Magnetism of iron-based superconductors

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Present talk:

I will not talk about the coexistence of AF and SC…

In order to stimulate the discussion on the normal state of iron-based superconductors, I would like to introduce

RA and H. Ikeda, JPSJ78, 113707 (2009)
"Is Fermi-surface nesting the origin of superconductivity in iron pnictides?"

P. Hansmann, RA, *et al.*, PRL104 197002 (2010)
"Dichotomy between large local and small ordered magnetic moment in Iron-based superconductors"

RA and H. Ikeda, JPSJ78, 113707 (2009)

(plain) FLEX for pnictides has a problem which we usually do not mention/discuss

What is the problem ? How are we treating this ?
Is there any better ways to treat it ?

P. Hansmann, RA, et al., PRL104 197002 (2010)

How magnetism is described in LDA+DMFT ?
(in the context of the localized vs itinerant picture)

Orbital dependent nesting in RPA

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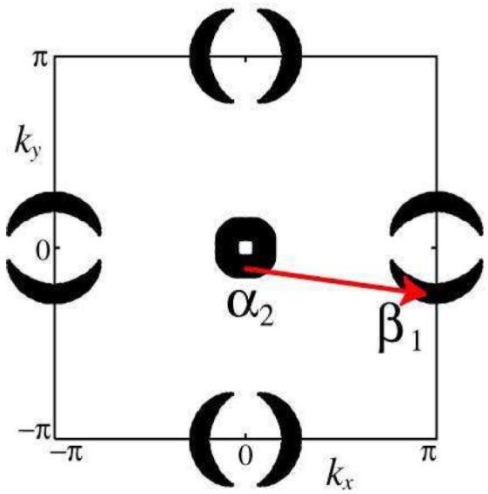
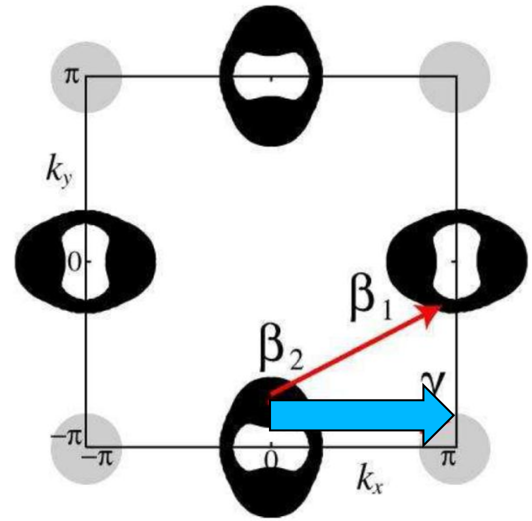
yz / xz



x^2-y^2



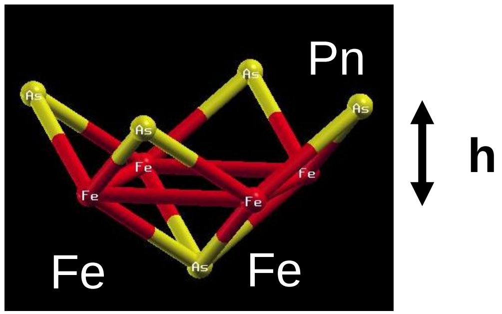
x/y axis points to As

x^2-y^2 at (π,π) is the key to understand the material dependence of SC in Fe-pnictides

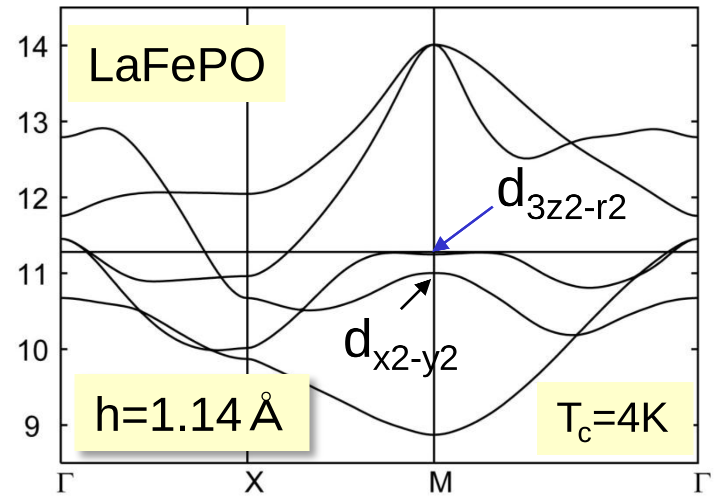
K. Kuroki's talk (yesterday)

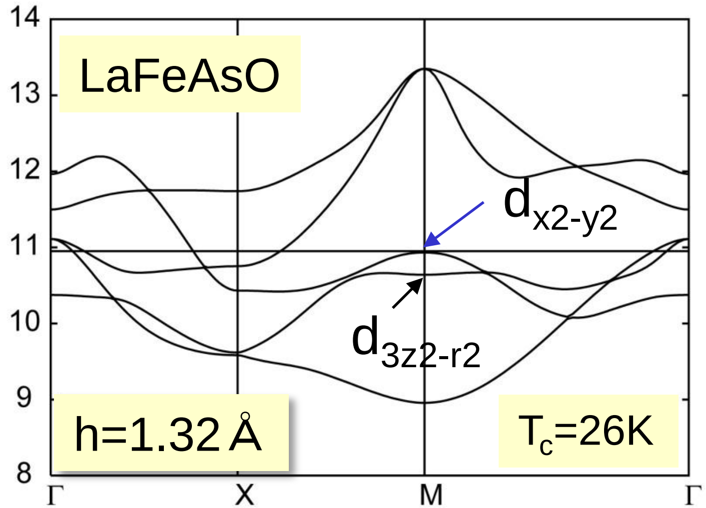
LDA band of 1111 compounds

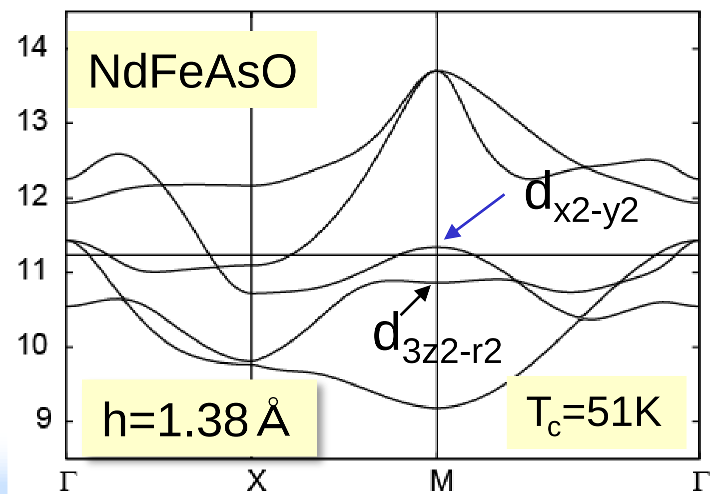
Whether we have x^2-y^2 at (π,π) sensitively depends on the crystal structure



Large h $\rightarrow x^2$-y^2 tends to make FS







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Orbital dependent nesting: LaFeAsO vs LaFePO

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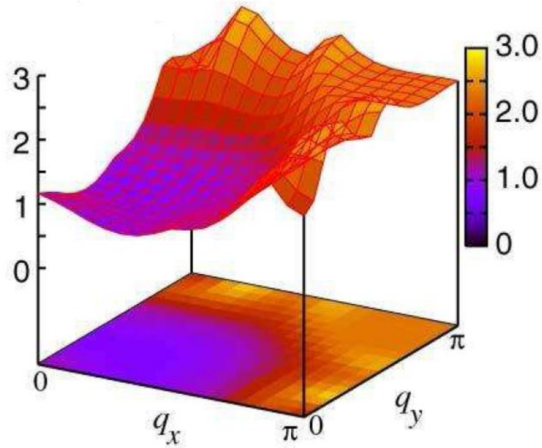
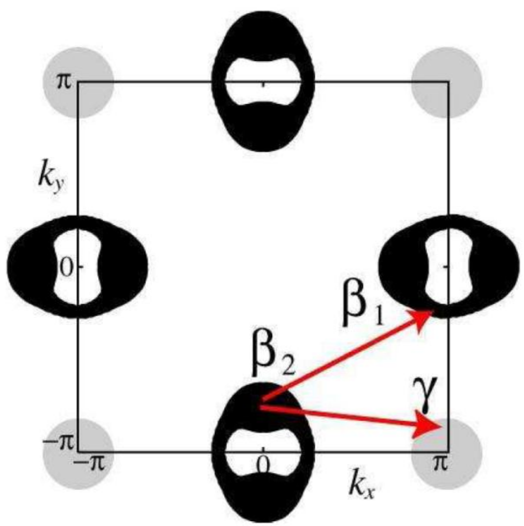
χ_{s0}^{iiii}

$i = x^2 - y^2$

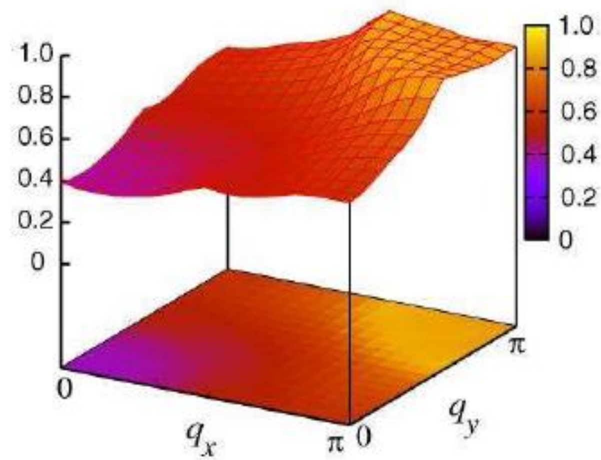
LaFeAsO



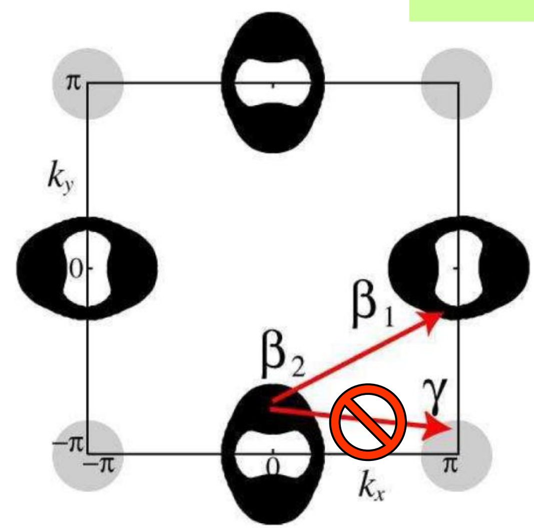
peak at (π,0)



LaFePO



No structure at (π,0)

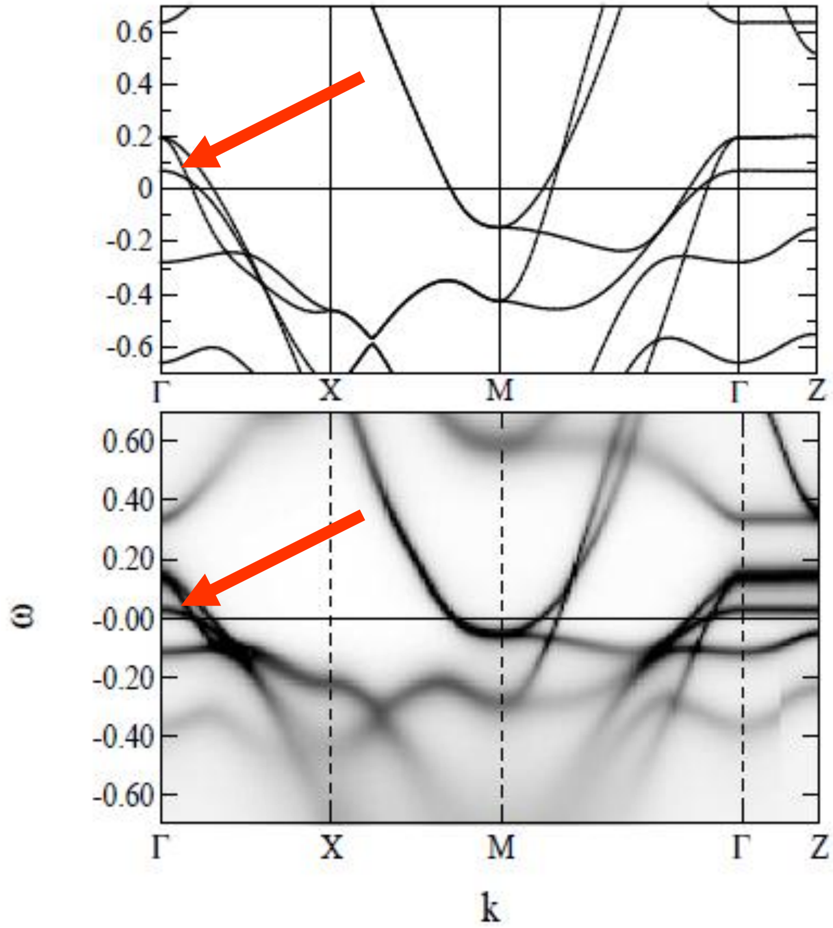


In RPA,

SC sensitively depends on whether we have x^2-y^2 FS at (π,π)

<u>x^2-y^2 FS at (π,π) robust against Σ ?</u>

DMFT self energy $\Sigma_{ij}(\omega)$ correction to ε_{LDA}



Aichhorn et al., PRB80 085101(2009)

<u>Σ changes the position of d_{x2-y2} at (π,π)</u>

0.08 eV (LDA) →0.02 eV (DMFT)

Momentum dependent $\Sigma_{ij}(\boldsymbol{k},\omega)$?

FLEX/self consistent 2nd order perturbation

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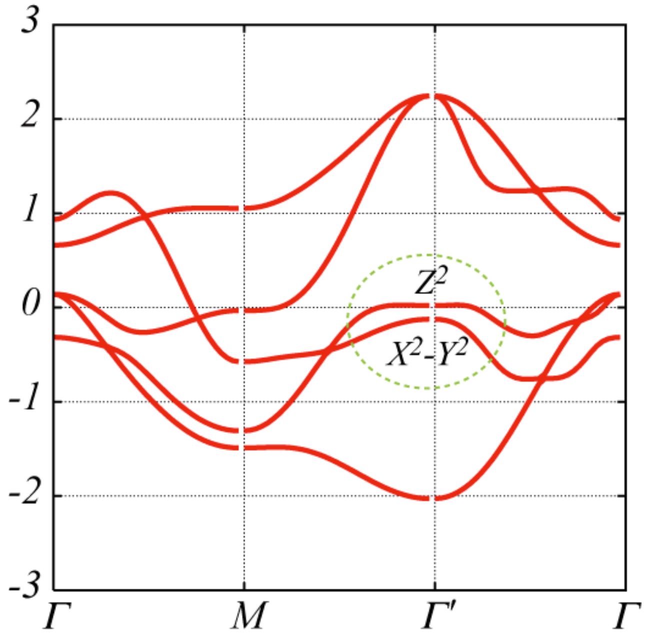
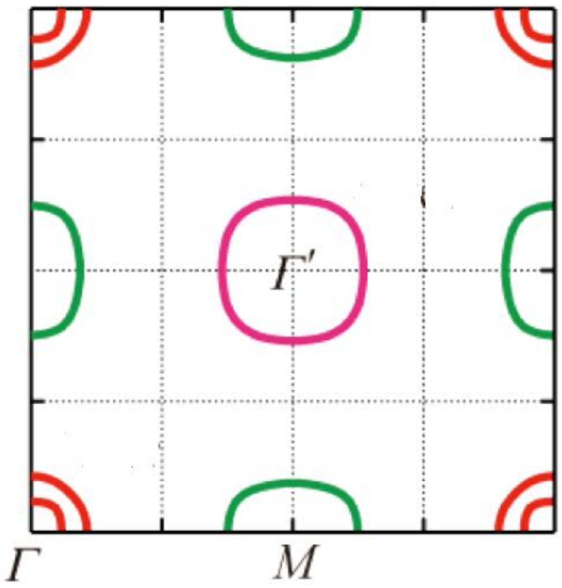
H. Ikeda, JPSJ 77 123707 (2008)





If we consider Σ, z^2 makes Large FS

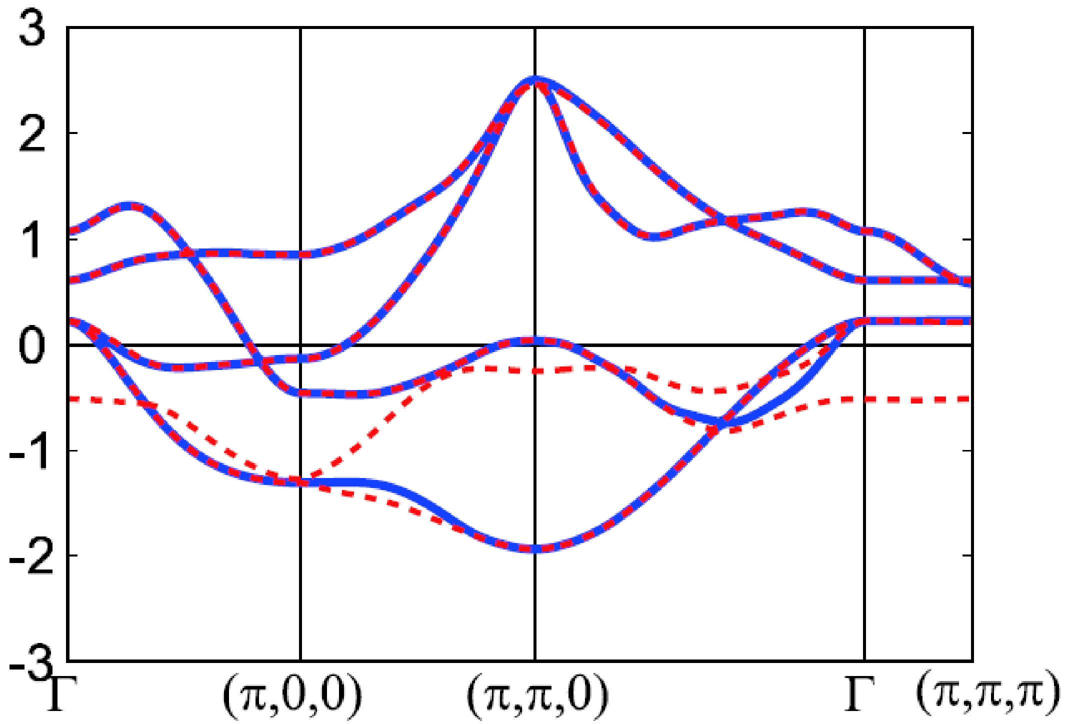
(π,0) fluctuation is weak

(π,π) fluctuation is dominant

→ introduction of artificial level shift for z^2

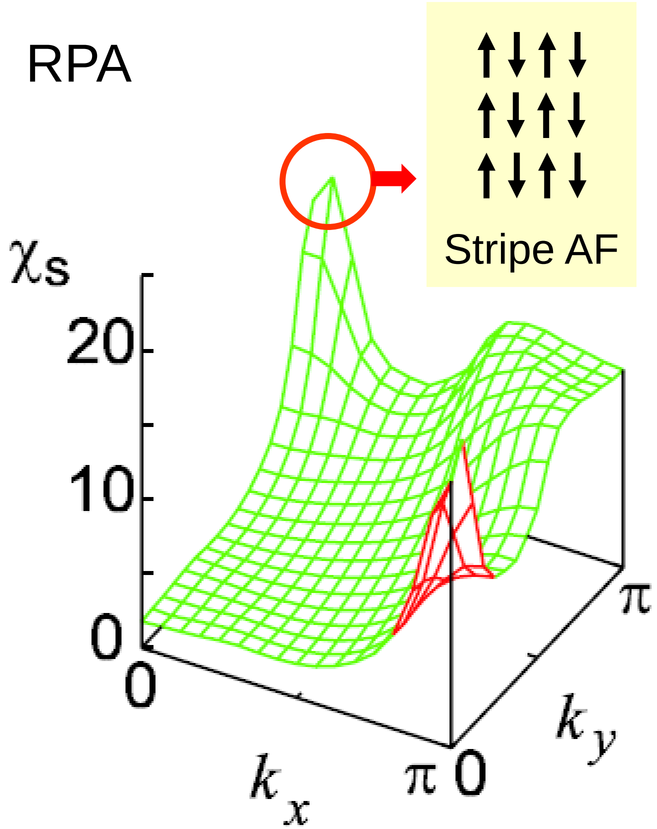
4 orbital model

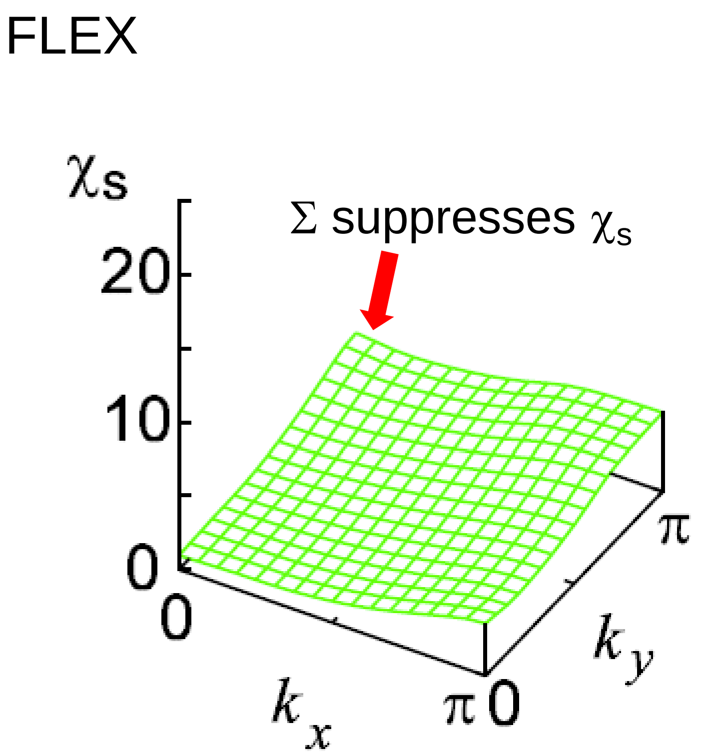
Let us assume that z^2 is not a key player and we can forget about it
Let us consider a model without dz^2…



RPA vs FLEX: spin susceptibility

U=1.2, U'=0.9, J=0.15 eV





Moderately large *U* needed to induce strong AF instability

Electron Correlation vs Anion Height

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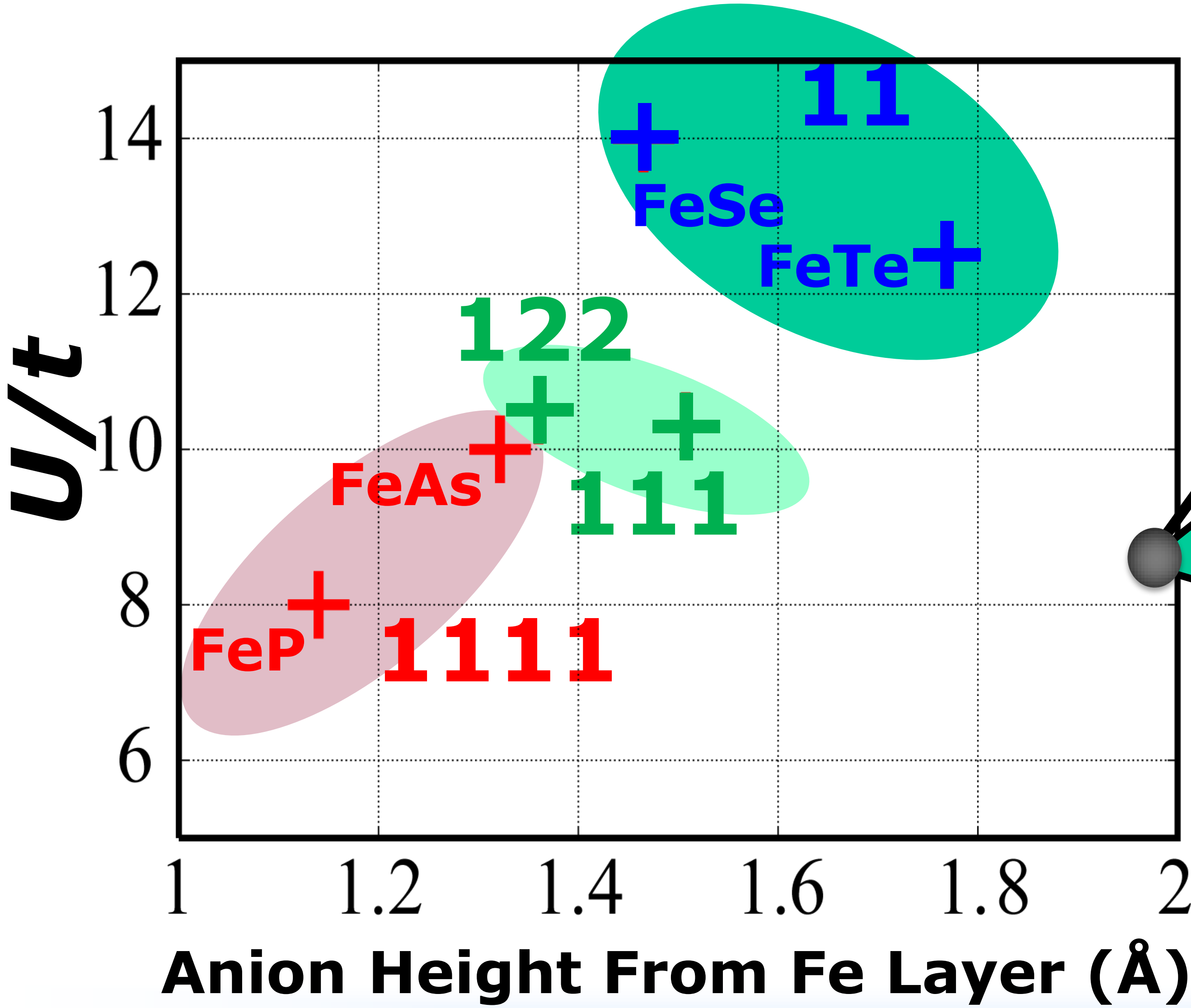
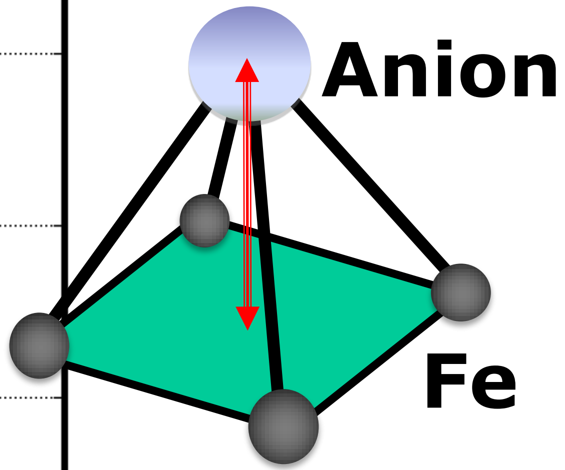
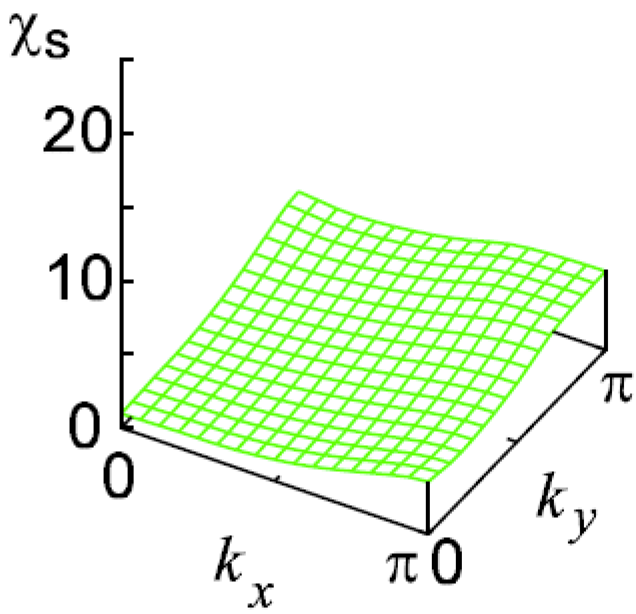
Miyake-Nakamura-RA-Imada, JPSJ09



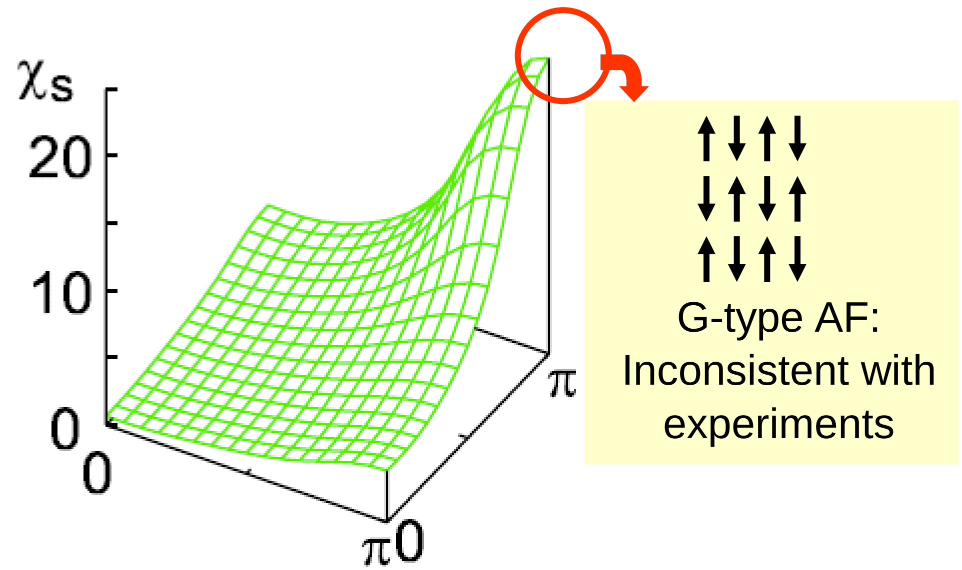


FLEX for realistic *U*

U=1.2, U'=0.9, J=0.15 eV



U=1.8, U'=1.2, J=0.3 eV



In moderately correlated regime, FS nesting does not favor S-type AF

FLEX for realistic U: $|G(\boldsymbol{k},i\omega_1)|$ of x^2-y^2

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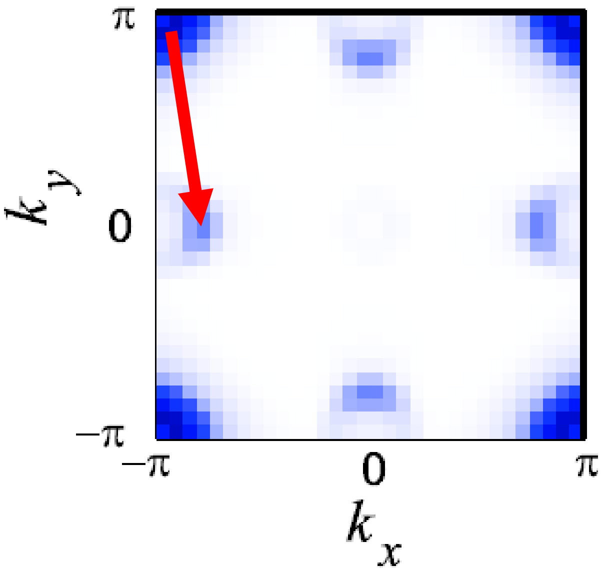
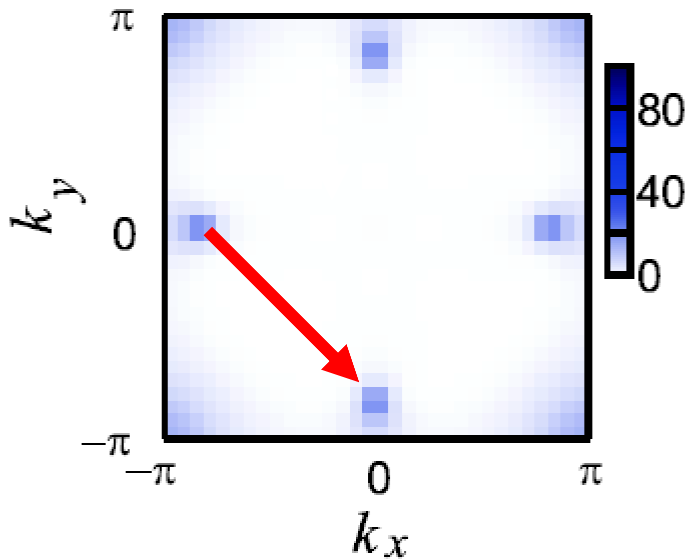
RPA ($U=1.2, J=0.15$)



$|G(\boldsymbol{k},i\omega_1)|$ is large at (π,π)

(π,0) nesting is dominant

FLEX ($U=1.8, J=0.3$)



$|G(\boldsymbol{k},i\omega_1)|$ is small at (π,π)

(π,π) nesting is dominant

(plain) FLEX can not explain stripe AF in moderately correlated regime ?

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So, what we are doing now in FLEX ?

H. Ikeda, R. Arita, and J. Kunes

"Phase diagram and Gap anisotropy in iron-pnictide superconductors"
Phys. Rev. B 81 054502 (2010)

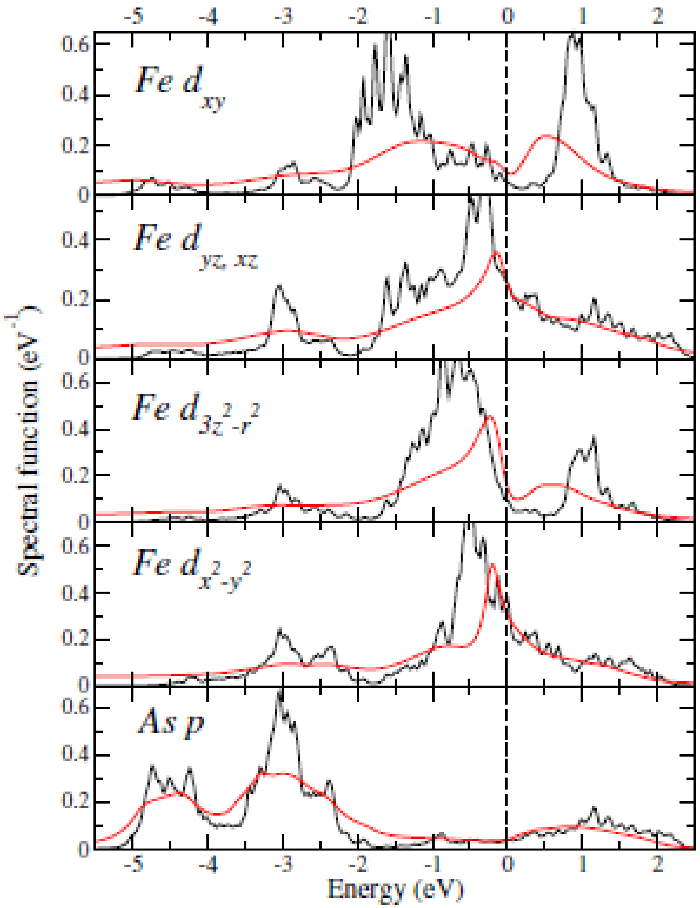
"Doping dependence of spin fluctuations and electron correlations in iron pnictides"
Phys. Rev. B 82 024508 (2010)

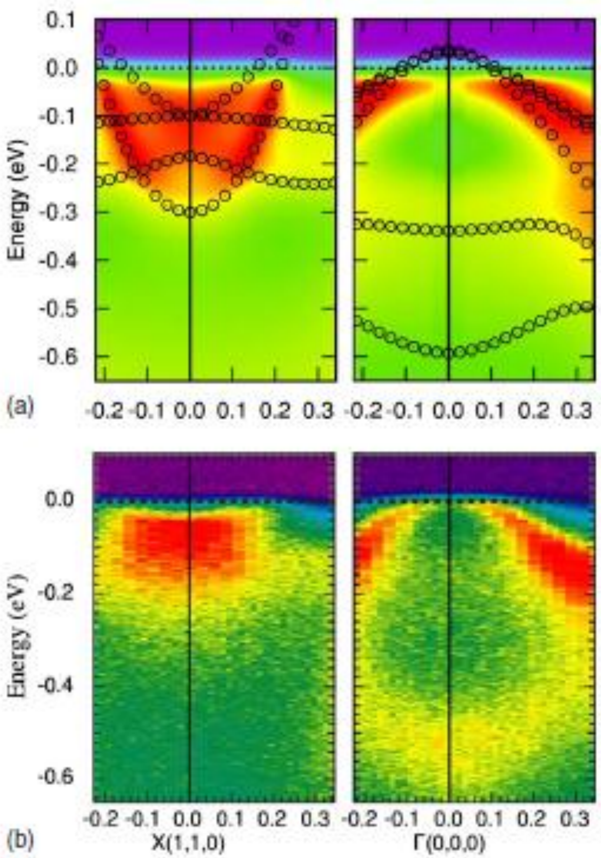
A constraint "Re Σ_{ij} (k, ω=0)=0" introduced

Are there any better treatments ?

LDA+DMFT

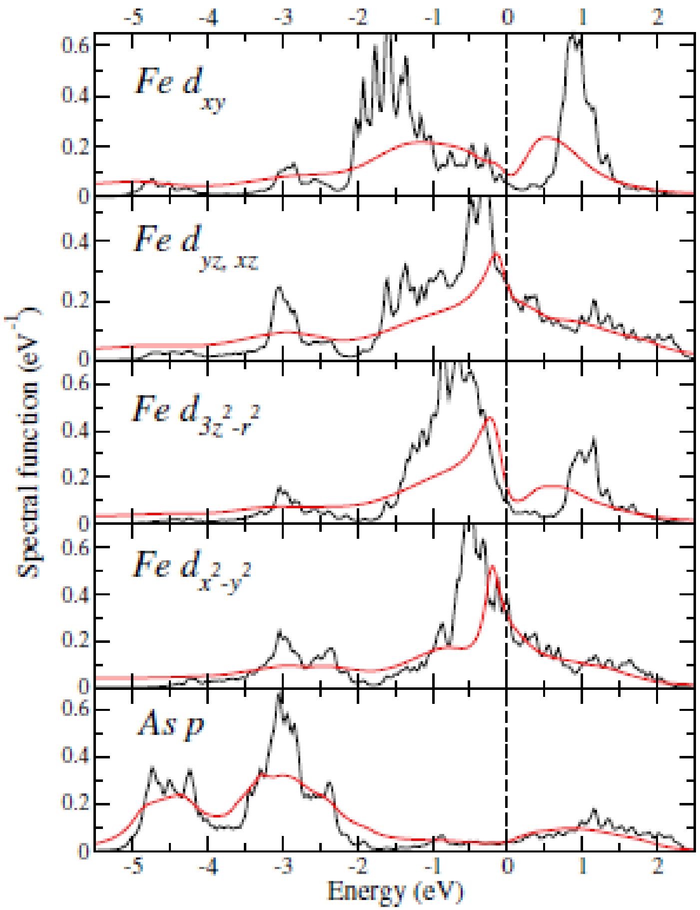
dpp model (Skornyakov et al. 09, cf Aichhorn et al. 09)

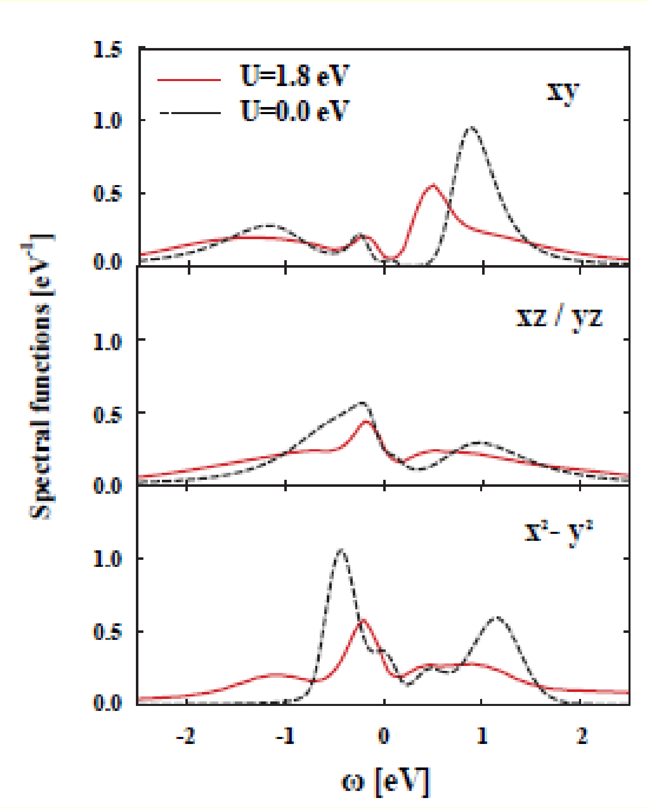




m*/m~2

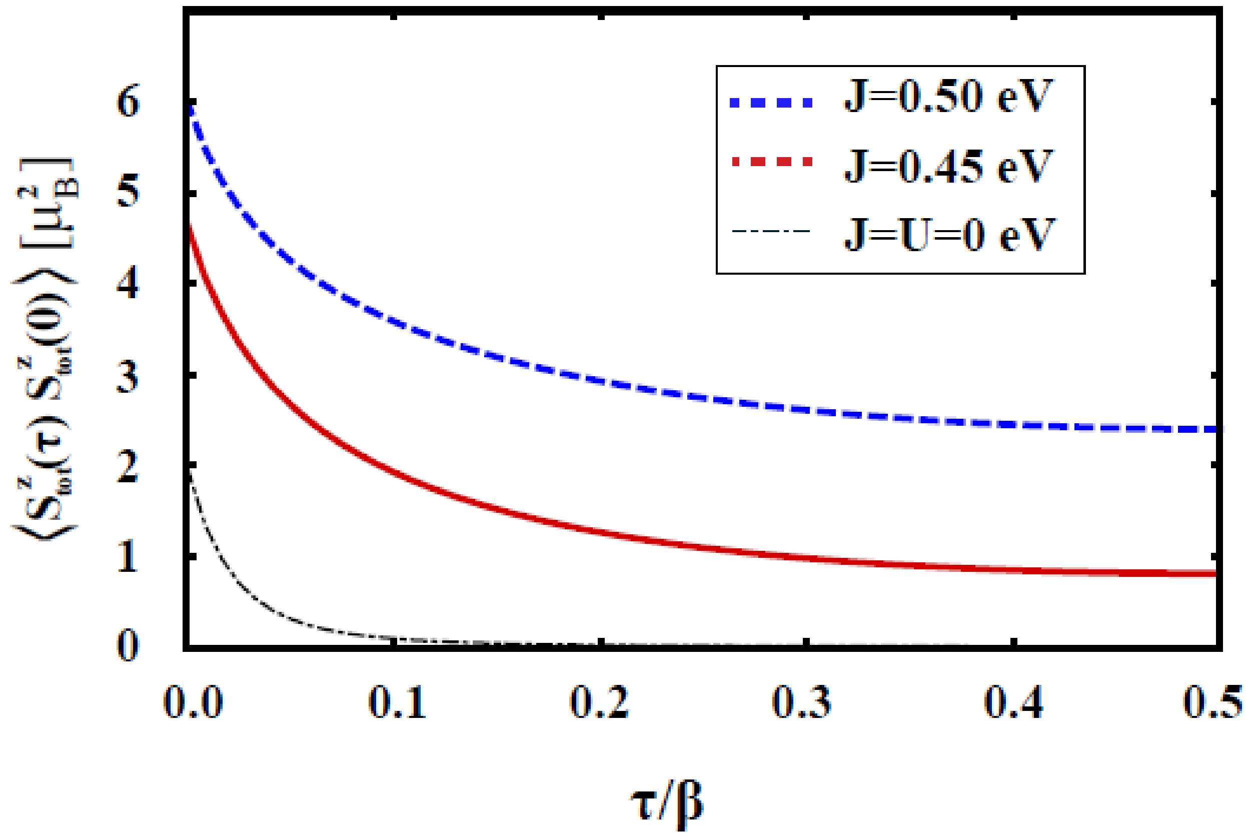
LDA+DMFT: dpp vs 4 orbital model





How about spin-spin correlation ?

LDA+DMFT: spin-spin correlation



In the moderately correlated regime (Z~0.5)
Local moment at t=τ=0 is about $2\mu_B$
(~LSDA ordered moment)

Correlation effect is not so significant in

One-particle quantity

But can be visible in two-particle quantity

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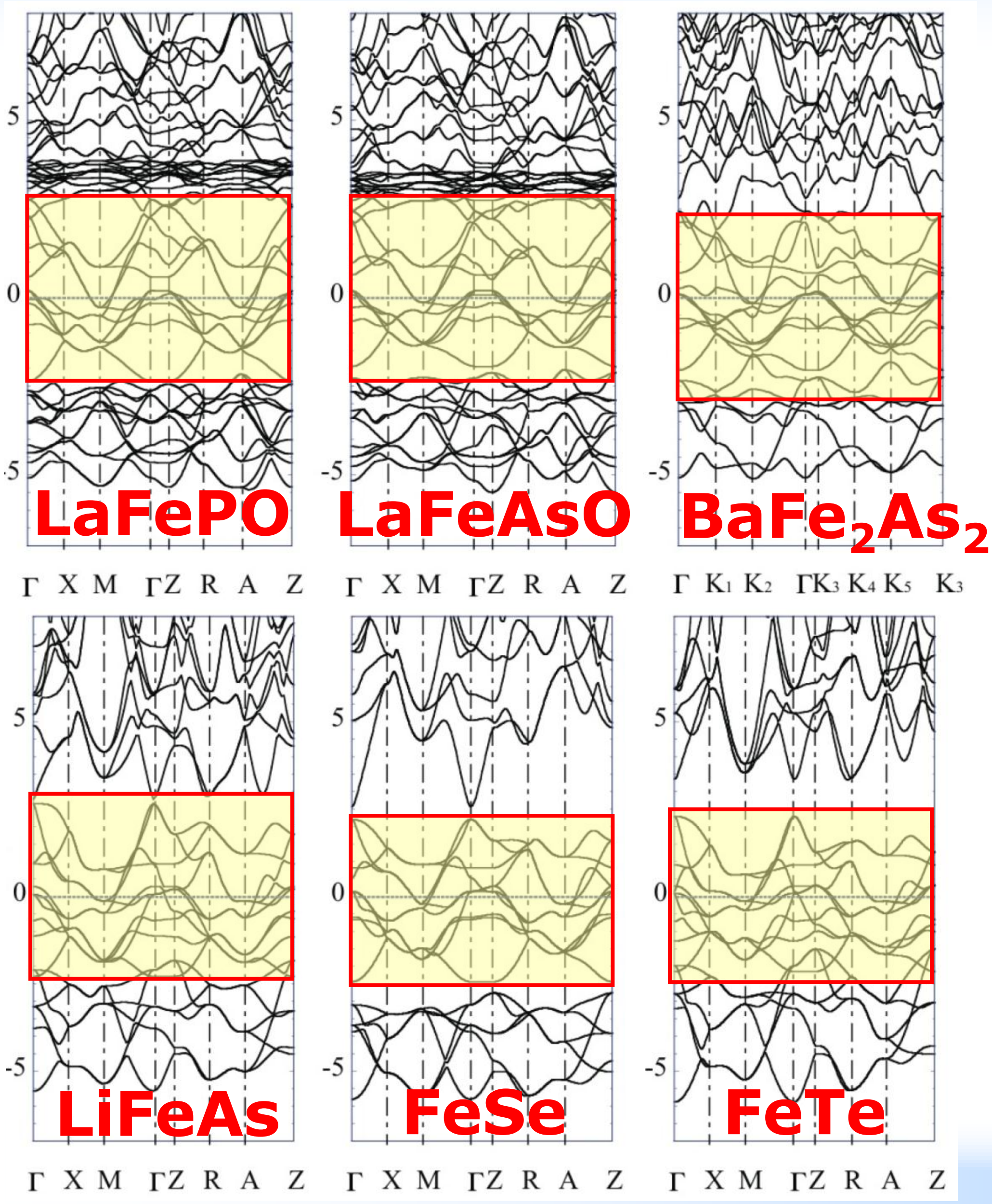
ab initio derivation of low-energy Hamiltonians for Iron-based superconductors

Miyake-Nakamura-RA-Imada, JPSJ79, 044705 (2010)

Band Structure of iron-based superconductors



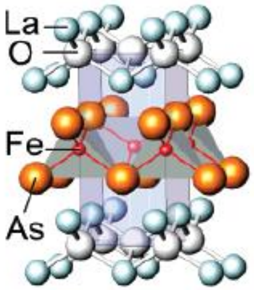
Similar structure around E_F

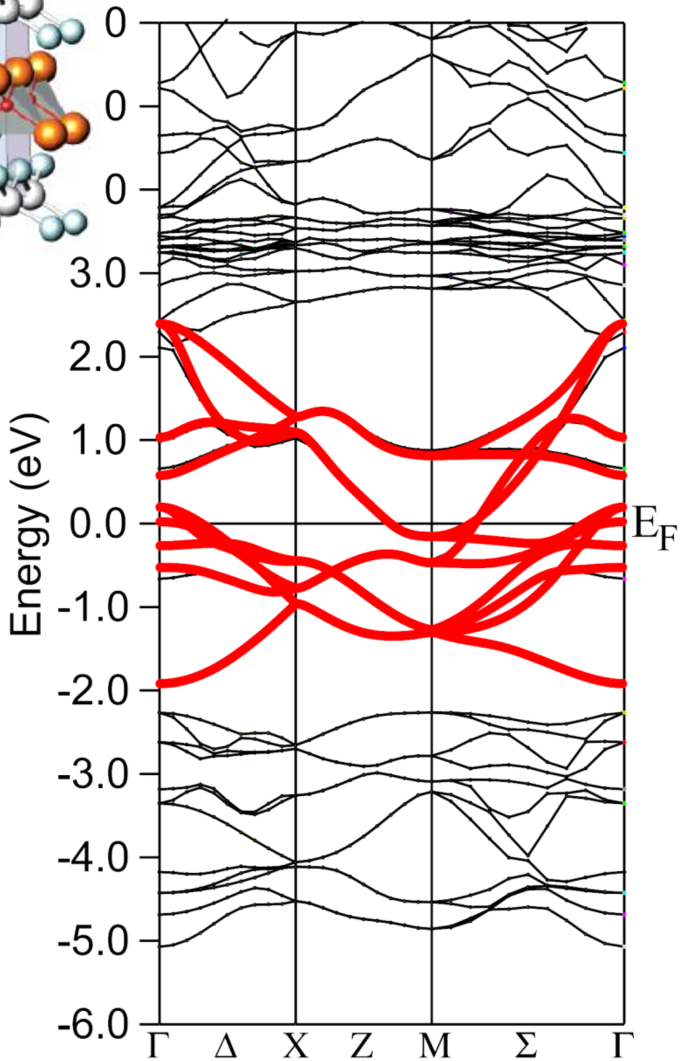
Band Width:

LaFePO	4.9 eV
LaFeAsO	4.4 eV
$BaFe_2As_2$	4.4 eV
LiFeAs	5.1 eV
FeTe	4.5 eV
FeSe	4.6 eV

Family dependence of interaction parameters ?

d-only model for iron-based superconductors



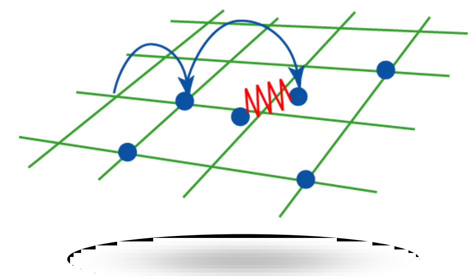


La 4f

Fe 3d

O 2p
As 4p

$$H_0 = \sum_{\sigma} \sum_{RR'} \sum_{nm} t_{mRnR'} c^{\dagger}_{\sigma nR} c_{\sigma mR'}$$



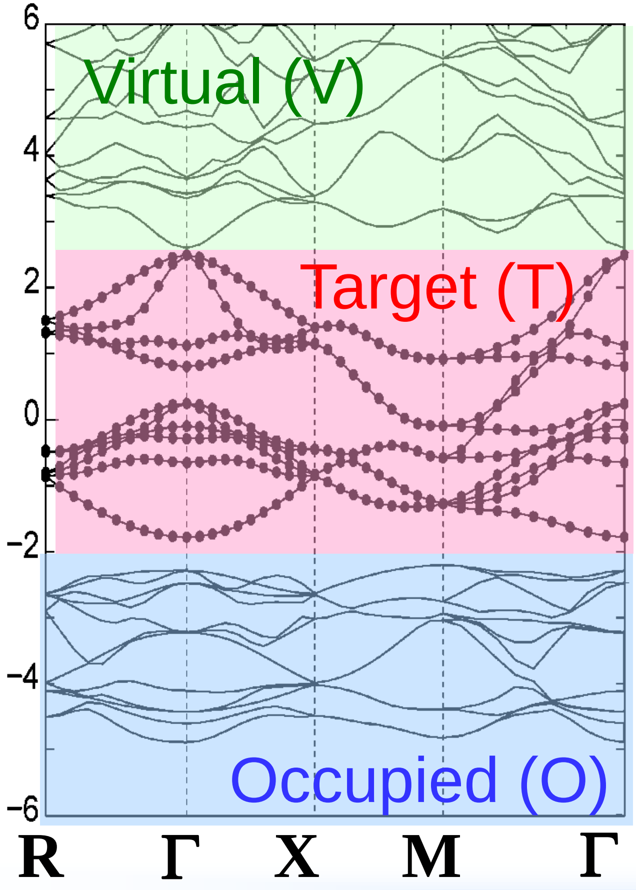
$$|w_{\sigma nR}\rangle = c^{\dagger}_{\sigma nR} |0\rangle$$

MaxLoc Wannier

Kuroki, Onari, RA et al.
Phys. Rev. Lett. 101 087004 (08)

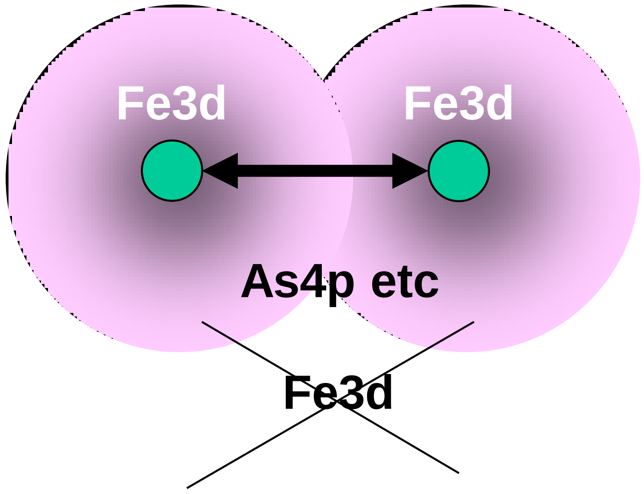
Constrained RPA

$$W = (1 - v\chi)^{-1} v$$



Full RPA polarizability:

$$\chi = \sum_{i}^{occ} \sum_{j}^{unocc} \frac{\psi_i(r)\psi_j^*(r)\psi_i^*(r')\psi_j(r')}{\omega - \varepsilon_j + \varepsilon_i \pm i\delta}$$

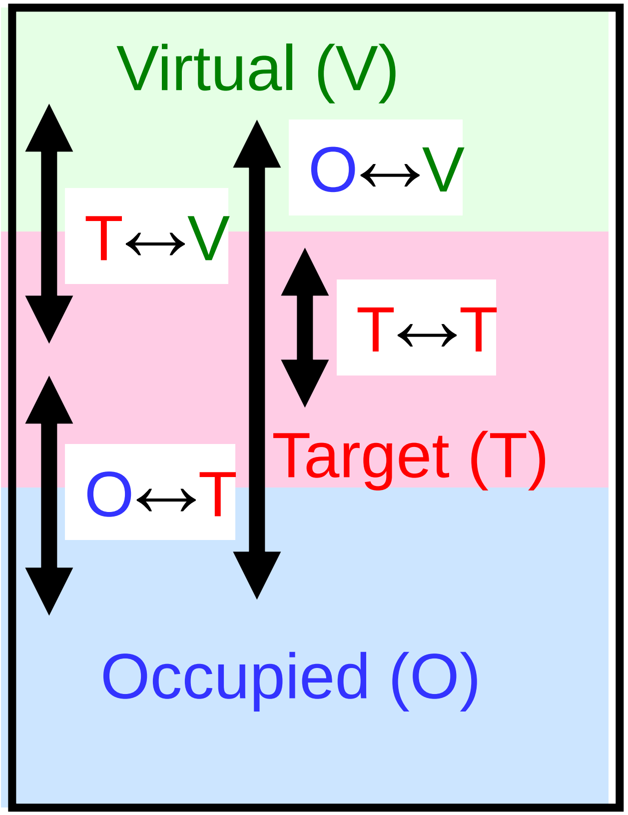


Constrained RPA method

Aryasetiawan et al, PRB 70, 195104 (2004)
Solovyev-Imada, PRB 71, 045103 (2005)

Constrained RPA

$$W = (1 - v\chi)^{-1} v$$



Full RPA polarizability:

$$\chi = \sum_{i}^{occ} \sum_{j}^{unocc} \frac{\psi_i(r)\psi_j^*(r)\psi_i^*(r')\psi_j(r')}{\omega - \varepsilon_j + \varepsilon_i \pm i\delta}$$

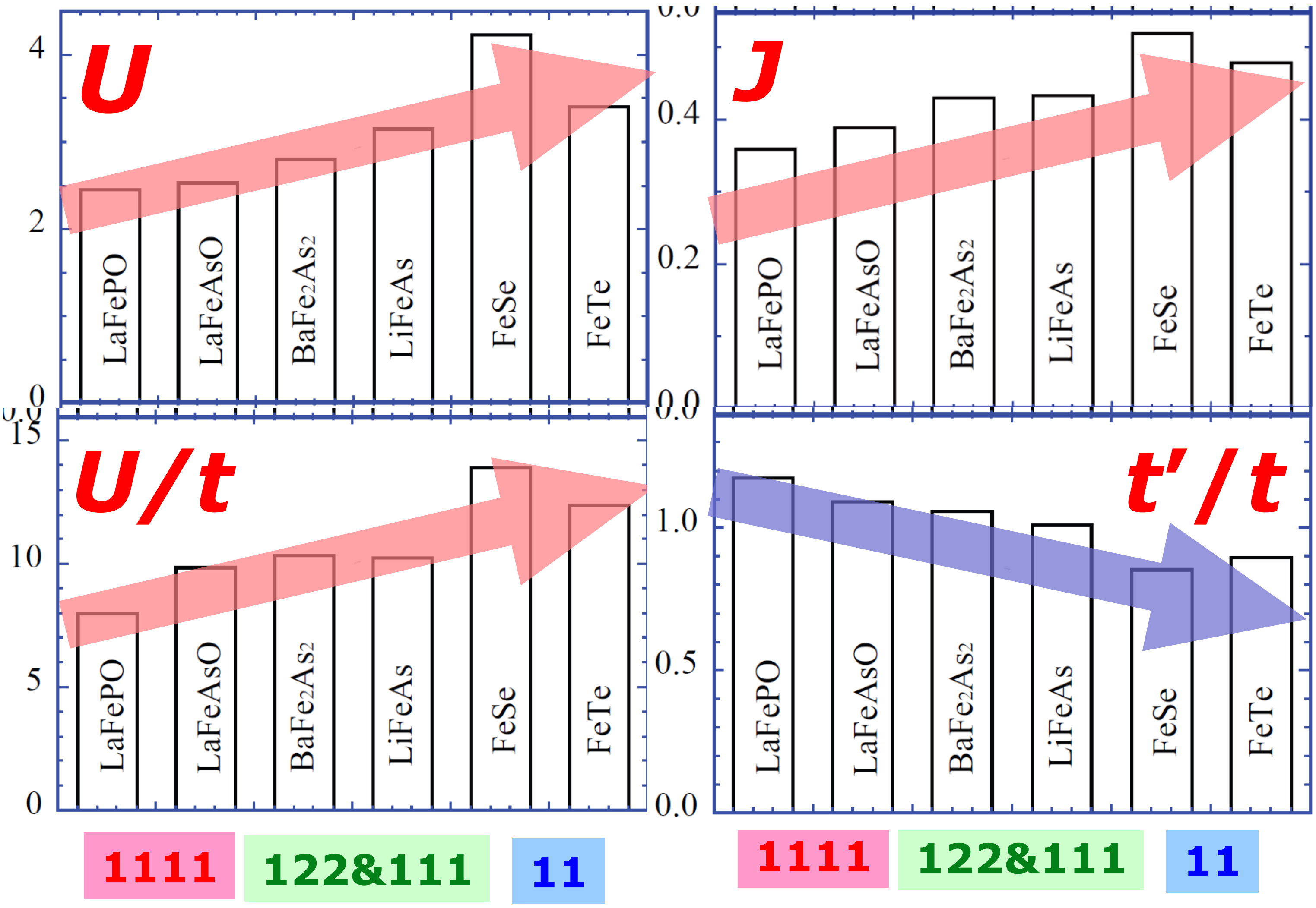
$$\chi = \sum_{O\leftrightarrow T} + \sum_{T\leftrightarrow V} + \sum_{O\leftrightarrow V} + \sum_{T\leftrightarrow T}$$

$$\chi_{\mathrm{r}} = \sum_{O\leftrightarrow T} + \sum_{T\leftrightarrow V} + \sum_{O\leftrightarrow V} \qquad \chi_{\mathrm{d}} = \sum_{T\leftrightarrow T}$$

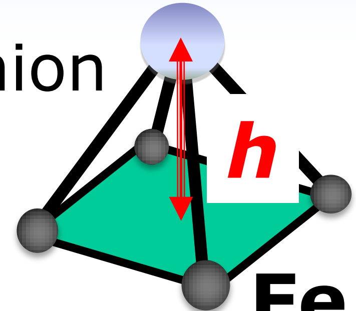
$$W_{eff} = (1 - v\chi_{\mathrm{r}})^{-1} v$$

$$U_{\mathbf{R}} = \langle w_{\mu\mathbf{0}} w_{\mu\mathbf{0}} | W_{eff} | w_{\nu\mathbf{R}} w_{\nu\mathbf{R}} \rangle$$

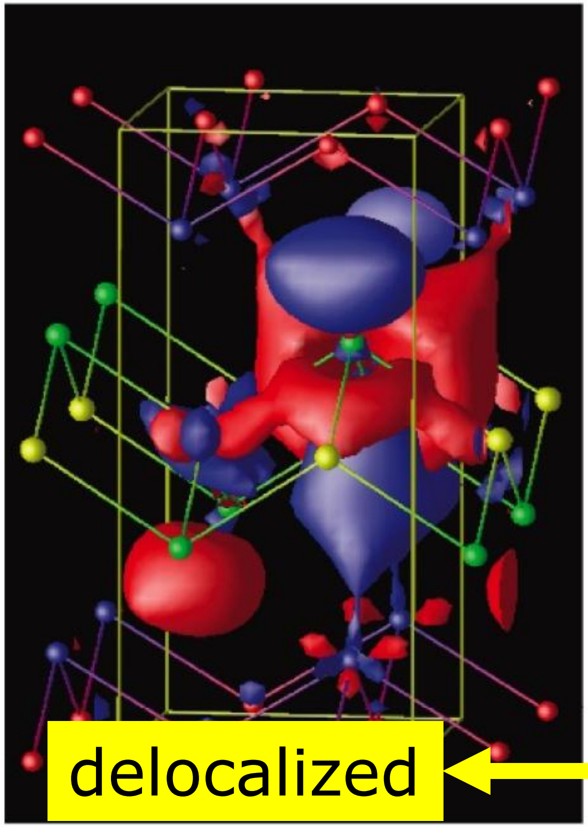
Family Dependence of model parameters



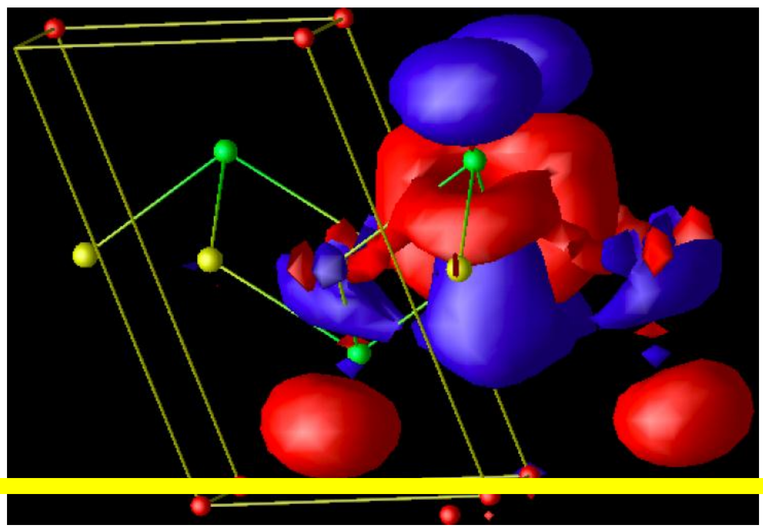
Spread of MaxLoc Wannier



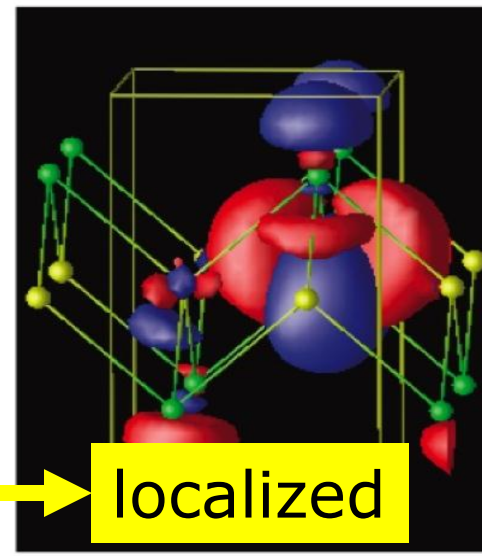
LaFeAsO



$BaFe_2As_2$



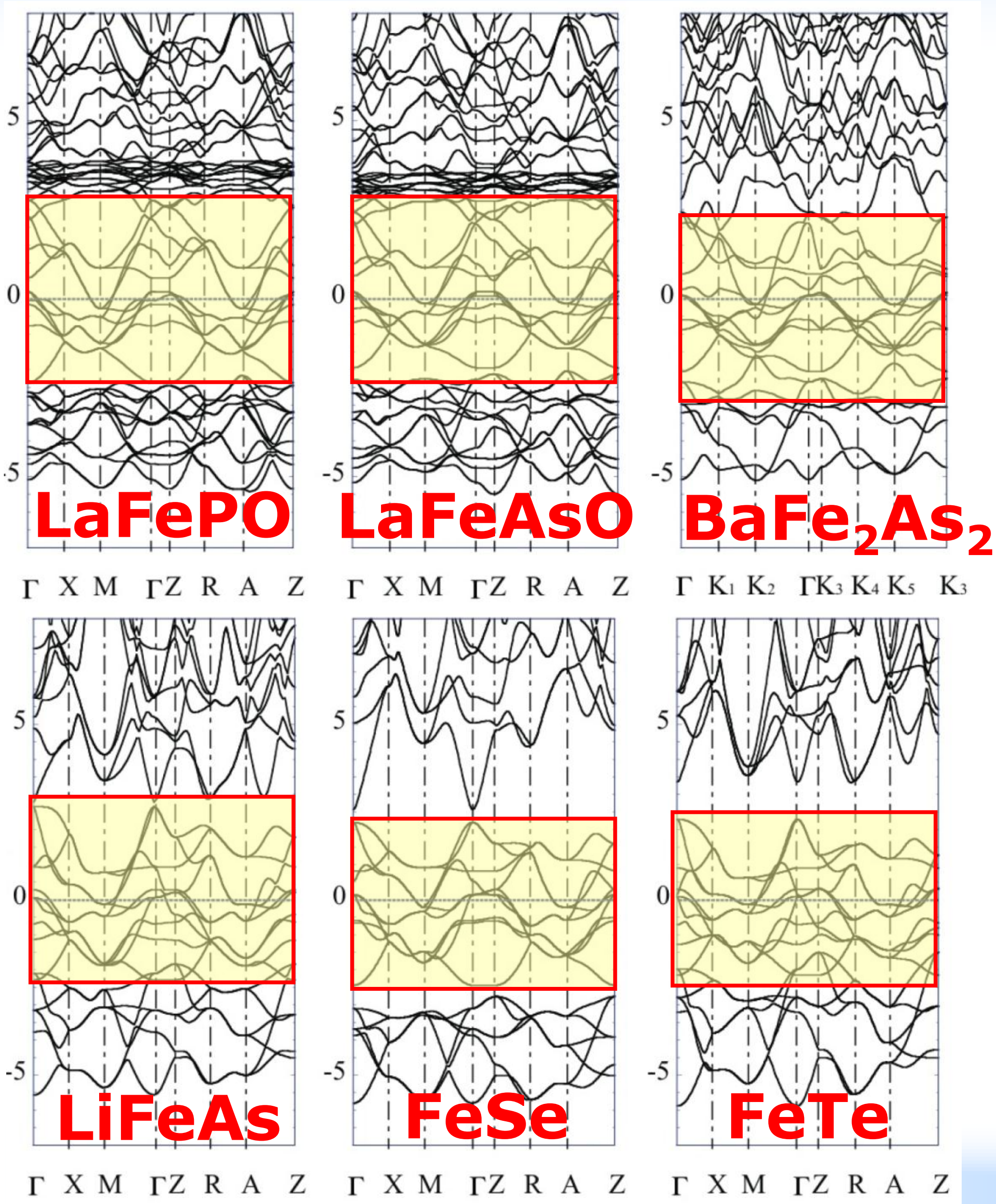
FeTe



LaFeAsO	$BaFe_2As_2$	FeTe
h=1.32 Å	h=1.36 Å	h=1.77 Å
U_{bare}=14.9 eV	U_{bare}=15.6 eV	U_{bare}=16.9 eV

R.Arita

Band Structure of iron-based superconductors



# of screening channels
Small for 11 systems
→ stronger correlation

Summary: Family dependence of int. parameters

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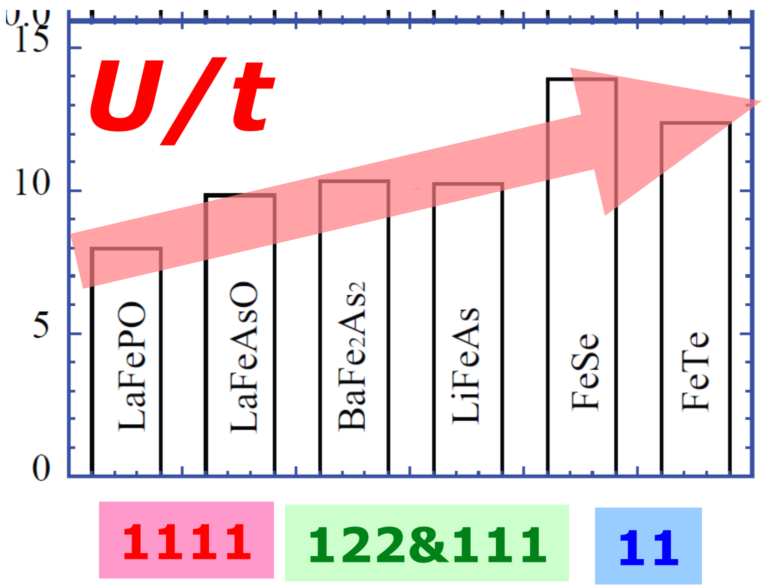

- Electron correlations in iron-based superconductors:
  - LaFeAsO, 122, 111 are moderately correlated
  - Correlation in 11 system is stronger
  - LaFePO is weakly correlated