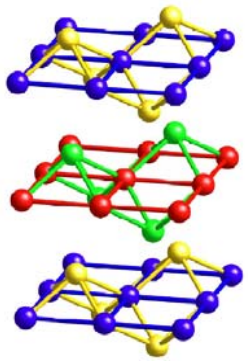
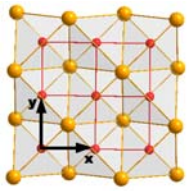


Electronic Structure of Fe-based superconductors: Magnetism and electron-phonon interaction

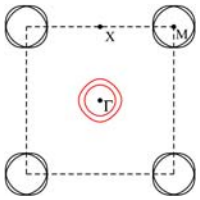
L.Boeri, O.V. Dolgov, O.K. Andersen,
MPI-FKF, Stuttgart, Germany
A.A. Golubov, *Univ. Twente, the Netherlands*
M. Calandra, F. Mauri, *UPMC, Paris, France*
I.I. Mazin, *NRL Washington, USA*

KITP, Santa Barbara, 17/1/2011

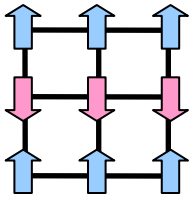
DFT in Fe-based superconductors: What is special?



Chemistry:
Two details are crucial: presence and geometry of Fe(Pn/Ch) planes + band filling (d^6).

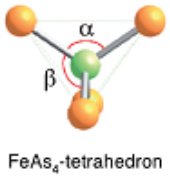


Non-magnetic (NM) Electronic Structure:
Presence of strongly nested hole-electron pockets, with nearly free-electron like masses.



Magnetism:
LSDA gives the correct AFM ground state; the value of the magnetic moment, and the doping dependence, is overestimated.

WHY?

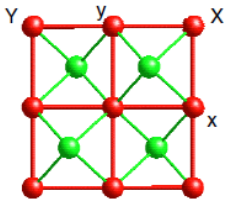


$FeAs_4$-tetrahedron

Lattice Properties:
The e-ph coupling estimated in the NM case is weak; BUT there is a strong sensitivity of the lattice properties to magnetism and vice-versa.

What are the consequences on the e-ph interaction?

Non-magnetic Electronic Structure

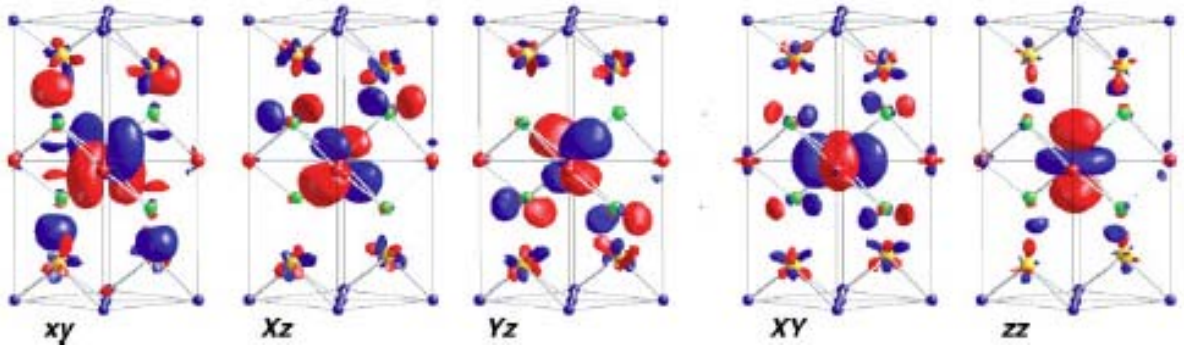


Geometry of the Fe-As planes:

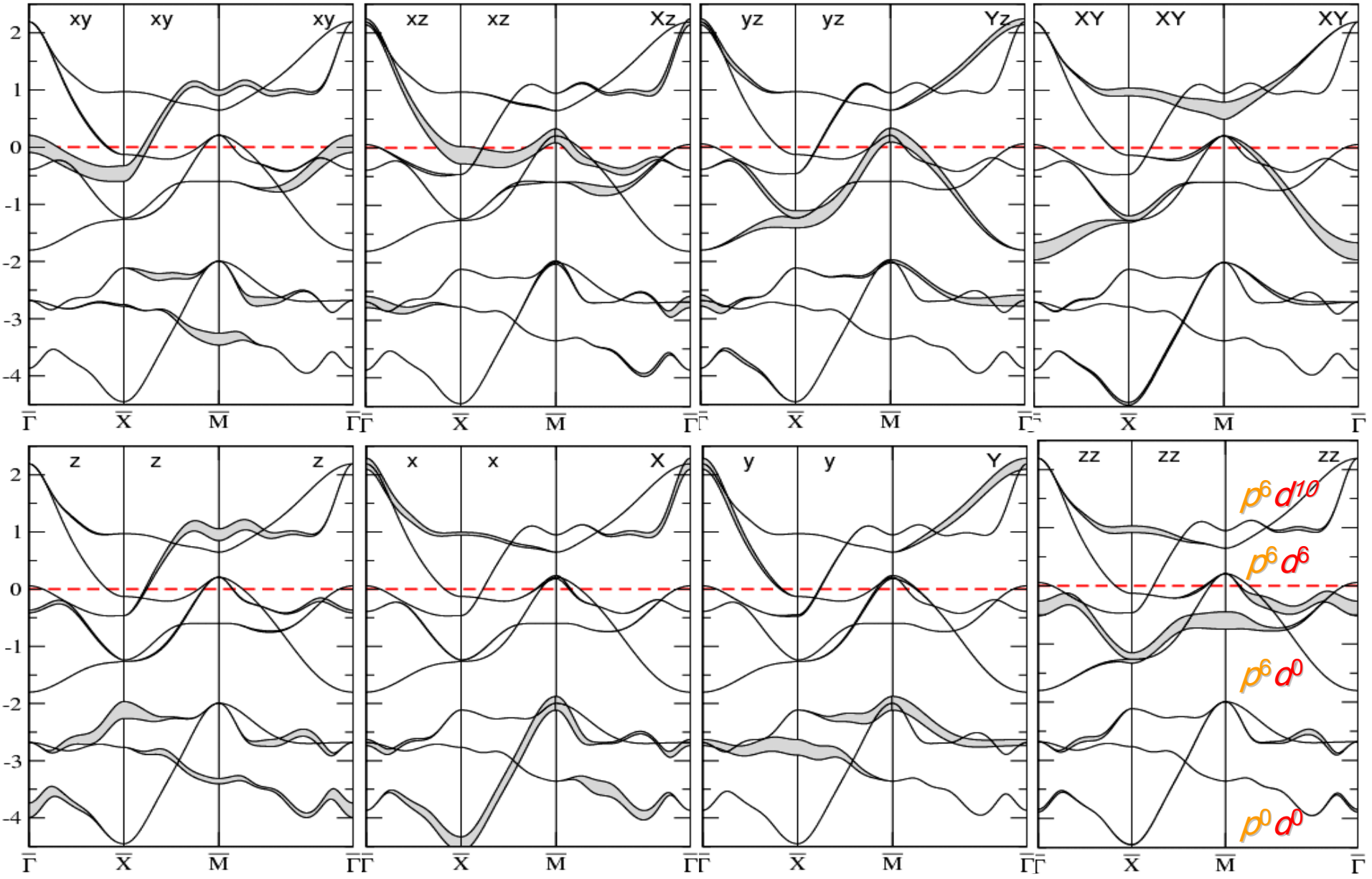
d-p + direct *d-d* hopping

d-p hopping is large and sensitive to tetrahedral distortion

+ small (e-t) crystal field splitting (max crystal field splitting is (e-t) is 0.2 eV).

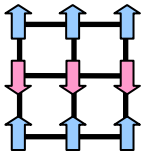


Long hopping ranges due to incomplete pairing of orbitals, i.e. the bonding is partly covalent and partly metallic.



Non-magnetic band structure of LaOFeAs, from ab-initio p-d TB model.

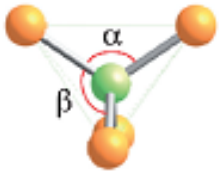
DFT, magnetism:



The ground state is a **striped AFM metal (m~2.0 μ_B).**
The **magnetic** transition is accompanied by a **structural** distortion.

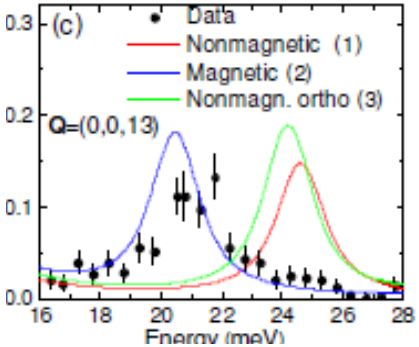
GOOD, BUT

Electrons: The tendency to magnetism is **overestimated** in DFT; the calculated magnetic moments are 2-5 times larger than those measured by neutrons, μ_{SR}; magnetism survives at high dopings, where the samples are **paramagnetic**.



$FeAs_4$-tetrahedron

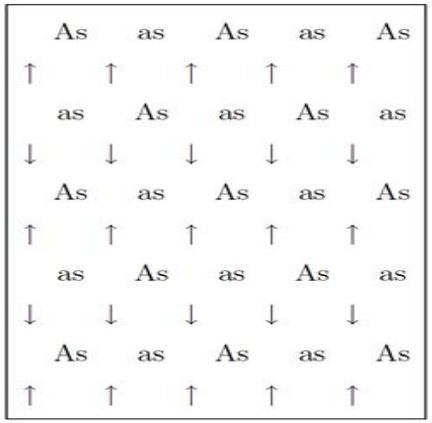
Structure: DFT calculations reproduce the "right" exp structure only if large magnetic moments are present; the $FeAs_4$ **tetrahedral angle** is very sensitive to the value of the magnetic moment.



Phonons: Phonon frequencies of both paramagnetic and SDW samples are well reproduced only from spin-polarized calculations with large magnetic moments…

Zbiri et al., PRB 2008; Yildirim, Physica C 2009, Reznik et al., PRB 2009

How can we understand the LSDFT magnetic response?



$$\mathbf{H}_{stripe} = \begin{bmatrix} \mathbf{H}(k_x, k_y) & \frac{1}{2}\mathbf{\Delta} \\ \frac{1}{2}\mathbf{\Delta} & \mathbf{H}(k_x, k_y + \pi) \end{bmatrix}$$

SDW Hamiltonian

$$\text{with } \mathbf{\Delta} = \Delta \times \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

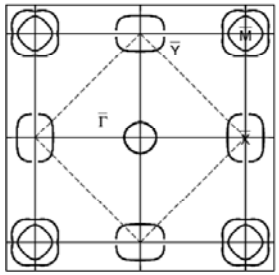
Exchange splitting

$$m(\Delta) = \sum_{\alpha=1}^{5} m_\alpha(\Delta) = \sum_{\alpha=1}^{5} \sum_{i\mathbf{k}} c_{\alpha,i\mathbf{k}} c^*_{\alpha,i\mathbf{k}+\mathbf{Q}} \qquad \Delta = m(\Delta)\, I$$

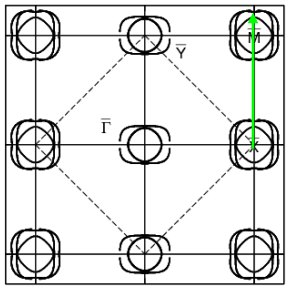
Magnetic moment

Self-consistency condition

I is the Stoner- or Hund's-rule exchange coupling constant for Fe

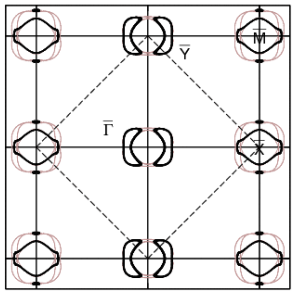


1) Start from PM bands

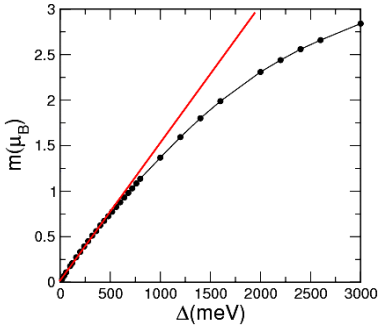


2) Fold in …

q



3) Couple with Δ…

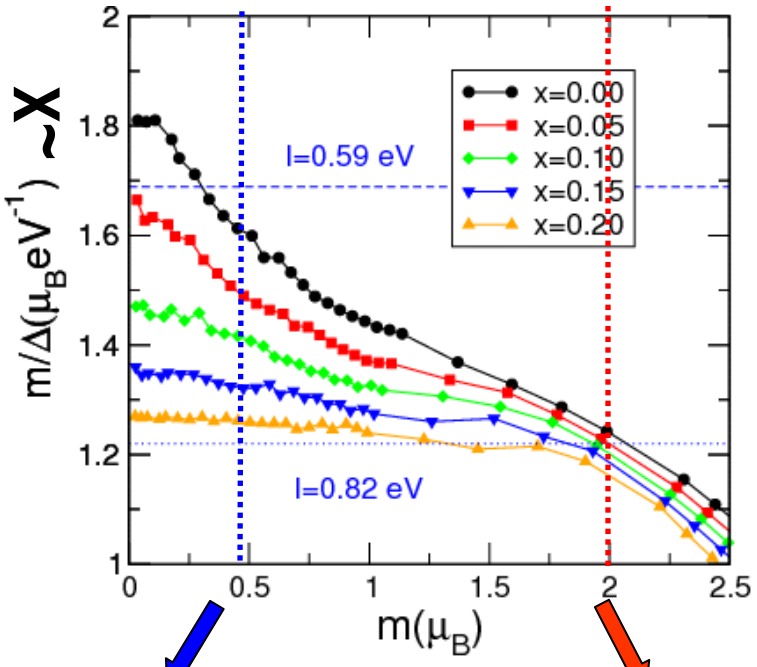


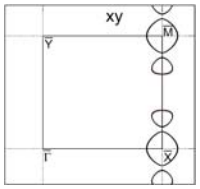
4) Compute $m(\Delta)$

5) Solve $m(\Delta) = \Delta/I$

Itinerant Magnetism: linear response and strong-coupling regime

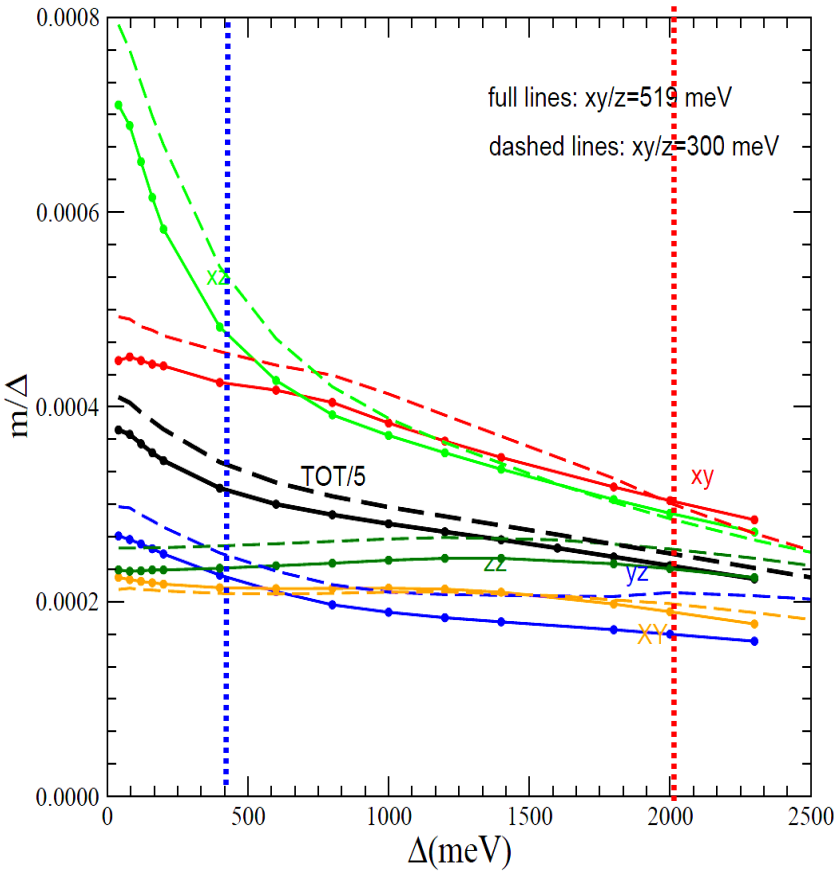
$$\Delta = mI$$





Linear response (nesting)

Intermediate couping (LSDFT)



Orbital polarization is small and decreases with Δ !

In summary…

Non-Magnetic Electronic Structure: **Long-range p-d interactions +Small crystal field splittings:** hard to extract localized TB models of the band structure with less than 5 d orbitals; strong sensitivity of the band structure to tetrahedral angle.

Magnetism: LSDFT corresponds to an **intermediate coupling** regime **–** no nesting in strict sense; Orbital polarization is moderate -> hard to extract localized models.

What can we say about superconductivity?

Spin Fluctuations:

Mostly sensitive to intra-orbital χ of bands near E_F: Strong material dependence!

Mazin et al., PRL 2008, Kuroki et al., PRL 2008, Korshunov and Eremin, PRB 2008, Graser, Maier, Hirschfeld, Scalapino PRB 2008

Electron-Phonon Coupling:

Intrinsically weak due to non-bonding character of bands at EF;

Boeri et al., PRL 2008; *Mazin et al., PRL 2008; Subedi et al., PRB 2008.*

BUT

could be relevant for orbital fluctuation models, or to "switch" between almost degenerate gap symmetry solutions...

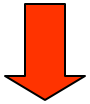
What can we say about the magnitude of the e-ph interaction in Fe pnictides?

Step 0 (2008): Estimate the magnitude of the e-ph coupling in the **non-magnetic state**; The coupling is low -> WHY?

BUT

The description of the lattice properties in non-spin polarized calculations is bad

The description of the lattice properties in spin-polarized calculations with large moments is good..



Local moment scenario

Step 1 (2010): Estimate the magnitude of the e-ph coupling in the **AFM state**; understand the relation between phonon softening, e-ph coupling, sensitivity of the magnetic moments to the crystal structure.

Step 2 (2010): Construct a model for the **Paramagnetic** state.

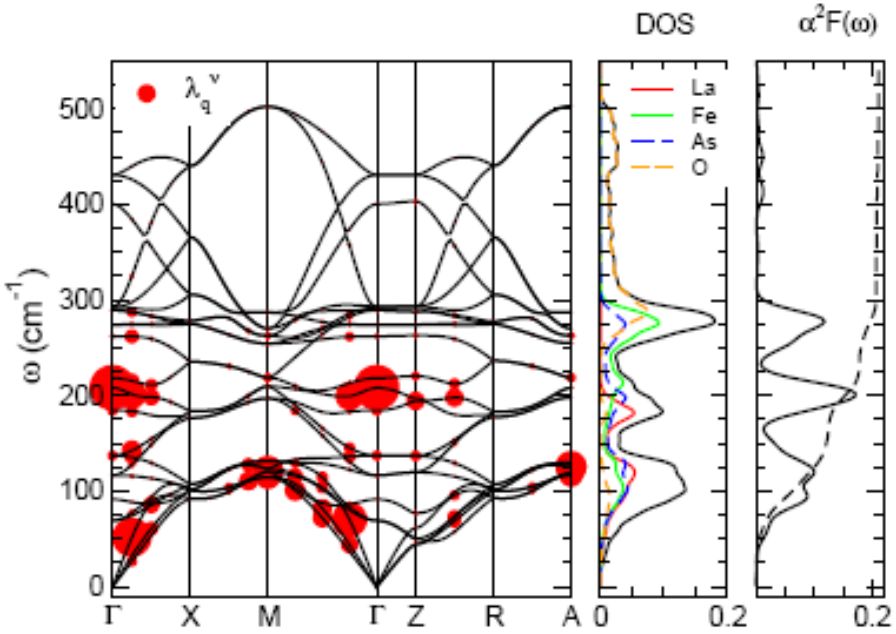
Step 0: Estimate the coupling in the NM state:

PRL 101, 026403 (2008) PHYSICAL REVIEW LETTERS week ending 11 JULY 2008

Is $LaFeAsO_{1-x}F_x$ an Electron-Phonon Superconductor?

L. Boeri,[1] O. V. Dolgov,[1] and A. A. Golubov[2]

NO!



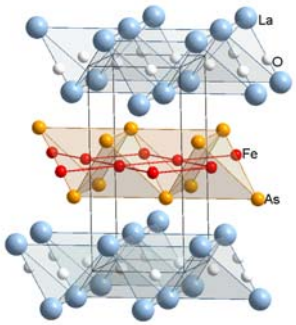
$$\lambda = 0.21$$
$$\omega_{\log} = 206K$$
$$T_c^{ME}(\mu^* = 0) = 0.5K$$

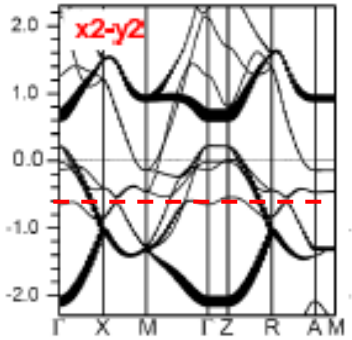
- The coupling is uniformly distributed over Fe-As modes.
- E-ph interaction: λ~0.2 is too small to account for T_c
- N(0) is large, λ is small because of **small e-ph matrix elements**.

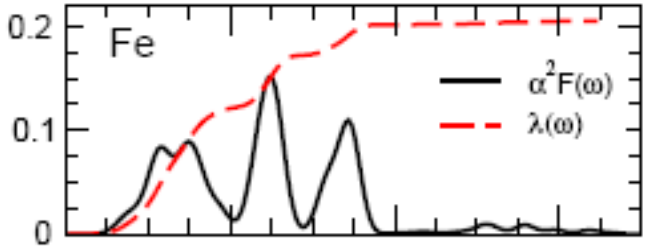
See also Mazin et al, PRL 2008, A. Subedi et al, PRB 2008, J. Nossinger et al, PRL 2009

... and what about phonons: why is the coupling so small ?

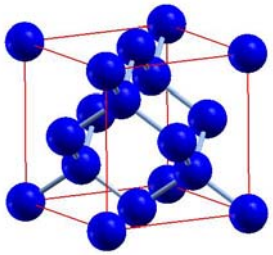
Because the only bands derived from ***directed Fe-Fe bonds*** *sit* ***far*** *from* E_F…

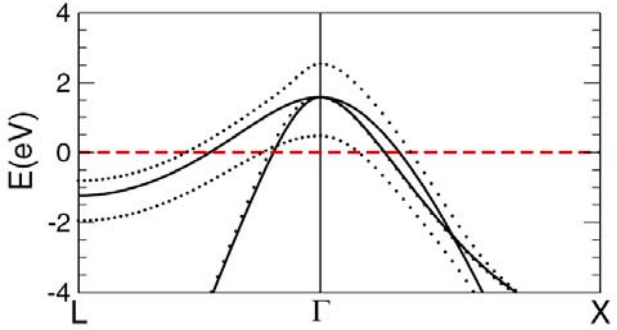


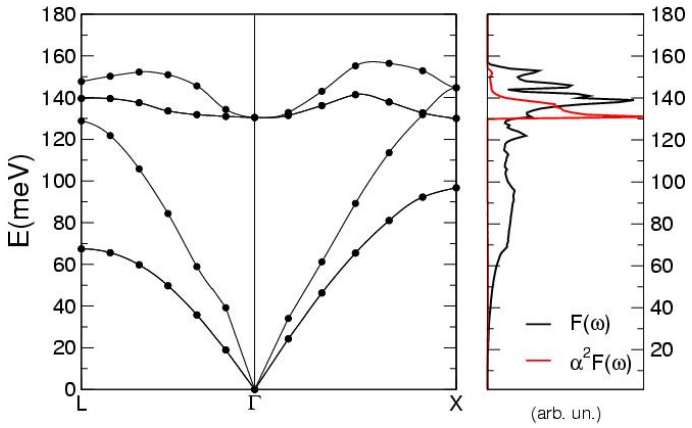




In contrast to good e-ph superconductors, where strongly covalent bonds couple to bond-stretching phonons…



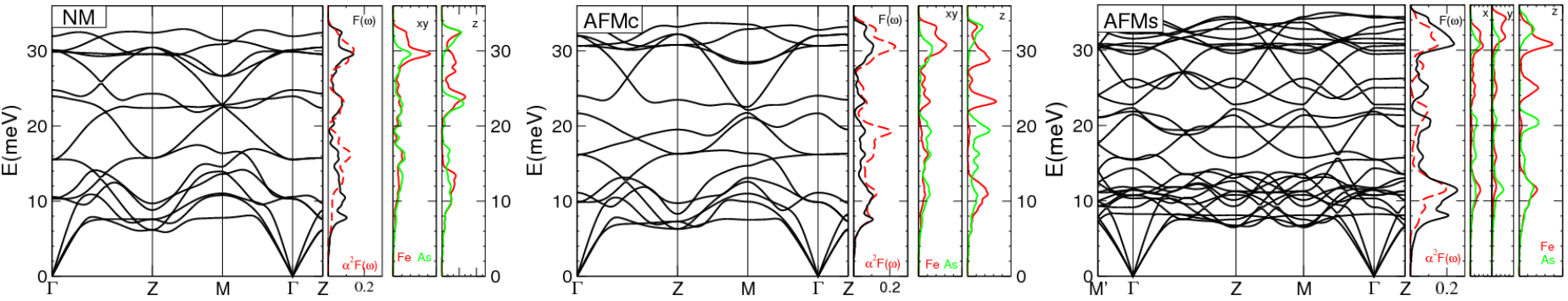




Hole-doped diamond *is an extreme example …*

Step 1: Effect of Magnetism:

Non-magnetic (NM) ***Checkerboard (AFMc)*** ***Stripe (AFMs)***



$\lambda = 0.18$

$N(0) = 1.18 ev^{-1}$

$m = 0$

$\lambda = 0.33$

$N(0) = 1.36 ev^{-1}$

$m = 2.4 \mu_B$

$\lambda = 0.18$

$N(0) = 0.68 ev^{-1}$

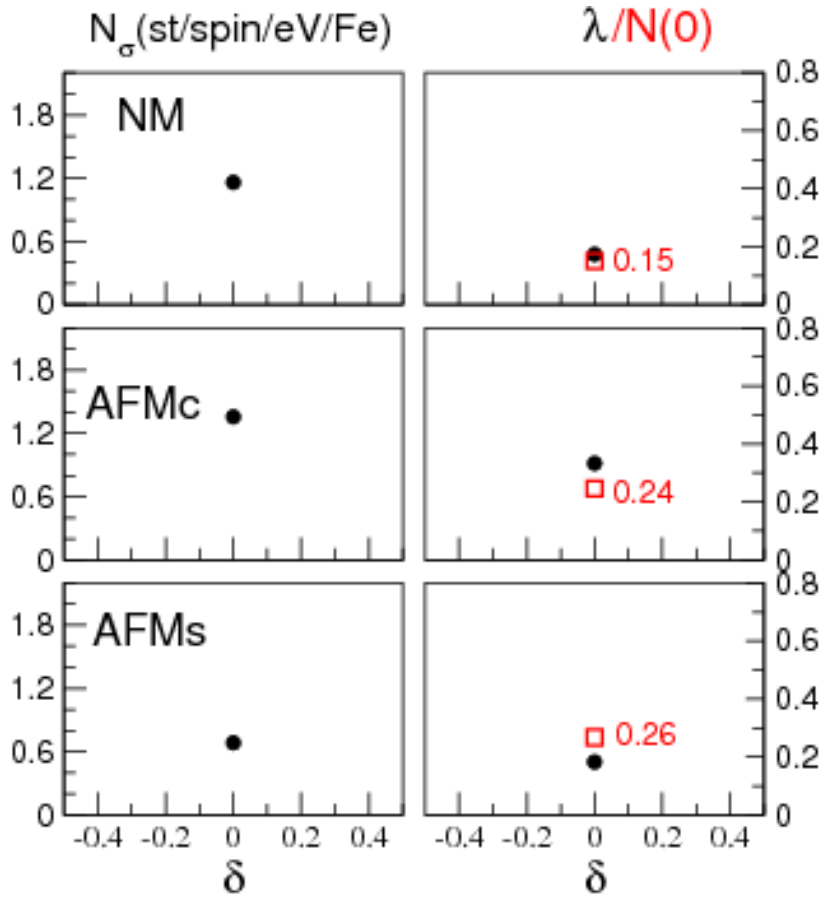
$m = 2.6 \mu_B$

Phonon Dispersions: *AFM causes a strong shift of Fe and As modes (change of Fe-As bonding); in-plane polarized modes are sensitive to the direction of the AFM wave-vector.*

Electron-phonon coupling: *AFM and NM Eliashberg functions have the same three-peak structure; the values of λ are too small to explain Tc.*

$$\lambda \approx \frac{N(0)I^2}{M\omega^2}$$

Electron-Phonon Coupling:



AFMc and AFMs have larger λ/N(0) than NM...

Can we use this information to estimate the coupling in the paramagnetic state?

Paramagnetic State

Large local moments + **Disorder**

LDA: **AFM phonon frequencies (bonding)** **NM Fermi surfaces (wavefunctions)**

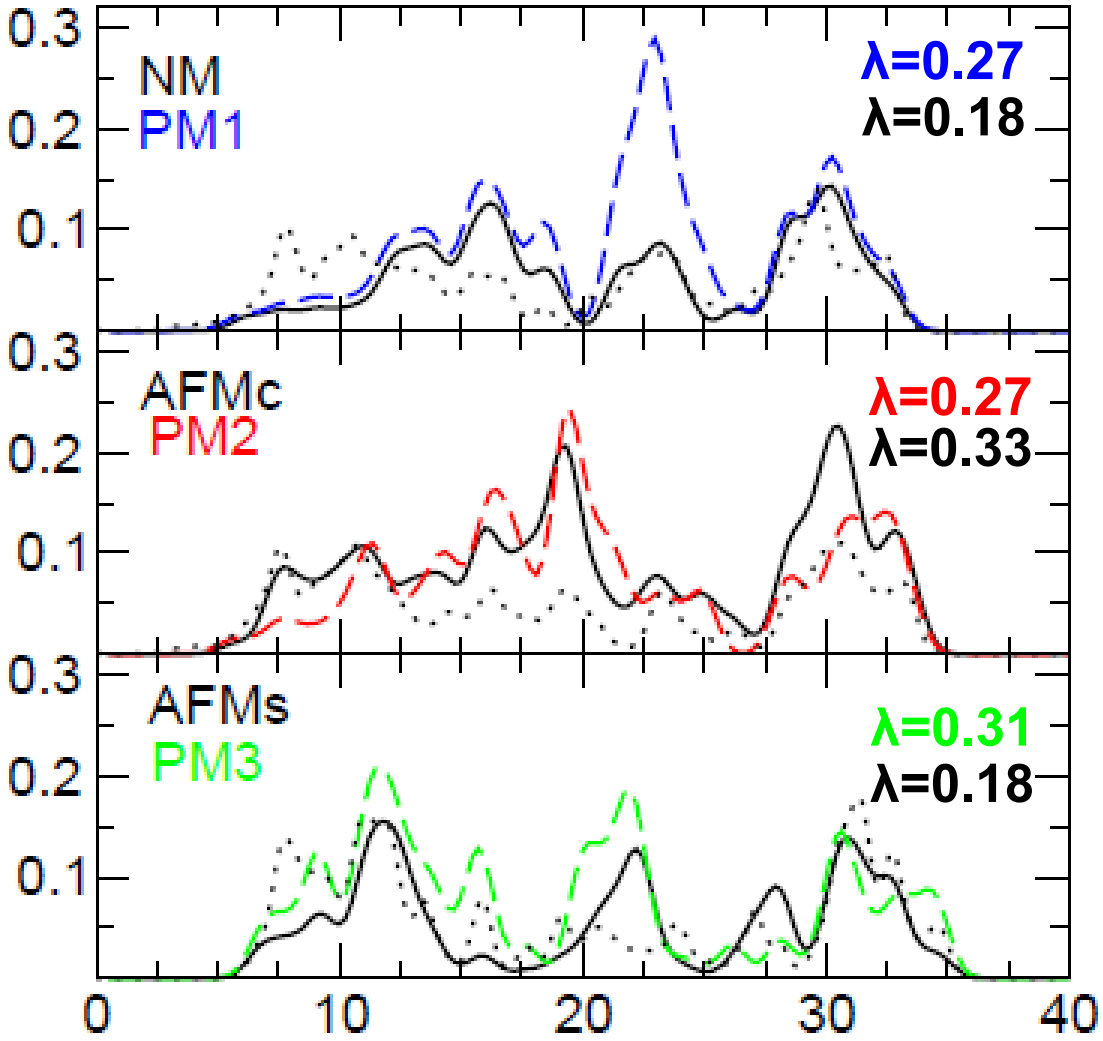
IDEA:

E-ph properties are given by AFM potentials and frequencies and NM wavefunctions

$$\alpha^2 F(\Omega) = \frac{1}{N(0)} \sum_{\mathrm{kk}',\alpha} \delta(\varepsilon_{\mathrm{k}}) \delta(\varepsilon_{\mathrm{k}'}) \mid g^{\alpha}_{\mathrm{kk}'} \mid^2 \delta(\Omega - \omega_{\mathrm{k}-\mathrm{k}'})$$

$$g^{\mathbf{q}\nu}_{\mathbf{k}+\mathbf{q}j',\mathbf{k}j} = \left\langle \mathbf{k}+\mathbf{q}j' \middle| \delta^{\mathbf{q}\nu} V_{sc} \middle| \mathbf{k}j \right\rangle$$

”Paramagnetic” model:

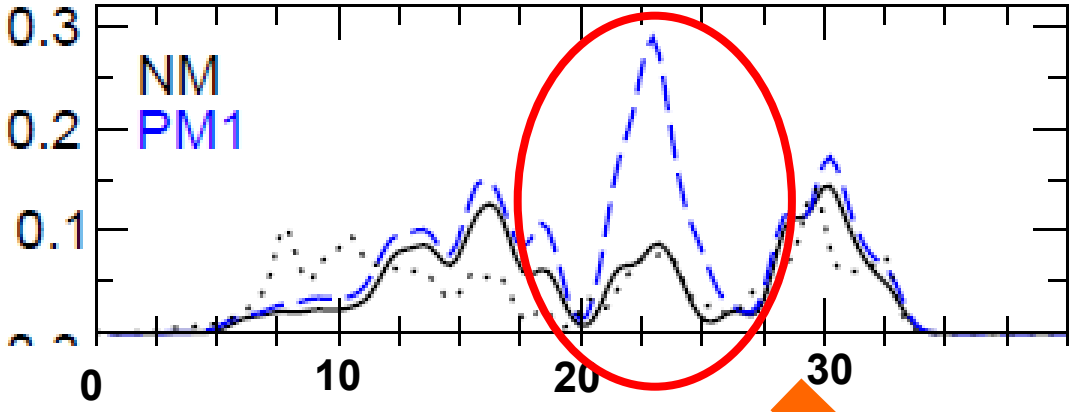


PM1:
NM wf + AFMc V + NM ω

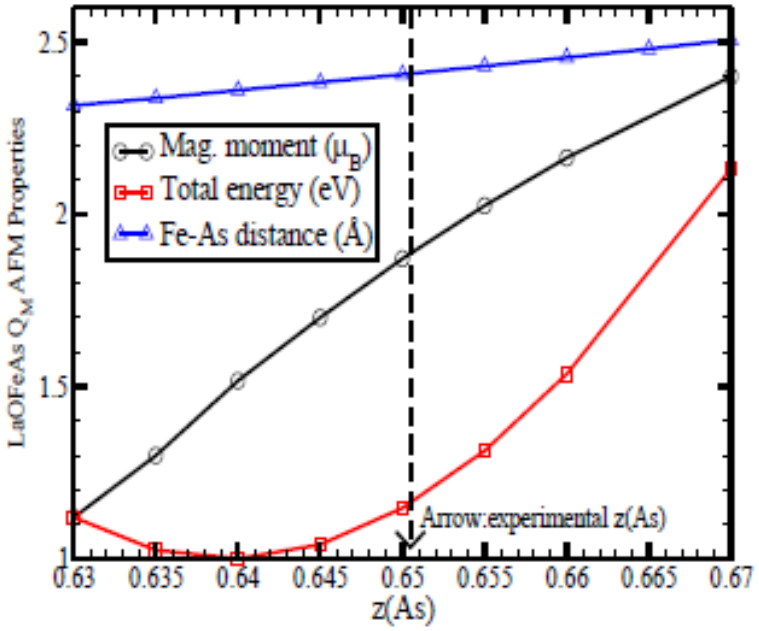
PM2:
NM wf + AFMc V + AFMc ω

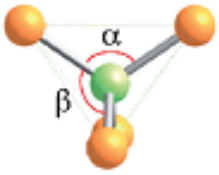
PM3:
NM wf + AFMs V + AFMs ω

Where does the increase in λ come from?



The modes at 20 meV modulate the FeAs4 tetrahedra...

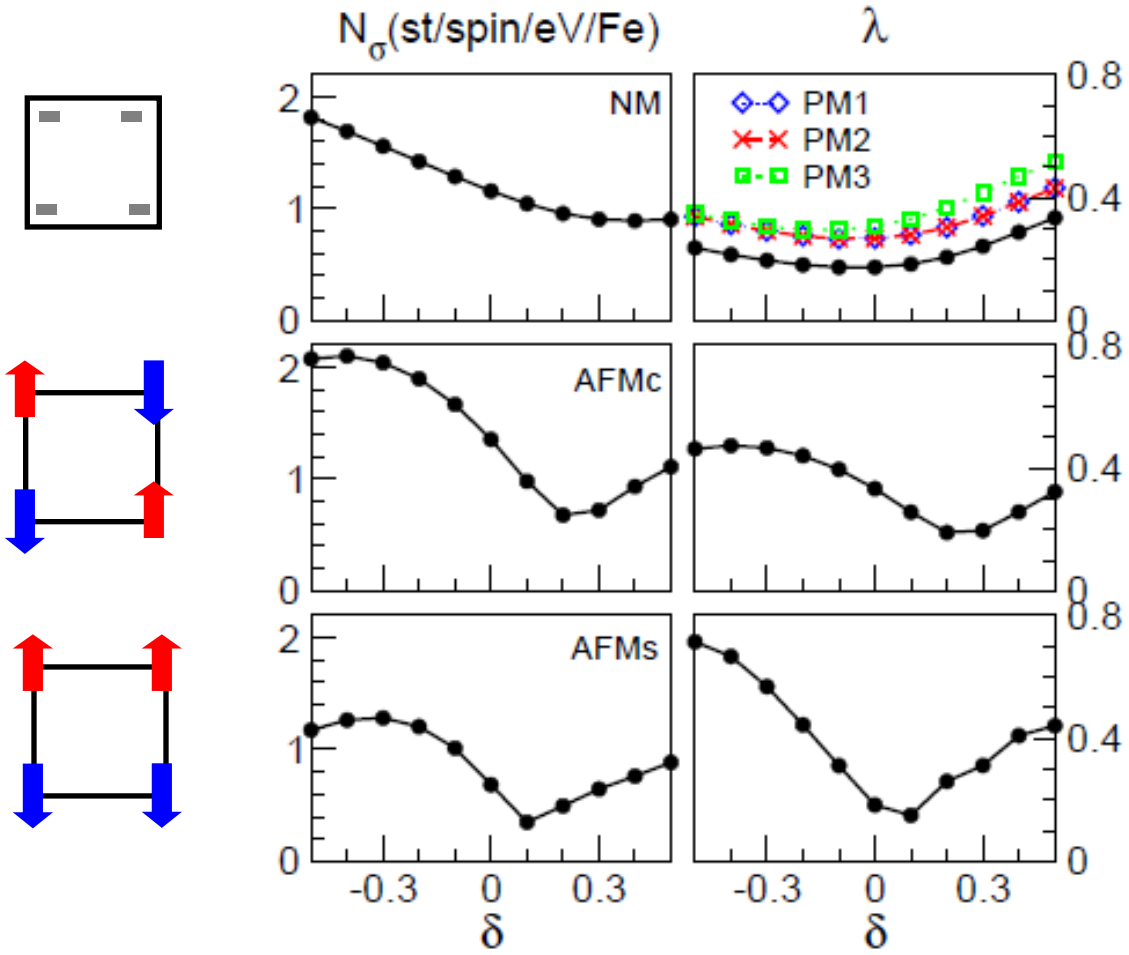




$FeAs_4$-tetrahedron

Which in turn modulate the magnetic moment!

Results:



Paramagnetic model: AFM potentials cause an almost uniform 50 % increase of the coupling.

Effect of doping: (Rigid-band) The coupling does not simply follow the shape of the DOS – matrix elements are important!

In the relevant range of dopings the e-ph coupling is always ≤ 0.35!!!

... In Summary...

Early estimates of the **e-ph coupling** in Fe-based superconductors are **extremely small (λ~0.2): non-magnetic (NM) calculations!**

BUT

Can we trust these estimates if NM calculations give a poor description of lattice dynamics?

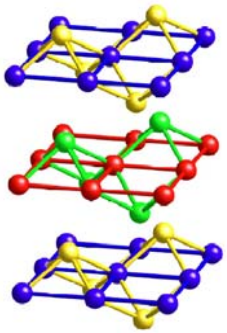
Linear response calculations of lattice dynamics and e-ph coupling in Ba-122

? What is the **effect of magnetism** on the phonon dispersion and e-ph coupling constant? *Strong **renormalization of Fe-As modes** (change of bonding);*
***~ 50 % increase** of the e-ph coupling **matrix element**.*

? Can we model the **paramagnetic** state? *Combine AFM potentials and NM wavefunctions.*

? Can we estimate an upper bound for λ in Fe-based SC?

For realistic values of doping λ≤0.35!



What next?

More than 300 RETMPnO compounds exist ...

Electronic and magnetic properties of Mn, Fe, Co, Ni and Zn in LaTPnO

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr

TM	Mn		Fe		Co		Ni		(Cu)	Zn	
Pn	P	As	P	As	P	As	P	As		P	As
Elect. Prop.	Mott Insulator		Superconductor		Metal		Superconductor		–	Semiconductor	
Magnetism	AFM				FM				–	Non-magnetic	
E_g	~1 eV		–		–		–		–	~1.5 eV	
T_C (SC) $T_{N,C}$(Mag.)	> 400 K		Undoped: 4 K	F-doped: 26 K	43 K	66 K	Undoped: 3 K	Undoped: 2.4 K		–	
Ref.	Yanagi et al JAP (submitted)		Kamihara et al. JACS(2006), Kamihara et al. JACS (2008)		Yanagi et al. PRB (2008)		Watanabe et al. IC (2007), Watanabe et al. JSSC (2007)		–	Kayanuma et al. PRB (2007), Kayanuma et al. TSF (2008)	

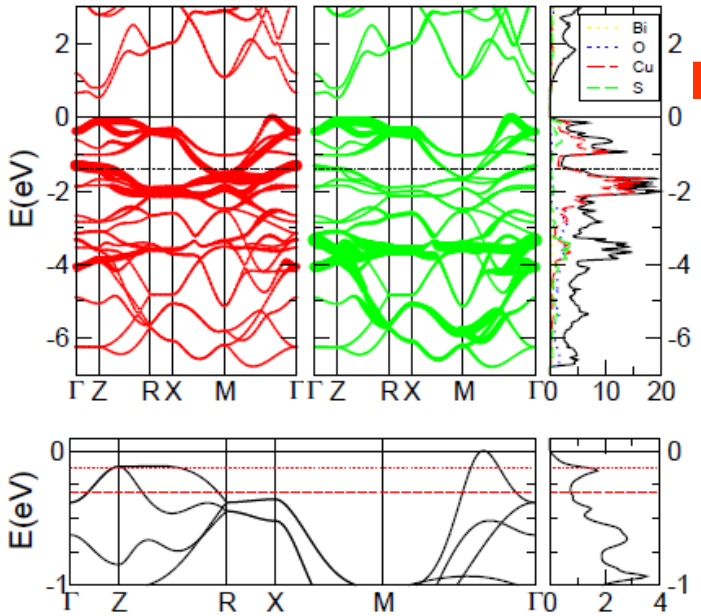
Fig. 10. Electromagnetic and optical properties elucidated in LaT_xPnO.

Due to the rich electronic structure the magnetic and SC properties can be tuned by doping/pressure...

TM pnictides represent an ideal playground to study the interplay between magnetism, SC and e-ph interaction...

A related example: $BiOCu_{1-x}S$, cond-mat/0911.5305

A related example: $BiOCu_{1-x}S$, cond-mat/1012.5761



Same crystal structure as LaOFeAs.

Cu-S layers play the role of FeAs layers.

Superconductivity is observed at x=0.5

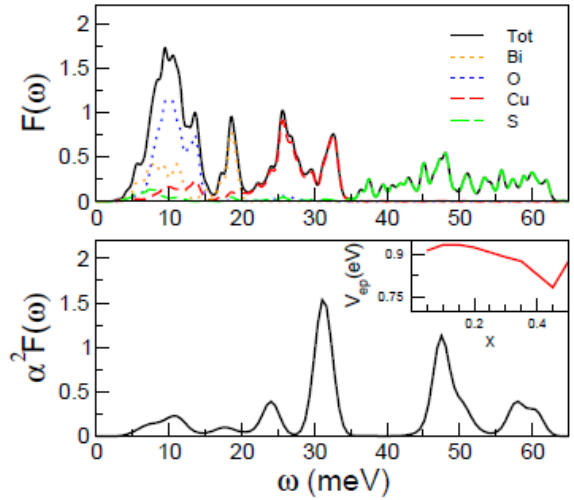
Electron count is d^{10-x}.

The Fermi level sits in the S antibonding region.

LSDFT gives:

-> Instability to magnetism (FM) (Cu)

Large e-ph interaction (S/Cu hybridization)



Competition of SF (FM) and e-ph interaction?

References:

- **On the e-ph interaction in Fe and Ni-based pnictides:**
  L. Boeri, O.V. Dolgov and A. Golubov, Phys. Rev. Lett 2008 and Physica C 2009.

- **On problems connected with DFT in FeBSC:**
  I.I. Mazin, M. D. Johannes, L. Boeri, K. Koepernik, and D. J. Singh,
  Phys. Rev. B 78, 085104 (2008).

- **On the AFM e-ph coupling in Fe-BSC:**
  L. Boeri, M. Calandra, I. I. Mazin, O. V. Dolgov, and F. Mauri,
  Phys. Rev. B 82, 020506R (2010)

- **On the electronic structure and magnetism in Fe-BSC**
  O.K. Andersen and L. Boeri, cond-mat/1011.1658.

- **On the superconductivity of BiOCuS,**
  L. Ortenzi et al., arXiv:1012.4761

THANK YOU!

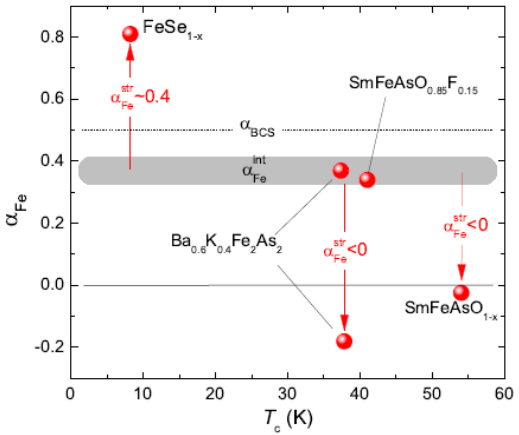
Experimental estimates of the e-ph interaction

$$T_c = \frac{\omega_{\log}}{1.2}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right]$$

$T_c = 5-55K$ ⇒ $\lambda \approx 0.5-1.5,\ \omega_{\log} \approx 200K$

The *e-ph* coupling has been estimated by various **exp techniques**:

- Pump-probe ARPES (cond-mat/1008.1561), Pump-probe optics(PRB **82**, 024513 (2010)), Raman (PRB **78**, 212503 (2008)), ... $\lambda \approx 0.2-0.4$
- ARPES *(cond-mat/1002.3149)*, Raman (*PRB **80**, 064509 (2009)*) $\lambda \approx 1.0-1.5$



The isotope effect is also controversial…

Khasanov et al.,cond-mat/1008.4540