VOLUME 3, NUMBER 12 PHYSICAL REVIEW LETTERS DECEMBER 15, 1959

BARDEEN-COOPER-SCHRIEFFER THEORY OF SUPERCONDUCTIVITY IN THE CASE OF OVERLAPPING BANDS

H. Suhl, B. T. Matthias, and L. R. Walker
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received November 16, 1959)

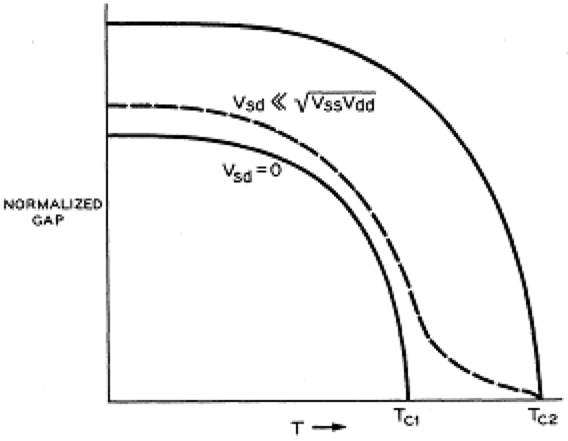
$$H = \sum_{\mathrm{k}\sigma} \epsilon_{\mathrm{k}s} c_{\mathrm{k}\sigma}{}^{*} c_{\mathrm{k}\sigma} + \sum_{\mathrm{k}\sigma} \epsilon_{\mathrm{k}d} d_{\mathrm{k}\sigma}{}^{*} d_{\mathrm{k}\sigma} - \sum_{\mathrm{kk}'} V_{ss} c_{\mathrm{k}\uparrow}{}^{*} c_{-\mathrm{k}\downarrow}{}^{*} c_{-\mathrm{k}'\downarrow} c_{\mathrm{k}'\uparrow} - V_{dd} \sum_{\mathrm{kk}'} d_{\mathrm{k}\uparrow}{}^{*} d_{-\mathrm{k}\downarrow}{}^{*} d_{-\mathrm{k}'\downarrow} d_{\mathrm{k}'\uparrow}$$

$$- V_{sd} \sum_{\mathrm{kk}'} (c_{\mathrm{k}\uparrow}{}^{*} c_{-\mathrm{k}\downarrow}{}^{*} d_{-\mathrm{k}'\downarrow} d_{\mathrm{k}'\uparrow} + d_{\mathrm{k}\uparrow}{}^{*} d_{-\mathrm{k}\downarrow}{}^{*} c_{-\mathrm{k}'\downarrow} c_{\mathrm{k}'\uparrow})$$

$$F(A) = \int_0^{\hbar\omega} d\epsilon \tanh\left[\frac{(\epsilon^2 + A^2)^{1/2}}{2kT}\right] \Big/ (\epsilon^2 + A^2)^{1/2}$$

$$A[1 - V_{ss} N_s F(A)] = B V_{sd} N_d F(B)$$

$$B[1 - V_{dd} N_d F(B)] = A V_{sd} N_s F(A)$$



- Multiband Superconductivity was considered immediately after BCS theory, in connection with transition metals.

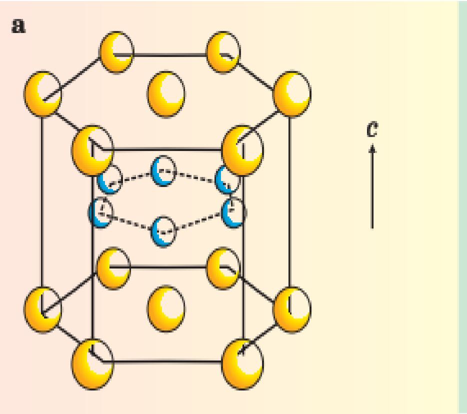
- The physics of multiple gaps is best understood in terms of the quasi-spin model.

Magnesium Diboride: Better Late than Never

Paul C. Canfield and George W. Crabtree

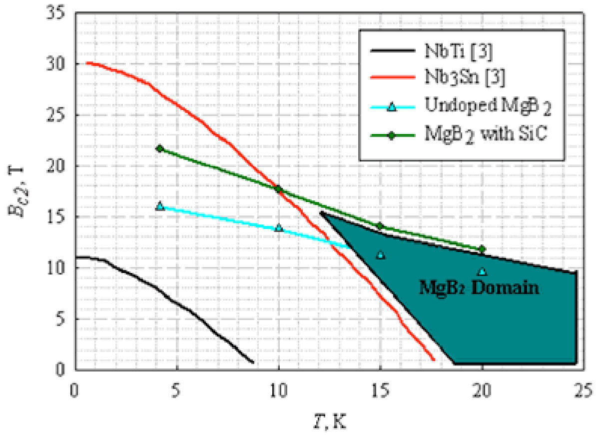
34 March 2003 Physics Today

M. Swift, D. White, *J. Am. Chem. Soc.* **79**, 3641 (1957).



Searching for ferromagnetism, superconductivity at 40 K was discovered

Nagamatsu, Nakagawa, Muranaka, Zenitani, and Akimitsu, Nature **410**, 63 (2001)



A. Gurevich et al. Supercond. Sci. Technol. 2004, 17, 278-286

- Within months of the discovery theory and expteriment had converged on an answer.

J. M An and W. Pickett PRL (2001)

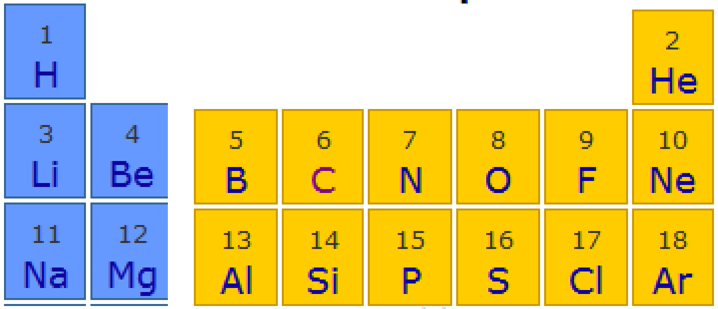
Kortus and Mazin PRL (2001)

Y Kong O V Dolgov O Jepsen and O Andersen Phys. Rev. B 64, 020501 (2001)

- And applications followed.

VOLUME 86, NUMBER 19 PHYSICAL REVIEW LETTERS 7 MAY 2001

Superconductivity of MgB$_2$: Covalent Bonds Driven Metallic



J. M. An and W. E. Pickett

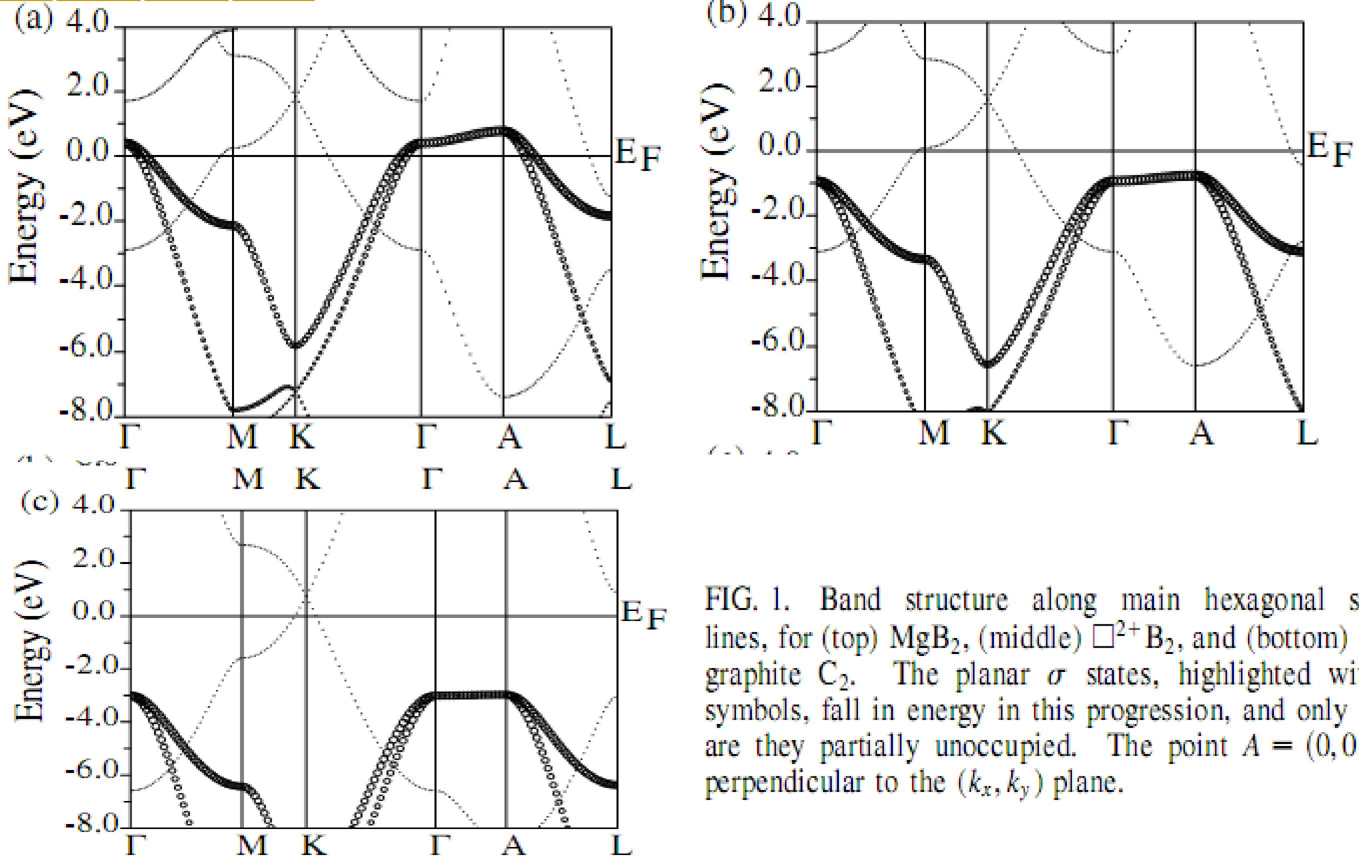
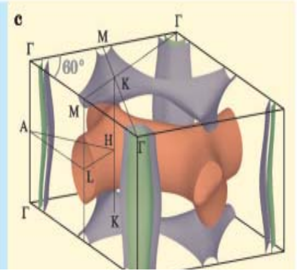


FIG. 1. Band structure along main hexagonal symmetry lines, for (top) MgB$_2$, (middle) $\square^{2+}B_2$, and (bottom) primitive graphite C$_2$. The planar σ states, highlighted with larger symbols, fall in energy in this progression, and only in MgB$_2$ are they partially unoccupied. The point $A = (0, 0, \pi/c)$ is perpendicular to the (k_x, k_y) plane.



Basic Physics of MgB2

Two very different set of bands sigma (2d) and pi (3d). Two types of Electrons.

Two types of Fermi Surfaces.

Sigma bonds very strong. Deformation potential 13 3v/A amazing for a metal.

Only a fraction of the electrons are strongly coupled to those phonons.

Two gaps.

A case clear case of momentum space differentiation.

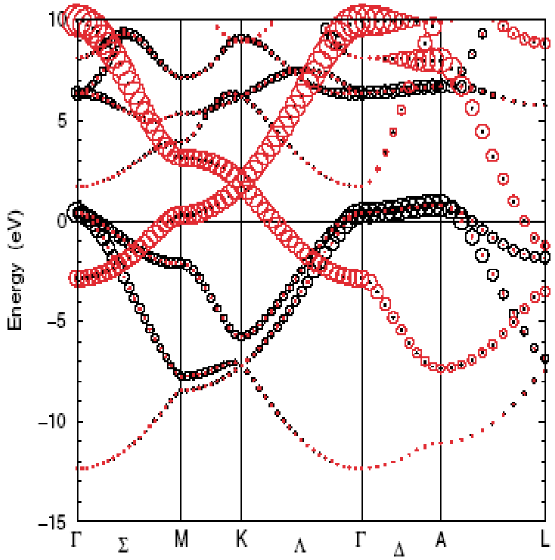


FIG. 1 (color). Band structure of MgB_2 with the B p character. The radii of the red (black) circles are proportional to the B p_z (B $p_{x,y}$) character.

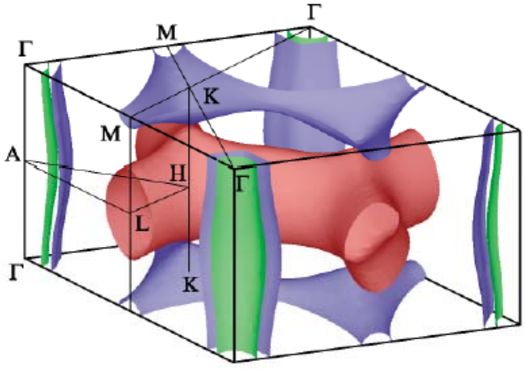
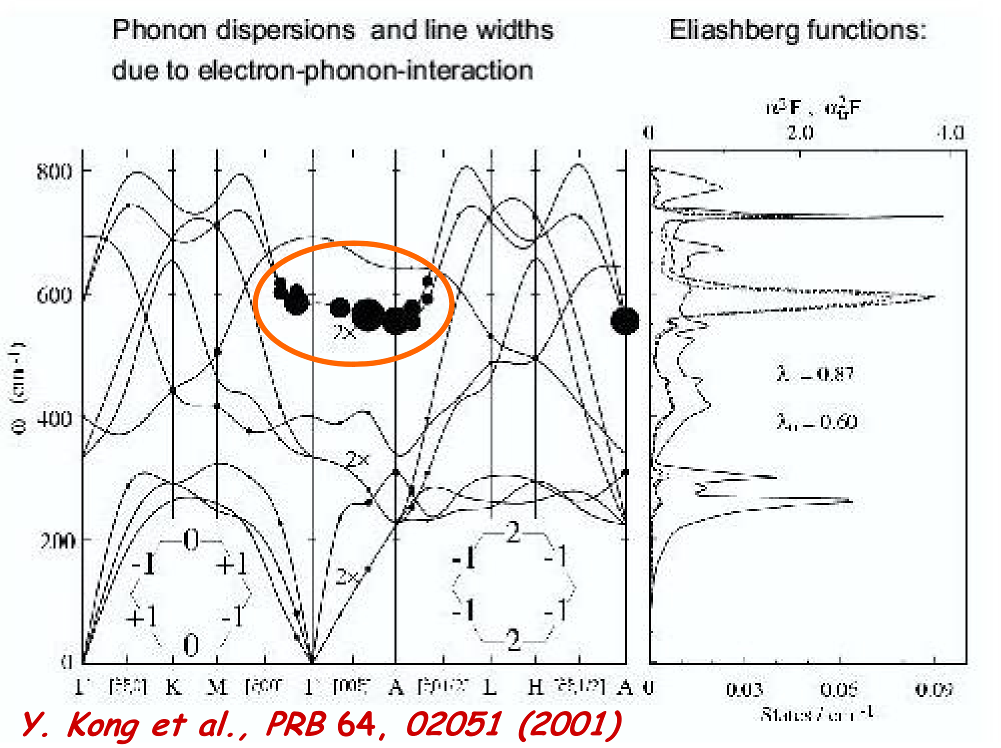


FIG. 3 (color). The Fermi surface of MgB_2. Green and blue cylinders (holelike) come from the bonding $p_{x,y}$ bands, the blue tubular network (holelike) from the bonding p_z bands, and the red (electronlike) tubular network from the antibonding p_z band. The last two surfaces touch at the K point.

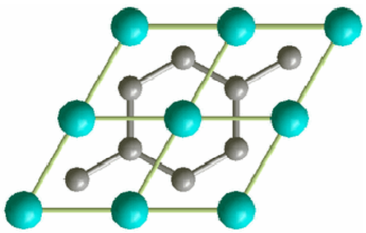
J. M An and W. Pickett PRL (2001)
Kortus and Mazin PRL (2001)
Y Kong O V Dolgov O Jepsen and O Andersen Phys. Rev. B 64, 020501 (2001)

Visualizing the electrons and phonons in interaction in MgB$_2$ Lamda is a matrix.

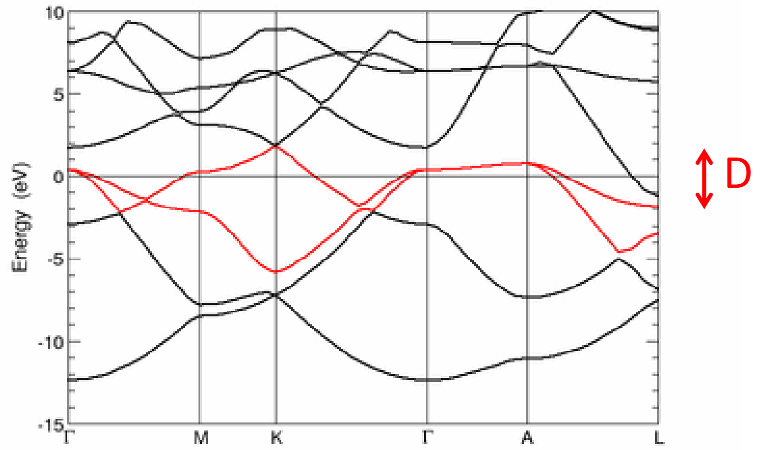


Y. Kong et al., PRB 64, 02051 (2001)

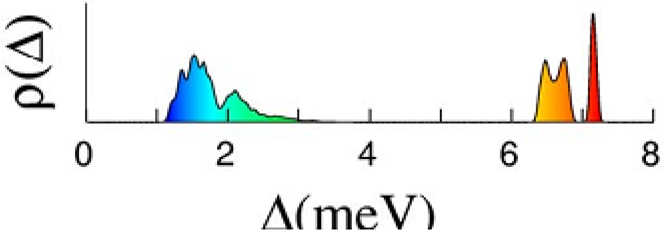
The total e-ph coupling **λ=0.8-0.9** is concentrated in a doubly-deg. bond-stretching mode . Deformation potential is large. Few phonons have large linewidth. [Electrons affect phonons] . Only sigma electrons are strongly coupled. Eliashberg function.

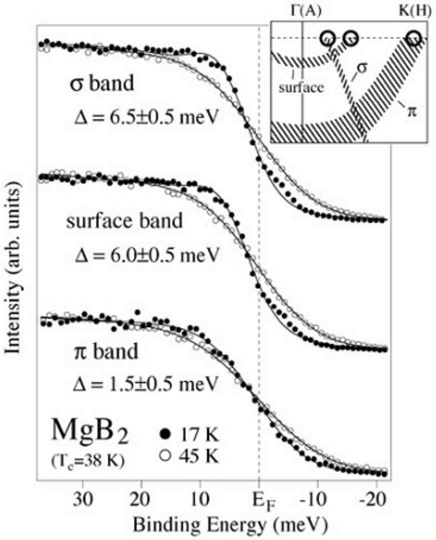


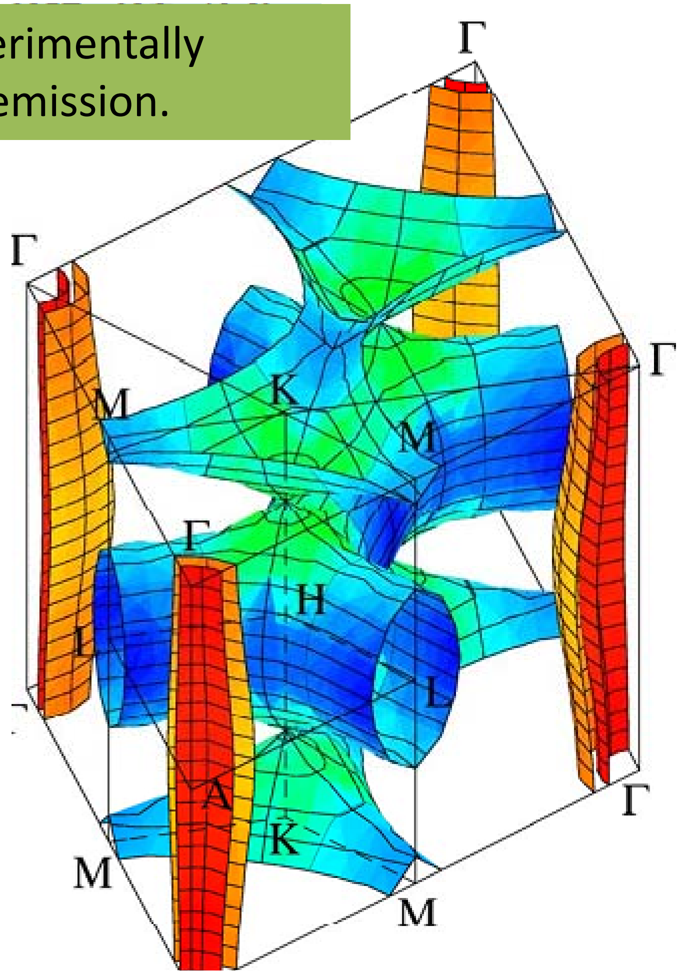
Strong coupling between bond-stretching modes and stiff σ bonds



Two Gap Superconductivity: tested experimentally Using many probes. For example photoemission.







ARPES STUDIES OF
MULTIPLE SUPERCONDUCTING GAPS IN MgB$_2$

S. Souma[1], Y. Machida[2], T. Sato[1], H. Matsui[1], T. Takahashi[1], S.-C. Wang[3], H. Ding[3], A. Kaminski[4], J. C. Campuzano[5], S. Sasaki[2], and K. Kadowaki[6]

Experimental verification of the two gap picture by many photoemission groups in the world.

Excitations in a Superconductor

- Anderson Bogolubov quasiparticles. Can be imaged directly by ARPES.
- Bogolubov Anderson density oscillations. Phase fluctuations, pushed to the plasma frequency by long range interactions. Would be Goldstone mode that got Higgsed.
- Amplituded mode. [“Higgs boson”] first observed in NbSe2.

Zooryakumar and Klein PRL 45, 660 (1980). Littlewood and Varma PRL 47, 811 (1981).

- Out of phase oscillations of the phase mode. First pointed out by Leggett. Prog Theor Phys 36, 901 (1966)
- Possibly measured in MgB2 by Raman. PRL 99, 227002 (2007)

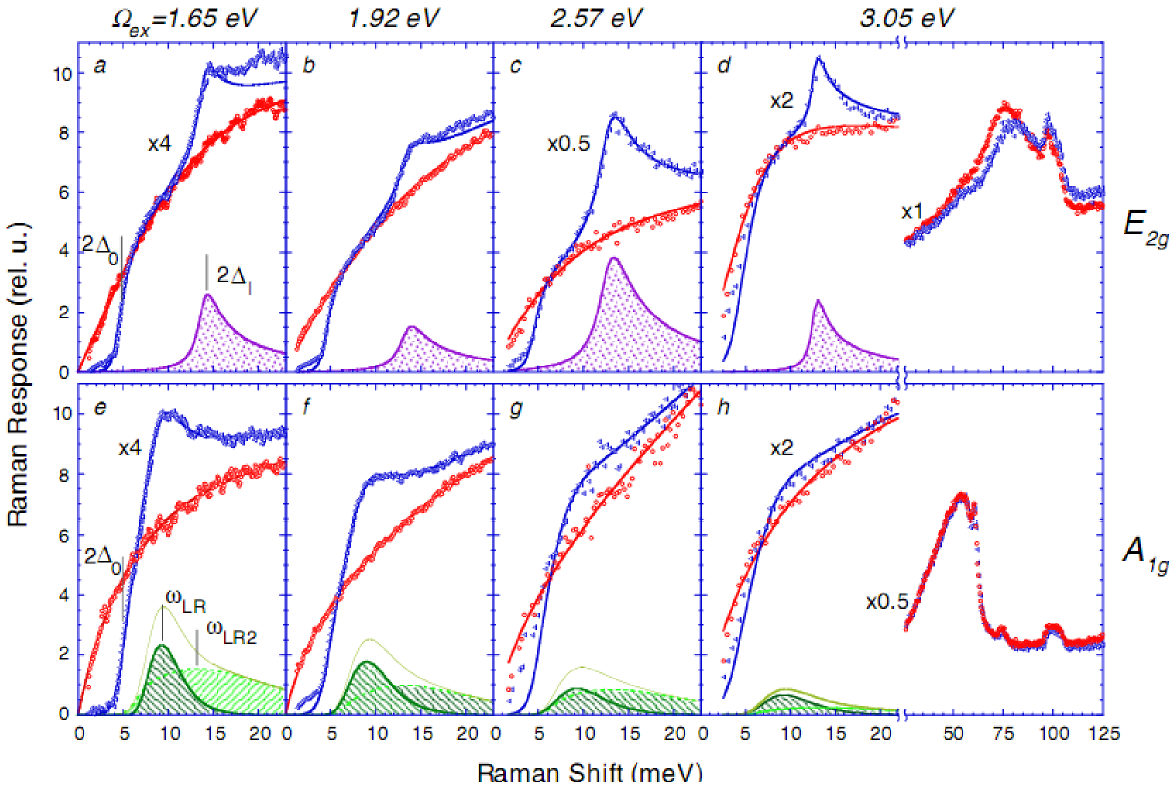
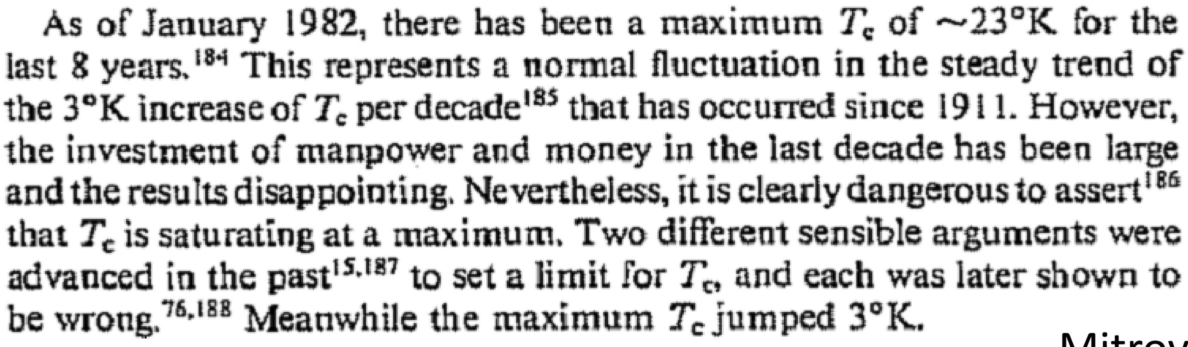


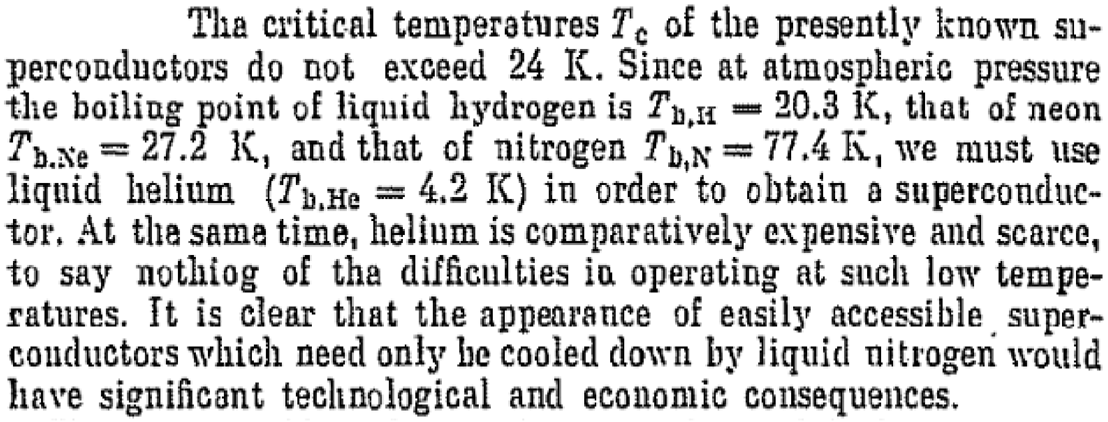
FIG. 1 (color online). The Raman response spectra of an MgB$_2$ crystal in the normal (red) and SC (blue) states for the E_{2g} (top row) and A_{1g} (bottom row) scattering channels. The E_{2g} channel is accessed by RL (a)–(c) or VH (d) polarization and the A_{1g} channel by RR (e)–(h) polarization. The low temperature data are acquired at 5–8 K. The normal state has been achieved either by increasing the crystal temperature to 40 K (d) or by applying a 5 T magnetic field parallel to the *c*-axis [(a)–(c), (e)–(h)] [32]. The columns are arranged in the order of increasing excitation energy Ω_{ex}. Solid lines are fits to the data points. The normal state continuum is fitted with $\omega/\sqrt{a + b\omega^2}$ function. The data in the SC state is decomposed into a sum of a gapped normal state continuum with temperature broadened $2\Delta_0 = 4.6$ meV gap cutoff, the SC coherence peak at $2\Delta_l = 13.5$ meV (shaded in violet), and the collective modes at $\omega_{\mathrm{LR}} = 9.4$ meV and $\omega_{\mathrm{LR2}} = 13.2$ meV (shaded in dark and light green). The solid hairline is the sum of both modes. To fit the observed shapes the theoretical BCS coherence peak singularity $\chi'' \sim 4\Delta_l^2/(\omega\sqrt{\omega^2 - 4\Delta_l^2})$ is broadened by convolution with a Lorentzian with HWHM = 5%–12% of $2\Delta_l$ [22]. The collective mode ω_{LR} is fitted with the response function shown in Fig. 3. Panels (d) and (h) also show the high energy part of spectra for respective symmetries. The broad E_{2g} band at 79 meV is the boron stretching mode, the only phonon that exhibits renormalization below T_C [25]. For the A_{1g} channel the spectra are dominated by two-phonon scattering.

Historical Note: just before the discovery of cuprate superconductivity (1986) there was not much going on in terms of increasing Tc.

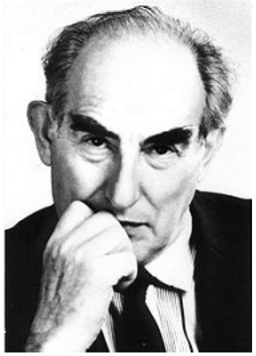


As of January 1982, there has been a maximum T_c of ~23°K for the last 8 years.[184] This represents a normal fluctuation in the steady trend of the 3°K increase of T_c per decade[185] that has occurred since 1911. However, the investment of manpower and money in the last decade has been large and the results disappointing. Nevertheless, it is clearly dangerous to assert[186] that T_c is saturating at a maximum. Two different sensible arguments were advanced in the past[15,187] to set a limit for T_c, and each was later shown to be wrong.[76,188] Meanwhile the maximum T_c jumped 3°K.

Mitrovic and Allen in Solid State Physics



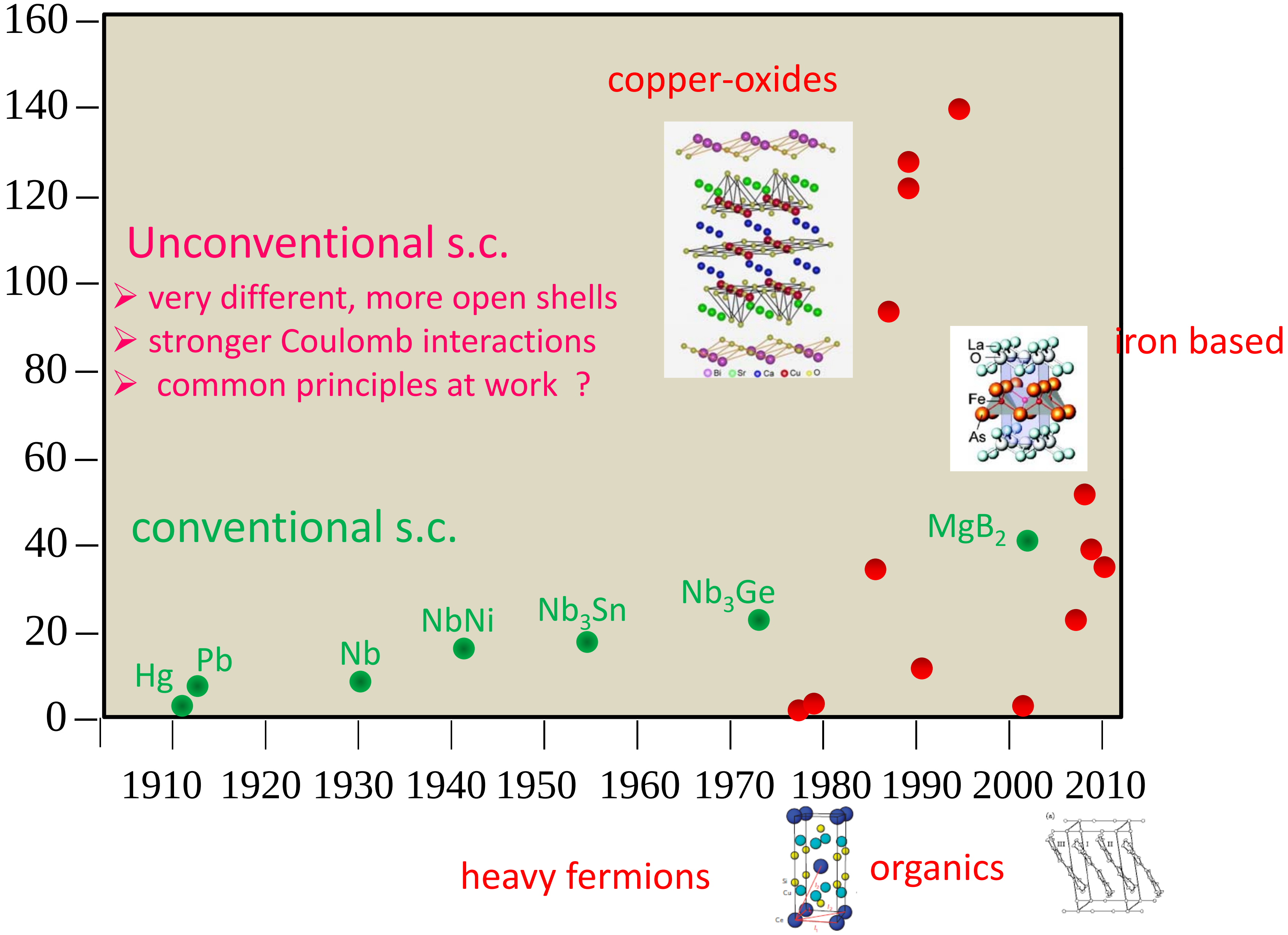
The critical temperatures T_c of the presently known superconductors do not exceed 24 K. Since at atmospheric pressure the boiling point of liquid hydrogen is $T_{b,H} = 20.3$ K, that of neon $T_{b,Ne} = 27.2$ K, and that of nitrogen $T_{b,N} = 77.4$ K, we must use liquid helium ($T_{b,He} = 4.2$ K) in order to obtain a superconductor. At the same time, helium is comparatively expensive and scarce, to say nothing of the difficulties in operating at such low temperatures. It is clear that the appearance of easily accessible superconductors which need only be cooled down by liquid nitrogen would have significant technological and economic consequences.



High-temperature Superconductivity

V.L.Ginzburg and D.A.Kirzhnits

timeline of discoveries



Unconventional s.c.

- ➢ very different, more open shells
- ➢ stronger Coulomb interactions
- ➢ common principles at work ?

conventional s.c.

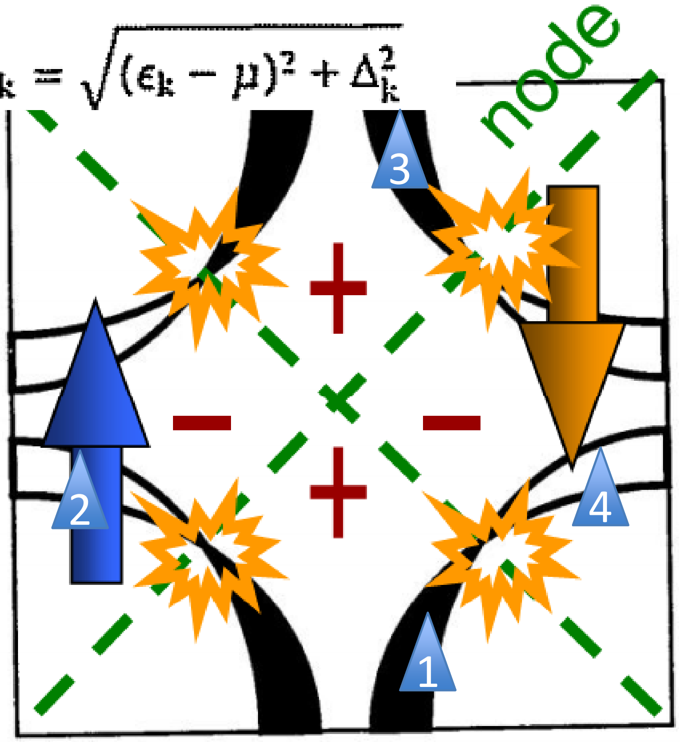
Superconductivity from Repulsion

$$\Delta_{\mathbf{k}} = -\frac{1}{N}\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}\tanh\frac{\beta E_{\mathbf{k}'}}{2}$$

$\Delta(k) = \Delta(\text{Cos}(kx)\text{-Cos}(ky))$

where

$$E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}}-\mu)^2+\Delta_{\mathbf{k}}^2}$$



Vkk' can resembles and exchange constant J(k-k')or a spin suscepbility χ (k-k')

separable model scatters only between triangles. V12, V23, V14, V34 >0

Real Space Picture . On site interaction strongly repulsive. Nearest neighbor attractive. Oscillatory in space.

Contrast with phonon mediated which oscillates in time, since at short times is repulsive.

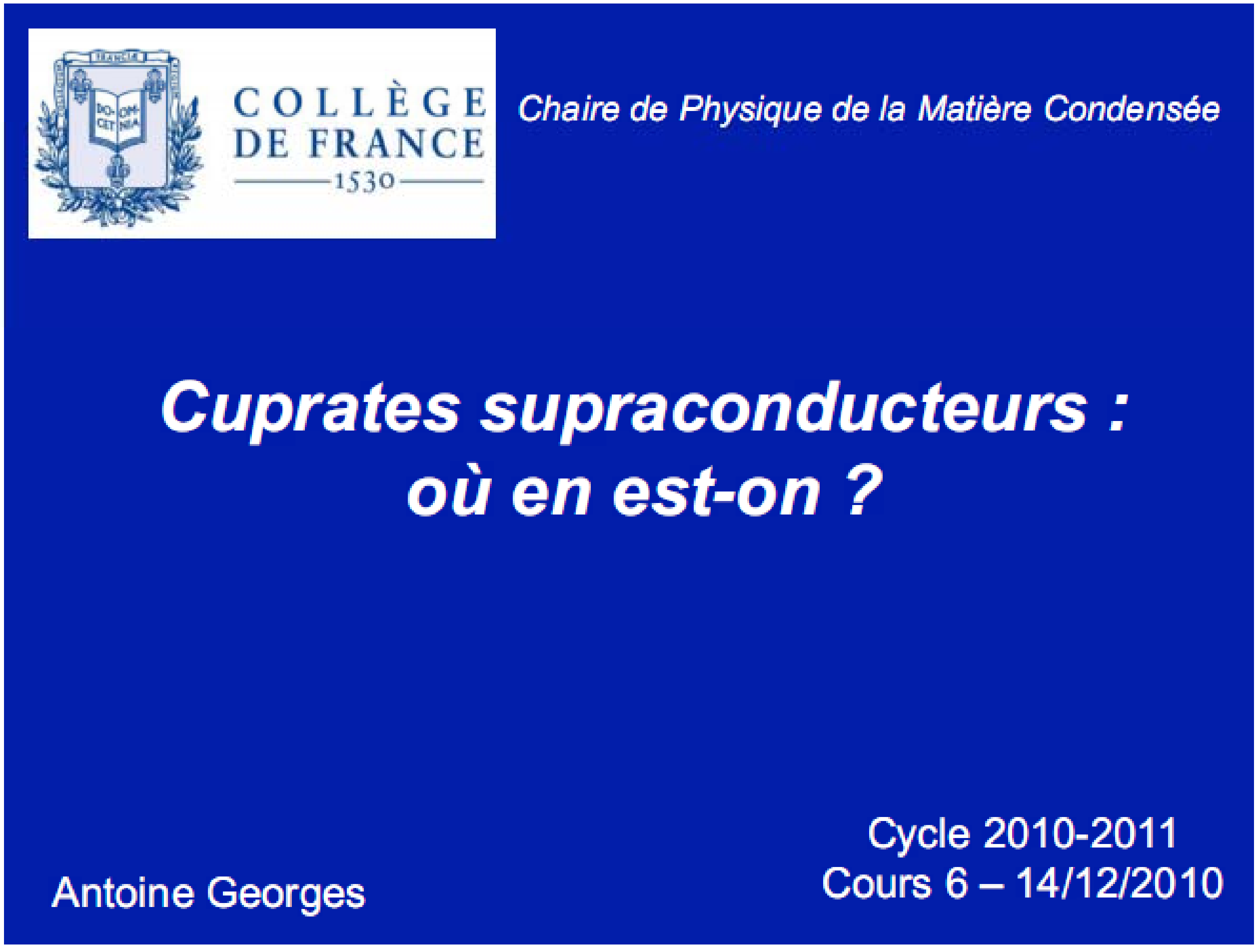
Correlated Superconductivity

- Order parameter transforms according to non trivial representation of the symmetry group of the crystal. K dependence.
- Higher energy scales are involved. Fermi liquid state has not been reached, near Tc optimal.
- New tools will probably be needed!!
- Cluster DMFT, a natural generalization of the ME theory.
- Model Hamiltonian: identify common features
- System Specific Calculations: identify materials trends.

Look at superconductivity in cuprates with the tools we have.

What controls Tcmax ?

Fortunately the background material has been covered in Antoine Georges earlier course . See last two lectures in



COLLÈGE DE FRANCE
1530

Chaire de Physique de la Matière Condensée

Cuprates supraconducteurs : où en est-on ?

Antoine Georges

Cycle 2010-2011
Cours 6 – 14/12/2010

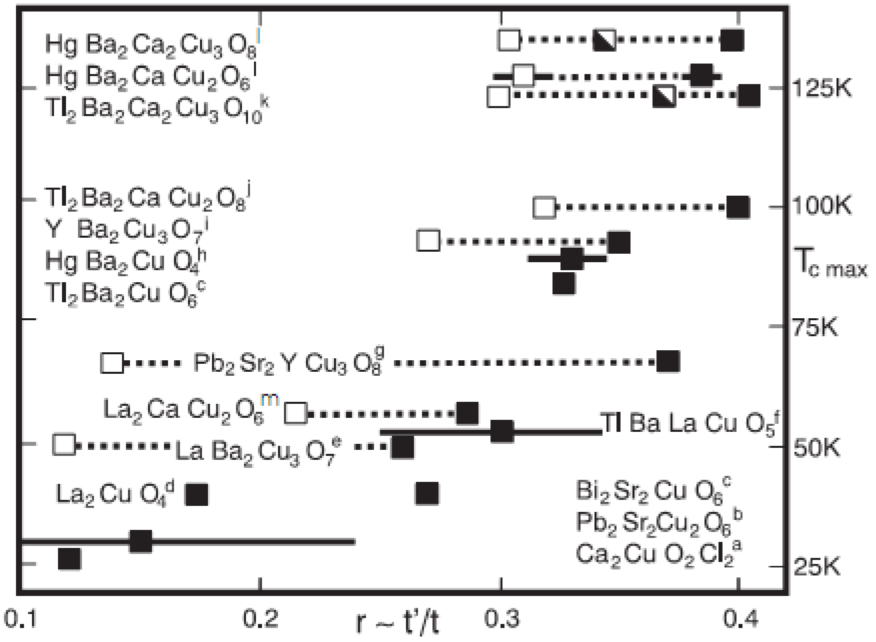
Material Dependence of Tc

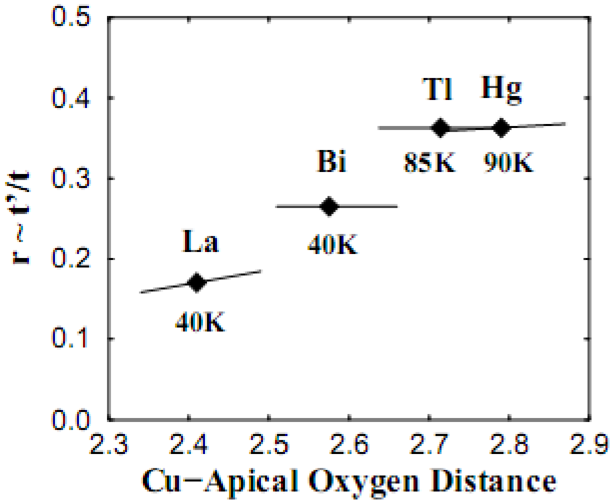
Band-structure trend in hole-doped cuprates and correlation with $T_{c\,\max}$.

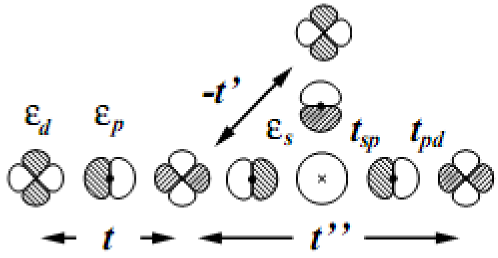
E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, and O.K. Andersen.

Phys. Rev. Lett. 87, 047003 (2001)

As the apical oxygen is pulled out of the plane Tcmax goes UP!



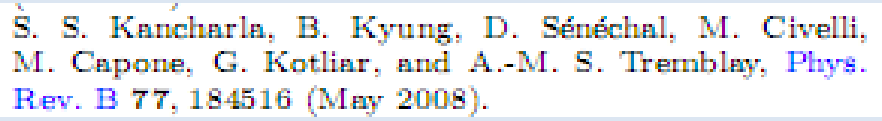




Theoretical issues with Andersen's proposal.

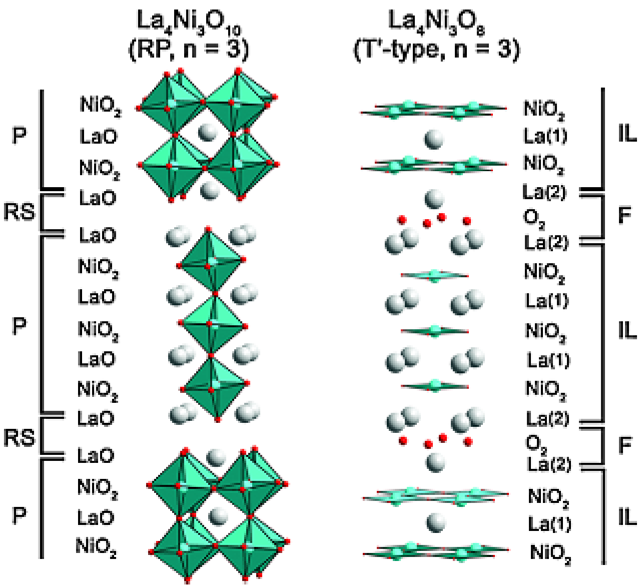
Within Slave Boson MFT, t-J model. Tcmax decreases as t' /t increases.

Within Hubbard model cluster DMFT studies of superconductivity Tcmax decreases as t'/t increases. In many studies, for example in CDMFT



S. S. Kancharla, B. Kyung, D. Sénéchal, M. Civelli, M. Capone, G. Kotliar, and A.-M. S. Tremblay, Phys. Rev. B 77, 184516 (May 2008).

Earlier DMRG for ladders, White and Scalapino reached identical conclusion.



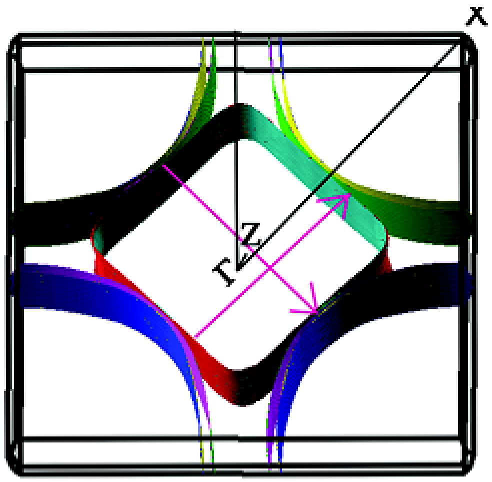
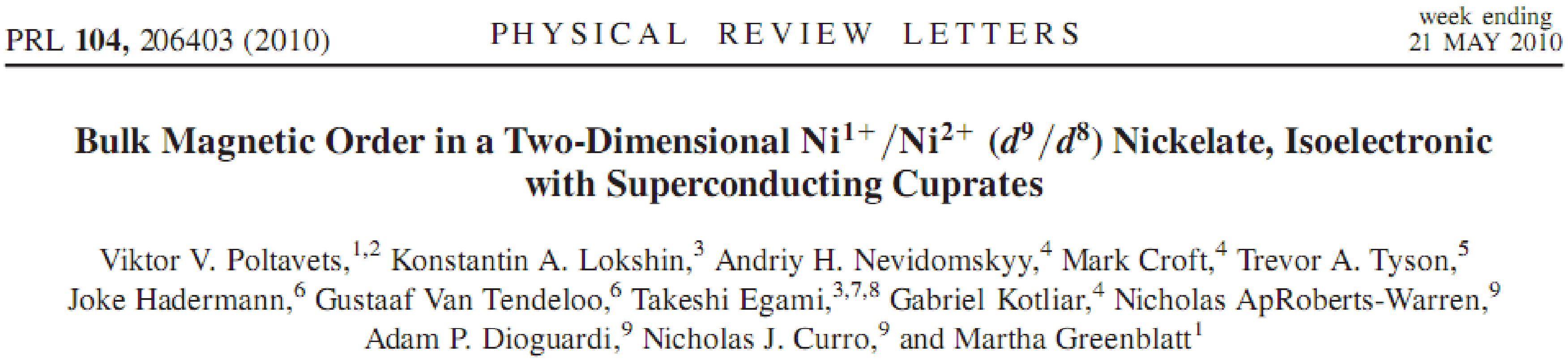


FIG. 4 (color online). Fermi surface of $La_4Ni_3O_8$ in reciprocal space with nesting vectors (arrows).

Larger t'/t than cuprates but no Tc



PRL **104**, 206403 (2010) PHYSICAL REVIEW LETTERS week ending 21 MAY 2010

Bulk Magnetic Order in a Two-Dimensional Ni^{1+}/Ni^{2+} (d^9/d^8) Nickelate, Isoelectronic with Superconducting Cuprates

Viktor V. Poltavets,[1,2] Konstantin A. Lokshin,[3] Andriy H. Nevidomskyy,[4] Mark Croft,[4] Trevor A. Tyson,[5] Joke Hadermann,[6] Gustaaf Van Tendeloo,[6] Takeshi Egami,[3,7,8] Gabriel Kotliar,[4] Nicholas ApRoberts-Warren,[9] Adam P. Dioguardi,[9] Nicholas J. Curro,[9] and Martha Greenblatt[1]

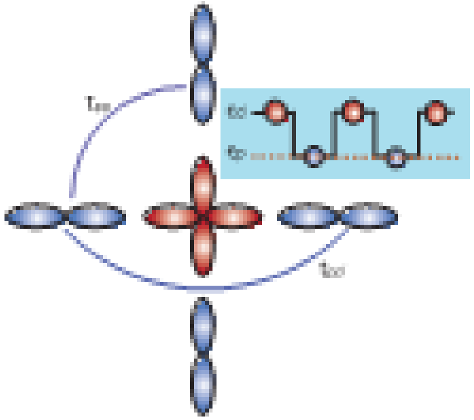
New Proposal: C. Weber C. Yee K. Haule GK cond-mat arXiv:1108.3028

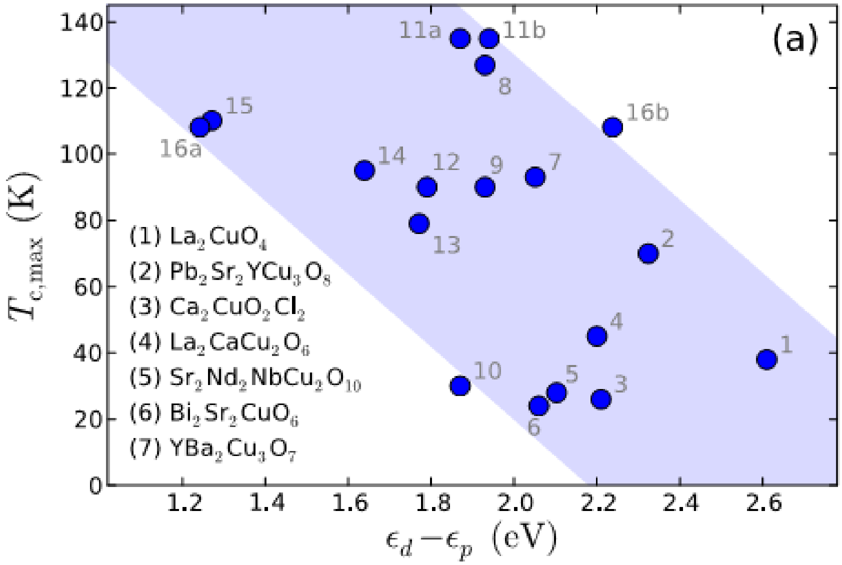
The main effect of the distance of the apical oxygen to the plane is to control the charge transfer gap: ed-ep

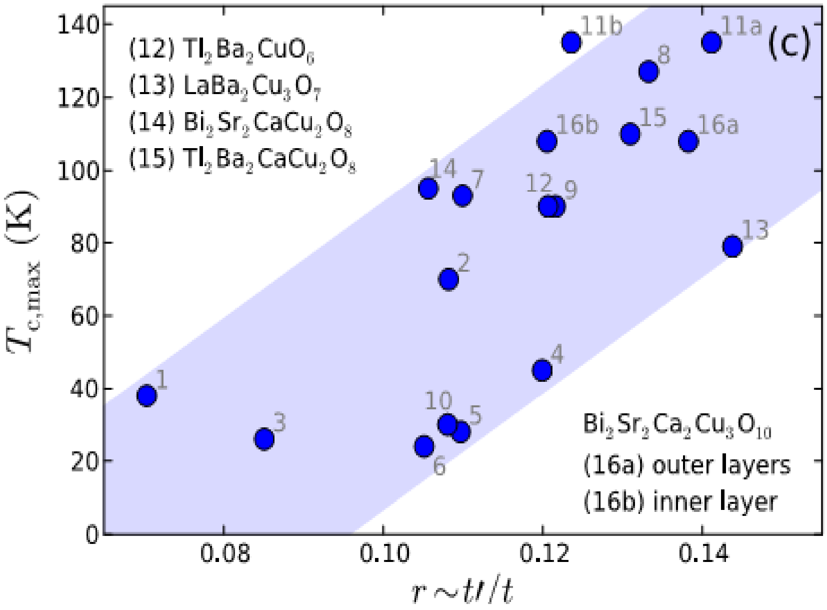
Moving the apical oxygen away from the plane reduces the charge transfer gap and increases Tc.

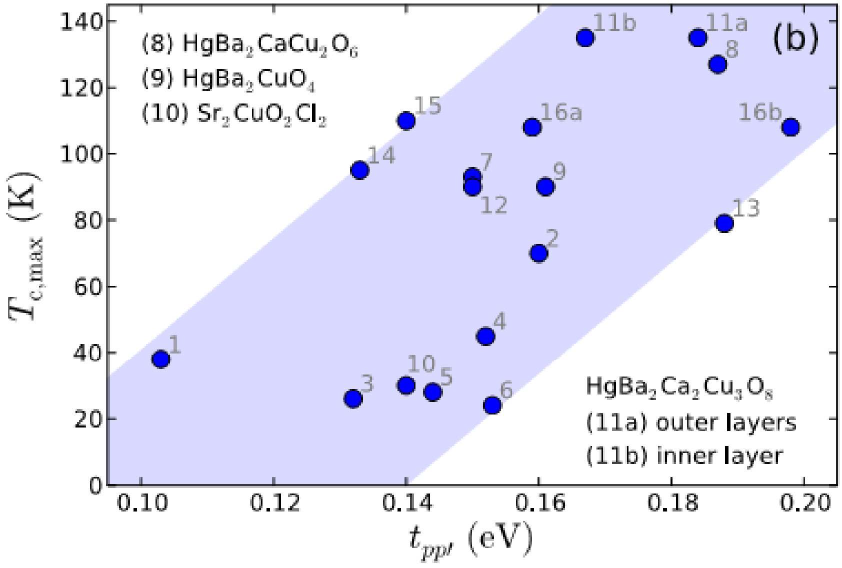
Moving the apical oxygen away from the plane ALSO increases tpp’ as Andersen pointed out. But the increase of tpp’ is detrimental to Tc. [Correlation is not the same as causation]

Correlations: deriving the starting Hamiltonian to do LDA+DMFT gives parameters.

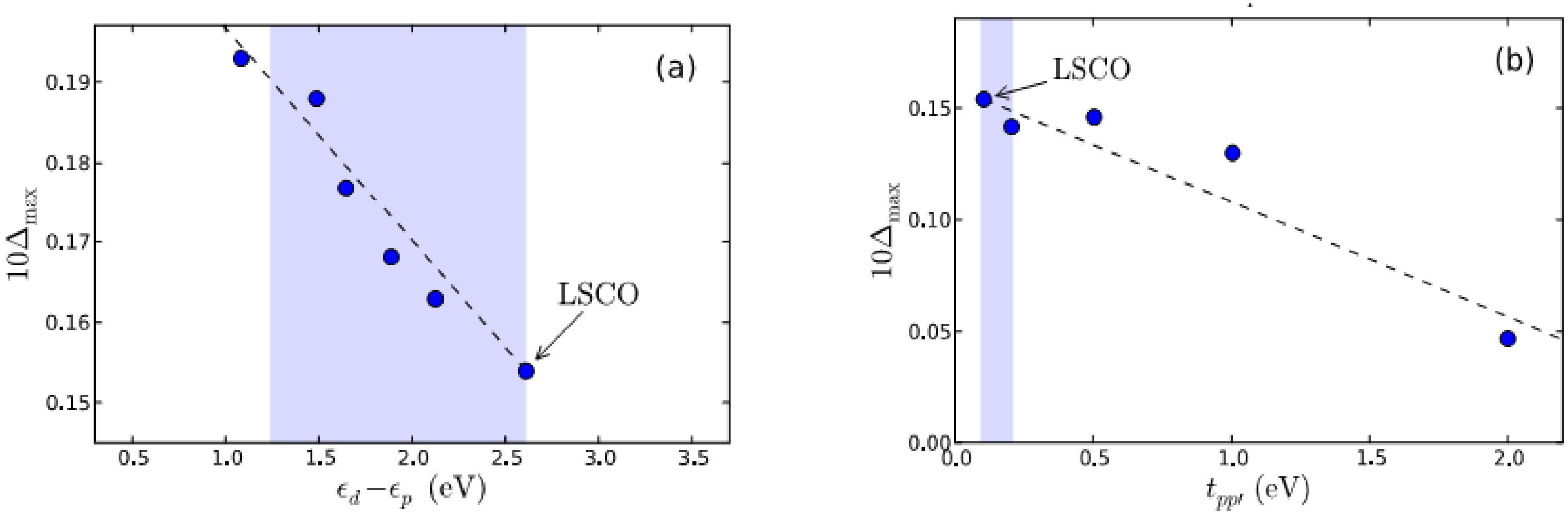








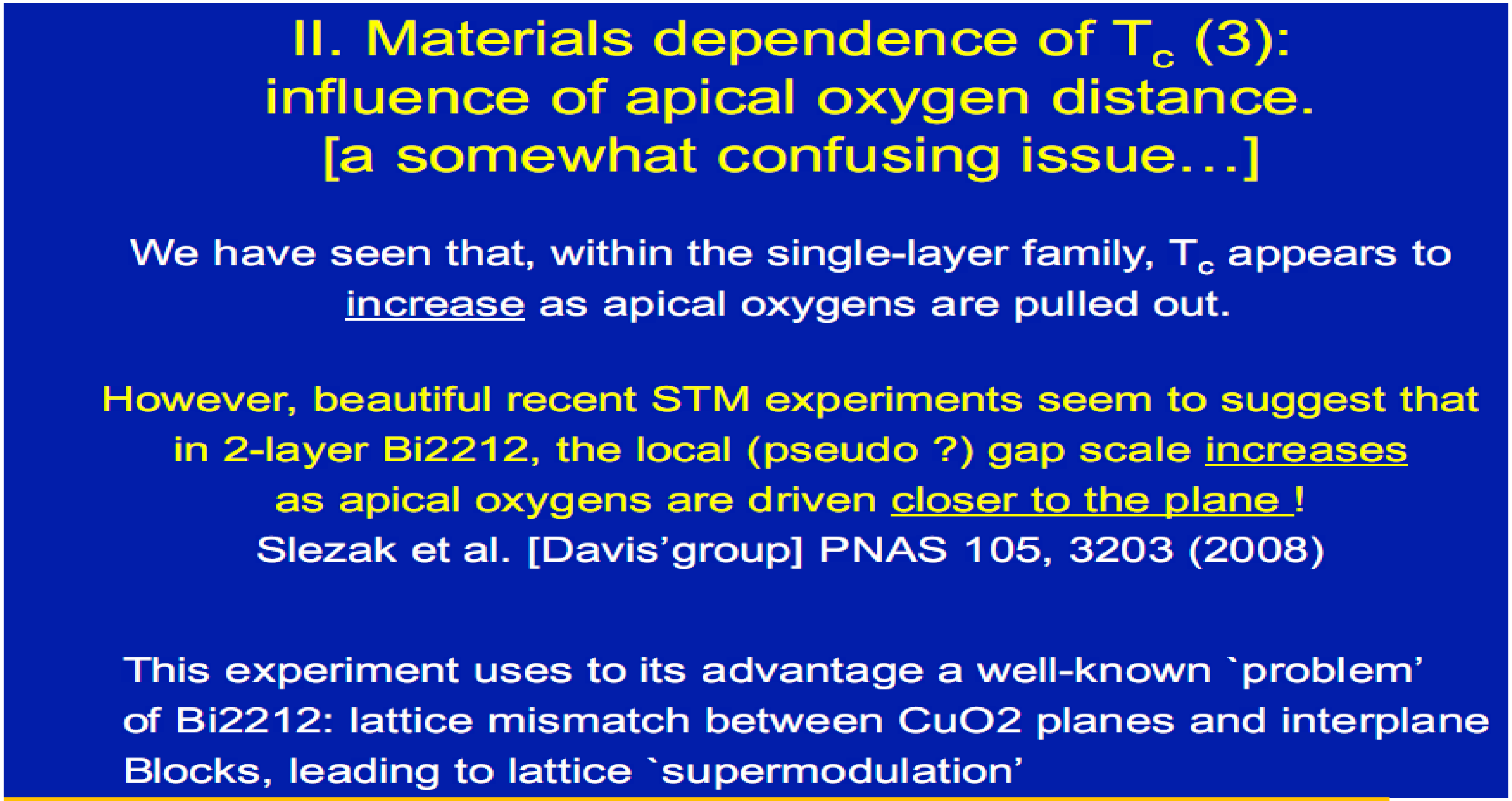
Causation: Reducing ed-ep helps Tc (pushing apical away from the plane)



Increasing tpp’ hurts Tc

Moving the apical oxygen away form the plane reduces ed-ep but also increases tpp’ . We believe the reduction of ep-ed is dominant.

Another difficulty with Andersen’s proposal. [Antoine Georges College de France lectures : cuprates superconducteurs ou en et est on]



II. Materials dependence of T_c (3): influence of apical oxygen distance. [a somewhat confusing issue…]

We have seen that, within the single-layer family, T_c appears to increase as apical oxygens are pulled out.

However, beautiful recent STM experiments seem to suggest that in 2-layer Bi2212, the local (pseudo ?) gap scale increases as apical oxygens are driven closer to the plane !
Slezak et al. [Davis’group] PNAS 105, 3203 (2008)

This experiment uses to its advantage a well-known `problem’ of Bi2212: lattice mismatch between CuO2 planes and interplane Blocks, leading to lattice `supermodulation’

Insight: driving the apical oxygens closer to the plane INCREASES the charge transfer gap , thus making the material locally correlated/ insulating , thus INCREASING the pseudogap scale.

The superconductivity landscape.

- Using two theoretical approaches, ME theory, cluster DMFT, we examined some aspects of the landscape of superconducting systems.
- Interesting spots around the BCS-BEC crossover. [Continuum better than lattice ?] . Instantaneous attractive interaction among particles (and QP)].
- Phonon mediated superconductivity. Tc=40 K in MgB_2. Used two types of phonons and electrons. Still limited in frequency range.
- Electronic superconductivity. Requires spatial structure of the interaction among (electrons ? QP ?)
- Control parameter, charge transfer gap. Can we improve beyond what has been found so far ?
- Possible roles of momentum space differentiation. 1) avoiding alternative instabilities that would have occurred in a more uniform situation. 2) achieve larger coupling by focusing it on smaller number of electrons ?
- McMillan Formula and the Material Design issue. Formulae in terms of renormalized parameters are not that useful. Needed, formula in terms of bare parameters that can be controlled.

Since MgB2 many superconductors have been recognized as having two gaps.