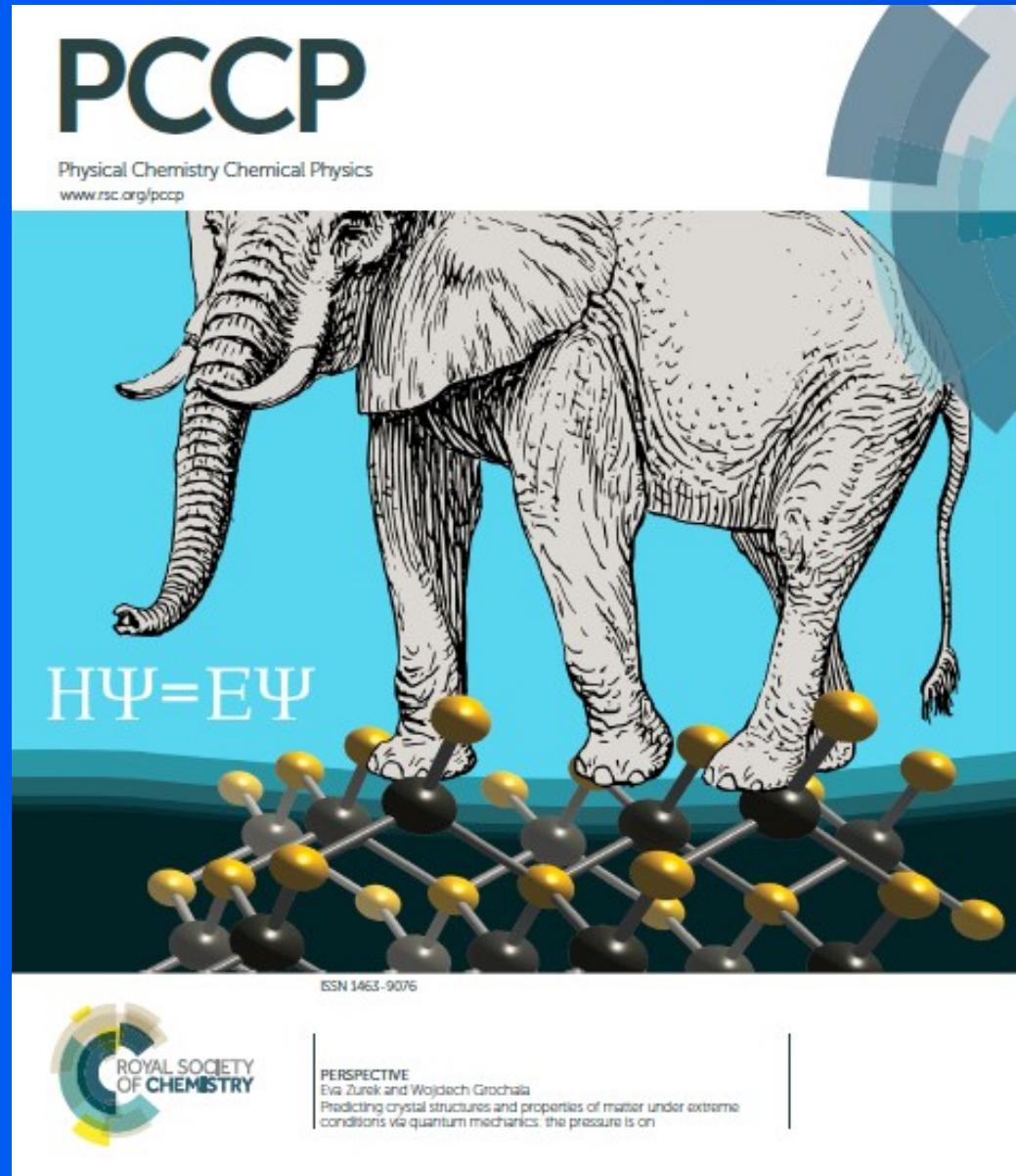


Chemistry Under Pressure

Eva Zurek
SUNY Buffalo

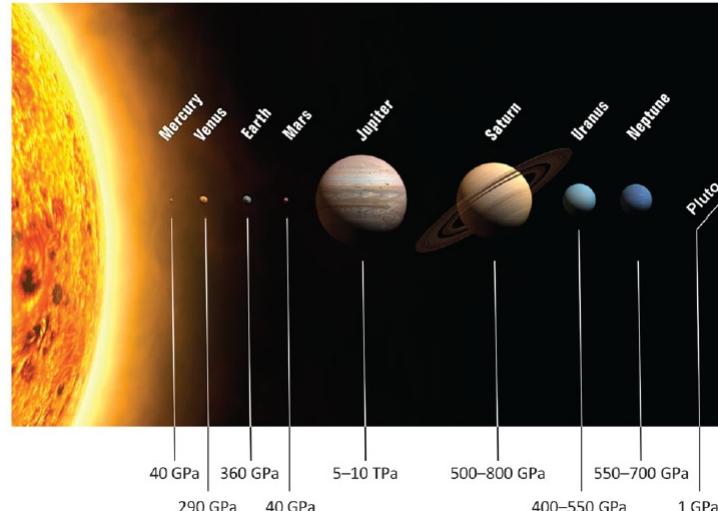


Under Pressure

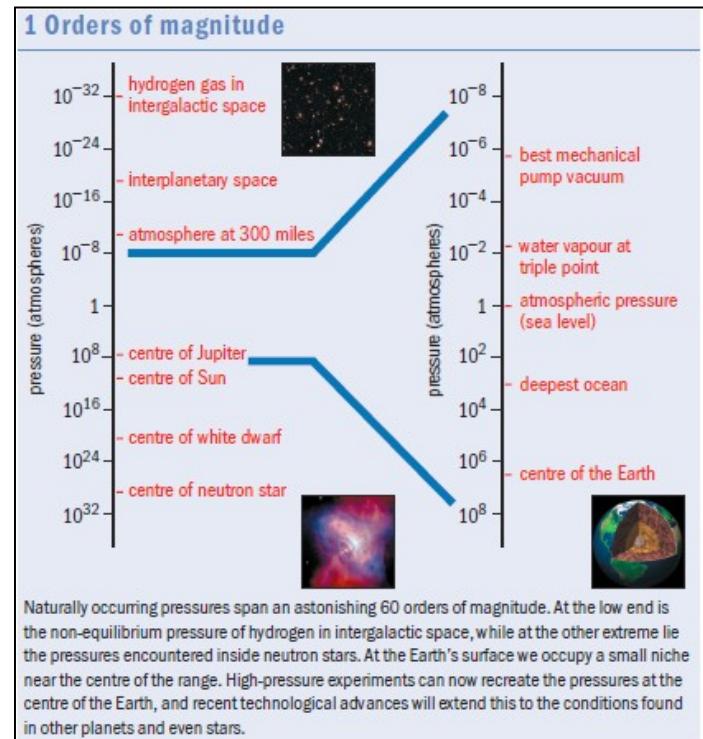
1 atmosphere



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

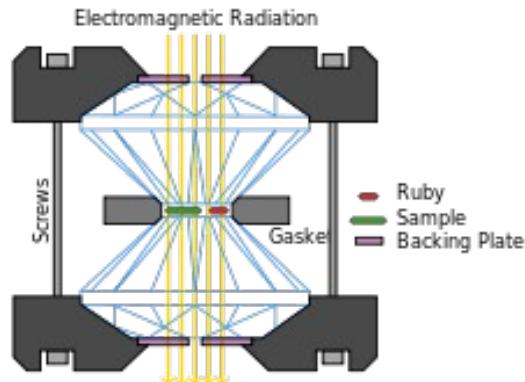


- geosciences
- planetary sciences
- nuclear weapons
- basic science
- high pressure chemical synthesis
- superhard materials
- superconductors
- metallic hydrogen (the holy grail of high pressure research)



Achieving High Pressure

Static Pressure: Diamond Anvil Cells

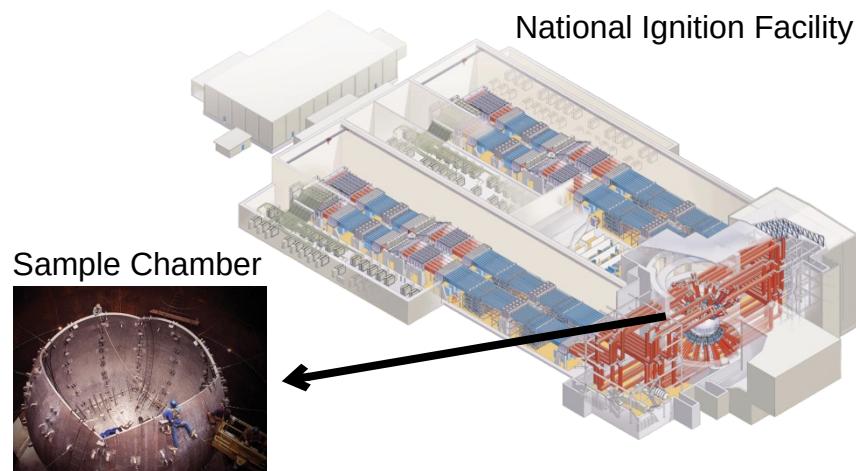


$$\text{Pressure} = \frac{\text{Force}}{\text{Area}}$$

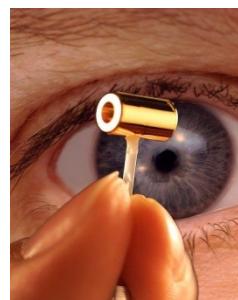
Computations: Changing the Volume!

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

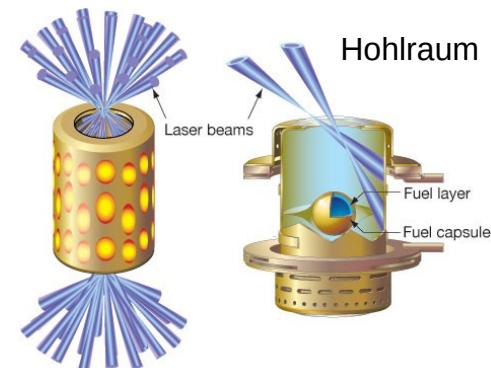
Dynamic Pressure: Shock Compression



Lasers & Sample

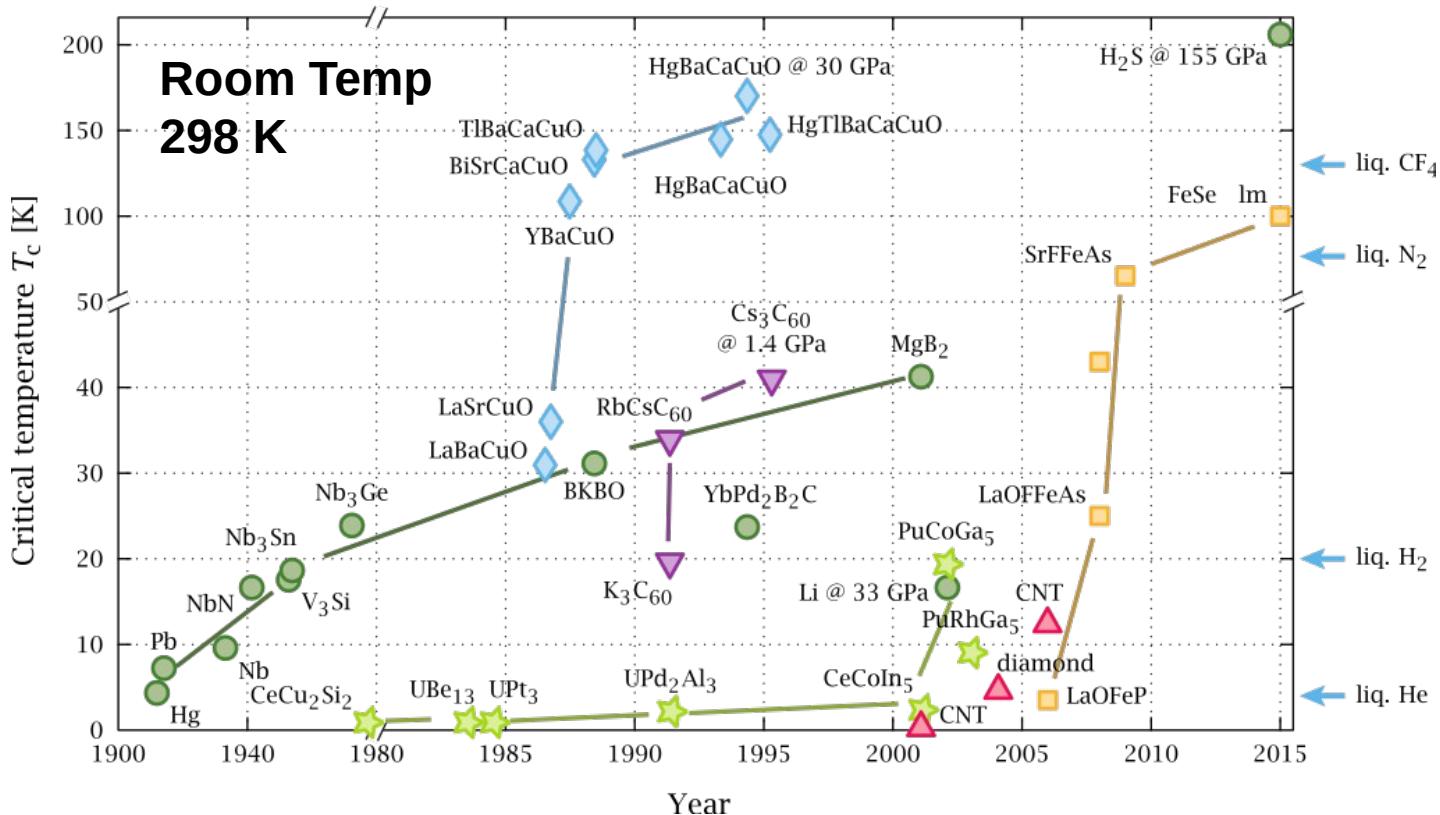


Hohlraum

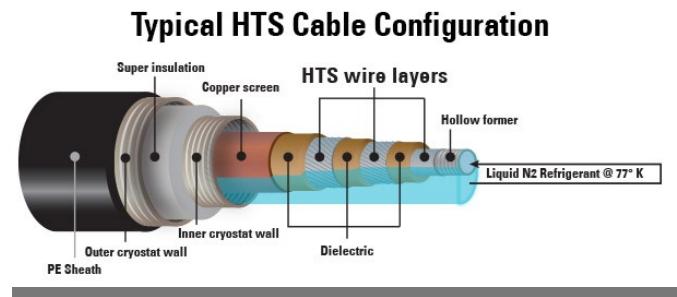
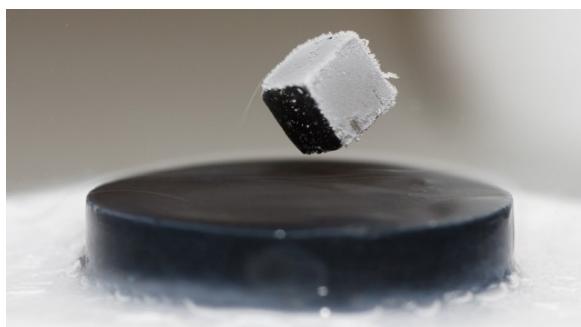


ICF Fusion Microcapsule

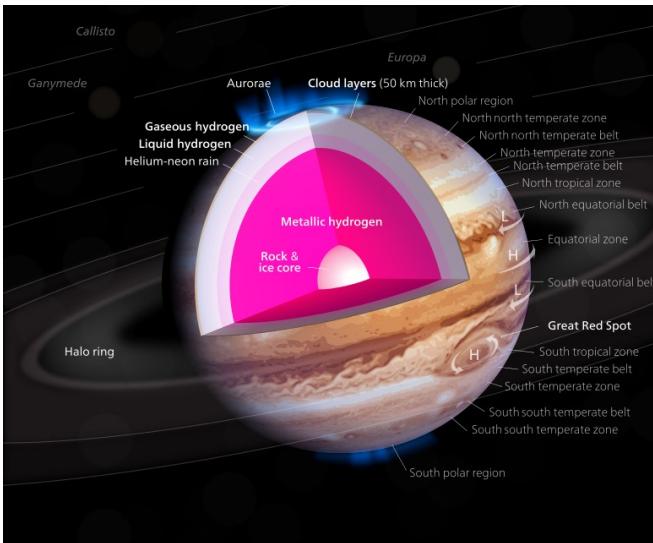
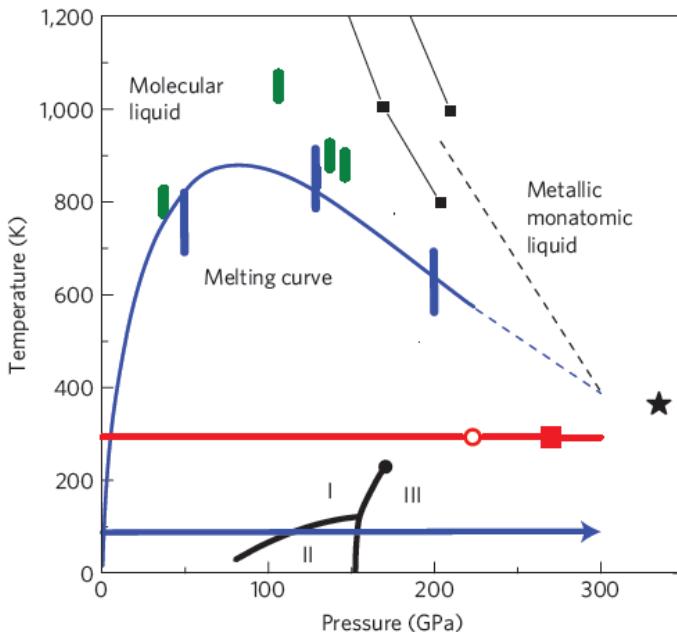
Superconductivity



By PJRay - Own work, CC BY-SA 4.0, <https://commons.wikimedia.org/w/index.php?curid=46193149>



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).

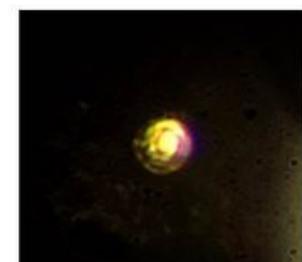
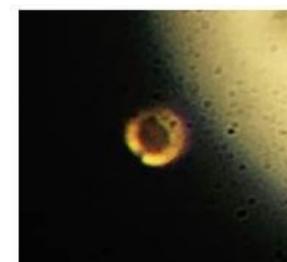
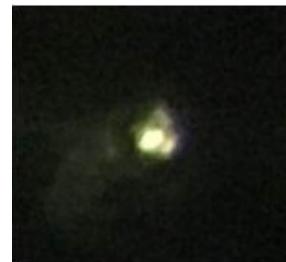
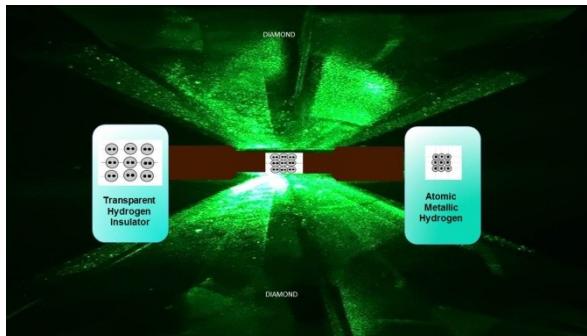
Observation of the Wigner-Huntington transition to metallic hydrogen

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.

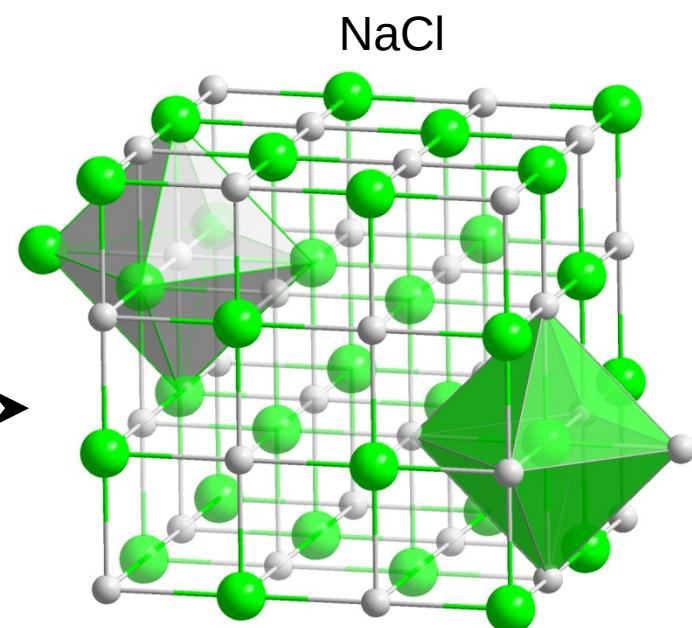


Chemical Reactivity Under Pressure

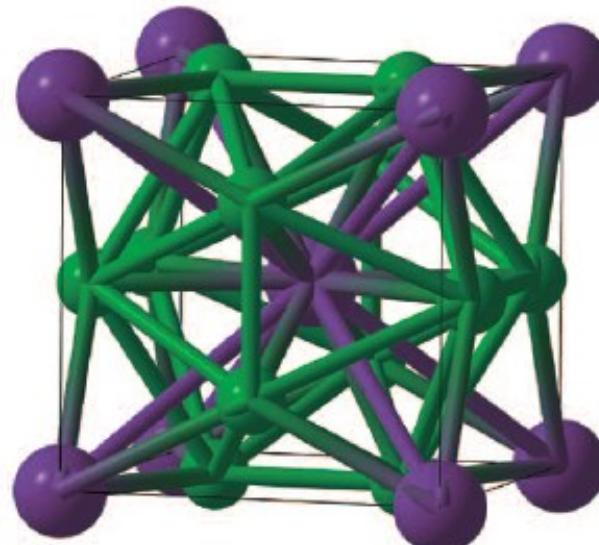
Table Salt



1 atmosphere crystal
structure



Under pressure NaCl₃
can be made!



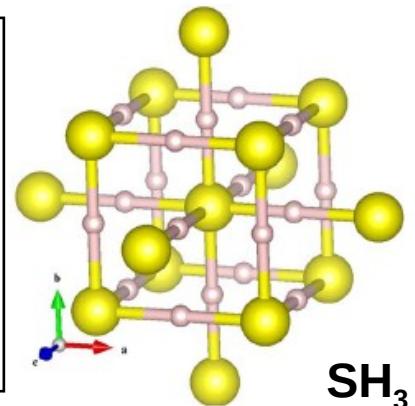
Recent Experimental Measurements

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



PHYSICAL REVIEW LETTERS 122, 027001 (2019)

Editors' Suggestion

Featured in Physics

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

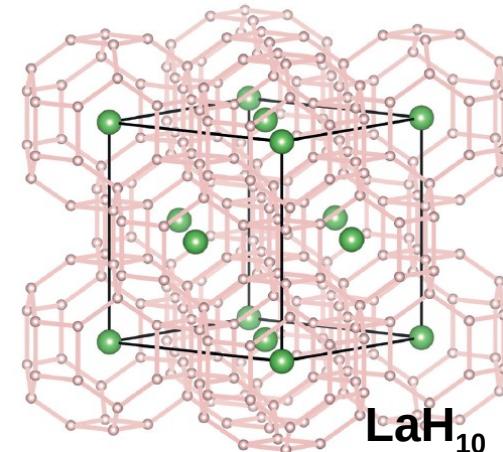
Maddury Somayazulu,^{1,*} Muhtar Ahart,¹ Ajay K. Mishra,^{2,‡} Zachary M. Geballe,² Maria Baldini,^{2,§} Yue Meng,³ Viktor V. Struzhkin,² and Russell J. Hemley^{1,†}

LETTER

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

Superconductivity at 250 K in lanthanum hydride under high pressures

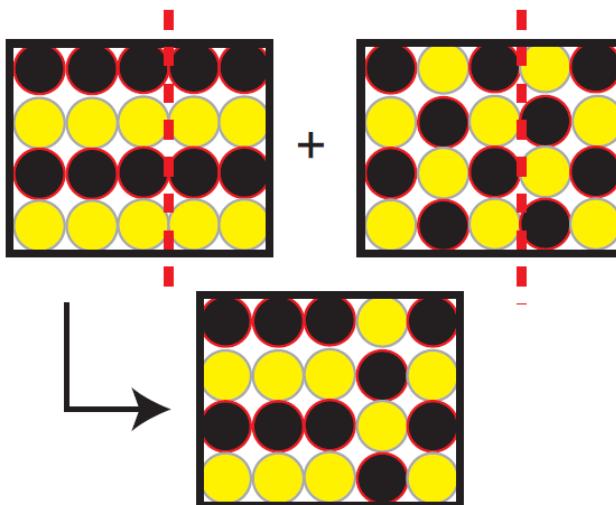
A. P. Drozdov^{1,7}, P. P. Kong^{1,7}, V. S. Minkov^{1,7}, S. P. Besedin^{1,7}, M. A. Kuzovnikov^{1,6,7}, S. Mozaffari², L. Balicas², F. F. Balakirev³, D. E. Graf², V. B. Prakapenka⁴, E. Greenberg⁴, D. A. Knyazev¹, M. Tkacz⁵ & M. I. Eremets^{1*}



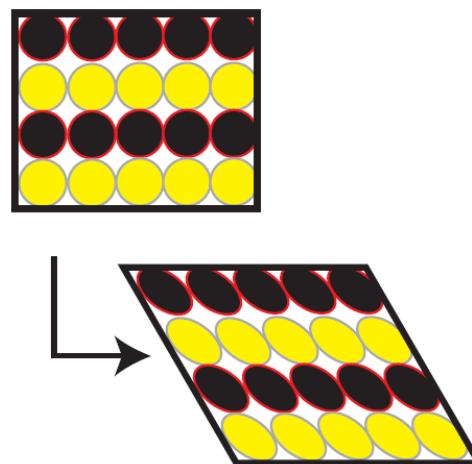
LaH_{10}

Evolutionary Structure Prediction: XtalOpt

1. Crossover

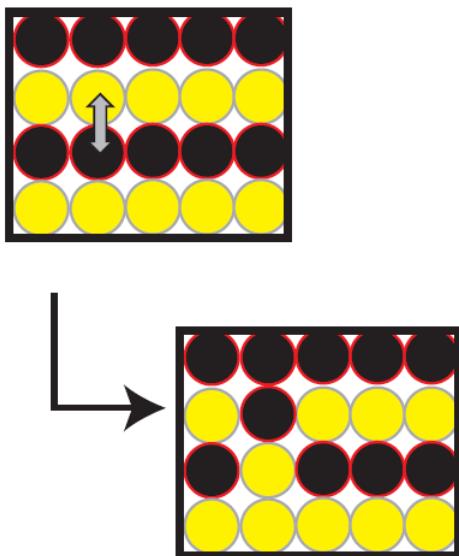


2. Strain

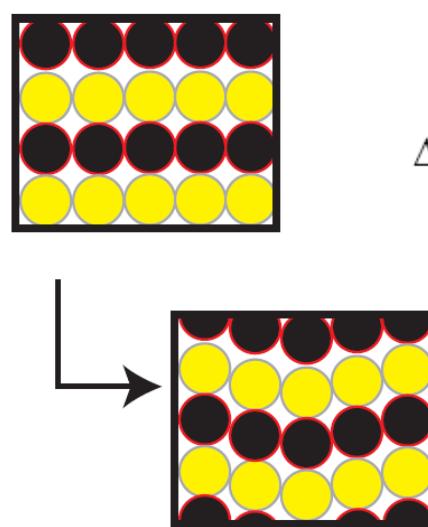


$$\mathbf{v}_{\text{new}} = \begin{bmatrix} 1 + \varepsilon_{11} & \frac{\varepsilon_{12}}{2} & \frac{\varepsilon_{13}}{2} \\ \frac{\varepsilon_{12}}{2} & 1 + \varepsilon_{22} & \frac{\varepsilon_{23}}{2} \\ \frac{\varepsilon_{13}}{2} & \frac{\varepsilon_{23}}{2} & 1 + \varepsilon_{33} \end{bmatrix}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

3. Exchange

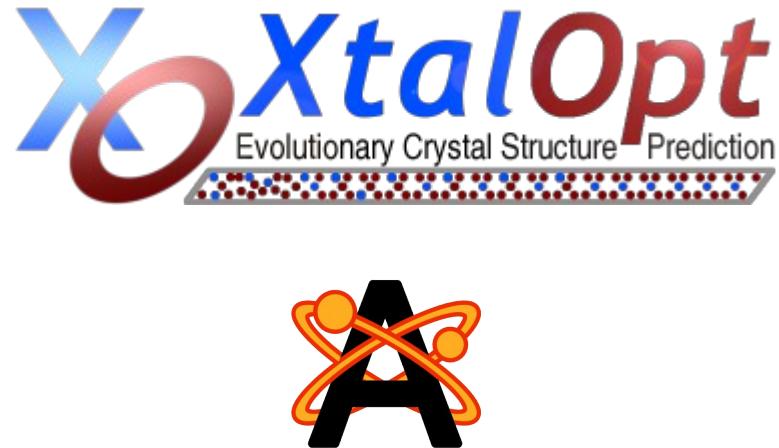
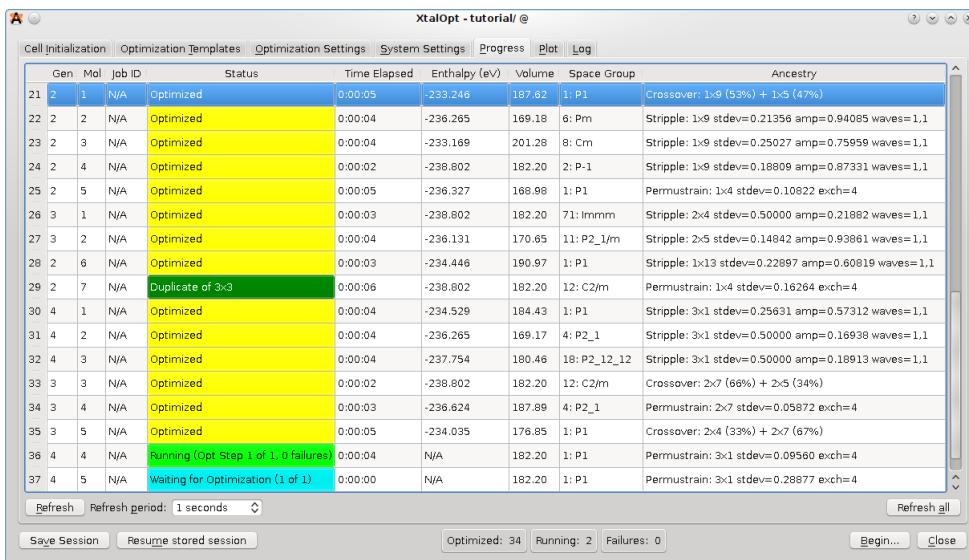


4. Ripple



XtalOpt: Visualization

Website: xtalopt.github.io



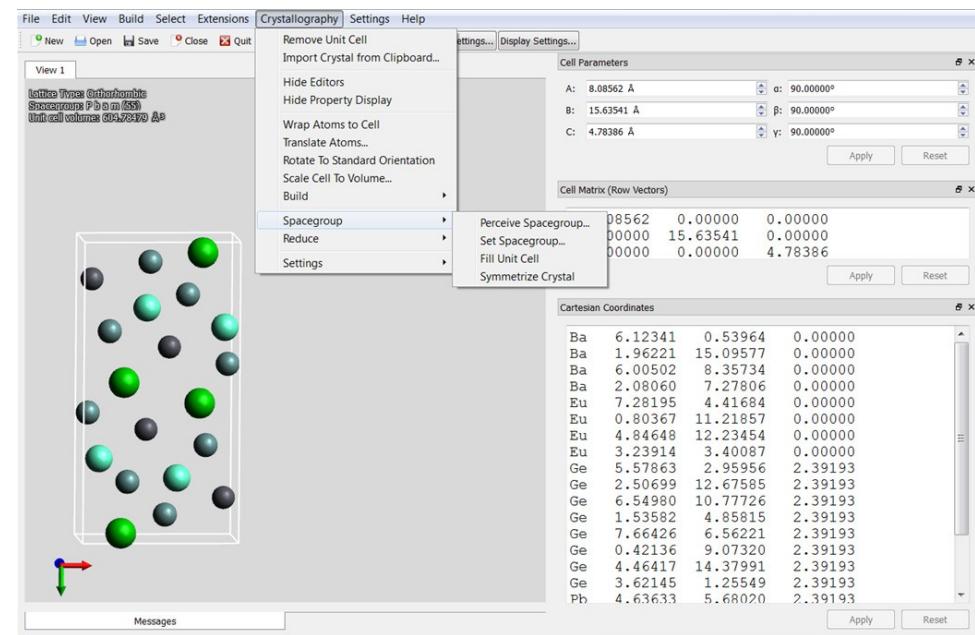
Platforms & Queue Interface

- 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
latticeMins      = 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>

Yet Another extended Hückel MO Program

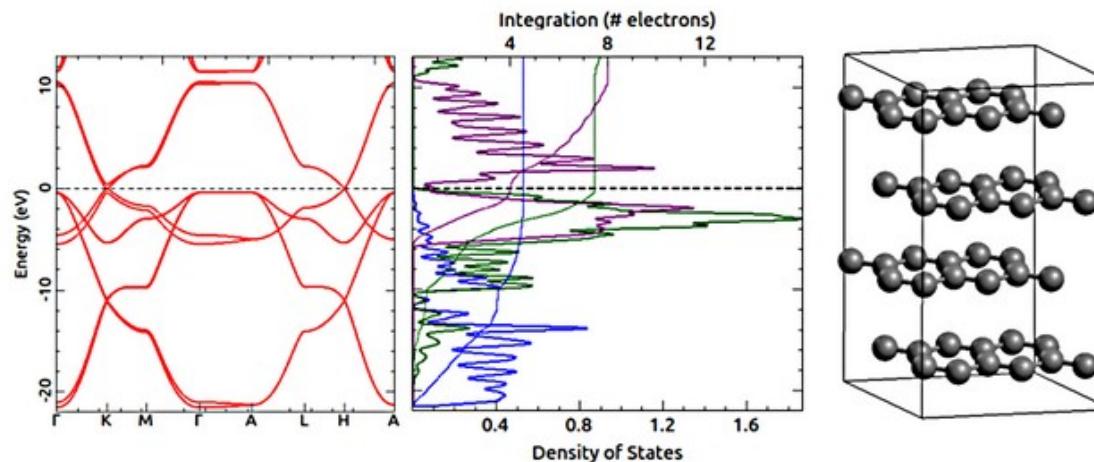
Avogadro with YAeHMOP

Windows

Mac OS X

Linux

YAeHMOP is an extended Hückel package that can be found [here](#).
It has been interfaced with the open-source molecular editor [Avogadro](#).



A tutorial is available [here](#).



<http://avogadro-yaehmop.github.io>

Avery, Ludowieg, Autschbach,, Zurek. 2018, *J. Chem. Educ.* **95**, 331-337.

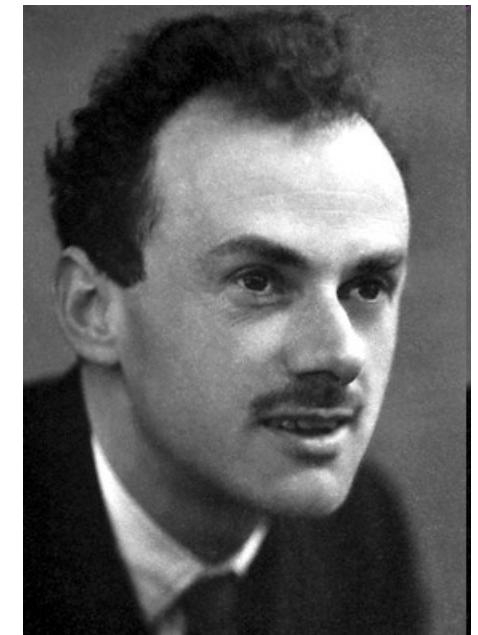
Quantum Mechanics

The Non-Relativistic Schrödinger Equation:

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

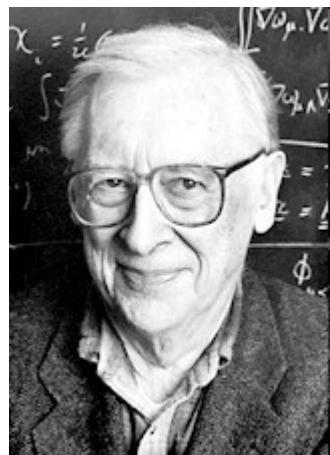
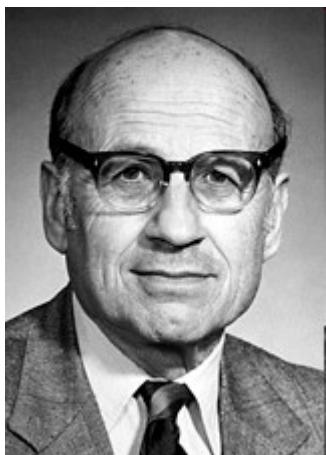
The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

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".

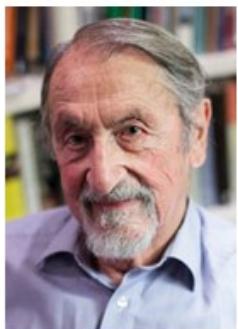
Nobel Prize in Chemistry 2013



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".

[Share](#) | [Tell a Friend](#) | [Comments](#)

To cite this page

MLA style: "The Nobel Prize in Chemistry 2013". [Nobelprize.org](#). Nobel Media AB 2013.

[Q](#) | [Terms](#)

Copyright © Nobel Media AB 2013

I

New York Times:

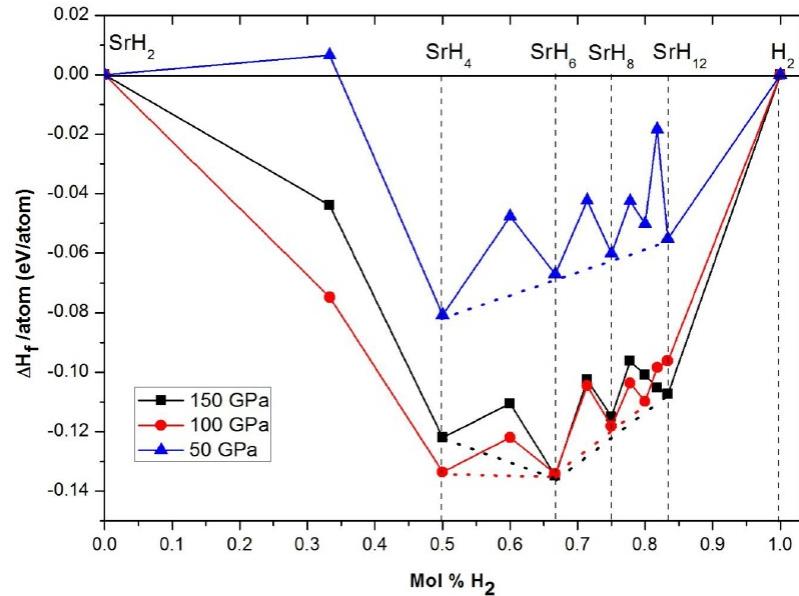
Chemistry, meet computer science.

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.

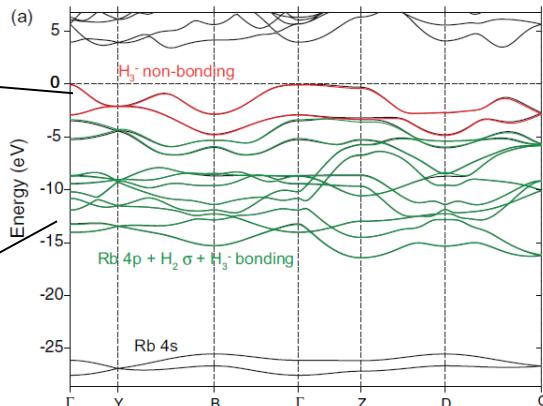
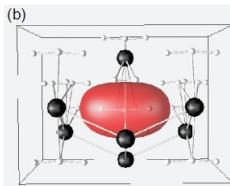
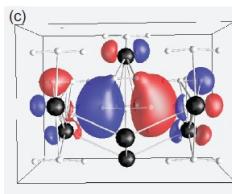
Exploring Chemical Trends



Stoichiometry



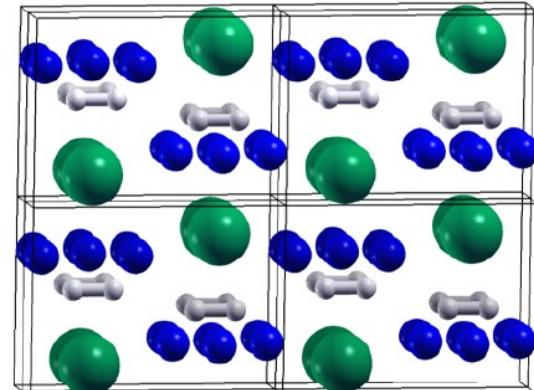
Mol % H_2



Energy (eV)

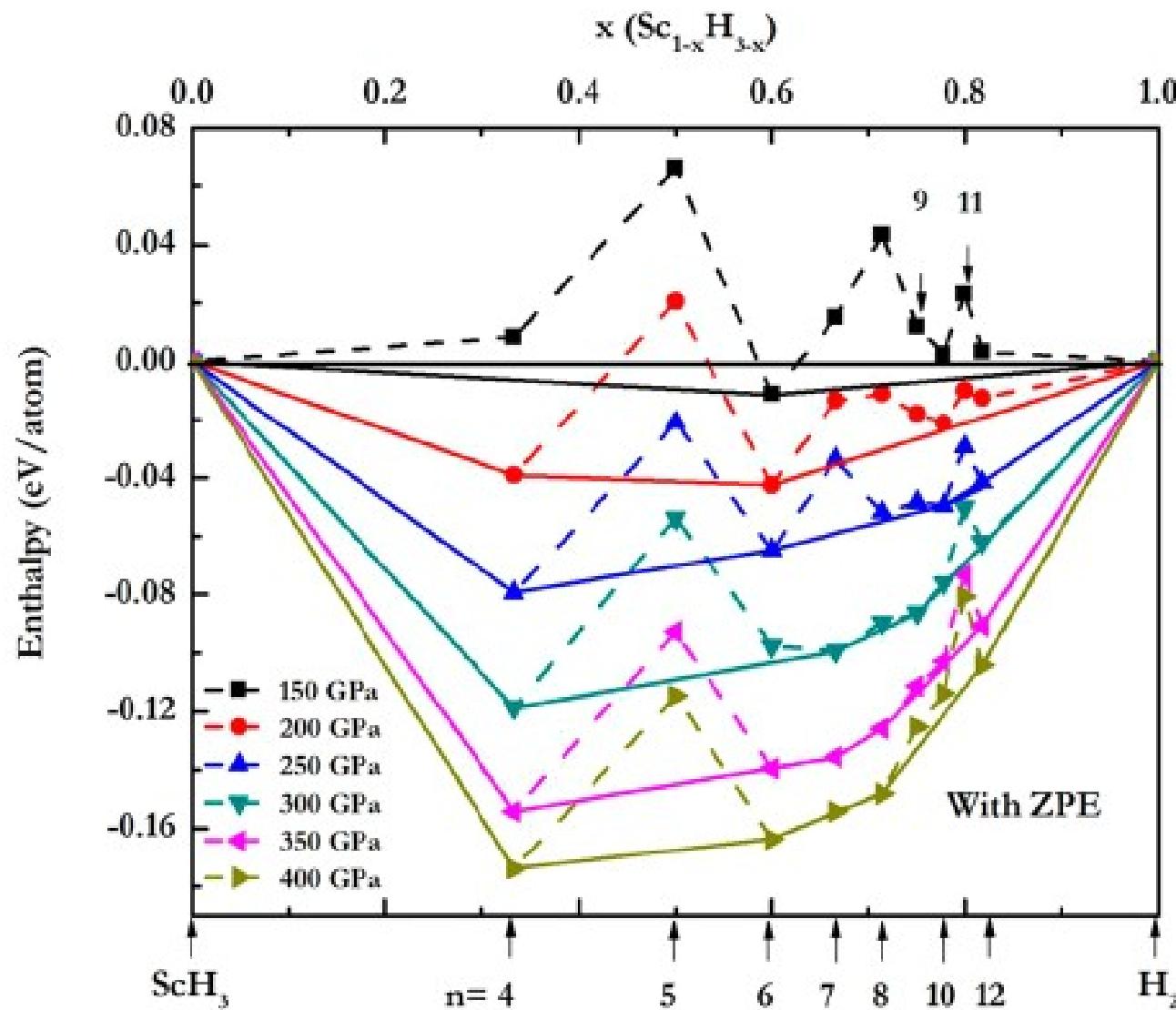
Properties

Electronic Structure

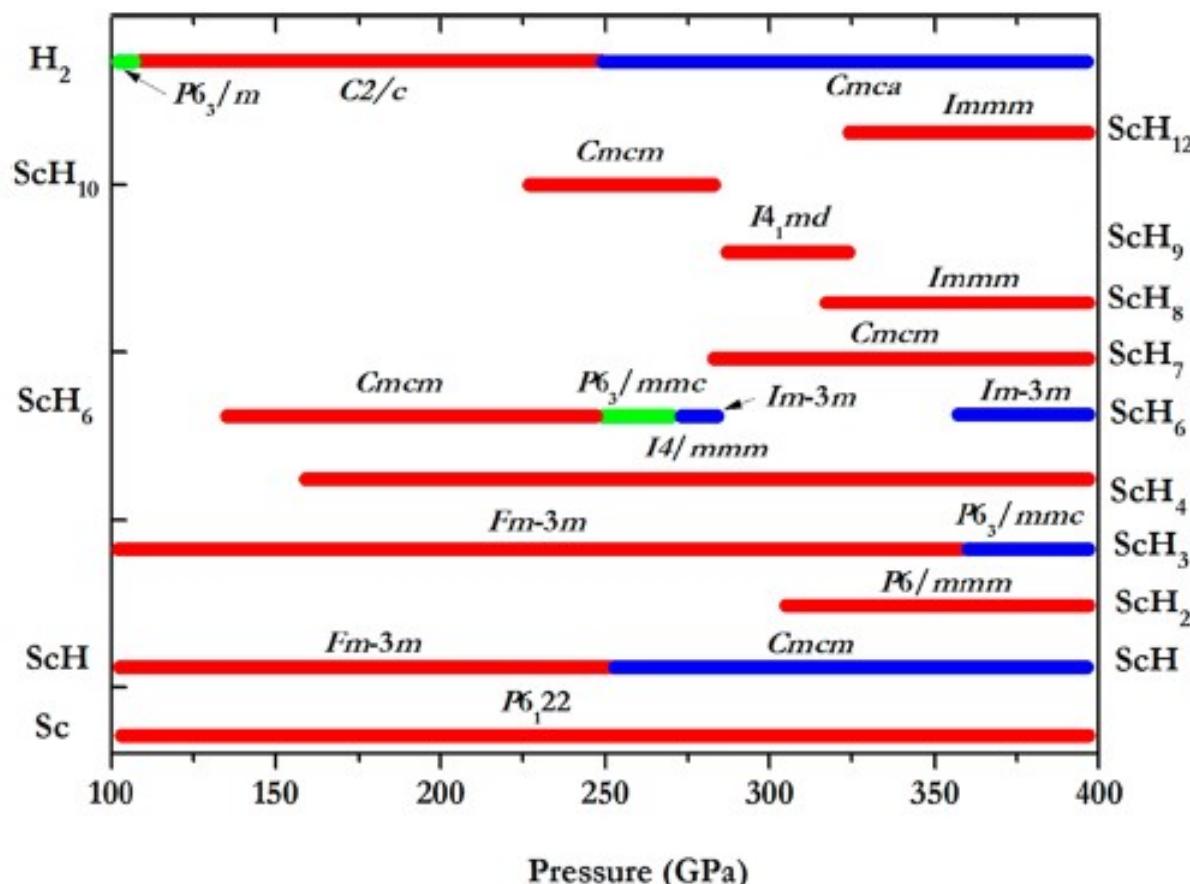


Structure

Polyhydrides of Scandium?



Many Stable Polyhydrides...



New Structures Predicted Here:

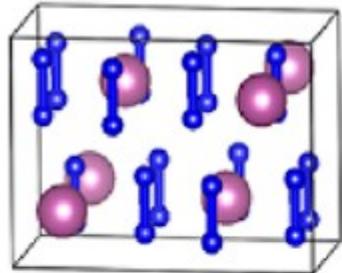
- Cmcm ScH₆
- Cmcm ScH₇
- I4₁md ScH₉
- Immm ScH₁₂

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

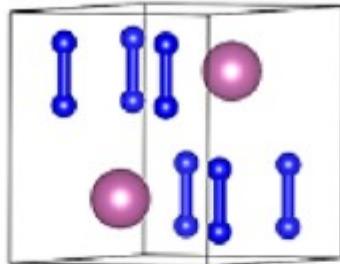
ScH₄ - ScH₈: Qian et al. PRB. 2017, 96, 094513.

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

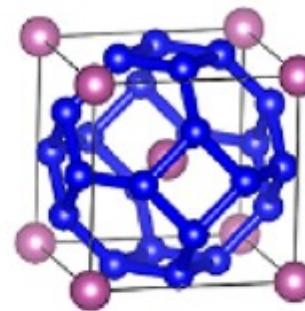
Stable Phases of ScH_6



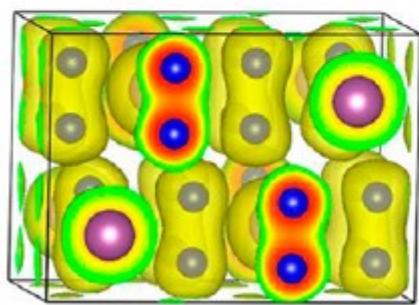
(a) $Cmcm$, 200 GPa



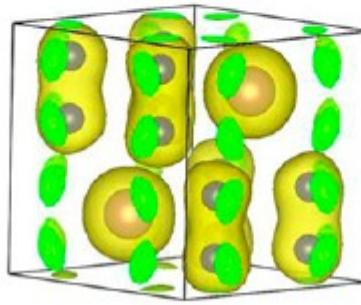
(b) $P6_3/mmc$, 250 GPa



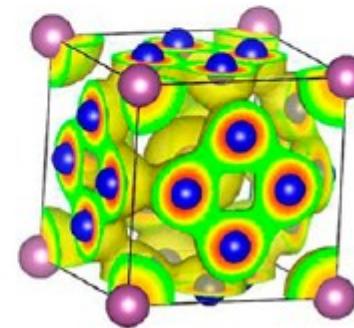
(c) $Im\text{-}3m$, 250 GPa



(d) $Cmcm$, 200 GPa



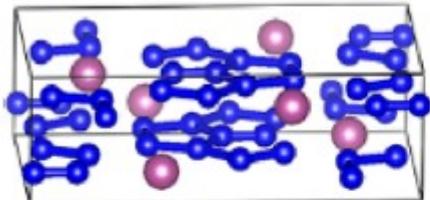
(e) $P6_3/mmc$, 250 GPa



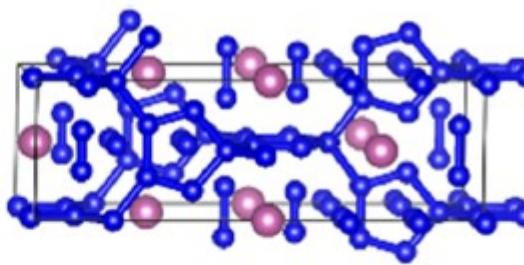
(f) $Im\text{-}3m$, 250 GPa

- “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)

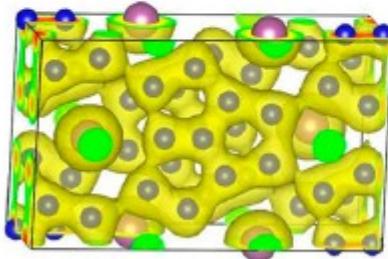
$\text{H}_5^{\delta^-}$ -” Motifs in ScH_9 and ScH_{10}



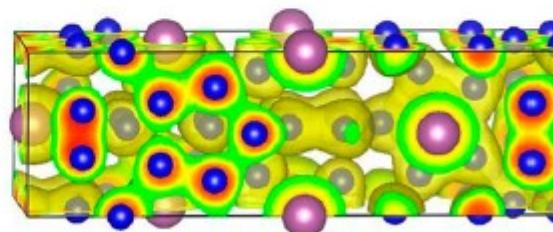
(a) $\text{ScH}_{10}, Cmcm$, 250 GPa



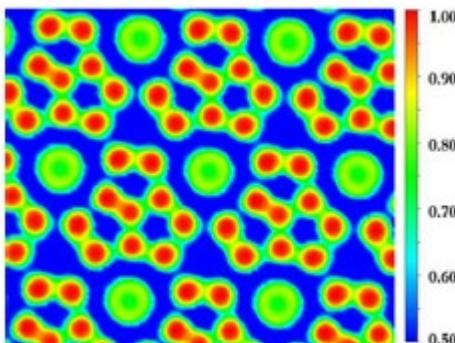
(b) $\text{ScH}_9, I4_1md$, 300 GPa



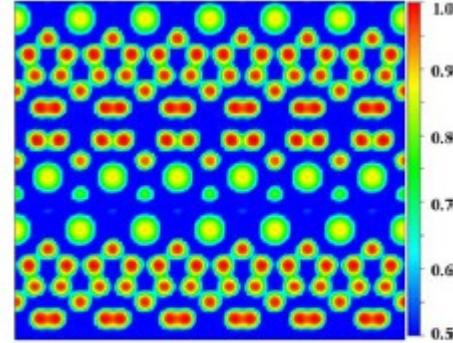
(c) $\text{ScH}_{10}, Cmcm$, 250 GPa



(d) $\text{ScH}_9, I4_1md$, 300 GPa



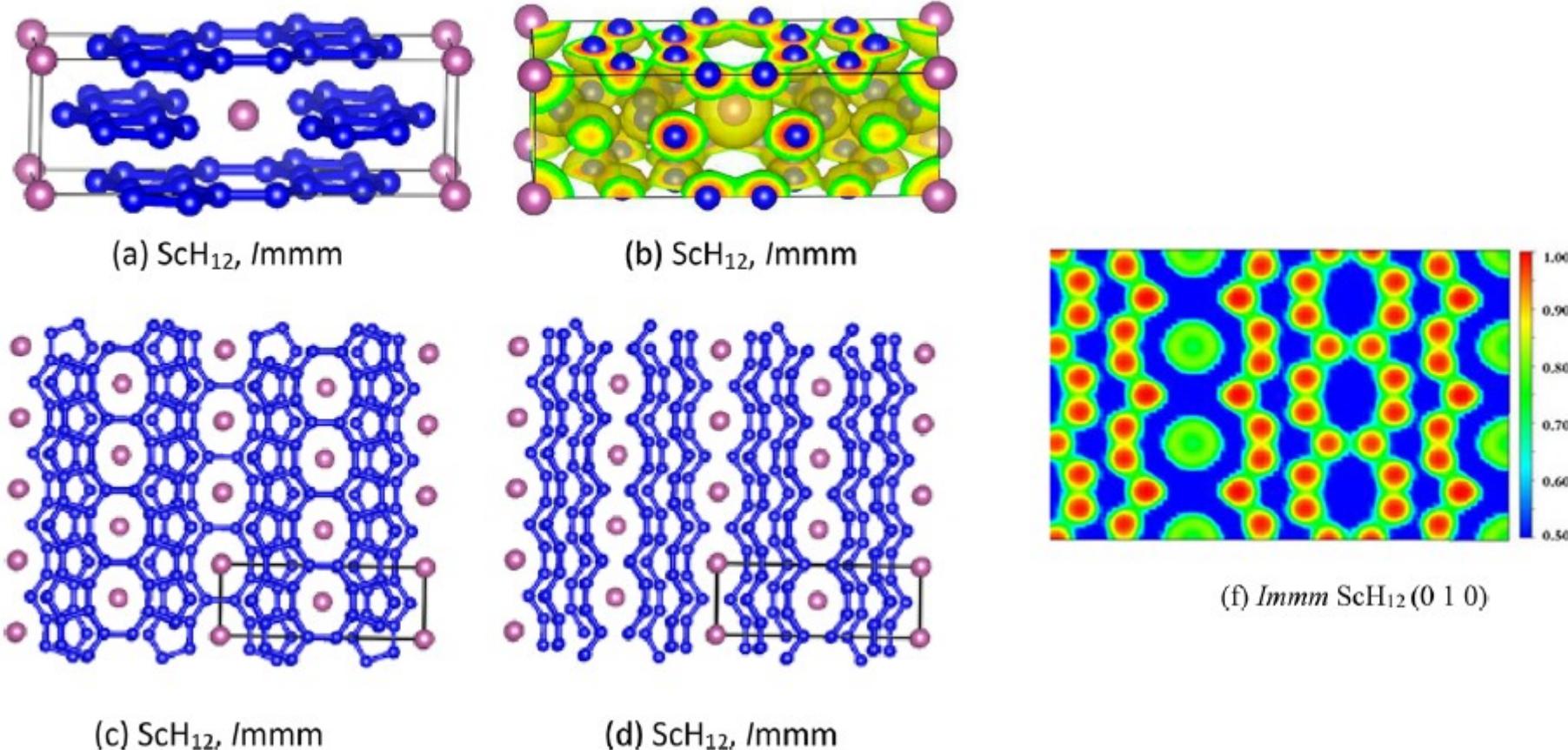
(e) $Cmcm$ $\text{ScH}_{10} (0\ 0\ 1)$



(f) $I4_1md$ $\text{ScH}_9 (0\ -1\ 0)$

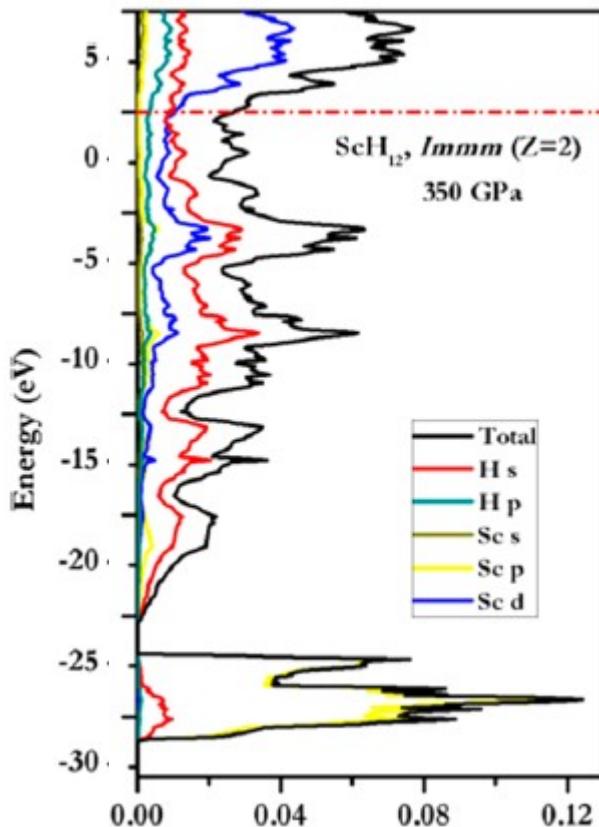
- In ScH_{10} , 10 hydrogen atoms form 0-D edge-fused $\text{H}_5^{\delta^-}$ motifs
- In ScH_9 , 1-D chains of edge-fused $\text{H}_5^{\delta^-}$ and H_2
- These “ $\text{H}_5^{\delta^-}$ ” motifs have not been observed in other hydrides

1-Dimensional Chains in ScH₁₂

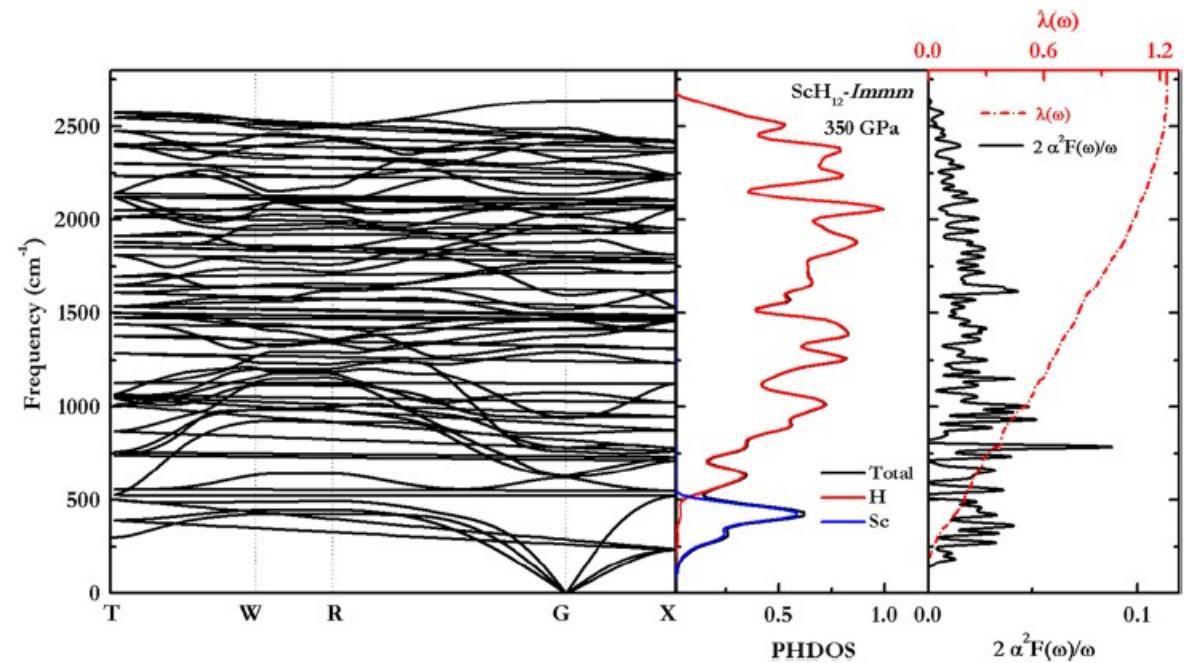


- In ScH₁₂, 1-D chains formed from or H₈^{δ-} “octagons” edge-shared with three H₅^{δ+} “pentagons” (H-H “bond” distance is 1.20 Å in (c) and 1.05 Å in (d))
- Such a motif has not been observed in other hydrides

Electronic and Phonon DOS



$I\bar{m}mm$ ScH_{12} at 350 GPa



- All of the phases are good metals
- Sc 3d and H 1s overlap – strong hybridization
- Doping with Sc has metallized hydrogen!
- Sc based phonon modes 23% and H based phonon modes 73% of EPC, 1.23

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>P</i> 6/ <i>mmm</i> ScH ₂ | 300 | 0.44 | 543.5 | 4(–) | H [–] |
| <i>P</i> 6 ₃ / <i>mmc</i> ScH ₃ | 400 | 0.17 | 571.8 | <1(–) | H [–] |
| <i>I</i> 4/ <i>mmm</i> ScH ₄ | 120 | 1.68 | 734.3 | 92 (163) | H [–] , H ₂ ^{δ–} |
| <i>I</i> 4/ <i>mmm</i> ScH ₄ | 250 | 0.81 | 1891.8 | 68 (78) | H [–] , H ₂ ^{δ–} |
| <i>P</i> 6 ₃ / <i>mmc</i> ScH ₆ | 250 | 0.57 | 1439.8 | 29 (43) | H ₂ ^{δ–} |
| <i>I</i> m-3 <i>m</i> ScH ₆ | 350 | 1.25 | 1433.4 | 135 (169) | 3-D |
| <i>C</i> mcm ScH ₇ | 300 | 1.84 | 1245.2 | 169 (213) | H [–] , H ₂ ^{δ–} |
| <i>I</i> 4 ₁ <i>md</i> ScH ₉ | 300 | 1.94 | 1156.2 | 163 (233) | H ₅ ^{δ–} and H ₂ ^{δ–} |
| <i>C</i> mcm ScH ₁₀ | 250 | 1.17 | 1366.8 | 120 (143) | H ₁₀ ^{δ–b} |
| <i>I</i> mmm ScH ₁₂ | 350 | 1.23 | 1525.3 | 141 (194) | 1-D |

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

Superconductivity in Phosphine?

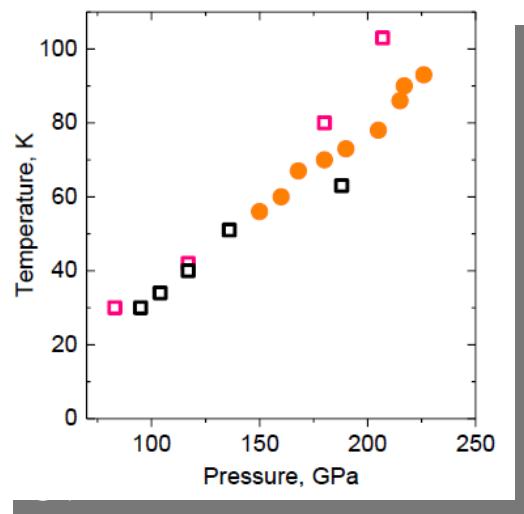
arXiv:1502.06224

Superconductivity above 100 K in PH₃ at high pressures

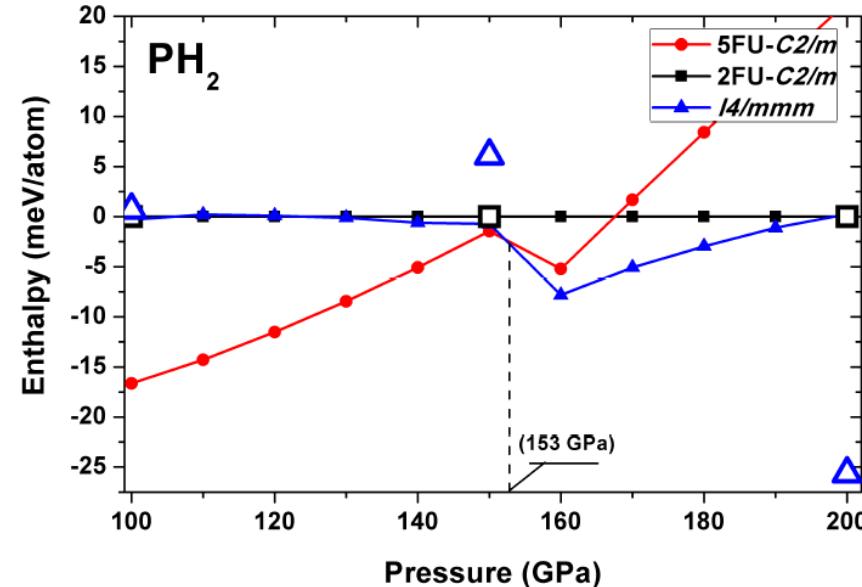
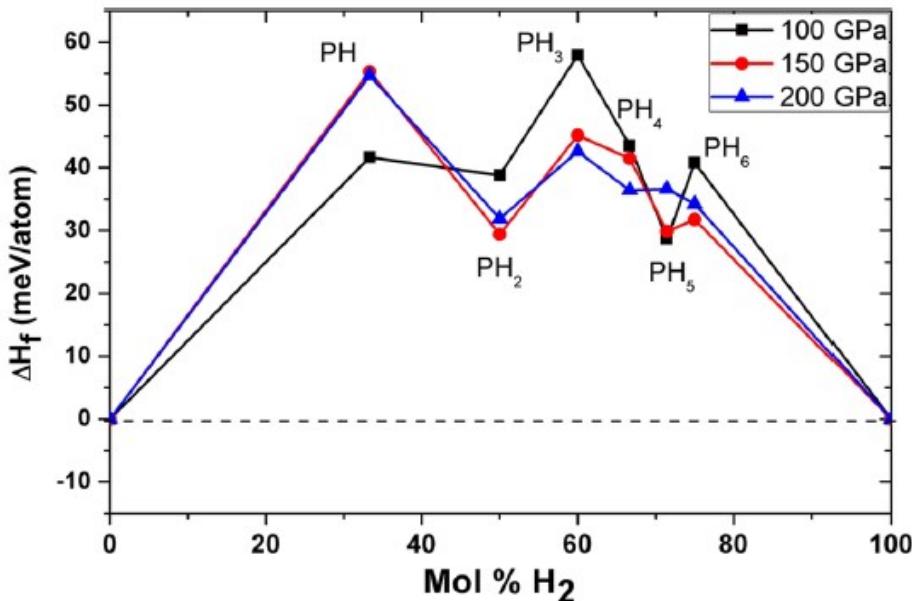
A. P. Drozdov, M. I. Eremets and I. A. Troyan

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

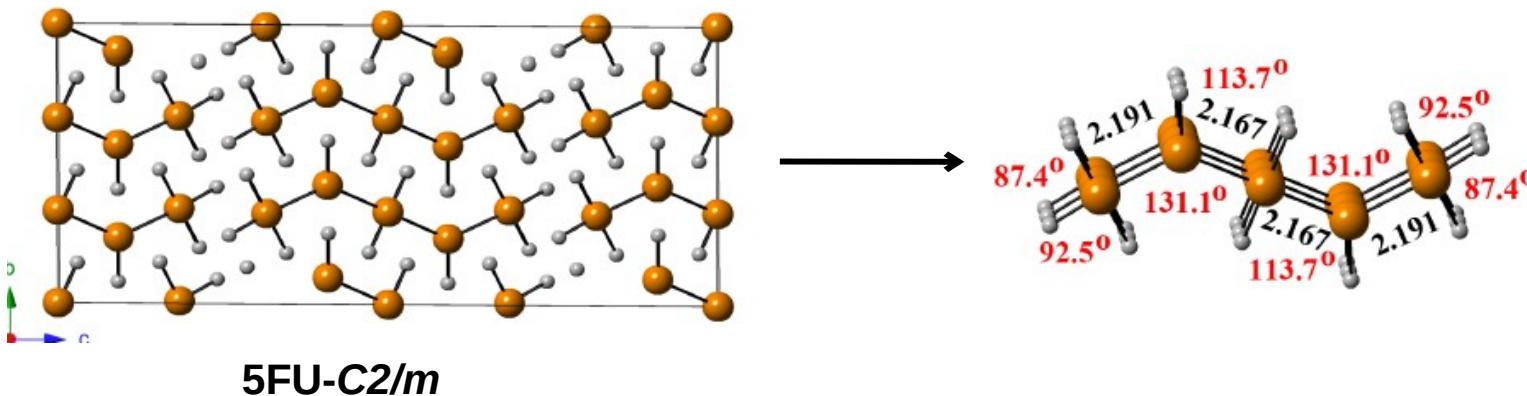
Following the recent discovery of very high temperature conventional superconductivity in sulfur hydride (critical temperature T_c of 203 K, Ref¹) we searched for superconductivity in other hydrides and found that a covalent hydride phosphine (PH₃) also exhibits a high $T_c > 100$ K at pressure $P > 200$ GPa as determined from four-probe electrical measurements.



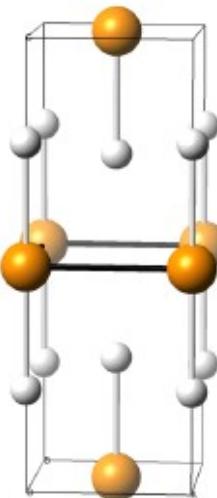
Phosphine Decomposition Under Pressure



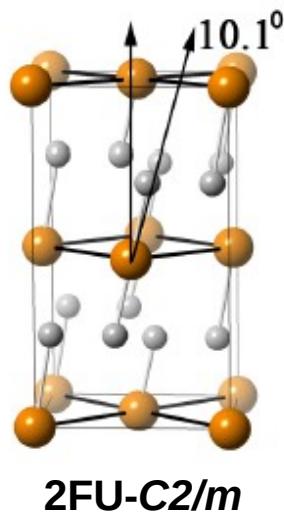
150 GPa, $\Delta(\text{H} + \text{ZPE}) + 45.8 \text{ meV/atom}$



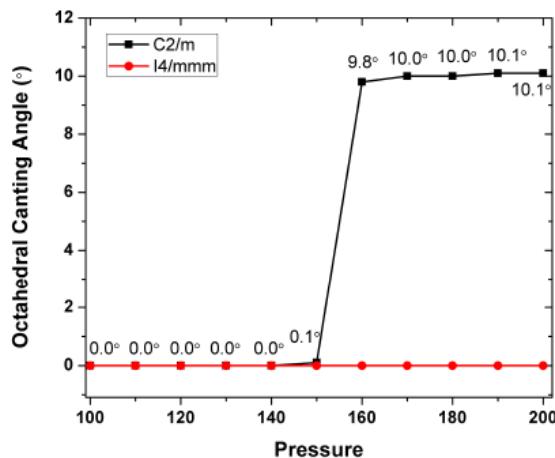
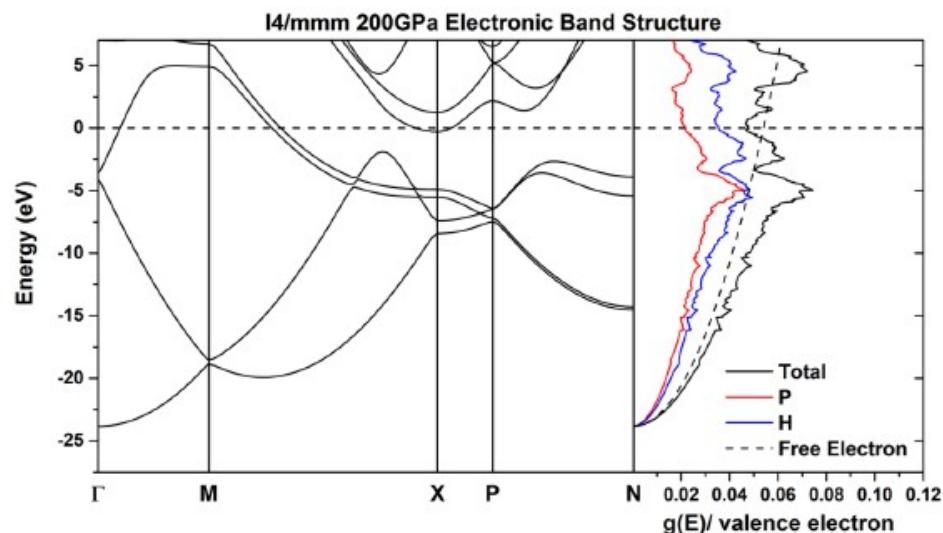
PH_2 Structure and Electronic Structure



$\text{C}2/m$

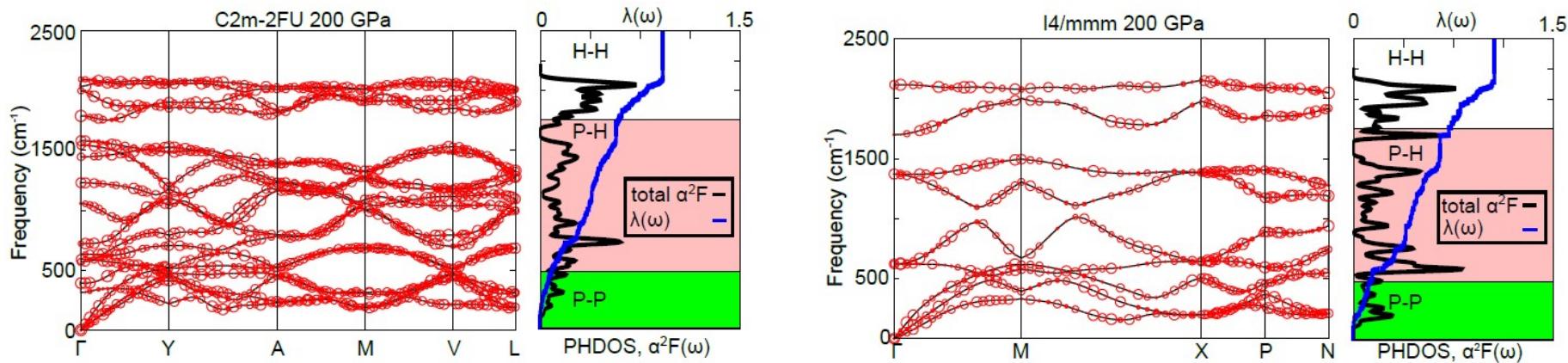


$\text{I}4/\text{mmm}$



- 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 |

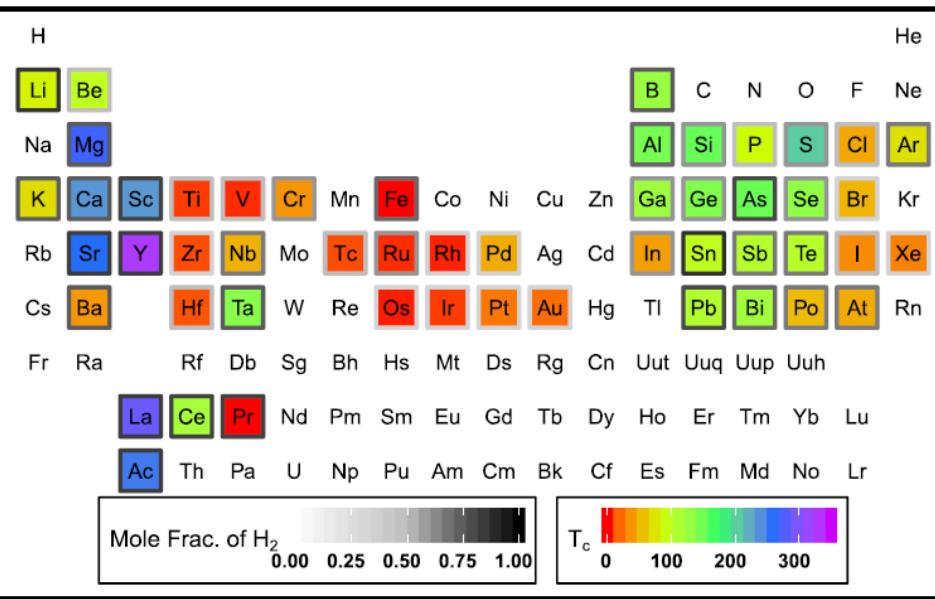
Flores-Livas et al. PRB. 2016, 93, 020508.

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

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

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

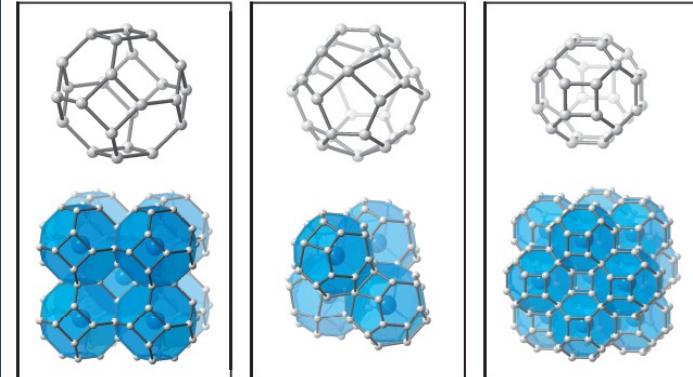
Periodic Table of Superconducting Hydrides



| System | P (GPa) | λ | μ^* | T _c (K) |
|--------------------------------|---------|-----------|-----------|--|
| MgH ₆ | 300 | 3.29 | 0.12 | 263 ^a 169 |
| CaH ₆ ^c | 150 | 2.69–2.71 | 0.13–0.10 | 220–235 ^b 168,170 |
| SrH ₆ ^c | 250 | 110 | 0.10 | 156 ^b 63 |
| ScH ₆ | 350 | 1.25 | 0.10 | 135 ^a 171, 169 ^b 171 |
| ScH ₆ ^d | 285 | 1.33 | 0.13–0.10 | 130–147 ^a 172 |
| ScH ₆ ^d | 300 | 1.20 | 0.13–0.10 | 90–100 ^b 173 |
| YH ₆ | 120 | 2.93 | 0.13–0.10 | 251–264 ^b 173,174 |
| YH ₆ | 120 | 3.19 | 0.10 | 247 ^b 170 |
| ZrH ₆ ^f | 295 | 1.20 | 0.13 | 114 ^b 175 |
| LaH ₆ | 100 | 2.00 | 0.13–0.10 | 150–160 ^b 173 |
| ScH ₉ | 400 | 1.50 | 0.13–0.10 | 150–190 ^b 173 |
| YH ₉ ^g | 150 | 4.42 | 0.13–0.10 | 253–276 ^b 173 |
| CeH ₉ | 200 | 2.30 | 0.10 | 117 ^a 176 |
| YH ₁₀ | 400 | 2.41 | 0.13–0.10 | 287–303 ^b 173 |
| YH ₁₀ | 250 | 2.58 | 0.13–0.10 | 244–265 ^a 177, 305–326 ^b 177 |
| YH ₁₀ | 250 | 2.67 | 0.10 | 291 ^b 170 |
| LaH ₁₀ ^g | 200 | 2.28 | 0.10 | 288 ^a 173 |
| LaH ₁₀ | 210 | 3.41 | 0.13–0.10 | 219–238 ^a 177, 274–286 ^b 177 |
| LaH ₁₀ | 300 | 1.74 | 0.10 | 231 ^b 170 |
| LaH ₁₀ ^h | 200 | 3.57 | 0.13–0.10 | 218–200 ^a 178, 245–229 ^b 178 |
| AcH ₁₀ ⁱ | 200 | 3.46 | 0.15–0.10 | 177–204 ^a 179, 226–251 ^b 179 |

The Journal
of Chemical Physics

scitation.org/journal/jcp



Volume 150, Issue 5, 7 Feb. 2019

High-temperature superconductivity
in alkaline and rare earth
polyhydrides at high pressure:
A theoretical perspective

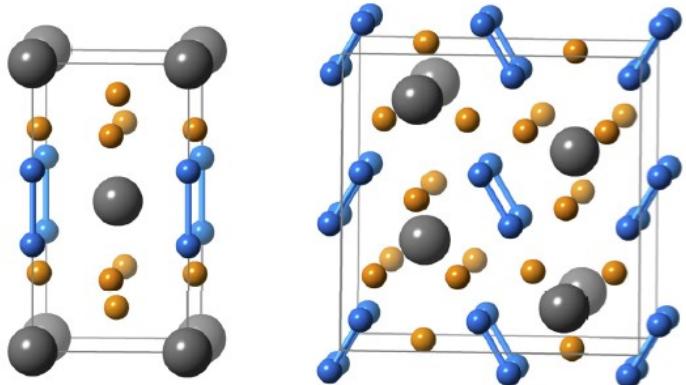
J. Chem. Phys. 150, 050901 (2019); doi.org/10.1063/1.5079225

Eva Zurek and Tiange Bi



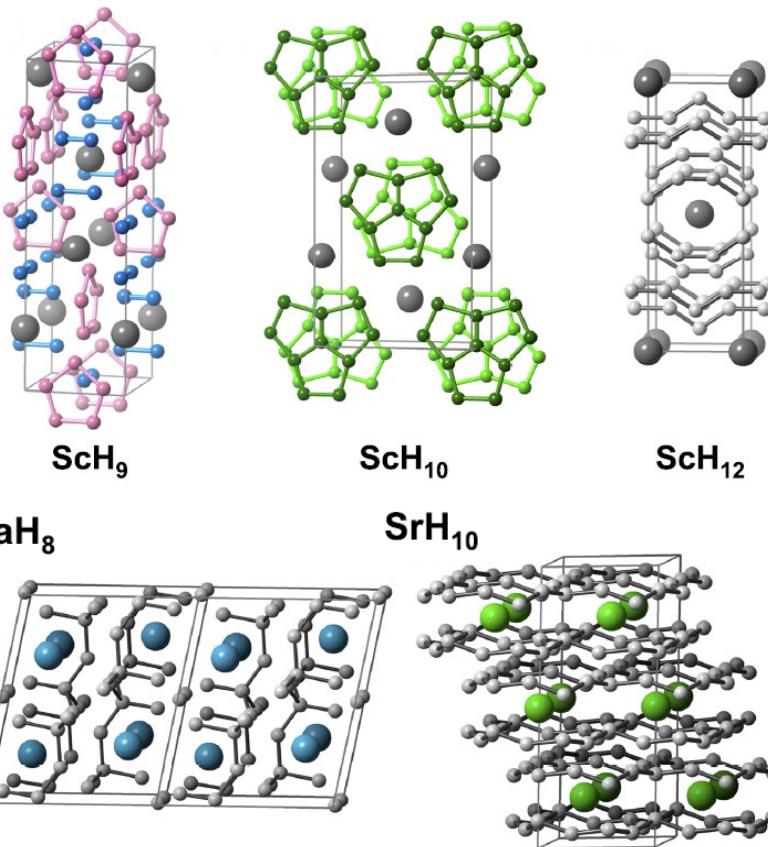
Other Structural Motifs

Mixed Molecular and Atomic Hydrogen



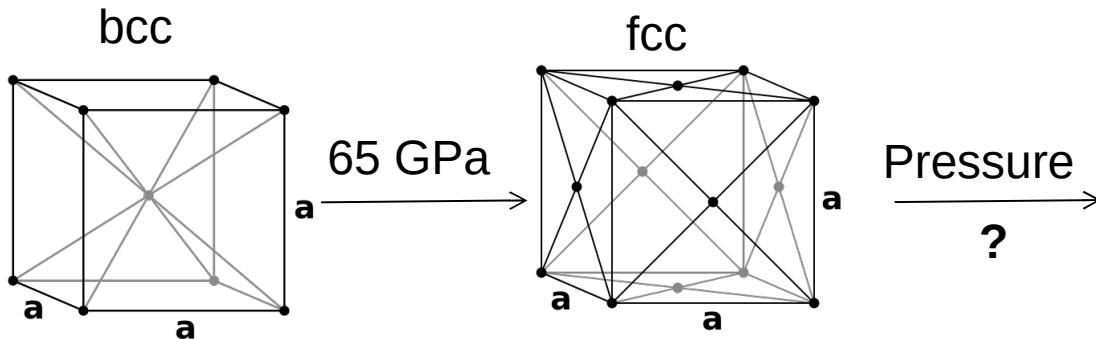
| System | P (GPa) | λ | μ^* | T _c (K) |
|------------------|---------|-----------|-----------|--|
| MgH ₄ | 255 | 0.88 | 0.13 | 81 ^a 175 |
| ScH ₄ | 120 | 1.68 | 0.10 | 92 ^b 171, 163 ^a 171 |
| | 195 | 0.89 | 0.13–0.10 | 67–81 ^b 172 |
| | 200 | 0.99 | 0.10 | 98 ^b 184 |
| | 120 | 1.01 | 0.13–0.10 | 84–95 ^a 174 |
| YH ₄ | | | | |
| ScH ₇ | 300 | 1.84 | 0.10 | 169 ^b 171, 213 ^a 171 |

Other Unique Hydrogenic Motifs



| System | P (GPa) | λ | μ^* | T _c (K) |
|-------------------------------------|---------|-----------|-----------|--|
| R̄3m SrH ₁₀ | 300 | 3.08 | 0.10 | 259 ^a 170 |
| I4 ₁ md ScH ₉ | 300 | 1.94 | 0.10 | 163 ^b 171, 233 ^a 171 |
| Cmcm ScH ₁₀ | 250 | 1.17 | 0.10 | 120 ^b 171, 143 ^a 171 |
| Immm ScH ₁₂ | 350 | 1.23 | 0.10 | 141 ^b 171, 194 ^a 171 |
| C2/m LaH ₈ | 300 | 1.12 | 0.13–0.10 | 114–131 ^b 177, 138–150 ^a 177 |

The “Simple” Metal Sodium Under Pressure



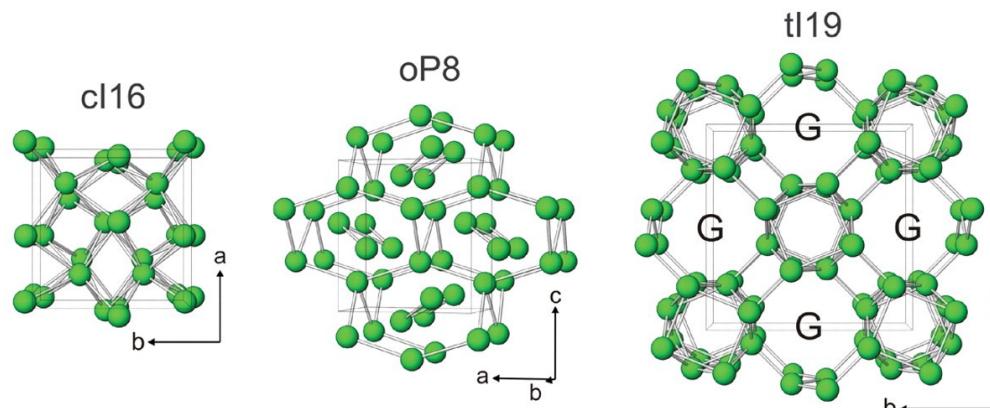
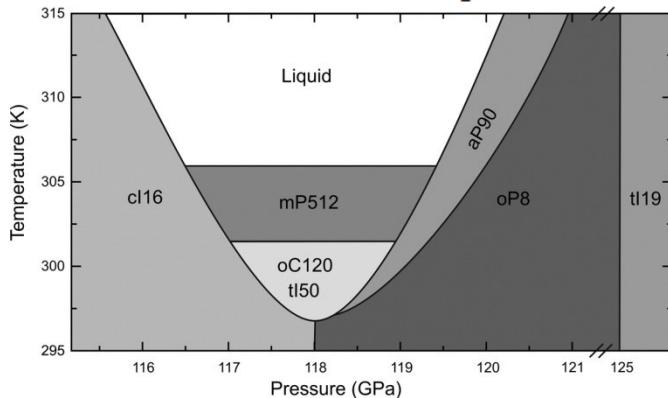
PHYSICAL REVIEW LETTERS

On the Constitution of Sodium at Higher Densities

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

2001, 86, 2830.

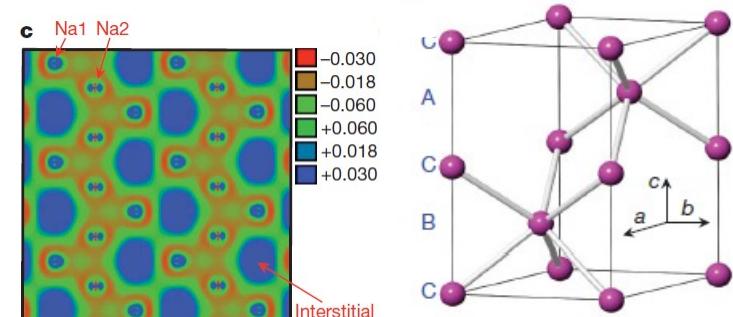
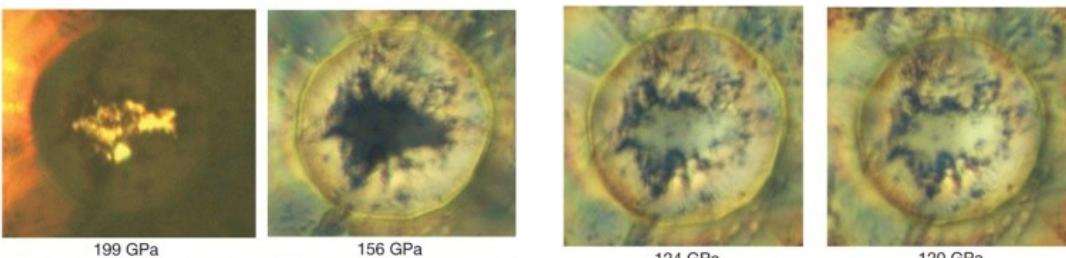
Structural Diversity of Sodium



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

Transparent dense sodium

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

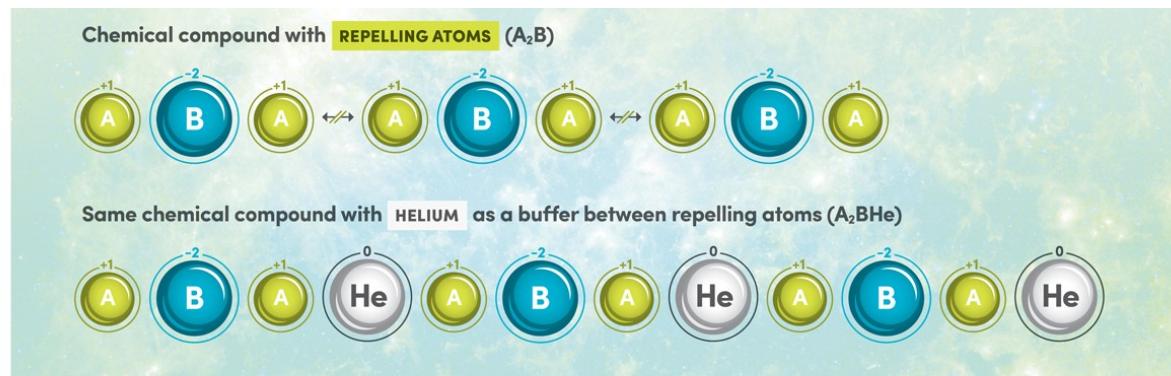
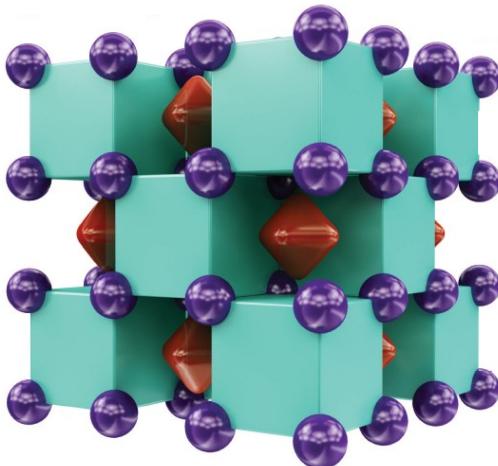


~200 GPa experiment shows Na becomes optically transparent and insulating

The “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

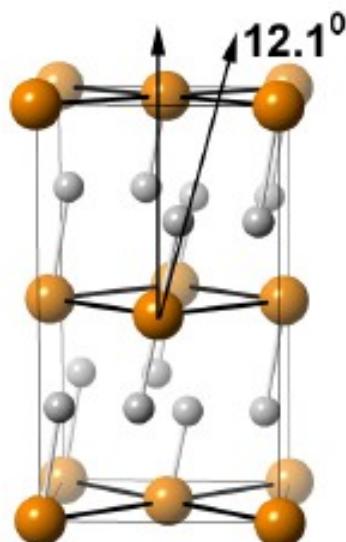


Nat. Commun. **9**, 951 (2018).

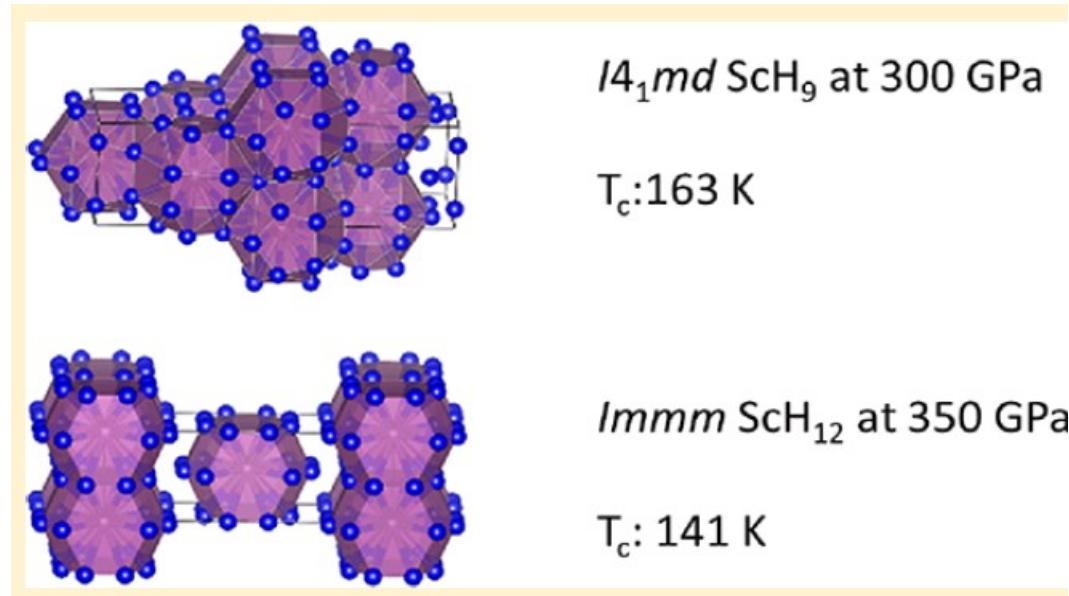
Nat. Chem., **9**, 440-445 (2017).

- 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).

New Pressure-Stabilized Materials?



PH_2 , $T_c = 82 \text{ K}$ at 200 GPa

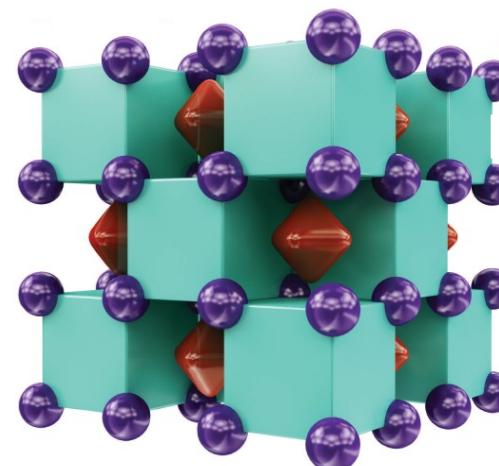


$I4_1md \text{ ScH}_9$ at 300 GPa

$T_c: 163 \text{ K}$

$Immm \text{ ScH}_{12}$ at 350 GPa

$T_c: 141 \text{ K}$



Na_2He

Acknowledgements

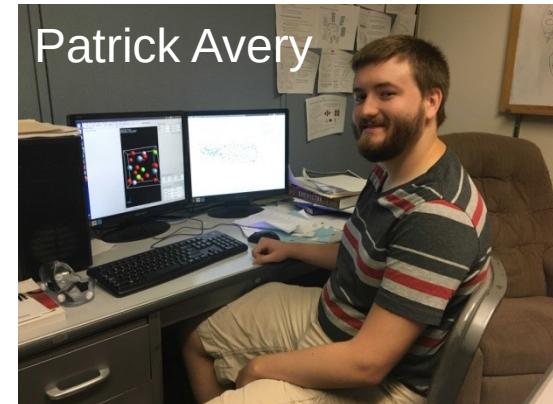
Tiange Bi



Niloofar Zarifi



Patrick Avery



Current Students

- Nisha Geng
- Xiaoyu Wang

Former Co-workers

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



High-P Collaborators

- Xiaoqui Ye
- Roald Hoffmann
- Neil Ashcroft
- Hanyu Liu
- Ajay Mishra
- Maddhury Somayazulu
- Russel Hemley

