Nadprzewodnictwo i nadciekłość, wykład oddziaływanie elektron-fonon, teoria Eliashberga i obliczenia ab-initio

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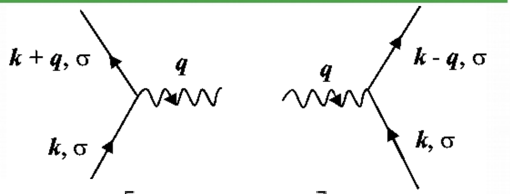
Electron-phonon interaction: formalism



- Fröhlich Hamiltonian for a system of interacting electrons and phonons

$$\hat{H}_F = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{ep}$$

$$\hat{H}_{el} = \sum_{\mathbf{k},i,\sigma} \epsilon(\mathbf{k}) a^\dagger_{\mathbf{k}\sigma i} a_{\mathbf{k}\sigma i} \qquad \hat{H}_{ph} = \sum_{\mathbf{q},\nu} \omega(\mathbf{q})(b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} + \frac{1}{2}) \qquad \hat{H}_{ep} = \sum_{\mathbf{k}\sigma\,\mathbf{q}\nu ij} g_{\mathbf{q}\nu}(\mathbf{k},i,j) a^\dagger_{\mathbf{k}+\mathbf{q},\sigma i} a_{\mathbf{k}\sigma j} \left[b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu} \right]$$

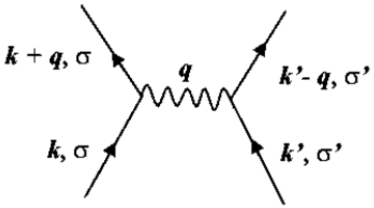
- Simplified solution: BCS reduced model

BCS theory

- From the Frohlich Hamiltonian to superconductivity: BCS theory

- Canonical transformation to the process of exchange of phonon between two electrons results in the effective Hamiltonian $\hat{H}_F^{\mathrm{eff}} = \sum_{\mathbf{k}\sigma} E(\mathbf{k}) a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\sigma\sigma'} V_{\mathrm{ep}} a^\dagger_{\mathbf{k}+\mathbf{q},\sigma} a^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'} a_{\mathbf{k}'\sigma'} a_{\mathbf{k}\sigma}$

  where
$$V_{\mathrm{ep}} = \sum_{\nu} \frac{\omega(\mathbf{q},\nu)|g_\nu(\mathbf{q},\nu)|^2}{[E(\mathbf{k}) - E(\mathbf{k}+\mathbf{q})]^2 - [\omega(\mathbf{q},\nu)]^2}$$



- Pair interaction – a pair of electrons exchange phonon and changes its momentum

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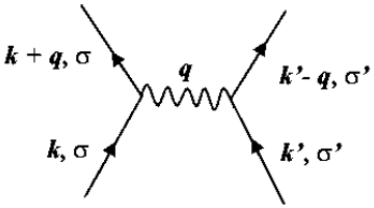

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- Pair interaction – a pair of electrons exchange phonon and changes its momentum
- This is the starting point to BCS model, where interaction is assumed to be weak, k independent, attractive and limited to the small energies around the Fermi surface

$$V_{\text{ep}} = V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -V, & |E(\mathbf{k}) - E_F| \leqslant \hbar\omega_D \\ 0, & \text{elsewhere} \end{cases}$$

- This leads to the electron pairing – electrons with opposite spins form a condensate of Cooper pairs, bounded with energy 2Δ, and gap opens in the electronic spectrum
- Condensate of pairs travels with no scattering at low T as the minimal energy is needed to break the pair. **Thus current is conducted with no resistivity = superconductivity is induced.**

BCS theory

- Critical temperature in the BCS model

- Gap equation $1 = \frac{V}{2}\sum_{\mathbf{k}}{}' \frac{1}{\sqrt{\tilde{E}(\mathbf{k})^2+\Delta^2}} \tanh \frac{\sqrt{\tilde{E}(\mathbf{k})^2+\Delta^2}}{2k_BT}$ $\tilde{E}(\mathbf{k}) = E(\mathbf{k}) - E_F$ $\sum_{\mathbf{k}}{}' \to N(E_F)\int_{-\hbar\omega_D}^{\hbar\omega_D} d\tilde{E}$

- T = 0 K solution: $\Delta(T=0) = 2\hbar\omega_D e^{-1/VN(E_F)}$

- Δ = 0 solution gives Tc: $k_BT_c = 1.13\hbar\omega_D e^{-1/VN(E_F)}$

- Tc depends on:
  - **Debye** frequency (temperature) = predicts **isotope effect** – the same material but made of lighter and heavier isotope will have different (lighter → larger) Tc $\omega_D \propto M^{-1/2}$ $T_C \propto M^{-1/2}$
  - **Interaction strength** $VN(E_F)$ (rather as a product, not separately, but large $N(E_F)$ is usually favorable for superconductivity)

- BCS model explains the phenomenon of superconductivity but to make practical calculations for real materials with real electron-phonon spectra and interactions we have to go to Eliashberg theory

fingerprints of superconductivity

1) Zero resistance

2) Diamagnetism

this defines the superconducting state

3) Anomaly in the specific heat:

always for ‘classical’ superconductor

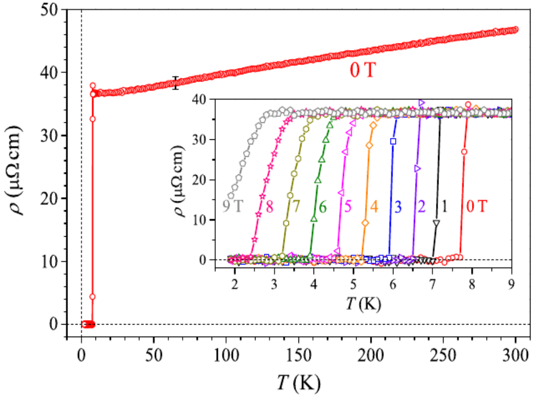
PRL **113,** 107001 (2014) PHYSICAL REVIEW LETTERS week ending 5 SEPTEMBER 2014

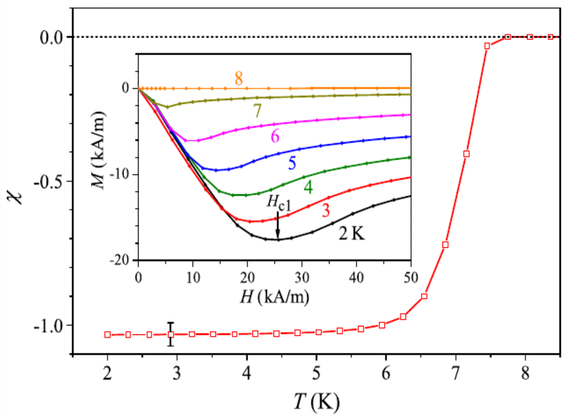
Discovery of a Superconducting High-Entropy Alloy

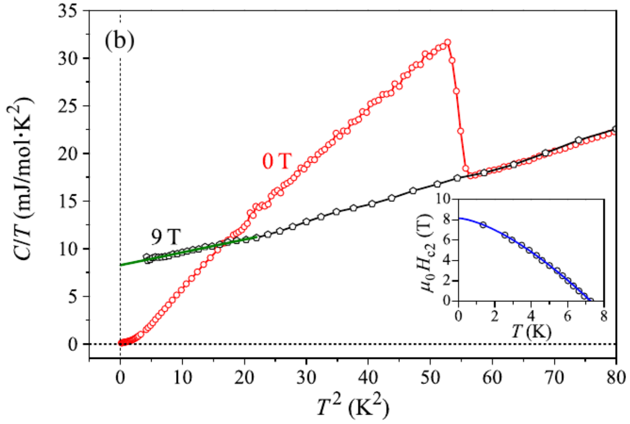
P. Koželj,[1] S. Vrtnik,[1] A. Jelen,[1] S. Jazbec,[1] Z. Jagličić,[2] S. Maiti,[3] M. Feuerbacher,[4] W. Steurer,[3] and J. Dolinšek[1,*]

$\mathbf{Ta_{0.34}Nb_{0.33}Hf_{0.08}Zr_{0.14}Ti_{0.11}}$

- bcc type structure with random occupation
- type-II superconductor (Hc_2 = 8.2 T)
- superconducting transition at Tc = 7.3 K
- specific heat jump: $\Delta C(T_c)/\gamma T_c = 1.63$ (weak-coupling BCS: 1.43)







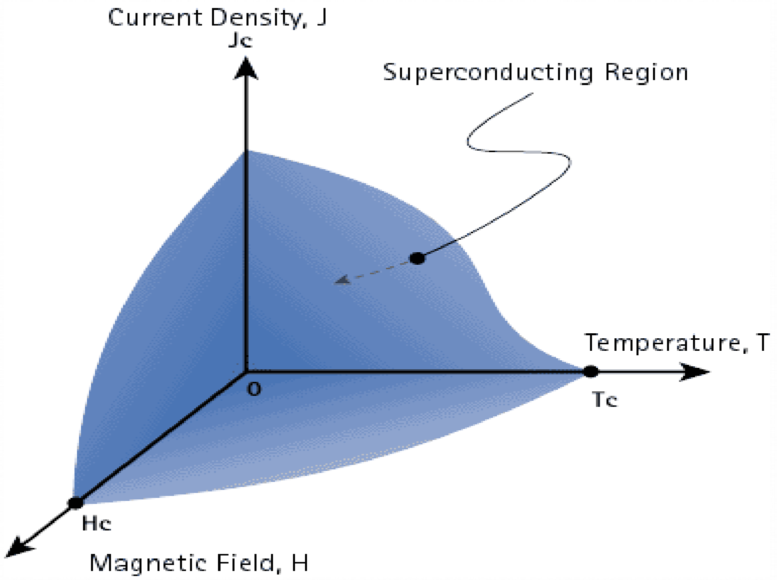
BCS theory

- Breaking the pairs in three ways

1) Current flows and pair has too large extra kinetic energy (critical current density)

2) In the external magnetic filed spin is flip or the orbital cyclotron energy is too large (critical magnetic field, Pauli or orbital mechanism)

3) The temperature is too large (critical temperature)



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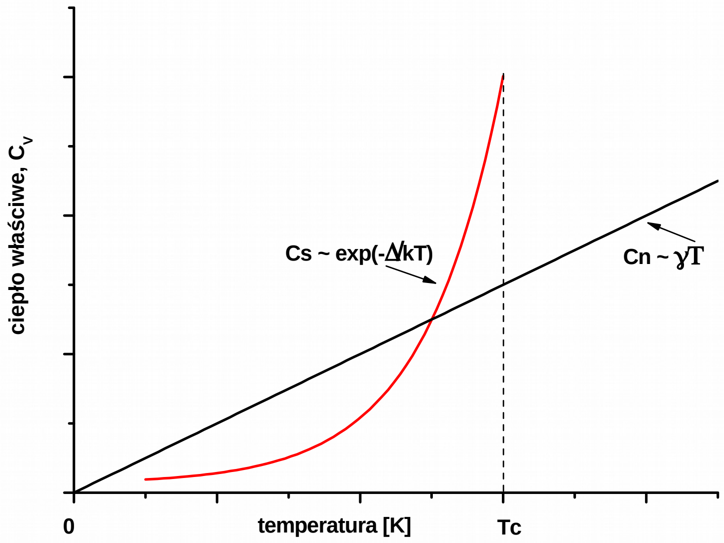
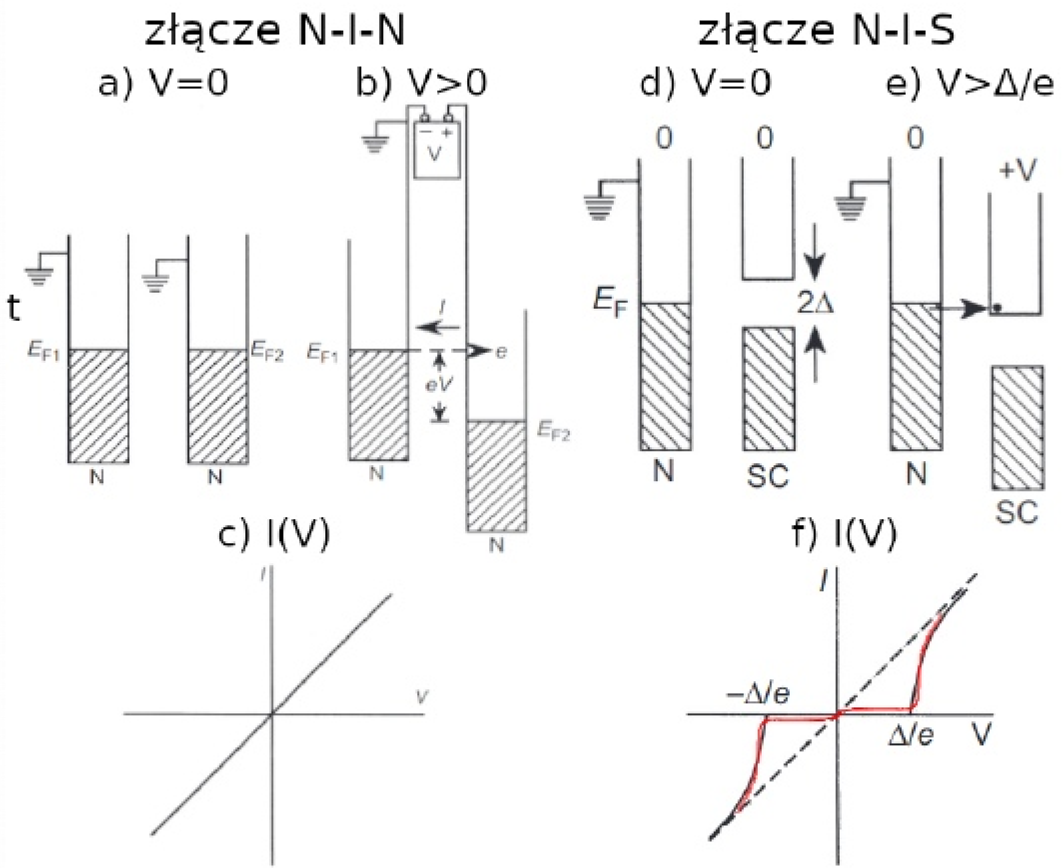




- Gap from specific heat
  (exponential only at very low T) or tunneling

BCS theory

- Isotope effect exponents are not necessarily 0.5

Table 6.2. Isotope Effect ($T_c \sim M^{-\alpha}$)

Element	α
Sn	0.46
Mg	0.5
Re	0.4
Ru	0 (±0.05)
Zr	0 (±0.05)
Os	0.21
Mo	0.33

- Characteristic ratios predicted by BCS theory (if observed in experiment we expect el-ph interaction to be the pairing interaction + interaction is weak)
- Specific heat jump at the transition $$\frac{\Delta C_e}{\gamma T_c} = 1.43$$
- Reduced gap magnitude $$\frac{2\Delta}{k_B T_c} = 3.53$$
- Deviations e.g. in Pb and Pb-Bi alloys: $\Delta C/\gamma T_c \sim 3$; $2\Delta/k_B T_c \sim 5$

Beyond the BCS theory

- What is missing in the BCS (reduced) model?

1) Frequency-dependent electron-phonon interaction with real phonon spectrum

2) Real electronic structure and non-spherical Fermi surface

3) Possibility of strong interactions

4) Multiband effects (more than 1 electronic band, many FS pockets)

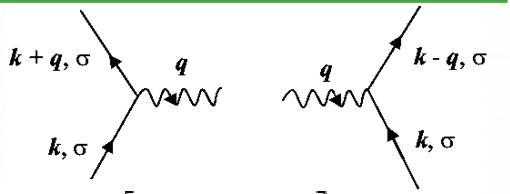
5) Electron-electron (retarded) repulsion in the Cooper pair (depairing effect)

- More accurate treatment: numerical calculations of the electronic structure, phonons and electron-phonon interaction (Density Functional Theory) +

  1) Isotropic Eliashberg theory
  2) Anisotropic Eliashberg theory
  3) Density functional theory for superconductors

Electron-phonon interaction from ab-initio

- Fröhlich Hamiltonian for a system of interacting electrons and phonons



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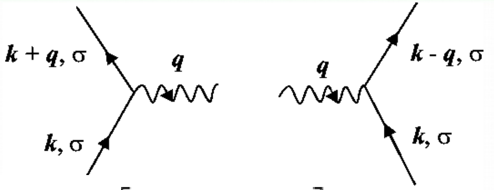

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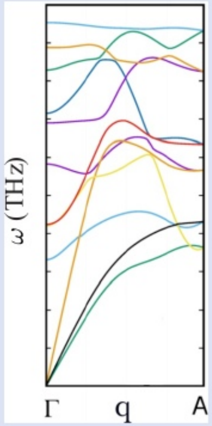
- Key quantity: matrix element *g*



phonons

phonon with wave vector **q**

n-th atom in the unit cell

Electrons in bands *i*, *j* with wave vectors **k**, **k + q**

$$g_{\mathbf{q}\nu}(\mathbf{k},i,j) = \left(\frac{\hbar}{2\omega_{\mathbf{q}\nu}}\right)^{1/2} \sum_n \frac{1}{\sqrt{M_n}} \langle \psi_{i,\mathbf{k}} | \frac{dV_{\mathrm{SCF}}}{d\hat{u}_{n,\nu}} \cdot \hat{\epsilon}_{n,\nu} | \psi_{j,\mathbf{k}+\mathbf{q}} \rangle$$

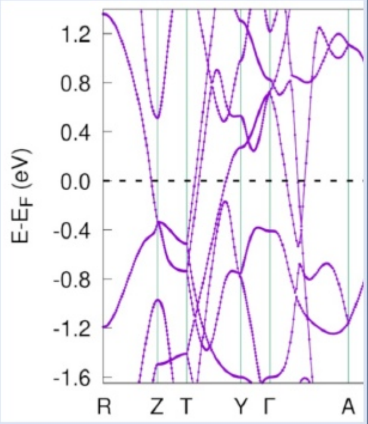
electrons

ν - phonon mode index

ω(q,ν) - phonon frequency

Perturbation of the electronic potential due to atomic displacement

Phonon eigenvector ε (atomic displacement)



- Perturbation of potential is computed using Density Functional Perturbation Theory in Quantum Espresso

Electron-phonon interaction from ab-initio

- From *g* we get the more global quantities, like phonon linewidths $\gamma_{\mathbf{q}\nu}$

$$\gamma_{\mathbf{q}\nu} = 2\pi\omega_{\mathbf{q}\nu} \sum_{ij} \int \frac{d^3k}{\Omega_{\mathrm{BZ}}} |g_{\mathbf{q}\nu}(\mathbf{k}, i, j)|^2 \times \delta(E_{\mathbf{k},i} - E_F)\delta(E_{\mathbf{k}+\mathbf{q},j} - E_F)$$

sum over all bands *i,j* + Fermi surface integral

phonons are emitted/absorbed by electrons so have a finite lifetime, $\Delta t \sim 1/\gamma$, $\Delta t \Delta E \sim \hbar$

- $\gamma_{\mathbf{q}\nu}$ does not depend on ω
- Phonon linewidths are computed in QE and characterize a strength on el-ph interaction mediated by selected phonon

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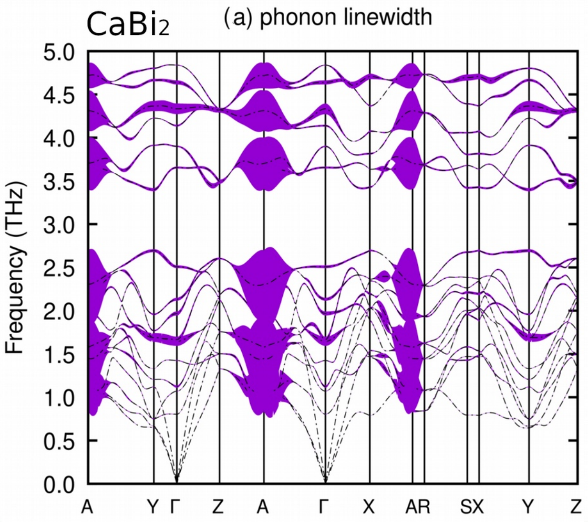
- Visualization possible, using band shading

linewidths here multiplied by 4.
typically ~ 1-100 GHz



CaBi2: S. Gołąb (Gutowska), B. Wiendlocha, PRB 2019

Electron-phonon interaction from ab-initio

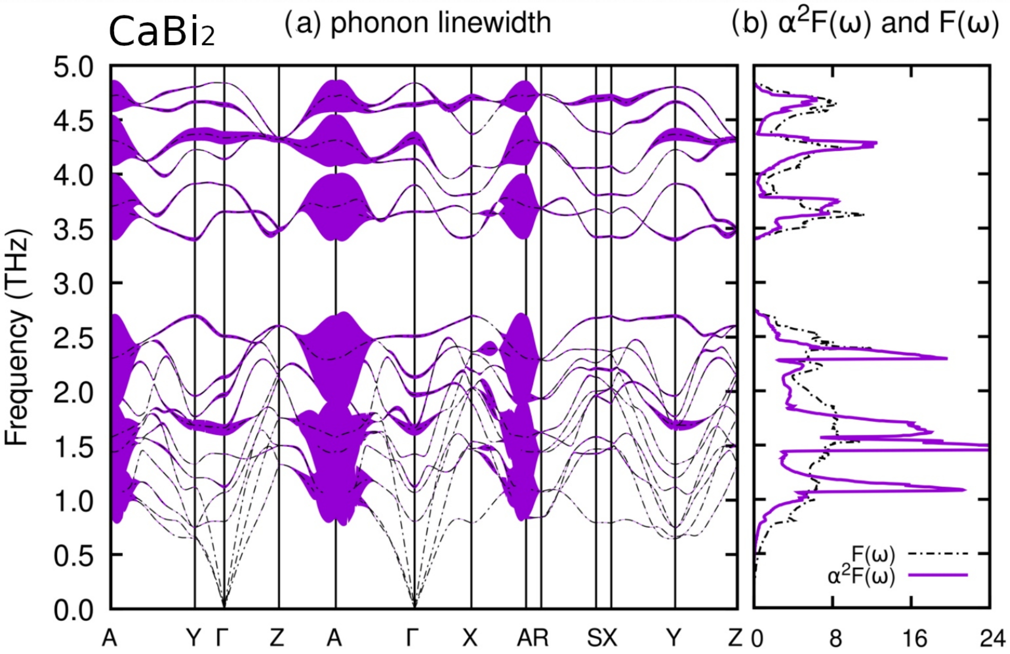
- Next more global quantity: Eliashberg function – summation over all phonons

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)} \sum_{\mathbf{q}\nu} \delta(\omega - \omega_{\mathbf{q}\nu}) \frac{\gamma_{\mathbf{q}\nu}}{\hbar\omega_{\mathbf{q}\nu}}$$

- Electron-phonon coupling parameter λ – integration over all frequencies

$$\lambda = 2\int_0^{\omega_{\max}} \frac{\alpha^2 F(\omega)}{\omega} d\omega, \qquad \lambda = \sum_{\mathbf{q},\nu} \frac{\gamma_{\mathbf{q}\nu}}{\pi \hbar N(E_F) \omega^2_{\mathbf{q},\nu}}$$

- λ: Electronic specific heat renormalization
- λ ~ 0 – 2 (Nb ~ 1, strong coupling)



- The same parameter λ determines the value of superconducting transition temperature Tc in the “classical” superconductors (where superconductivity is due to the electron-phonon interaction)

Eliashberg theory & McMillan/ Allen-Dynes formulas

- Takes into account the real, frequency-dependent electron-phonon interaction, described by Eliashberg function (isotropic Eliashberg)

- self-consistent equations for the (isotropic) superconducting energy gap as a function of temperature
- allow to determine the **thermodynamic** properties of the superconducting phase
- pairing = **electron-phonon** interaction
- **input** – Eliashberg function from first-principles calculations
- depairing in the **Coulomb pseudopotential** parameter μ^* (retarded e-e repulsion, $\mu^* = 0.1 – 0.2$)

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$$Z(i\omega_n) = 1 + \frac{\pi k_B T}{\omega_n} \sum_{n'} \frac{\omega_{n'}}{R(i\omega_{n'})} \lambda(n-n')$$

$$Z(i\omega_n)\Delta(i\omega_n) = \pi k_B T \sum_{n'} \frac{\Delta(i\omega'_n)}{R(i\omega'_n)} [\lambda(n-n') - \mu^* \theta(\omega_c - \omega'_n)]$$

$$\lambda(n-n') = \int_0^\infty d\omega \frac{2\omega\alpha^2 F(\omega)}{(\omega_n - \omega_{n'})^2 + \omega^2},$$

$$R(i\omega_n) = \sqrt{\omega_n^2 + \Delta^2(i\omega_n)}$$

$$i\omega_n = i(2n+1)\pi k_B T$$

- Aproximate analytic solution for Tc: McMillan (1968), Allen & Dynes (1970)

$$\lambda = 2 \int_0^{\omega_{\max}} \frac{\alpha^2 F(\omega)}{\omega} d\omega$$

$$\boxed{k_B T_c = \frac{\hbar\omega_D}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right]}$$

$$\boxed{k_B T_c = \frac{\hbar\langle\omega_{\log}^{\alpha^2 F}\rangle}{1.20} \exp\left\{-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right\}}$$

$$\langle\omega_{\log}^{\alpha^2 F}\rangle = \exp\left(\int_0^{\omega_{\max}} \alpha^2 F(\omega) \ln\omega \frac{d\omega}{\omega} \Big/ \int_0^{\omega_{\max}} \alpha^2 F(\omega) \frac{d\omega}{\omega}\right)$$

Eliashberg theory & McMillan/ Allen-Dynes formulas

- McMillan formula most often used to estimate λ from Tc

$$k_B T_c = \frac{\hbar\omega_D}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right]$$

1) Measure Tc
2) Measure specific heat
3) Calculate T_D
4) Estimate l from inverted McMillan formula assuming m* ~ 0.10 – 0.15 (0.13 most often)

Setting Θ_D = 157 K and T_c = 2.0 K, and making the common assumption that the Coulomb pseudopotential parameter $\mu^* = 0.13$, we can now calculate the electron–phonon coupling constant λ_{el-ph} using the modified McMillan formula:[41]

$$\lambda_{el-ph} = \frac{1.04 + \mu^* \ln\left(\frac{\Theta_D}{1.45 T_c}\right)}{(1 - 0.62\mu^*)\ln\left(\frac{\Theta_D}{1.45 T_c}\right) - 1.04} \qquad (2)$$

This yields λ_{el-ph} = 0.59, indicating that $CaBi_2$ is a moderate-coupling strength superconductor.

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Superconductivity in $CaBi_2$†

M. J. Winiarski,*[a] B. Wiendlocha,[b] S. Gołąb,[b] S. K. Kushwaha,[c] P. Wiśniewski,[d] D. Kaczorowski,[d] J. D. Thompson,[e] R. J. Cava[c] and T. Klimczuk*[a]

Electron-phonon interaction from experiment

- Electron-phonon coupling parameter λ affects the electronic specific heat (electrons seems to be “heavier”) - independent method of measuring λ if combined with first-principles calculations of density of states at the Fermi level

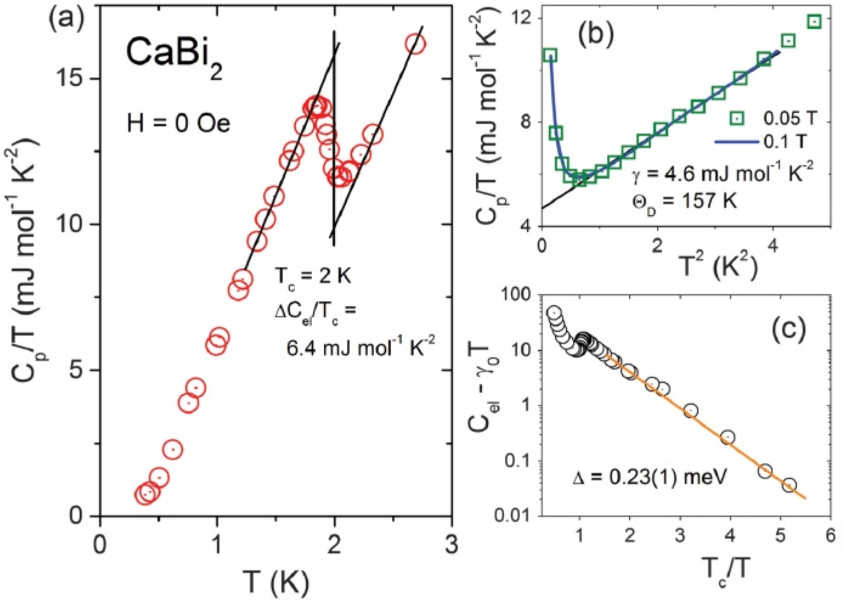
- Electronic specific heat C = γT, γ - Sommerfeld coefficient

‘bare’ bandstructure value: $$\gamma_0 = \frac{\pi^2}{3} k_B^2 N(E_F)$$

renormalized by the electron-phonon interaction:

$$\gamma = \gamma_0 \frac{m*}{m} = \gamma_0 (1 + \lambda_{\text{ep}})$$

CaBi2: calculated γ_0 = 2.59 mJ/mol K^2
measured: 4.1 mJ/mol K^2
renormalization: 4.1/2.59 = 1.58
λ_{ep} = 0.58
Calculated from Tc and McMillan formula:
λ_{ep} = 0.53
Calculated from Eliashberg function: 0.54



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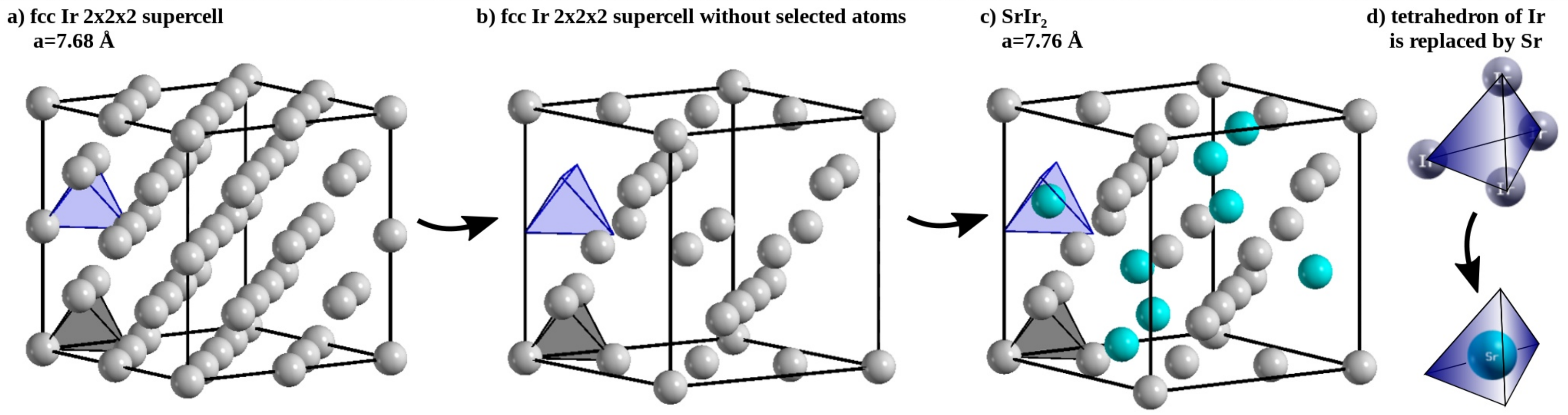
Superconductivity from *ab initio*

- Calculate electronic structure
- Calculate phonons and perturbation of potential
- Calculate electron-phonon matrix elements
- Calculate Eliashberg function
- Calculate λ
- Calculate Tc and other thermodynamic properties of superconducting phase (specific heat, critical fields, magnetic penetration depth)
  - Conclude on the mechanism of superconductivity (el-ph or not, isotropic/anisotropic)
  - Investigate how it changes e.g. under pressure or with the isotope substitution
  - Search for new superconductors
- Works very well in many various superconducting materials (including hydrogen-based high Tc high-pressure materials!)
- Becomes difficult for large systems and alloys
- We have some solution for alloys (simplified treatment via decoupling electrons from phonons)

Example

- Phonon engineering and superconductivity in SrIr2 (Laves phase, superconductor)

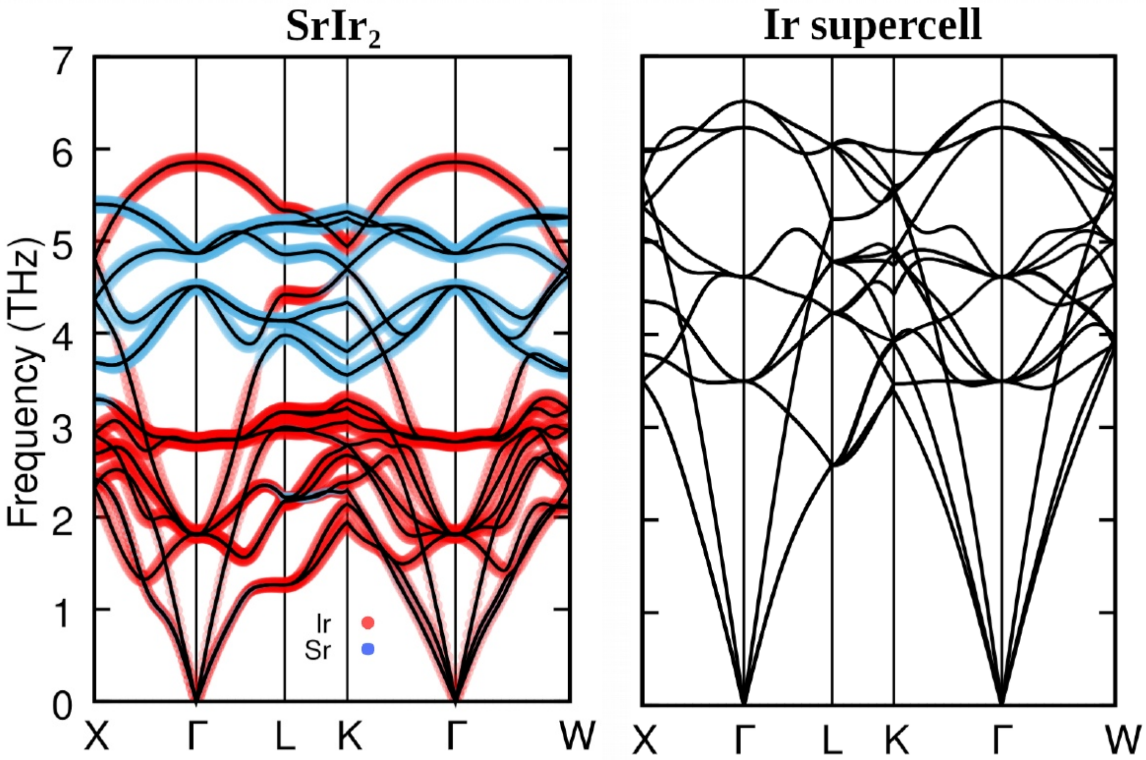
  - Crystal structure is closely related to metallic Ir fcc phase
  - Half of Ir4 tetrahedrons are replaced by Sr, located in the middle of the removed tetrahedron



- Why is $SrIr_2$ a strongly coupled superconductor with Tc =6 K, whereas Ir has Tc = 0.14 K?

Phonons: Ir vs $SrIr_2$

- SrIr2: highest phonon mode is from Ir!
- Mass: m(Ir) = 192 u, m(Sr) = 88 u but still Ir mode has a higher frequency



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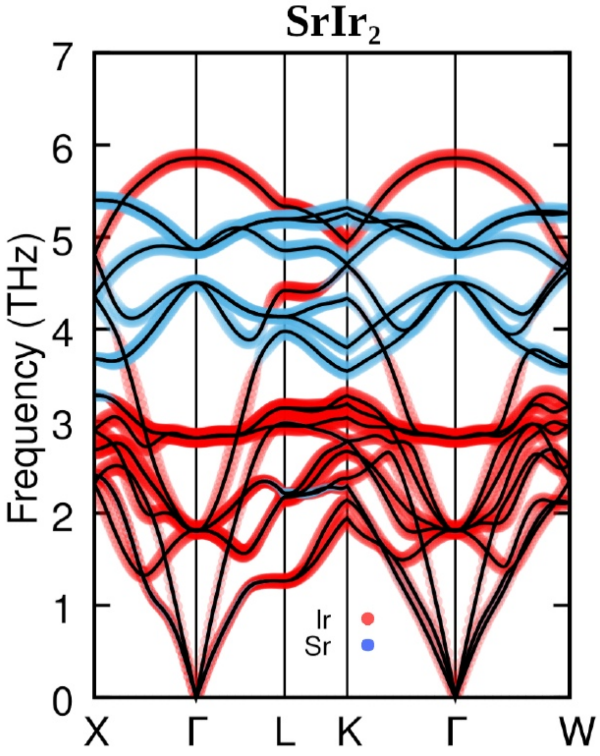
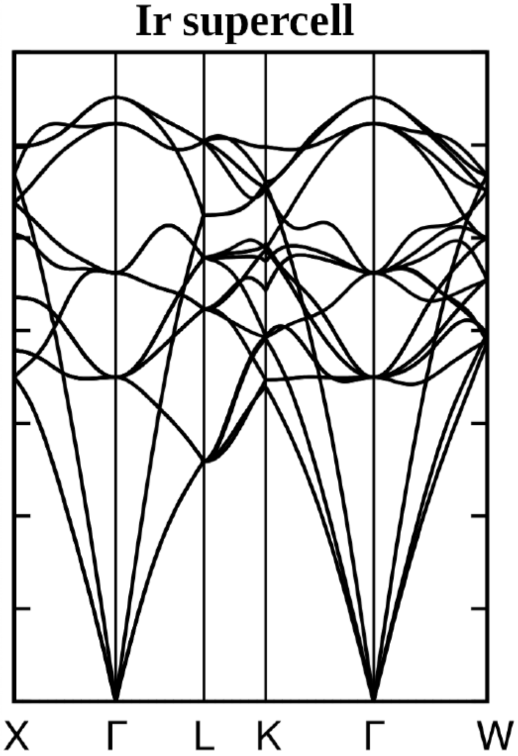
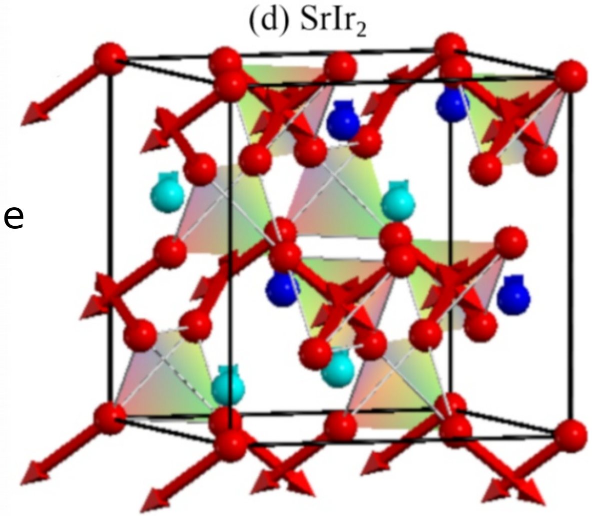


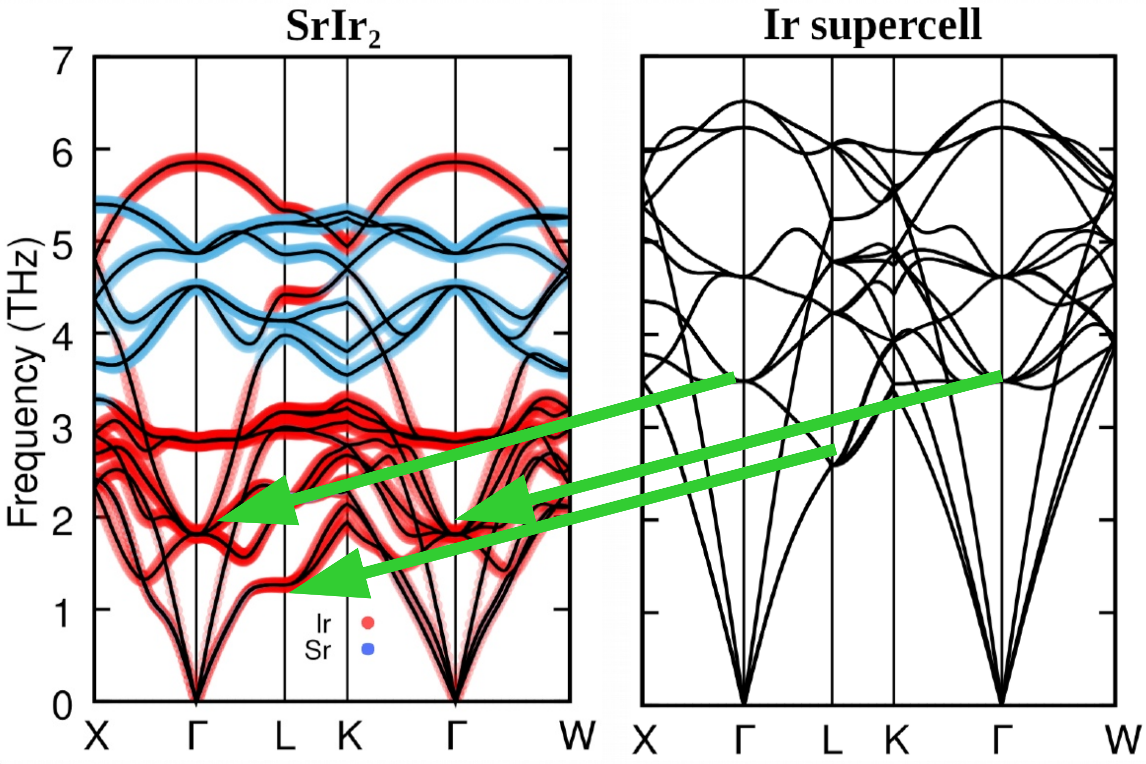


animation:
Ir vibrates to the center of tetrahedron, “breathing mode”

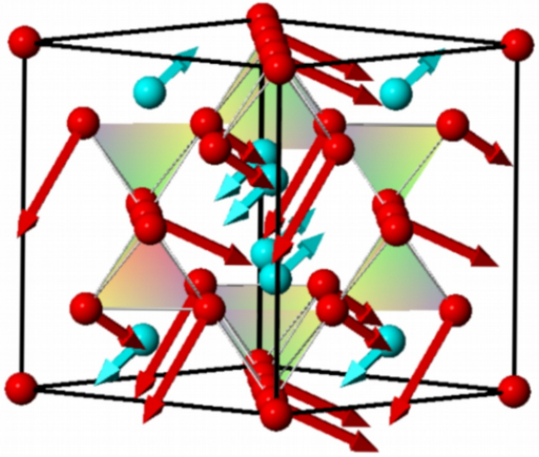


Phonons: Ir vs $SrIr_2$

- SrIr2: acoustic and lower optical modes go down! 50% lower ω
- Ir has more space around

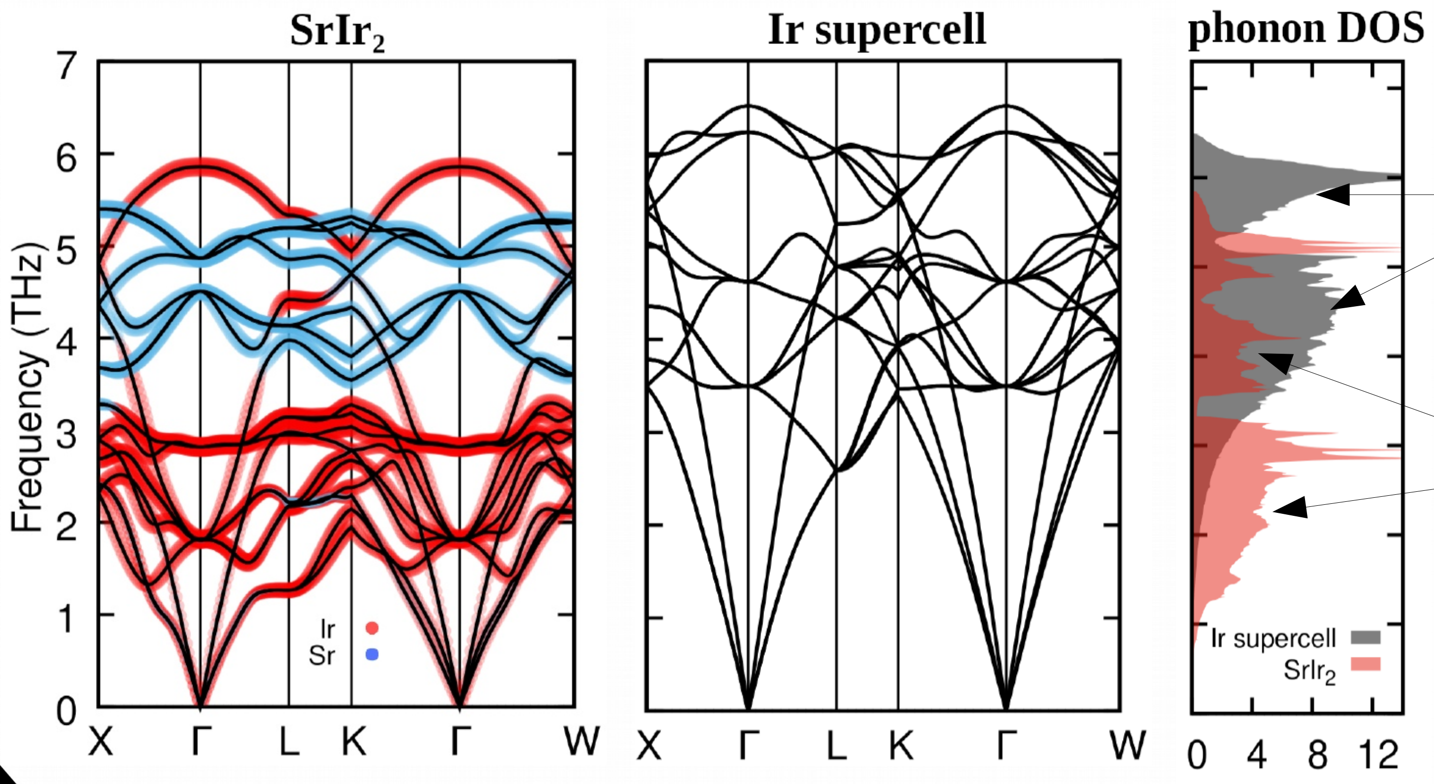


animation:
Ir vibrates
towards empty
space after
removing Ir
tetrahedrons



Phonons: Ir vs $SrIr_2$

- Phonon DOS – increase in population of lower-frequency phonons
- average frequency of Ir goes down



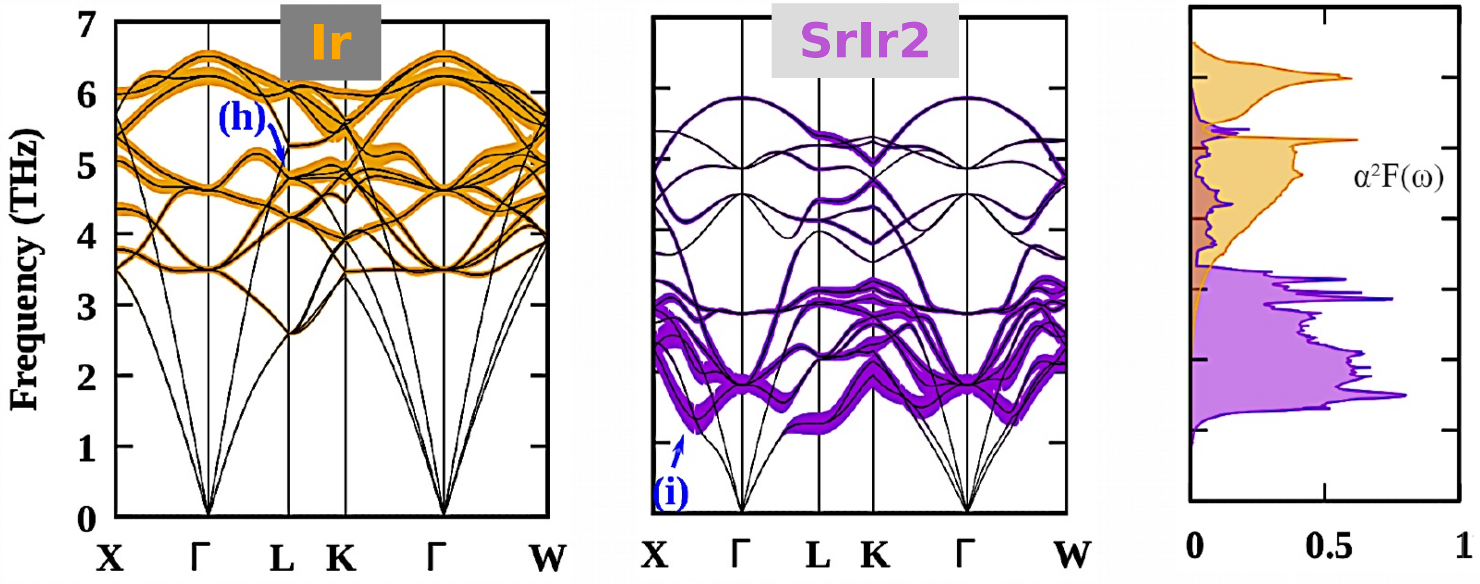
fcc Ir
$\langle\omega_{Ir}\rangle$ = 4.65 THz

$SrIr_2$
$\langle\omega_{Ir}\rangle$ = 2.96 THz

Electron-phonon coupling: Ir vs $SrIr_2$

- Ir has relatively large phonon linewidths but too high frequencies $\lambda \propto \frac{\gamma_{q\nu}}{\omega^2_{q\nu}}$

- $SrIr_2$ partially keeps large linewidths but at much lower ω



Superconductivity: Ir vs $SrIr_2$

Ir

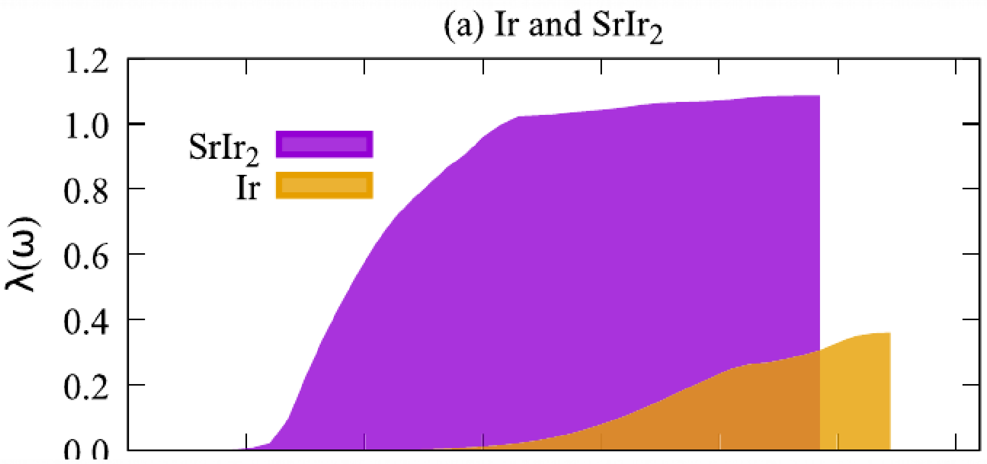
- $\lambda = 0.36$
- Tc = 0.17 K

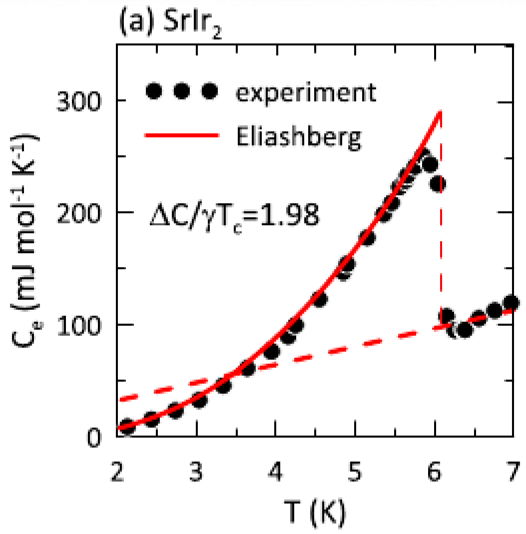
phonon engineering

$SrIr_2$

- $\lambda = 1.09$
- Tc = 6.88 K

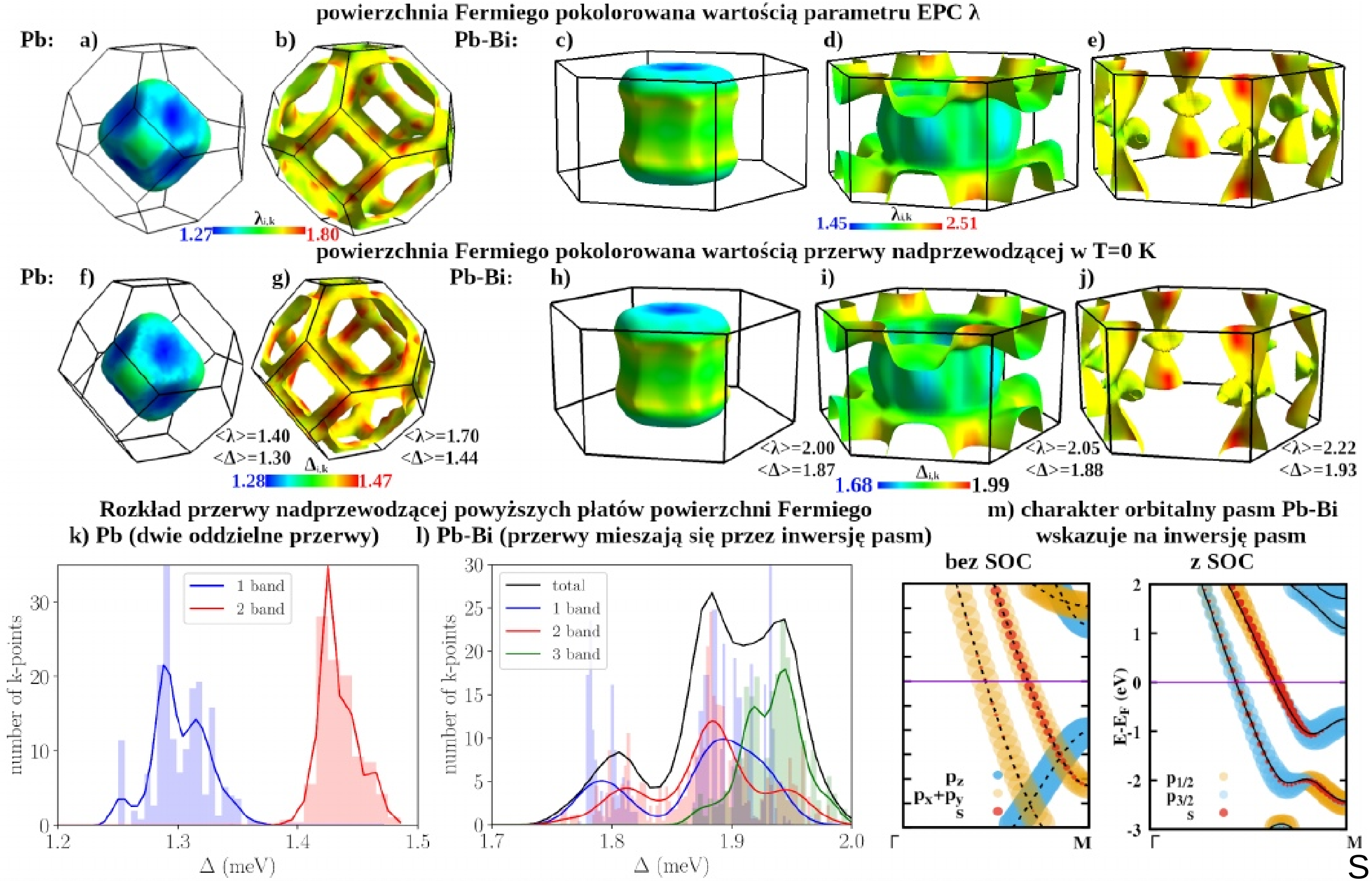
large low-frequency contribution to λ in SrIr2





specific heat in superconducting state by P. Wójcik

Anisotropy of the gap in Pb and Pb-Bi



S. Gutowska, PhD thesis

Hydrogenated high-temperature superconductors

- ‘Holy Grail’ of superconductivity: room-temperature superconductors
- 1968 – N. Ashcroft, suggestion that hydrogen @ high pressure (in metallic form) may be a high-temperature superconductor. Small mass+pressure = high Debye temperature of 3500 K may give high Tc

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)

$$\boxed{k_B T_c = 1.13\hbar\omega_D e^{-1/VN(E_F)}}$$

- high-temperature superconductors “cuprates”, first discovered in 1986 by Bednorz and Muller, have a record Tc of 138 K in (Hg0.8Tl0.2)Ba2Ca2Cu3O8.33 at ambient pressure and 164 K @ 30 GPa in $HgBa2Ca_{m-1}Cu_mO_{2m+2+\delta}$
- HTC – not the electron-phonon coupling mechanism. Commonly accepted theory is not yet formulated. These are strongly correlated materials with strong electronic interactions

Hydrogenated high-temperature superconductors

- 2015 – discovery of superconductivity in H2S/H3S under extreme pressure

LETTER

doi:10.1038/nature14964

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

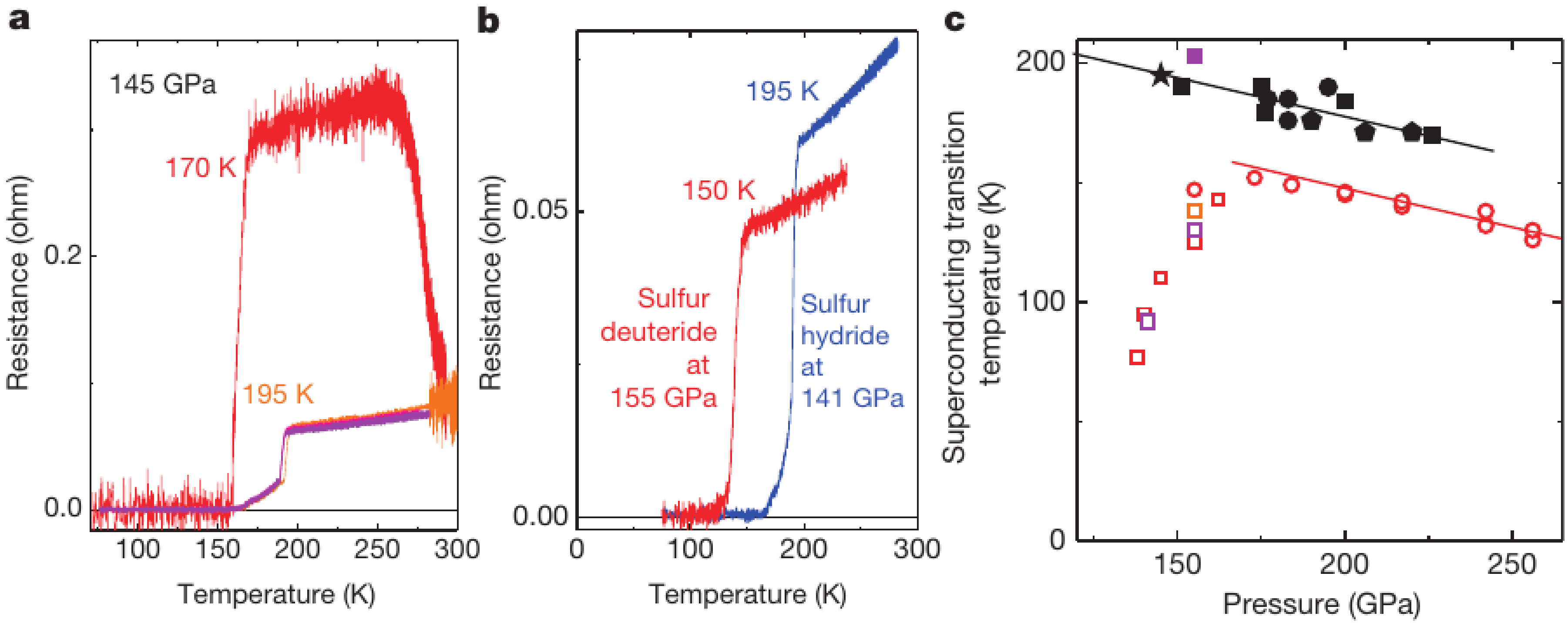
A. P. Drozdov[1]*, M. I. Eremets[1]*, I. A. Troyan[1], V. Ksenofontov[2] & S. I. Shylin[2]

of 17 kelvin has been observed experimentally[8]. Here we investigate sulfur hydride[9], where a T_c of 80 kelvin has been predicted[10]. 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

- 203 K @ 150 GPa (1GPa ~ 10 000 atm)
- Electron-phonon coupling and Eliashberg theory comes back!
- Predictions based on first-principles calculations were behind this discovery

Hydrogenated high-temperature superconductors

- 2015 – discovery of superconductivity in H2S/H3S under extreme pressure



- 2015 – explanation using Eliashberg theory and first-principles calculations

PRL **114**, 157004 (2015) PHYSICAL REVIEW LETTERS week ending 17 APRIL 2015

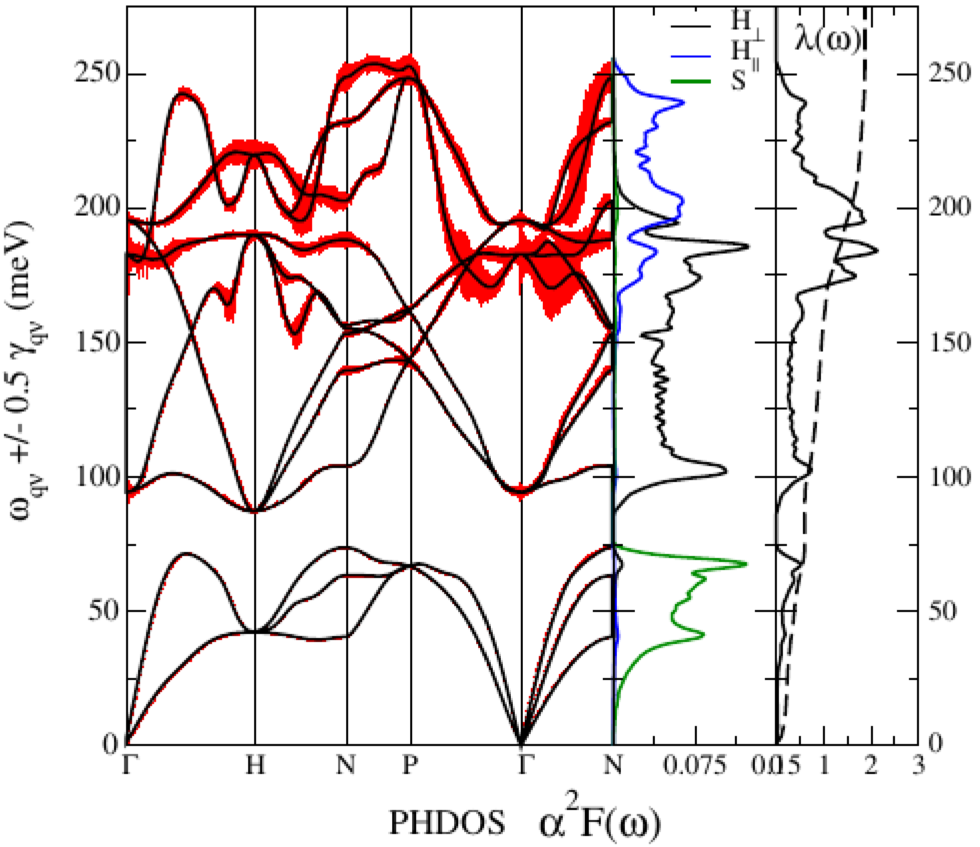
High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor

Ion Errea,[1,2] Matteo Calandra,[3,*] Chris J. Pickard,[4] Joseph Nelson,[5] Richard J. Needs,[5] Yinwei Li,[6] Hanyu Liu,[7] Yunwei Zhang,[8] Yanming Ma,[8] and Francesco Mauri[3]

TABLE II. Electron-phonon interaction and logarithmic averages of phonon frequencies, with and without anharmonic effects. The T_c's are calculated using the isotropic Migdal-Eliashberg equations (T_c^{ME}). A value of $\mu^* = 0.16$ is used. Data for T_c calculated with the McMillan equation are provided in the Supplemental Material [30]. Frequencies are in meV and T_c's are in K.

Compound	λ^{har}	$\omega_{\mathrm{log}}^{\mathrm{har}}$	λ^{anh}	$\omega_{\mathrm{log}}^{\mathrm{anh}}$	$T_c^{\mathrm{ME,har}}$	$T_c^{\mathrm{ME,anh}}$	T_c (expt.)
H_3S (200 GPa)	2.64	90.4	1.84	92.86	250	194.0	190
H_3S (250 GPa)	1.96	109.1	1.71	101.3	226	190	
D_3S (200 GPa)	2.64	68.5	1.87	73.3	183	152.0	90

- 2015 – explanation using Eliashberg theory and first-principles calculations



Hydrogenated high-temperature superconductors

- since 2015 – search for high-pressure high-temperature superconductors: both experimental and based on calculations
- 2019 – LaH10 (experiment after calculations) Tc = 250 K @ 170 Gpa (only -23 C !)

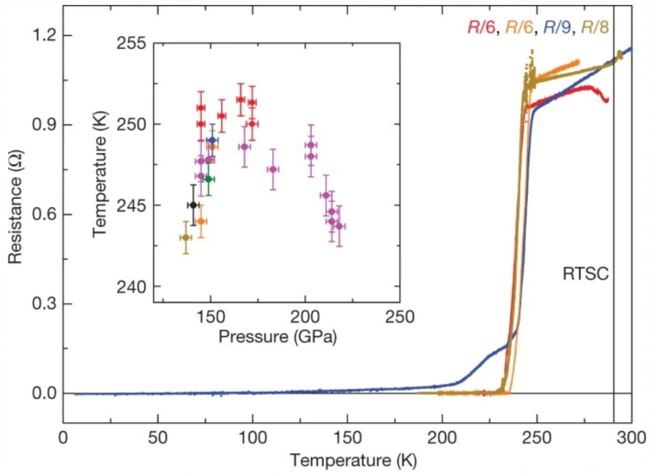
Letter | Published: 22 May 2019

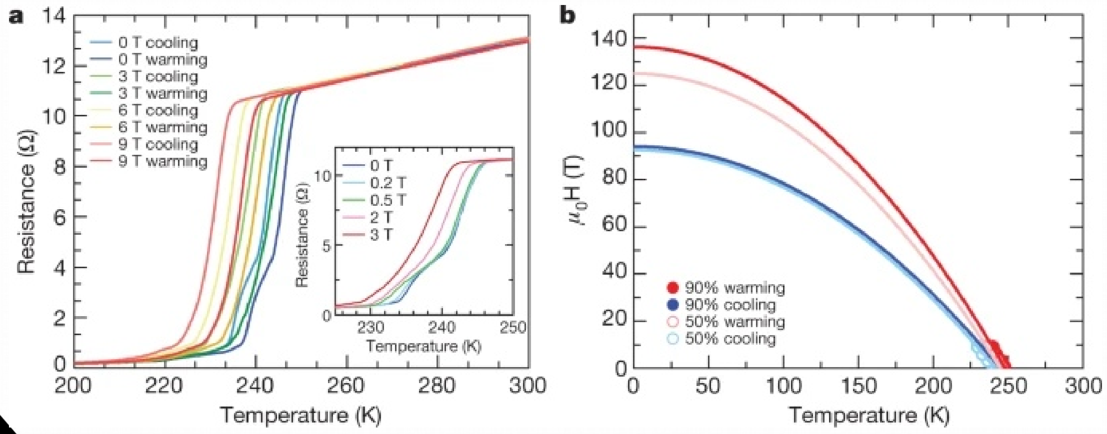
Superconductivity at 250 K in lanthanum hydride under high pressures

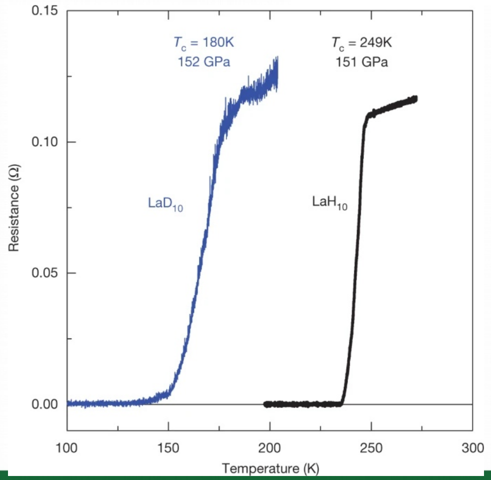
A. P. Drozdov, P. P. Kong, V. S. Minkov, S. P. Besedin, M. A. Kuzovnikov, S. Mozaffari, L. Balicas, F. F. Balakirev, D. E. Graf, V. B. Prakapenka, E. Greenberg, D. A. Knyazev, M. Tkacz & M. I. Eremets

Nature **569**, 528–531 (2019) | Cite this article

62k Accesses | **1458** Citations | **637** Altmetric | Metrics







Hydrogenated high-temperature superconductors

- since 2015 – search for high-pressure high-temperature superconductors: both experimental and based on calculations
- 2019 – LaH10 (experiment after calculations) Tc = 250 K @ 170 Gpa (only -23 C !)
- 2020 - carbonaceous sulfur hydride Tc = 287 K @ 267 Gpa. **Retracted**

Article | Published: 14 October 2020

RETRACTED ARTICLE: Room-temperature superconductivity in a carbonaceous sulfur hydride

Elliot Snider, Nathan Dasenbrock-Gammon, Raymond McBride, Mathew Debessai, Hiranya Vindana, Kevin Vencatasamy, Keith V. Lawler, Ashkan Salamat & Ranga P. Dias

- 2023 – N-doped lutetium hydride Tc = 294 K at 10 kbar (“only” 1 Gpa!) **Retracted**

Article | Published: 08 March 2023

RETRACTED ARTICLE: Evidence of near-ambient superconductivity in a N-doped lutetium hydride

Nathan Dasenbrock-Gammon, Elliot Snider, Raymond McBride, Hiranya Pasan, Dylan Durkee, Nugzari Khalvashi-Sutter, Sasanka Munasinghe, Sachith E. Dissanayake, Keith V. Lawler, Ashkan Salamat & Ranga P. Dias

This article was retracted on 07 November 2023

Hydrogenated high-temperature superconductors

- 2023 – “LK99” - claim of superconductivity with Tc ~ 400 K at ambient pressure

arXiv > cond-mat > arXiv:2307.12008

Search...

Help | Adva

Condensed Matter > Superconductivity

[Submitted on 22 Jul 2023]

The First Room-Temperature Ambient-Pressure Superconductor

Sukbae Lee, Ji-Hoon Kim, Young-Wan Kwon

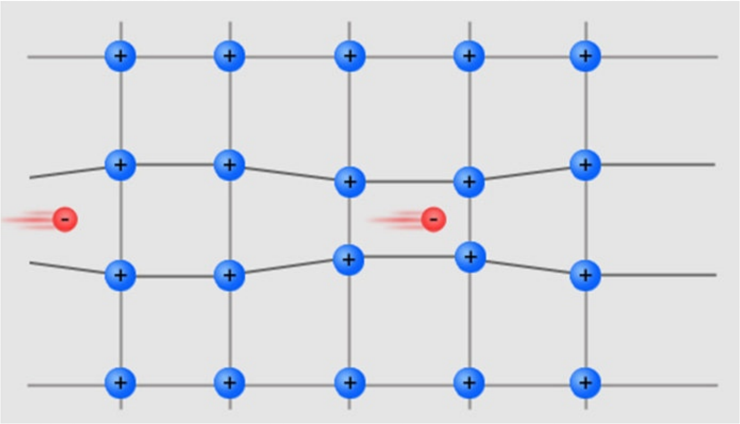
For the first time in the world, we succeeded in synthesizing the room-temperature superconductor ($T_c \geq 400$ K, 127 °C) working at ambient pressure with a modified lead-apatite (LK-99) structure. The superconductivity of LK-99 is proved with the Critical temperature (T_c), Zero-resistivity, Critical current (I_c), Critical magnetic field (H_c), and the Meissner effect. The superconductivity of LK-99 originates from minute structural distortion by a slight volume shrinkage (0.48 %), not by external factors such as temperature and pressure. The shrinkage is caused by Cu^{2+} substitution of Pb^{2+}(2) ions in the insulating network of Pb(2)-phosphate and it generates the stress. It concurrently transfers to Pb(1) of the cylindrical column resulting in distortion of the cylindrical column interface, which creates superconducting quantum wells (SQWs) in the interface. The heat capacity results indicated that the new model is suitable for explaining the superconductivity of LK-99. The unique structure of LK-99 that allows the minute distorted structure to be maintained in the interfaces is the most important factor that LK-99 maintains and exhibits superconductivity at room temperatures and ambient pressure.

- Unfortunately not confirmed by other experiments and theory

Summary

- Cooper pairs are formed in all superconductors
- Pairing mechanism in ‘classical’ superconductors is the electron-phonon interaction

- BCS theory explains superconductivity in case of el-ph coupling
- Eliashberg theory takes into account frequency-dependent and retarded nature of el-ph interaction and agrees quantitatively with experiment
- Anisotropy of interaction can be also taken into account
- high-temperature superconductors (cuprates) – pairing due to electronic correlations, no unified theory
- high-temperature-high pressure hydrites – pairing by phonons with Tc approaching the room temperature



what’s wrong in this picture?