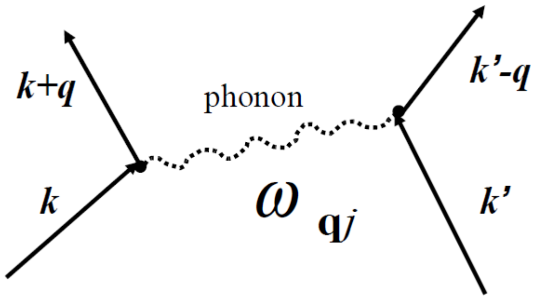
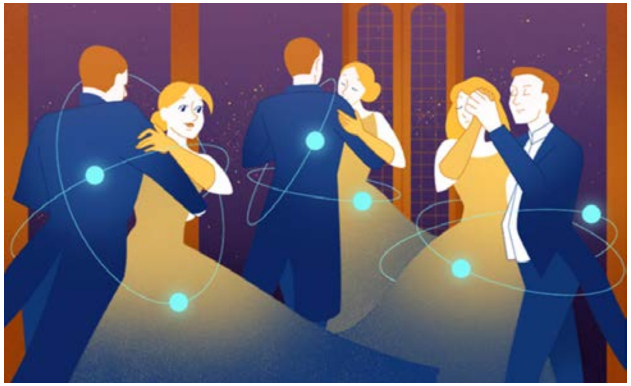
Why does compressed LaH10 have a room-temperature superconductivity?





Jun-Hyung Cho

Department of Physics
Hanyang University

Colloquium, POSTECH, Dec. 11, 2019

Outline

- ✓ **Introduction: BCS-type superconductivity**
- ✓ **Room-temperature superconductivity of LaH_{10}**

  - Electronic and phononic structures

  Phys. Rev. B **99**, 140501(R) (2019)

  - Pressure dependence of T_c

  Phys. Rev. B **100**, 060502(R) (2019)

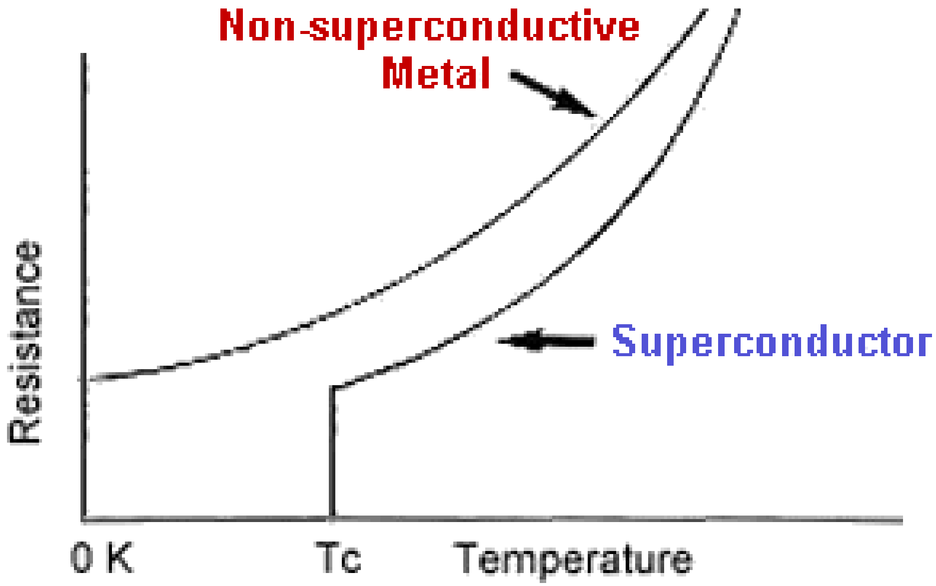
  - Multiband nature of superconductivity

  Phys. Rev. Lett. (submitted)

- ✓ **Conclusion**

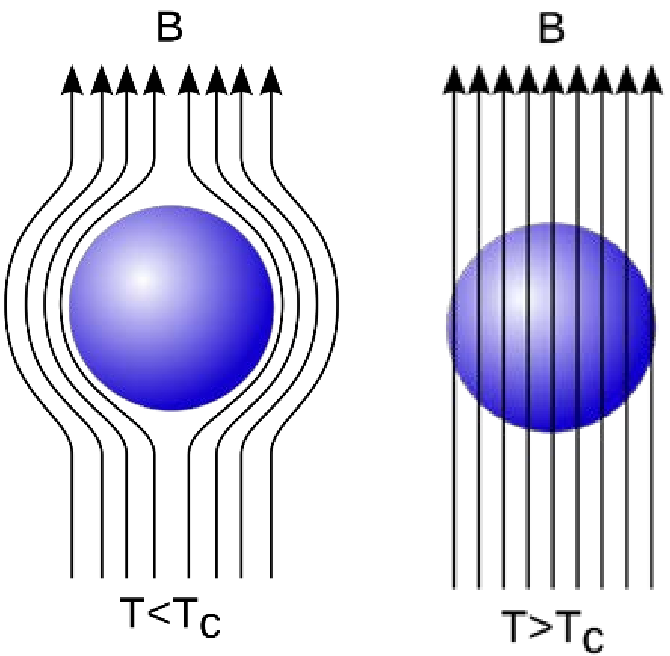
Properties of superconductors

Loss of electrical resistance



Expulsion of magnetic field

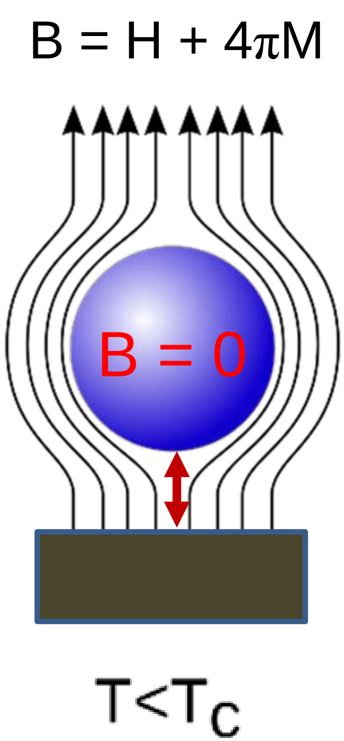
(Meissner effect)

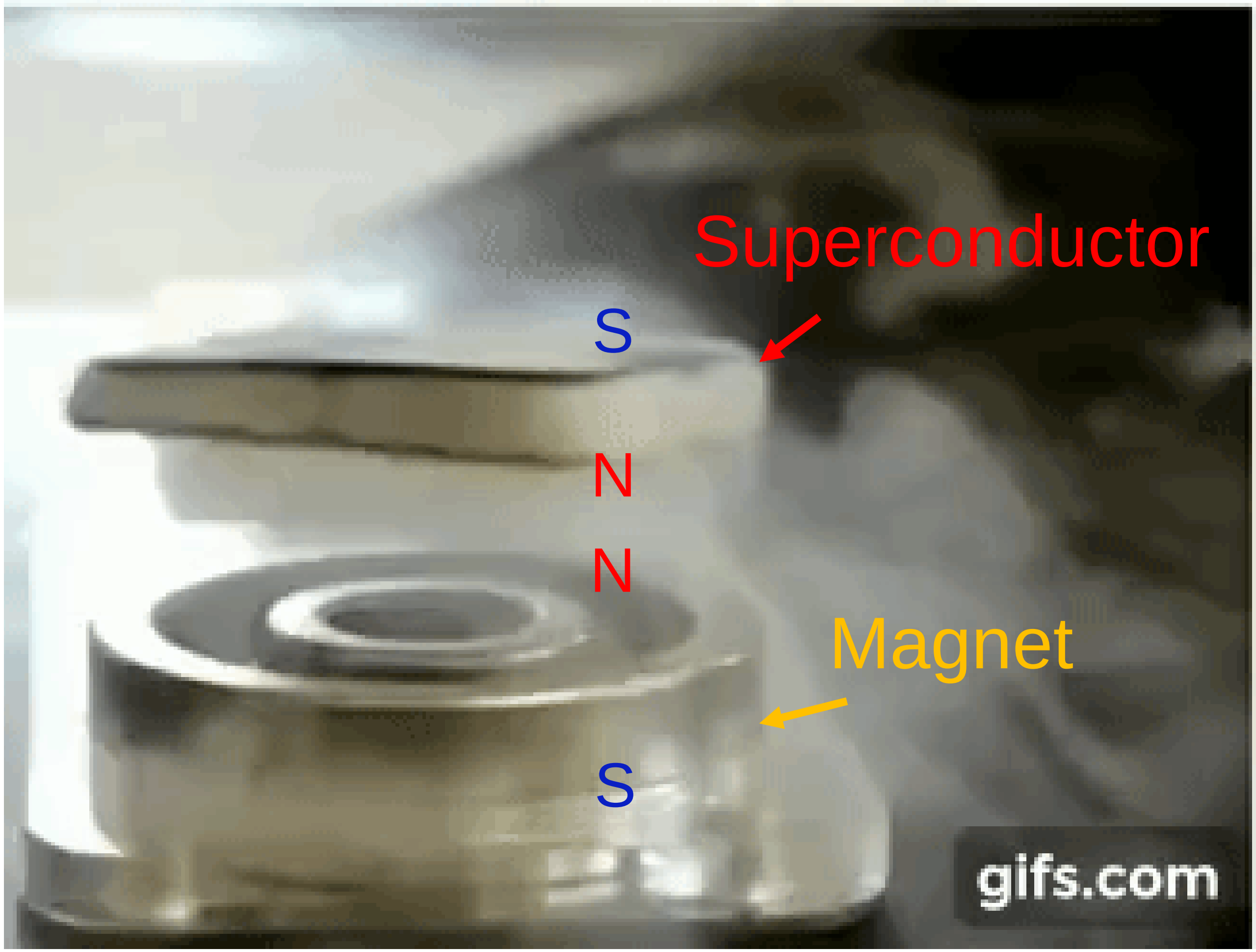


Superconducting Normal

Magnetic levitation of superconductors

Repulsive force between magnet and superconductor

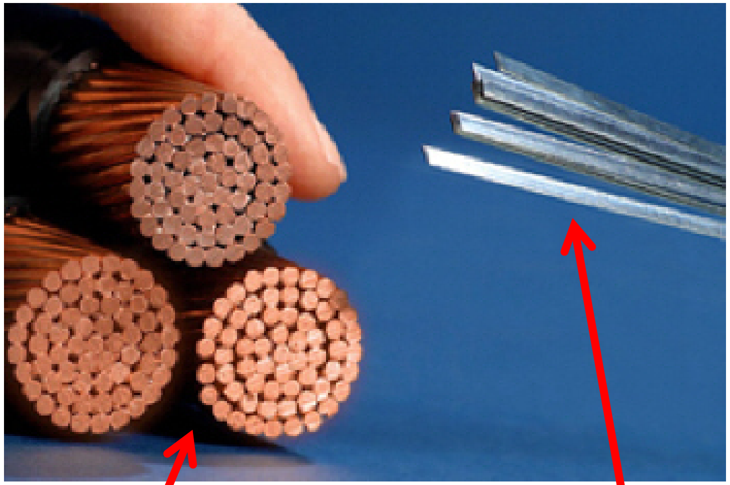




Applications of superconductors

Loss of electrical resistance

Power transmission



Superconducting wire

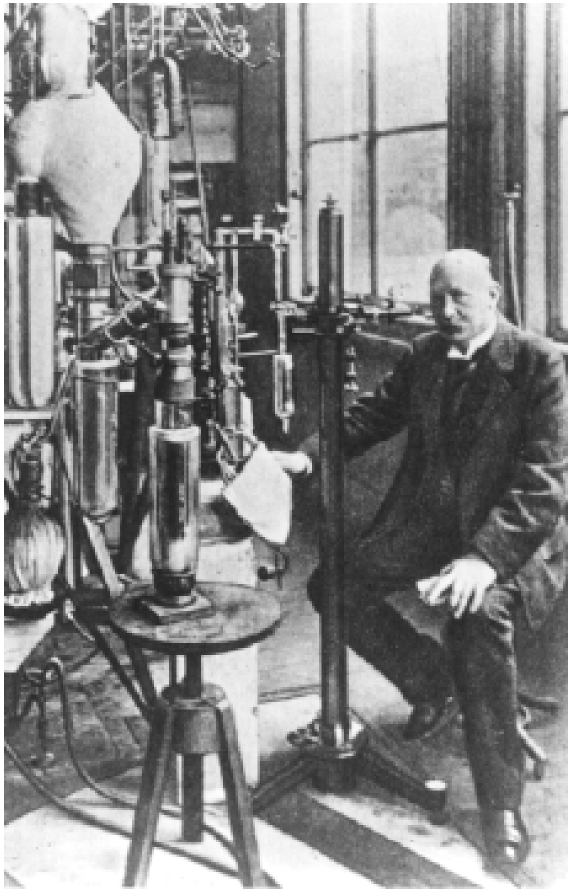
Conventional wire

Expulsion of magnetic field

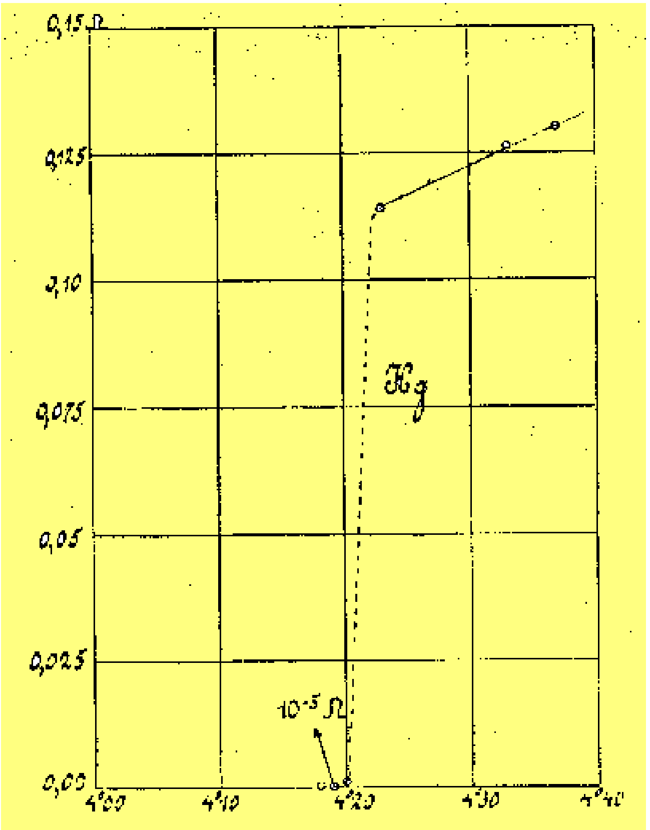
Ground transportation

600 km/h with little friction

Discovery of superconductivity in Hg

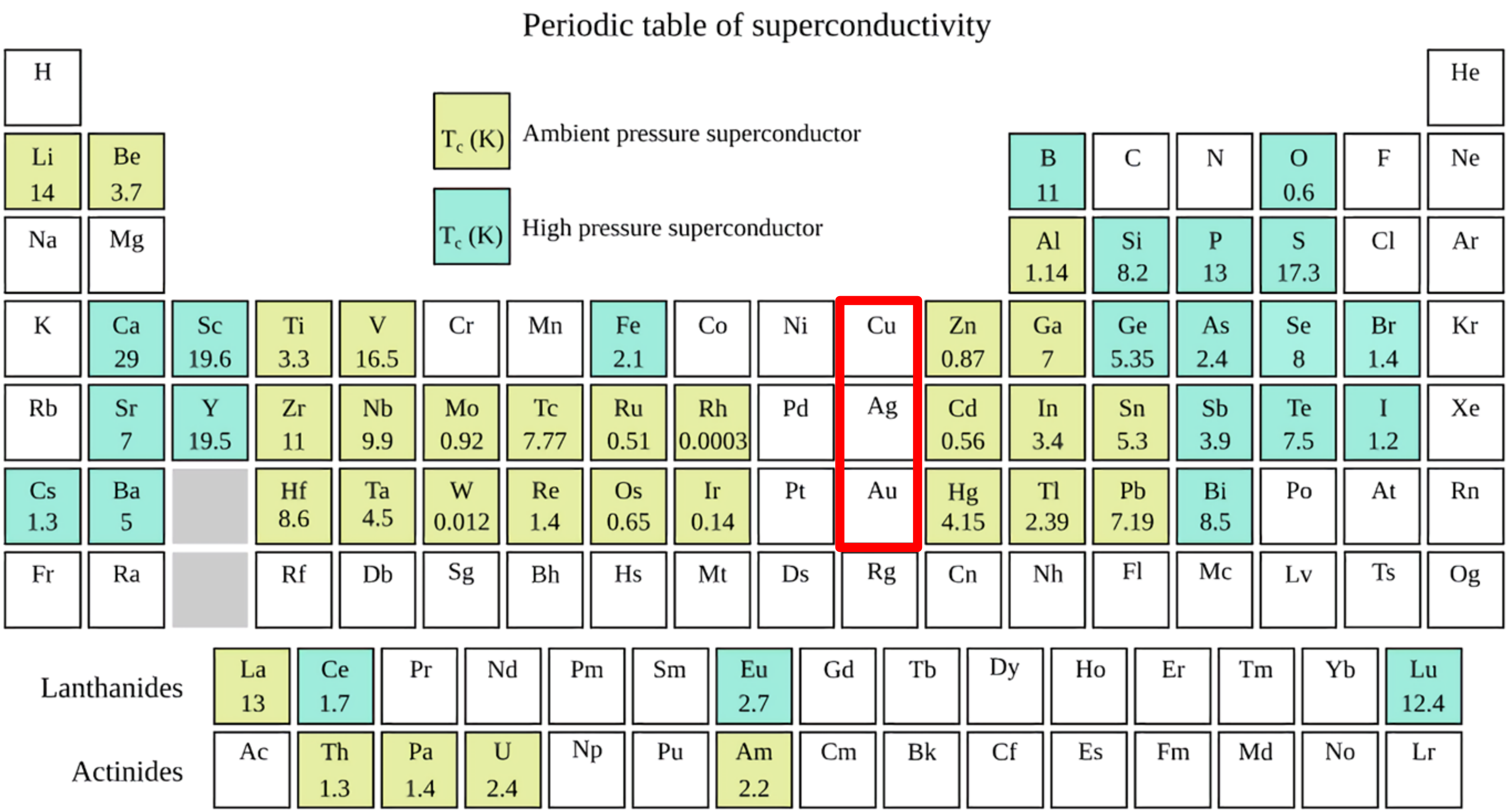


Heike K. Onnes (1911)



Resistivity = 0
below T_c = 4.2 K

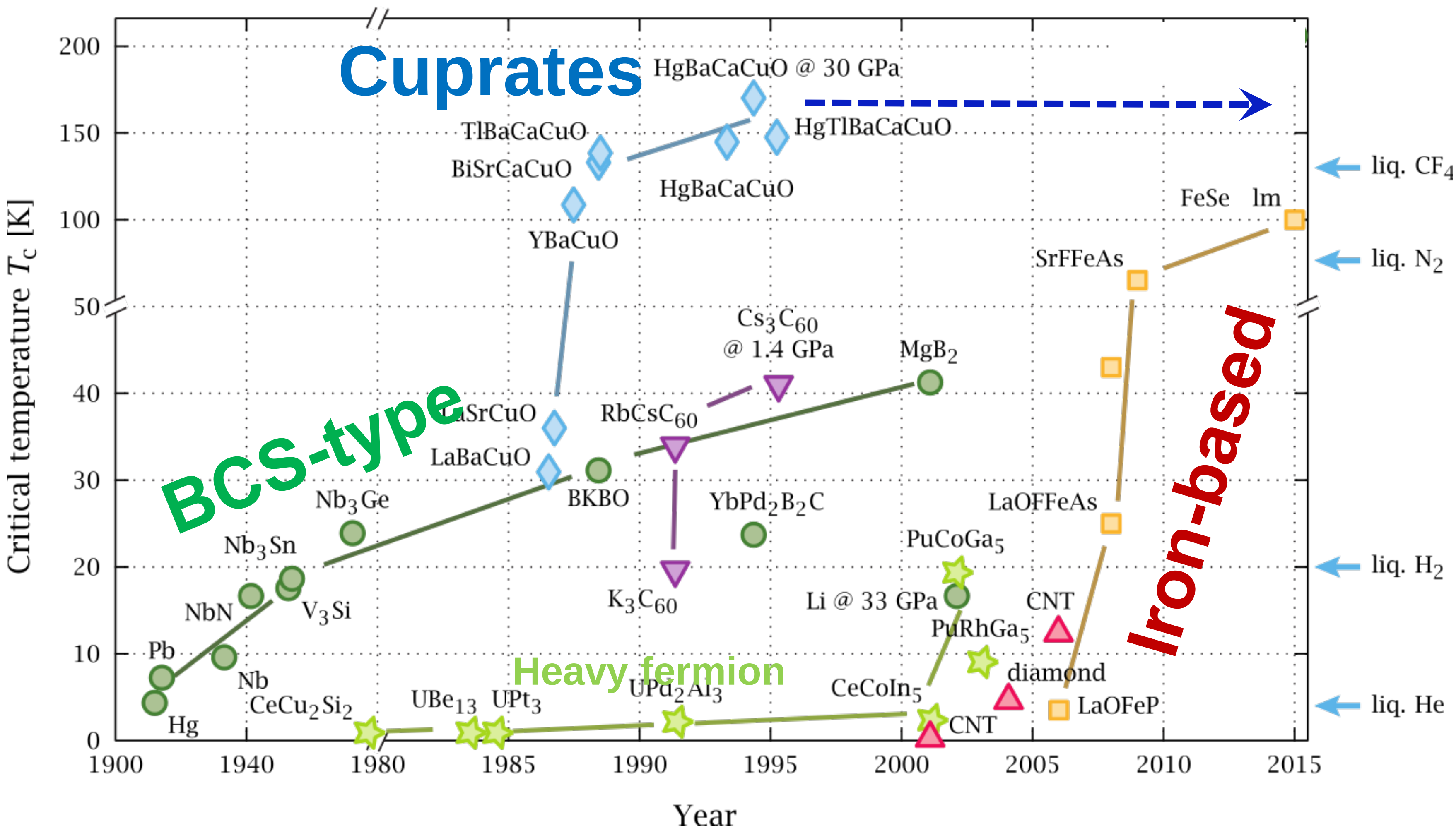
Superconducting transition temperature T_c



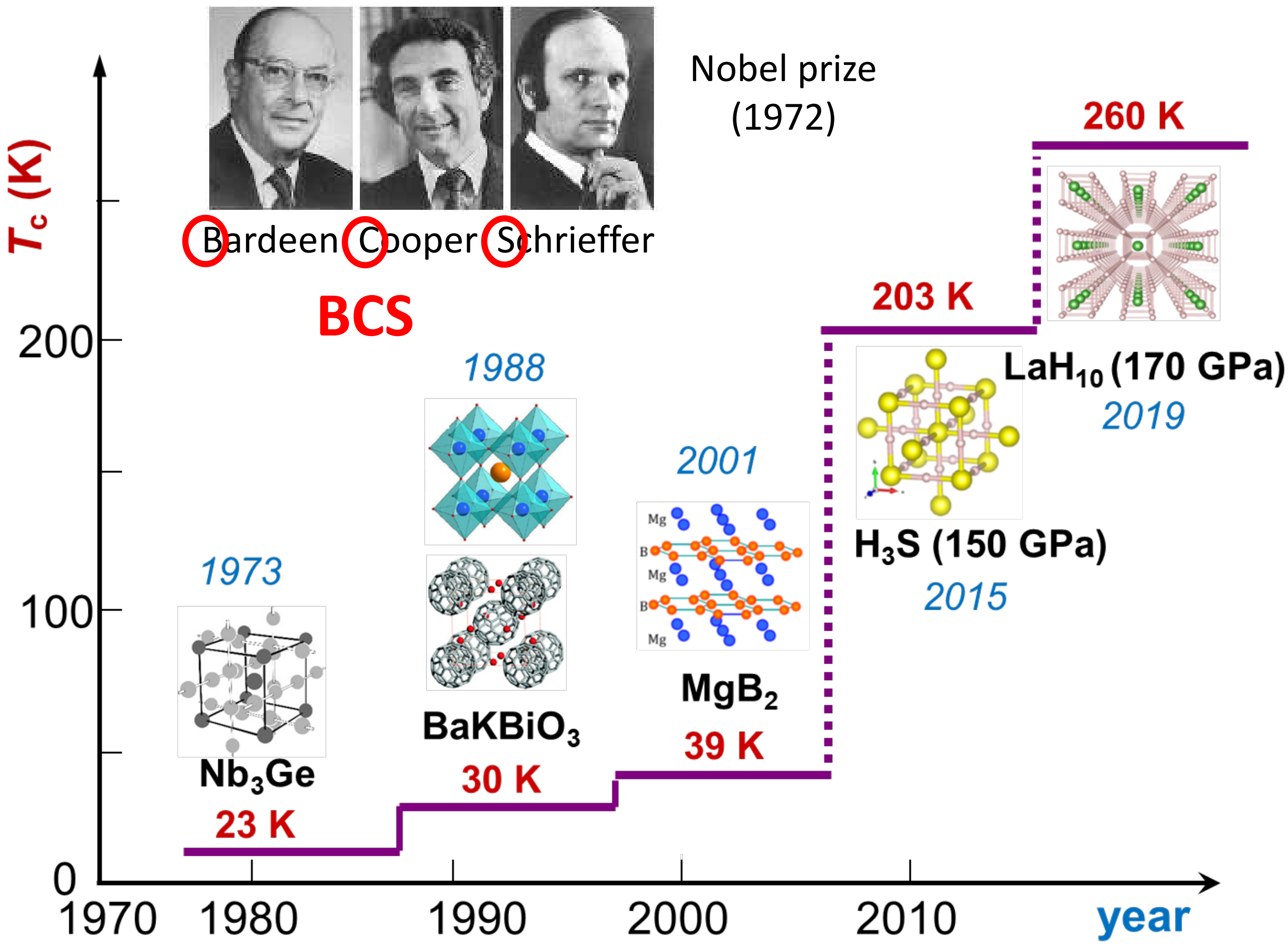
J. A. Flores-Livas *et al.*, arXiv:1905.06693

History of superconductors

T_c as a function of time

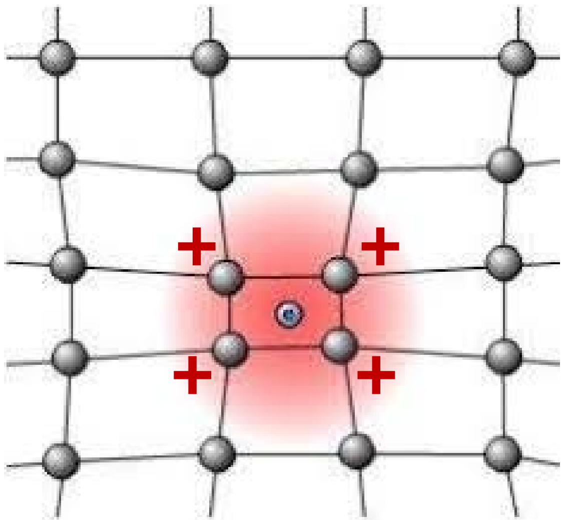


Conventional BCS-type superconductors

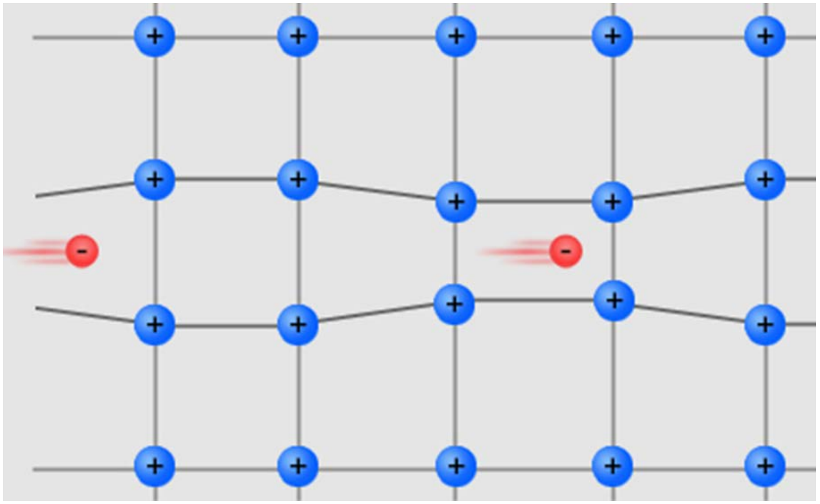


BCS theory: electron-phonon coupling (EPC)

Lattice deformation



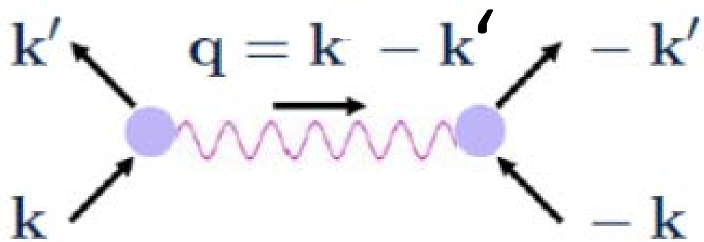
Cooper pair



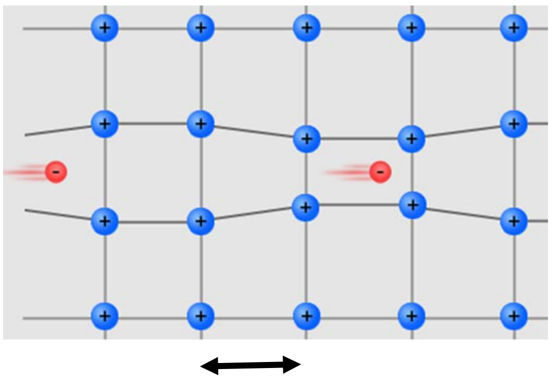
Attractive electron-electron interaction
mediated by “virtual” phonons !!

Cooper pair

Phonon exchange



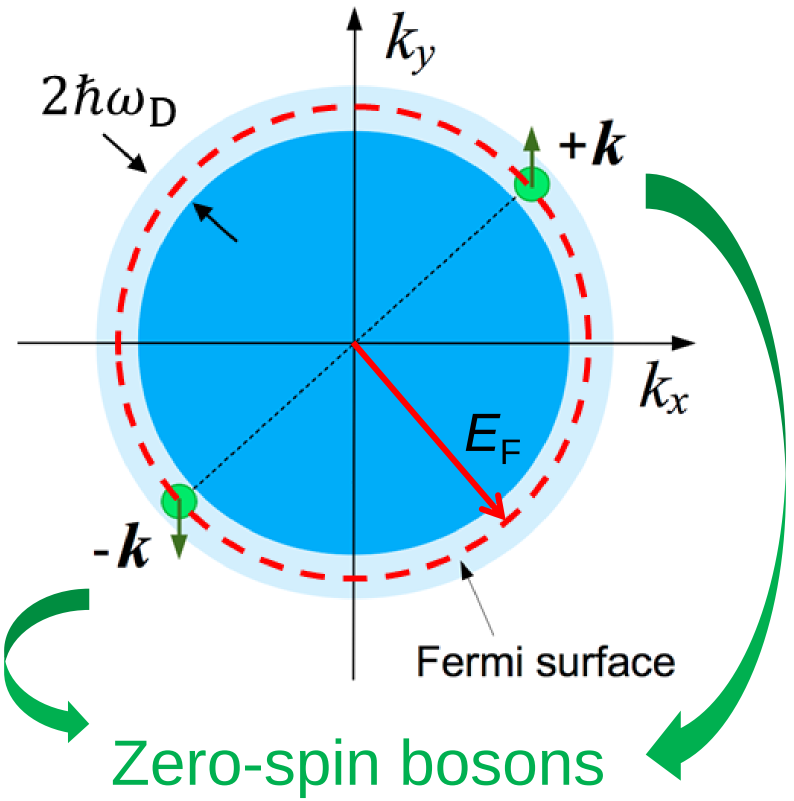
~ 100 nm ≈ $v_F \times 2\pi/\omega_D$



Lattice spacing
~ 0.3 nm

Cooper pairs in momentum space

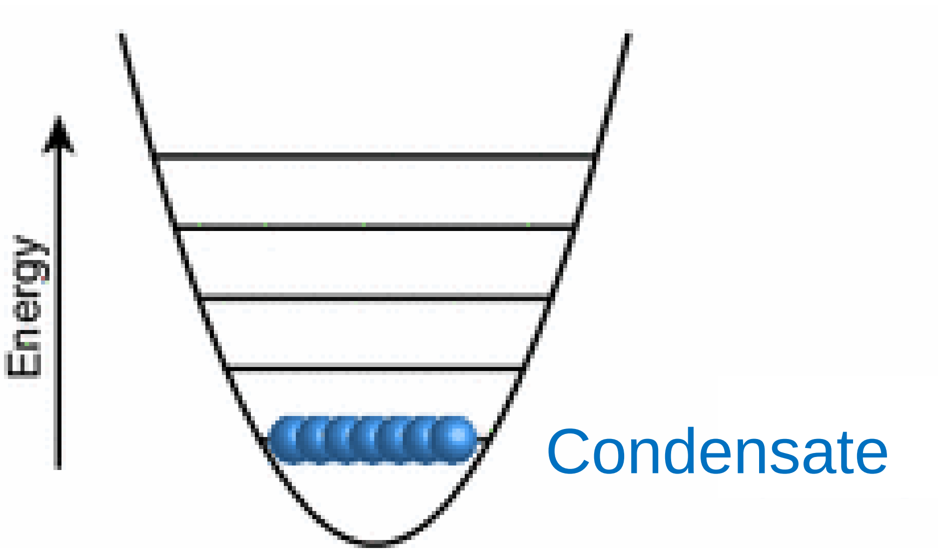
$|E - E_F| < \hbar\omega_D$



Zero-spin bosons

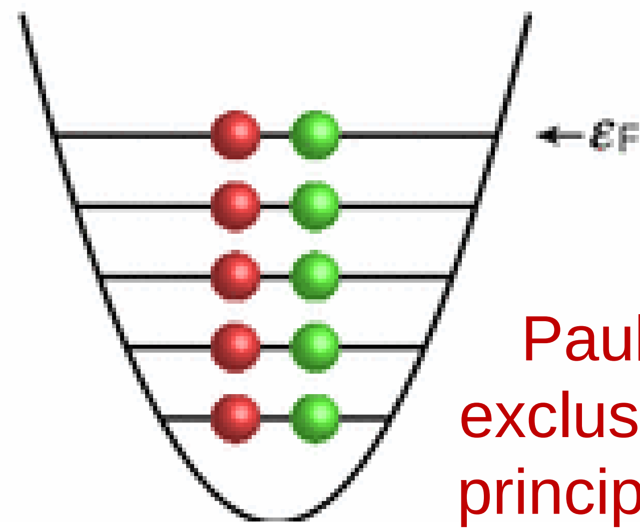
Bose condensation of Cooper pairs

Bosons
(integer spin)



Superconducting

Fermions
(half-integer spin)

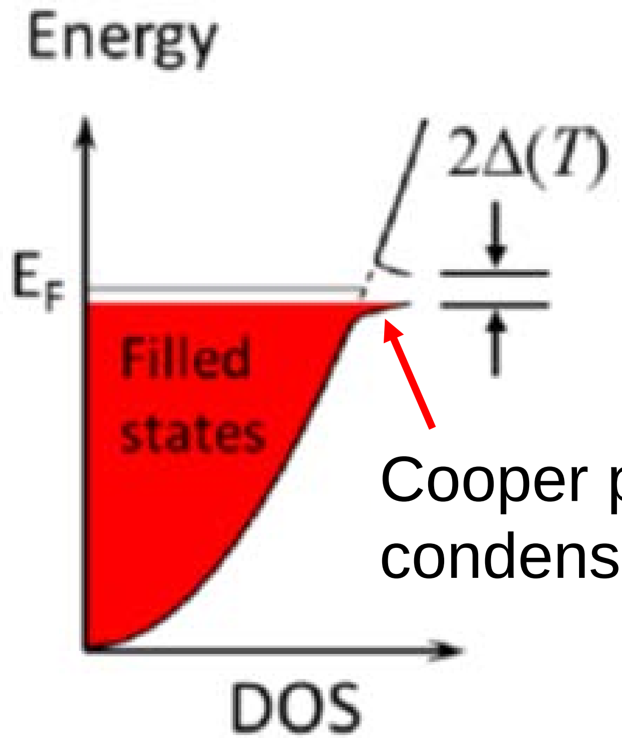


Pauli
exclusion
principles

Normal

BCS theory of superconductivity

Superconducting gap Δ and T_c



Cooper pairs condensate

$$|\Delta| = 2\hbar\omega_D \exp\left[-\frac{1}{N(0)V}\right]$$

$$k_B T_c = 1.14\hbar\omega_D \exp\left[-\frac{1}{N(0)V}\right]$$

Maximum $T_c < 25$ K

(Weak el-phonon coupling theory)

Cooper pairs in superconducting state

The Superconducting Dance Of Electron Pairs

Physicists link electron pair density to the temperature limit of superconductivity.

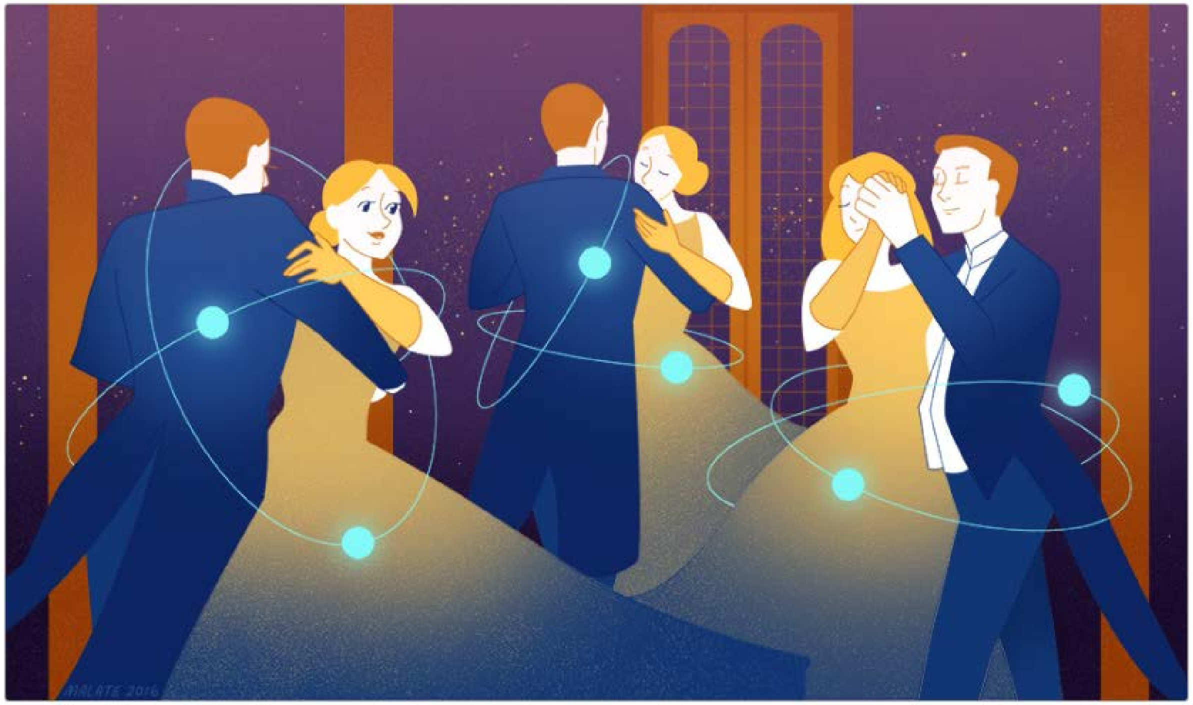
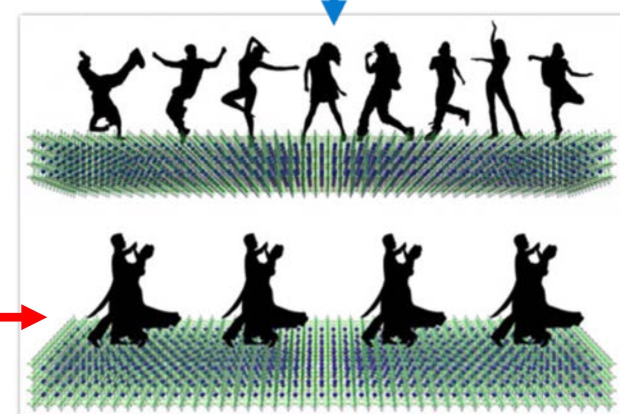


Image credits: Abigail Malate, *Staff Illustrator*

Normal
(independence)



Superconducting
(coherence)

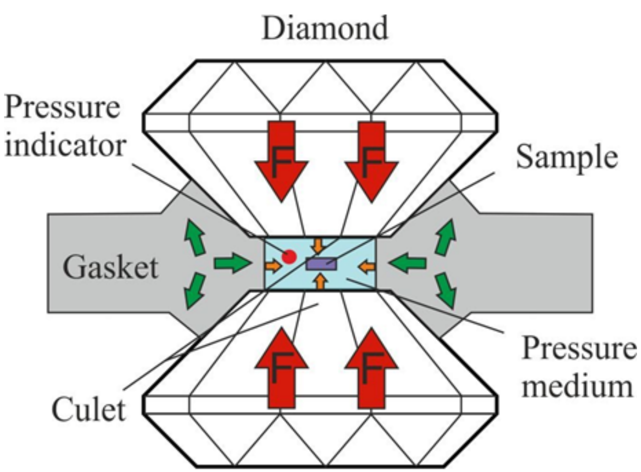
VOLUME 21, NUMBER 26 PHYSICAL REVIEW LETTERS 23 DECEMBER 1968

METALLIC HYDROGEN: A HIGH-TEMPERATURE SUPERCONDUCTOR?

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

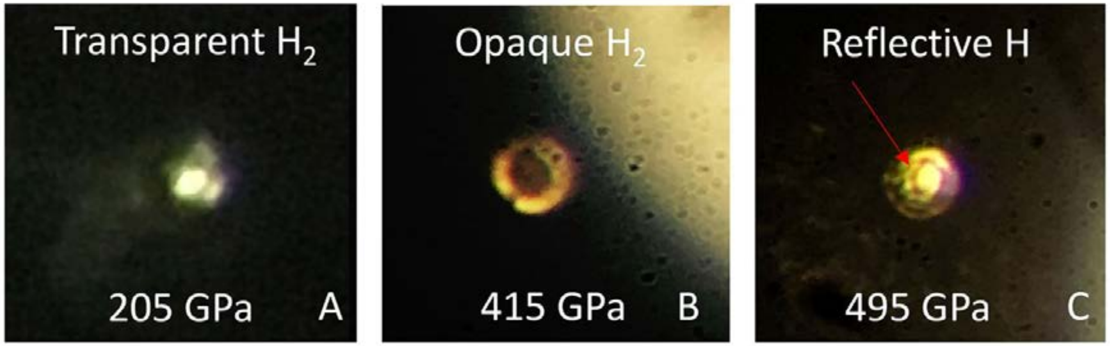
Application of the BCS theory to the proposed metallic modification of hydrogen suggests that it will be a high-temperature superconductor. This prediction has interesting astrophysical consequences, as well as implications for the possible development of a superconductor for use at elevated temperatures.

Possibility of room-temperature superconductor



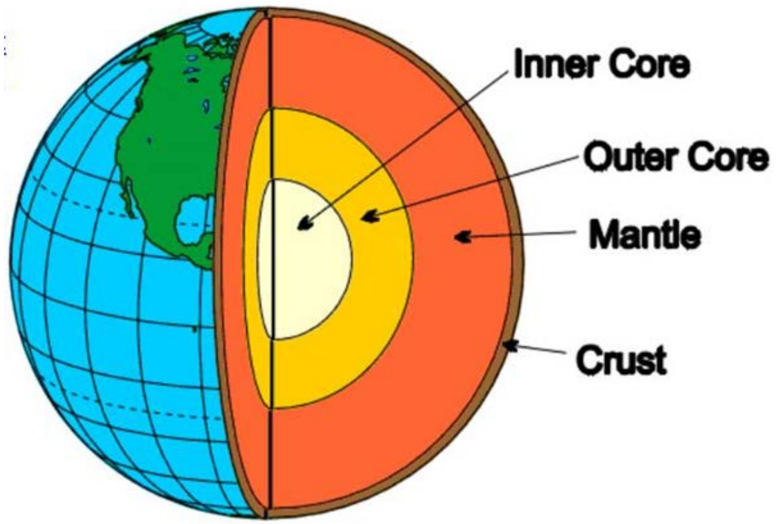
Diamond Anvil Cell

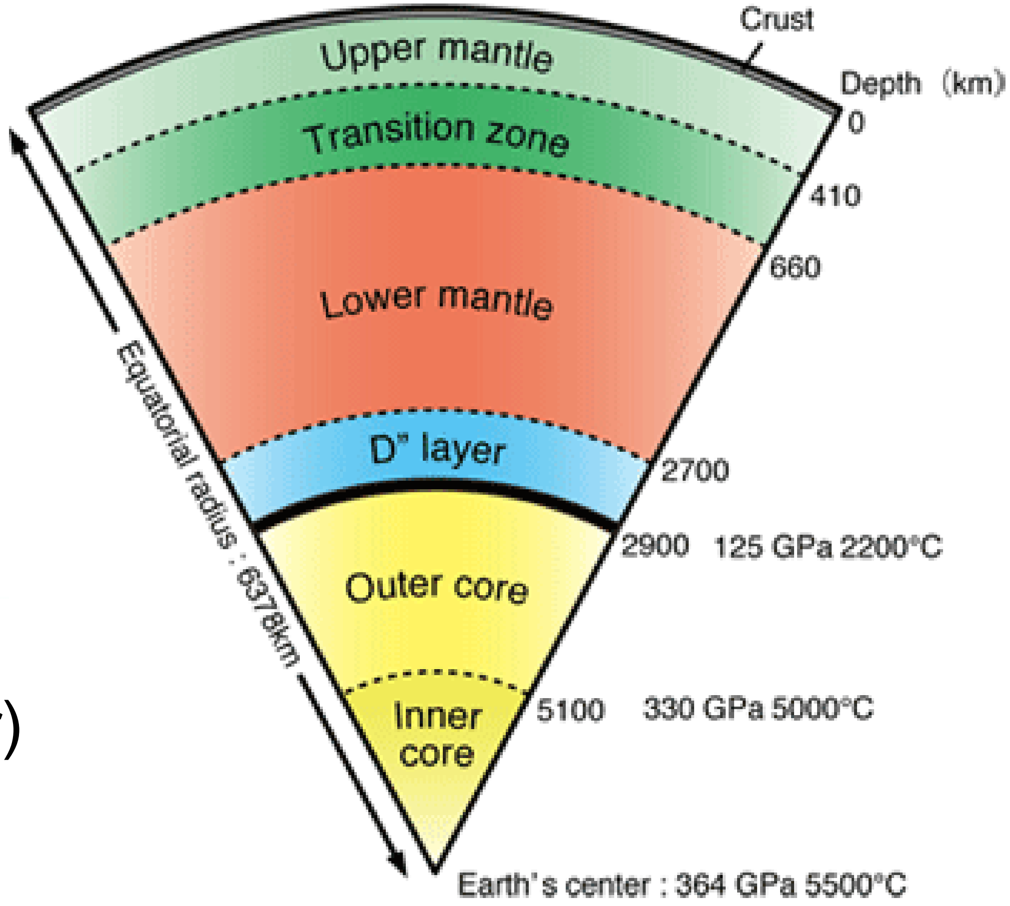
Insulator Semiconductor Metal



Dias and Silvera, Science (2017)

Pressure inside the Earth





1 GPa ≈ 10,000 atm (bar)

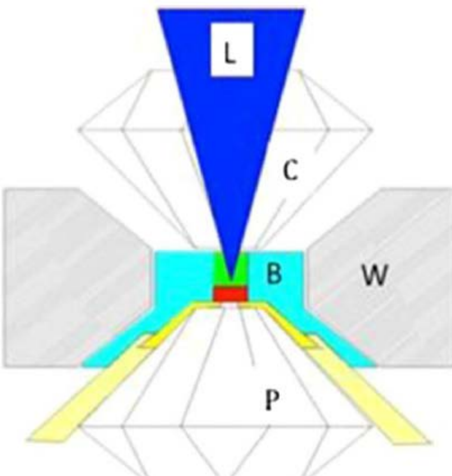
100 GPa ≈ 1 Mbar

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

Editors' Suggestion   Featured in Physics

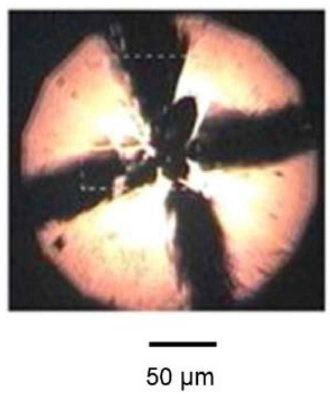
Evidence for Superconductivity above 260 K in Lanthanum Superhydride at Megabar Pressures

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,†]

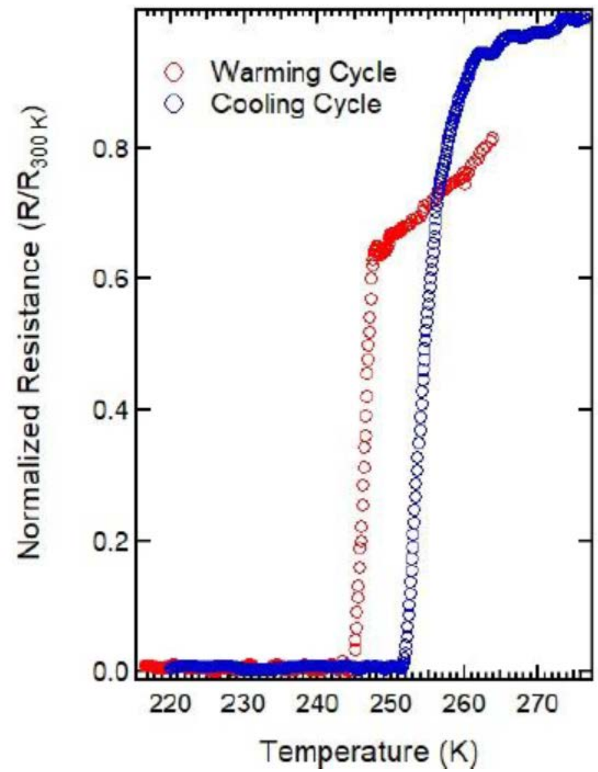


Diamond Anvil Cell

LaH_{10}



170 GPa



Nature (2019)

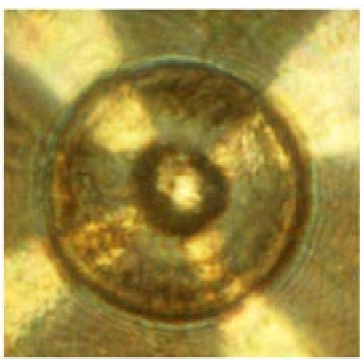
LETTER

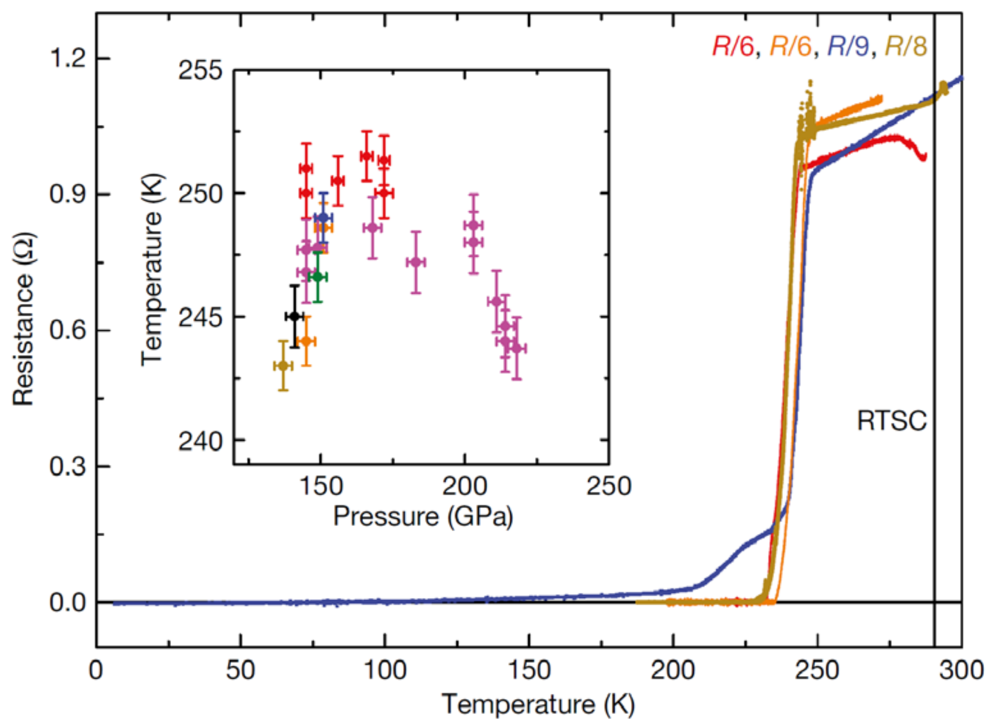
https://doi.org/10.1038/s41586-019-1201-8

Superconductivity at 250 K in lanthanum hydride under high pressures

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

LaH_{10}





Outline

- ✓ **Introduction**
- ✓ **Room-temperature superconductivity of LaH_{10}**

  - Electronic and phononic structures

  Phys. Rev. B **99**, 140501(R) (2019)

  - Pressure dependence of T_c

  Phys. Rev. B **100**, 060502(R) (2019)

  - Multiband nature of superconductivity

  Phys. Rev. Lett. (submitted)

- ✓ **Conclusion**

PHYSICAL REVIEW B **99**, 140501(R) (2019)

Rapid Communications

Microscopic mechanism of room-temperature superconductivity in compressed LaH_{10}

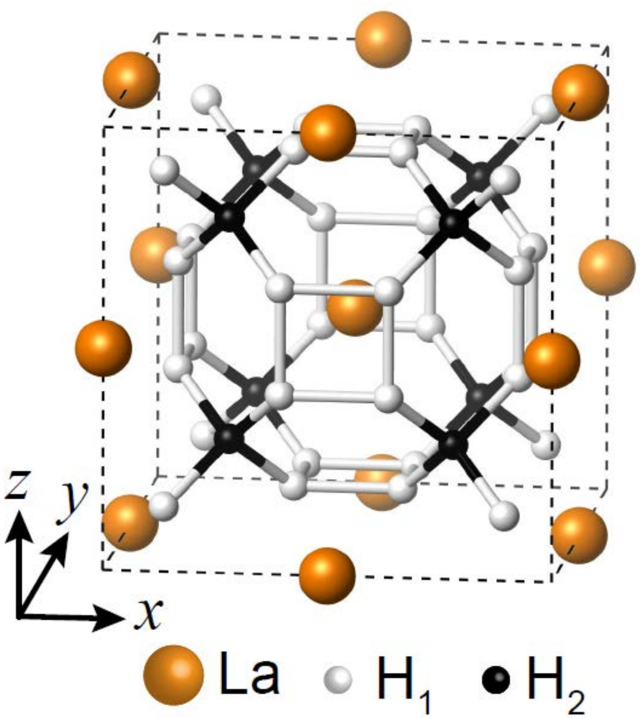
Liangliang Liu,[1,2] Chongze Wang,[1] Seho Yi,[1] Kun Woo Kim,[3] Jaeyong Kim,[1] and Jun-Hyung Cho[1,*]

[1]*Department of Physics, Research Institute for Natural Science, and HYU-HPSTAR-CIS High Pressure Research Center, Hanyang University, 222 Wangsimni-ro, Seongdong-Ku, Seoul 04763, Republic of Korea*

[2]*Key Laboratory for Special Functional Materials of Ministry of Education, Henan University, Kaifeng 475004, People's Republic of China*

[3]*Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon 34051, Republic of Korea*

(Received 11 November 2018; revised manuscript received 22 March 2019; published 4 April 2019)



Sodalite-like clathrate structure

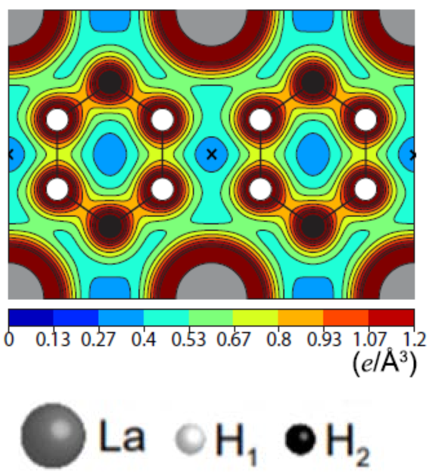
- ✓ La : fcc lattice
- ✓ H_1 and H_2 : H_{32} cage

High symmetry structure

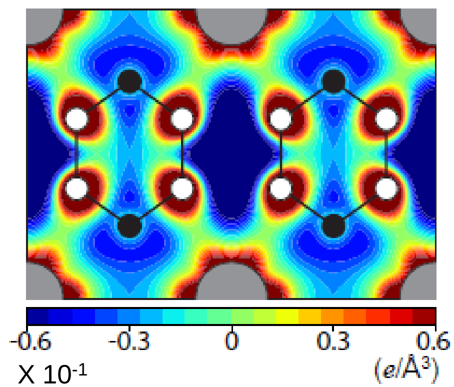
Intricate bonding nature of fcc LaH10

Polar covalent bonding

ρ_{tot}



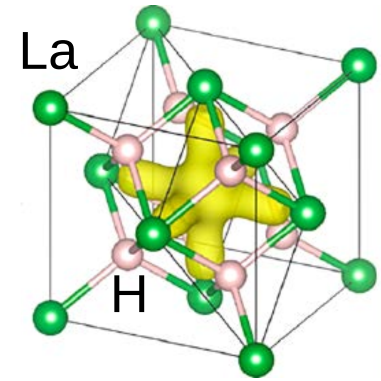
$\Delta\rho = \rho_{tot} - \rho_{La} - \rho_H$

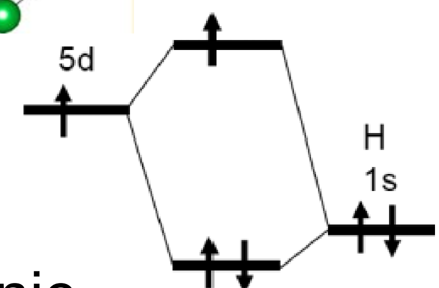


La & H_1 : anionic

H_2 : cationic

LaH_2: Ionic bonding





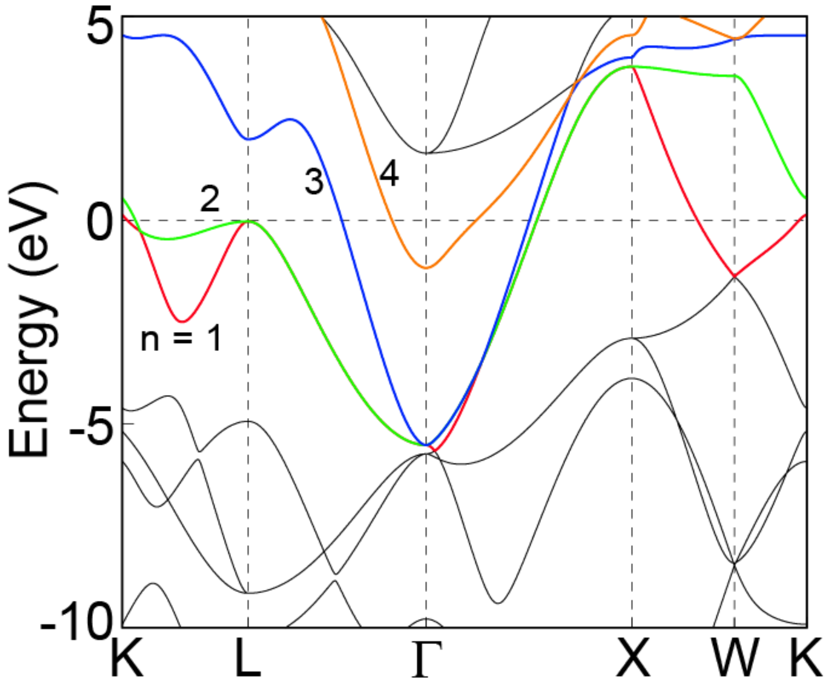
La: cationic

H: anionic

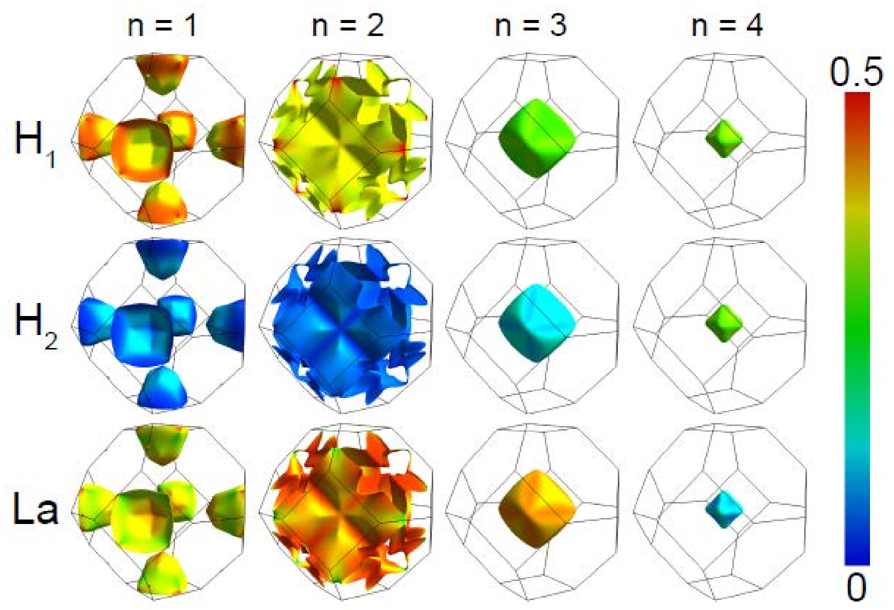
Mizoguchi *et al.*
Inorganic Chem. (2016)

Electronic structure of fcc LaH_{10}

Band structure (300 GPa)

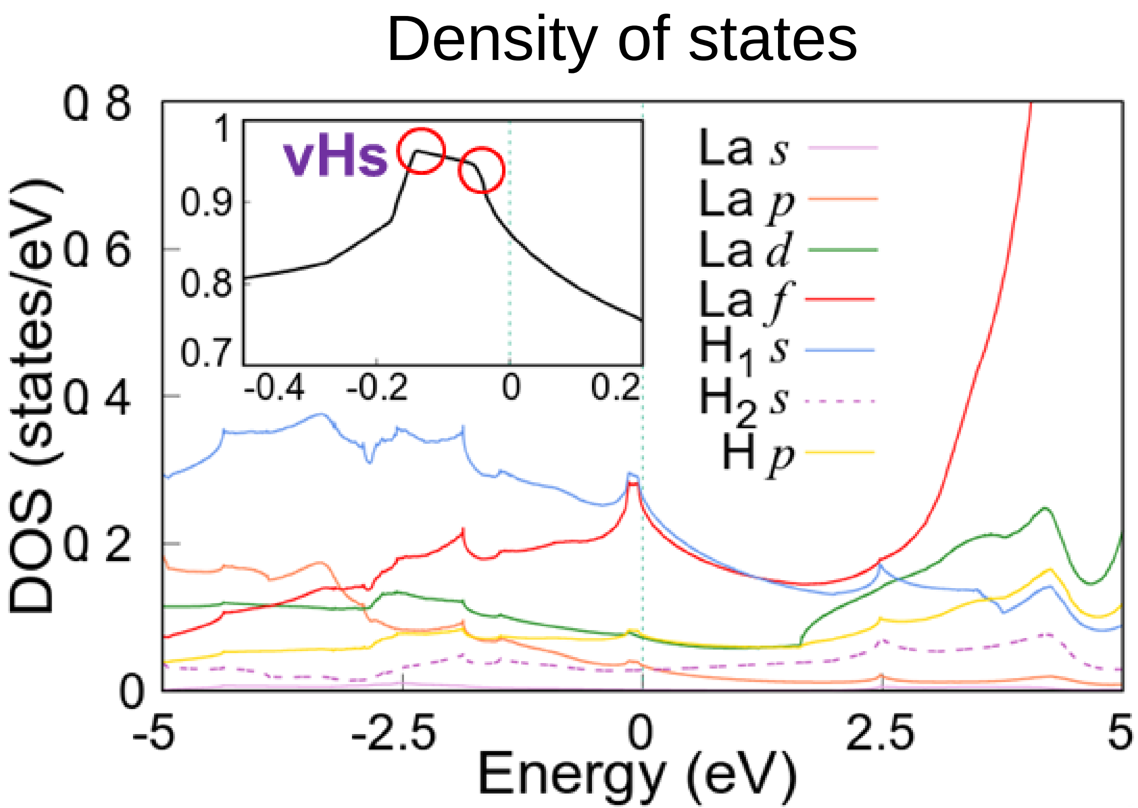


Fermi surface



✓ Multiband: four Fermi surface sheets provide many EPC channels.

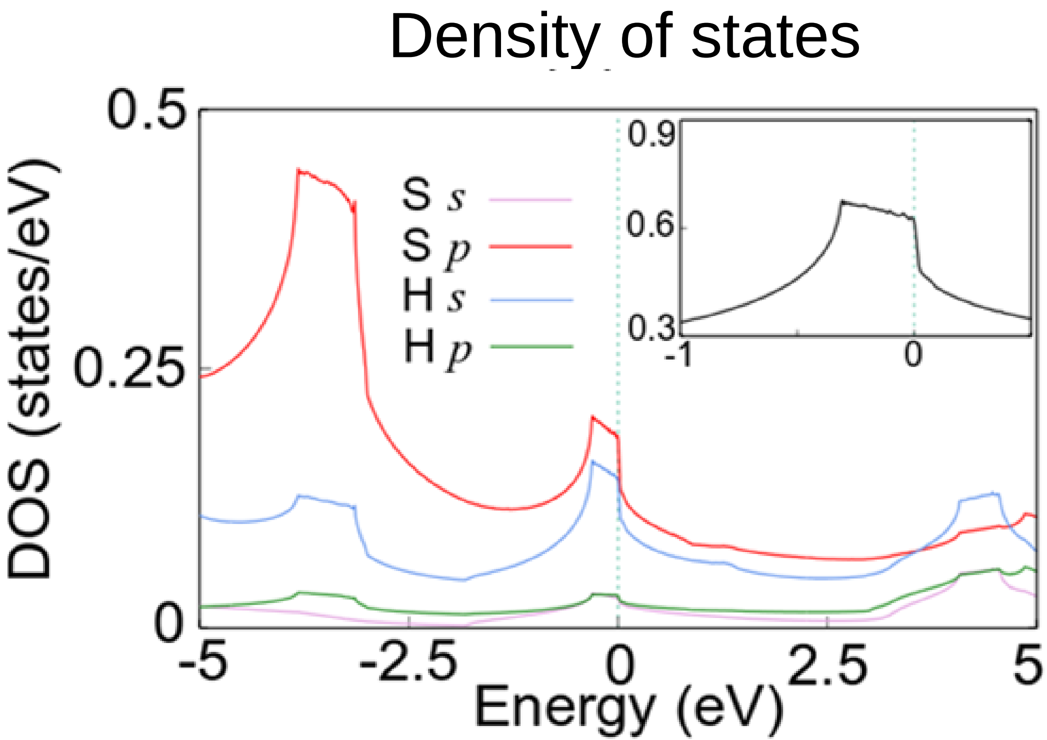
Density of electronic states of fcc LaH_{10}



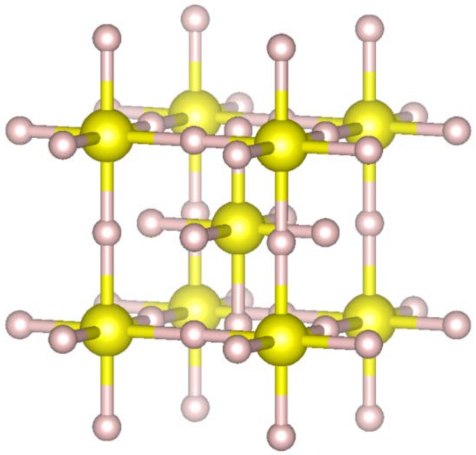
✓ Van Hove singularity (vHs): High DOS at the Fermi level

✓ Strong hybridization of La *f* and H_1 *s* orbitals at E_f

Density of electronic states of compressed H_3S



bcc structure



T_c = 203 K (150 GPa)

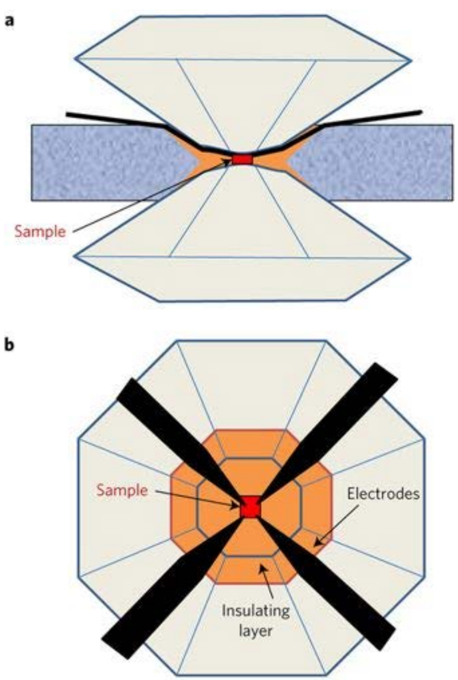
- ✓ Van Hove singularity: High DOS at the Fermi level
- ✓ Strong hybridization of S *p* and H *s* orbitals

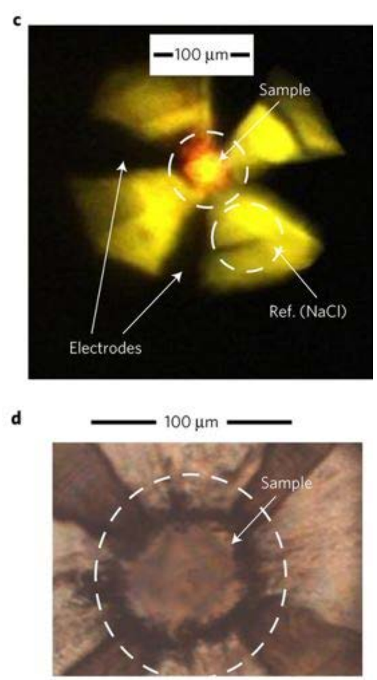
LETTER

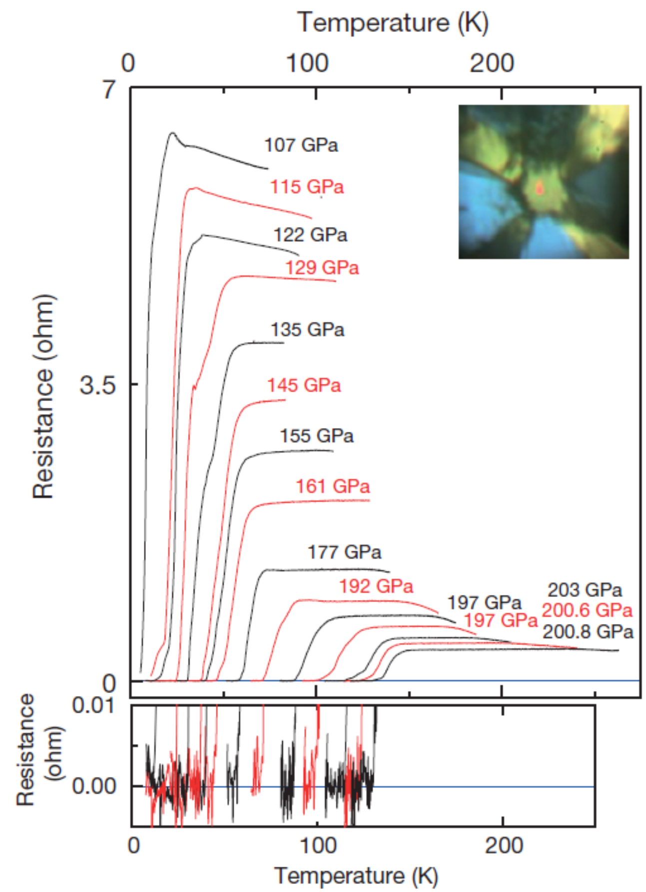
doi:10.1038/nature14964

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

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

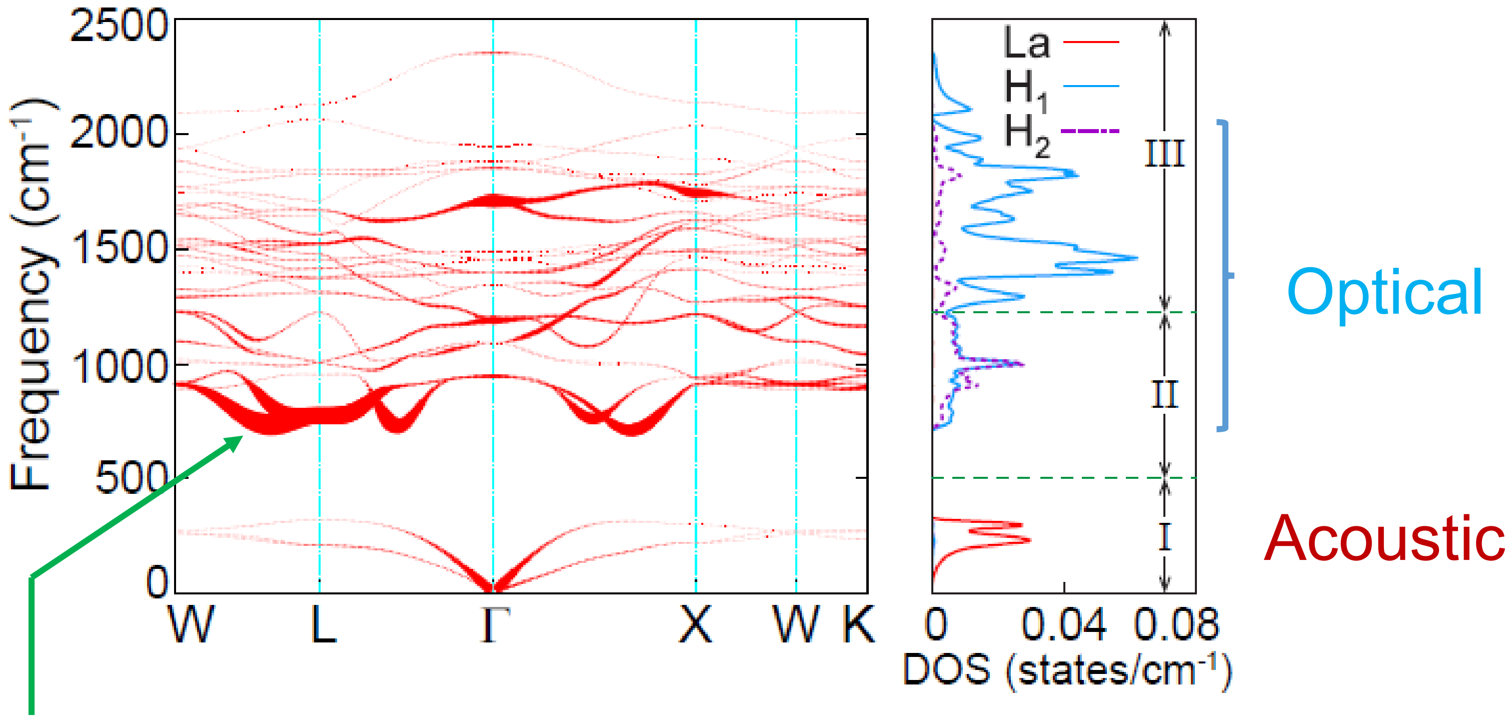






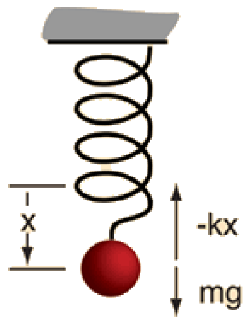
Phonon spectrum & phonon DOS of LaH_{10}

Phonon spectrum (at 300 GPa)



- ✓ The lowest optical phonon modes have large electron-phonon coupling strength.
- ✓ Optical modes arising from H_1 (anionic) and H_2 (cationic).

Comparison of phonon frequencies and T_c



Hooke's Law:

$$F_{spring} = -kx$$

$$\omega = \sqrt{\frac{k}{m}}$$

	Pb [1]	Nb_3Ge [2]	MgB_2 [3]	H_3S [4]	LaH_{10} [5]
ω_{max} (cm^{-1})	300	250	810	1800	2380
T_c (K)	4.2	23	39	200	233

[1] Brockhouse *et al.* Phys. Rev.(1962)

[2] Smith *et al.* PRB (1985)

[3] Margine *et al.* PRB (2013)

[4] Sci. Rep. (2014)

[5] Wang *et al.* PRB (2019)

Electron-phonon coupling constant $\lambda = 2\int \frac{\alpha^2 F(\omega)}{\omega} d\omega$

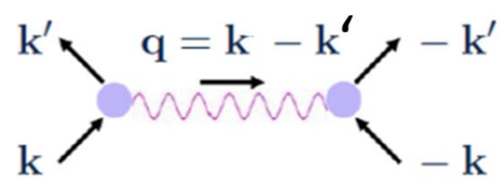
- ✓ Eliashberg spectral function

$$\alpha^2 F(\omega) = \frac{1}{N(E_F)} \sum_{\mathbf{q},j} \delta(\omega - \omega_{qj}) \sum_{n\mathbf{k},n'\mathbf{k}'} \left| g^{qj}_{nk,n'k'} \right|^2 \delta_{k+q,k'} \delta(\varepsilon_{nk}) \delta(\varepsilon_{n'k'})$$

- ✓ Phonon density of states $F(\omega) = \sum_{q,j} \delta(\omega - \omega_{qj})$

- ✓ Electron-phonon matrix elements

$$g^{qj}_{nk,n'k'} = \left\langle \psi_{n'k'} \left| \hat{\varepsilon}^{qj} \cdot \frac{\delta V_{eff}}{\delta \mathbf{u}(\mathbf{q}j)} \right| \psi_{nk} \right\rangle$$



Structural, electronic & phononic properties of fcc LaH_{10}

- ✓ Covalent H-H and La-H bonding characters
- ✓ High symmetry structure & vHs → high DOS
- ✓ Multiband & hybridized states at E_F
- ✓ High phonon frequencies of H atoms

Large electron-phonon coupling (EPC) constant

Room-temperature superconductivity

Outline

- ✓ **Introduction**
- ✓ **Room-temperature superconductivity of LaH_{10}**

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  Phys. Rev. B **99**, 140501(R) (2019)

  - Pressure dependence of T_c

  Phys. Rev. B **100**, 060502(R) (2019)

  - Multiband nature of superconductivity

  Phys. Rev. Lett. (submitted)

- ✓ **Conclusion**

LETTER

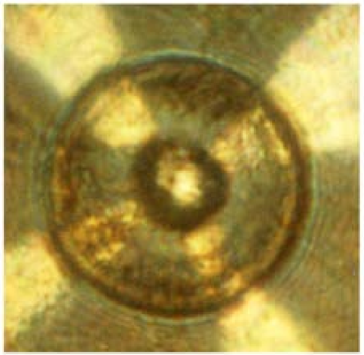
Nature (2019)

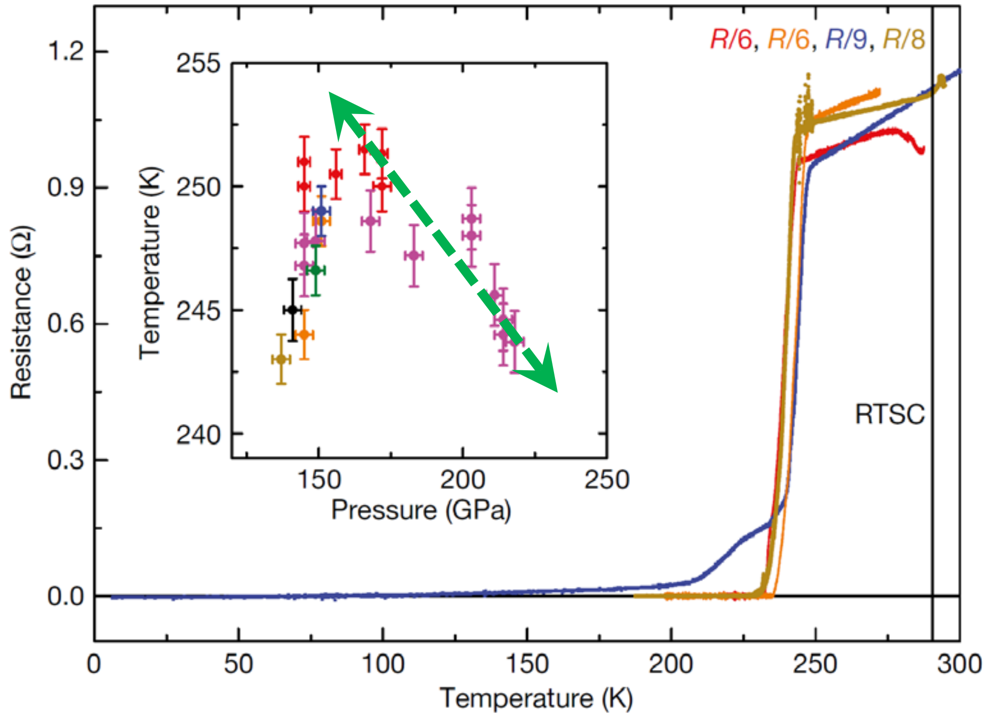
https://doi.org/10.1038/s41586-019-1201-8

Superconductivity at 250 K in lanthanum hydride under high pressures

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

LaH_{10}





✓ Why does T_c decrease with increasing pressure?

PHYSICAL REVIEW B **100**, 060502(R) (2019)

Rapid Communications

Pressure dependence of the superconducting transition temperature of compressed LaH_{10}

Chongze Wang, Seho Yi, and Jun-Hyung Cho*

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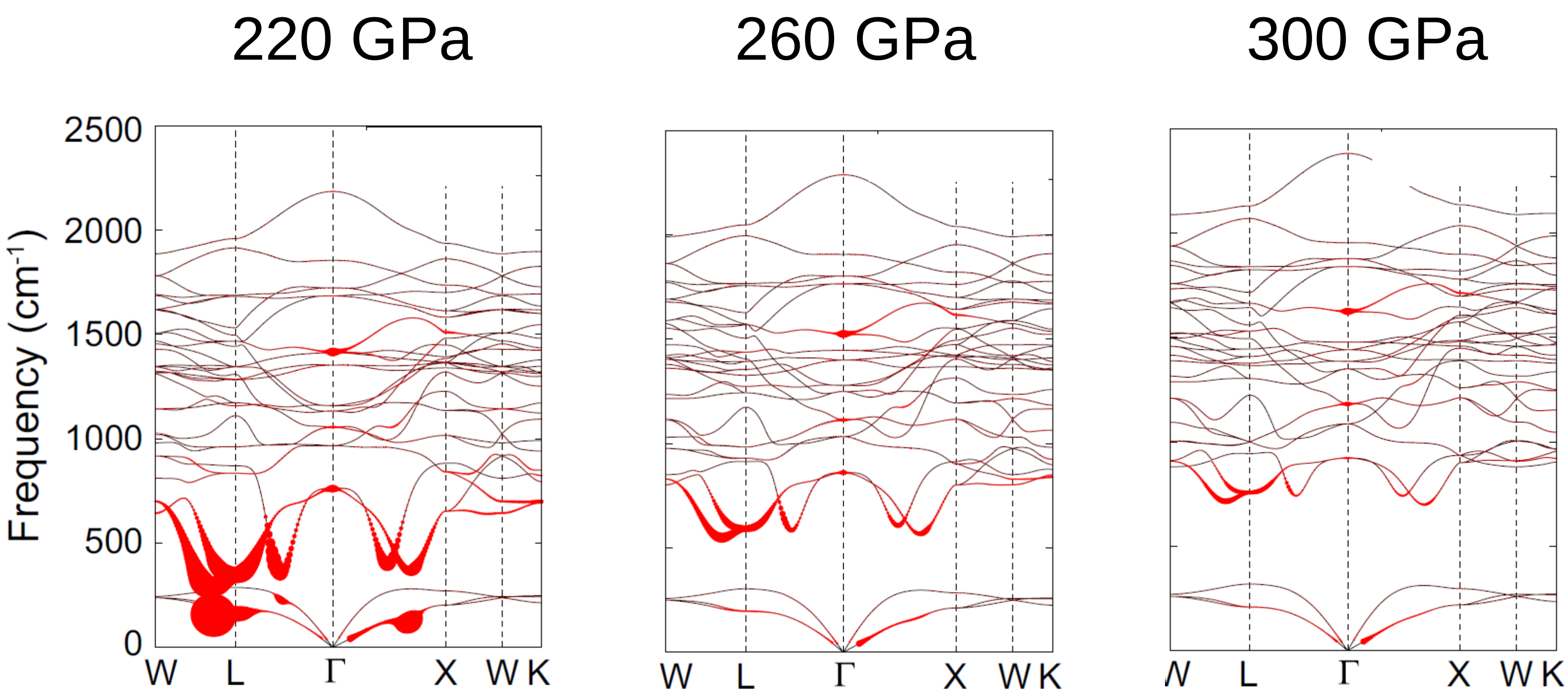
Two recent experiments [M. Somayazulu *et al.* Phys. Rev. Lett. **122**, 027001 (2019) and A. P. Drozdov *et al.*, Nature (London) **569**, 528 (2019)] reported the discovery of superconductivity in the fcc phase of LaH_{10} at a critical temperature T_c between 250 and 260 K under a pressure of about 170 GPa. However, the dependence of T_c on pressure showed different patterns, i.e., the former experiment observed a continuous increase of T_c up to ∼275 K on further increase of pressure to 202 GPa, while the latter one observed an abrupt decrease of T_c with increasing pressure. Here, based on first-principles calculations, we reveal that for the fcc-LaH_{10} phase, softening of the low-frequency optical phonon modes of H atoms dramatically occurs as pressure decreases, giving rise to a significant increase of the electron-phonon coupling (EPC) constant. Meanwhile, the electronic band structure near the Fermi energy is insensitive to change with respect to pressure. These results indicate that the pressure-dependent phonon softening is unlikely associated with Fermi-surface nesting, but driven by effective screening with the electronic states near the Fermi energy. It is thus demonstrated that the strong variation of EPC with respect to pressure plays a dominant role in the decrease of T_c with increasing pressure, supporting the measurements of Drozdov *et al.*

Phonon spectrum as a function of pressure

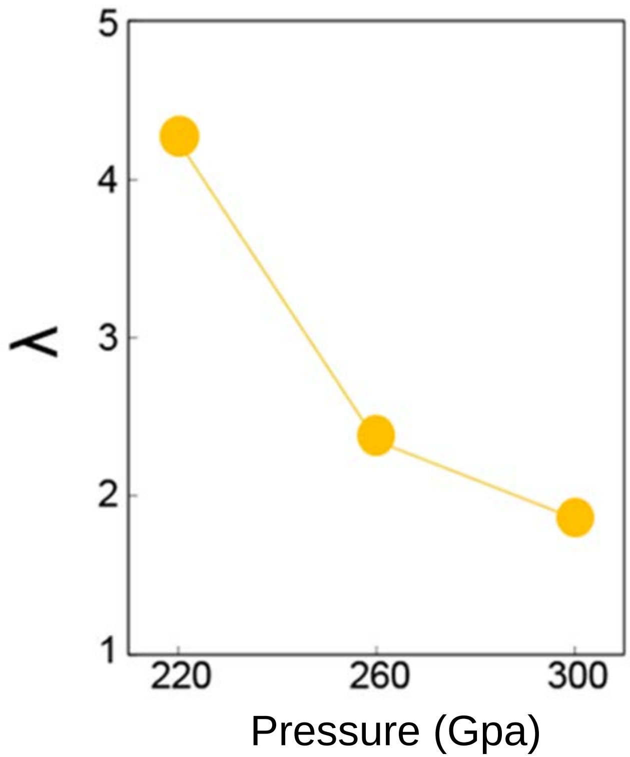


✓ The low-frequency optical phonon modes soften with decreasing pressure, increasing the EPC strength.

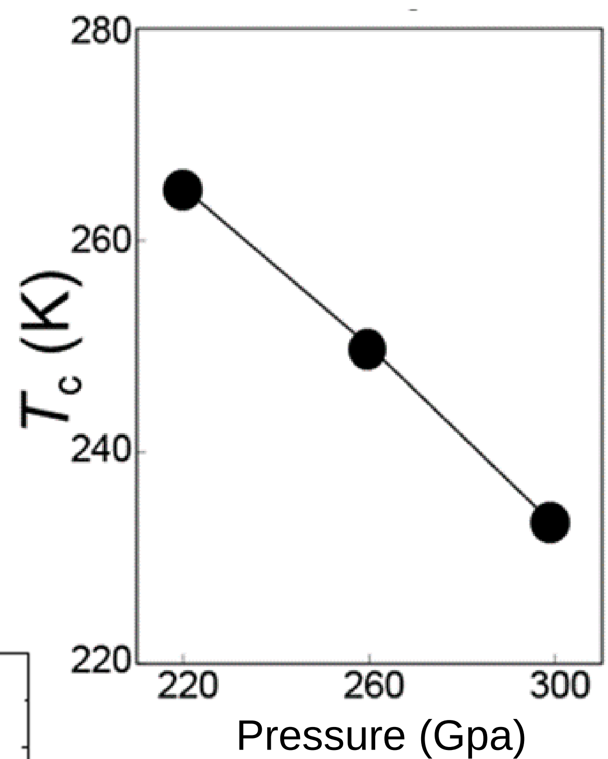
➡ Structural phase transition to a low-symmetry structure

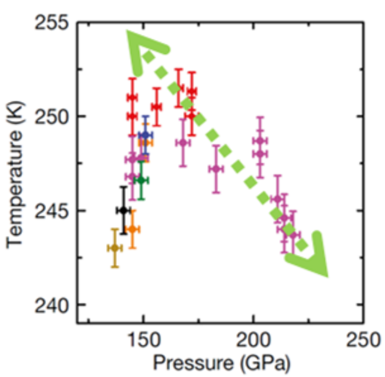
Pressure dependence of T_c in fcc-LaH_{10}

EPC constant



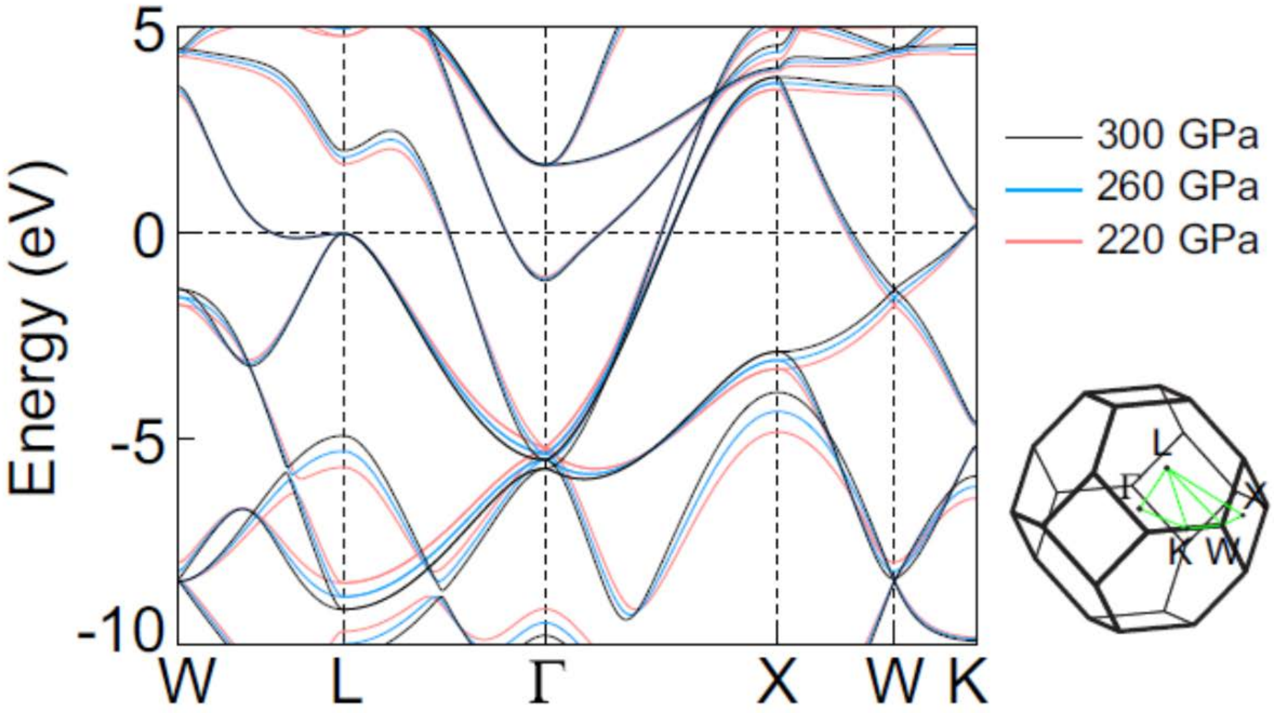
Migdal-Eliashberg equations





Drozdovar, *et al.* Nature (2019)

Band structure as a function of pressure



✓ Electronic states at E_f hardly change w.r.t pressure.

✓ Phonon softening is not due to Fermi-surface instability but is associated with electron-phonon coupling.

Outline

- ✓ **Introduction**
- ✓ **Room-temperature superconductivity of LaH_{10}**

  - Electronic and phononic structures

  Phys. Rev. B **99**, 140501(R) (2019)

  - Pressure dependence of T_c

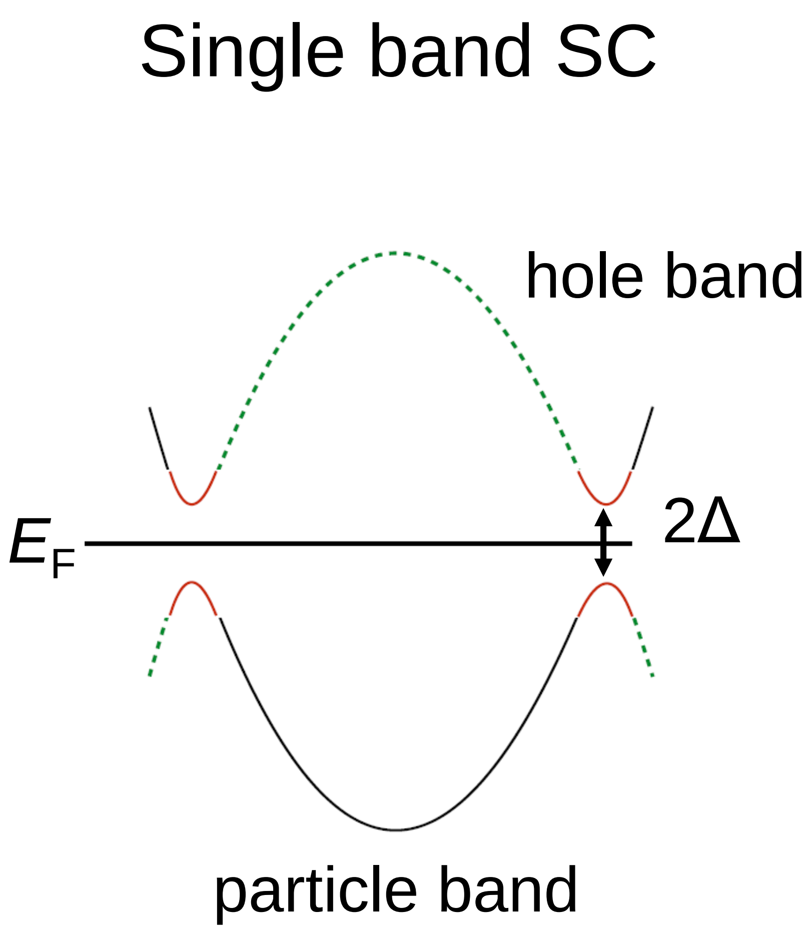
  Phys. Rev. B **100**, 060502(R) (2019)

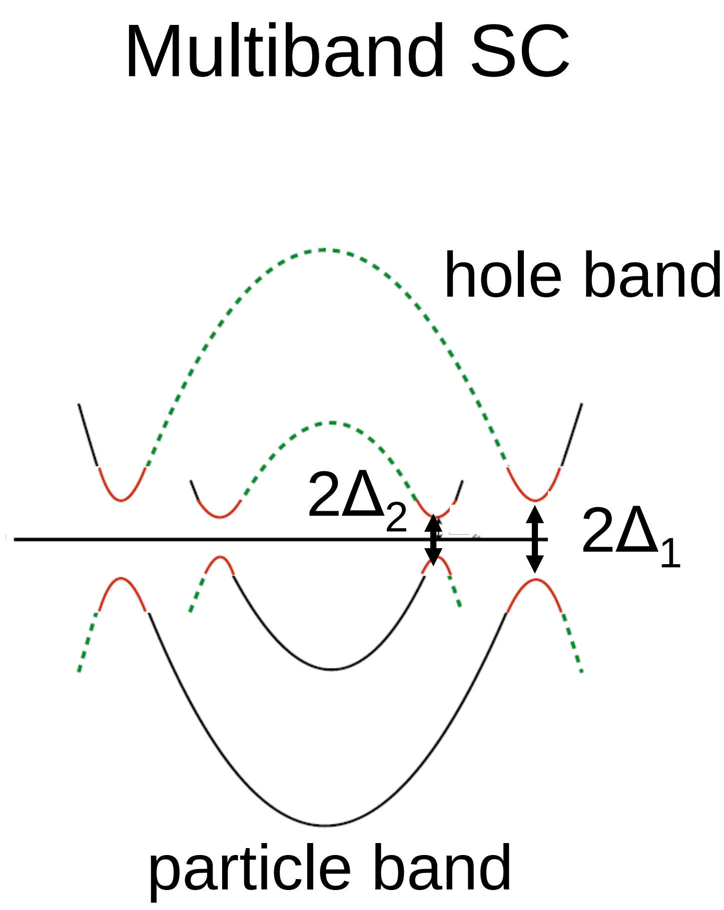
  - Multiband nature of superconductivity

  Phys. Rev. Lett. (submitted)

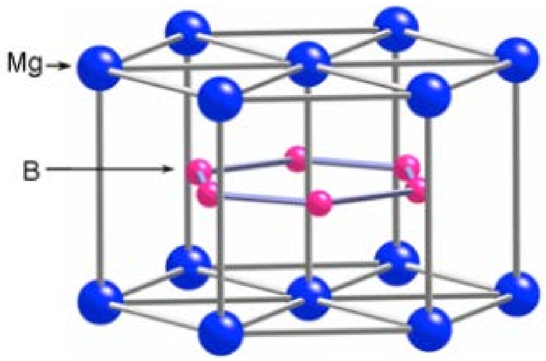
- ✓ **Conclusion**

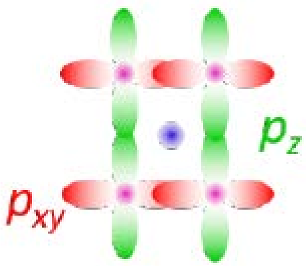
Multiband superconductivity

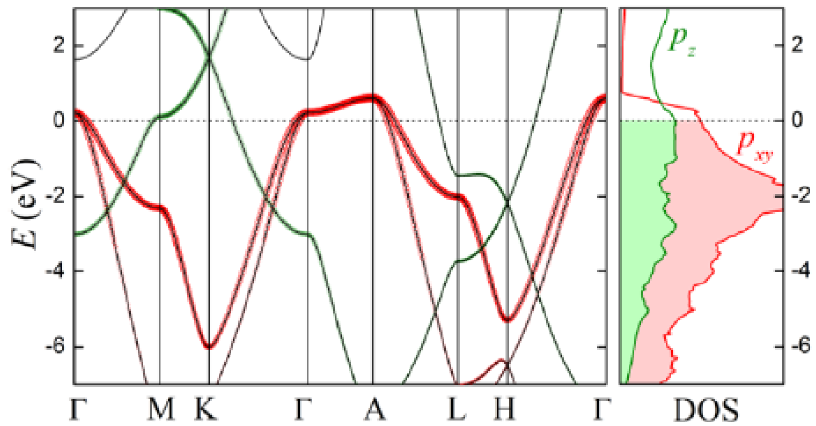


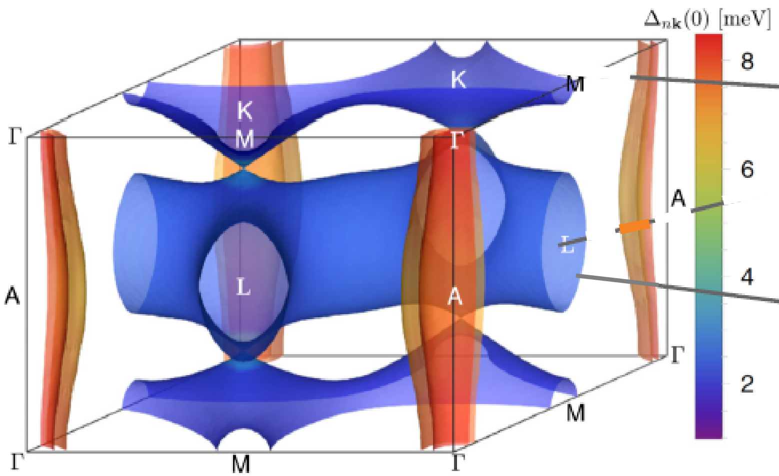


Multiband superconductivity in MgB_2

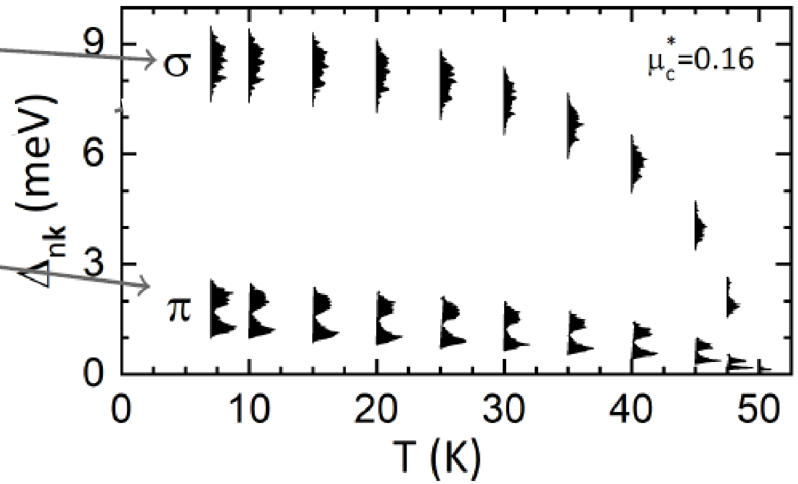








superconducting gap on FS



Margine & Giustino, PRB (2013)

PRL (Submitted)

Multiband Nature of the Room-Temperature Superconductivity in Compressed LaH_{10}

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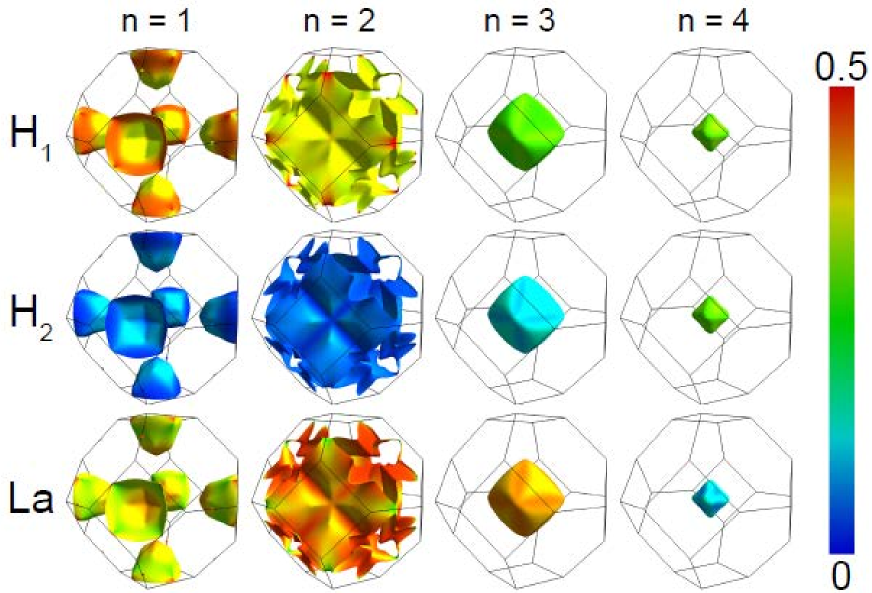
Four Fermi surface sheets



- ✓ n=1,2,3 bands :

  Hybridized states of H_1 & La

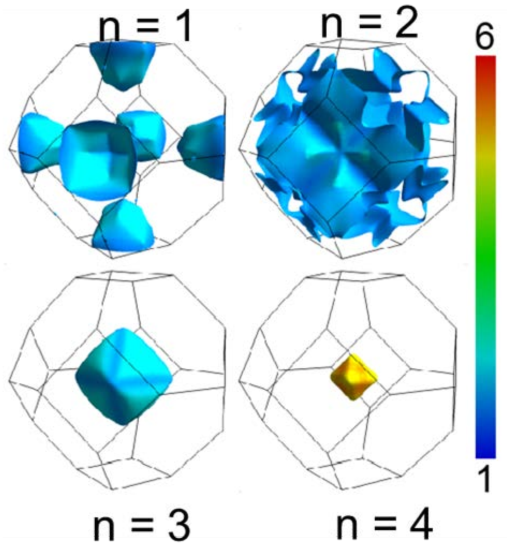
- ✓ n=4 band :

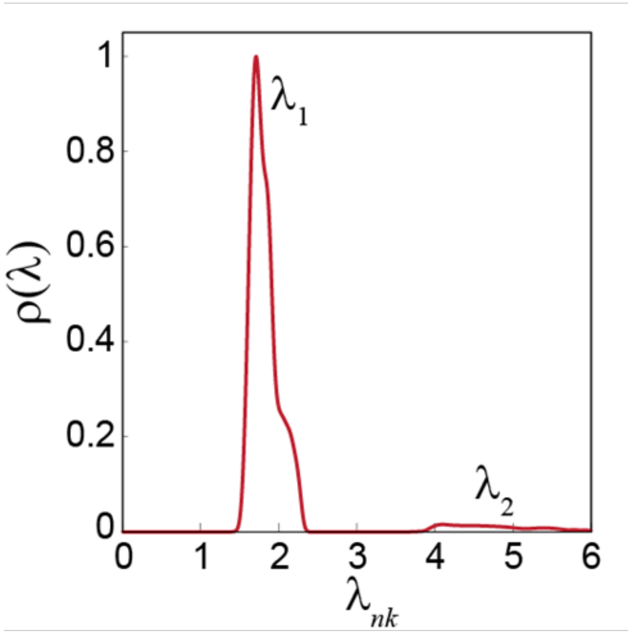
  Hybridized state of H_1 & H_2

Electron-phonon coupling (EPC) of LaH_{10}

Distribution of **k**-resolved EPC constant λ_{nk}

(Anisotropic Migdal-Eliashberg equations)

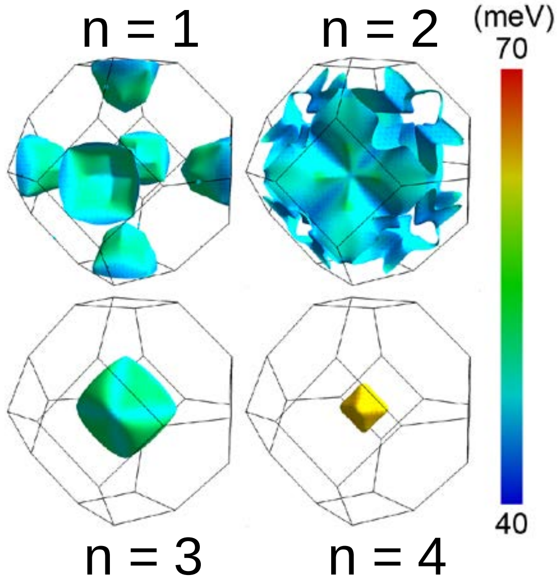




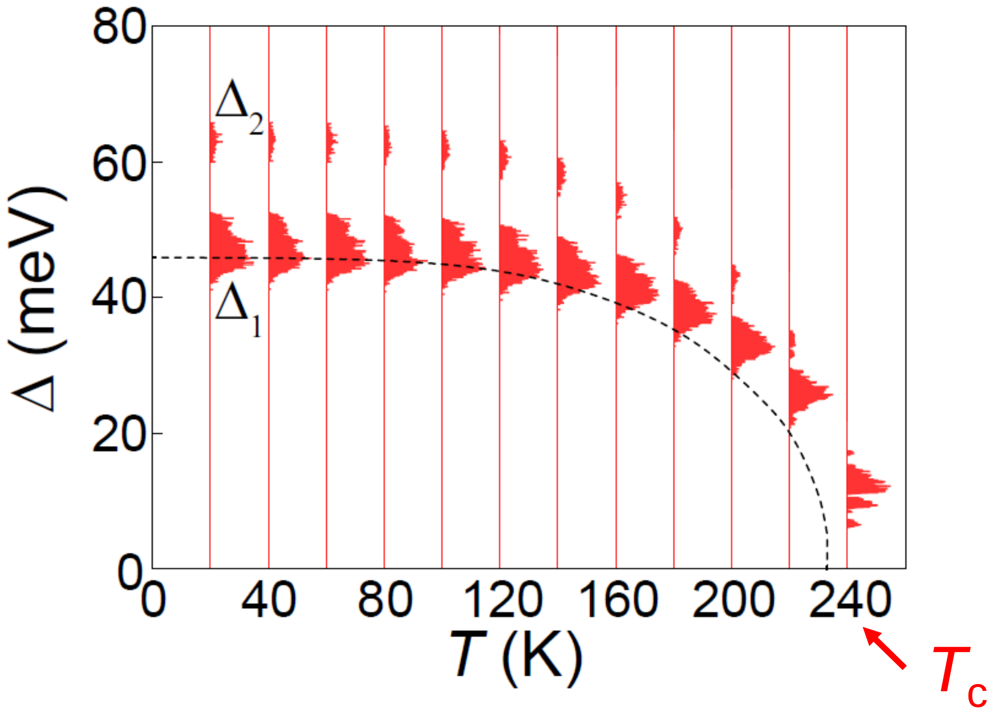
- ✓ The lower regime of λ_1 originates from n=1, 2, 3 bands.
- ✓ The upper regime of λ_2 originates from n=4 band.

Superconducting gap of fcc LaH_{10}

Energy distribution of **k**-resolved gap Δ_{nk}
(Anisotropic Migdal-Eliashberg equations)



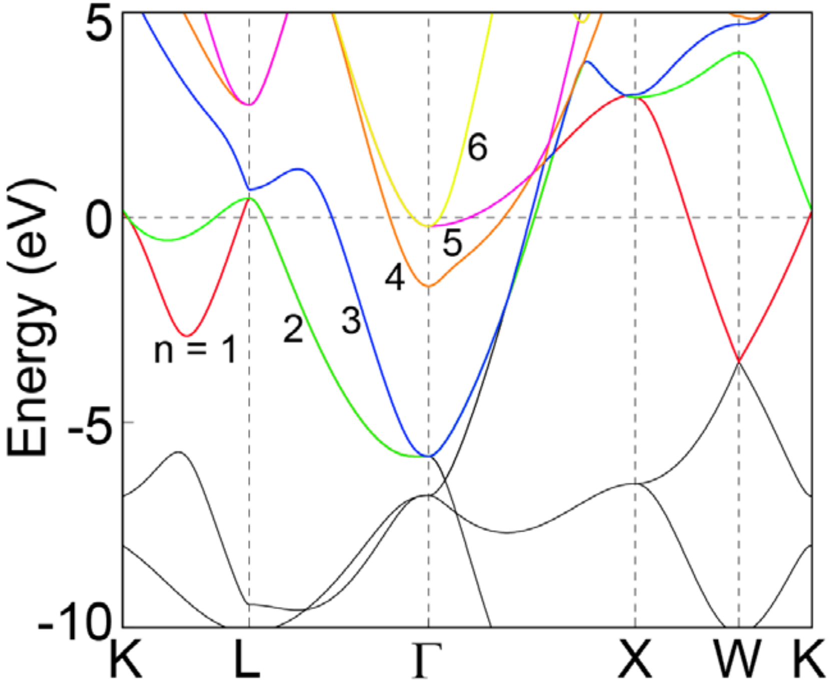
$T = 0$



✓ Anisotropic two-gap nodeless SC with *s*-wave symmetry

Multiple Fermi surface sheets in fcc YH_{10}

Band structure at 300 GPa

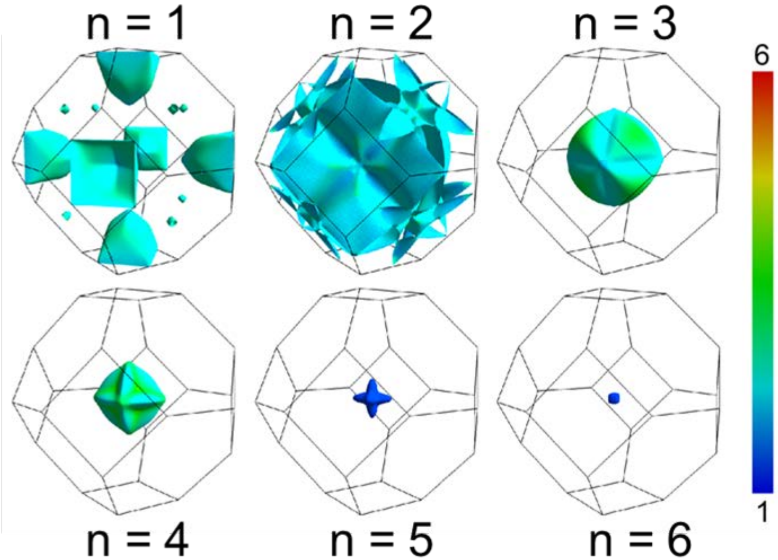


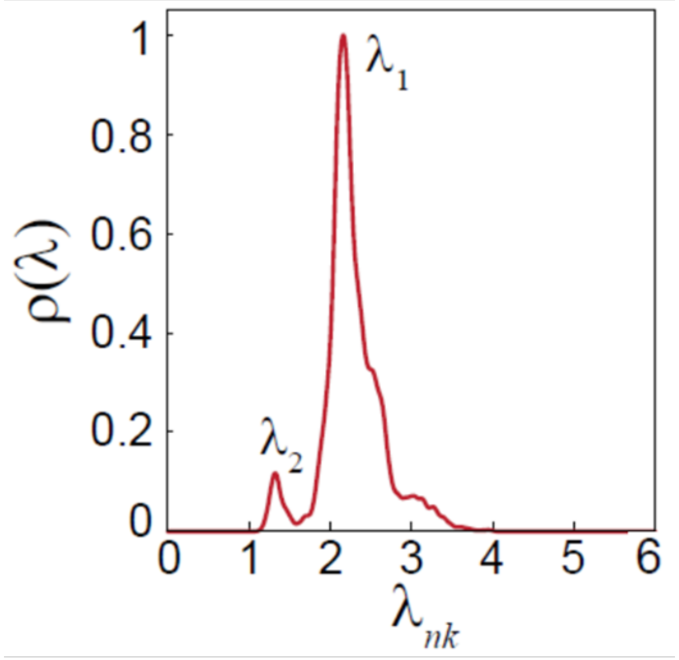
✓ Six bands cross at the Fermi energy.

✓ There are two more Fermi surface sheets than LaH10.

Electron-phonon coupling of YH_{10}

Distribution of **k**-resolved EPC constant λ_{nk}

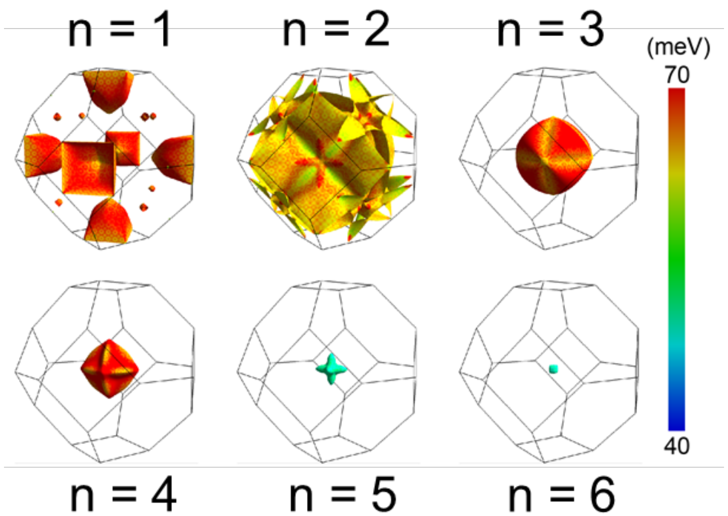




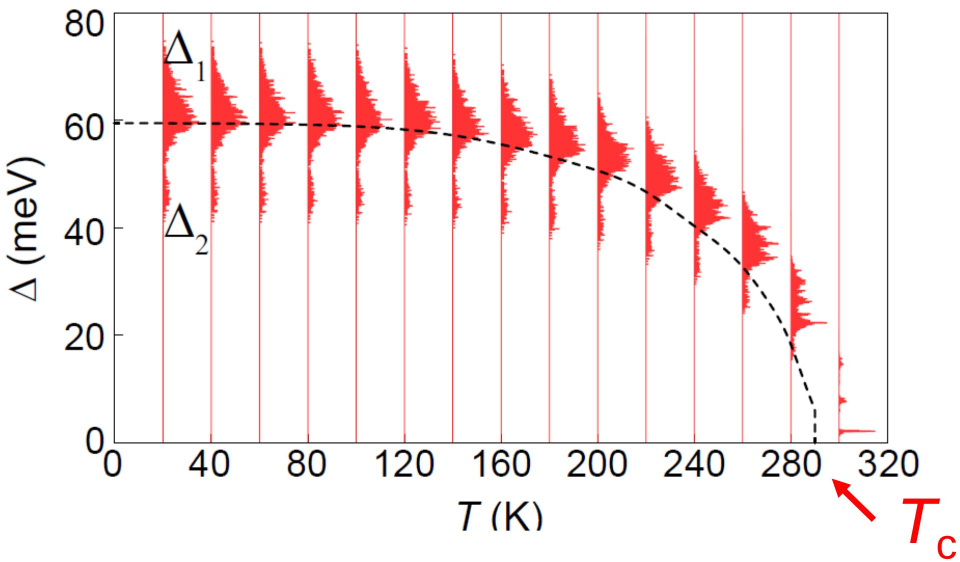
- ✓ The upper regime of λ_1 originates from n=1, 2, 3, 4 bands.
- ✓ The lower regime of λ_2 originates from n=5, 6 band.

Superconducting gap of fcc YH_{10}

Energy distribution of **k**-resolved gap Δ_{nk}



$T = 0$



- ✓ YH_{10} has T_c = 290 K at 300 GPa, higher than LaH_{10}.
- ✓ More Fermi surface sheets give higher T_c.

Why LaH_{10} has room-temperature SC ?

<u>Large EPC constant</u>

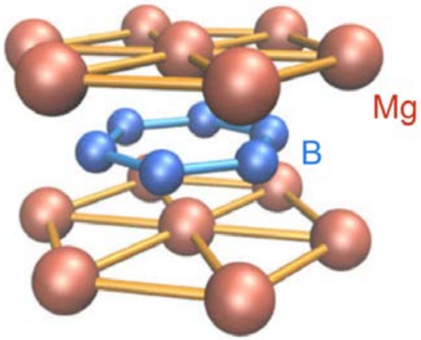
- ✓ Hybridized electronic states at E_F
- ✓ Multiband EPC channels
- ✓ Covalent H-H and La-H bondings

↓

Room-temperature superconductivity

High-T_c BCS-type superconductors

MgB_2



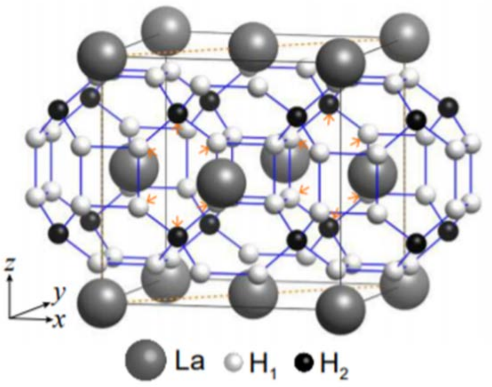
ω_{max}: 810 cm^{-1}

λ: 0.748

T_c: ~40 K

Margine *et al.* PRB (2013)

LaH_{10}



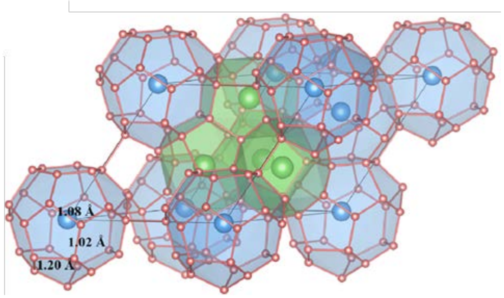
ω_{max}: 2380 cm^{-1}

λ: 1.86

T_c: ~233 K

Wang *et al.* PRB (2019)

Li_2MgH_{16}



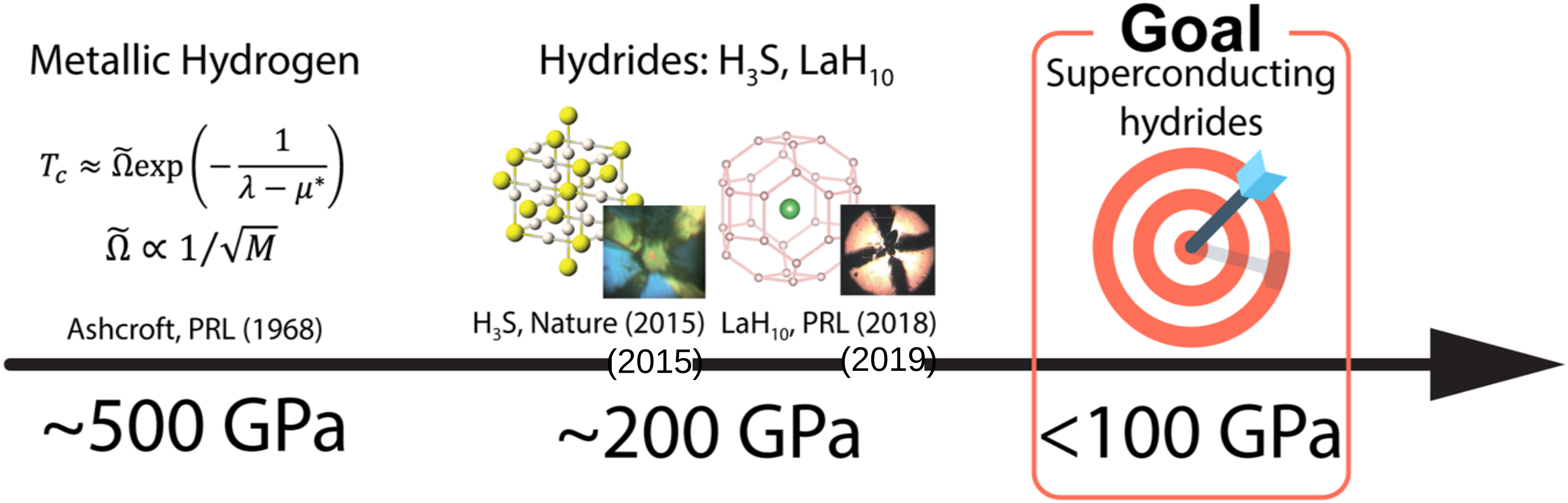
ω_{max}: 2400 cm^{-1}

λ: 3.35

T_c: ~473 K

Sun *et al.* PRL (2019)

Future direction of superconducting hydrides



✓ Room-temperature SC of hydrides at ambient pressure

The people behind this work

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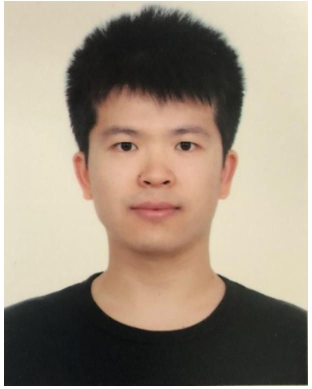

Seho Yi

Dr. Liangliang Liu


THANK
YOU