

V Escuela de Superconductividad

México, 27 noviembre 2021

Superconductividad en el MgB_2 : a 20 años del descubrimiento

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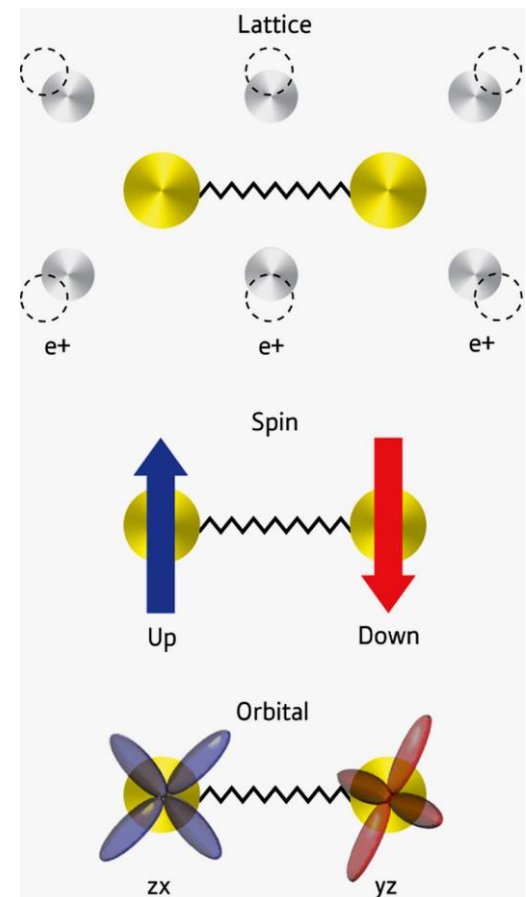


Funding: Conacyt-México
Grant No. 83604



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 - Two-gaps superconductivity.
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 - New materiales based on MgB_2 .



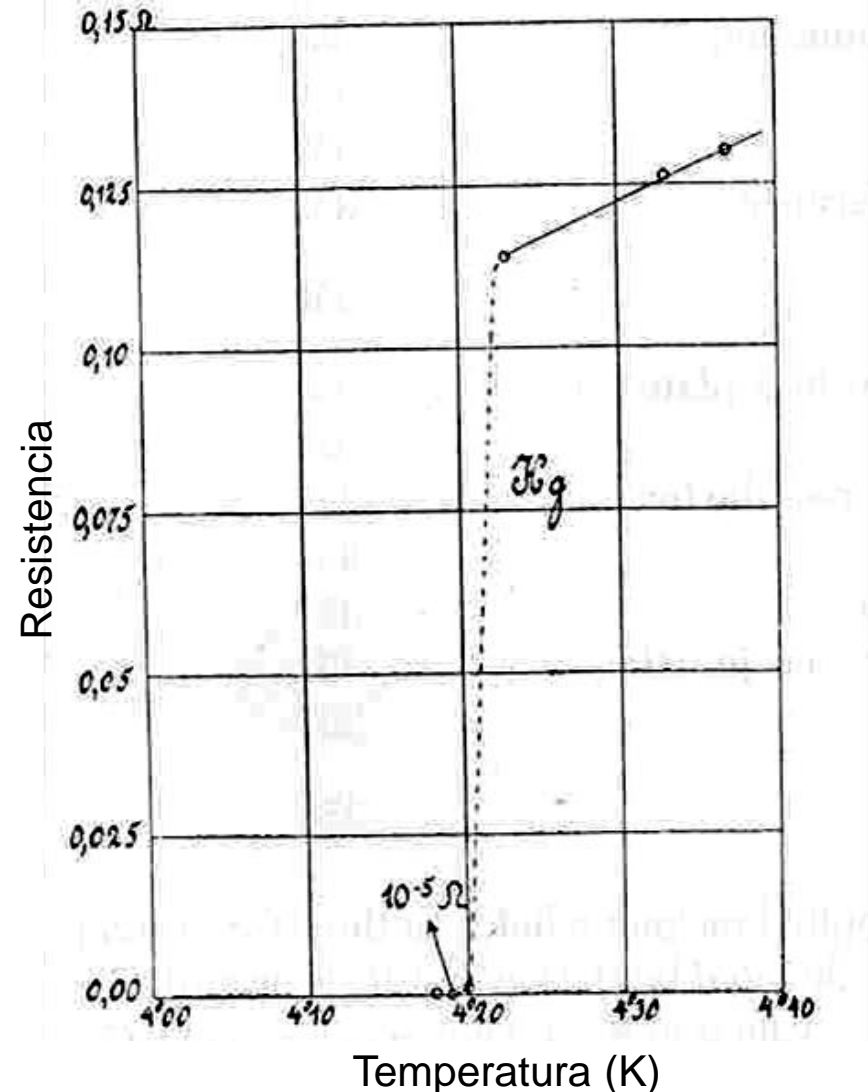
Descubrimiento de la superconductividad (1911)



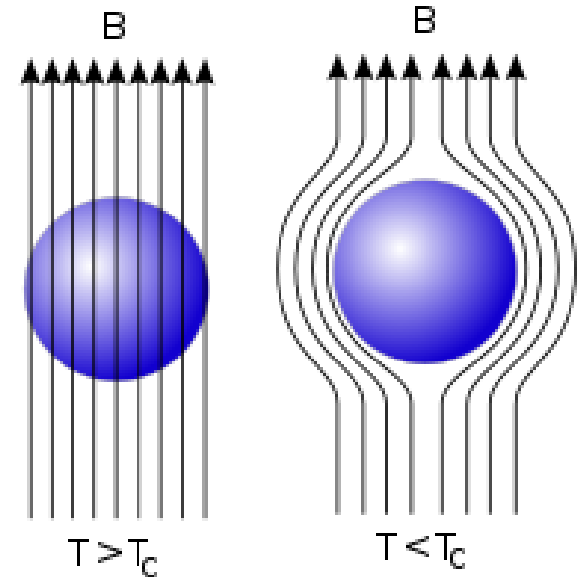
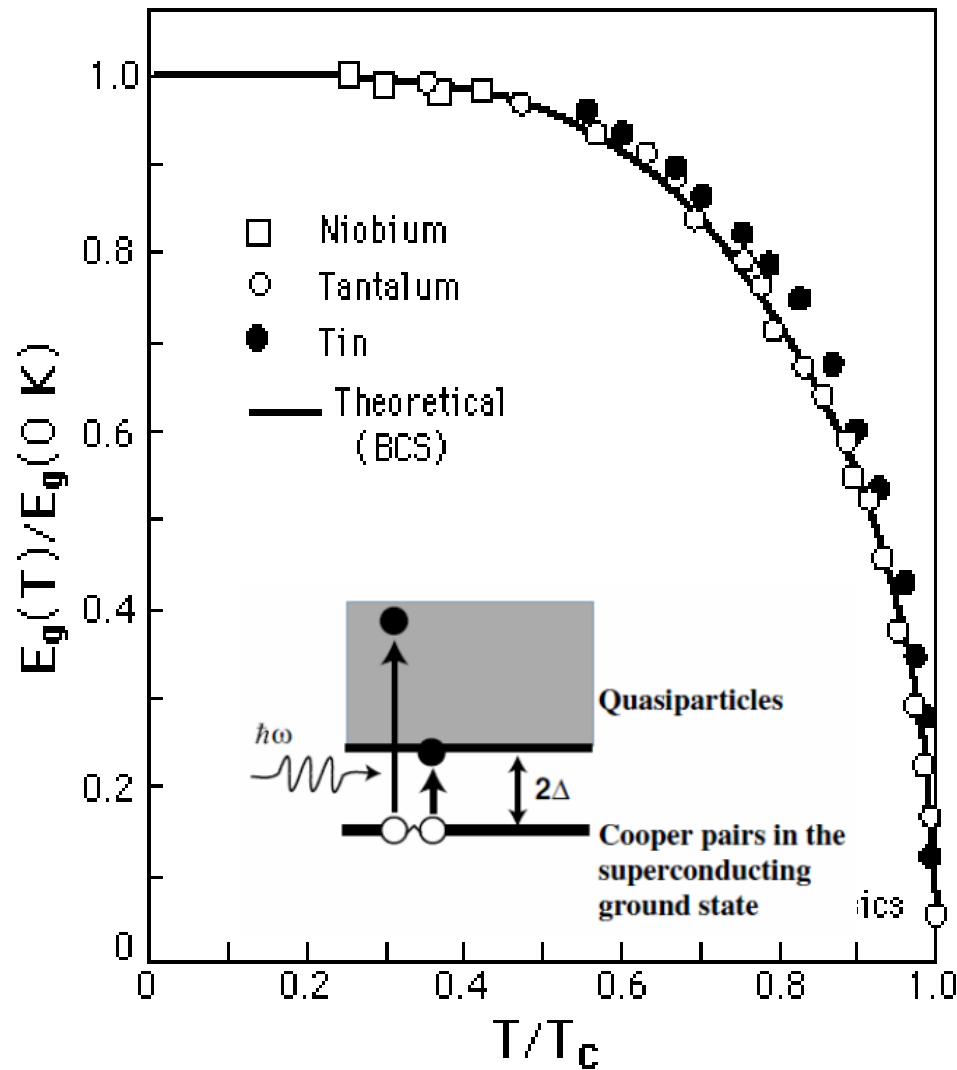
Resistencia eléctrica nula!!!

En 1911 Kamerling Onnes descubre que a la temperatura de 4.2 K el mercurio (Hg) pierde su resistencia eléctrica, a este fenómeno se denominó **superconductividad**.

Un material superconductor es mucho mas que un conductor perfecto.

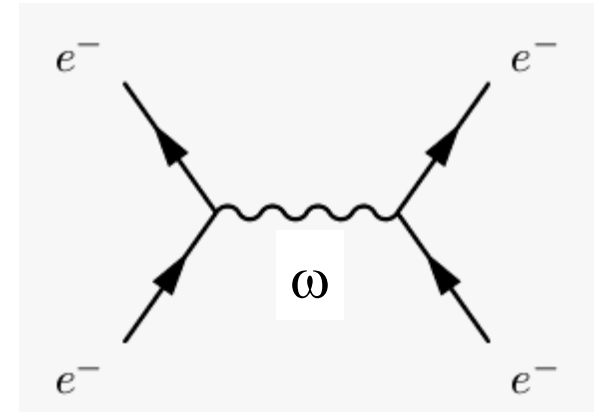


Brecha superconductor y Efecto Meissner



BCS Theory: electron-phonon interaction (1957)

BCS: Bardeen, Cooper and Schrieffer

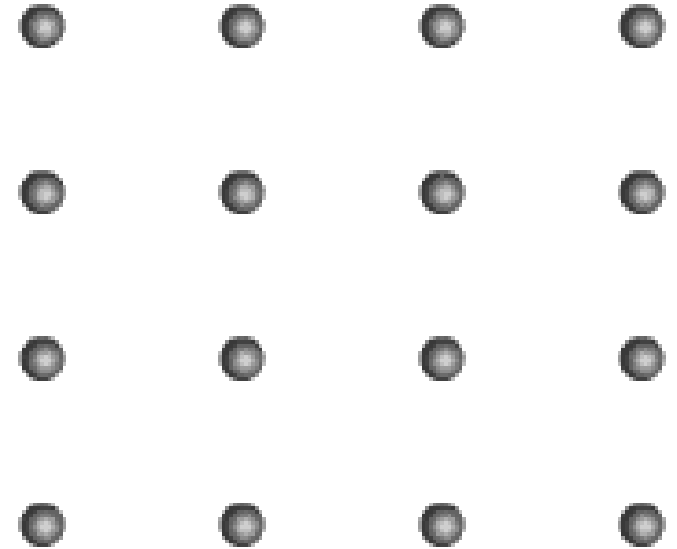


The Nobel Prize in Physics 1972

John Bardeen, Leon N. Cooper, Robert Schrieffer

The first widely-accepted theoretical understanding of superconductivity was advanced in 1957 by American physicists John Bardeen, Leon Cooper, and John Schrieffer (above). Their *Theories of Superconductivity* became known as the **BCS Theory**.

<https://www.nobelprize.org>



John Bardeen - Nobel Lecture 1972

ELECTRON-PHONON INTERACTIONS AND SUPERCONDUCTIVITY

Nobel Lecture, December 11, 1972

By JOHN BARDEEN

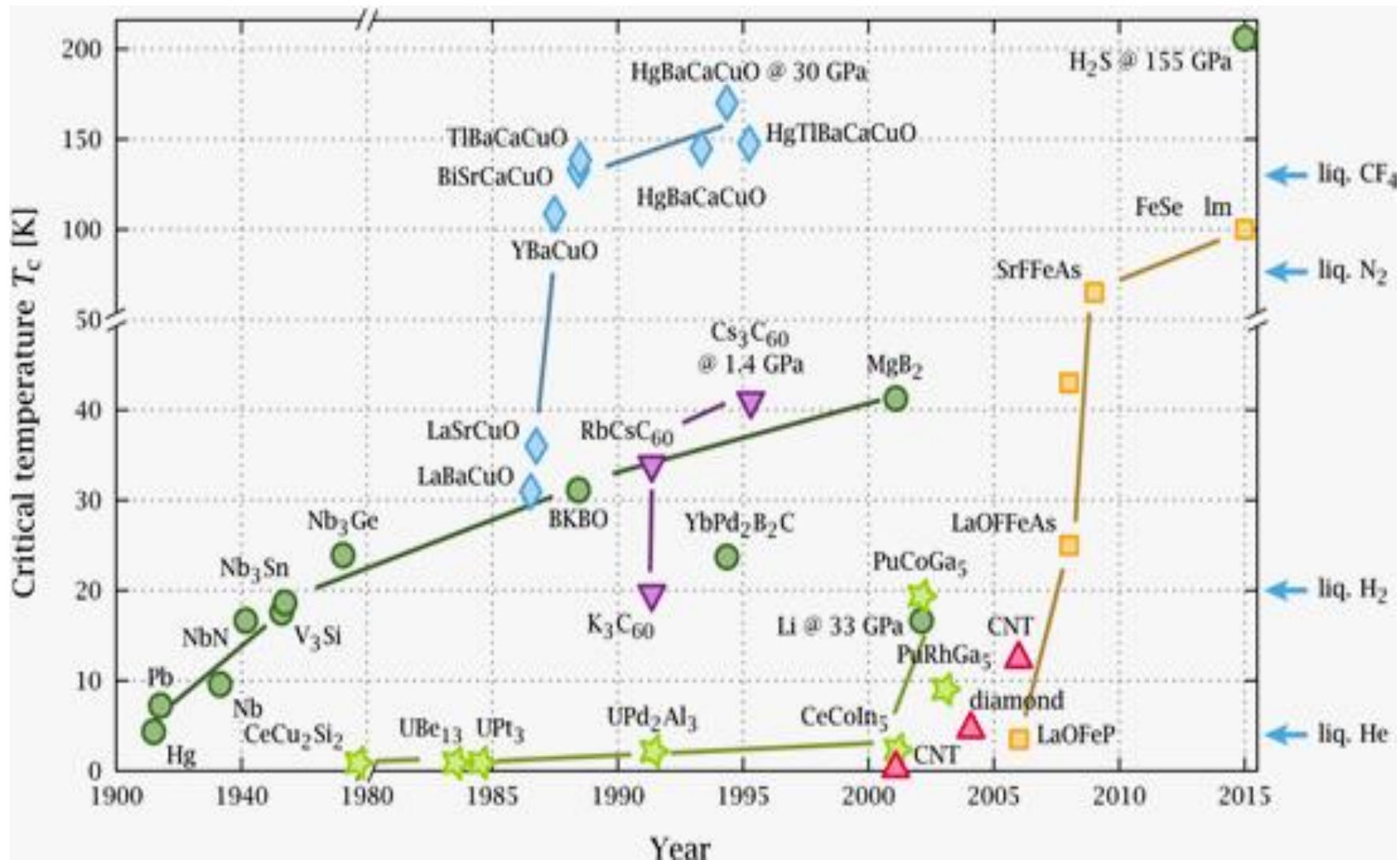
CONCLUSIONS

In this talk we have traced how our understanding of the role of **electron-phonon** interactions in superconductivity has developed from a concept to a precise quantitative theory.

All evidence indicates that the electron-phonon interaction is the dominant mechanism in the cases studied so far, which include many simple metals, transition metals, a rare earth, and various alloys and compounds. Except possibly for the metallic form of hydrogen, [35] which is presumed to exist at very high pressures, it is unlikely that the phonon mechanism will yield substantially higher transition temperatures than the present maximum of about 21 K for a compound of Nb, Al and Ge.

https://www.nobelprize.org/nobel_prizes/physics/laureates/1972/bardeen-lecture.html

Introduction: superconducting materials and T_c



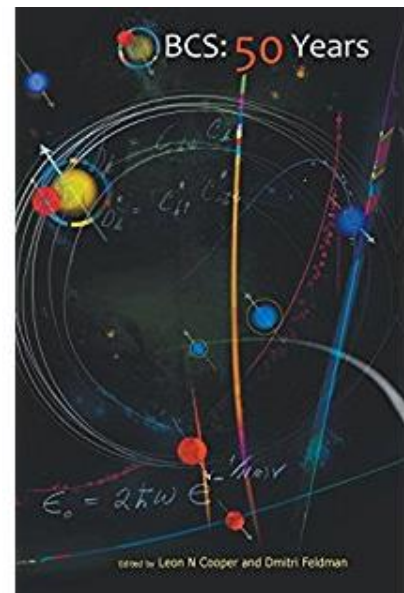
Introduction: Classes of Superconductors

- 1. BCS or Conventional:** Electron pairing induced by electron-phonon interactions. Experiments explained.

Materials: conventional metals, C60, some organics, doped semiconductors, MgB₂, hydrides

- 2. Exotic or Unconventional:** Many theories on the electron pairing, but no consensus on the mechanism.

Materials: cooper oxides, heavy fermion metals, some organics, dicalcogenides, (Fe,Ni) oxypnictides, FeSe,



Descrubrimiento de SC en el MgB_2

Superconductivity at 39 K in magnesium diboride

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Yuji Zenitani* & Jun Akimitsu*†

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0012, Japan

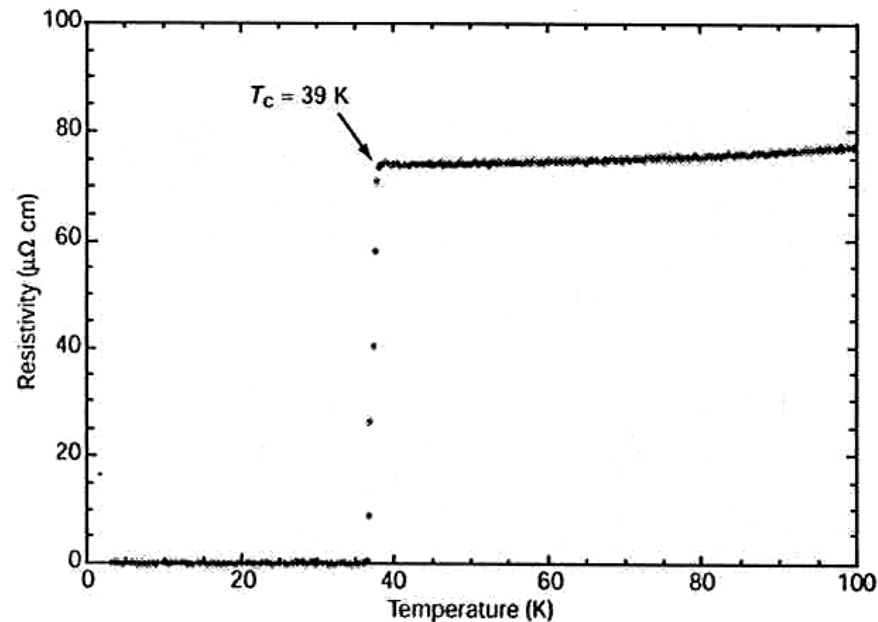
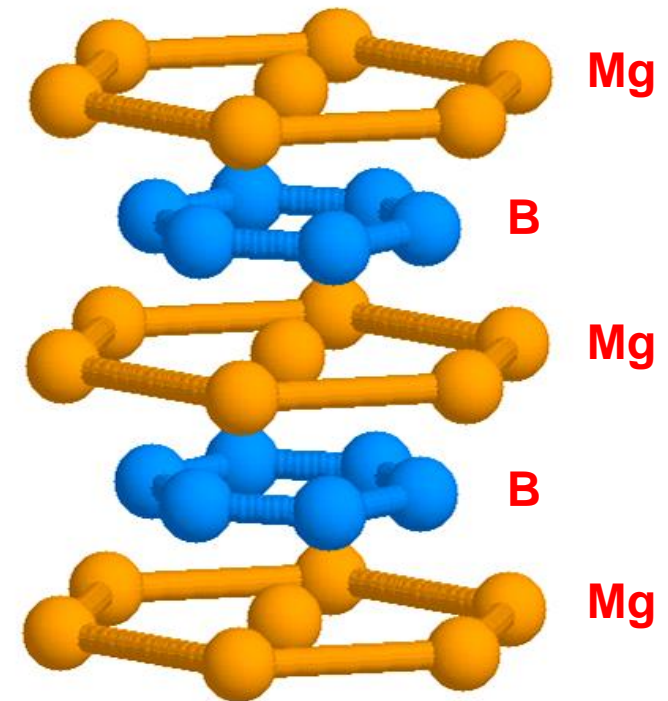


Figure 4 Temperature dependence of the resistivity of MgB_2 under zero magnetic field.

Nature **40**, 63 (1 march 2001).



Crystal Structure of MgB_2
Space group P6/mmm (no. 191)
 AlB_2 (ω phase)

MgB₂: magnesium diboride



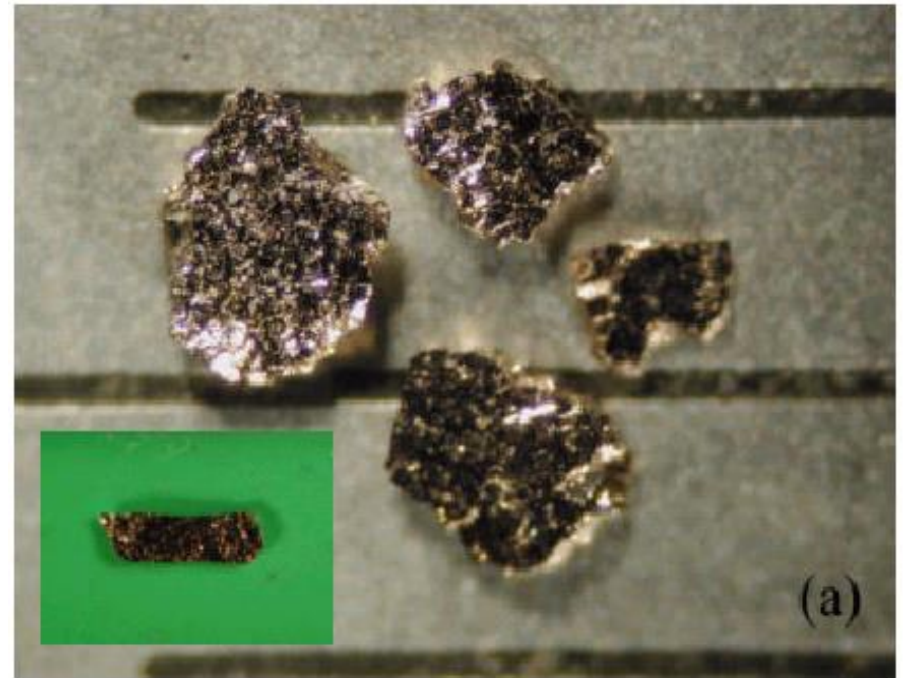
The compound MgB₂ has been known since 1953 !!!



Samples: crystals of Al and C-doped MgB_2



J. Karpinski et al.,
Cond-mat/ 0304658 (2003).



S. Lee et al.,
Cond-mat/ 0305485 (2003).

MgB₂: electronic and vibrational properties

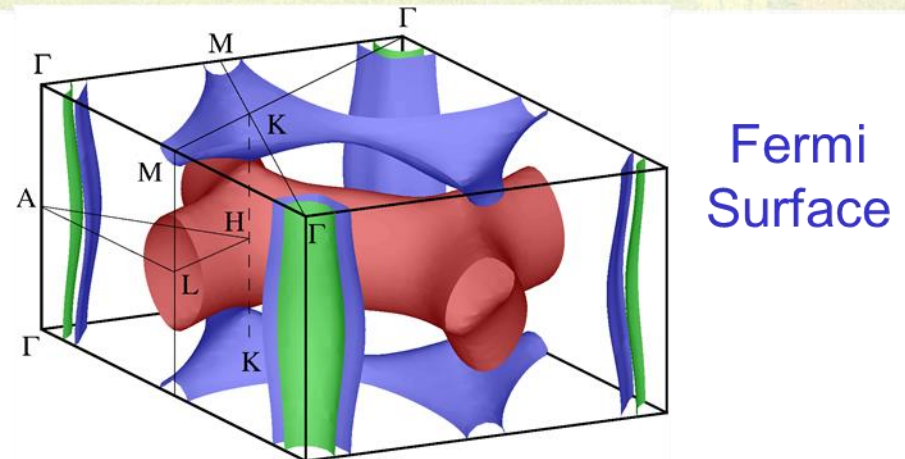
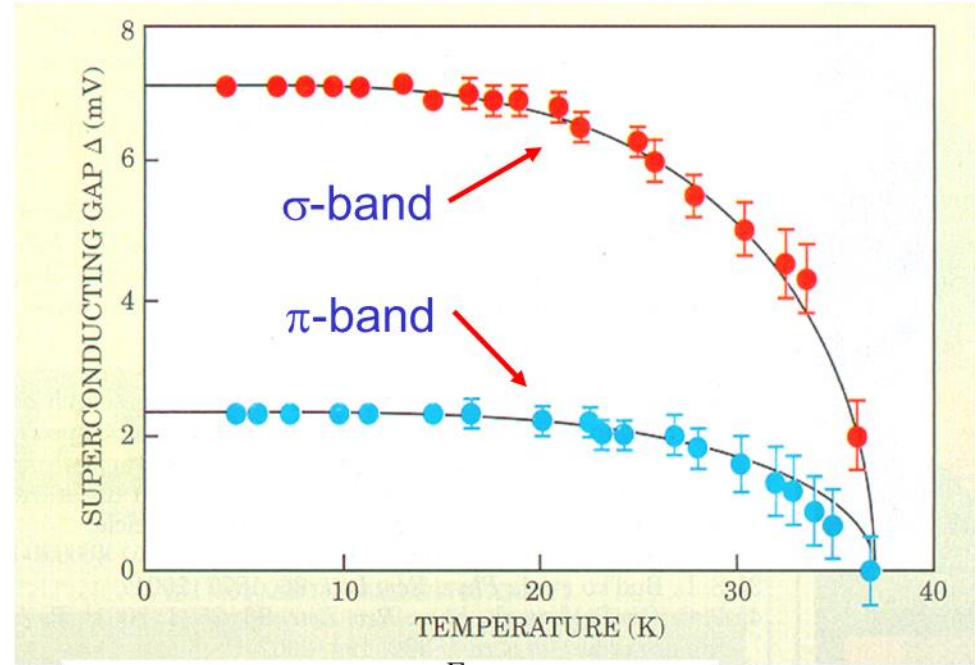
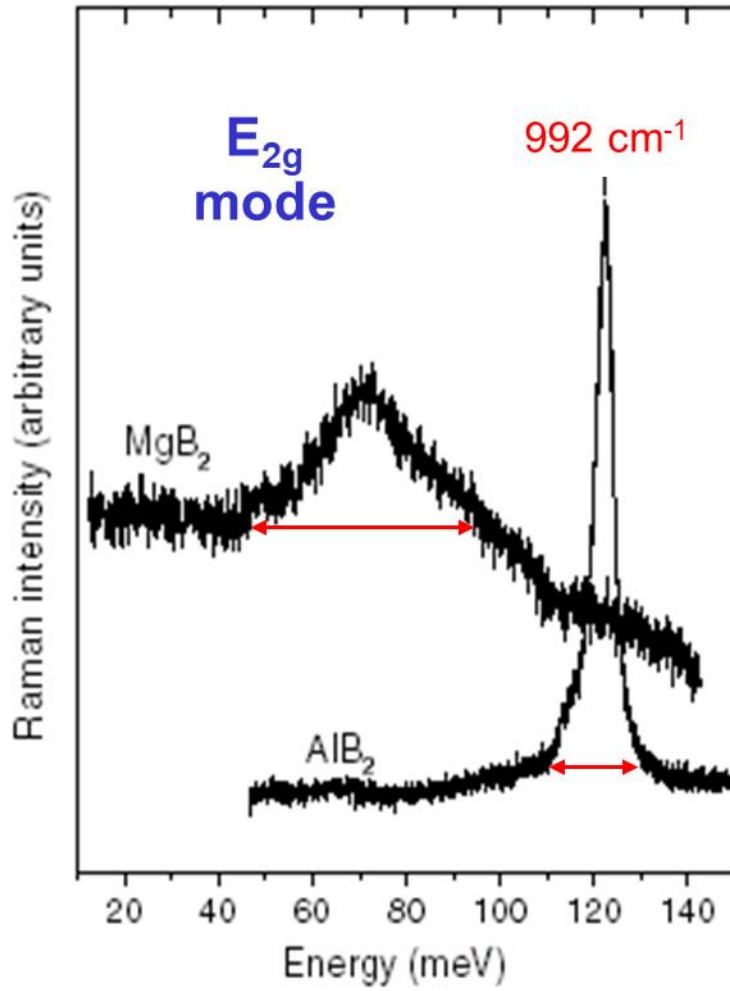
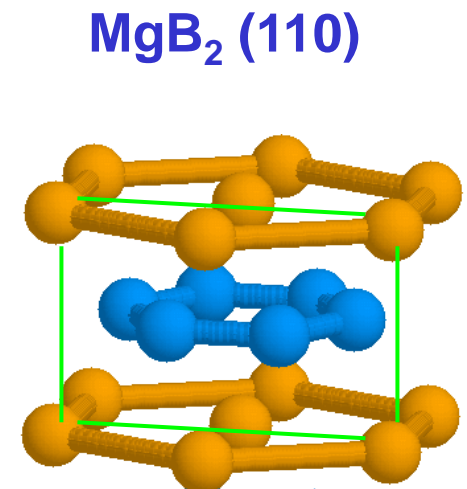
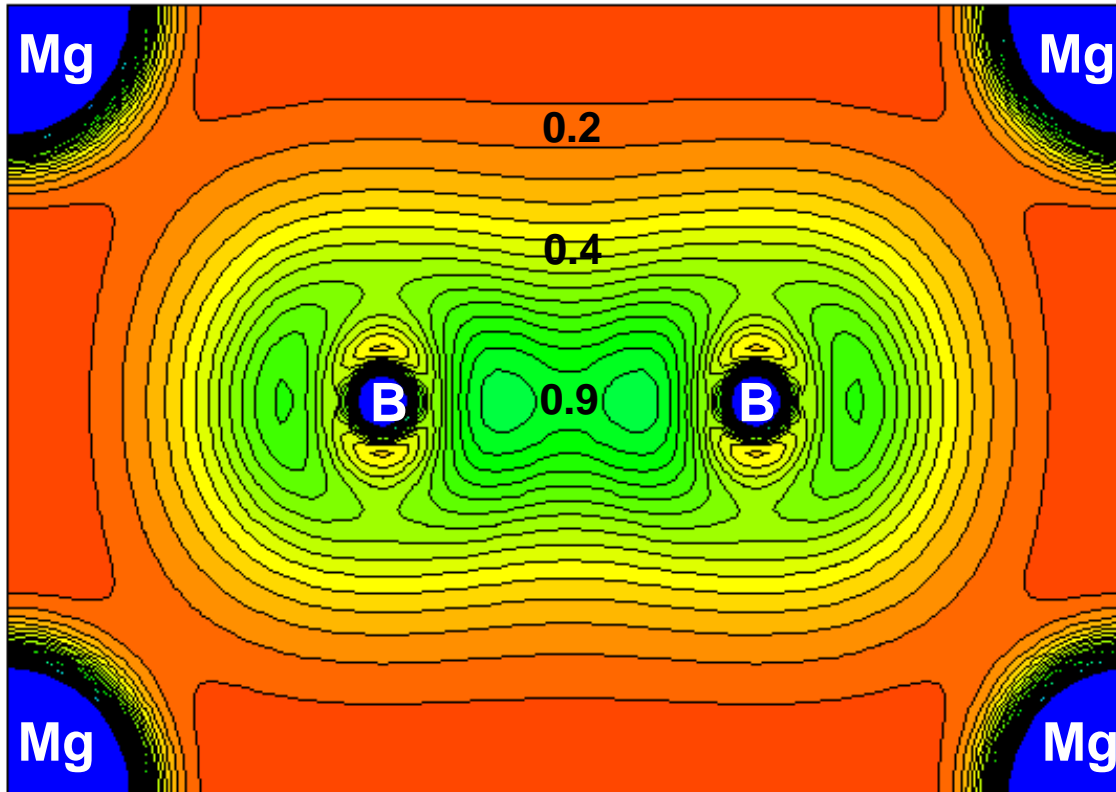


FIG. 1. Micro-Raman spectra obtained from polycrystalline grains of MgB₂ and AlB₂ at room temperature ($\lambda = 514.5$ nm).

MgB₂: enlace químico

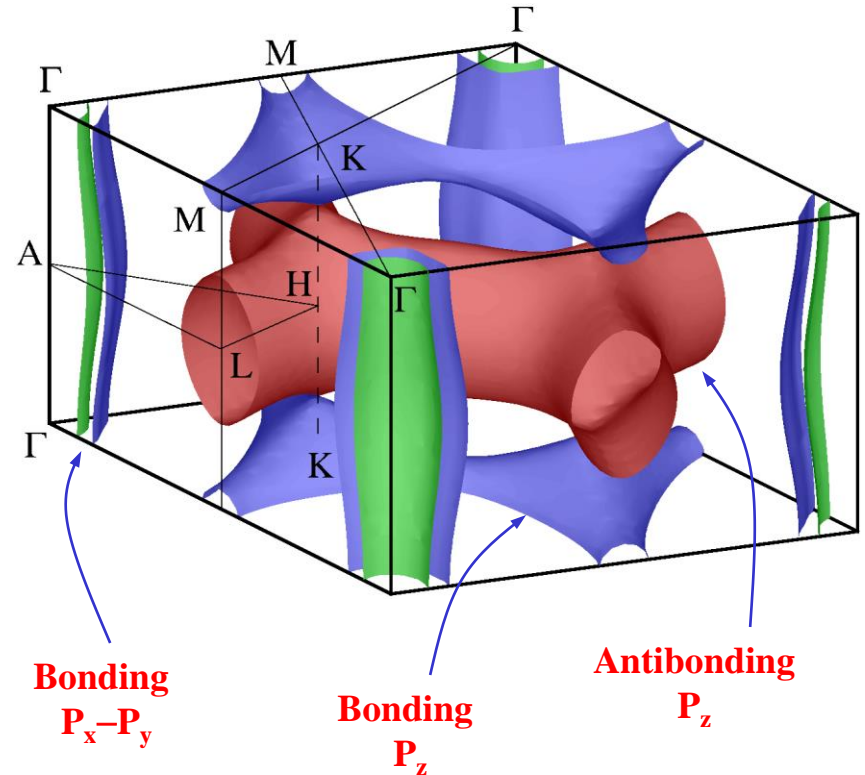
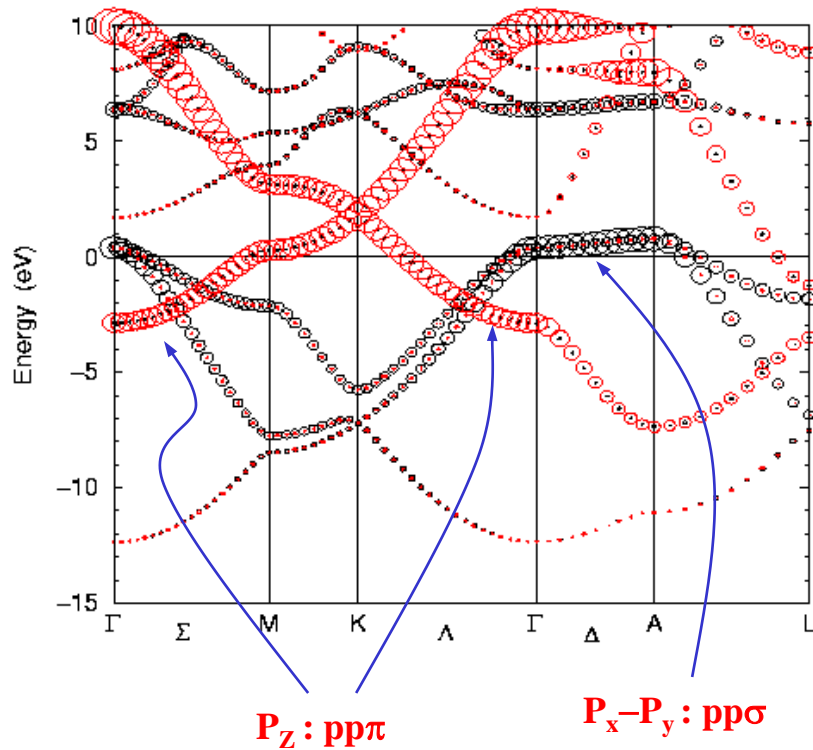


$$\Delta\rho=0.05 \text{ e}/\text{\AA}^3$$

A. Aguayo and R. de Coss (april 2001)
Cinvestav-Mérida, México.

MgB₂: estructura electrónica

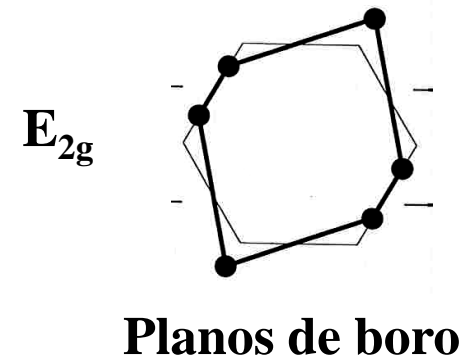
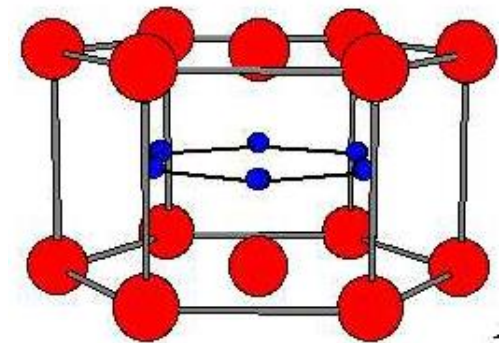
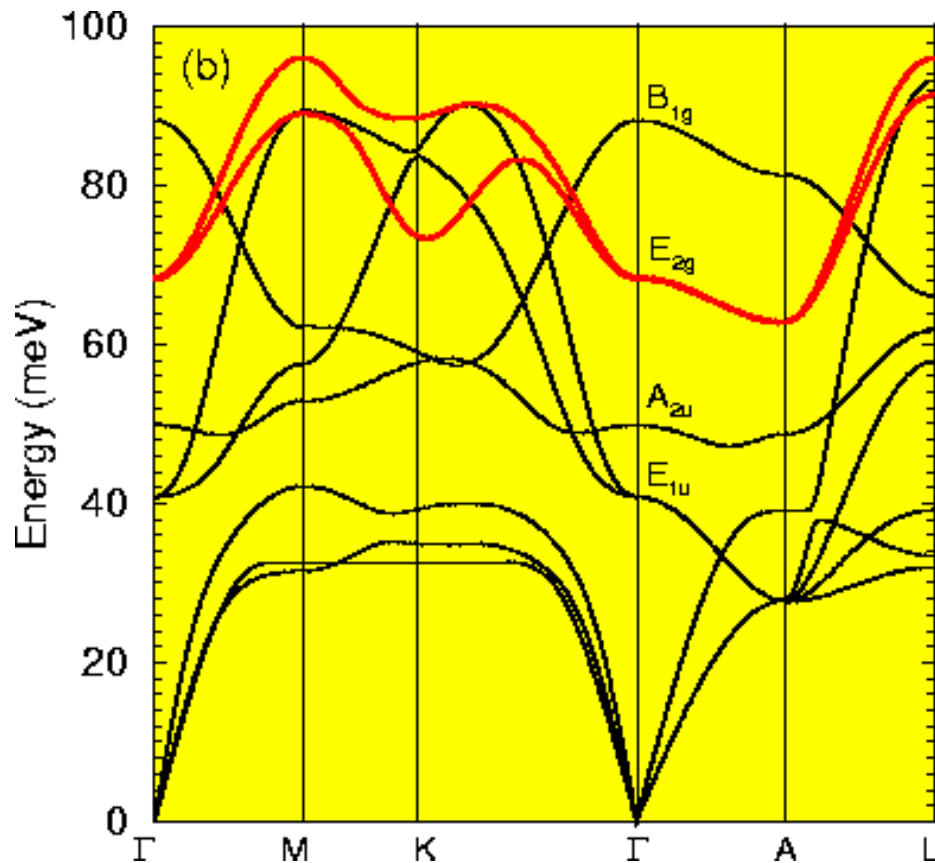
Band structure and Fermi surface of MgB₂ (FP-LAPW)



L. Kortus et al. *Phys. Rev. Lett.* **86**, 4656 (2001).

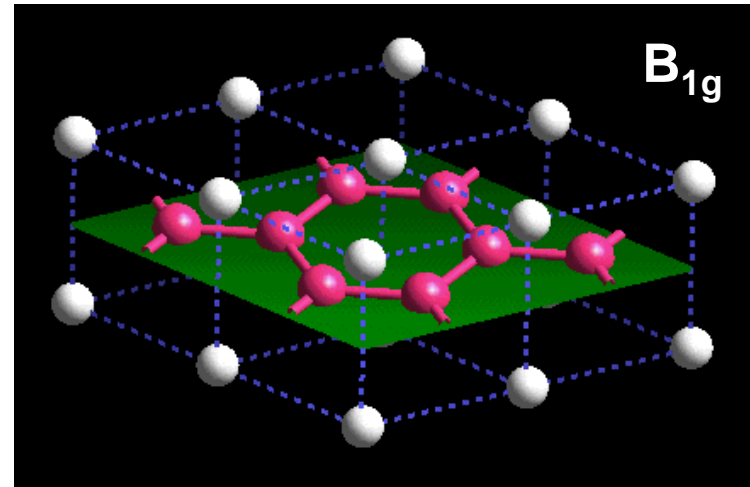
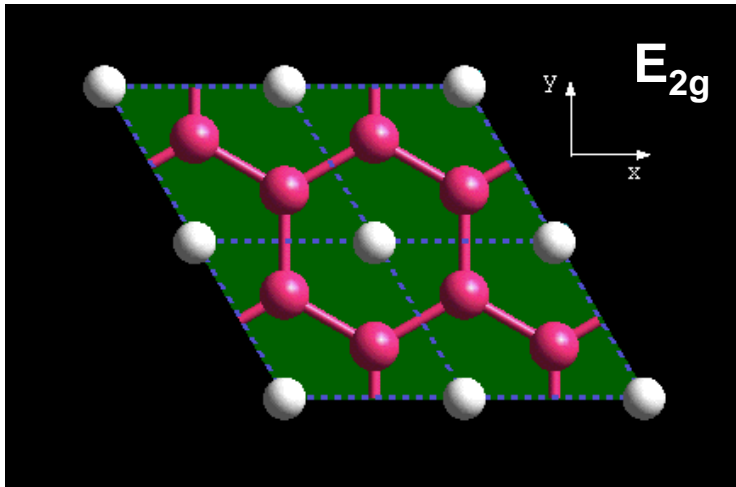
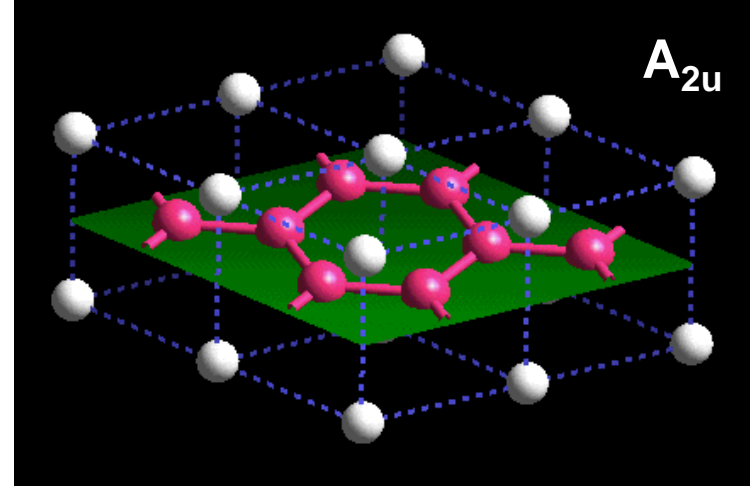
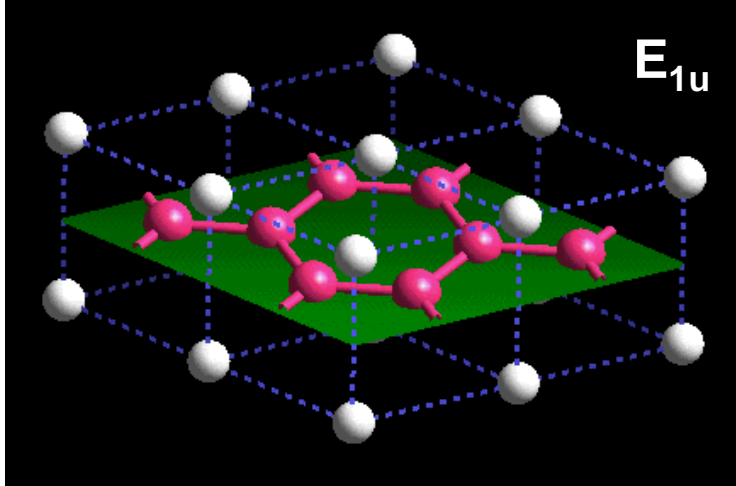
MgB₂: propiedades vibracionales

Estructura de bandas fonónicas calculadas: pseudopotenciales.



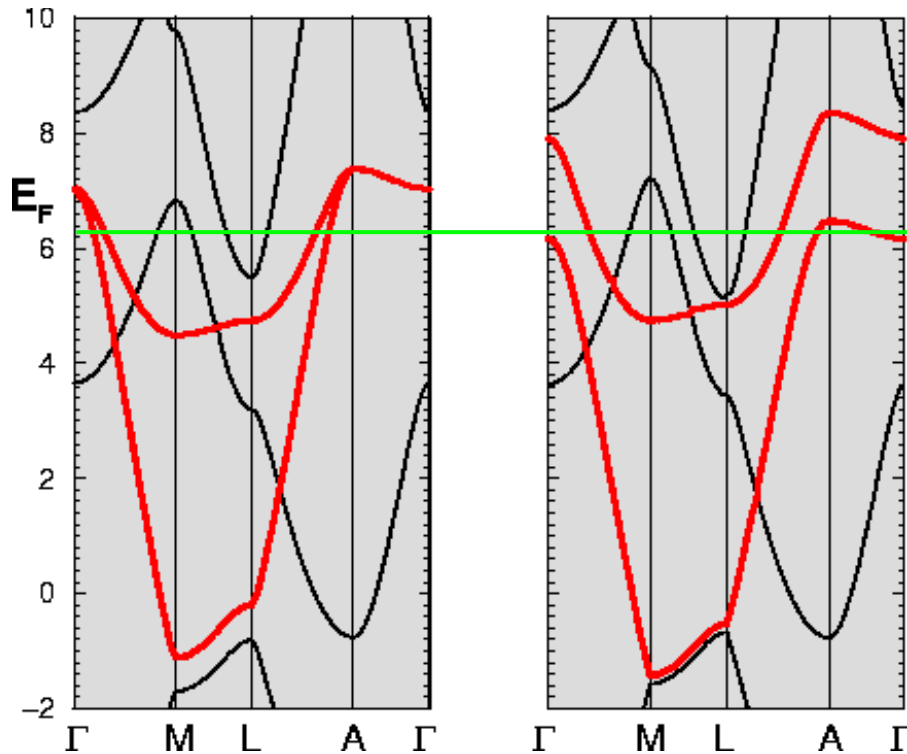
T. Yildirim et al., Phys. Rev. Lett. **87**, 37001 (2001).

MgB₂: modos vibracionales

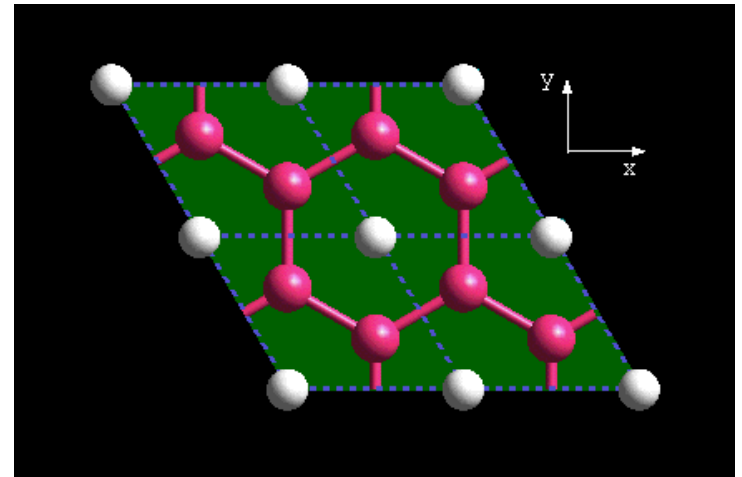


MgB₂: acoplamiento e-ph

Acoplamiento del modo E_{2g} con las bandas p_x-p_y

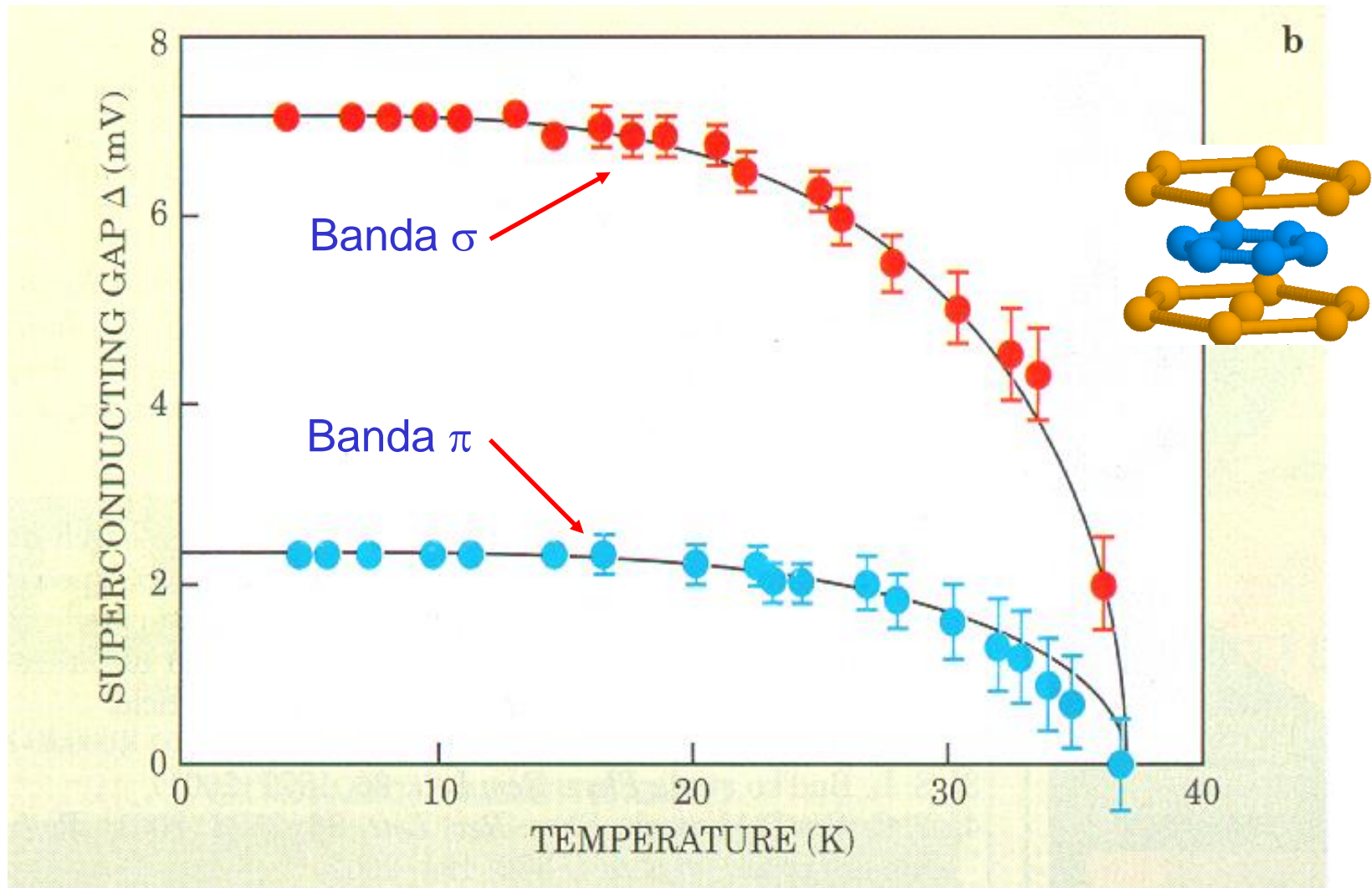


Modo E_{2g}



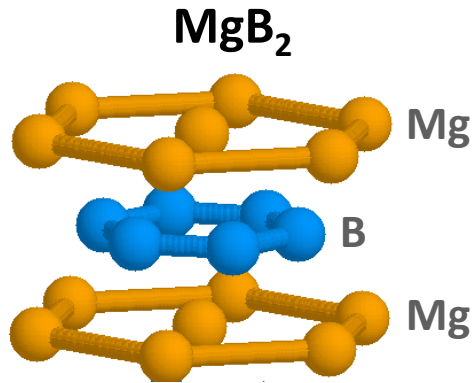
T. Yildirim et al., Phys. Rev. Lett. 87, 37001 (2001).
Home Page: <http://www.ncnr.nist.gov/staff/taner/mgb2/>

MgB₂: dos brechas superconductoras!!!

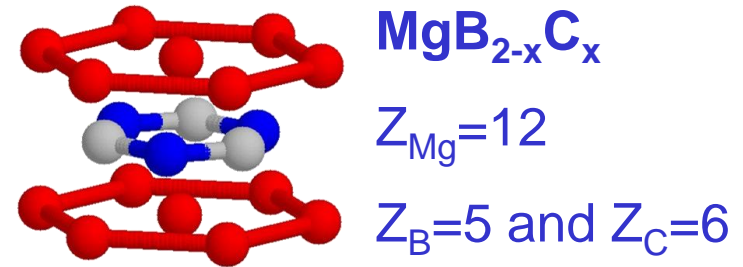
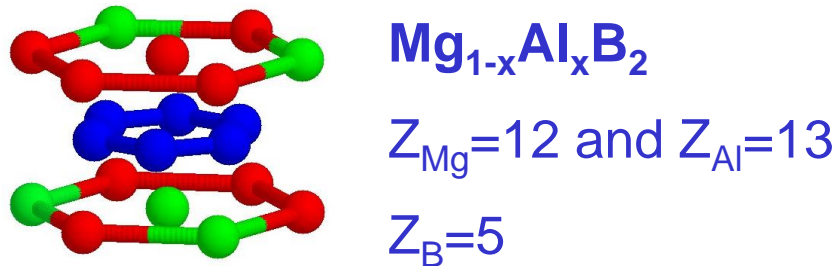


P.C. Canfield and G.W. Crabtree. *Physics Today* **56**, 34 (2003).

Our contributions: MgB₂ superconducting alloys



- Physical Review B **66**, 012511 (2002).
- Physical Review B **79**, 134523 (2009).
- Physical Review B **81**, 054519 (2010).
- Physical Review B **82**, 224508 (2010).
- Physics Procedia **36**, 479 (2012).



- ✓ **MgB₂ doped with Al and C:** We found that Al- and C-doping reduce drastically the DOS at the Fermi level and induce a strong phonon renormalization, producing a drop of T_c. In particular, we predict the loss of superconductivity for x(Al)=0.56, which was confirmed by experiments.



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Universidad Autónoma de Puebla



Dr. Rolf Heid
Karlsruhe Institute of Technology
Germany



Dr. Klaus-Peter Bohnen
Karlsruhe Institute of Technology
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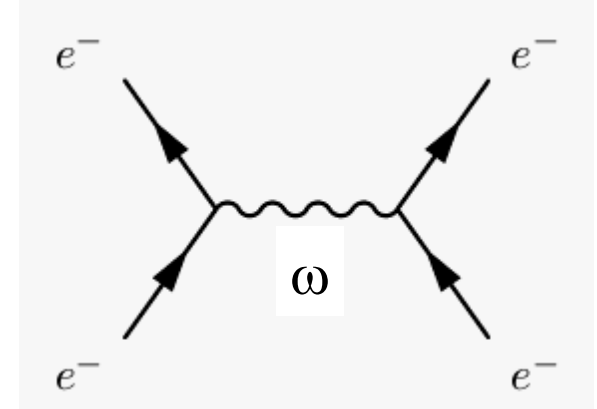


Predicting New Solids and Superconductors

Función isotrópica de Eliashberg

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(0)} \sum_{\mathbf{q}\lambda} \frac{\gamma_{\mathbf{q}\lambda}}{\omega_{\mathbf{q}\lambda}} \delta(\omega - \omega_{\mathbf{q}\lambda})$$

$\omega_{\mathbf{q}\lambda}$: frec. del modo fonónico ($\mathbf{q}\lambda$)



Ancho de línea del fonón

$$\gamma_{\mathbf{q}\lambda} = 2\pi\omega_{\mathbf{q}\lambda} \sum_{\mathbf{k}\nu\nu'} \left| g_{\mathbf{k}+\mathbf{q}\nu', \mathbf{k}\nu}^{\mathbf{q}\lambda} \right|^2 \delta(\epsilon_{\mathbf{k}\nu} - \epsilon_F) \delta(\epsilon_{\mathbf{k}+\mathbf{q}\nu'} - \epsilon_F)$$

Fórmula de Allen-Dynes: $T_c = \frac{\omega_{log}}{1.2} \exp\left(\frac{-1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)}\right)$

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

$$\omega_{log} = \exp\left(\frac{2}{\lambda} \int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} \ln(\omega)\right)$$

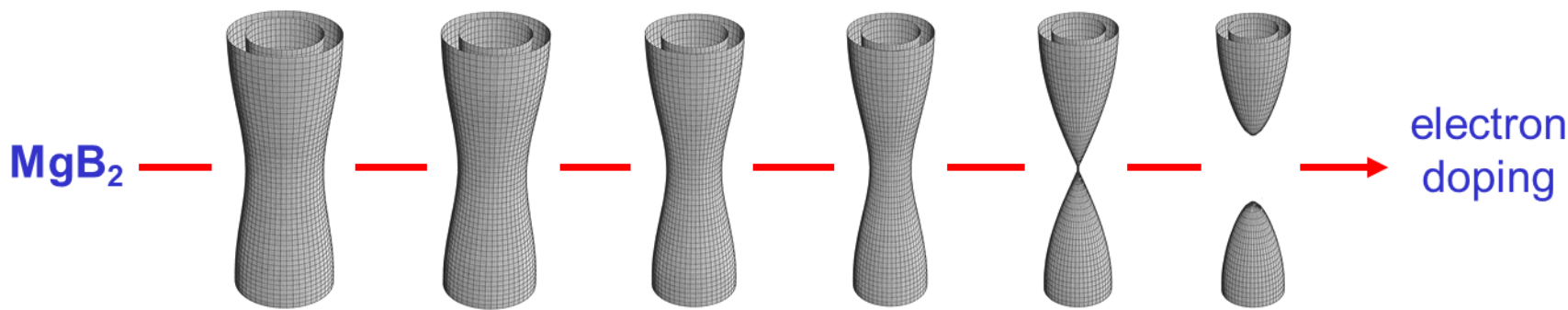
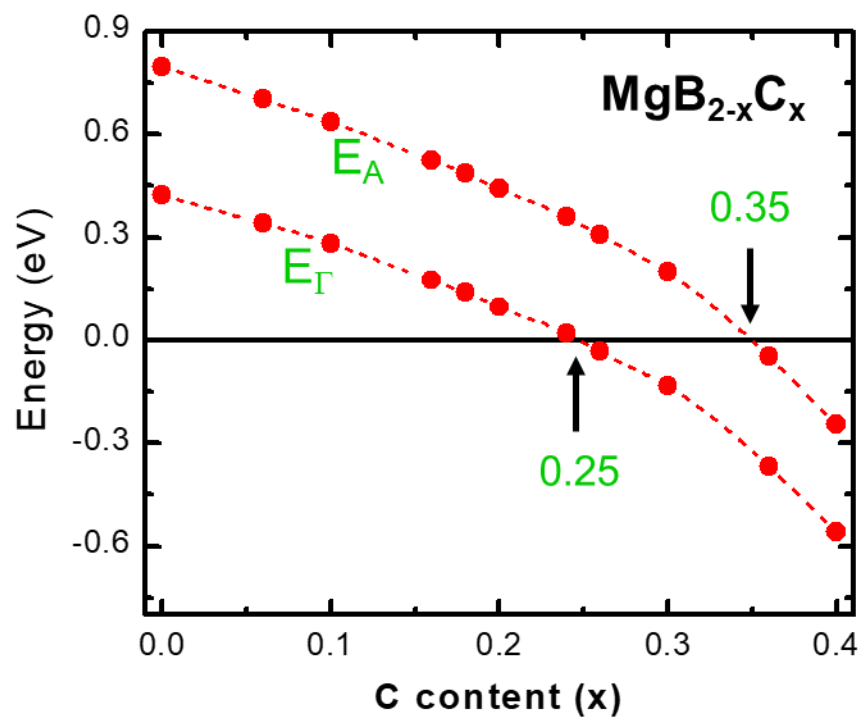
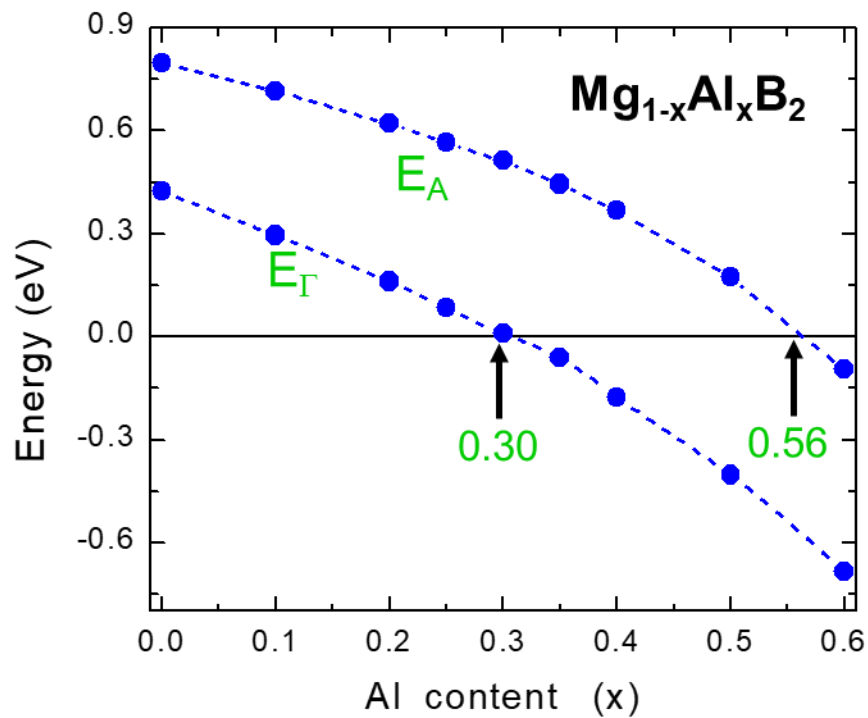
$N(0)$: DOS al nivel de Fermi

λ : constante de acoplamiento

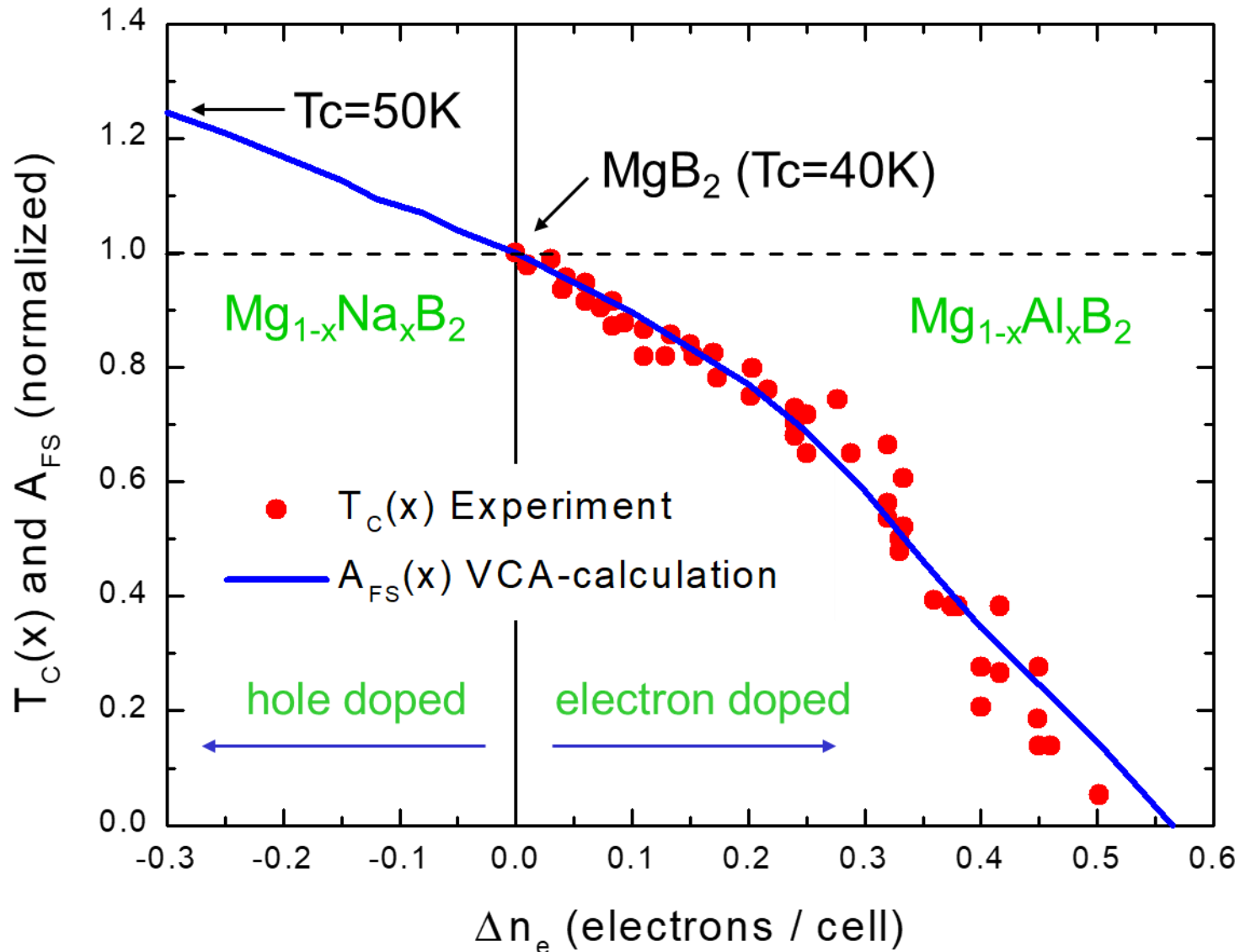
ω_{log} : frec. efectiva promedio

μ^* : inter. elec-elec apantallada

Fermi surface evolution of doped MgB_2

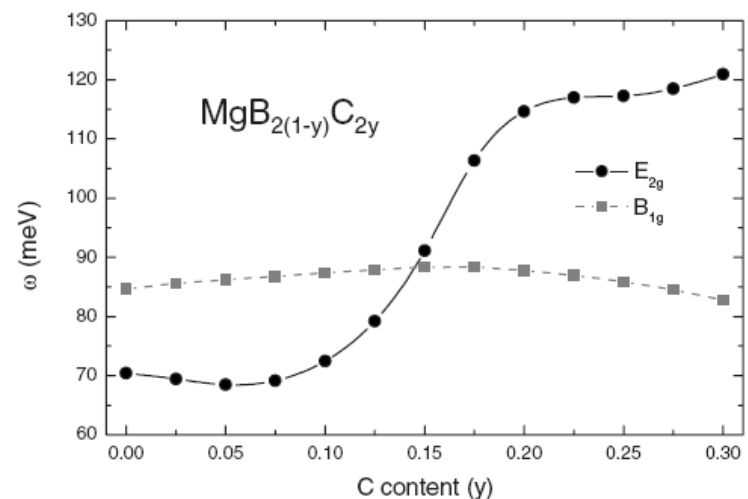
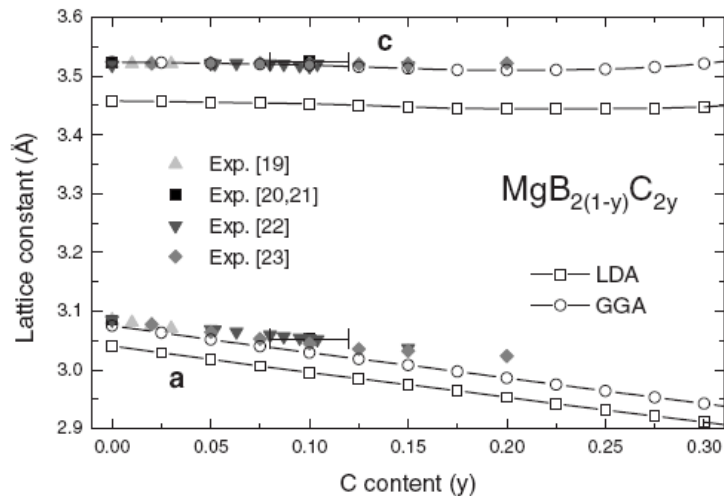
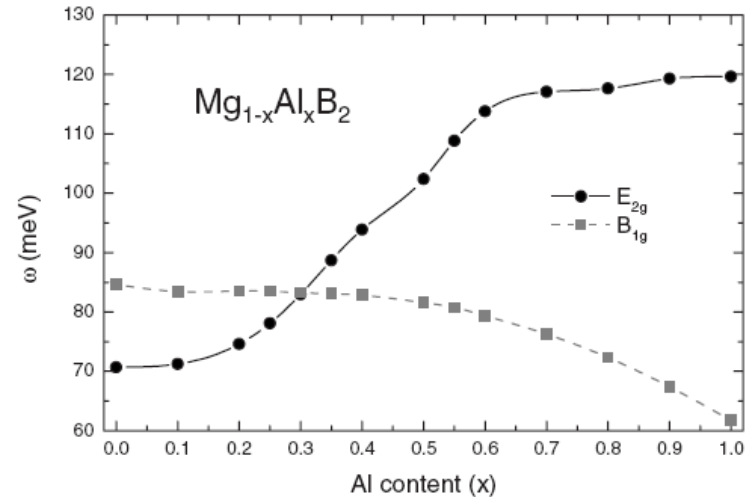
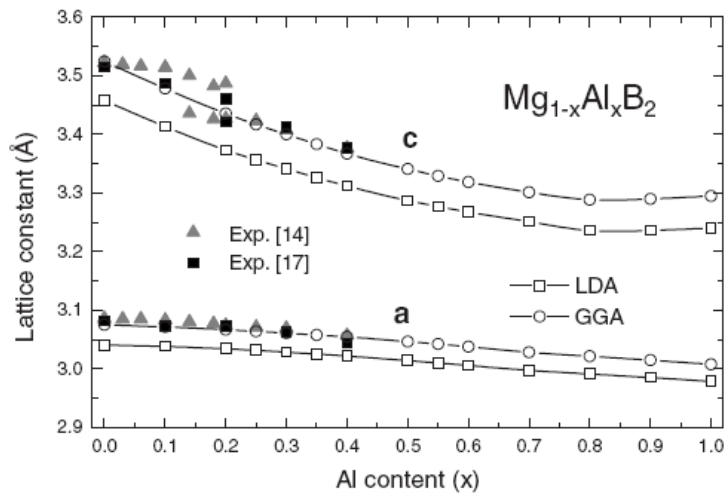


Fermi surface and T_c in doped MgB_2



Effects of Al and C doping on the electronic structure and phonon renormalization in MgB_2 O. De la Peña-Seaman,^{1,2} R. de Coss,¹ R. Heid,² and K.-P. Bohnen²¹*Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados del IPN, Apartado Postal 73 Cordemex 97310 Mérida, Yucatán, México*²*Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O. Box 3640, D-76021 Karlsruhe, Germany*

(Received 21 January 2009; revised manuscript received 10 March 2009; published 27 April 2009)



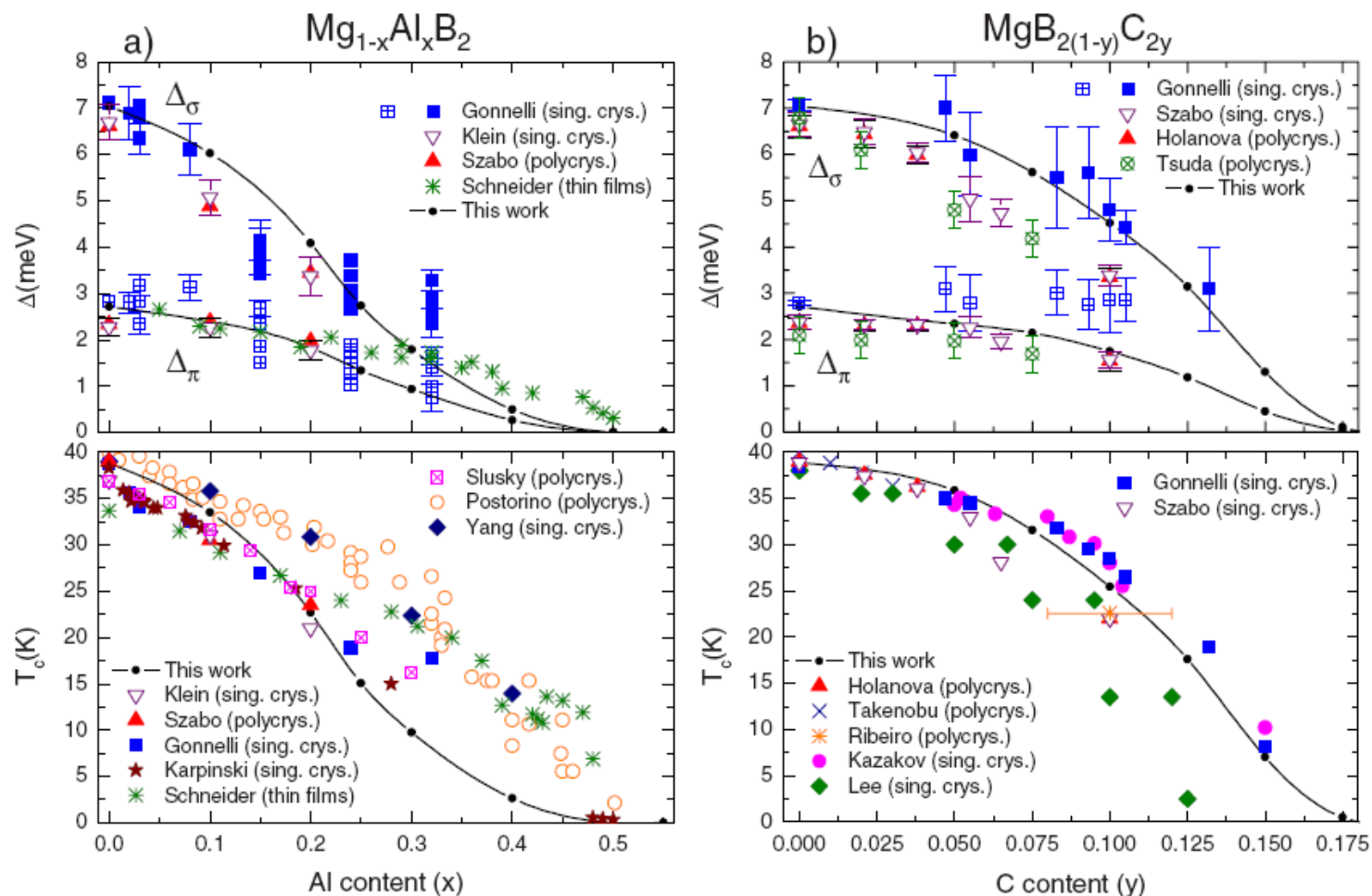
Electron-phonon coupling and two-band superconductivity of Al- and C-doped MgB₂

O. De la Peña-Seaman,^{1,2} R. de Coss,¹ R. Heid,² and K.-P. Bohnen²

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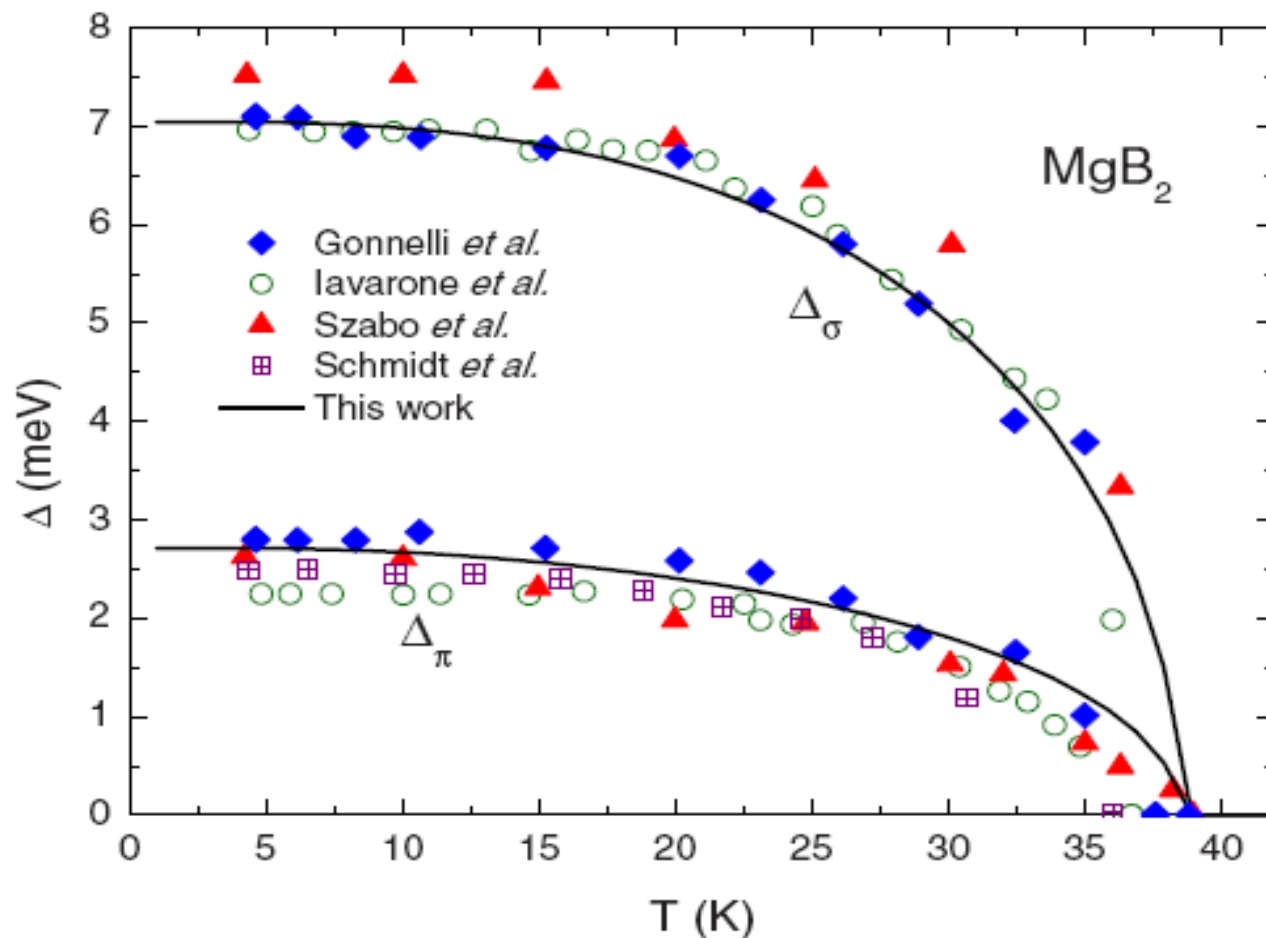
Electron-phonon coupling and two-band superconductivity of Al- and C-doped MgB₂

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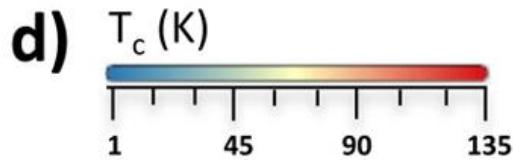
¹*Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados del IPN, Apartado Postal 73, Cordemex, 97310 Mérida, Yucatán, Mexico*

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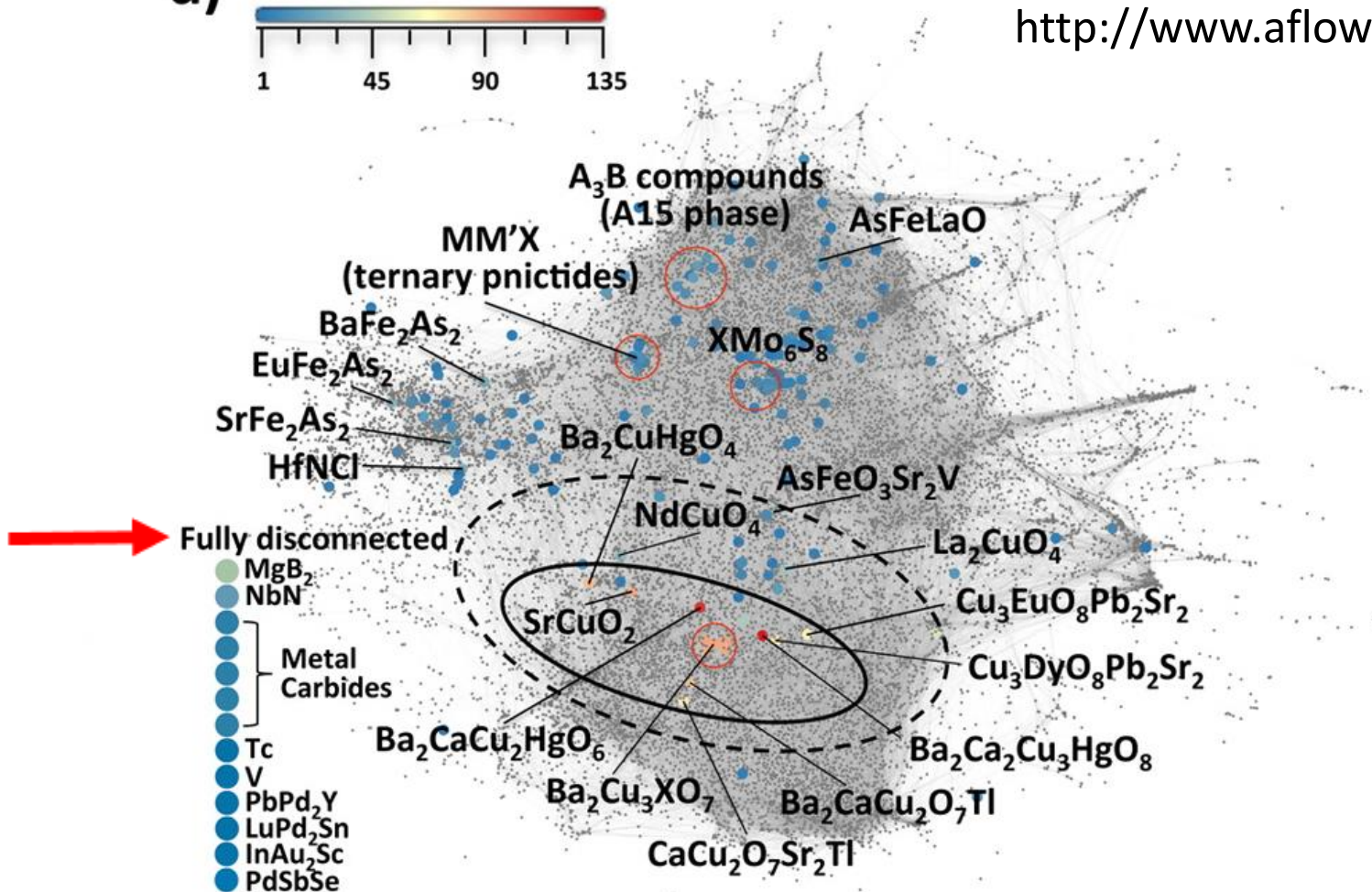
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Familias de compuestos superconductores



<http://www.aflowlib.org/>



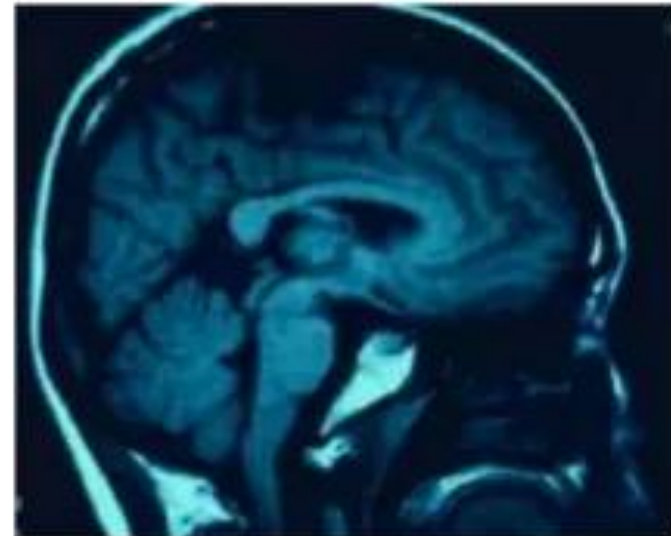
Aplicaciones de la superconductividad



- Particle Accelerators
- Generators
- Transportation
- Power Transmission
- Electric Motors
- Military
- Computing
- Medical
- B Field Detection (SQUIDS)

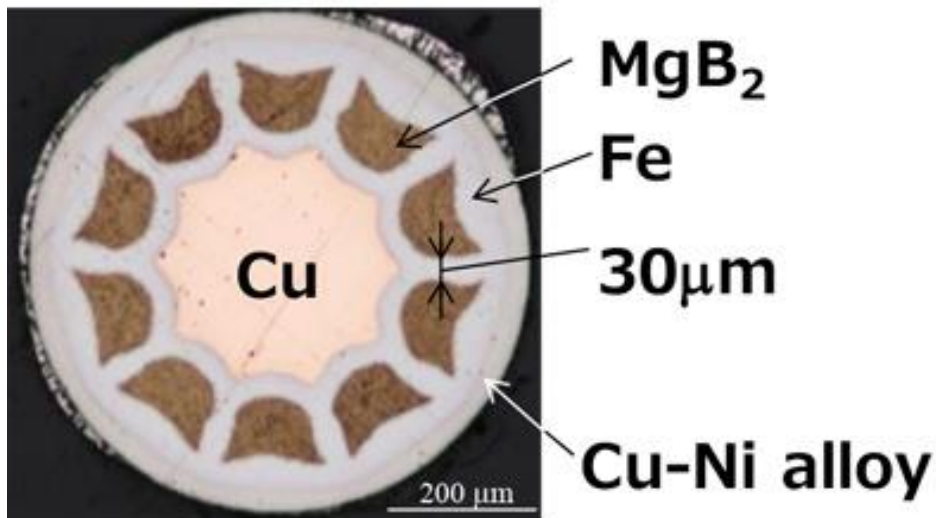


The Yamanashi MLX01 MagLev train





Development of 8-km-long Magnesium Diboride Superconducting Wire Reduces Cooling Power of Superconducting Magnet by Half

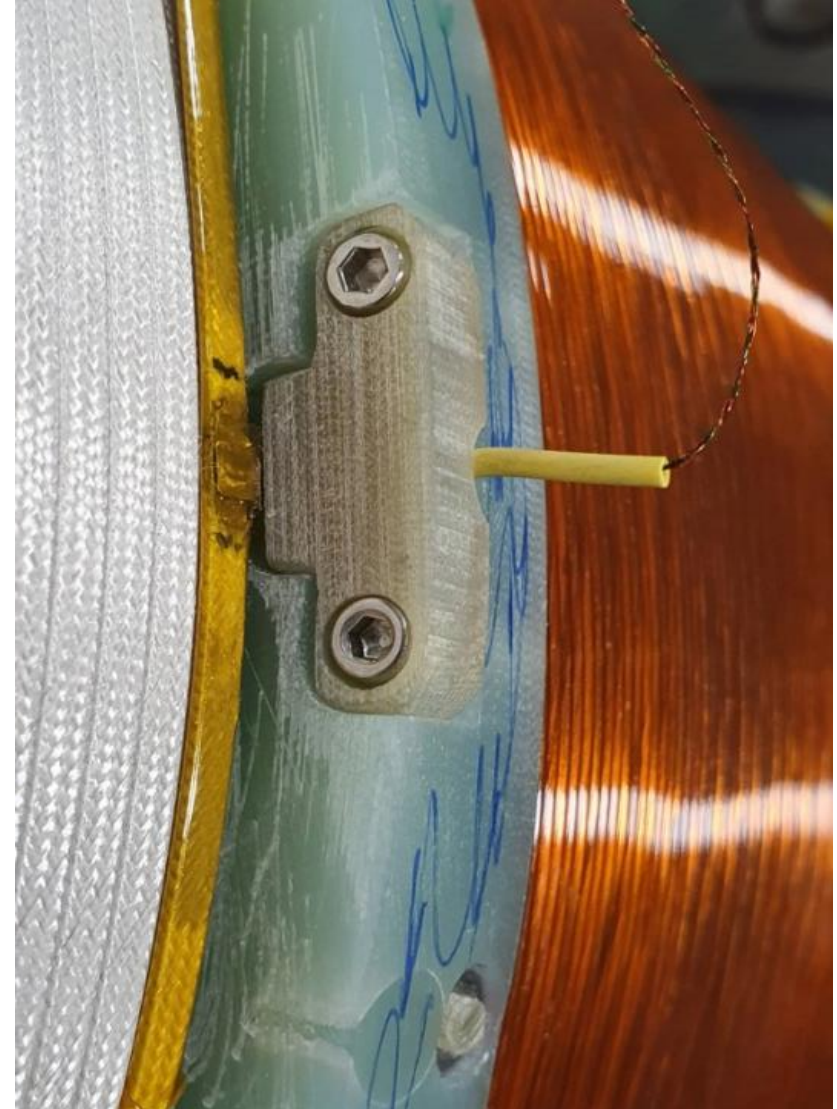




MgB_2 OPENS THE DOOR TO HIGH PERFORMANCE MAGNET RAMPING

Energy Storage, intraoperative MRI and particle therapy applications: empirical evidence shows MgB_2 confirms all theoretical expectations in carrying rapidly varying currents at 20K.

Alessio Capelluto and Lorenzo Mauro
ASG Superconductors S.p.A., R&D division, Genova, Italy





PHYSICAL REVIEW B **96**, 094510 (2017)

Evolution of multigap superconductivity in the atomically thin limit: Strain-enhanced three-gap superconductivity in monolayer MgB₂

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(Received 10 May 2017; revised manuscript received 18 July 2017; published 11 September 2017)

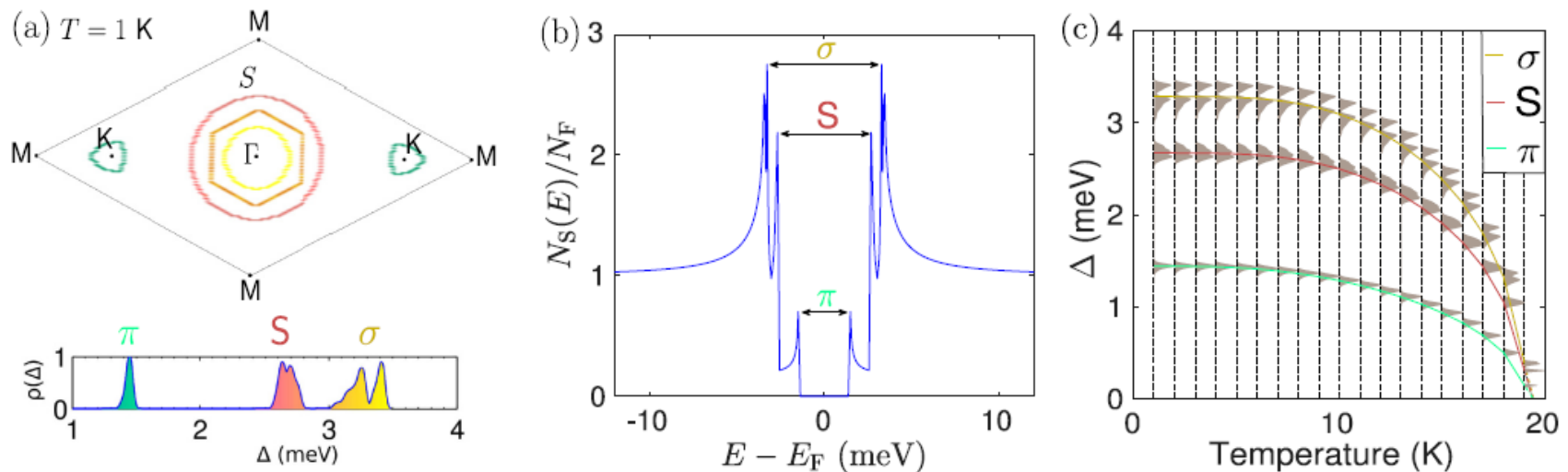


FIG. 1. The superconducting spectrum of one-ML MgB₂, calculated by anisotropic Eliashberg theory with *ab initio* input. (a) The distribution of the three superconducting gaps $\Delta(\mathbf{k}_F, T)$ on the Fermi surface: π , S (for surface), and σ , at $T = 1$ K. (b) The density of states in the superconducting state at $T = 1$ K, showing three distinct peaks corresponding to the three gaps. (c) The evolution of the gap spectrum with temperature, including the gap averages. The calculation shows that one-ML MgB₂ has $T_c \cong 20$ K.

Prediction of HTC in Hydrogenated M-MgB₂



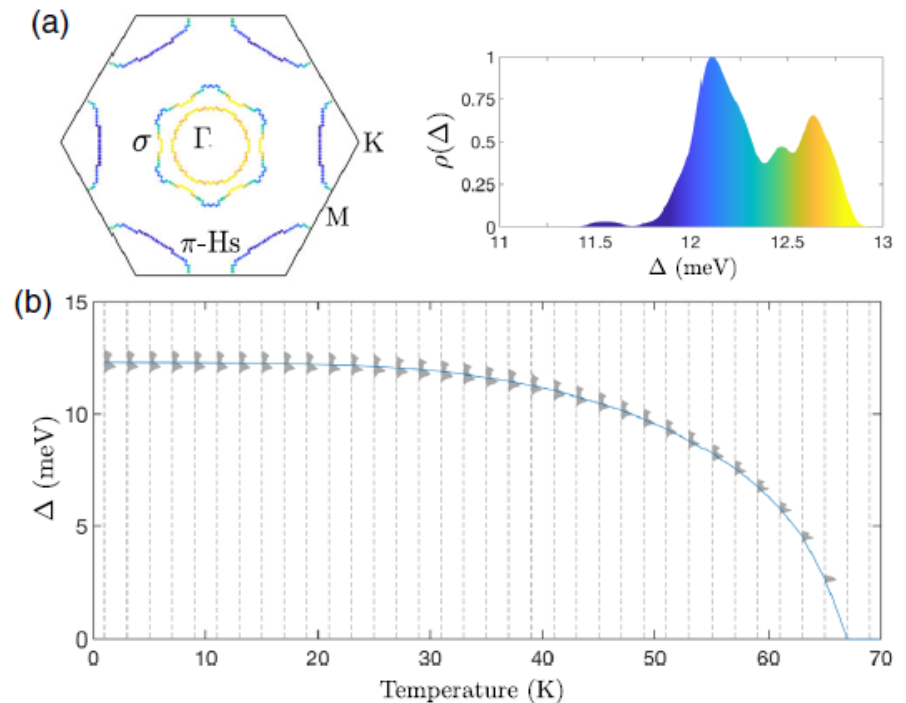
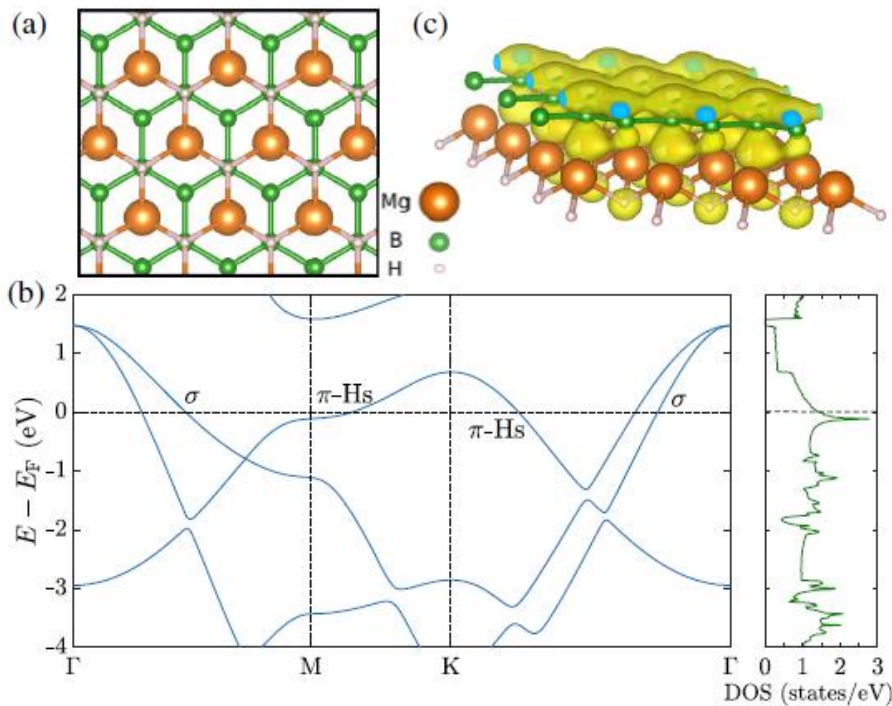
PHYSICAL REVIEW LETTERS **123**, 077001 (2019)

Hydrogen-Induced High-Temperature Superconductivity in Two-Dimensional Materials: The Example of Hydrogenated Monolayer MgB₂

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

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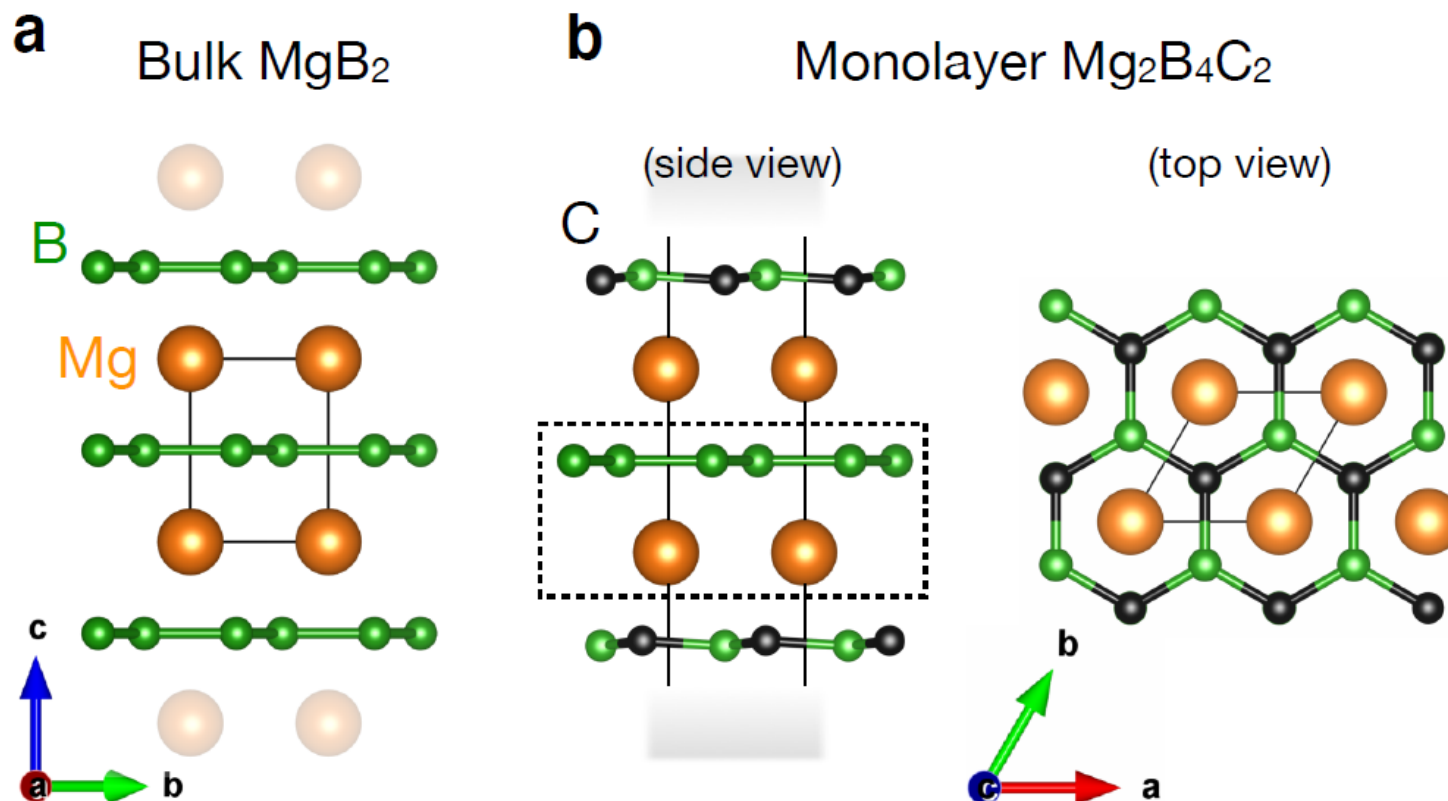


Prediction of superconductivity in M-MgB₂



High-temperature phonon-mediated superconductivity in monolayer Mg₂B₄C₂

Sobhit Singh,^{1,*} Aldo H. Romero,^{2,†} José D. Mella,^{3,4} Vitalie Eremeev,⁵ Enrique Muñoz,⁶ Anastassia N. Alexandrova,^{7,8} Karin M. Rabe,¹ David Vanderbilt,¹ and Francisco Muñoz^{4,9,‡}



Thank you for your attention

