Boson Induced Pairing:Horses and Zebras

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CLASSES OF SUPERCONDUCTORS

[1] BCS: conventional metals, C60, some organics, doped semiconductors, MgB2, …

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[2] EXOTIC: copper oxides, heavy fermion metals, some organics,

(Fe,Ni) oxypnictides ?, …

CURRENT SITUATION

CLASS [1]--- ELECTRON PAIRS
PAIRING INDUCED BY EL-PH INTERACTIONS

ALL EXPERIMENTS EXPLAINED

CLASS [2]---ELECTRON PAIRS

MANY THEORIES

BUT NO CONSENSUS ON THE MECHANISM

OUTLINE

[1] CLASS 1: PREDICTING NEW SUPERCONDUCTORS AND EXPLAINING PROPERTIES.

[2] POSSIBILITIES OF HIGHER TRANSITION TEMPERATURES IN CLASS 1.

[3] CLASS 2: HORSES AND ZEBRAS.

[4] A FEW CONCLUSIONS/COMMENTS.

HOW WELL CAN WE PREDICT THE EXISTENCE OF CLASS 1 SUPERCONDUCTORS AND EXPLAIN THEIR PROPERTIES?

A FEW EXAMPLES

PREDICTING

SEMIEMPIRICAL

GeTe, SnTe, $SrTiO_3$

SEMIEMPIRICAL

GeTe, SnTe, $SrTiO_3$

AB INITIO

high pressure:

sh Si, hcp Si, Ge(?),GaAs,

Nb_3Nb (SEMI-AB INITIO)

PREDICTIONS FOR Si

(Si at high pressures: sh and hcp)

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existence, stability, lattice constants, mechanical properties, electronic structures, phonon properties, electron-phonon coupling,

superconducting Tc's and their pressure dependences

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silicon may be the best understood superconductor!

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Schematic pictures of alkali and alkaline-earth doped C60 fullerides, (a) face-centered cubic phase observed in alkali fullerides A3C60
(A ¼ K, Rb, or mixture of Na, K, Rb, and Cs), (b) body-centered orthorhombic phase observed in Cs4C60, Sr4C60, and Ba4C60, (c) bodycentered
cubic phase observed in alkali fullerides A6C60 (A ¼ K, Rb, or Cs) and alkaline-earth fullerides Sr6C60 and Ba6C60, and (d) A15 phase
observed in Cs3C60 and Ba3C60.

[S.Saito, K.Umemoto, S.G.Loiuie, and M.L. Cohen (2004)]

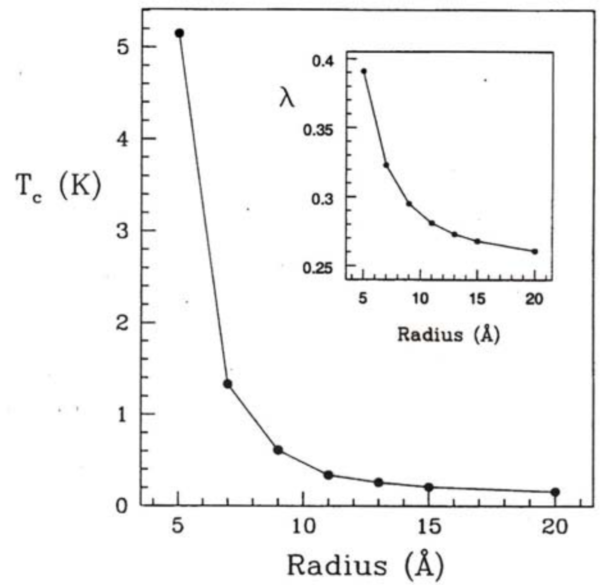
QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

(2008)

Electron-Phonon Coupling and Superconductivity in Carbon Nanotubes

THEORY:

[L. X. Benedict, V. H. Crespi, S. G. Louie and M. L. Cohen, PRB **52**, 14935 (1995)]



- Large curvature of small diameter tubes leads to enhanced λ.

- Tc can be in the range of 10-20 degrees Kevin for diameter d < 5 A.

EXP:

Z.K. TANG et al, Science 292, 2462 (2001)

EXPLAINING

“AFTER THE FACT”

(WITH SOME PREDICTIONS OF PROPERTIES)

Good example: MgB_2

Calculational Methods

Atomic numbers of Mg and B

⇓

Ab initio pseudopotentials for Mg and B

⇓

Density functional theory
(electronic structures of MgB_2)

⇓

Frozen-phonon method (phonon structure) ⇐ Atomic masses of Mg and B

⇓

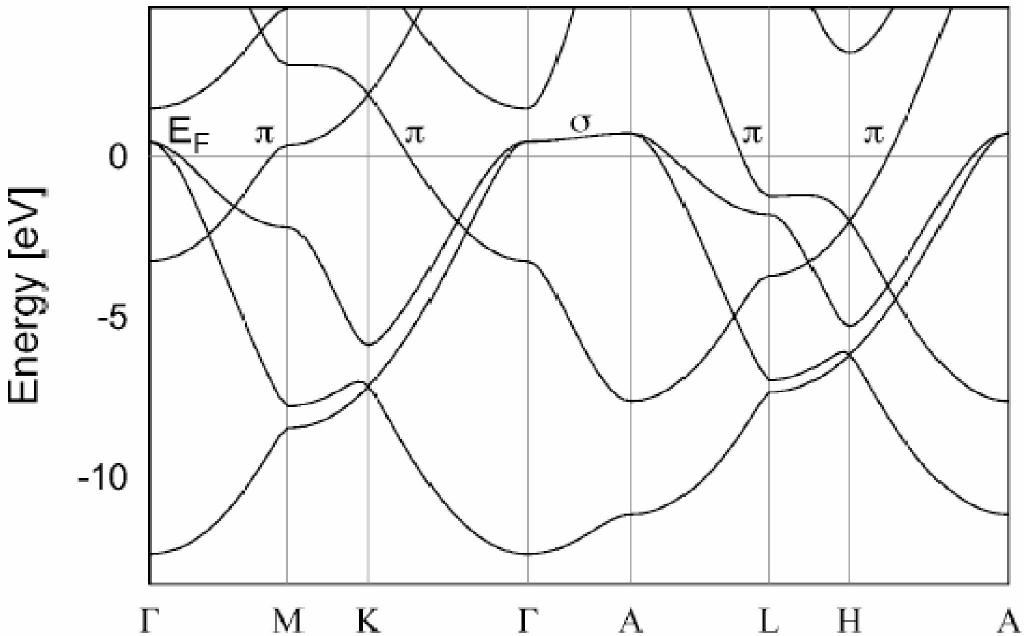
Electron-phonon interactions
(normal-state specific heat)

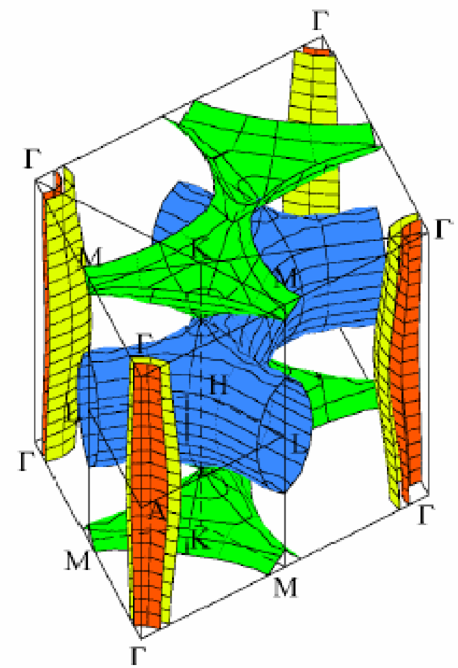
⇓

Eliashberg formalism ⇐ μ^*
(T_c, isotope effect, superconducting gap, specific heat)

Pristine MgB_2: Electronic structures and Fermi surface

- Band structure



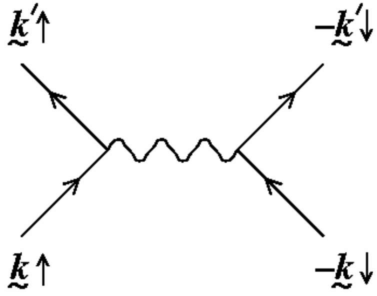


- Fermi surface consists of four sheets:
  two from σ-bonding boron $p_{x,y}$ orbitals
  and two from π-bonding boron p_z orbitals.

Also: An & Pickett, PRL 2001; Kortus, et al, PRL 2001; Liu, et al, PRL 2001;
Kong, et al, PRB 2001; …

Superconductivity in the Eliashberg Formalism

BCS Theory



Electron pairing
via phonon exchange

Main ingredient: momentum– and frequency-dependent Eliashberg function

$$\alpha^2 F(\vec{k},\vec{k}',\omega) \equiv N(\varepsilon_F) \sum_j \left| g^j_{\vec{k}\vec{k}'} \right|^2 \delta(\omega - \omega_{j\vec{q}})$$

where $N(\varepsilon_F)$ = density of states per spin at Fermi level

$g_{\mathbf{kk'}}$ = electron-phonon matrix element

$\omega_{\mathbf{jq}}$ = frequency of phonon in jth branch with **q**=**k**-**k'**

Equivalently:

$$\lambda(\vec{k},\vec{k}',n) \equiv \int_0^\infty d\omega \alpha^2 F(\vec{k},\vec{k}',\omega) \frac{2\omega}{\omega^2 + (2n\pi T)^2}$$

$\lambda = \langle \lambda(k, k', 0) \rangle$

Transition Temperature and Isotope Effect

	harmonic		anharmonic		experiment
	isotropic	anisotropic	isotropic	anisotropic	
T_c	28 K	55 K	19 K	39 K	39 K
α_B	0.42	0.46	0.25	0.32	0.26,0.30
α_{Mg}	0.04	0.02	0.05	0.03	0.02
λ	0.73		0.61		0.58, 0.62
ω_{ph}	62.7 meV		75.9 meV		75.9, 76.9

$\mu^*(\omega_c) = 0.12.$

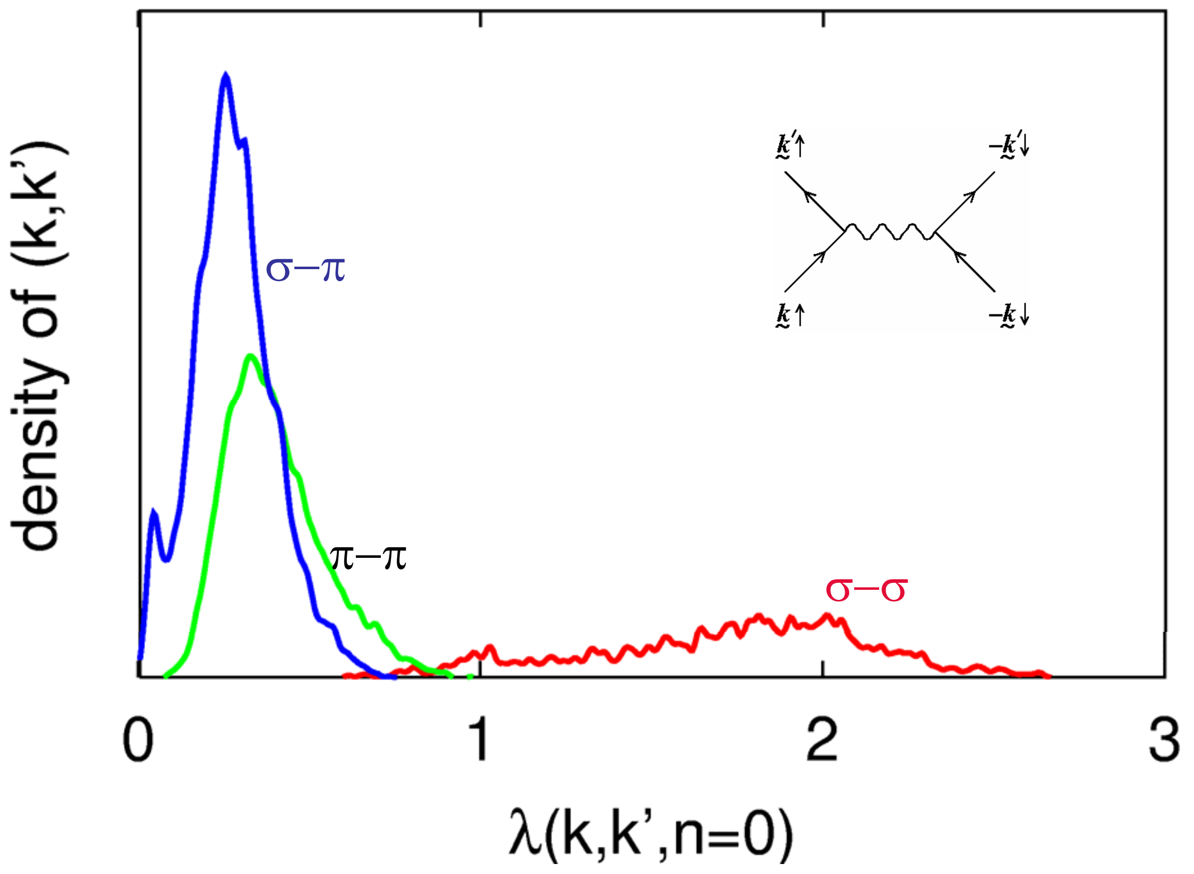
Anharmonicity --> small α_B

λ : averaged electron-phonon coupling.

ω_{ph} : frequency of the in-plane B–B stretching modes (E_{2g}) at Γ.

For $0.10 \leq \mu^*(\omega_c) \leq 0.14$, 41 K $\geq T_c \geq$ 37K

Distribution of Electron-Phonon Couplings

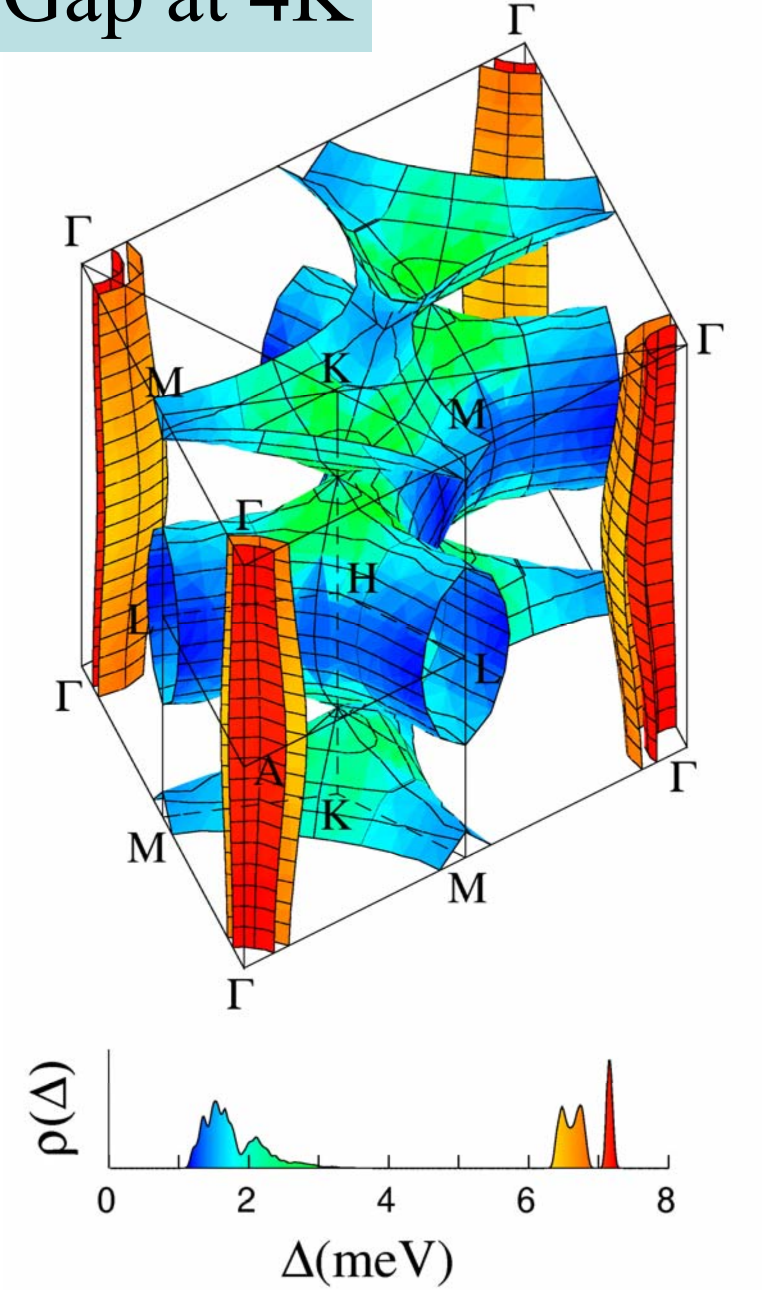


Notes: 1) most metals: $\lambda \sim 0.3$ - 0.5

2) MgB_2: **<λ> = 0.61**; specific heat data λ = 0.58, 0.62

Superconducting Gap at 4K

- $\Delta(\mathbf{k})$ on Fermi surface at T=4 K
- Large gap on cylindrical σ–sheets
- 2 dominant sets of gap values



CLASS [1]

ACHIEVING HIGHER TRANSITION TEMPERATURES

T_c formulas

$$T_c = 1.14\omega_{ph} \exp\left(\frac{-1}{N(0)V}\right)$$ BCS, 1957

$$T_c = \frac{T_D}{1.45} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)$$ McMillan, 1968

$$T_c = \frac{\langle\omega\rangle_{\log}}{1.20} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right) \quad \text{for } \lambda < 1.5$$

$$T_c = 0.183\sqrt{\lambda\langle\omega^2\rangle} \quad \text{for } \lambda > 10,\ \mu^*=0$$

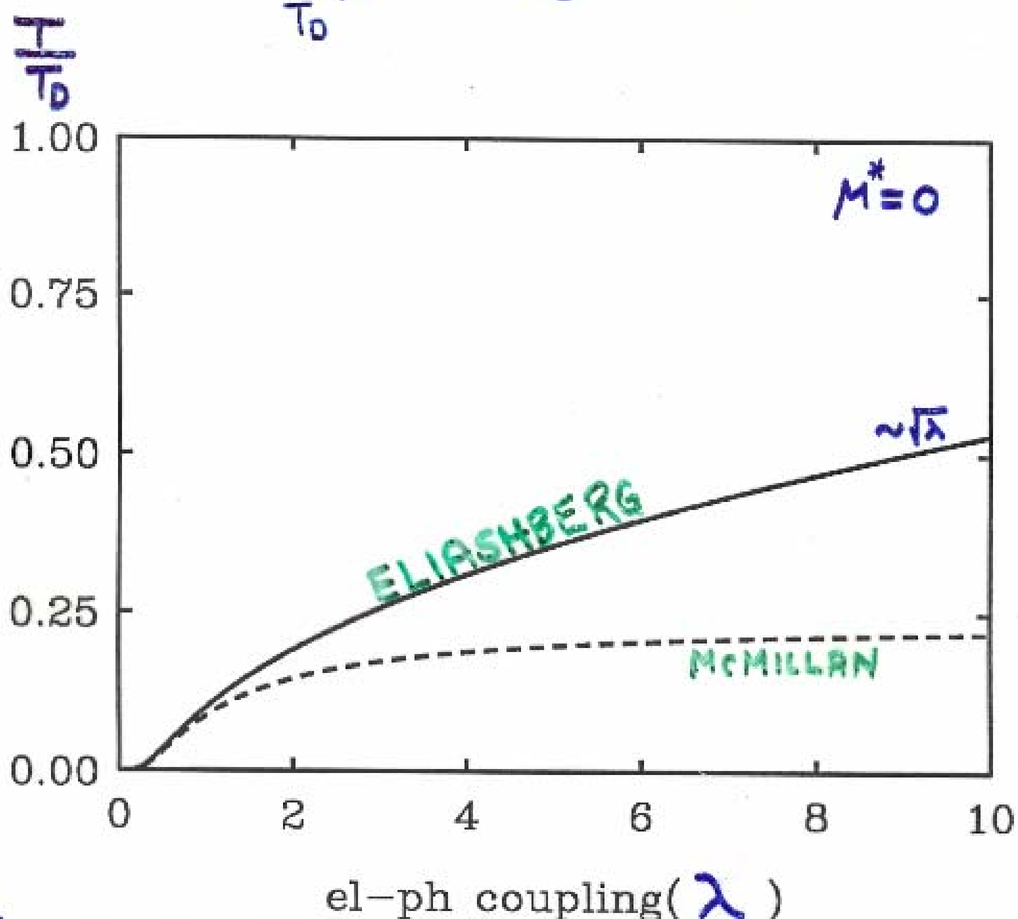
Allen and Dynes, 1975

$$\lambda \equiv 2\int_0^{\omega_{\max}} \alpha^2 F(\omega)\omega^{-1} d\omega$$

+ anisotropic electrons, anharmonic phonons, etc…

McMILLAN 1968

$$\frac{T_c}{T_D} \approx 0.69\, e^{-\frac{1}{\lambda^* - \mu^*}}$$



Kresin–Barbee–Cohen

$$\frac{T_c}{\langle\omega\rangle} = 0.26\,(e^{2/\lambda} - 1)^{-1}$$

AT THIS POINT, WE WANT..,

ROUGHLY SPEAKING

1] LARGE LAMBDAS

2] BUT NOT TOO LARGE TO AVOID INSTABILITIES, THEREFORE WE WANT

“CAGED” STRUCTURES OR OTHERS WITH

LATTICE INTEGRETY ASSURED BY “OTHER BONDS”

TO GO FURTHER, WE NEEDED A MORE QUANTITATIVE ASSESSMENT

Bloch to Wannier Representation

$$g(\mathbf{k},\mathbf{q}) = \sum_{\mathbf{R}_\mathrm{e},\mathbf{R}_\mathrm{p}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}_\mathrm{e}}\, \mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}_\mathrm{p}}\, u_\mathbf{q}\, U_{\mathbf{k}+\mathbf{q}}\, g(\mathbf{R}_\mathrm{e},\mathbf{R}_\mathrm{p})\, U^\dagger_\mathbf{k}$$

Bloch

Wannier

$$g(\mathbf{k},\mathbf{q}) = \sum_{\mathbf{R}_\mathrm{e},\mathbf{R}_\mathrm{p}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}_\mathrm{e}}\, \mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}_\mathrm{p}}\, u_\mathbf{q}\, U_{\mathbf{k}+\mathbf{q}}\, g(\mathbf{R}_\mathrm{e},\mathbf{R}_\mathrm{p})\, U^\dagger_\mathbf{k}$$

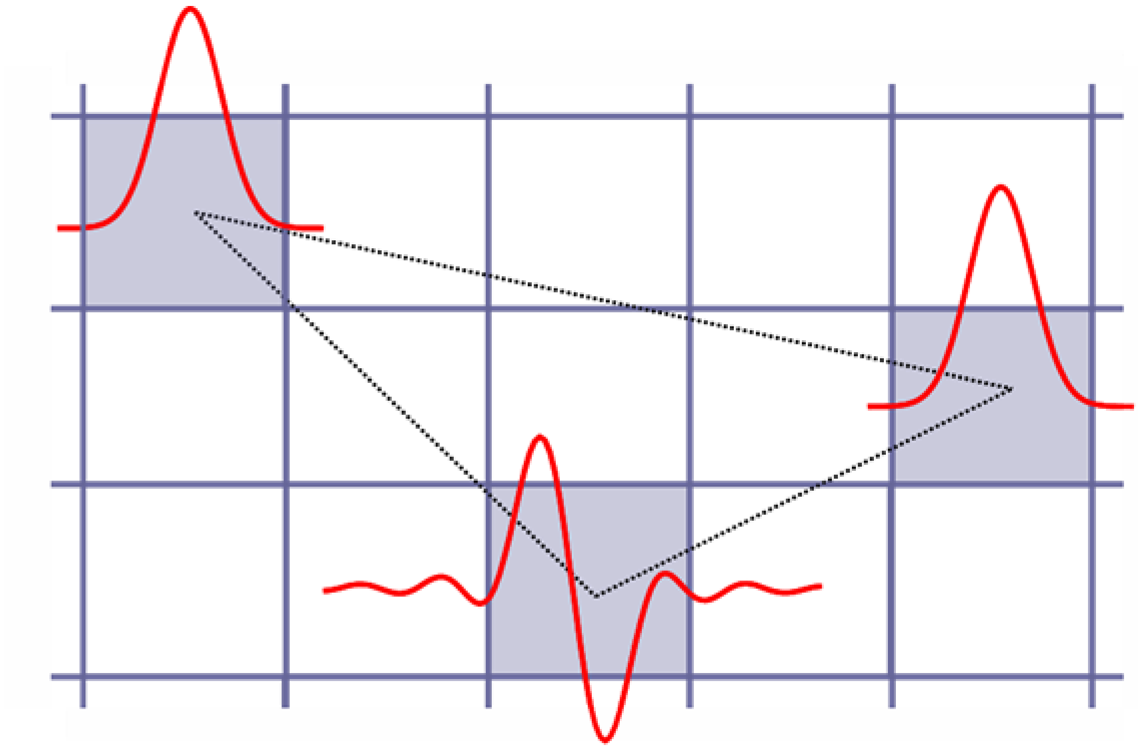
Bloch

Wannier

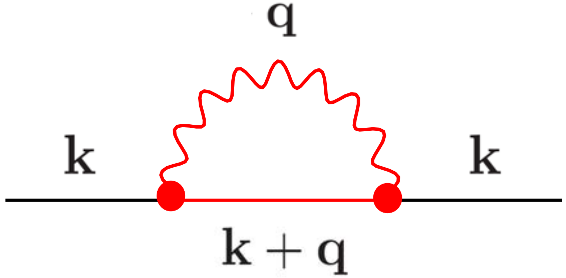
$$\langle m\mathbf{0}_\mathrm{e}|\,\Delta_{\kappa\alpha,\mathbf{R}_\mathrm{p}} V(\mathbf{r})|n\mathbf{R}_\mathrm{e}\rangle$$

Wannier Representation

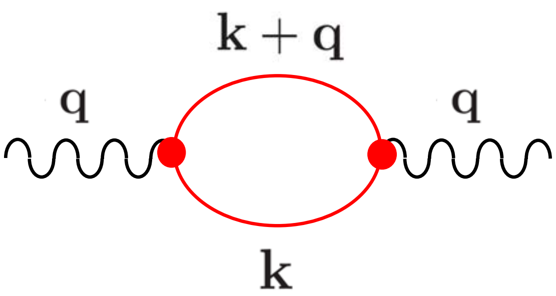
$\langle m\mathbf{0}_{\mathrm{e}}|$ $\quad \Delta_{\kappa\alpha,\mathbf{R}_{\mathrm{p}}} V(\mathbf{r}) \quad$ $|n\mathbf{R}_{\mathrm{e}}\rangle$



Electron and Phonon Self-energy



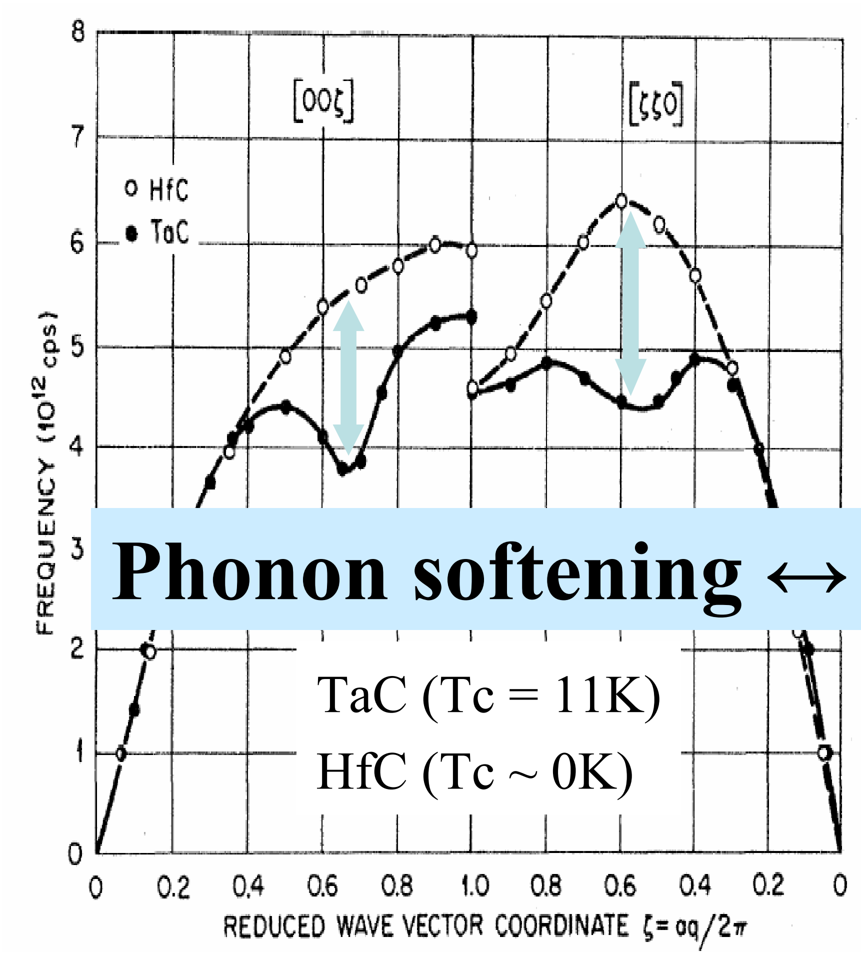
$$\Sigma = i \int \frac{d\,2}{(2\pi)^4} \, |g(1,2)|^2 \, D(1-2) \, G(2)$$

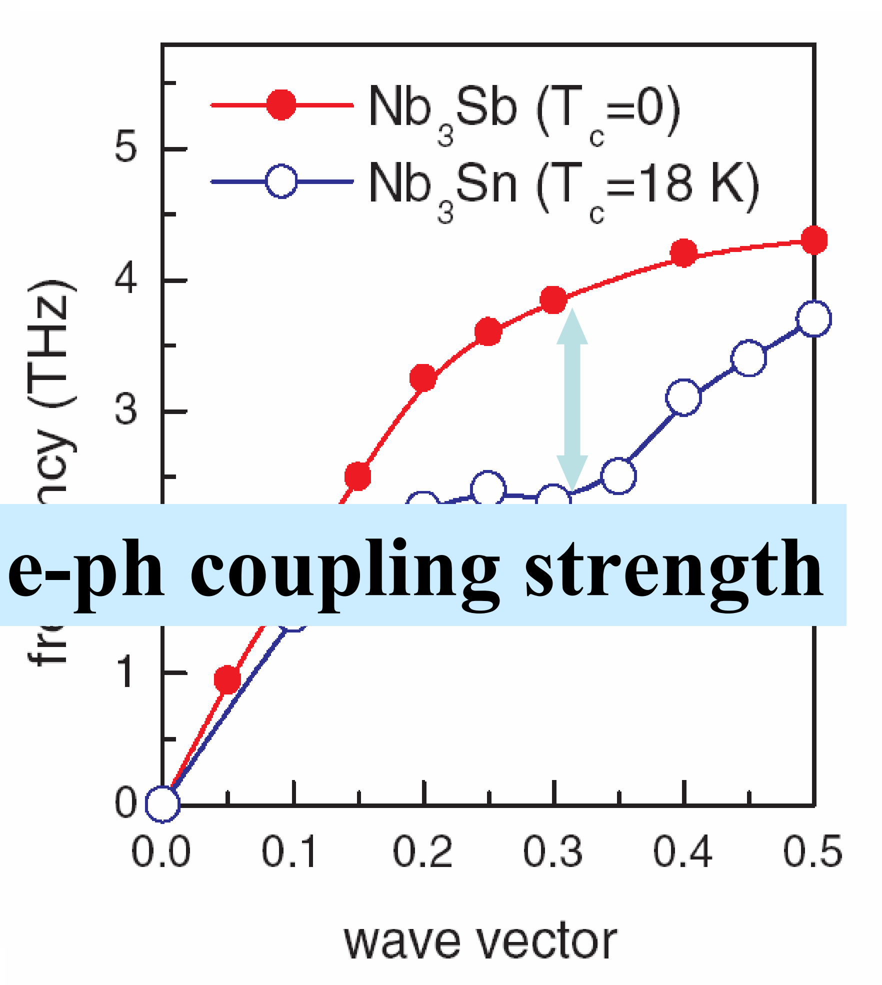


$$\Pi = -2\, i \int \frac{d\,1}{(2\pi)^4} \, |g(1,2)|^2 \, G(1) \, G(2)$$

TaC and HfC

Phonon softening in superconductors





Phonon softening ↔ e-ph coupling strength

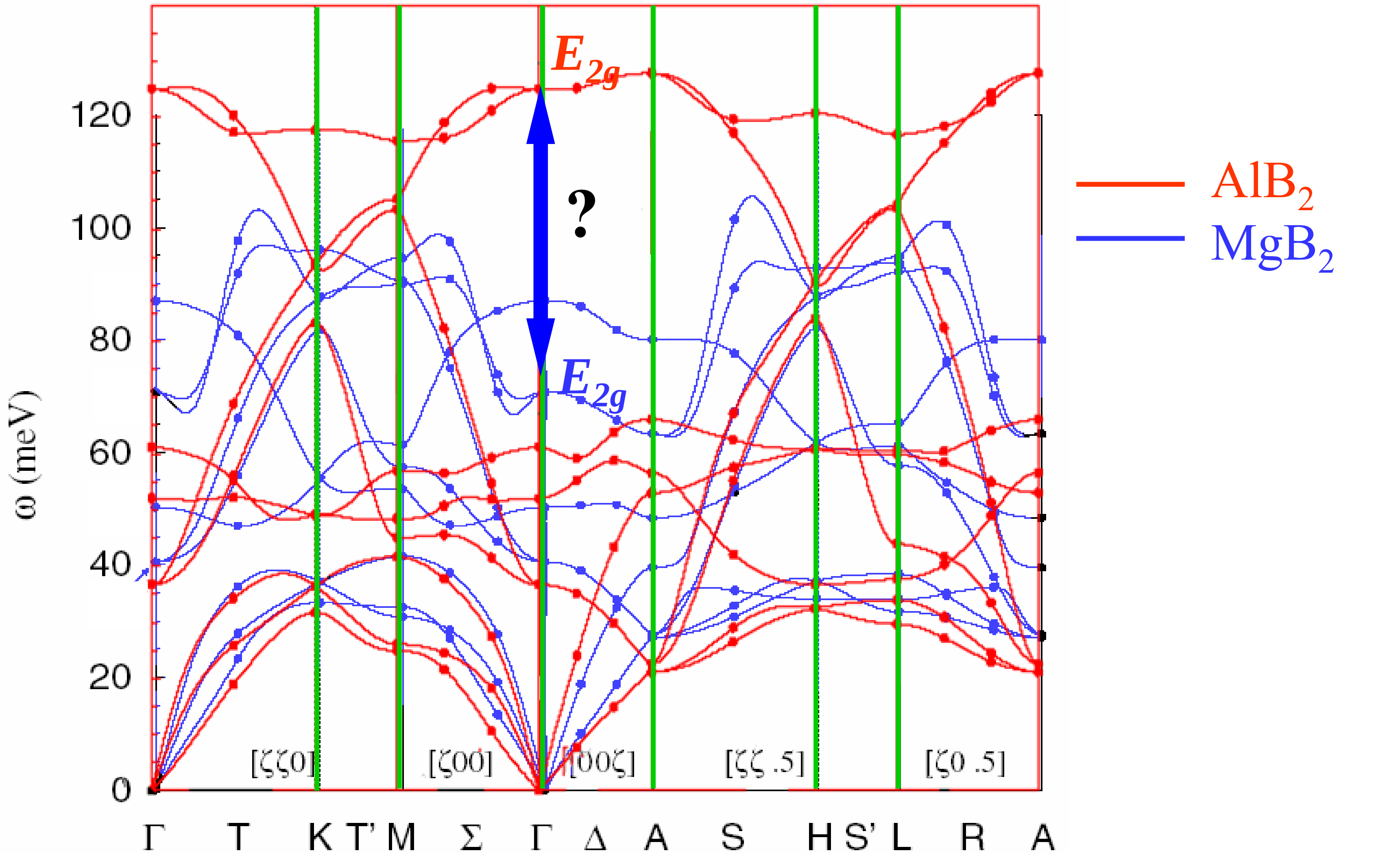
H. G. Smith and W. Glaser, PRL 25, 1611 (1970).

L. Pinstchovius et al., PRL 54, 1260 (1985)
L. Pinstchovius et al. PRB 28, 5866 (1983)
L. Pintschovius, phys. stat. sol. (b) 242, 30 (2005)

WHAT ABOUT MgB_2?

DOPING, PRESSURE, ETC.

E_{2g} phonon in MgB_2 and AlB_2



K. P. Bohnen, R. Heid, and B. Renker, PRL 86, 5771 (2001).

RAISING Tc

WE TRIED TO USE THEORY TO SUGGEST HOW TO INCREASE THE TRANSITION TEMPERATURE OF MAGNESIUM DIBORIDE SIGNIFICANTLY BUT FAILED!

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THIS RESULT IS CONSISTENT WITH EXPERIMENTS UP TO NOW.

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THIS RESULT IS CONSISTENT WITH EXPERIMENTS UP TO NOW.

BUT WE ARE STILL TRYING--RECENTLY WE FIND ABOUT A 10K INCREASE FOR CaB_2 .

CLASS 1

MORE GENERAL CONSIDERATIONS FOR INCREASING T_c

ELECTRON-PHONON COUPLING

$$\lambda\left\langle \omega^2 \right\rangle = \sum_i \frac{\eta_i}{M_i}$$

SO λ CAN BE VIEWED AS THE RATIO OF AN ELECTRONIC SPRING CONSTANT η AND A LATTICE SPRING CONSTANT

Values of η

	η (eV/Å^2)	$0.183\sqrt{\lambda\langle\omega^2\rangle}$(K)	EXP
C (diamond)*	54	290	~ 10
C (graphite)*	48	270	?
BN*	36	240	?
Si*	10	82	~10

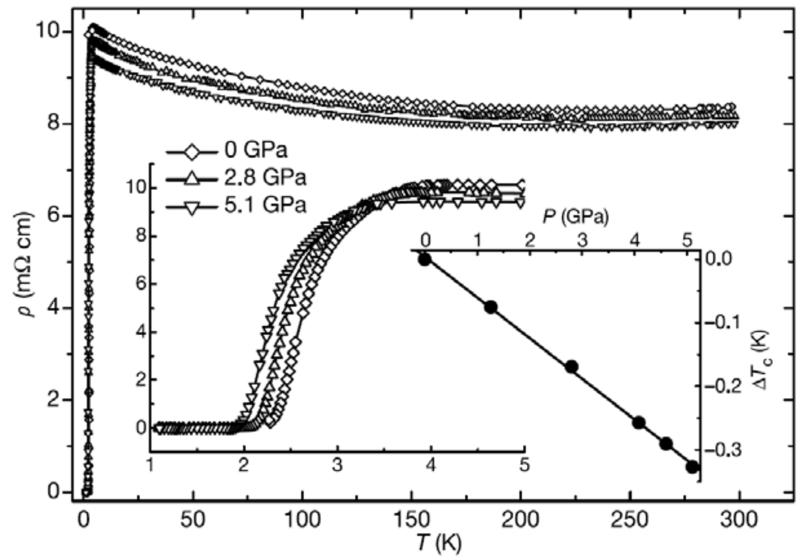
*at peak of η(E)

Superconductivity in diamond

E. A. Ekimov[1], V. A. Sidorov[1], E. D. Bauer[2], N. N. Mel'nik[3], N. J. Curro[2], J. D. Thompson[2] & S. M. Stishov[1]

[1]*Vereshchagin Institute for High Pressure Physics, Russian Academy of Sciences, 142190 Troitsk, Moscow region, Russia*
[2]*Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[3]*Lebedev Physics Institute, Russian Academy of Sciences, 117924 Moscow, Russia*

NATURE | VOL 428 | 1 APRIL 2004 | www.nature.com/nature



CLASS 2

HORSES AND ZEBRAS

WHEN YOU HEAR HOOFBEATS ON THE BRIDGE,

WHEN YOU HEAR HOOFBEATS ON THE BRIDGE,

DON’T THINK OF ZEBRAS

IT IS IMPORTANT TO TEST FOR CLASS [1] SIGNATURES (HORSES)

CUPRATES

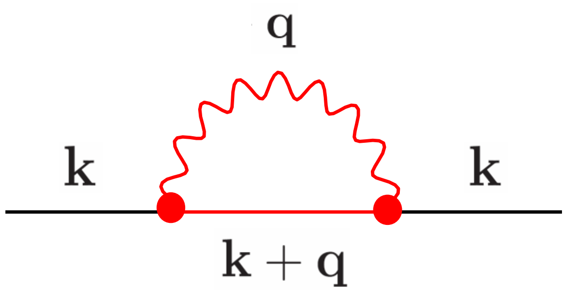
ELECTRONIC STRUCTURE

PHONON ENERGIES

ELECTRON-PHONON COUPLINGS

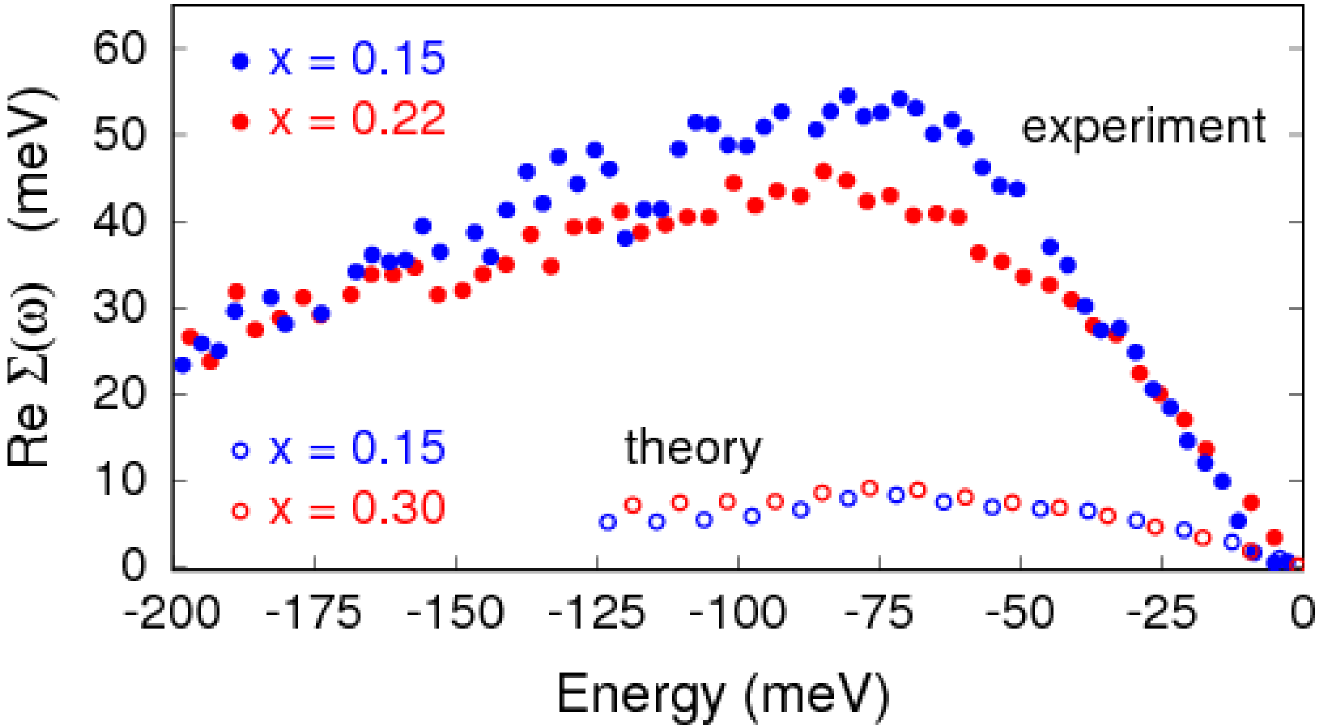
KINKS

Electron Self-energy



$$\Sigma = i \int \frac{d\,2}{(2\pi)^4}\, |g(1,2)|^2\, D(1-2)\, G(2)$$

YIELDS A MASS ENHANCEMENT AND ASSOCIATED "KINK" AT THE FERMI SURFACE."KINKS" HAVE BEEN OBSERVED IN ARPES DATA AND INTERPRETETED AS SIGNATURES OF STRONG ELECTRON-PHONON COUPLING.



x = 0.15
x = 0.22
experiment
x = 0.15
x = 0.30
theory
Re Σ(ω) (meV)
Energy (meV)
60
50
40
30
20
10
0
-200
-175
-150
-125
-100
-75
-50
-25
0

CONCLUSION

BASED ON THE WANNIER FORMALISM FOR CALCULATING ELECTRON-PHONON SELF-ENERGIES, THE COUPLING IS 1/7 OF WHAT IS NEEDED TO REPRODUCE THE OBSERVED ARPES “KINKS”

IT IS IMPORTANT TO TEST FOR CLASS [1] SIGNATURES (HORSES)

PNICTIDES

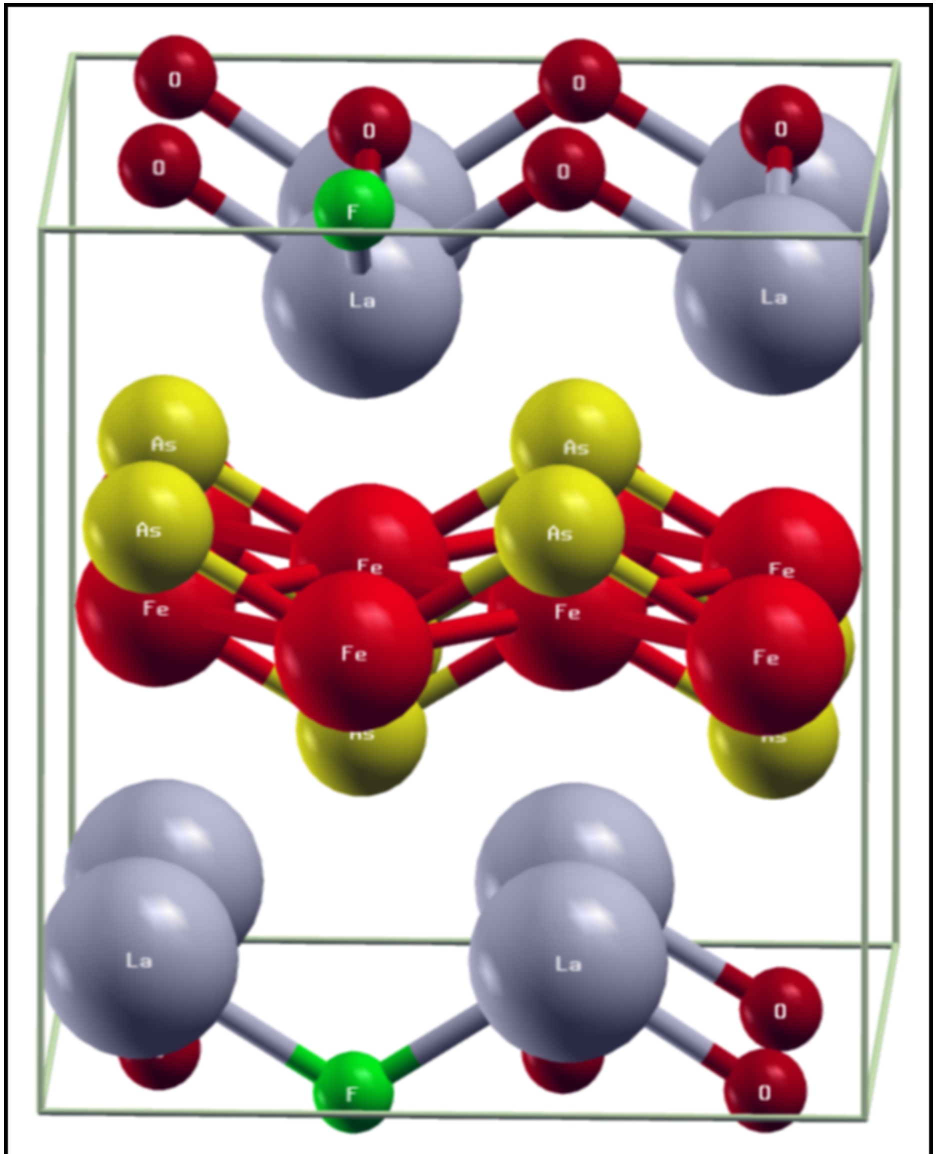
ELECTRONIC STRUCTURE

(LDA, SPIN POL GGA)

PHONON ENERGIES

(BOTH CALCULATED WITH AND WITHOUT DOPING USING A VIRTUAL XTAL AND A SUPERCELL APPROACH)

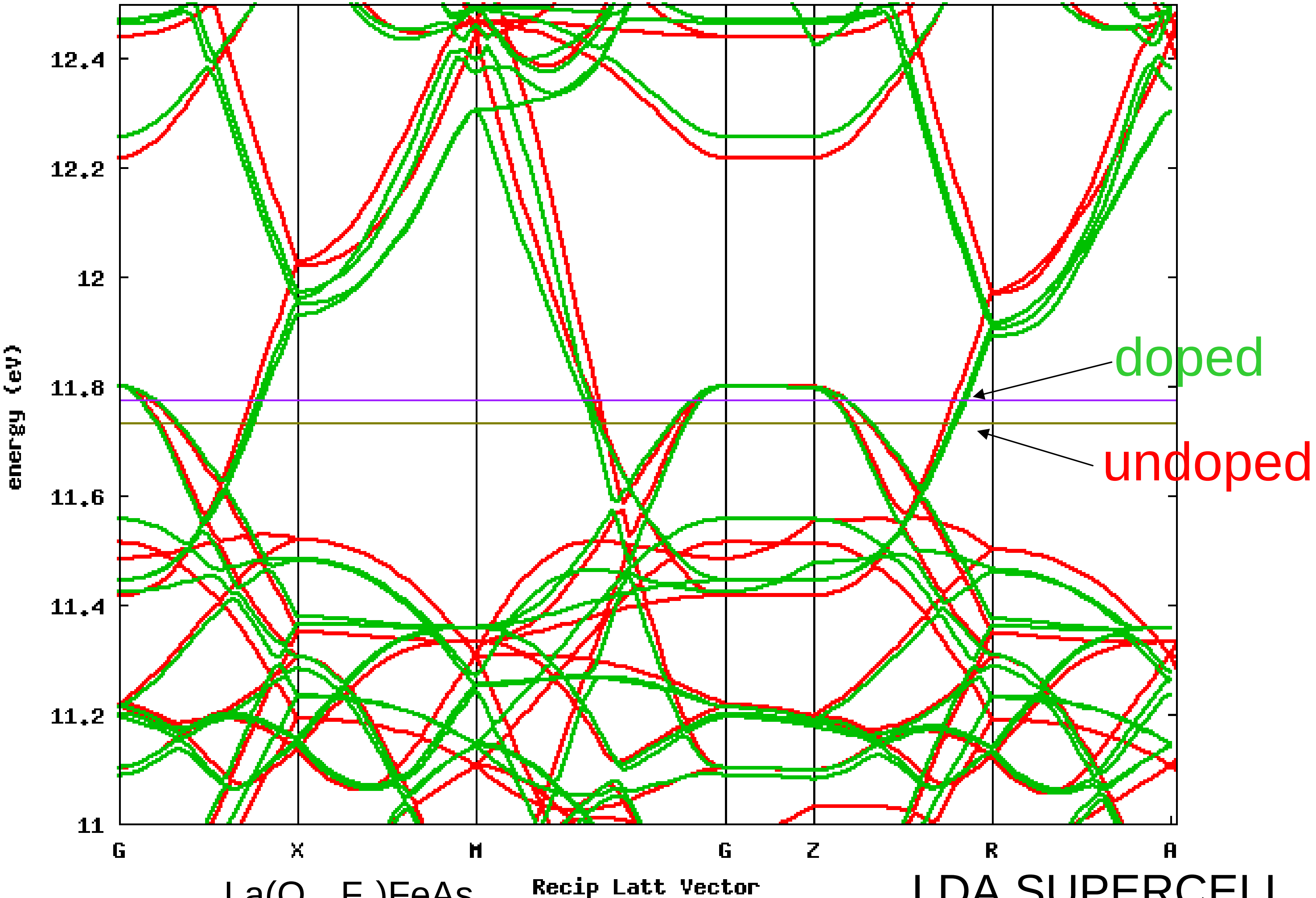
ELECTRON-PHONON COUPLINGS



$La(O_{1-x}F_x)FeAs$

$x = 0.125$

32 ATOM CELL



$La(O_{1-x}F_x)FeAs$

LDA SUPERCELL

Difference in Planar Integrated Charge Density Along z-axis When Doped

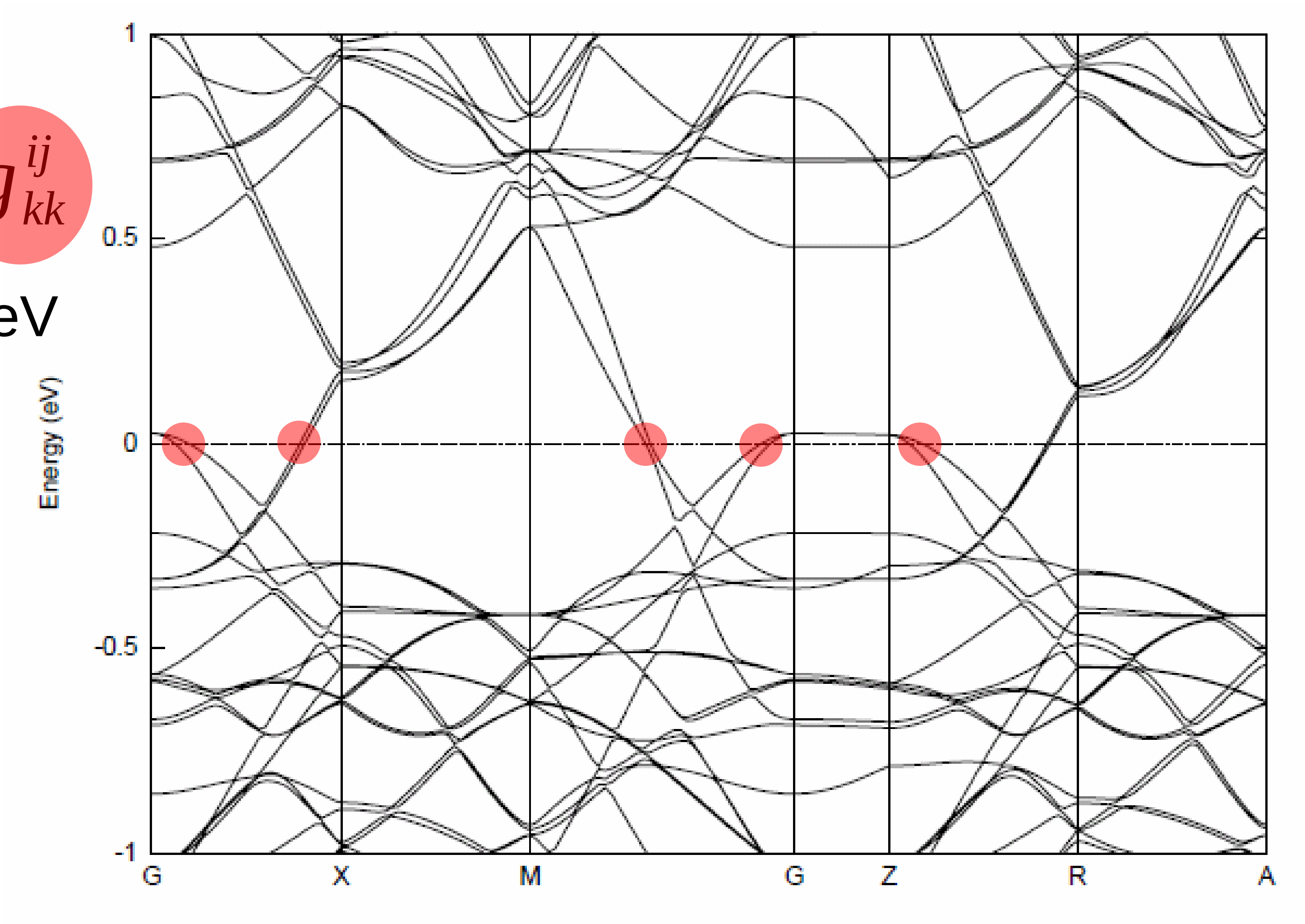
QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Noffsinger et al

ELECTRONIC STATES COUPLED TO PHONONS

Maximum g_{kk}^{ij}

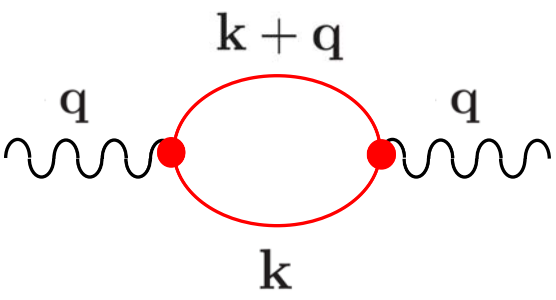
$= 20 \pm 7$ meV



TENTATIVE CONCLUSIONS FOR LAMBDA

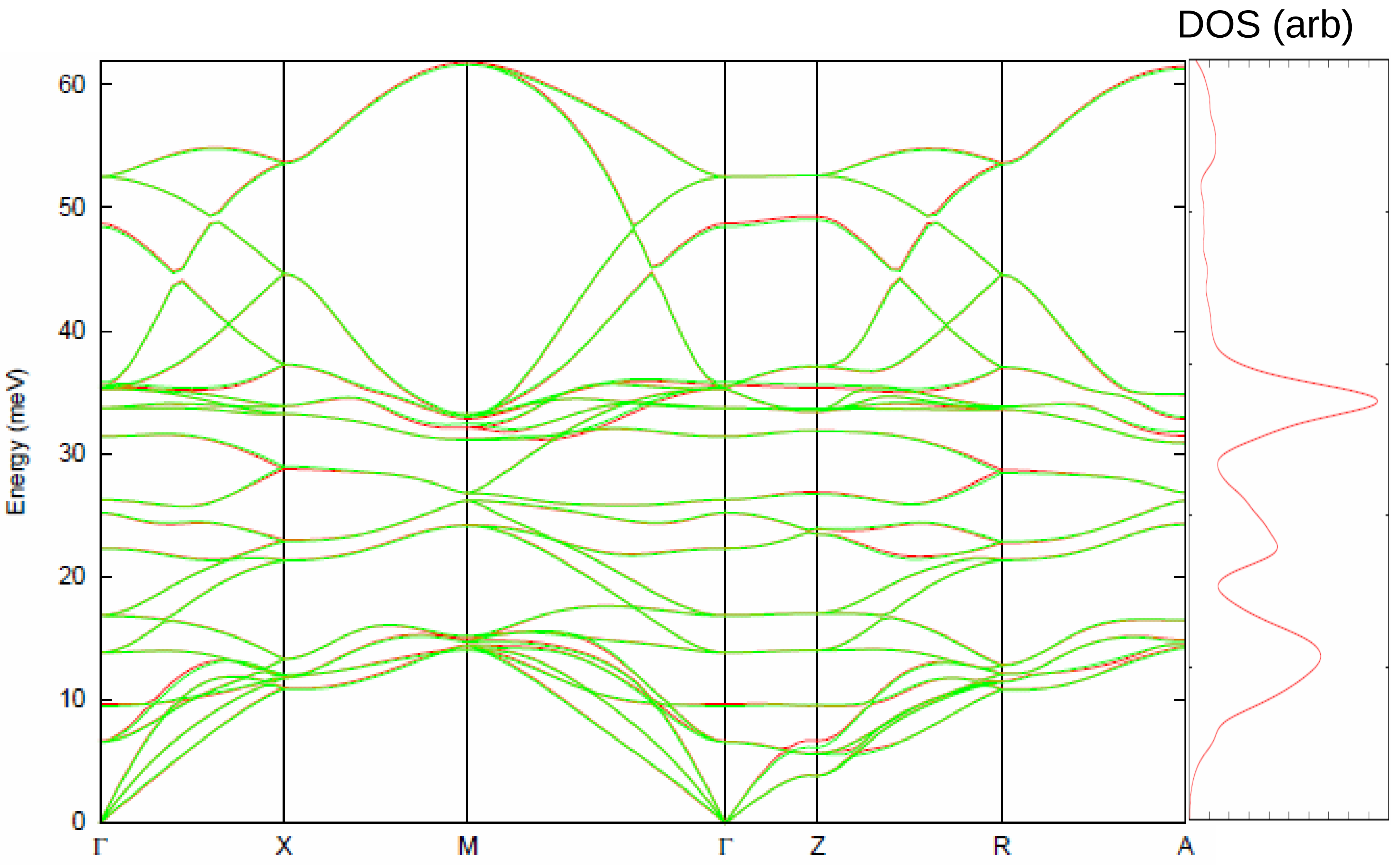
BASED ON THESE CALCULATIONS OF THE ELECTRON-PHONON g’s, OUR ESTIMATES OF LAMBDA (~0.18) ARE IN LINE WITH THOSE CALCULATED BY OTHERS USING A VIRTUAL CRYSTAL MODEL.

What about Phonon Self-energies?



$$\Pi = -2\,i \int \frac{d\,1}{(2\pi)^4}\,|g(1,2)|^2\, G(1)\, G(2)$$

Phonon Dispersion: Red = undoped, green = 12% rigid band doped



EXPERIMENT

M. Le Tacon, M. Krisch, A. Bosak, J.-W. G. Bos, S. Margadonna, arXiv:0809.2898

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

THEORY

Noffsinger et al

TENTATIVE CONCLUSIONS FOR DOPING SHIFTS IN PHONONS

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TENTATIVE CONCLUSIONS FOR DOPING SHIFTS IN PHONONS

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2] IT IS INTERESTING THAT SOME OF THE DOPING SHIFTS (e.g. SOFTENING) OCCUR FOR THE LOWER FREQUENCY PHONONS (BY INFLUENCING THE BONDS TO THE HEAVIER ELEMENTS) IN ADDITION TO THE MORE OR LESS EXPECTED CHANGES SEEN FOR THE HIGHER OXYGEN FREQUENCIES.

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3] THE SHIFTS DO NOT APPEAR TO ARISE FROM STANDARD EL-PH SELF-ENERGY THEORY VIA INCREASED ELECTRON CONCENTRATION.

GENERAL CONCLUSIONS/COMMENTS

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1) CLASS [1] IS UNDERSTOOD AND SHOWS PROMISE FOR HIGHER Tc.

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3) CAUTIONS FOR BOSON MECHANISMS

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CAUTIONS FOR BOSON MECHANISMS

1] WATCH BOSON RENORMALIZATION AND STABILITY.

2] BE CAREFUL IF YOUR MODE IS TRANSVERSE (e.g. EXCITONS).

3] LOCAL FIELDS ARE IMPORTANT.

4] THE Q-DEPENDENCE IS CRUCIAL FOR AN ATTRACTIVE INTERACTION TO WORK (e.g. DEMONS).

GENERAL CONCLUSIONS/COMMENTS

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1) CLASS [1] IS UNDERSTOOD AND SHOWS PROMISE FOR HIGHER Tc.

2) THE Fe SYSTEMS PROBABLY BELONG IN CLASS [2].

3) CAUTIONS FOR BOSON MECHANISMS

4) CLASS [2] HAS INTRODUCED INTERESTING NEW PHYSICS, BUT THERE IS NO AGREEMENT ON THE THEORY AS YET. ZEBRAS APPEAR LIKELY, BUT MULES (HYBRIDS) MAY BE POSSIBLE.

"Can we start over? Like, from 1987, say?"

• •

THE END

1. In the case of electron-electron interactions, is the concept of a pairing "glue" even meaningful?   YES

2. If your theory advocates an instantaneous interaction, does this mean the pairs have no dynamics, or just that the theory has not developed to the extent to address this question? RETARDED

3. If your theory ignores phonons, can you really get away with that? Do you think phonons are even relevant? NO, YES

4. What is the spectroscopic signatures predicted for your theory? Is a McMillan-Rowell inversion or related procedure possible for your theory? Is this question meaningful? YES

5. What would your theory predict in regards to collective modes? Is this even an important question? NO