma et al, *Nature* 2009, 458, 182.



~200 GPa experiment shows Na becomes optically transparent and insulating

The Quest for Metallic Hydrogen



- High-temperature superconductor! Predicted $T_c \sim 242$ K (Cudazzo et al. *Phys. Rev. Lett.* 2008, 100, 257001).
- Using DAC solid hydrogen turns black at 320 GPa, but remains insulating at the highest pressures reached so far 342 GPa (Loubeyre et al. *Nature*, 2002, 416, 613 & Narayana et al. *Nature*, 1998, 393, 16.)
- Using DAC conductivity measured in DAC at room temperature $P > 200$ GPa (Eremets, Troyan, *Nature*, 2011). Phase IV observed (Howie et. al., *PRL*, 2012) in this range.
- Liquid hydrogen has been metallized in shock-wave experiments (for a microsecond, at 3000 K), via shock wave experiments (Weir et al. *Phys. Rev. Lett.* 1996, 76, 1860).

Metallic Hydrogen for Real?

Science

REPORTS

Cite as: R. P. Dias *et al.*, *Science* 10.1126/science.aal1579 (2017).

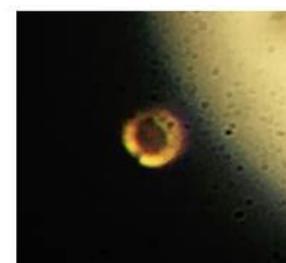
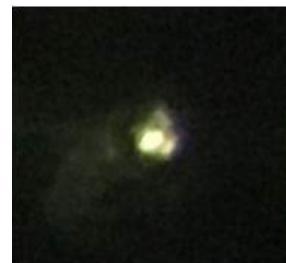
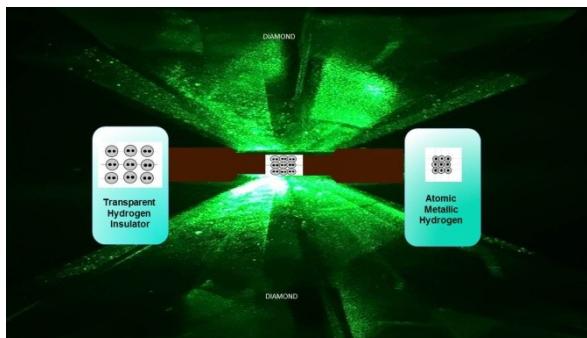
Observation of the Wigner-Huntington transition to metallic hydrogen

Ranga P. Dias and Isaac F. Silvera*

Lyman Laboratory of Physics, Harvard University, Cambridge, MA 02138, USA.

*Corresponding author. Email: silvera@physics.harvard.edu

Producing metallic hydrogen has been a great challenge to condensed matter physics. Metallic hydrogen may be a room temperature superconductor and metastable when the pressure is released and could have an important impact on energy and rocketry. We have studied solid molecular hydrogen under pressure at low temperatures. At a pressure of 495 GPa hydrogen becomes metallic with reflectivity as high as 0.91. We fit the reflectance using a Drude free electron model to determine the plasma frequency of 32.5 ± 2.1 eV at $T = 5.5$ K, with a corresponding electron carrier density of $7.7 \pm 1.1 \times 10^{23}$ particles/cm³, consistent with theoretical estimates of the atomic density. The properties are those of an atomic metal. We have produced the Wigner-Huntington dissociative transition to atomic metallic hydrogen in the laboratory.



Hydrogen Rich Systems & Superconductivity

LETTER

doi:10.1038/nature14964

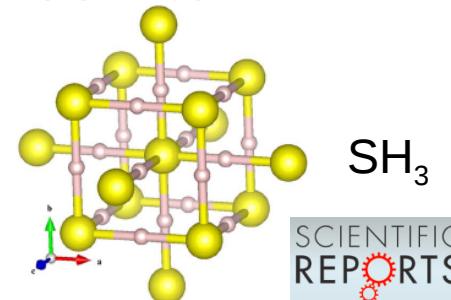
Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov^{1*}, M. I. Eremets^{1*}, I. A. Troyan¹, V. Ksenofontov² & S. I. Shylin²

A superconductor is a material that can conduct electricity without resistance below a superconducting transition temperature, T_c . The highest T_c that has been achieved to date is in the copper oxide system¹: 133 kelvin at ambient pressure² and 164 kelvin at high pressures³. As the nature of superconductivity in these materials is still not fully understood (they are not conventional superconductors), the prospects for achieving still higher transition temperatures by this route are not clear. In contrast, the Bardeen–Cooper–Schrieffer theory of conventional superconductivity gives a guide for achieving high T_c with no theoretical upper bound—all that is needed is a favourable combination of high-frequency phonons, strong electron–phonon coupling, and a high density of states⁴. These conditions can in principle be fulfilled for metallic hydrogen and covalent compounds dominated by hydrogen^{5,6}, as hydrogen atoms provide the necessary high-frequency phonon modes as well as the strong electron–phonon coupling. Numerous calculations support this idea and have predicted transition temperatures in the range 50–235 kelvin for many hydrides⁷, but only a moderate T_c of 17 kelvin has been observed experimentally⁸. Here we investigate sulfur hydride⁹, where a T_c of 80 kelvin has been predicted¹⁰. We find that this system transforms to a metal at a pressure of approximately 90 gigapascals. On cooling, we see signatures of superconductivity: a sharp drop of the resistivity to zero and a decrease of the transition temperature with magnetic field, with magnetic susceptibility measurements confirming a T_c of 203 kelvin. Moreover, a pronounced isotope shift of T_c in sulfur deuteride is suggestive of an electron–phonon mechanism of superconductivity that is consistent with the Bardeen–Cooper–Schrieffer scenario. We argue that the phase responsible for high- T_c superconductivity in this system is likely to be H_3S , formed from H_2S by decomposition under pressure. These findings raise hope for the prospects for

Pressure-induced metallization of dense $(H_2S)_2H_2$ 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



nature
physics

LETTERS

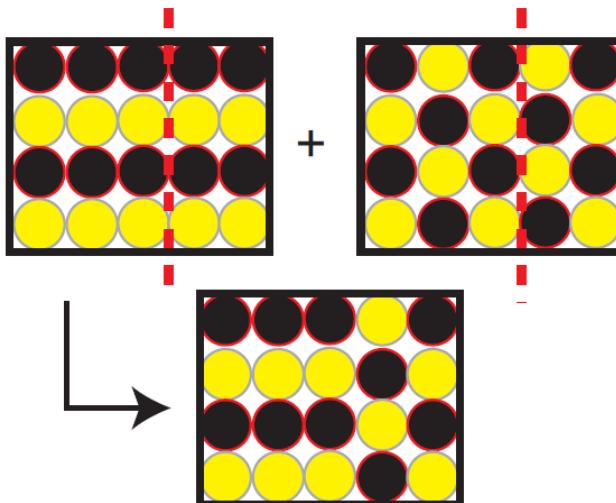
PUBLISHED ONLINE: 9 MAY 2016 | DOI: 10.1038/NPHYS3760

Crystal structure of the superconducting phase of sulfur hydride

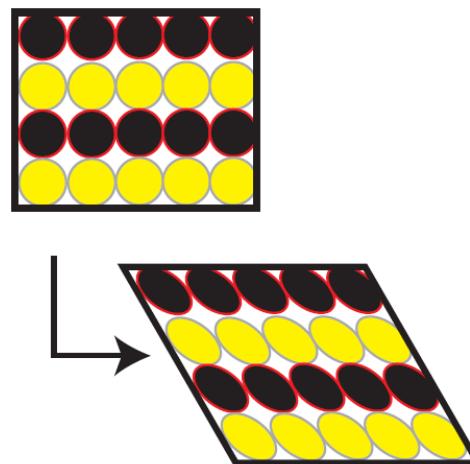
A superconducting critical temperature above 200 K has recently been discovered in H_2S (or D_2S) under high hydrostatic pressure^{1,2}. These measurements were interpreted in terms of a decomposition of these materials into elemental sulfur and a hydrogen-rich hydride that is responsible for the superconductivity, although direct experimental evidence for this mechanism has so far been lacking. Here we report the crystal structure of the superconducting phase of hydrogen sulfide (and deuterium sulfide) in the normal and superconducting states obtained by means of synchrotron X-ray diffraction measurements, combined with electrical resistance measurements at both room and low temperatures. We find that the superconducting phase is mostly in good agreement with the theoretically predicted body-centred cubic (bcc) structure for H_3S ³. The presence of elemental sulfur is also manifest in the X-ray diffraction patterns, thus proving the decomposition mechanism of H_2S to $H_3S + S$ under pressure^{4–6}.

Evolutionary Structure Prediction: XtalOpt

1. Crossover

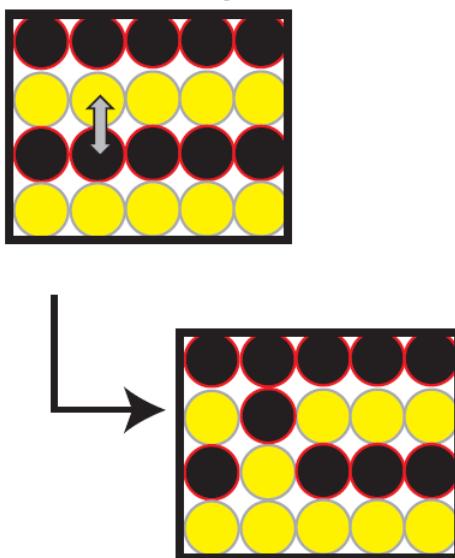


2. Strain

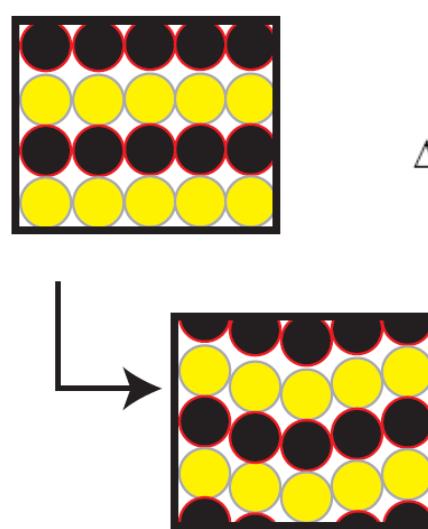


$$\mathbf{v}_{\text{new}} = \begin{bmatrix} 1 + \varepsilon_{11} & \frac{\varepsilon_{12}}{2} & \frac{\varepsilon_{13}}{2} \\ \frac{\varepsilon_{12}}{2} & 1 + \varepsilon_{22} & \frac{\varepsilon_{23}}{2} \\ \frac{\varepsilon_{13}}{2} & \frac{\varepsilon_{23}}{2} & 1 + \varepsilon_{33} \end{bmatrix} \mathbf{v}$$

3. Exchange

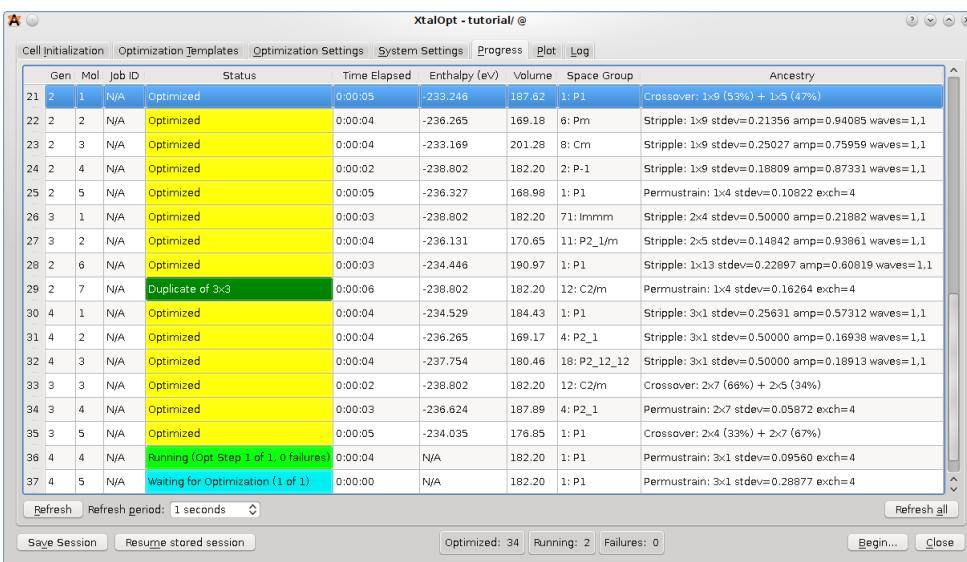


4. Ripple



XtalOpt: Visualization

Website: xtalopt.github.io



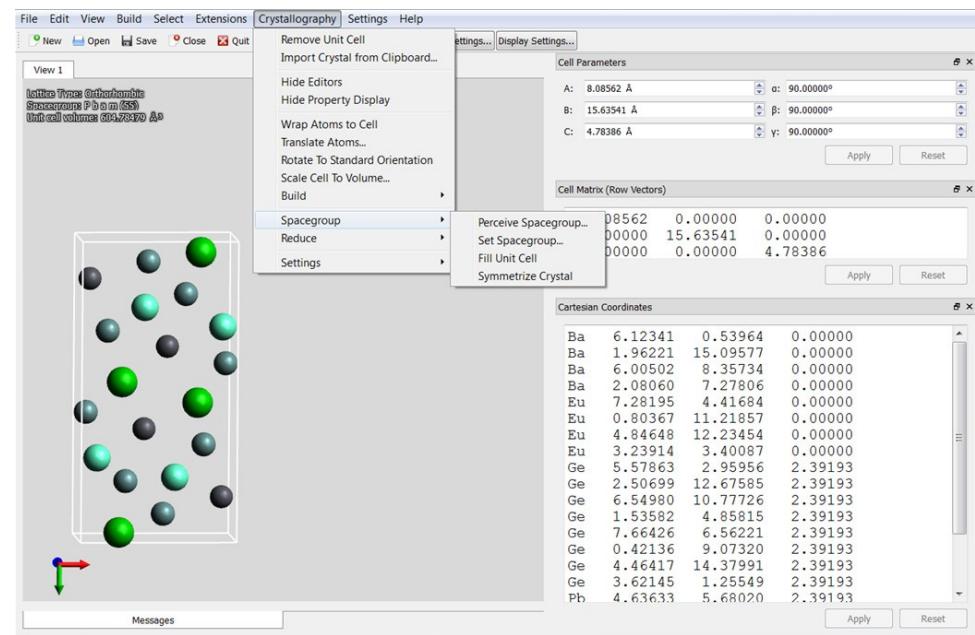
Platforms & Queue Interface

- Linux, Windows
- PBS, SGE, SLURM, local computer

Codes

- GULP, VASP, PW-SCF, CASTEP, SIESTA, ADF BAND

GPL & BSD Licenses



Other Tools

XtalComp Web Interface: Enter POSCAR files

Paste a POSCAR file into each of the following boxes and hit "Compare" to let **XtalComp** determine if they describe the same structure.

Tolerance for position / length comparisons. Same units as cell matrix. (default = 0.05):

Angular tolerance for lattice comparisons (default = 0.25 degrees):

Notes:

- The POSCAR format is specified [here](#).
- Each structure **must have the same number of atoms**, and the order of the atom type counts (line 6) must be the same in each POSCAR.
- Update:** you may now compare different crystals with different formula units (e. g. TiO₂ and Ti₂O₄). The crystals will be reduced to their primitive form using functions from spglib before the comparison. However, the order of atoms **must** still match.

RandSpg: Generate Random Crystals with Specific Spacegroups

A sample input is given in the text area below. Change it around as needed and click "submit" when you are ready for **RandSpg** to generate the crystal structures!

```
First line is a comment line
# Anything to the right of a hash is a comment
# Composition is set by atomic symbols followed by number as such:
composition      = Mg4Al2

# Which spacegroups to generate are set as follows (hyphens and commas work)
spacegroups      = 1-6, 10, 25

# lattice mins and maxes set constraints on the lattice to be generated.
# Distances are in Angstroms and angles are in degrees.
#          a,   b,   c, alpha, beta, gamma
latticeMins      = 3.0, 3.0, 3.0, 60.0, 60.0, 60.0
latticeMaxes     = 10.0, 10.0, 10.0, 120.0, 120.0, 120.0

# minVolume and maxVolume specify constraints on the volume in Angstroms
# If the volume is not within this range, it will be rescaled so that it is
# If you remove minVolume or specify it to be -1, there will be no minVolume
# Same goes for maxVolume
minVolume        = 450
maxVolume        = 500

# numOfEachSpgToGenerate tells us how many crystals of each spg to generate
numOfEachSpgToGenerate = 3

# For advanced users: by default, the program will only generate a spacegroup
# for a crystal if it can use the most general Wyckoff position at least
# once. This is because the spacegroup is not guaranteed if the most
# general Wyckoff position is not used at least once. The user, however,
```

Notes:

- Since this program is running on a server that runs other programs, it may run too slow (depending on the settings) and time out. If you'd like to run it at full speed, please obtain and compile the program from [the Github repository](#) and run the executable on your local computer.
- The POSCAR format is specified [here](#).
- If you wish to visualize the crystal using the [Avogadro](#) molecular editor, copy the POSCAR of the crystal, click the "Crystallography" menu at the top of Avogadro, and select "Import Crystal from Clipboard...".
- If you wish to use another format, you may convert it using [OpenBabel](#).

<http://xtalopt.openmolecules.net/xtalcomp/xtalcomp.html>

<http://xtalopt.openmolecules.net/randSpg/randSpg.html>

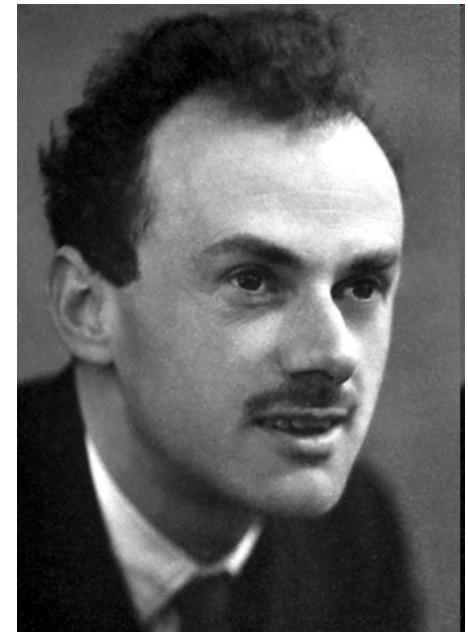
Quantum Mechanics

The Non-Relativistic Schrödinger Equation:

$$\left[-\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + \sum_{i=1}^N V_{ext}(\mathbf{r}_i) + \frac{1}{2} \sum_{j \neq i=1}^N \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right] \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = E \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N),$$

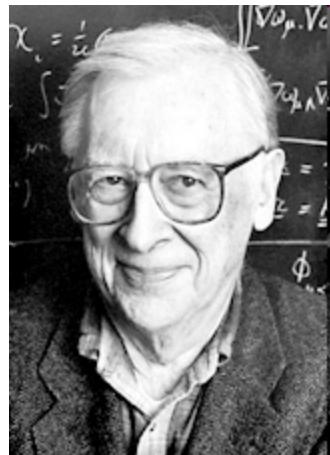
The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

Approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.



Nobel Prize in Chemistry 1998

$$\begin{aligned}E_{KS}[n] &= T[n] + U[n] + V[n] \\&= T_s[\phi_i[n]] + U_H[n] + E_{xc}[n] + V_{ext}[n] \\&= T_s[n] + \int n(\mathbf{r}) \left[V_{ext}(\mathbf{r}) + \frac{1}{2} V_C(\mathbf{r}) \right] d\mathbf{r} + E_{xc}[n]\end{aligned}$$



The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn *"for his development of the density-functional theory"* and John A. Pople *"for his development of computational methods in quantum chemistry"*.

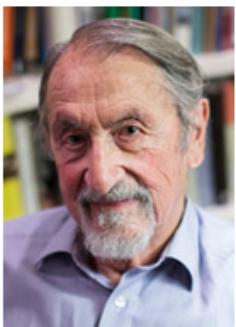
Nobel Prize in Chemistry 2013



The Nobel Prize in Chemistry 2013

Martin Karplus, Michael Levitt, Arieh Warshel

The Nobel Prize in Chemistry 2013



© Nobel Media AB
Martin Karplus



Photo: Keilana via
Wikimedia Commons
Michael Levitt



Photo: Wikimedia
Commons
Arieh Warshel

The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*.

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New York Times:

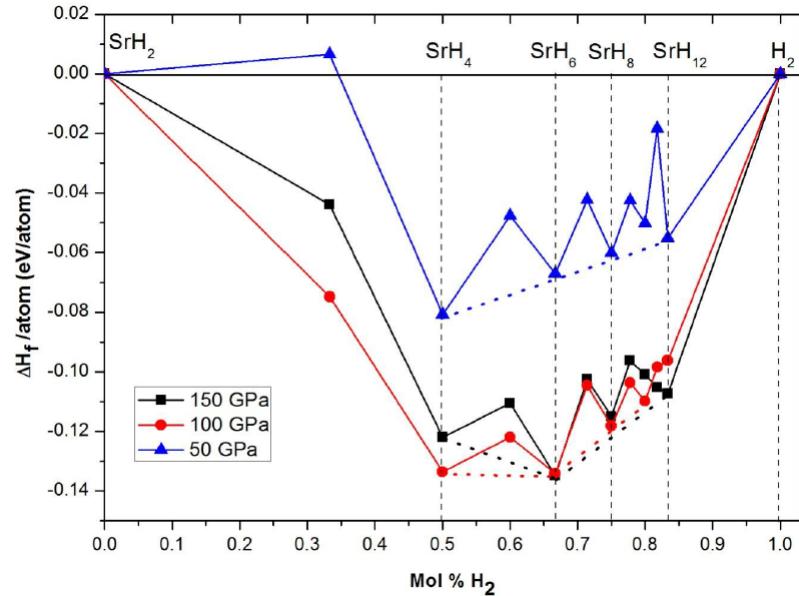
Chemistry, meet computer science.

This year's Nobel Prize in Chemistry was awarded to three researchers for work that did not involve test tubes or lab coats. Instead, they explored the world of molecules virtually, with computers. Such numerical simulations enable the closer study of complex reactions like photosynthesis and combustion, as well as the design of new drugs.

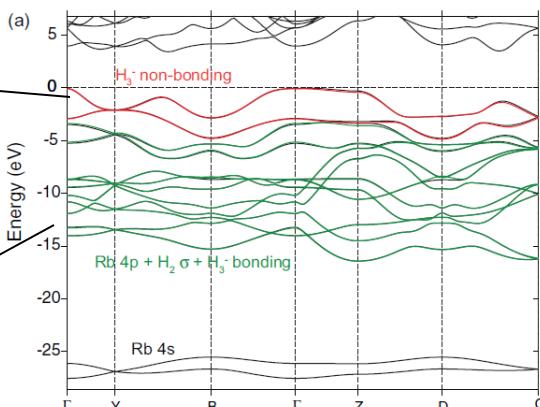
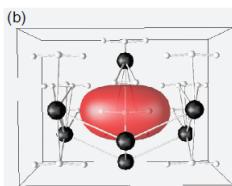
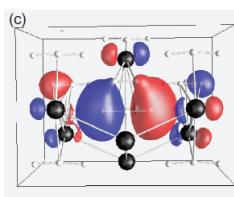
Exploring Chemical Trends



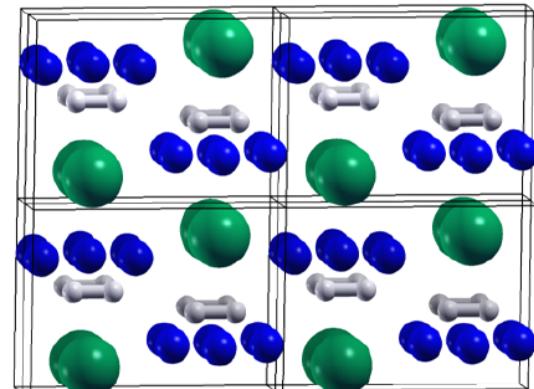
Stoichiometry



Mol % H_2



Properties



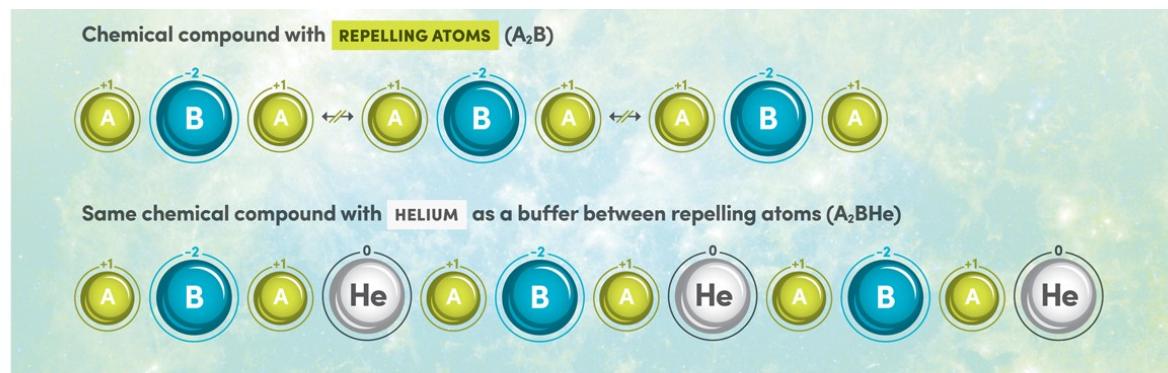
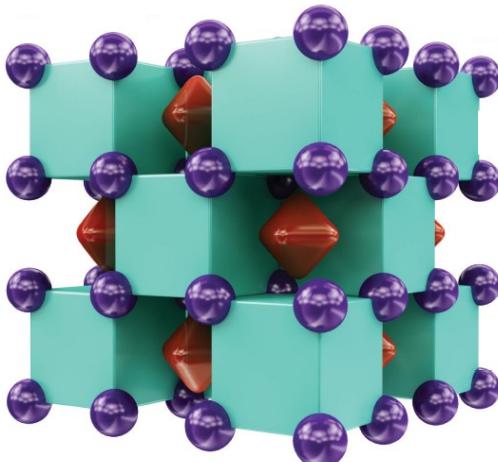
Electronic Structure

Structure

The “Noble” Gas Helium Under Pressure

- At 1 atm helium is unreactive because of its filled shell electron configuration, zero electron affinity, and high ionization potential.

Na_2He stable above 113 GPa



Nat. Chem., **9**, 440-445 (2017).

- Calculations predicted that systems with uneven ratio of positively and negatively charged ions may react with helium under at pressures as low as 30 GPa.
- Helium is light, so it tends to float away. Therefore it was believed there is not much helium stored in the Earth. Because many of the mantle elements are ionic, this might not be the case!
- This might be used to make new porous materials!
- Could helium be mined?!? (The world uses 8 billion cubic feet of He each year – LHC, nuclear reactors, MRIs, superconductors).

Superconductivity in Phosphine?

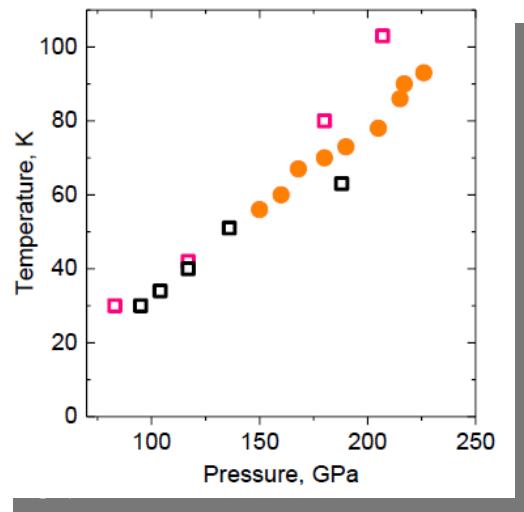
arXiv:1508.06224

Superconductivity above 100 K in PH₃ at high pressures

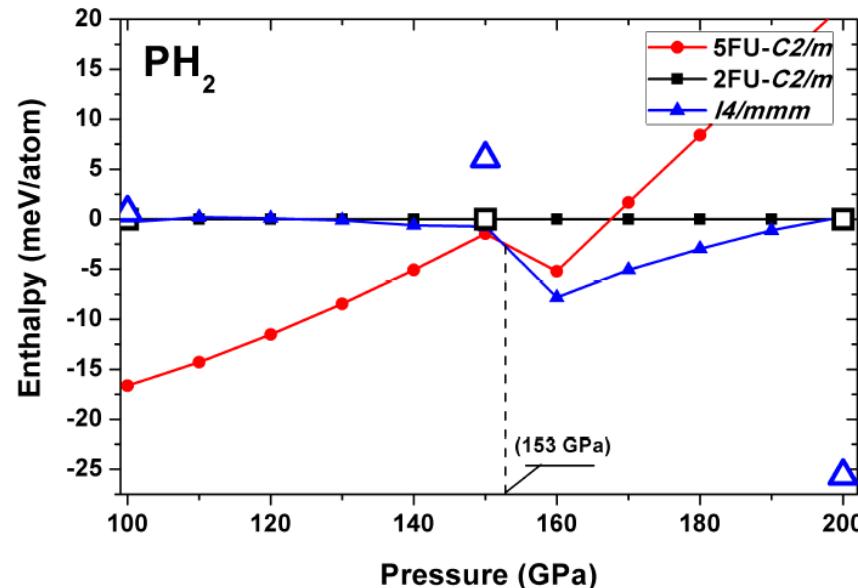
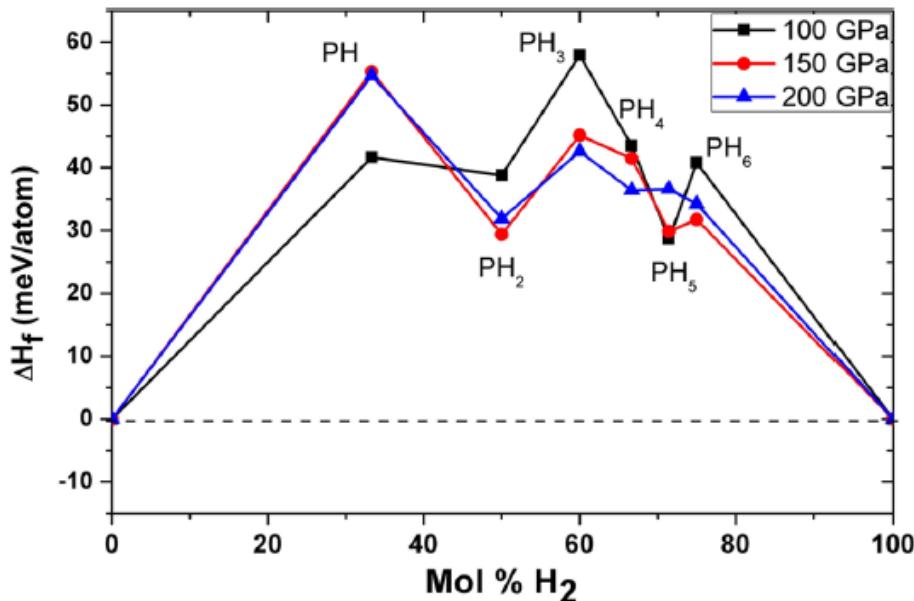
A. P. Drozdov, M. I. Eremets and I. A. Troyan

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

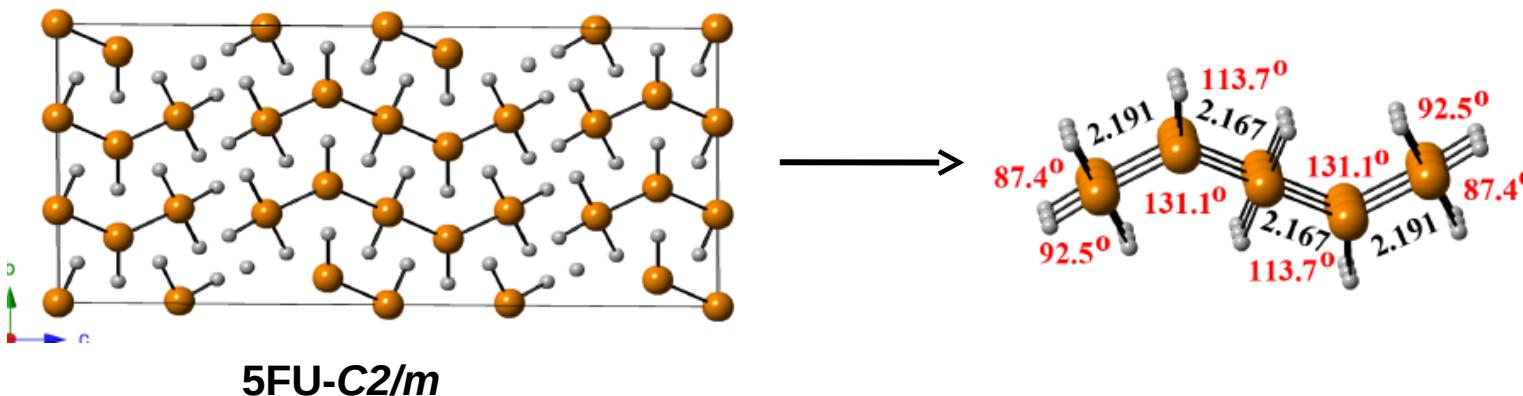
Following the recent discovery of very high temperature conventional superconductivity in sulfur hydride (critical temperature T_c of 203 K, Ref⁴) we searched for superconductivity in other hydrides and found that a covalent hydride phosphine (PH₃) also exhibits a high $T_c > 100$ K at pressure $P > 200$ GPa as determined from four-probe electrical measurements.



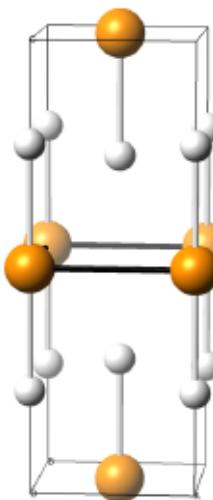
Phosphine Decomposition Under Pressure



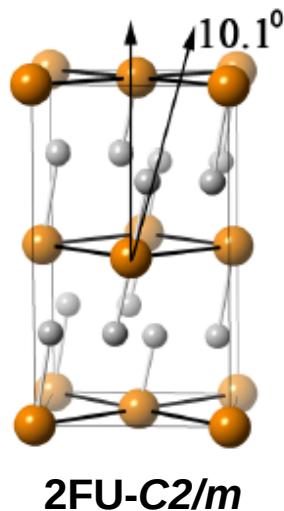
150 GPa, $\Delta(\text{H}+\text{ZPE}) + 45.8 \text{ meV/atom}$



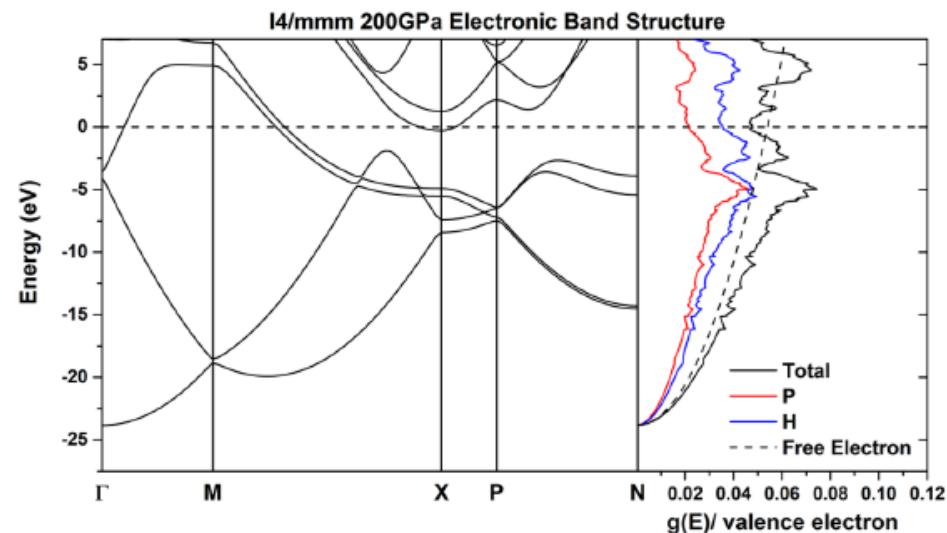
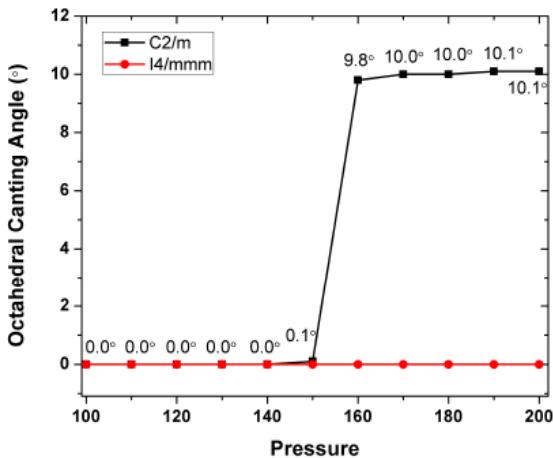
PH_2 Structure and Electronic Structure



$\text{C}2/m$

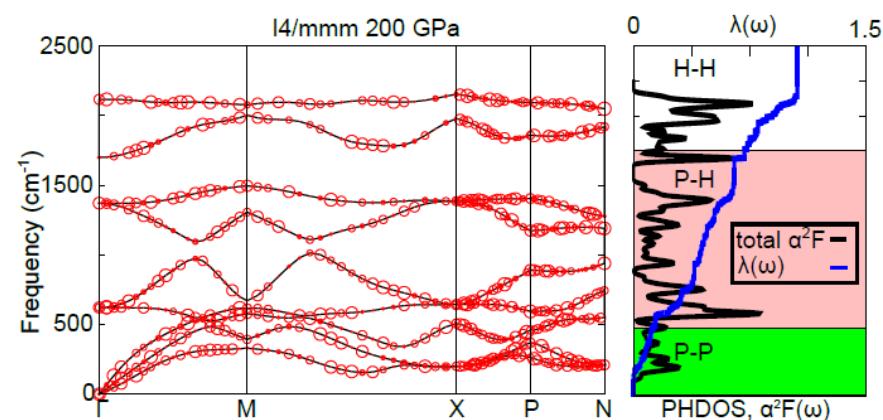
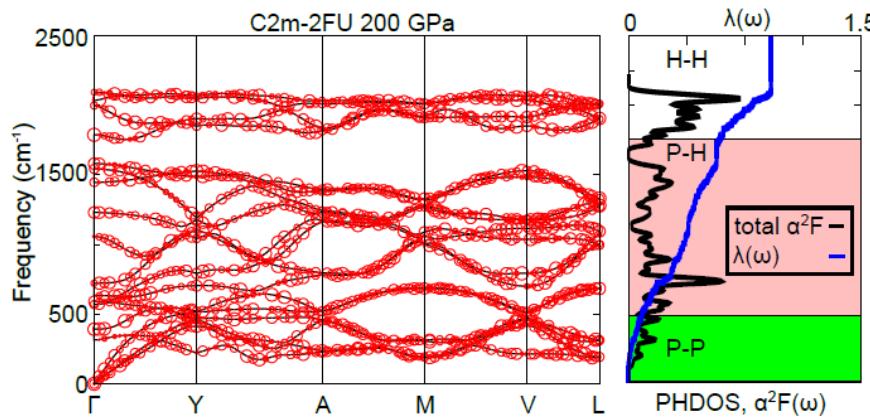


$\text{I}4/\text{mmm}$



- Dynamically stable 100-200 GPa
- Canting in $\text{C}2/m$ decreases the volume
- DOS is nearly-free-electron like

Superconductivity in PH₂ at 150-200 GPa



System	Pressure (GPa)	λ	ω_{\log} (K)	$T_c^{\mu^*=0.1}$ (K)	$T_c^{\mu^*=0.18}$ (K)
S.C. P	100	0.66	521.7	15.9	6.4
S.H. P	150	0.21	575.6	0.00	0.00
S.H. P	200	0.13	671.8	0.00	0.00
5FU- <i>C2/m</i>	100	1.05	655.1	49.0	32.1
5FU- <i>C2/m</i>	150	1.00	798.1	55.5	35.2
2FU- <i>C2/m</i>	200	1.04	1026.5	75.6	49.2
<i>I4/mmm</i>	150	0.86	946.2	50.6	28.3
<i>I4/mmm</i>	200	1.13	851.6	70.4	48.0

Flores-Livas et al. PRB. 2016, 93, 020508.

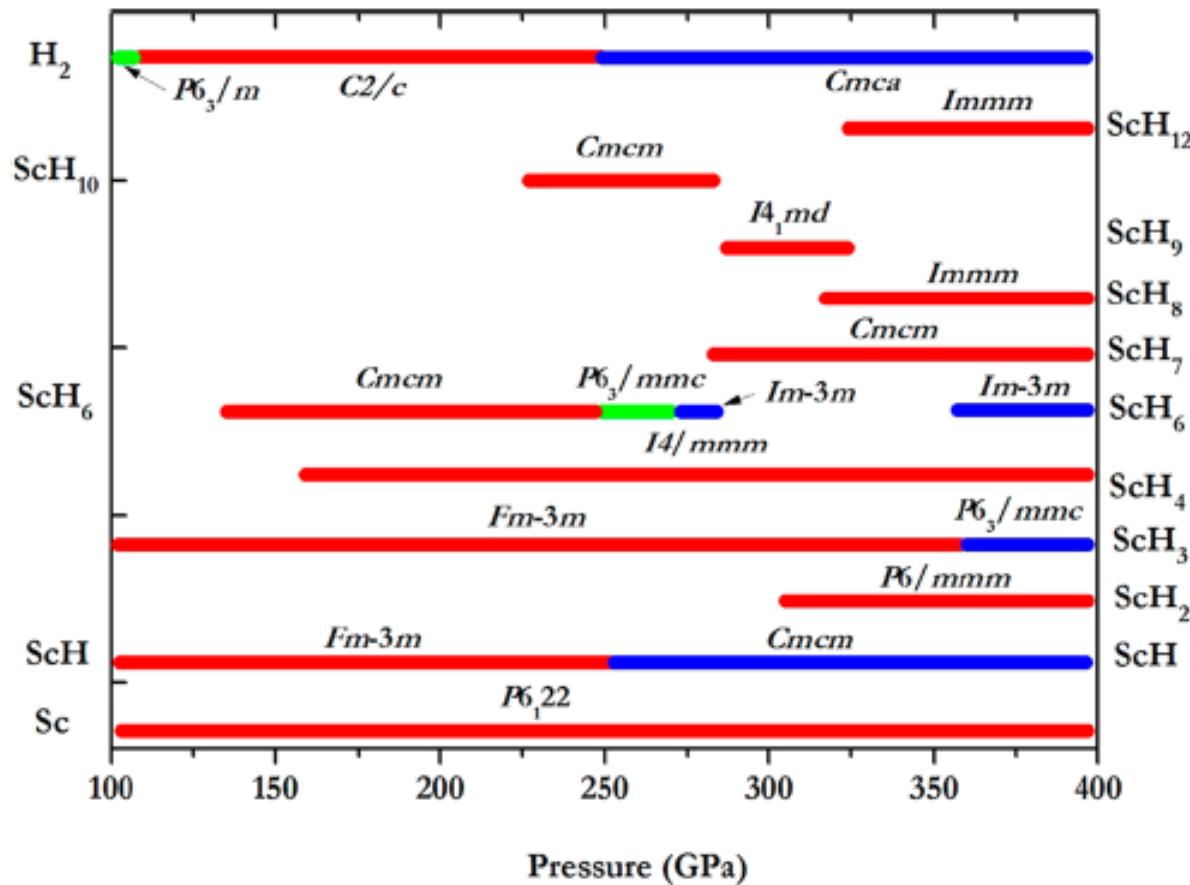
Fu, Y et al. Chem. Mater. 2016, 28, 1746.

Liu, H. et al. J. Phys. Chem. C, 2016, 6, 3458.

$$T_c = \frac{\omega_{\log}}{1.2} \exp \left[-\frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right]$$

Polyhydrides of Scandium?

Ye, Zarifi, Zurek, Hoffmann, Ashcroft. 2018, *J. Phys. Chem. C* **122**, 6298-6309.



New Structures Predicted Here:

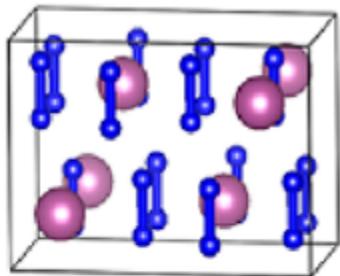
- Cmcm ScH₆
- Cmcm ScH₇
- I4₁md ScH₉
- Immm ScH₁₂

ScH₄ - ScH₆: Abe. PRB. 2017, 96, 144108.

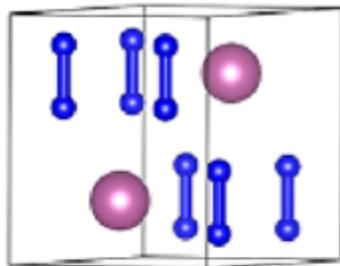
ScH₄ - ScH₈: Qian et al. PRB. 2017, 96, 094513.

ScH₄ - ScH₁₂: Peng. et al. Phys. Rev. Lett. 2017, 119, 107001.

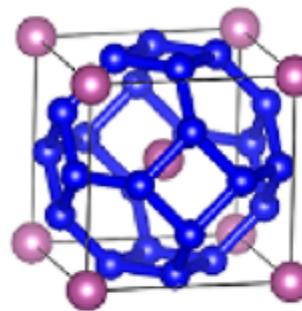
Stable Phases of ScH_6



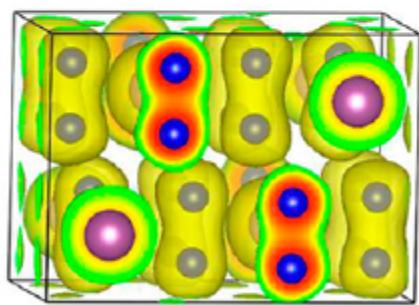
(a) $Cmcm$, 200 GPa



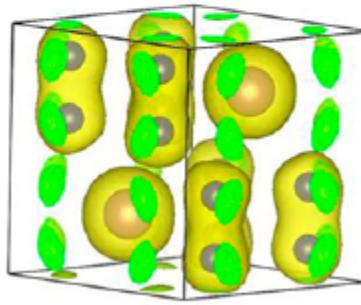
(b) $P6_3/mmc$, 250 GPa



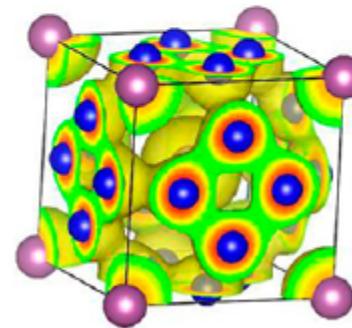
(c) $Im\text{-}3m$, 250 GPa



(d) $Cmcm$, 200 GPa



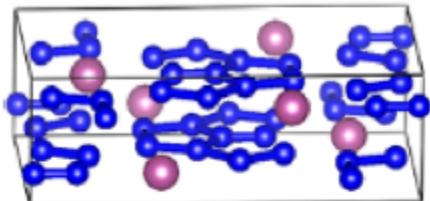
(e) $P6_3/mmc$, 250 GPa



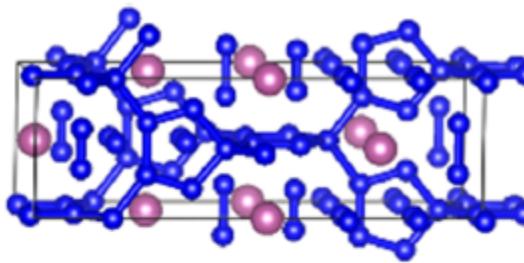
(f) $Im\text{-}3m$, 250 GPa

- “Sodalite” structure with H-H distances of 1.15 Å at 250 GPa
- Stable in a narrow pressure range around 275 GPa
- Same structure predicted for: CaH_6 (150 GPa), YH_6 (110 GPa), LaH_6 (100 GPa), MgH_6 (150 GPa)

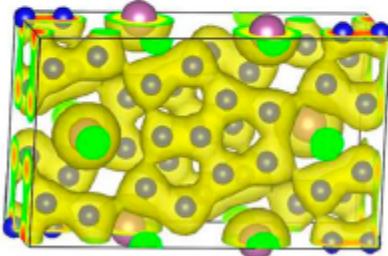
$\text{H}_5^{\delta-}$ Motifs in ScH_9 and ScH_{10}



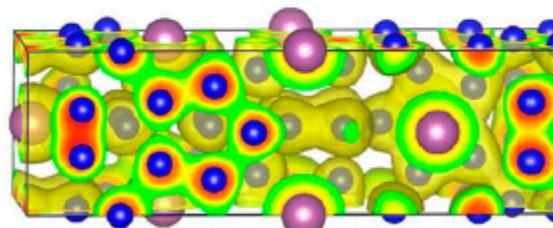
(a) $\text{ScH}_{10}, \text{Cmcm}, 250 \text{ GPa}$



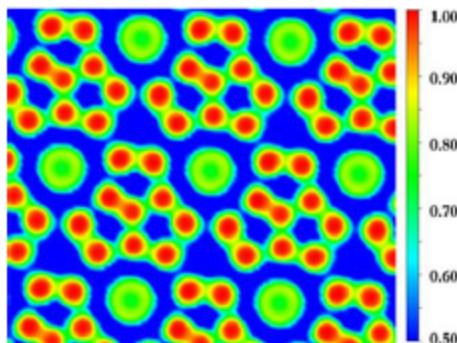
(b) $\text{ScH}_9, \text{I}4_1\text{md}, 300 \text{ GPa}$



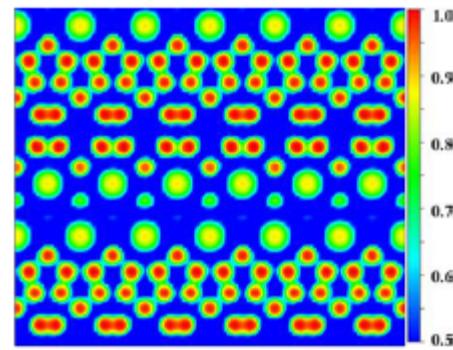
(c) $\text{ScH}_{10}, \text{Cmcm}, 250 \text{ GPa}$



(d) $\text{ScH}_9, \text{I}4_1\text{md}, 300 \text{ GPa}$

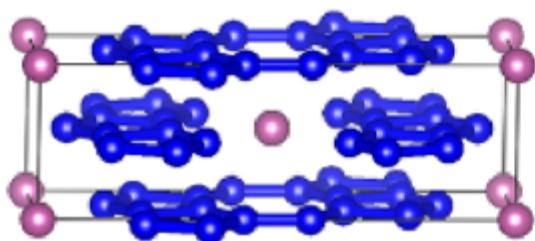


(e) $\text{Cmcm } \text{ScH}_{10} (0\ 0\ 1)$

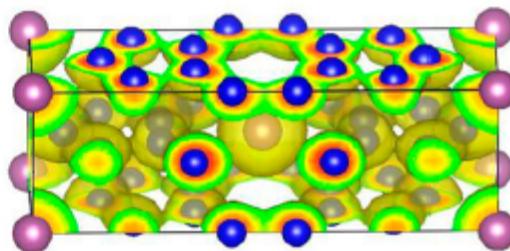


- In ScH_{10} , 10 hydrogen atoms form 0-D edge-fused $\text{H}_5^{\delta-}$ motifs
- In ScH_9 , 1-D chains of edge-fused $\text{H}_5^{\delta-}$ and H_2
- These $\text{H}_5^{\delta-}$ motifs have not been observed in other hydrides

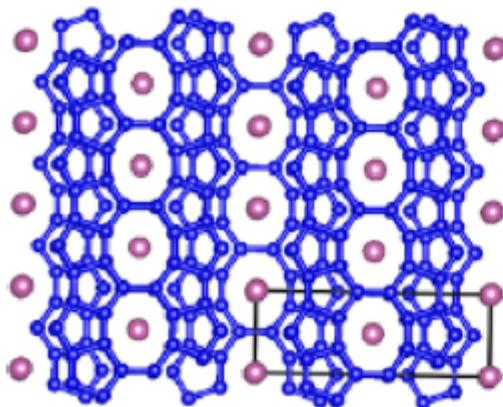
1-Dimensional Chains in ScH_{12}



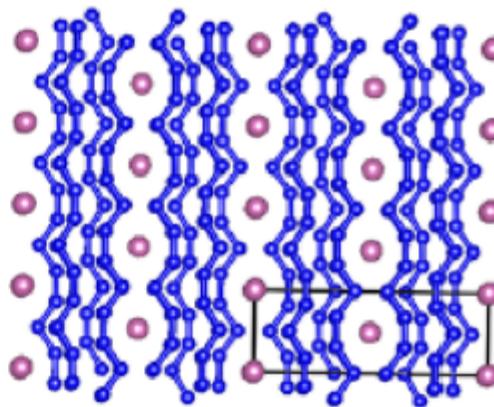
(a) ScH_{12} , $I\bar{m}mm$



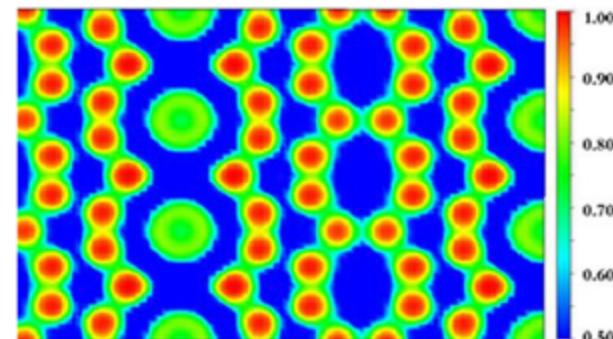
(b) ScH_{12} , $I\bar{m}mm$



(c) ScH_{12} , $I\bar{m}mm$



(d) ScH_{12} , $I\bar{m}mm$



(f) $I\bar{m}mm$ $\text{ScH}_{12}(0\ 1\ 0)$

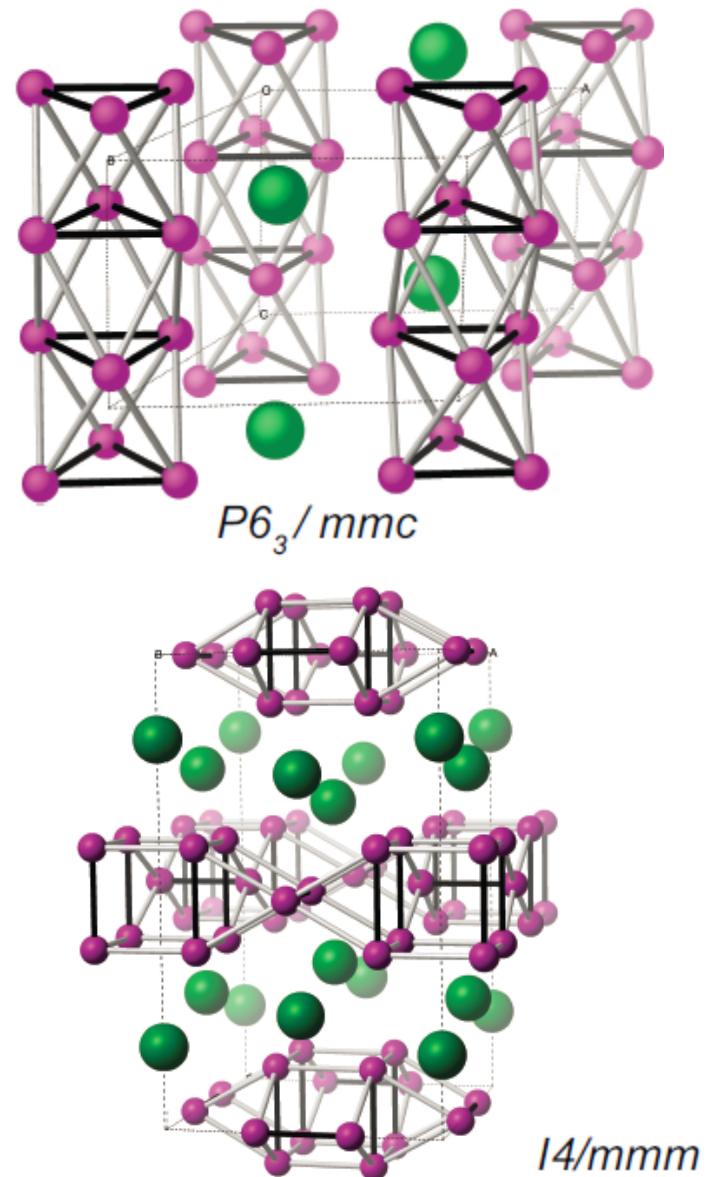
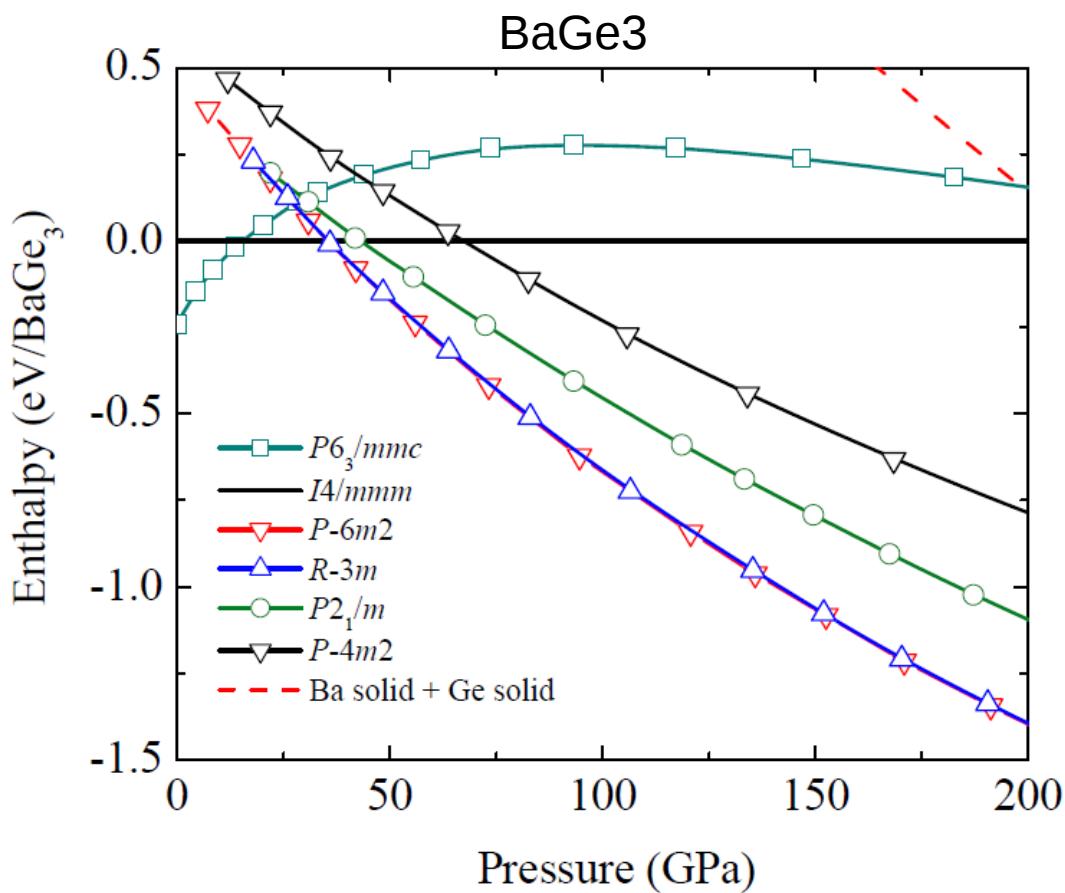
- In ScH_{12} , 1-D chains formed from or $\text{H}_8^{\delta-}$ “octagons” edge-shared with three $\text{H}_5^{\delta-}$ “pentagons” (H-H “bond” distance is 1.20 Å in (c) and 1.05 Å in (d))
- Such a motif has not been observed in other hydrides

Superconductivity Under Pressure

Superconducting Critical Temperature, T_c , as Estimated using the Modified McMillan Equation with $\mu^*=0.1$. The Numerical Solution of the Eliashberg Equation is Provided in Parentheses.

system	pressure (GPa)	λ	ω_{\log} (K)	T_c (K)	hydrogenic motifs ^a
<i>P6/mmm</i> ScH ₂	300	0.44	543.5	4/-	H ⁻
<i>P6₃/mmc</i> ScH ₃	400	0.17	571.8	<1/-	H ⁻
<i>I4/mmm</i> ScH ₄	120	1.68	734.3	92 (163)	H ⁻ , H ₂ ^{$\delta-$}
<i>I4/mmm</i> ScH ₄	250	0.81	1891.8	68 (78)	H ⁻ , H ₂ ^{$\delta-$}
<i>P6₃/mmc</i> ScH ₆	250	0.57	1439.8	29 (43)	H ₂ ^{$\delta-$}
<i>Im-3m</i> ScH ₆	350	1.25	1433.4	135 (169)	3-D
<i>Cmcm</i> ScH ₇	300	1.84	1245.2	169 (213)	H ⁻ , H ₂ ^{$\delta-$}
<i>I4₁md</i> ScH ₉	300	1.94	1156.2	163 (233)	H ₅ ^{$\delta-$} and H ₂ ^{$\delta-$}
<i>Cmcm</i> ScH ₁₀	250	1.17	1366.8	120 (143)	H ₁₀ ^{$\delta-b$}
<i>Imm</i> ScH ₁₂	350	1.23	1525.3	141 (194)	1-D

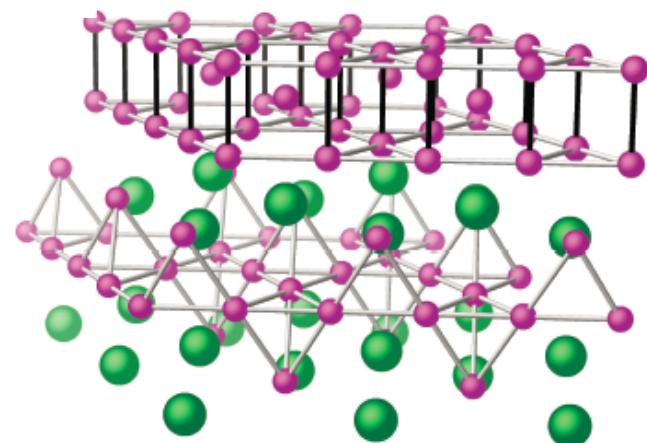
Polar Intermetallic Compounds



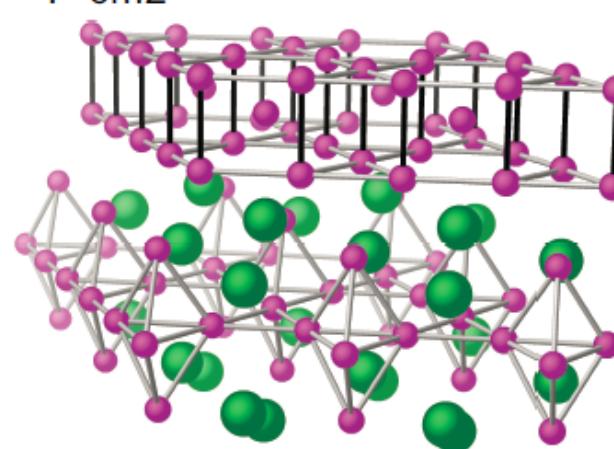
- $P6_3/mmc$: BaGe₃ synthesized 3-13 GPa, T_c 4.0 K
- $I4/mmm$: CaGe₃, CaSi₃, YSi₃, LuSi₃

Two New Phases of BaGe₃ Above 50 GPa

R-3m

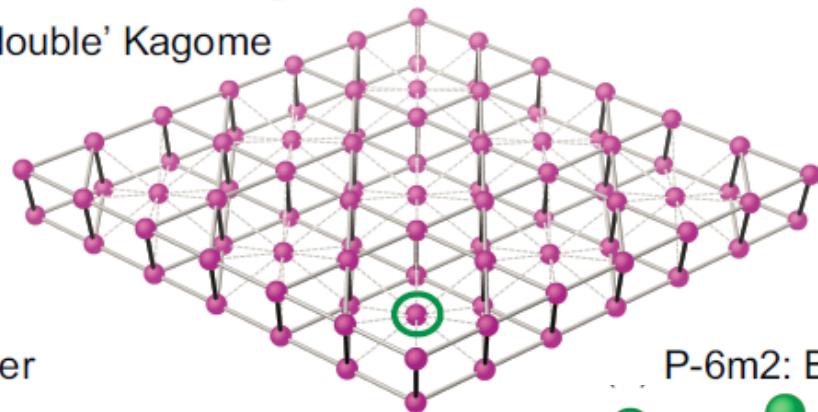


P-6m2

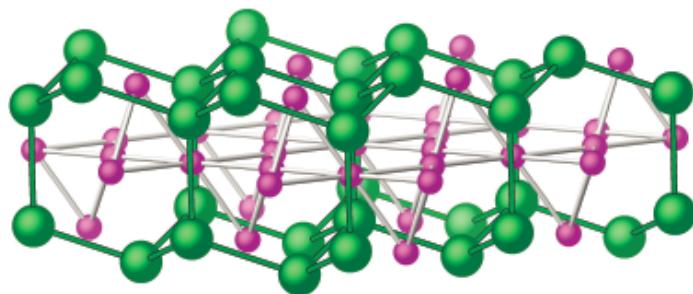


Zurek, E.; Yao, Y. *Inorg. Chem.* **54**, 2875 (2015)

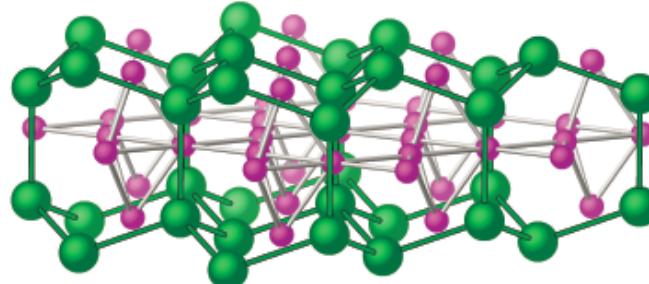
'double' Kagome



R-3m : Ba/Ge layer

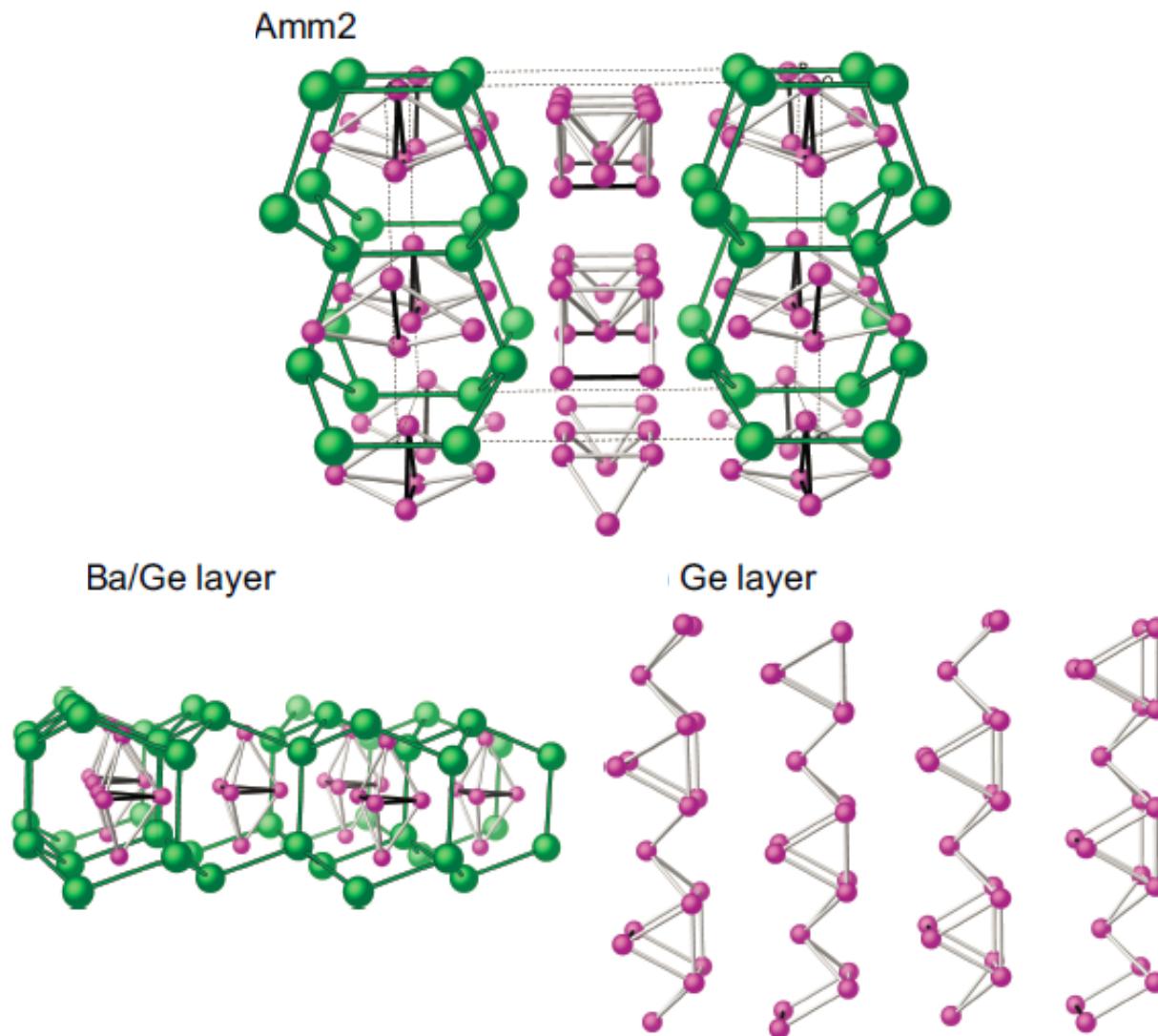


P-6m2: Ba/Ge layer



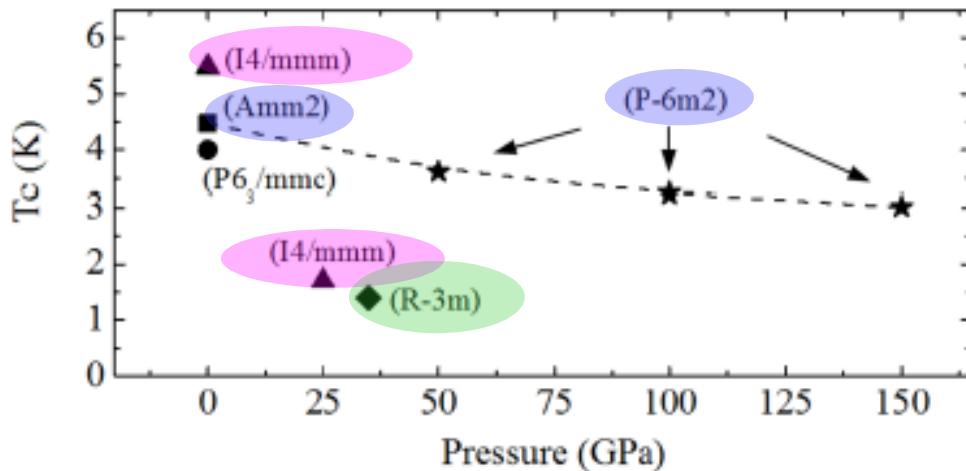
Isostructural with Laves phases MgCu₂ (R-3m) and MgZn₂ (P-6m2)

Decompression to 1 atm



Upon decompression to 1 atm $P-6m2$ transforms to dynamically stable Amm2

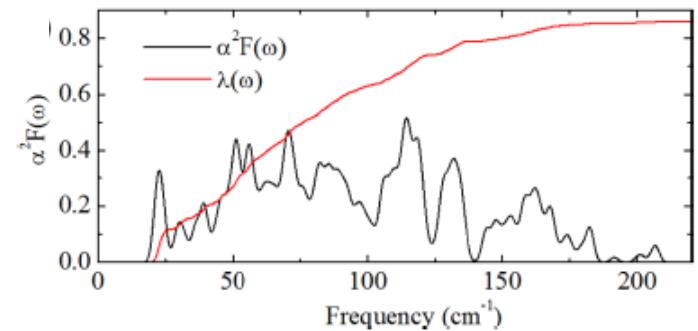
Superconductivity



phase	pressure	λ	ω_{\log} (K)	T_c (K)
$P6_3/mmc$	1 atm	0.73	122.4	4.0
$Amm2$	1 atm	0.86	95.3	4.5
$I4/mmm$	1 atm	0.86	116.2	5.5
$I4/mmm$	25 GPa	0.51	179.7	1.7
$R\bar{3}m$	35 GPa	0.48	209.1	1.4
$P\bar{6}m2$	50 GPa	0.68	133.6	3.6
$P\bar{6}m2$	100 GPa	0.66	134.2	3.2
$P\bar{6}m2$	150 GPa	0.64	138.8	3.0

Large electron-phonon coupling and considerable DOS at E_F compensates for the low vibrational frequencies (ω_{\log}) induced by the heavy atomic masses of Ba and Ge.

Isotropic electron-phonon coupling.



Newly predicted $I4/mmm$ and $Amm2$ $BaGe_3$ have a T_c slightly higher than $P6_3/mmc$ at 1 atm, primarily because of larger λ .

Recent Experimental Results

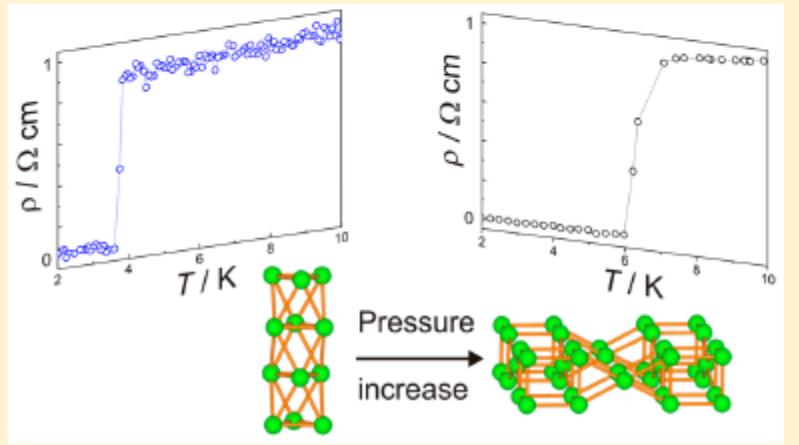
Germanium Dumbbells in a New Superconducting Modification of BaGe₃

Rodrigo Castillo, Alexey I. Baranov, Ulrich Burkhardt, Raul Cardoso-Gil,[†] Walter Schnelle, Matej Bobnar, and Ulrich Schwarz*

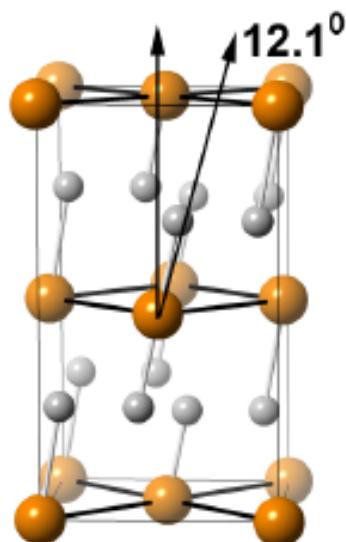
Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden, Germany

 Supporting Information

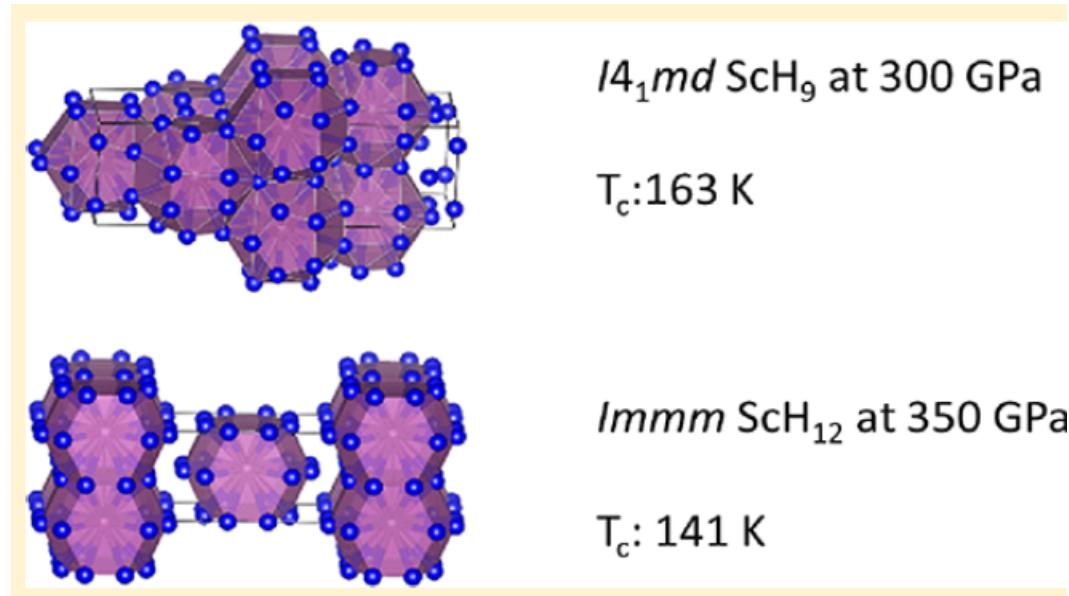
ABSTRACT: We report the high-pressure high-temperature synthesis ($P = 15$ GPa, $T = 1300$ K) of BaGe₃(*tf32*) adopting a CaGe₃-type crystal structure. Bonding analysis reveals layers of covalently bonded germanium dumbbells being involved in multicenter Ba–Ge interactions. Physical measurements evidence metal-type electrical conductivity and a transition to a superconducting state at 6.5 K. Chemical bonding and physical properties of the new modification are discussed in comparison to the earlier described hexagonal form BaGe₃(*hP8*) with a columnar arrangement of Ge₃ triangles.



New Pressure-Stabilized Materials?



PH₂, T_c = 82 K at 200 GPa

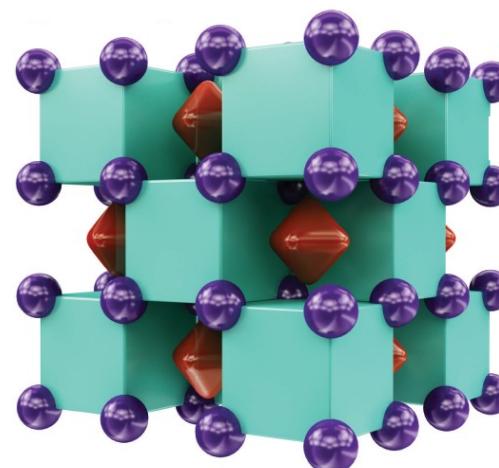


I4₁md ScH₉ at 300 GPa

T_c: 163 K

Immm ScH₁₂ at 350 GPa

T_c: 141 K



Na₂He

Acknowledgements

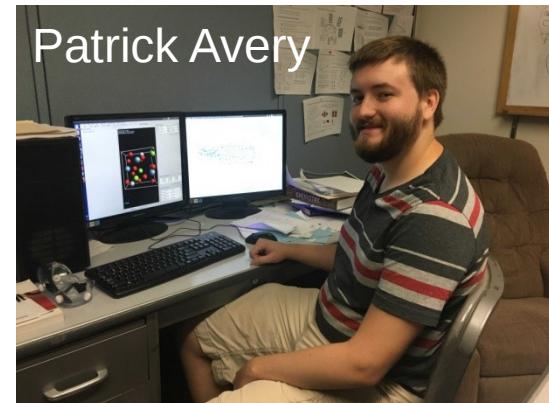
Tiange Bi



Niloofar Zarifi



Patrick Avery



Former Co-workers

- Dr. James Hooper (Krakow)
- Dr. David Lonie (Kitware)
- Dr. Pio Baettig (Zurich)
- Dr. Bahadir Altintas (Turkey)
- Dr. Tyson Terpstra (Buffalo)
- Dr. Zack Falls (Buffalo)
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