Do the Pinctides point to other possible mechanisms for high Tc?

George Sawatzky

arXiv:0808.1390 2008 EPL 8 6, 1 7 00 6 2009 G.A. Sawatzky, I.S. Elfimov, J. van den Brink, J. Zaanen
Ar X iv: 08 1 1 .021 4v 1 2008 Mona Berciu, Ilya Elfimov and George A sawatzky PRB in Press

Meinders et al PRB 52, 2484 (1995)
Van den Brink et al PRL 75, 4658 (1995)
J. van den Brink et al Europhysics Letters 50, 447 (2000)

collaborators

Experiment

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- N.Ingle UBC
- H.Wadati UBC
- J. Geck Dresden
- K. Shen Cornell

Theory

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- Subhra Gupta

Most papers on the pnictide superconductors Refer to similarities with the Cuprates. Are they really similar?

.

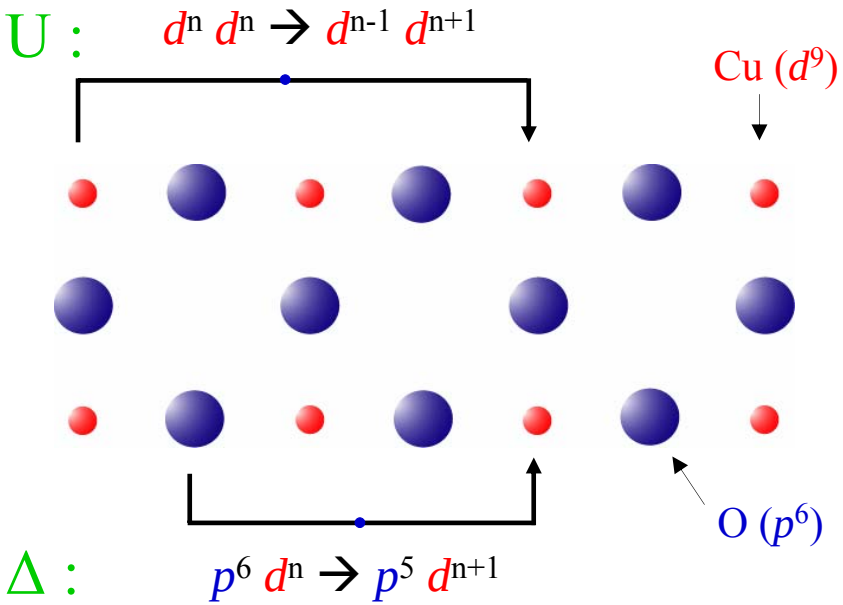
Cuprates

- Local moments
- Large superexchange,
- Charge transfer gaps not Mott Hubbard
- Charge carriers mostly of anion p character
- Strong Cu 3d-O 2p hybridization
- 2 Dimensional

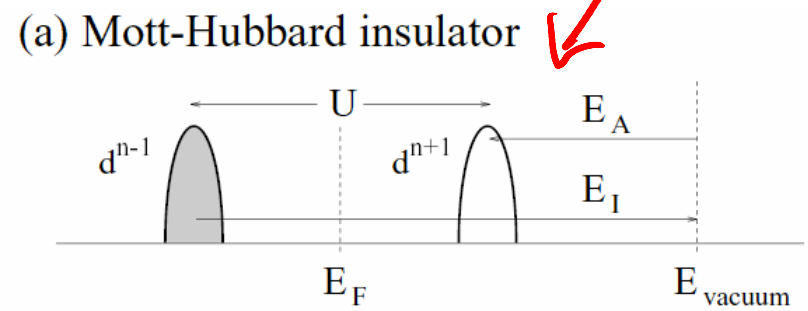
Pnictides

- Small amplitude SDW
- Some evidence of large spin wave dispersion
- Reports support small Mott Hubbard gap if any
- Charge carriers Fe d electrons and holes
- Relatively weak Fe 3d-As 4p hybridization
- Weak anisotropy

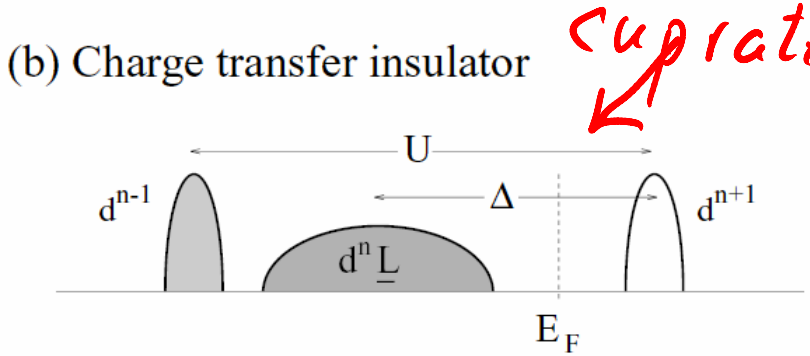
Correlated Electrons in a Solid



Pnictides



cuprates



$$U = E_I^{TM} - E_A^{TM} - Epol$$

$$\Delta = E_I^{O} - E_A^{TM} - Epol + \delta E_M$$

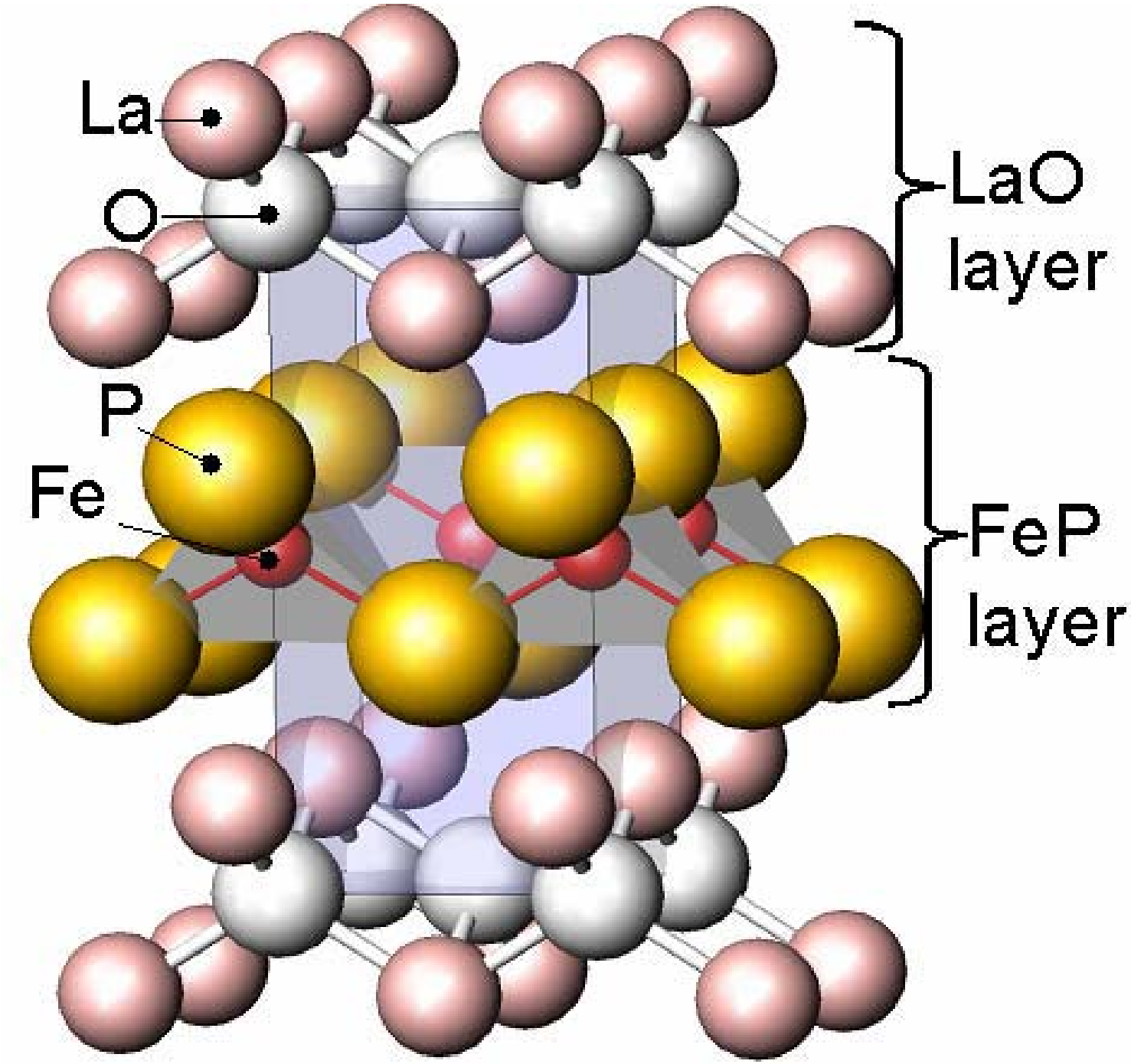
If $\Delta < (W+w)/2$ → Self doped metal

E_I ionization energy
E_A electron affinity energy
E_M Madelung energy

Epol depends on surroundings!!! $E_p = \frac{ze^2\alpha}{R^4}$

- **J.Hubbard, Proc. Roy. Soc. London A 276, 238 (1963)**
- **ZSA, PRL 55, 418 (1985)**

Since the pure pnictides like LaFeAsO, BaFe2As2, etc are (bad) metals we would have to conclude that U<the 3d band width


La
O
P
Fe
LaO
layer
FeP
layer

What would the Fe 3d states look like if we started in the same way as in the Cuprates?

Not layered like TiS2

As drawn this presents a Surface

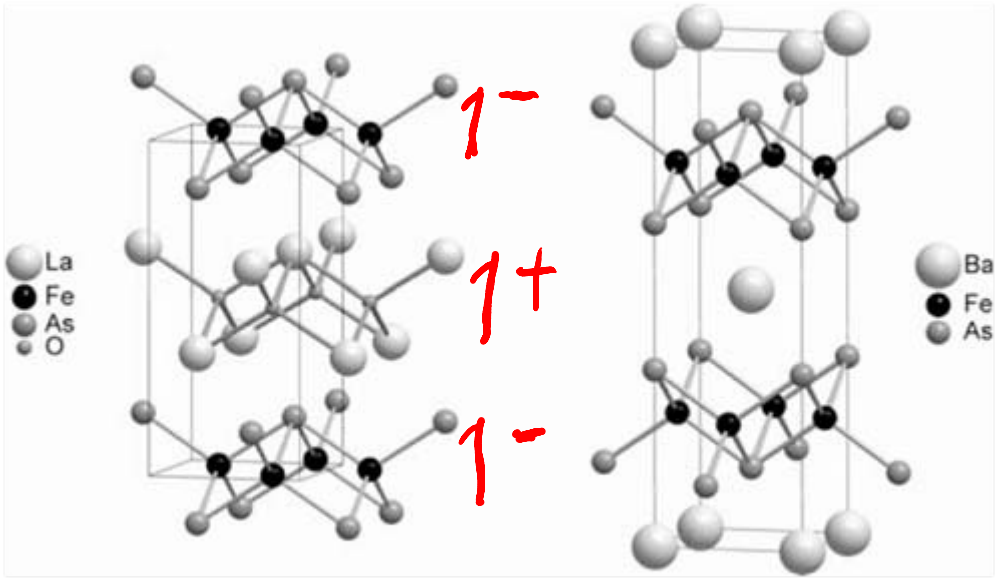
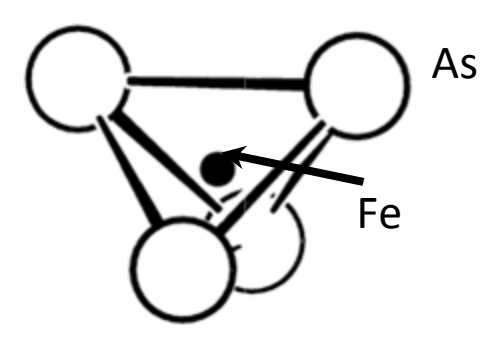
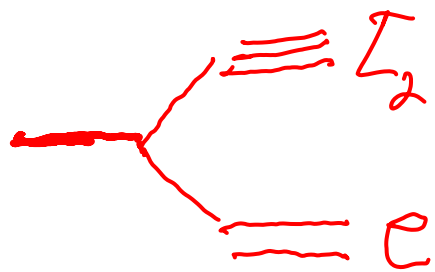


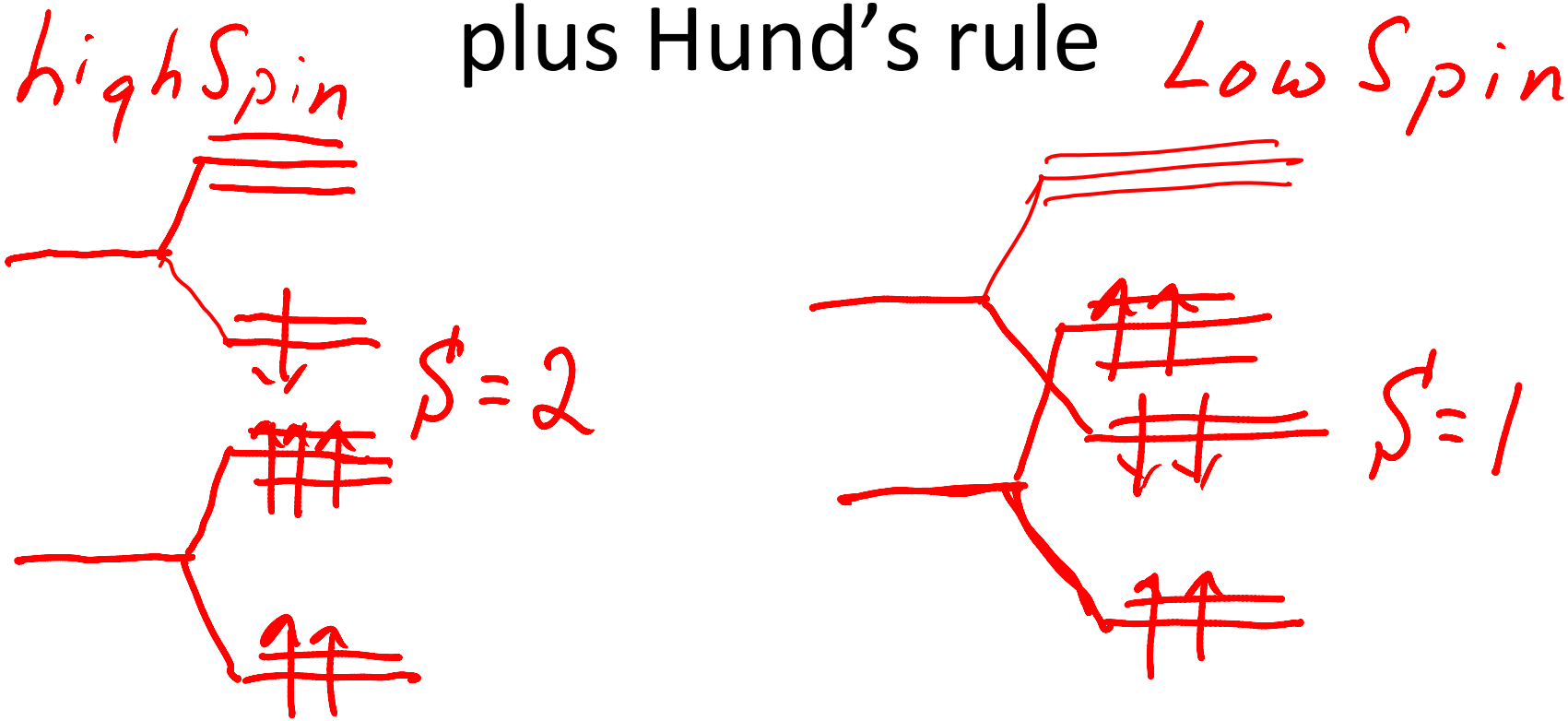
Figure 1 . Crystal structures of LaFeAsO (left) and $BaFe_2As_2$ (right)



~ Tetrahedral coordination
Crystal field splitting
Is inverted as compared to Octahedral



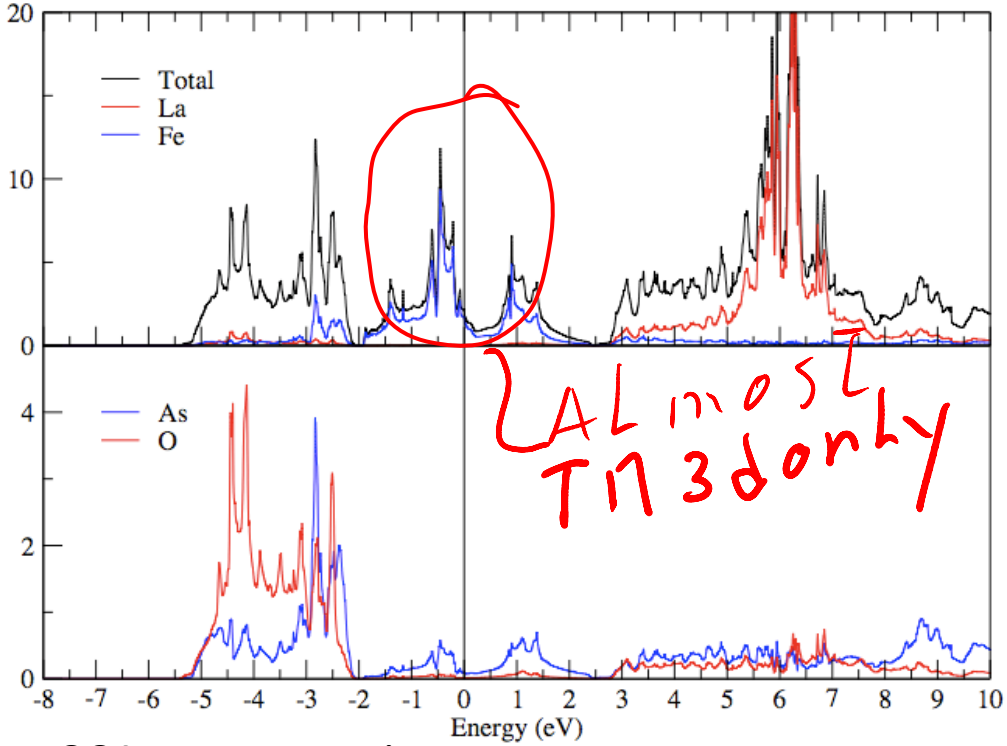
Local crystal/ ligand field picture plus Hund's rule



Band theory - Crystal/ligand field splitting is not very large
And less important than the 3d band structure.

Very different from the cuprates!!

Electronic Structure of LaOFeAs band theory (Elfimov)

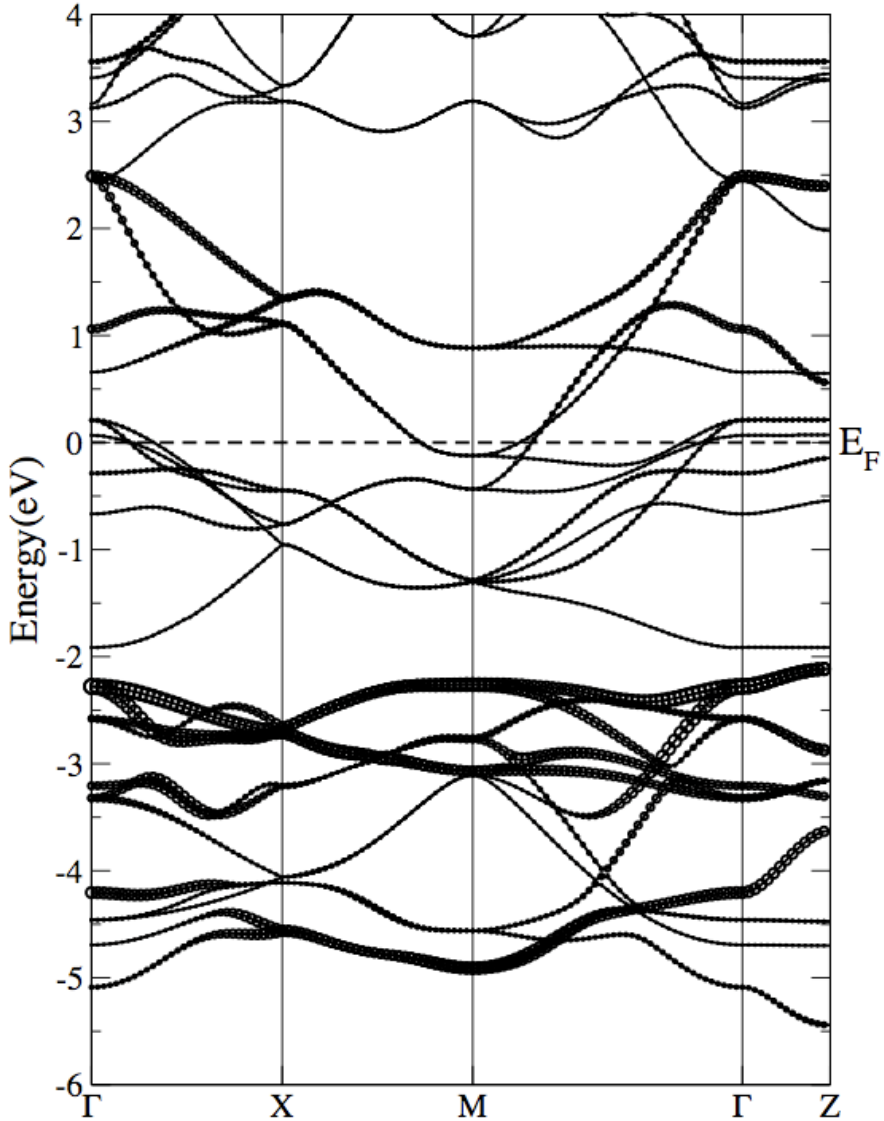


GGA; non magnetic

Fat bands show As 4p character

MT Radii (A) :

La	1.22
Fe	1.01
As	1.38
O	1.11



How can we explain the low VARIABLE magnetic moment? Since the hybridization is small?

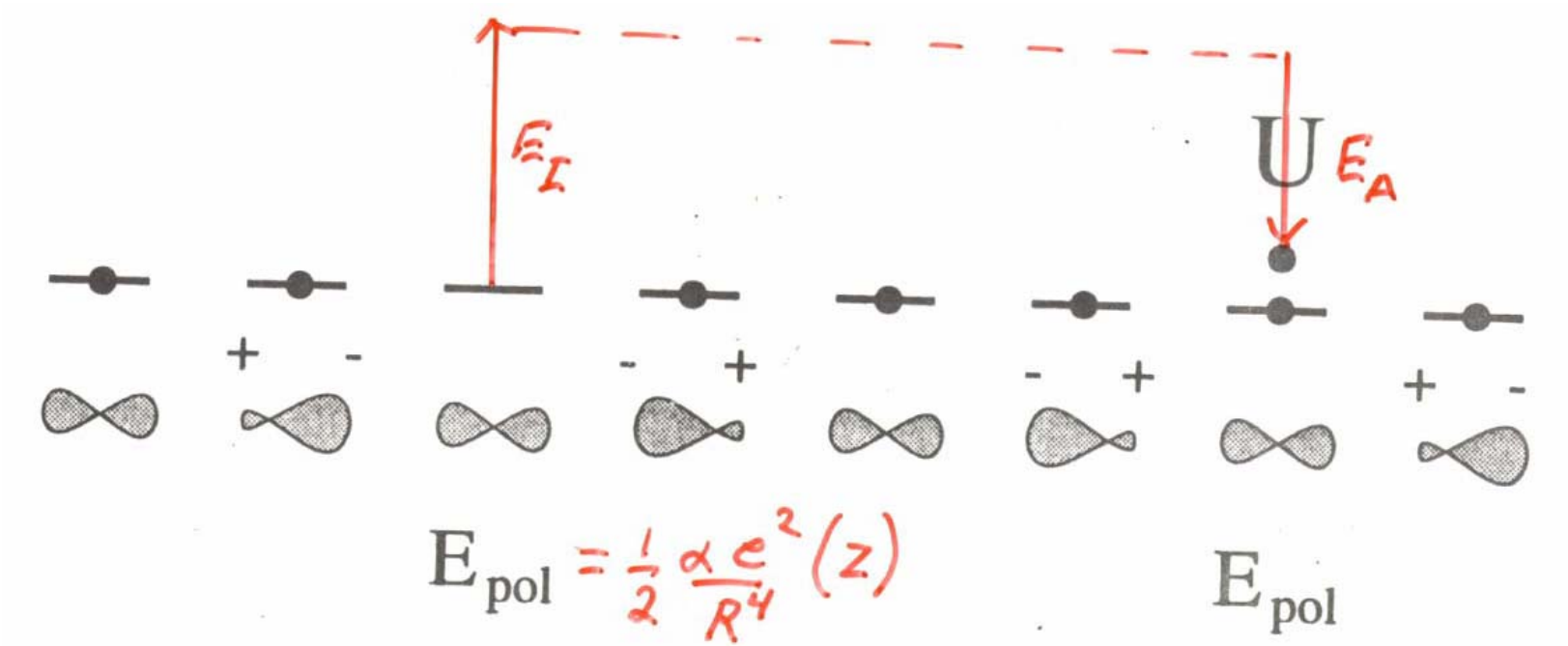
- Low Hubbard U i.e. U< 3d band width
- Band width is about 2-3 eV so U~2-3eV?
- How do we reduce an on site interaction from about 20eV in the free ion to less than 2 eV?
- A large contribution is the Polarizability of the anion!!!

Effective Hamiltonians can be misleading

- Hubbard like models are based on the assumption that longer range coulomb interactions are screened and the short range on site interactions remain
- However U for the atom is about 20 eV but U as measured in the solid is only of order 5 eV and for the pnictides even less than this
- IF WE RENORMALIZE WILL NEW TERMS APPEAR?

Reduction of onsite interactions and changing the nearest neighbor interactions with polarizable ions in a lattice

Van den Brink et al



We assume that the hole and electron move slowly compared to the response time of the polarizability of the atoms.

Note the oppositely polarized atoms next to the hole and extra electron

You can write the interaction Hamiltonian as

$$H_{\text{int}} = (U - 2zP)\sum_{i} n_{i\uparrow} n_{i\downarrow} + 2P\sum_{l,i} n_l n_{l+2a_i}$$

So the reduction of the Hubbard U in a polarizable medium like this introduces a strong
Next nn repulsive interaction. This changes our model!!

For a different geometry actually the intersite interaction can also be strongly reduced perhaps even Attractive (Fe Pnictides)

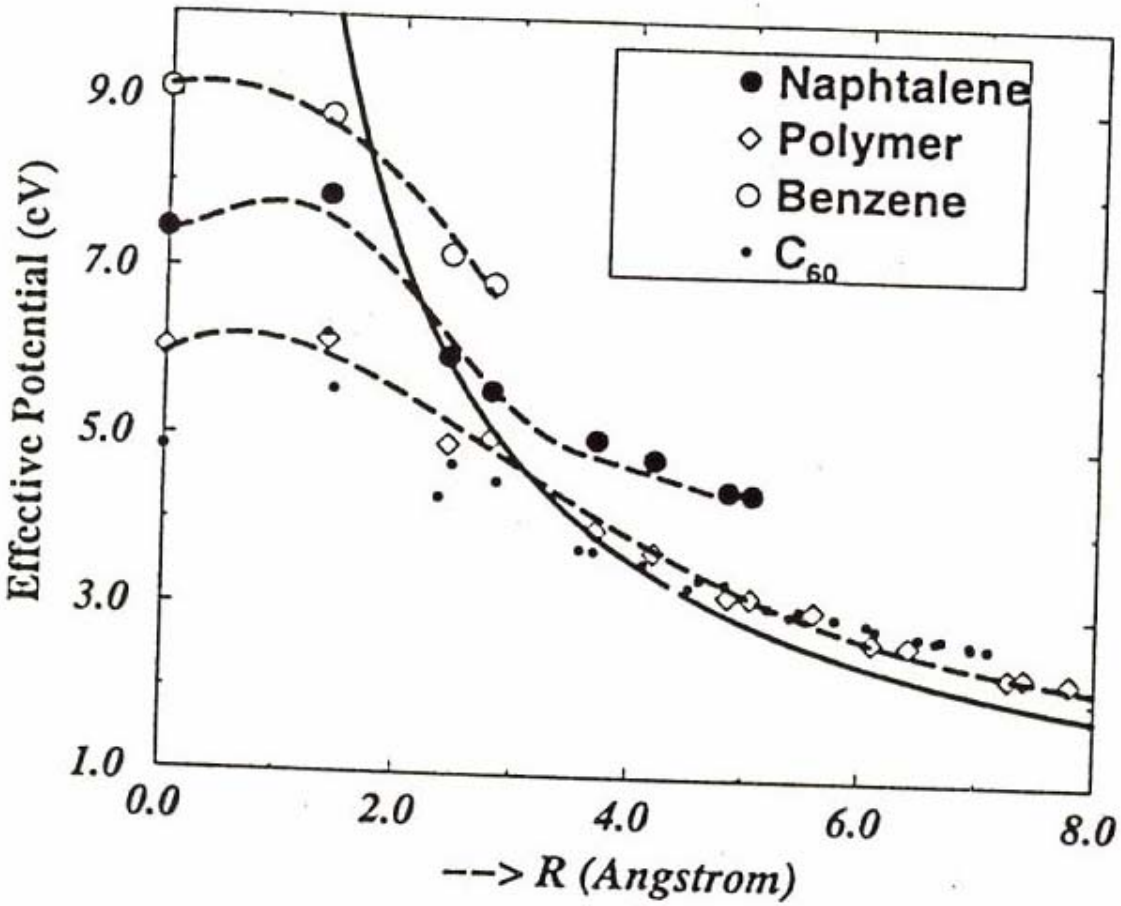


FIG. 5. The effective Coulomb interaction on different organic molecules. The carbon polarizability is 0.56 Å^3. The full line represents the bare Coulomb repulsion. The dashed lines are guides for the eye.

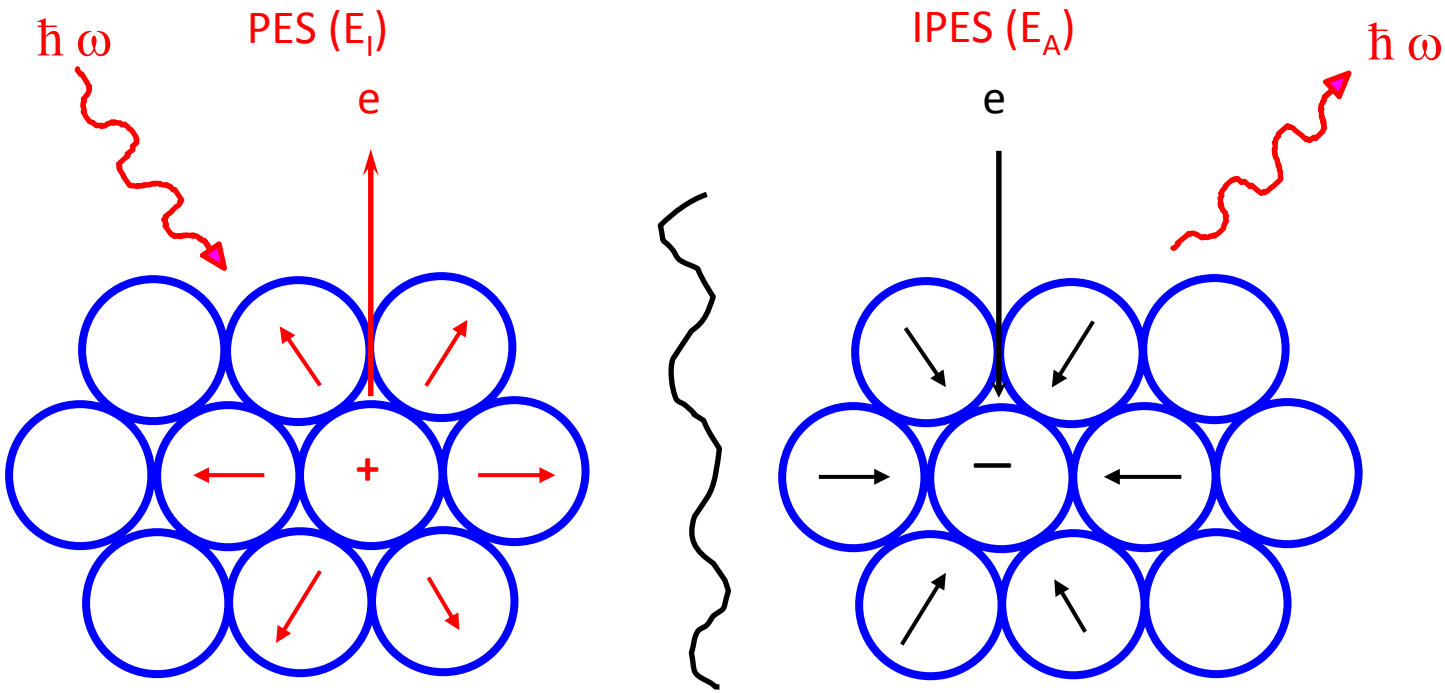
Note short range interactions are reduced “ screened ” and intermediate range interactions are enhanced or antiscreened-quite opposite to conventional wisdom in solid state physics

Jeroen van den Brink Thesis U of Groningen 1997

remember that

- The polarizability of anions results in a strong reduction of the Hubbard on site U
- The charged carriers living on transition metal ions are dressed by virtual electron hole excitations on the anions resulting in electronic polarons
- **The nearest neighbor coulomb interactions can be either repulsive or attractive depending on the details of the structure**

A Picture of Solvation of ions in a polarizable medium



Full polarization can develop provided that Dynamic Response Time of the polarizable medium is faster than hopping time of the charge

ΔE (polarizability) > W ; $\Delta E \approx$ MO energy splitting in molecules, plasma frequency in metals-----

We are alive because of Solvation

Ions both positive and negative in our bodies regulate most everything

Reduction of U due to polarizability of O2- or As3- (SOLVATION)

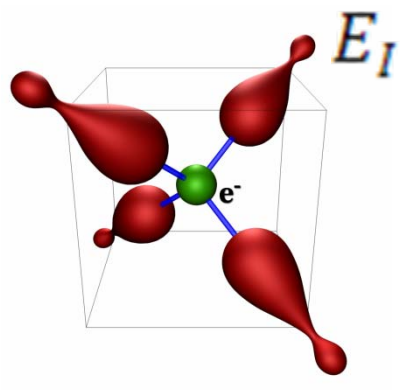
$U = E_I^{TM} - E_A^{TM}$ -2Epol $Epol = Z\,P \cdot F$

Z=nnn, P= ionduced dipole, F=electric field

E_I ionization energy

E_A electron affinity energy

$Epol = \frac{1}{2}\sum_i \sum$



$$E_I = E_I^0 - \sum_i \frac{1}{2}\alpha_i F_i^2 \qquad E_A = E_A^0 + \sum_i \frac{1}{2}\alpha_i F_i^2$$

$$\text{Epol} = 2\sum_i \frac{1}{2}\alpha_i F_i^2$$

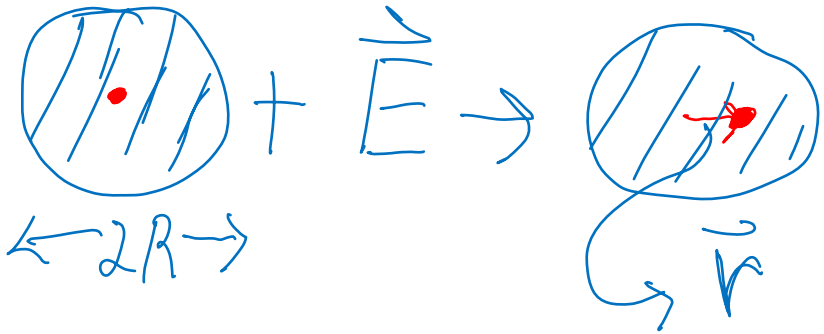
For 6 nn of O2- ~ 13eV

For 4 nn As3- ~17 eV

ELECTONIC POLARON

Rough estimate
Atomic or ionic polarizability ~volume

- Consider atom = nucleus at the center of a uniformly charge sphere of electrons
- In a field E a dipole moment is induced P=αE



$$F = e^2\left(\frac{r^3}{R^3}\right)\left(\frac{\vec{r}}{r^3}\right)$$

- For Z = 1 and 1 electron restoring force = $(e^2/R^3)\,\vec{r}$

$$\vec{p} = -e\vec{r} = \frac{e^2}{f}E = \alpha E \qquad \alpha = R^3$$

f

Whats the importance of As or P?

- Very large anions
- Electronic polarizabilities roughly equal to volume

$\alpha(P^{3-}) \simeq 6-8\,\text{Å}^3$ $\alpha(As^{3-}) \simeq 10-12\,\text{Å}^3$

$\alpha(O^{2-}) \simeq 1-3\,\text{Å}^3$

- 4p orbitals have 2 radial nodes –very diffuse
- Weak hybridization with highly directed local Fe 3d orbitals (from band theory)
- Large polarizability strongly reduces U on Fe and the nearest neighbor interaction V between Fe 3d

What about intersite interaction V?

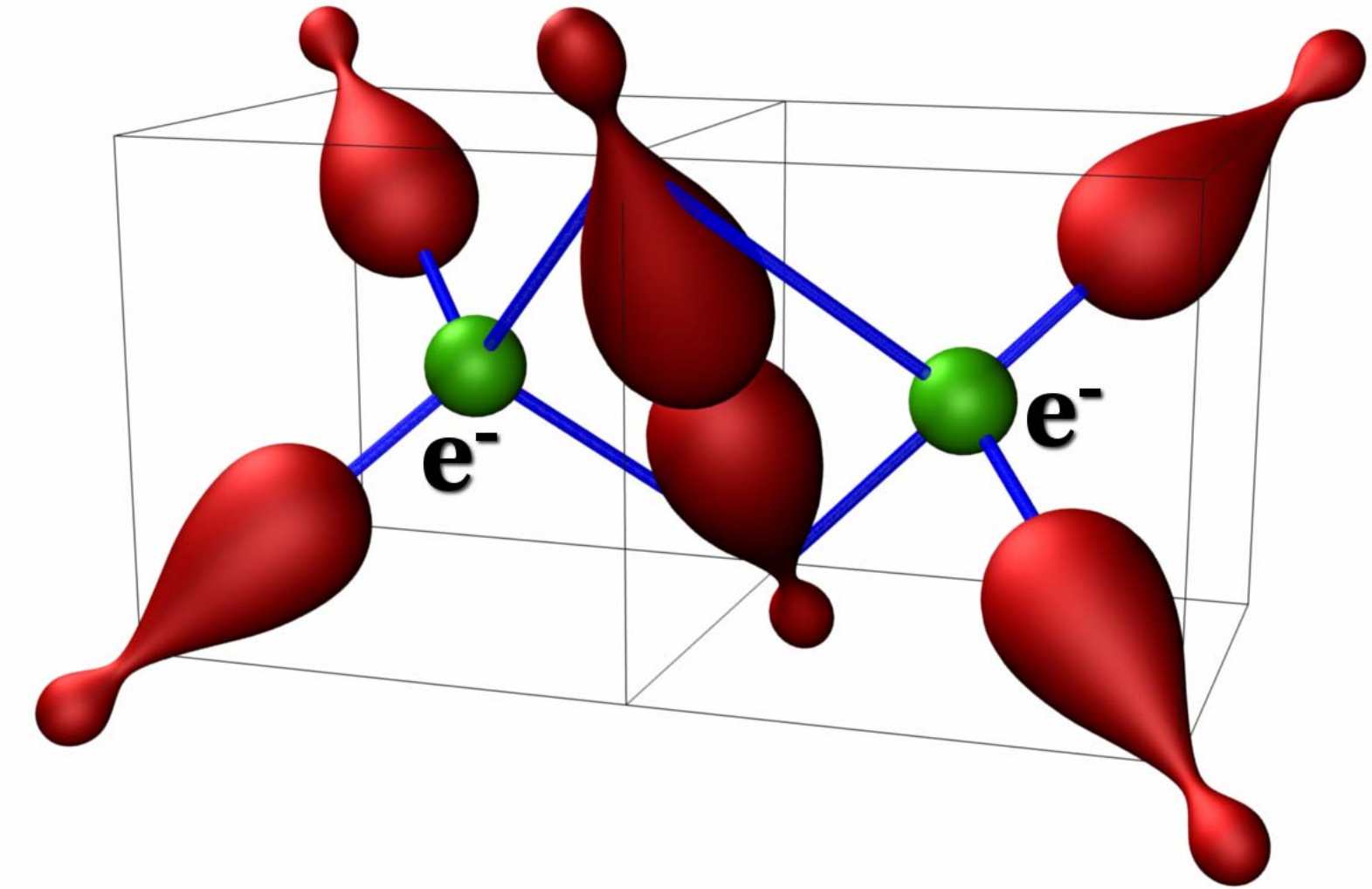
$$V = V_0 - \frac{1}{2} \sum_{common} \alpha[(\mathbf{E}_1 + \mathbf{E}_2)^2 - E_1^2 - E_2^2],$$

which reduces to $V = V_0 - 2\alpha \mathbf{E}_1 \cdot \mathbf{E}_2$, where 2 ref

For the cuprates the Cu-O-Cu bond angle is 180 degrees therefore the repulsive interaction is enhanced!
i.e. larger than in free space

For pnictides the Fe-As-Fe nn bond angle is ~70 degrees
Therefore the contribution to V is attractive ~4 eV

Polarization cloud For Two charges on Neighboring Fe “ELECTRONIC BIPOLARON



2 level model for the dynamic high frequency polarizability and motion of the polaron/bipolaron

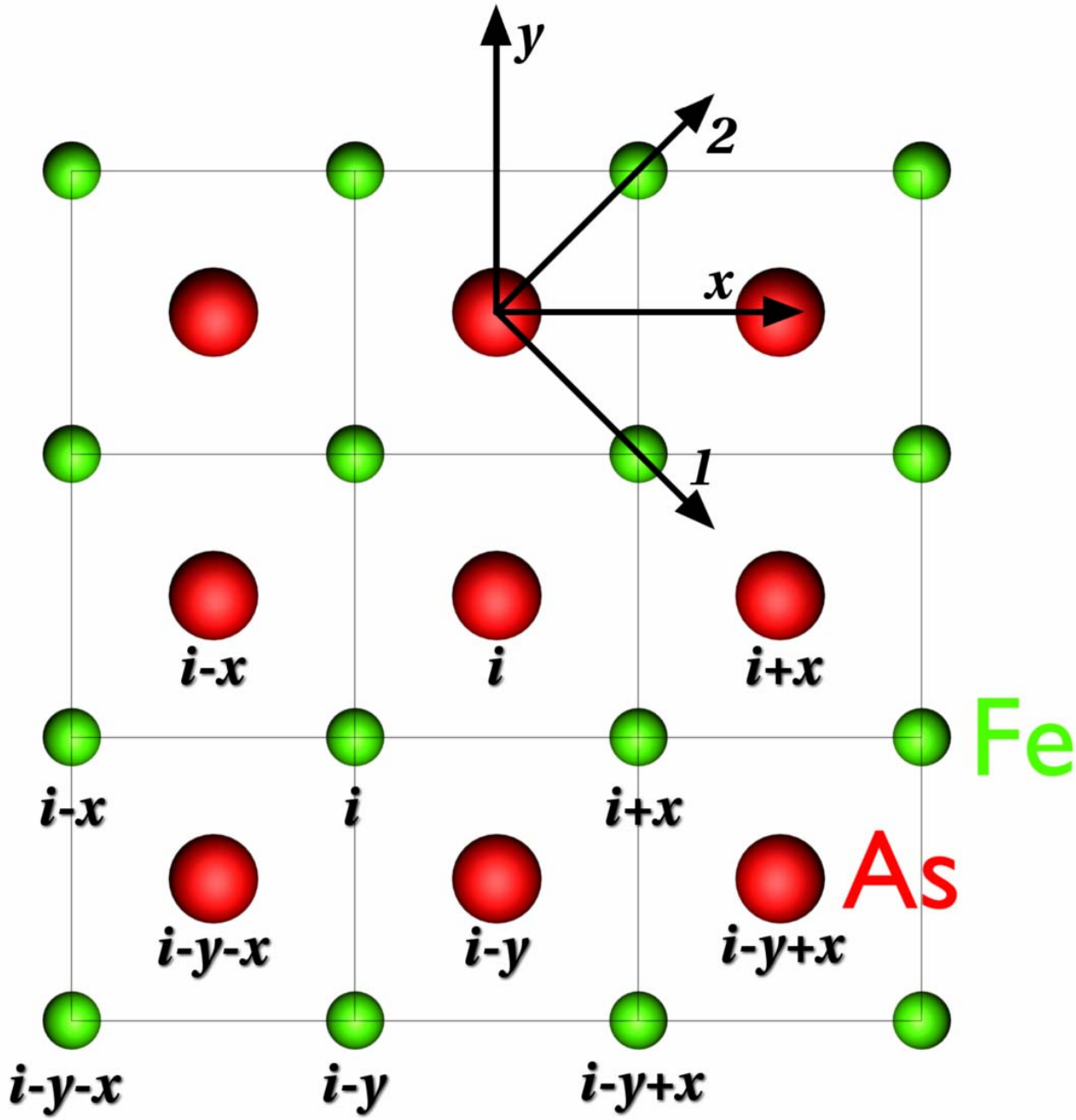
PHYSICAL REVIEW B VOLUME 29, NUMBER 8 15 APRIL 1984

Exciton satellites in photoelectron spectra

D. K. G. de Boer, C. Haas, and G. A. Sawatzky
Laboratories of Inorganic and Physical Chemistry, Materials Science Centre of the University, Nijenborgh 16, 9747-AG Groningen, The Netherlands
(Received 6 September 1983)

Use a two level model of As i.e. 4p occupied and 5s empty. In an electric field due to the point charge they mix yielding The pictures we draw of the polarization cloud.

Mona Berciu et al PRB in press


y
2
x
1
i-x
i
i+x
Fe
i-x
i
i+x
As
i-y-x
i-y
i-y+x
i-y-x
i-y
i-y+x

$$\mathcal{H}_{\mathrm{Fe}} = -\sum_{i,j,\sigma}\left(t_{ij}c^{\dagger}_{i,\sigma}c_{j,\sigma} + h.c.\right) + U_H\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

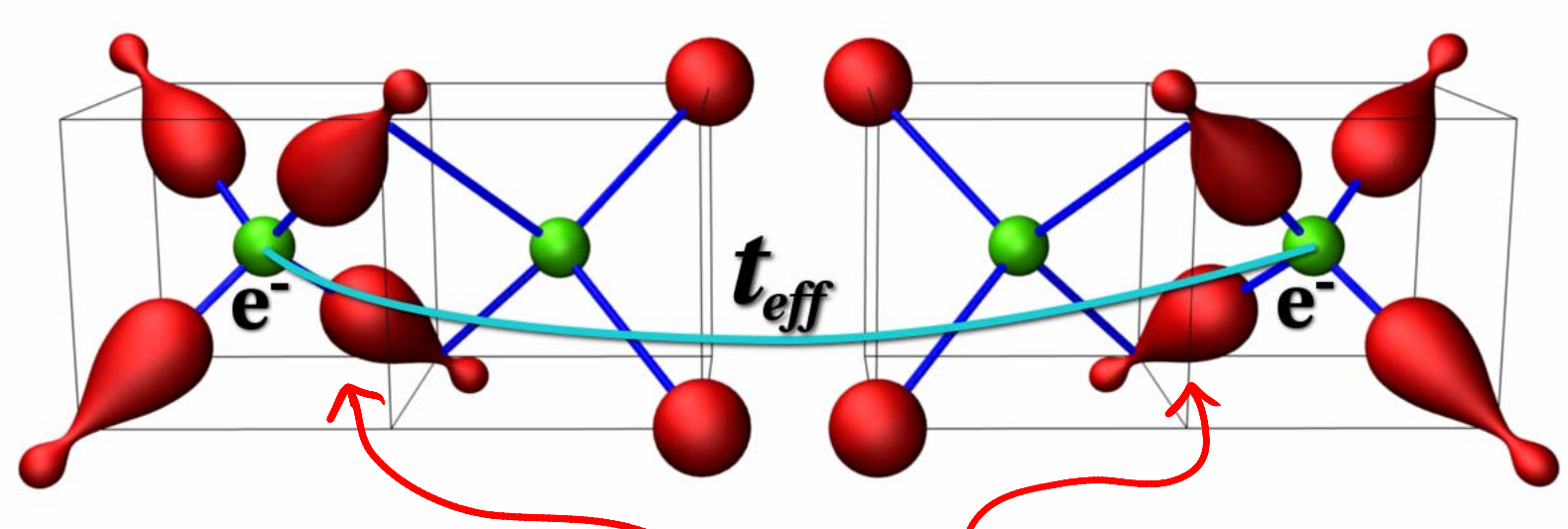
$$\mathcal{H}_{\mathrm{As}} = \Omega\sum_{i,\lambda,\sigma} p^{\dagger}_{i,\lambda,\sigma}p_{i,\lambda,\sigma}\,,$$

= 4p-5s excitation energy

$$\begin{aligned}\mathcal{H}_{\mathrm{int}} \quad &= g\sum_{i,\sigma}\hat{n}_i\Big[s^{\dagger}_{i,\sigma}\left(-\sin\theta p_{i,2,\sigma} + \cos\theta p_{i,3,\sigma}\right)\\ &+ s^{\dagger}_{i-y,\sigma}\left(-\sin\theta p_{i-y,1,\sigma} + \cos\theta p_{i-y,3,\sigma}\right)\\ &+ s^{\dagger}_{i-x-y,\sigma}\left(\sin\theta p_{i-x-y,2,\sigma} + \cos\theta p_{i-x-y,3,\sigma}\right)\\ &+ s^{\dagger}_{i-x,\sigma}\left(\sin\theta p_{i-x,1,\sigma} + \cos\theta p_{i-x,3,\sigma}\right) + h.c.\Big] \quad (3)\end{aligned}$$

Because Omega is a high energy we can use perturbation theory in t as the smallest
We assume only one particle so that U is not active

The Motion of a single quasi particle
These move like electronic polarons



$$\tau_{eff} \sim t |\langle \phi_1 | \phi_2 \rangle|^2$$

i.e. the overlap integral of the polarization clouds

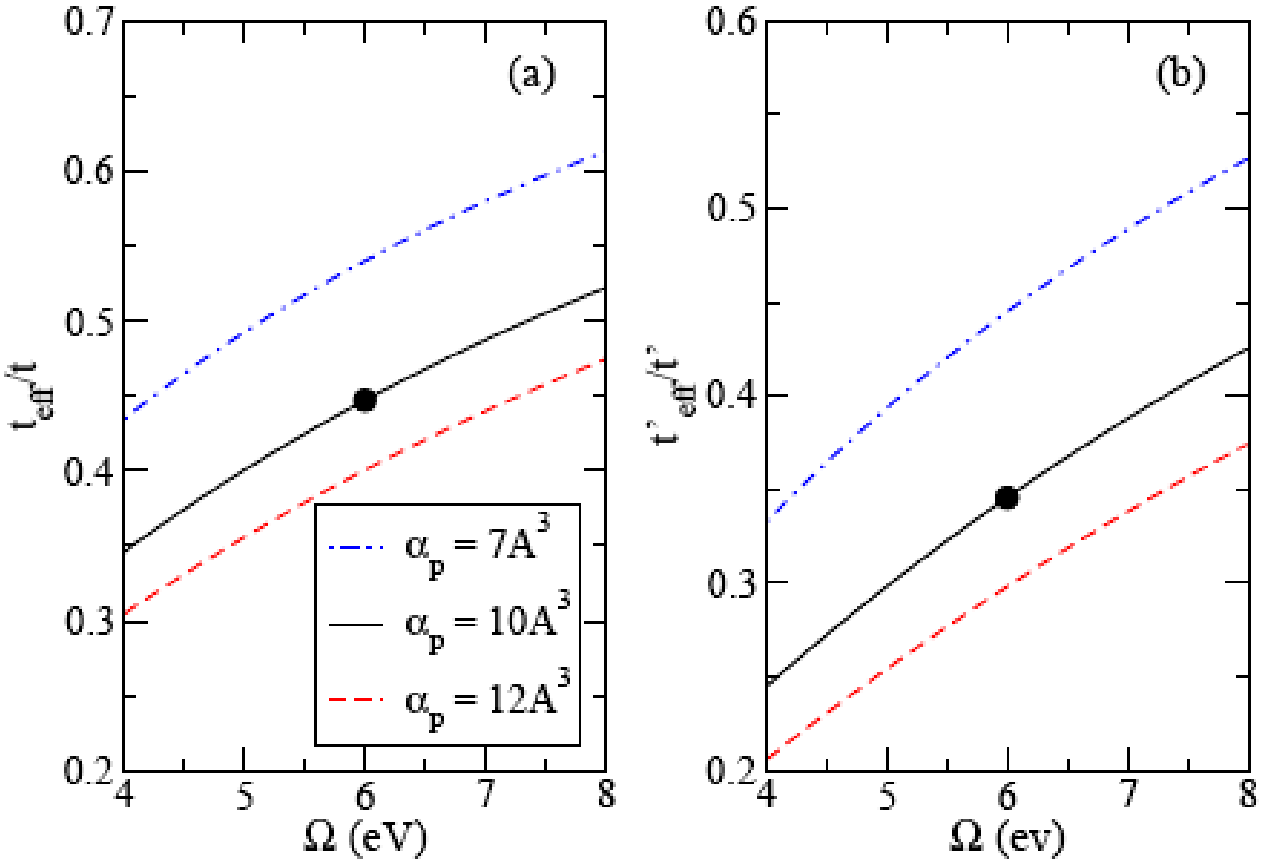


FIG. 3: (a) $t_{\rm eff}/t$ and (b) $t'_{\rm eff}/t'$ vs. Ω, for a polarizability $\alpha_p = 7, 10$ and $12\mathring{A}^3$. The dots show the values used here.

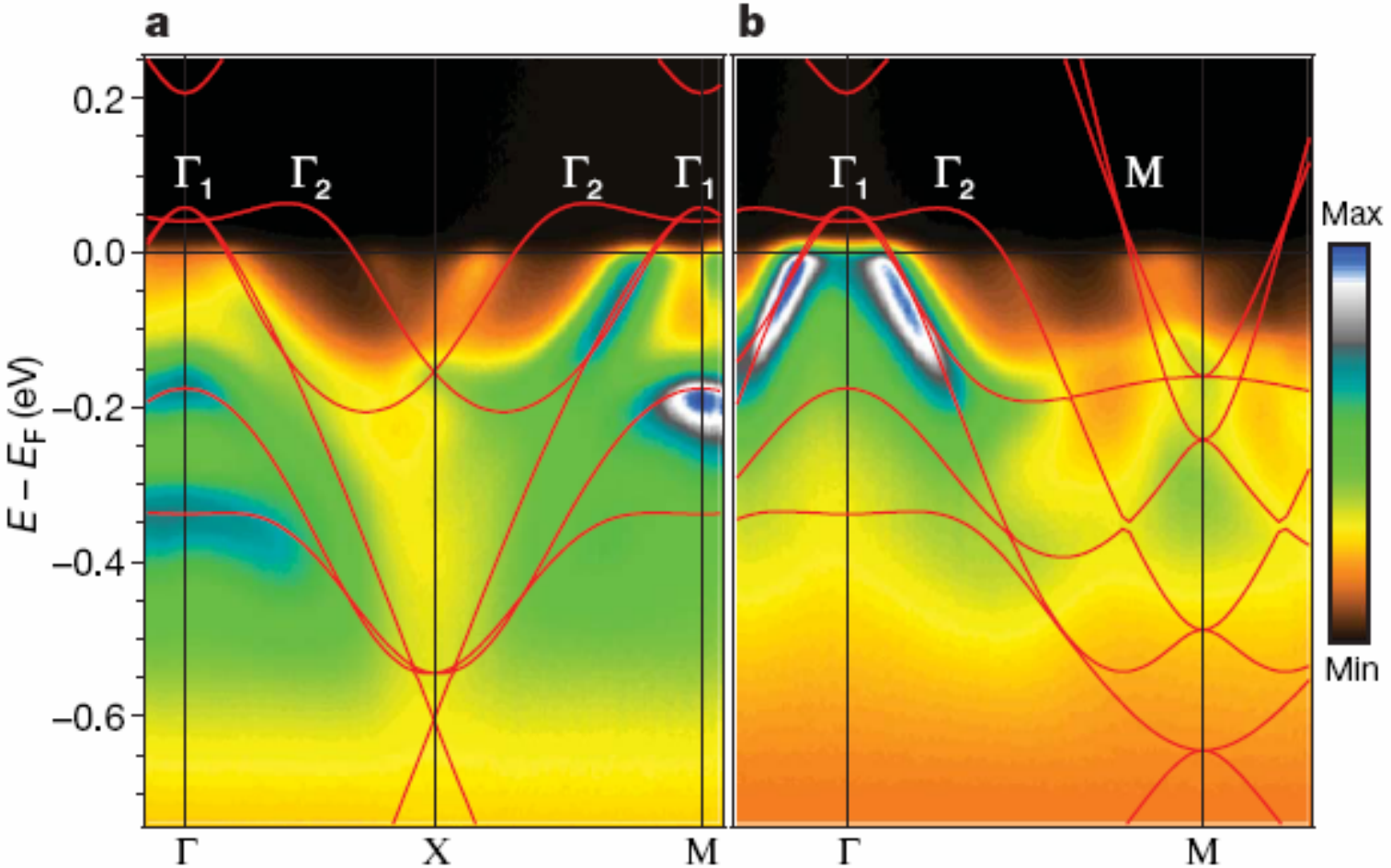
The effective polaron mass is simply t/teff =2.2 this is light compared to conventional lattice polaron masses

Angular resolved phtoemission comparison with LDA LaFePO

Lu et. al Nature 455, 81 2008

close to our 1/z ~ 2

NOTE The band theory result has been shifted up by 0.11 eV and scaled down by a factor of 2.2



What about the nn interaction? Can this lead to bipolaronic bound states? And if so what is their mass

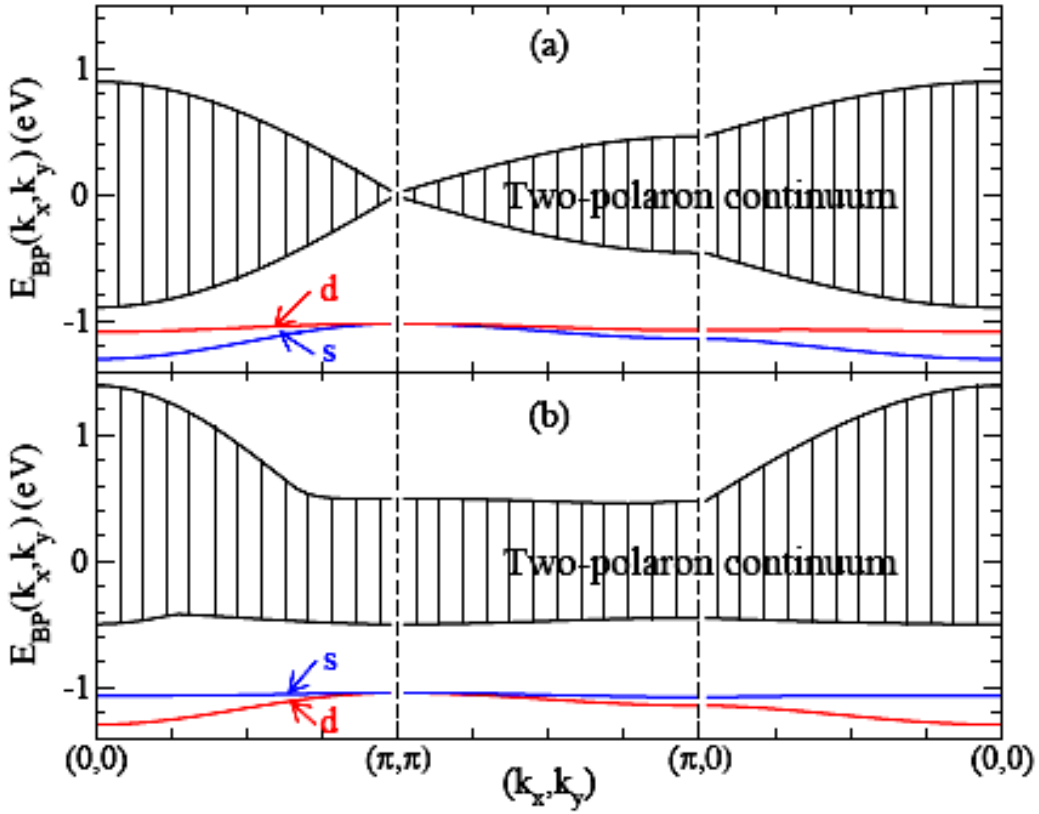


FIG. 7: Dispersion of the two bound bipolaron states along high-symmetry axes in the Brillouin zone, for (a) $t' = 0$ and (b) $t' = -t/2$. The two-polaron continuum is also shown. Parameters are $U_H = 10$ eV, $\alpha_p = 10\mathring{A}^3, \Omega = 6$ eV (similar results are found for all $\alpha_p = 7 - 12\mathring{A}^3, \Omega = 4 - 8$ eV). The symmetry of the ground state changes from s to d if $t' \neq 0$.

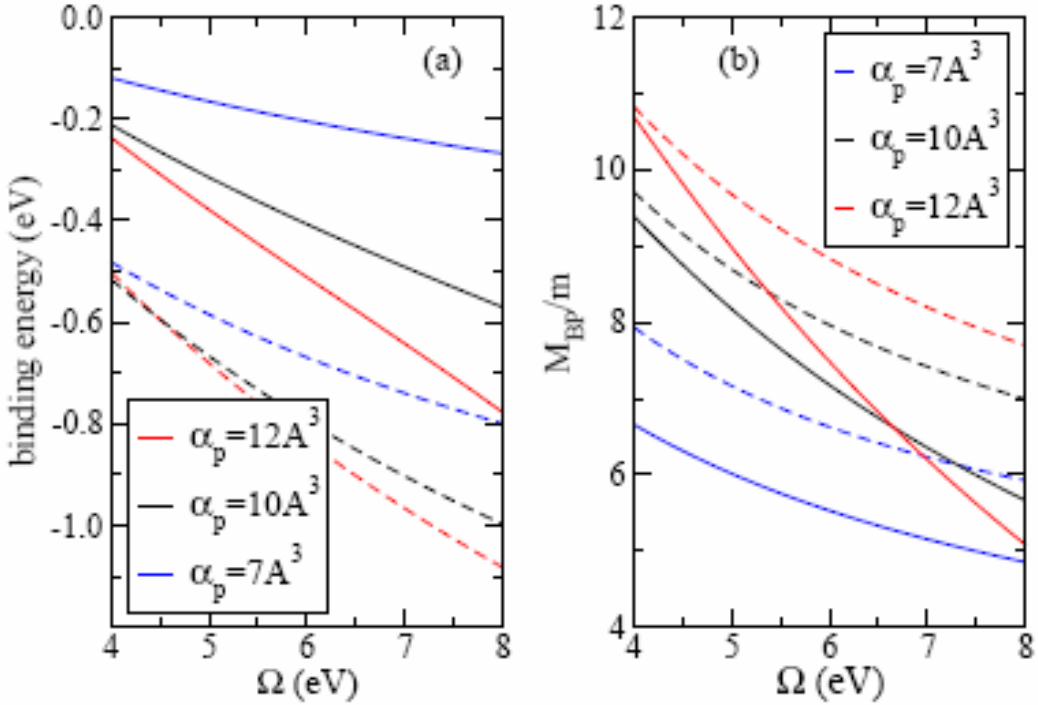


FIG. 8: Ground-state bipolaron (a) binding energy, and (b) effective mass in units of the free carrier mass vs. Ω, for various polarizabilities. The full lines correspond to $t' = 0$, dashed lines to $t' = -t/2$. Here $U_H = 10$eV.

Note that the bipolaron mass is only 8 times the free particle mass this Is again much lighter than for lattice bipolarons allowing for an eventual high Bose Einstein condensation T.

Systematics of Tc

- Tc variation with bond angles bond lengths and polarizabilities
- Note that often the As-Fe-As bond angle is used or the orthorhombic distortion in the plane or the Fe-As-Fe diagonal bond angle is used for systematics.
- Our model suggests rather using bond lengths and the Fe-As-Fe nearest neighbor bond angle

Effective interaction plotted vs log Tc

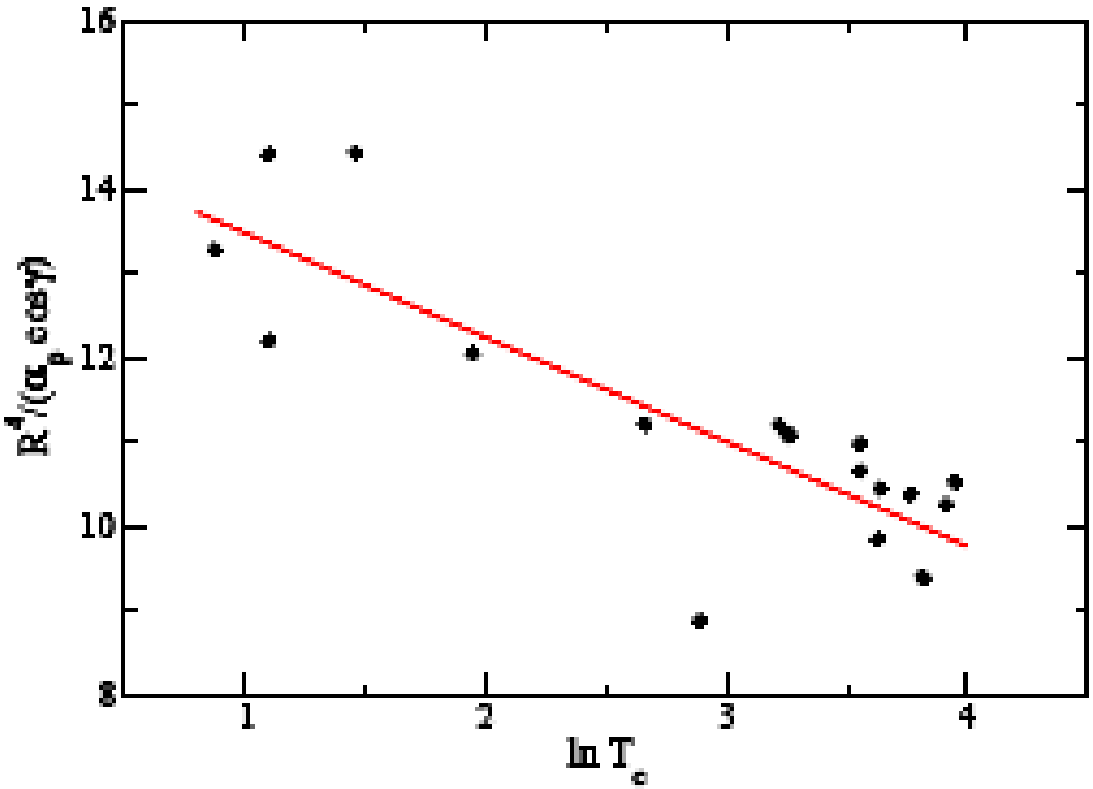


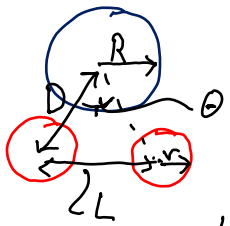
FIG. 13: Linear fit of $\ln T_c$ vs. $\frac{R^4}{\alpha_p^2 \cos^2\gamma}$. The data points are taken from Refs. 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16.

Conclusions

- The Fe pnictides and heavy anion chalcogenides are very different from the cuprates with regard to low energy scale properties: spin, charge, orbital, and lattice degrees of freedom
- Hybridization covalency involving Fe 3d is weak crystal and ligand fields are small, electronic structure given by band structure with weak correlation
- We suggest that the As 4p – Fe 4s and 4p hybridization and especially the Arsenic ELECTRONIC polarizability set the scene for a band structure approach.
- The quasi particles are electronic polarons with a modest mass of about 2-3 with possibly an attractive nn interaction resulting in bipolarons with s,or d wave superconductivity and also a modest mass

- DESIGN (ARTIFICIAL) STRUCTURES USING HIGHLY POLARIZABLE ATOMS OR SMALL MOLECULES ALTERNATING WITH NARROW BAND METAL FILM FOR HIGHER Tc's?

Material design and limitations



$D_{min} = R + r$ $\quad Z$ = n common polarizable neighbors

$$Interaction = Z\alpha\left(\frac{1}{R+r}\right)^4 \cos(\theta) > \frac{1}{L} \quad \text{(bare repulsion)}$$

$L = 2(R+r)\sin\theta$ $\quad 2Z\alpha\left(\frac{1}{R+r}\right)^3 \cos\theta\sin\theta > 1$

$\alpha = CR^3$ $\quad \simeq 2ZC\frac{1}{(1+\frac{r}{R})^3}\cos\theta\sin\theta > 1$

For $r = 0.5\,\text{Å}$ $\quad R = 2\,\text{Å}$ $\quad \simeq 2ZC\frac{1}{2}\cos\theta\sin\theta > 1$

Can be attractive for $Z \geq 2$

Need to maximize Z and minimize θ

Z is limited by R i.e Anion-Anion $> 2R$

Fe pnictides do a good job of this

What about the magnetic properties

- Strongly increasing magnetic susceptibility with temperature above the SDW transition and above Tc indicates a activated nature of the local spins
- The bipolarons we suggest are singlets in the ground state they would exhibit an increasing susceptibility with temperature.
- The bipolarons could condense into a SDW of low amplitude because of Bipolaron- Bipolaron exchange interactions
- Or they could condense into a BEC like superconductor

Previous Models using electronic polarizabilities

PHYSICAL REVIEW VOLUME 134, NUMBER 6A 15 JUNE 1964

Possibility of Synthesizing an Organic Superconductor*

W. A. LITTLE
Department of Physics, Stanford University, Stanford, California
(Received 13 November 1963; revised manuscript received 27 January 1964)

PHYSICAL REVIEW B VOLUME 7, NUMBER 3 1 FEBRUARY 1973

Model for an Exciton Mechanism of Superconductivity*

David Allender,† James Bray, and John Bardeen
Department of Physics and Materials Research Laboratory, University of Illinois, Urbana, Illinois 61801
(Received 7 August 1972)

Both concentrated on on site interactions reguiring huge retardation effects to Compensate for the on site repulsive interaction. !!!

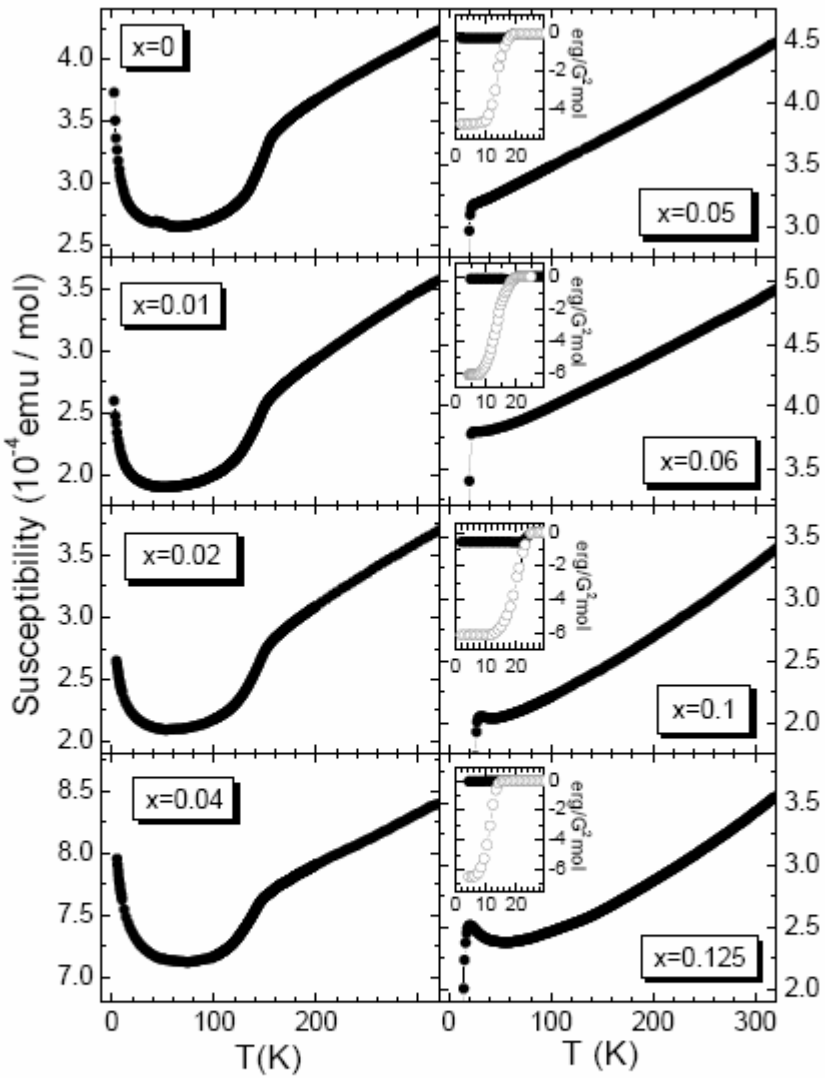


FIG. 3: Static susceptibility $\chi = M/B$ of $LaFeAsO_{1-x}F_x$, for different doping level between $0 \leq x \leq 0.125$ at $B = 1\,\mathrm{T}$. Note, that for all graphs the ordinate covers the range $\Delta\chi = 2\,\mathrm{emu/mol}$. Insets: M vs T for $B = 2\,\mathrm{mT}$.

Some other experimental results

- Neutron scattering yields ordered moments ranging from very small to 0.9 μ B
- Magnetic ordering is antiferromagnetic SDW like 1D ferromagnetic chains coupled antiferromagnetically
- Neutron inelastic scattering yields a large spin wave velocity i.e. large J but also a large spin wave gap of 10 meV and the spin waves are heavily damped above about 30 meV. " Stoner Continuum?"