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First-principles study of the electronic structure of the Iron-based pnictides

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First-principles study of the electronic structure of the iron-based pnictides

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arXiv:0803.3325, to appear in Phys. Rev. Lett.
arXiv:0806.3285, to appear in Phys. Rev. B
arXiv:0806.3860, to appear in J. Phys. Soc. Jpn
arXiv:0806.4750, to appear in J. Phys. Soc. Jpn

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- H. Usui (Univ. Electro-Commun.)
- H. Kontani (Nagoya Univ.)
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Outline

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- Introduction
- Construction of an effective model from first-principles
  - Minimal model which describes low energy physics:
    Which d-orbitals are involved?
  - Estimation of interaction parameters:
    How large is *U, U', J* ?
- Multi-band RPA study on unconventional superconductivity
  - Symmetry of Δ

Iron-based layered superconductor

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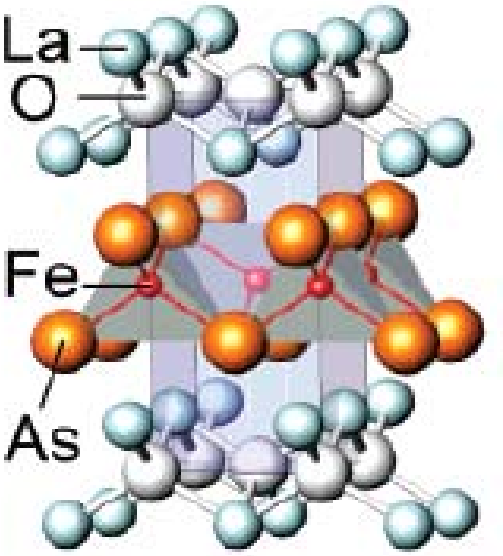
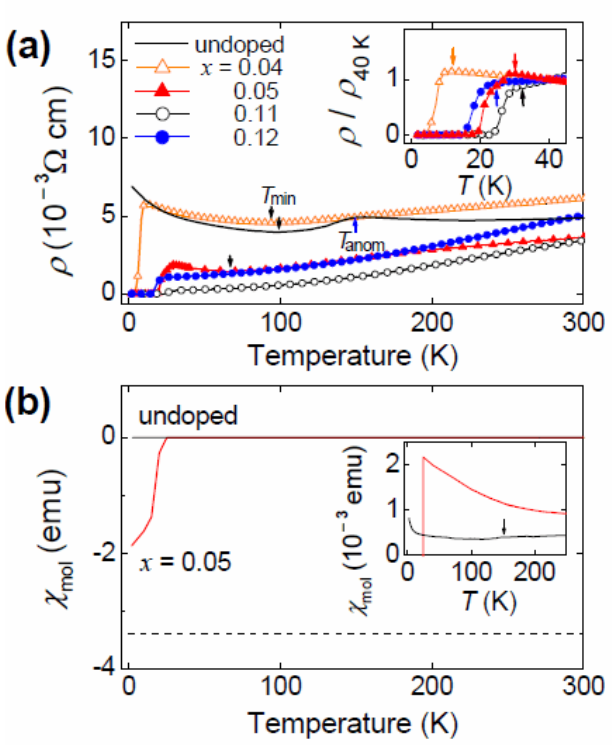
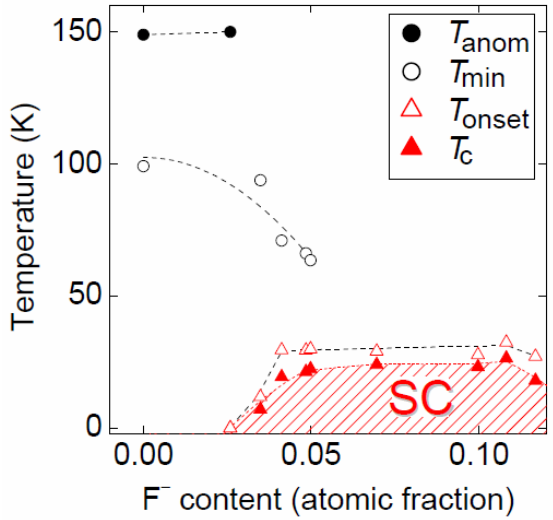
Kamihara et al, JACS 130 3296 (2008)

LaFeAs [$O_{1-x}F_x$] (x=0.05-0.12)







T_c~26K

High T_c: raising up to ~55K

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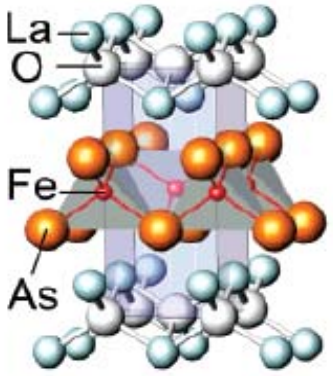
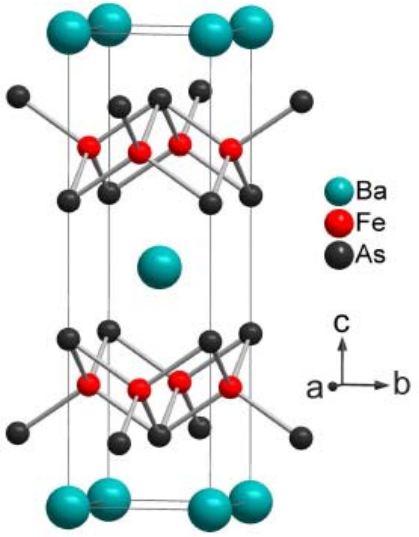
- $RFeAsO_{1-x}F_x$
  - Substitution of La with other rare-earths
    Tc=51K (R=Nd), 55K (R=Sm), etc.
- $RFeAsO_{1-\delta}$
  - Oxygen vacancies instead of F doping
- "122", $ThCr_2Si_2$-type
  - AFe_2As_2, A=alkaline earth metal
- "111", PbFCl-type
  - LiFeAs (without chemical doping)
- "11", PbO-type
  - FeSe
- Under pressure
  - $LaFeAsO_{1-x}F_x$: Tc=26K → 43K
  - Undoped 122-type: Tc=0K → 30K
  - Undoped 11-type: Tc=8K →27K



"1111" (RFeAsO)



"122" (AFe_2As_2)

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Problems in DFT calculations

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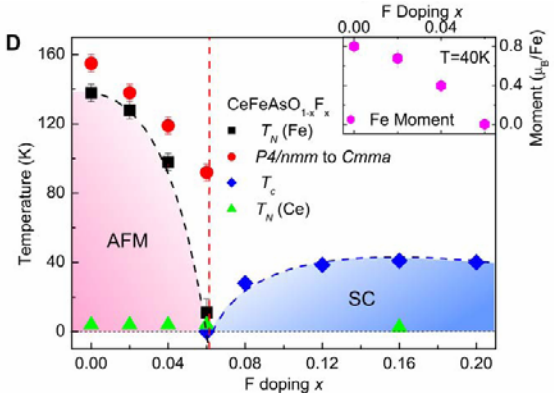
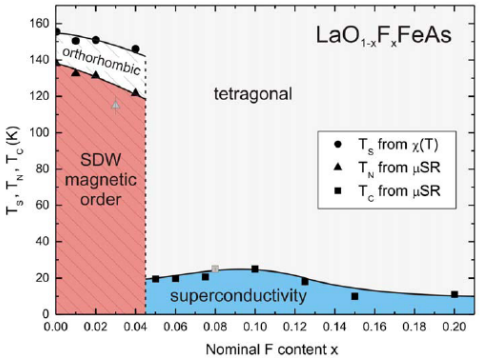
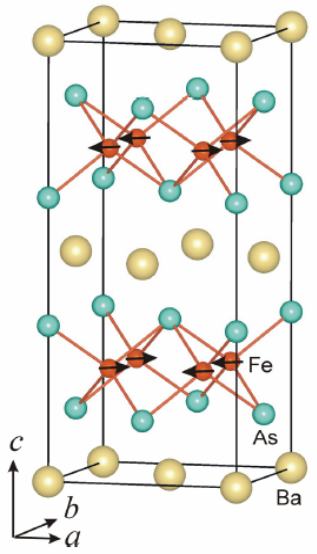
- Magnetic moment overestimated
  - 1.5-2.0 μ_B, whether in doped or undoped cases
  - Experimentally, AF is observed only at very low doping levels and is weak (~0.3μ_B for LaFeAsO, ~0.9μ_B for NdFeAsO, ~0.9μ_B for $BaFe_2As_2$)



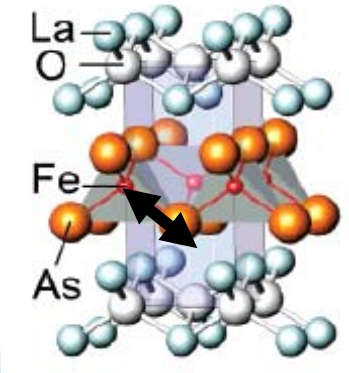
Zhao et al, arXiv:0806.2528



Luetkens et al, arXiv:0806.3533



- Fe-Pn bond length
  - Underestimated in structure optimization (up to 0.15Å)



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LDA: a good starting point for theoretical studies?

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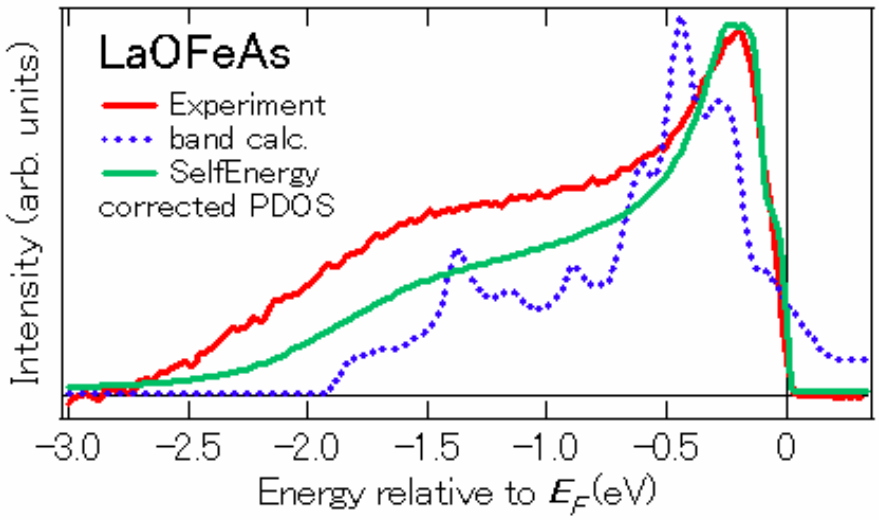
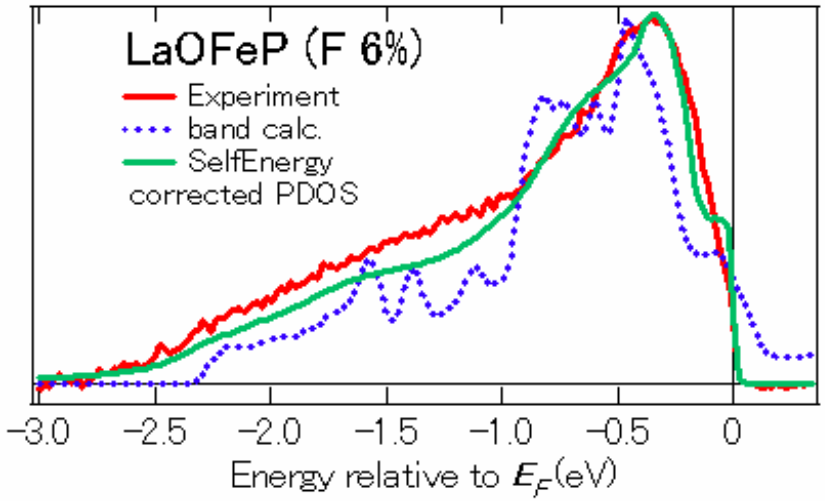
- PES Yoshida et al, arXiv:0806.3860, to appear in J. Phys. Soc. Jpn





LDA DOS qualitatively agree with PES
No Hubbard band observed

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LDA: a good starting point for theoretical studies?

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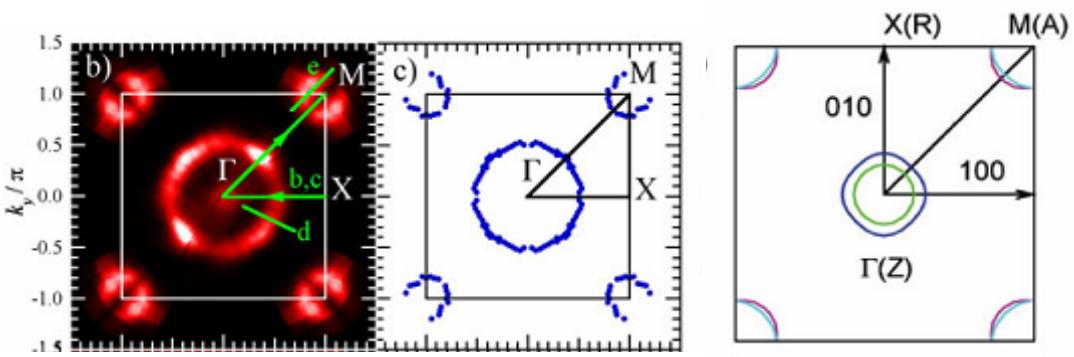
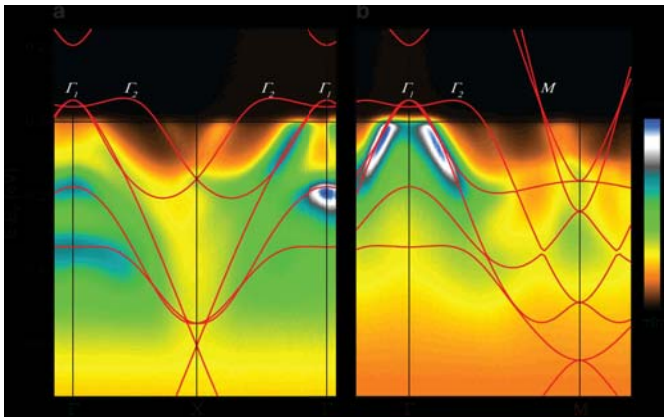
- ARPES
  - $NdFeAsO_{1-x}F_x$



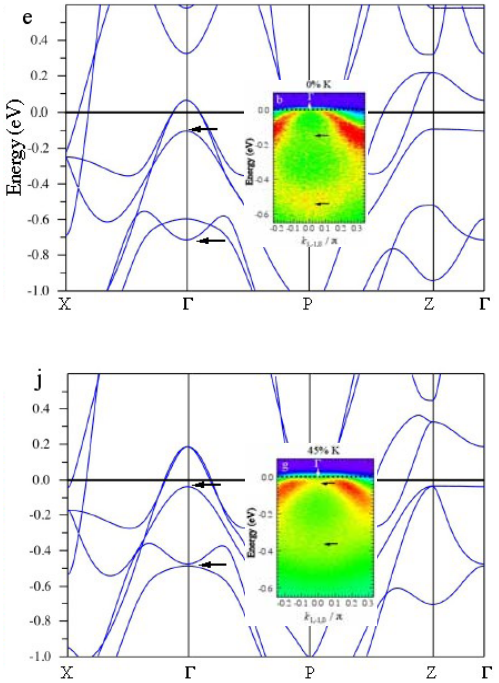
Liu et al, arXiv:0807.2009

  - LaFeOP



Liu et al, arXiv:0806.3453

  - $Ba_{1-x}K_xFe_2As_2$



Liu et al, arXiv:0806.3453

LDA captures essential features of ARPES

LDA band structure & MaxLoc Wannier functions

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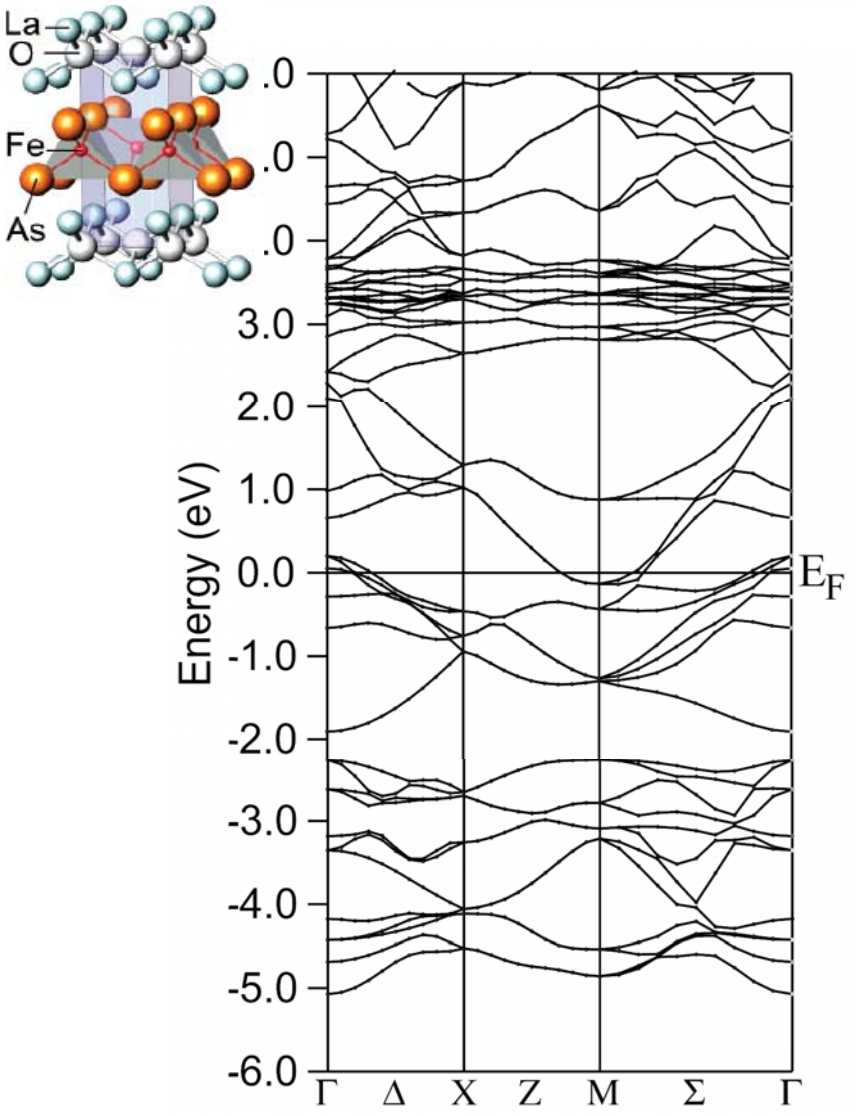

Complicated band structure
10 bands around E_F
(2 Fe atoms in the unit cell)

LDA band structure & MaxLoc Wannier functions

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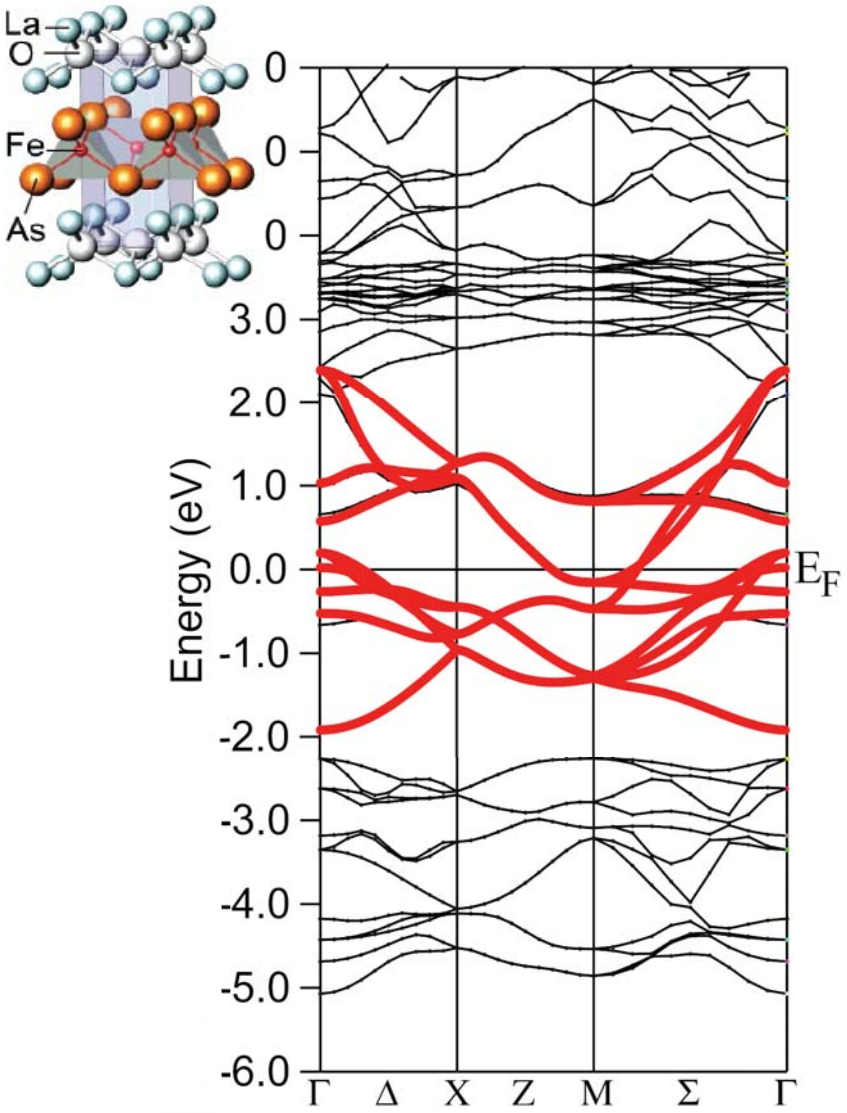

La 4f

Fe 3d

O 2p
As 4p

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

10 band model

5 band model (BZ unfolding)

4,3,2 band model ?

LDA band structure & MaxLoc Wannier functions

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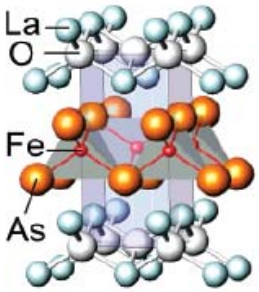

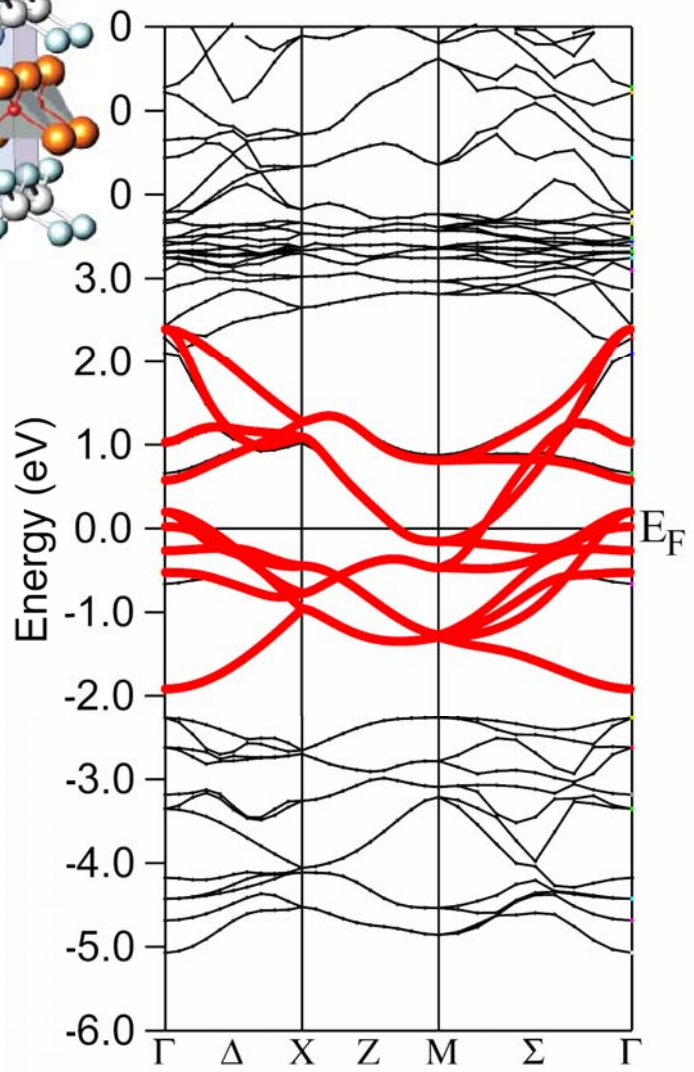

La 4f

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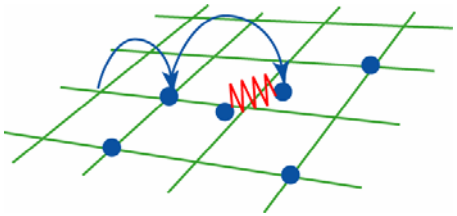
$$H_0 = \sum_{\sigma} \sum_{RR'} \sum_{nm} t_{mRnR'} c^{\dagger}_{\sigma nR} c_{\sigma mR'}$$



$$c^{\dagger}_{\sigma nR} |0\rangle \quad ?$$

Maximally localized Wannier functions

(Marzari-Vanderbilt, 97)

LDA band structure & MaxLoc Wannier functions

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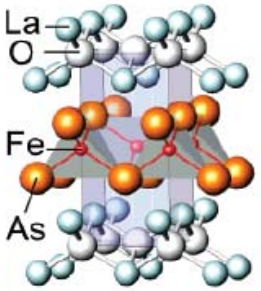
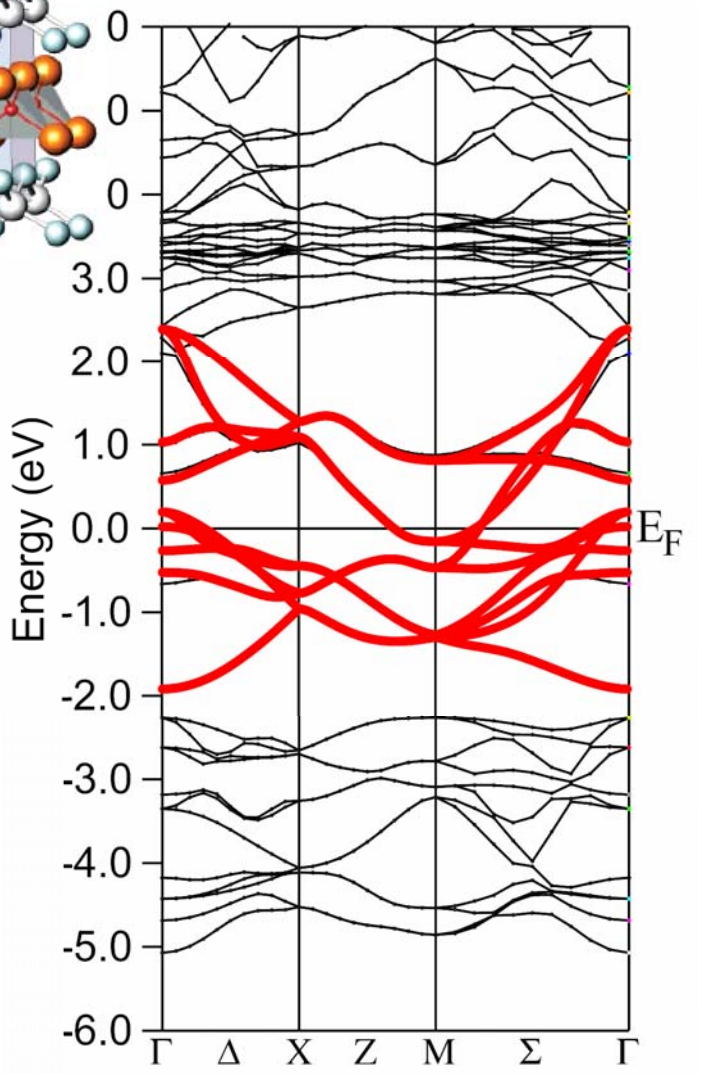
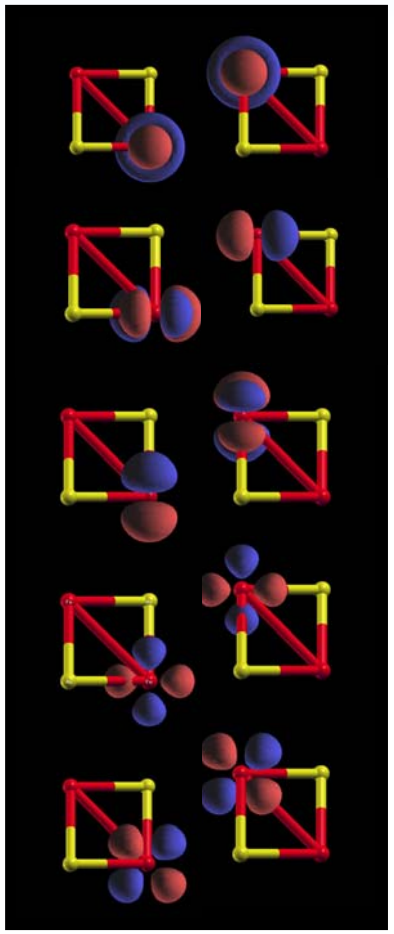




La 4f

Fe 3d

O 2p
As 4p



$$\langle \phi_{\alpha k} | H_{KS} | \phi_{\alpha k} \rangle \Rightarrow \langle w_{\mu i} | H_{KS} | w_{\nu j} \rangle$$

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Transfer hoppings

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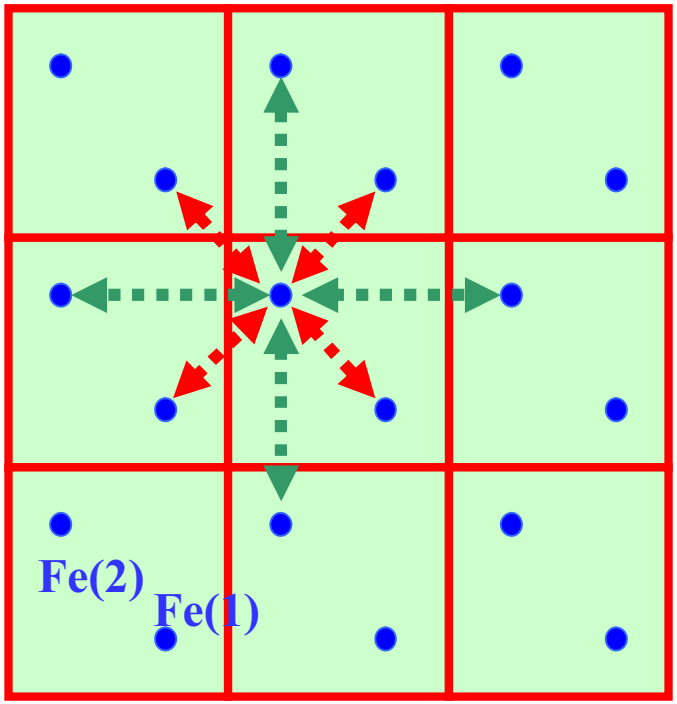
$$t_{\mu i \nu j} = \left\langle w_{\mu i} \middle| H_{KS} \middle| w_{\nu j} \right\rangle$$

Kuroki, RA et al, arXiv:0803.3325 to appear in PRL
Nakamura-RA-Imada, arxiv:0806.4750 to appear in JPSJ



Nearest

	xy	yz	z^2	zx	x^2-y^2
xy	-0.315	-0.255	-0.299	-0.254	0.000
yz	-0.255	-0.211	-0.077	-0.134	0.176
z^2	-0.299	-0.077	0.076	-0.077	-0.000
zx	-0.254	-0.134	-0.077	-0.211	-0.176
x^2-y^2	0.000	0.176	-0.000	-0.176	-0.185

Next Nearest

-0.059	-0.141	-0.000	0.000	0.000
0.141	0.148	0.000	0.000	0.000
-0.000	0.000	-0.003	-0.145	-0.181
0.000	0.000	0.145	0.331	-0.011
0.000	0.000	-0.181	0.011	0.131

in eV

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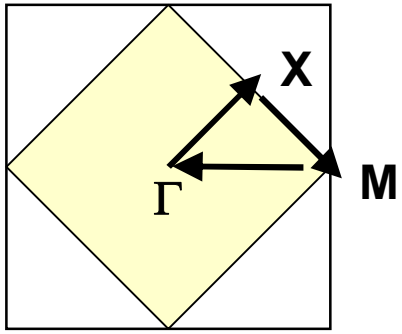
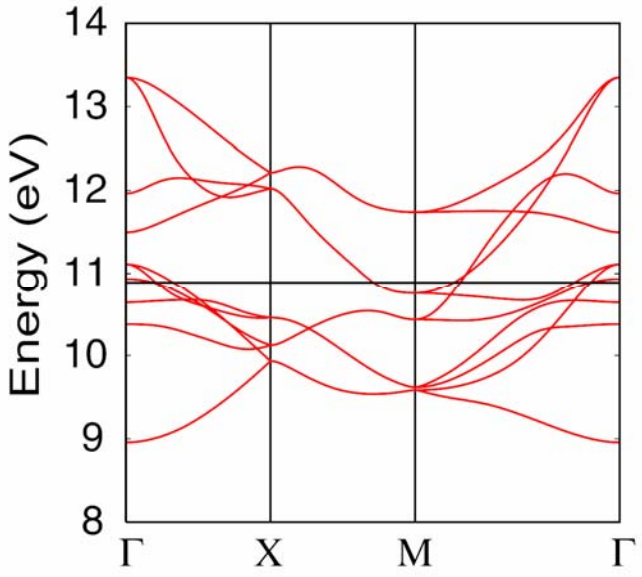
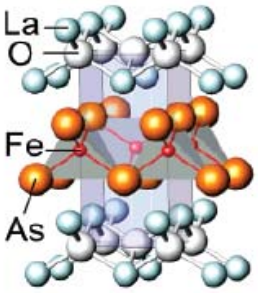
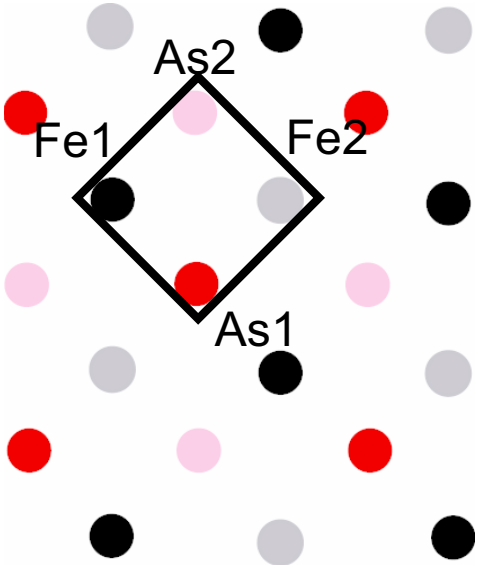
BZ unfolding



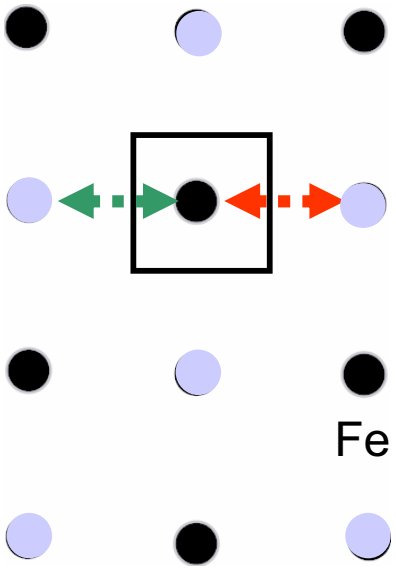


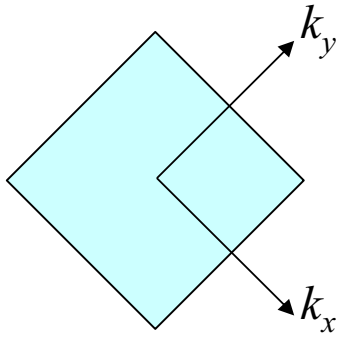
BZ unfolding

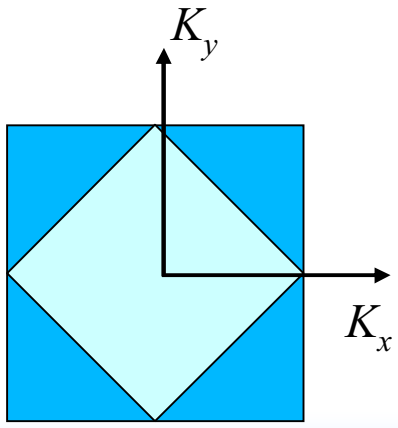




2 Fe atoms sit on the same Wyckoff position







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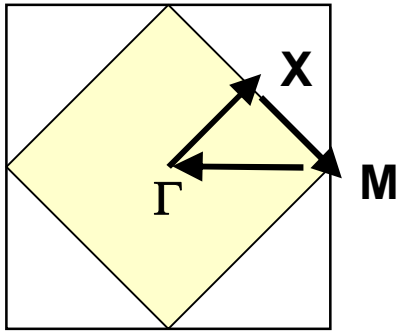

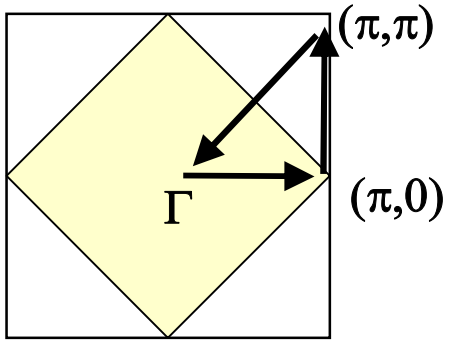

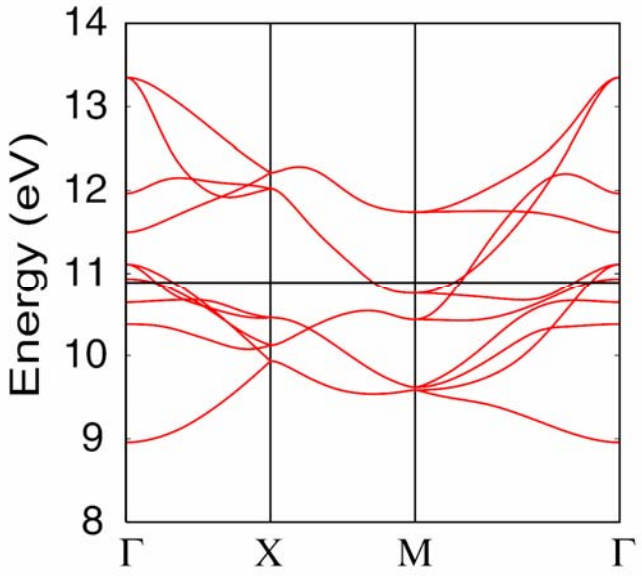

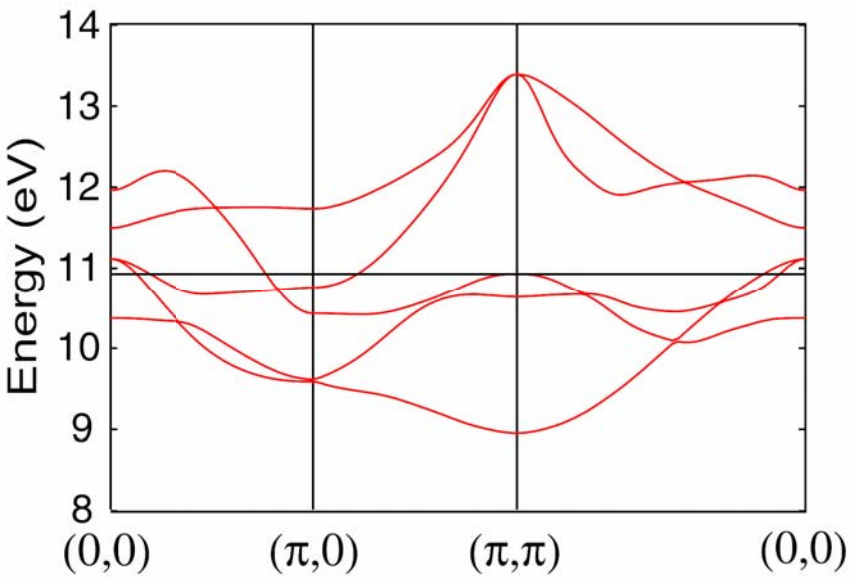

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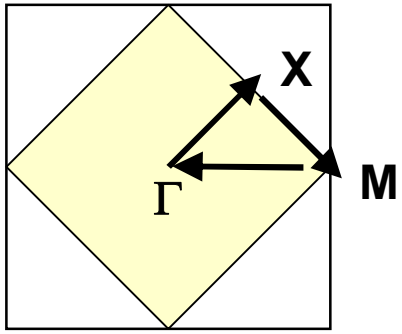

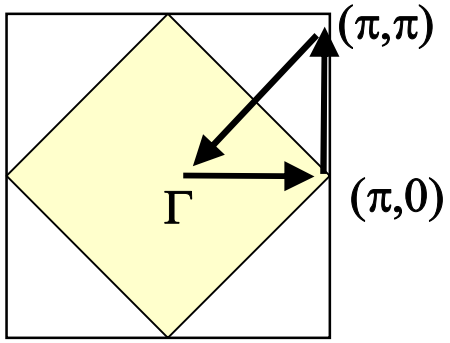

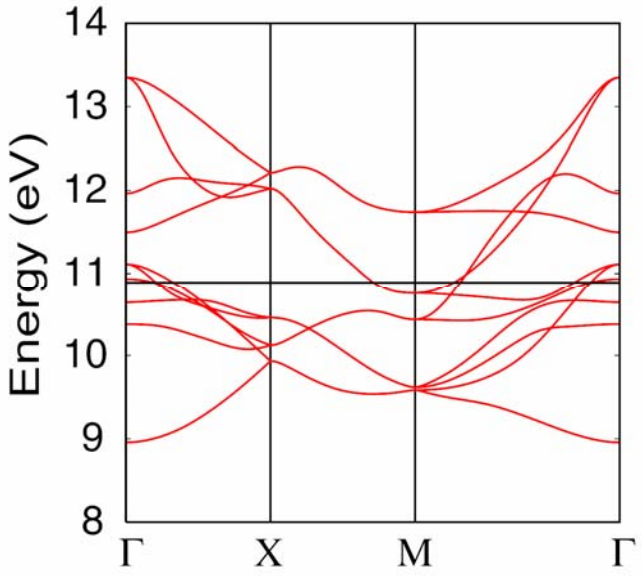

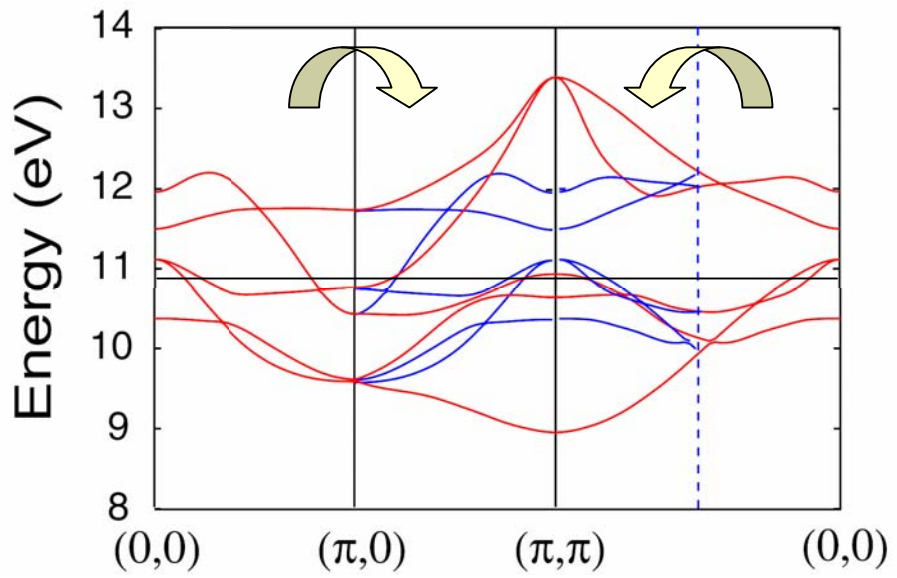

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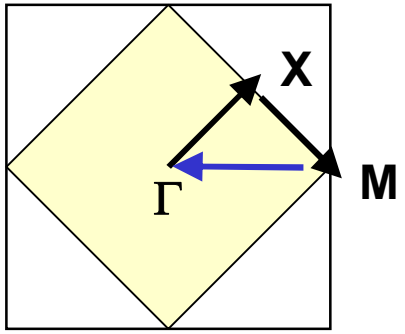

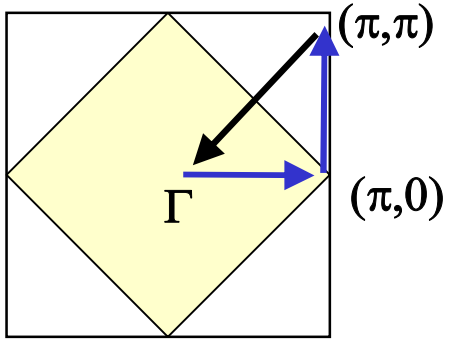

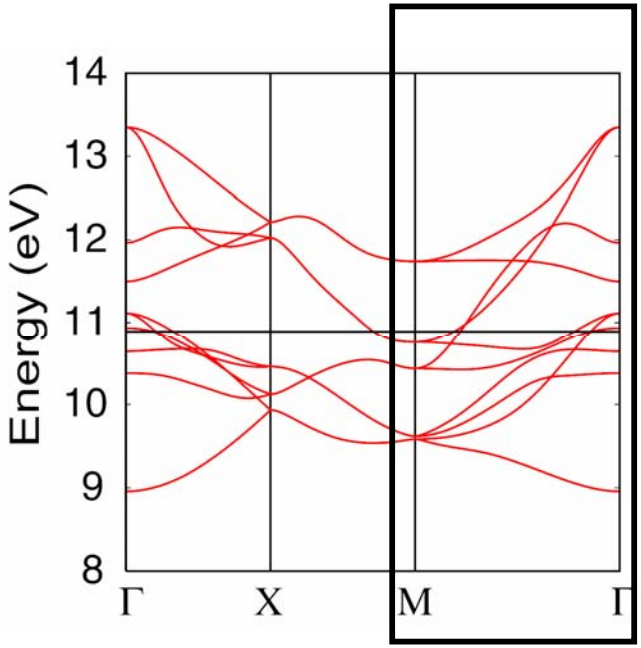

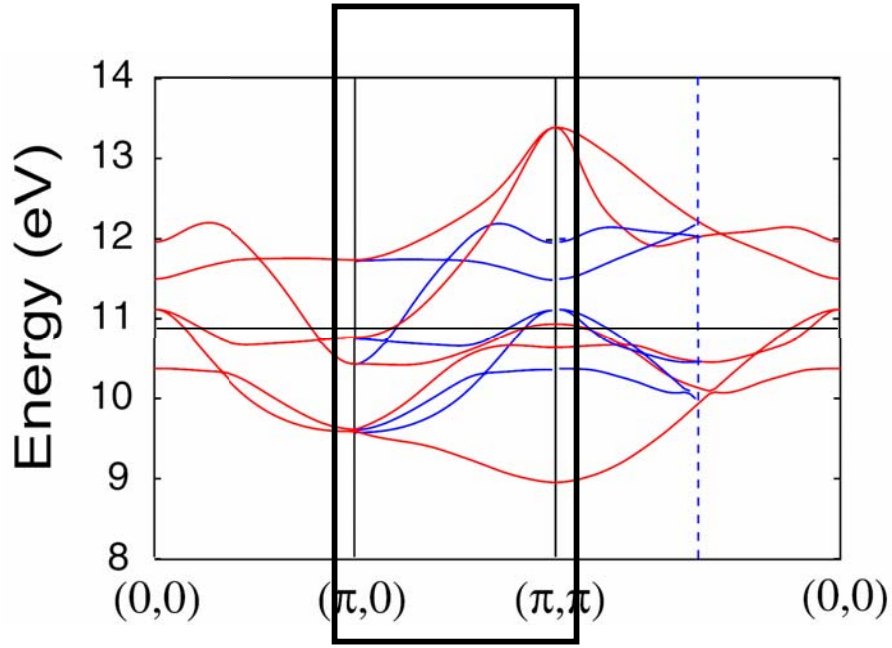

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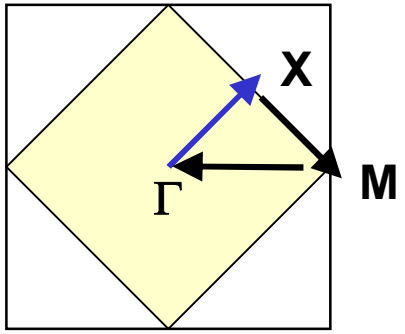

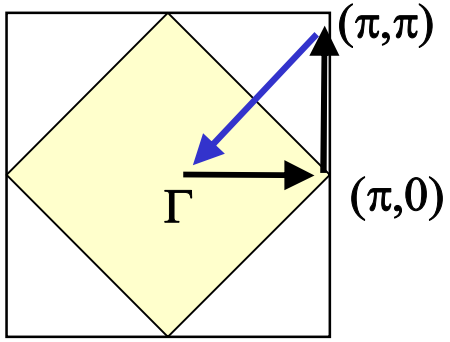

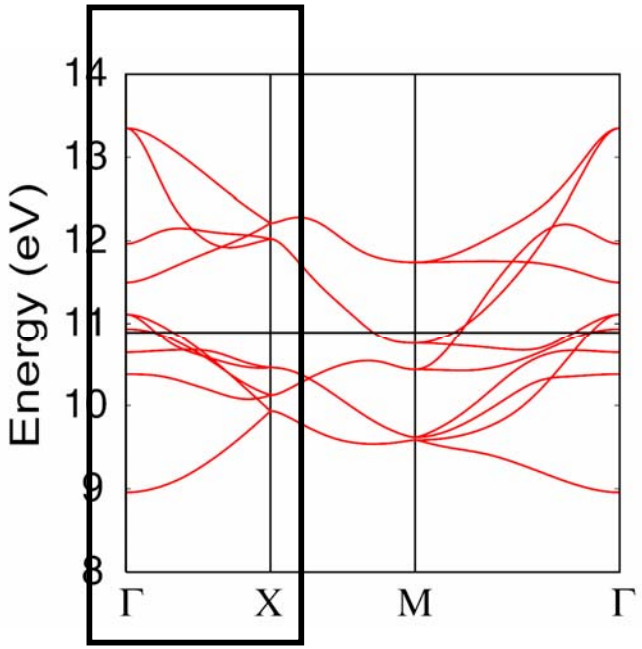

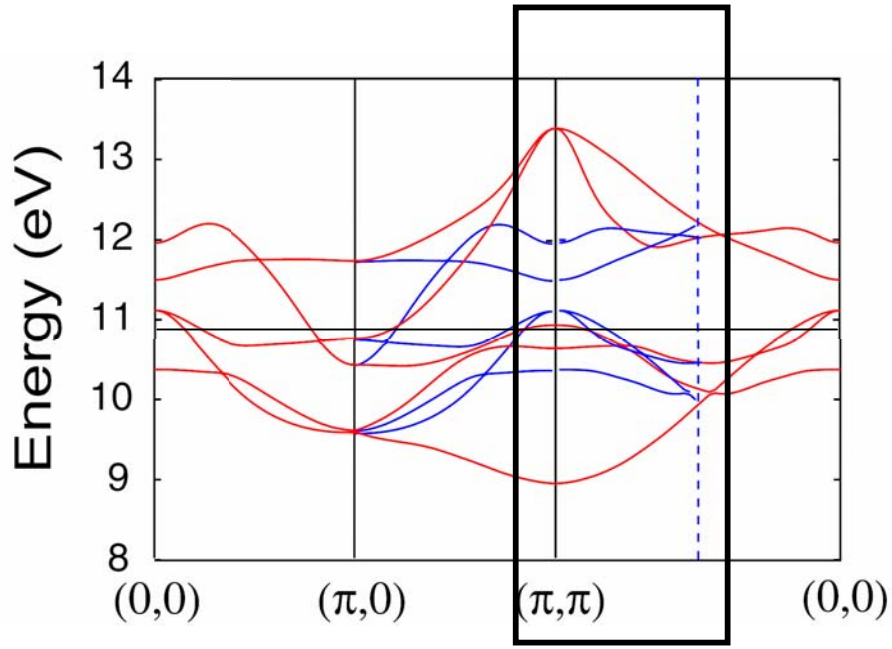

2 band model (d_{yz}+d_{xz})

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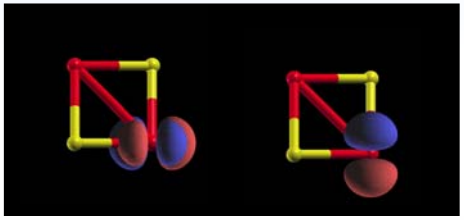
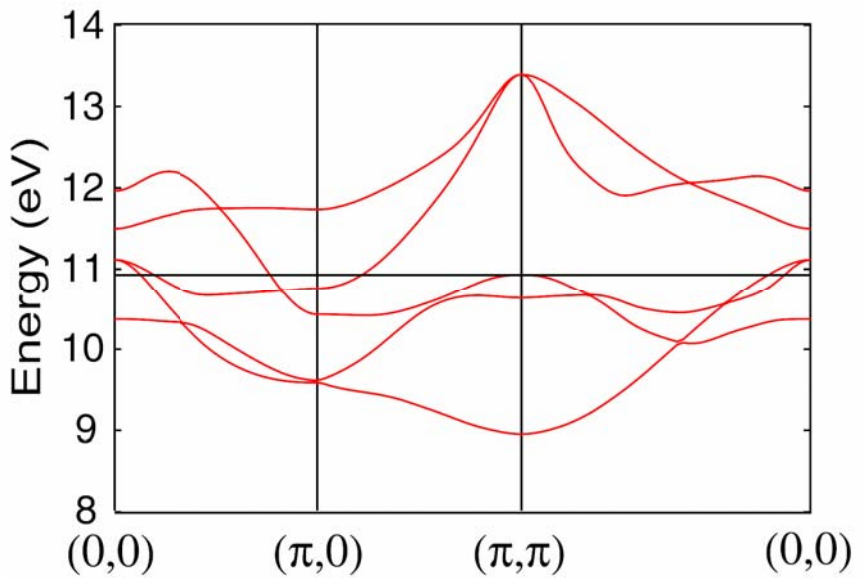
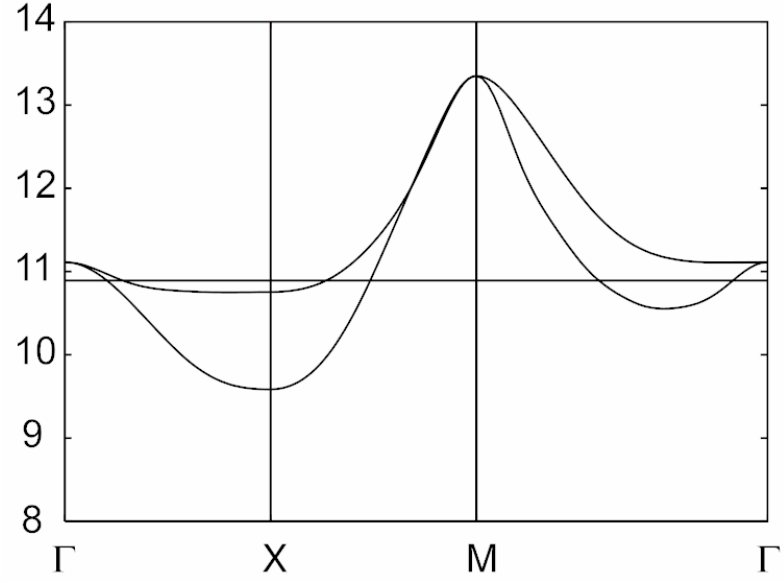
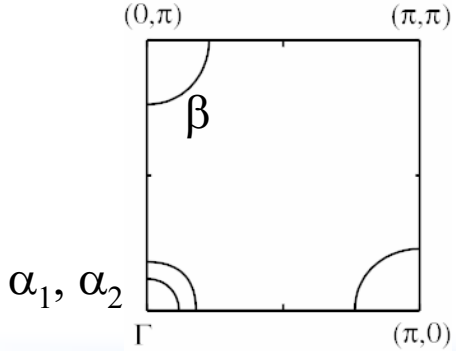
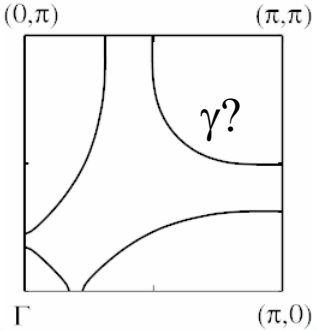








- α_2 absent
- Large β
- γ ?



n=6.1 (10% dope)

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2 band model (d_{yz}+d_{xz})

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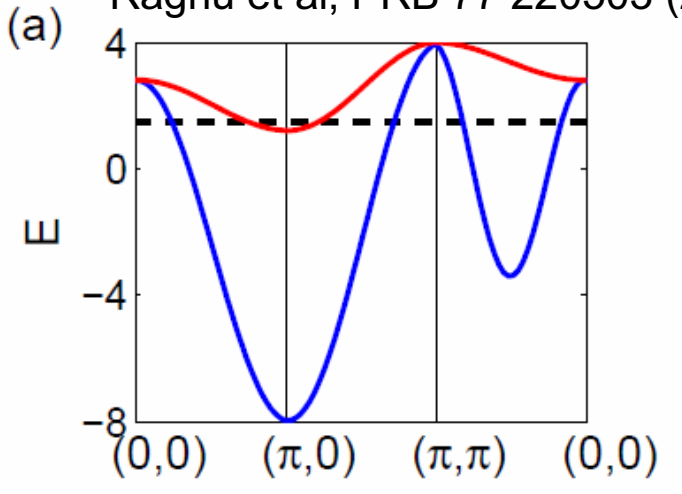
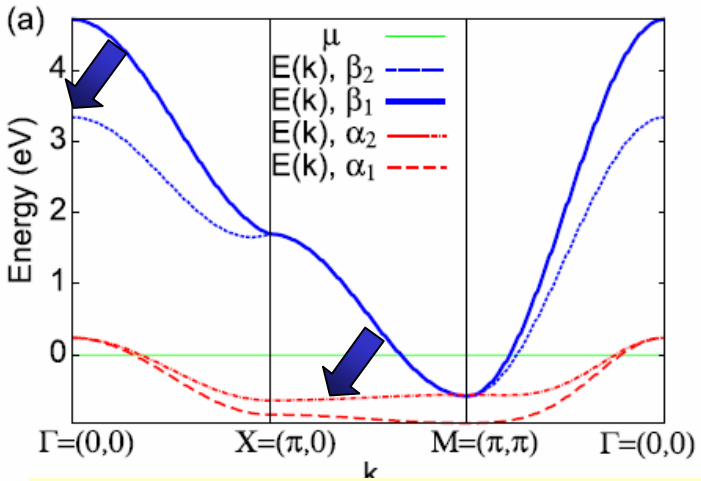
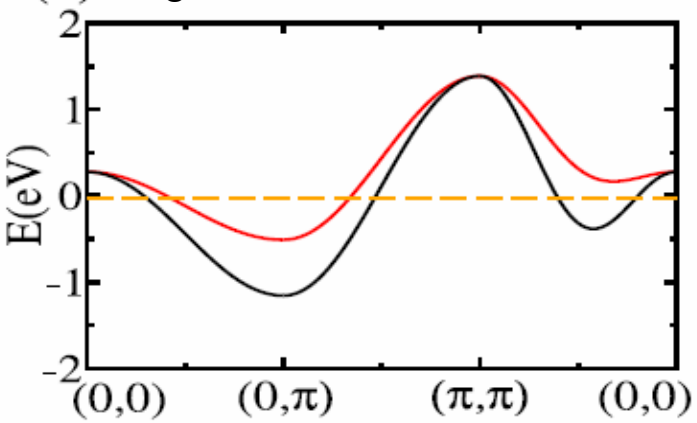
Raghu et al, PRB 77 220503 (2008)



Korshunov et al, arXiv:0804.1793

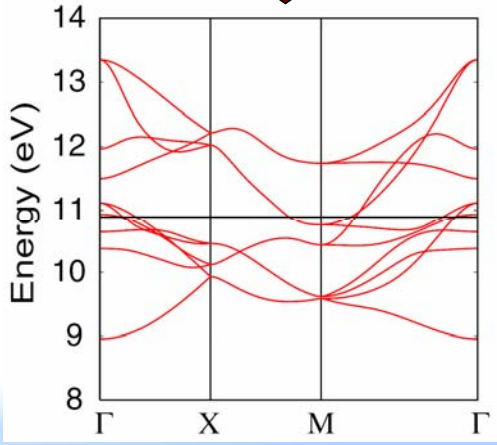


(b) Daghofer et al, arXiv:0805.0148



one FS around Γ
FS appears around (π,π)

4 band model from 10 bands
Bonding-antibonding split along X-M



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2 band model (d_{yz}+d_{xz})

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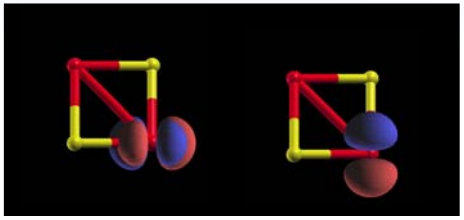
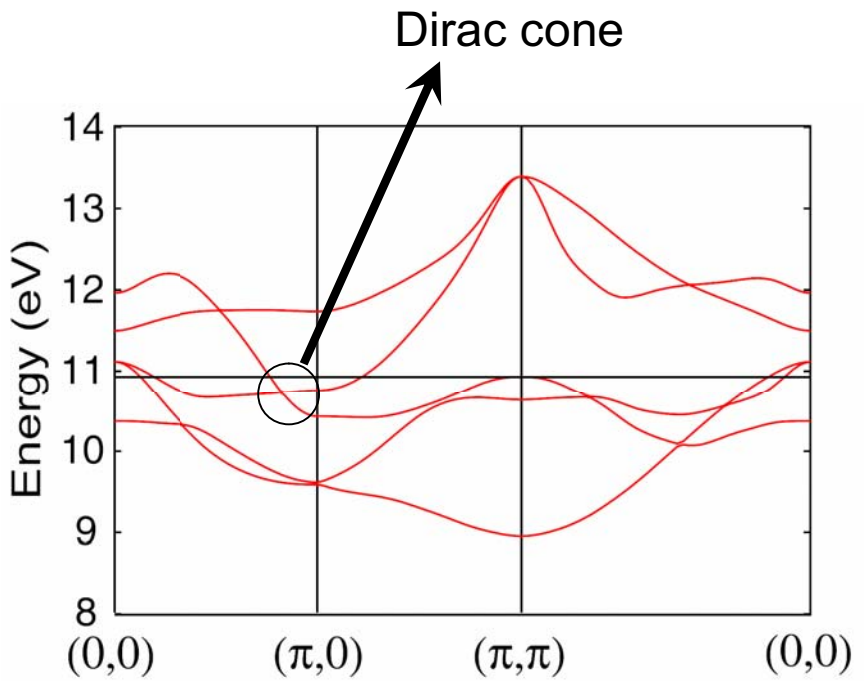
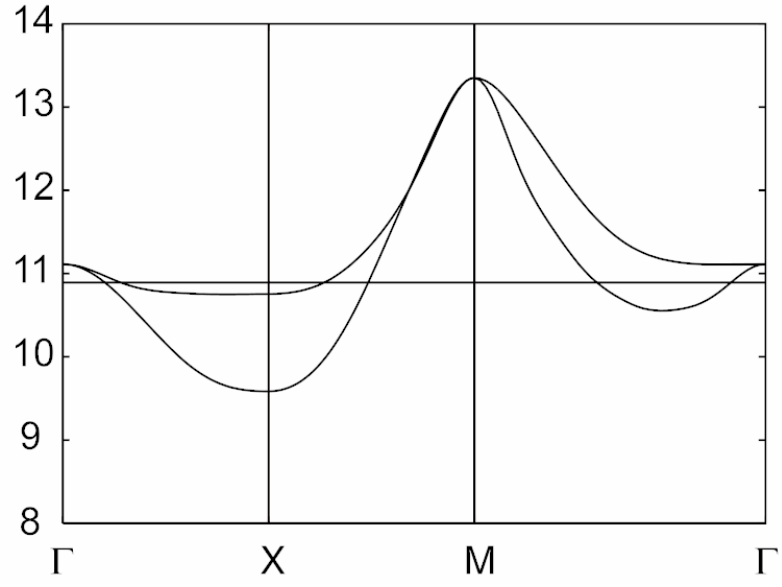
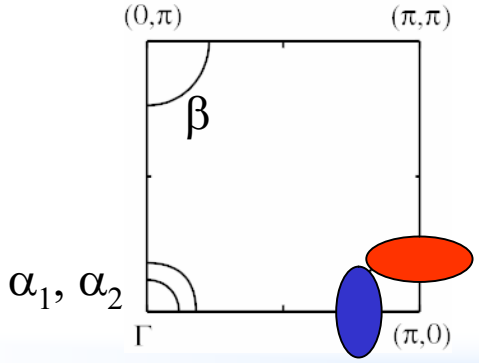
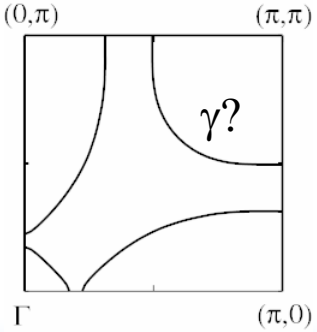








- α_2 absent
- Large β
- γ ?



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3 band model (d_{yz}+d_{xz}+d_{x2-y2})

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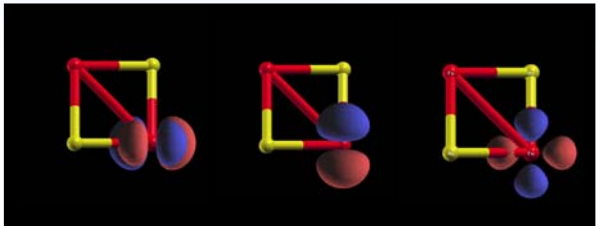
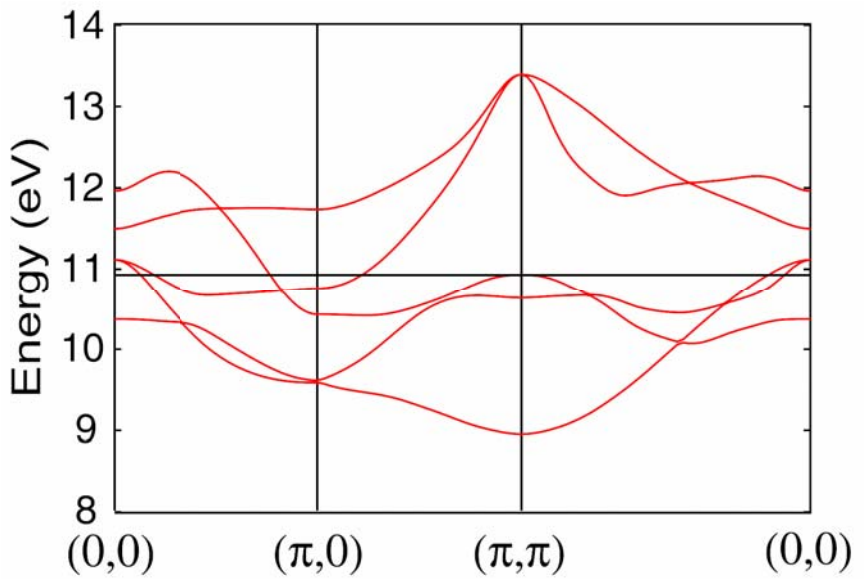
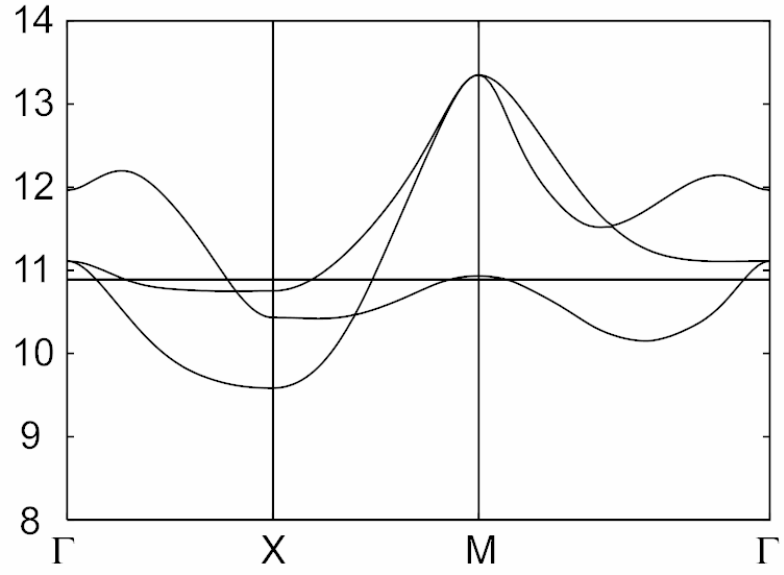
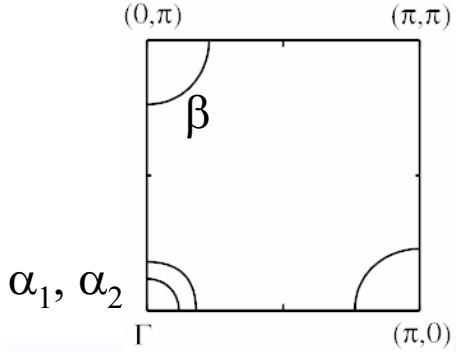




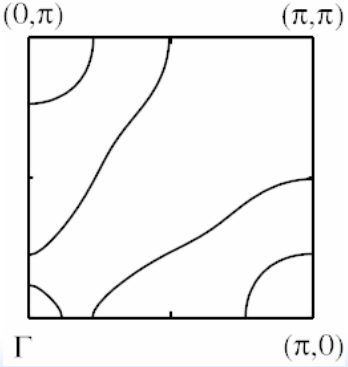




✘ α_2 absent

✘ γ ?

✓ Small β



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3 band model (d_{yz}+d_{xz}+d_{x2-y2})

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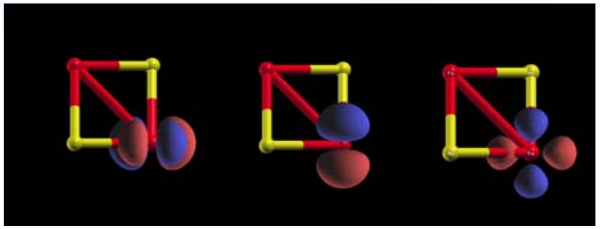
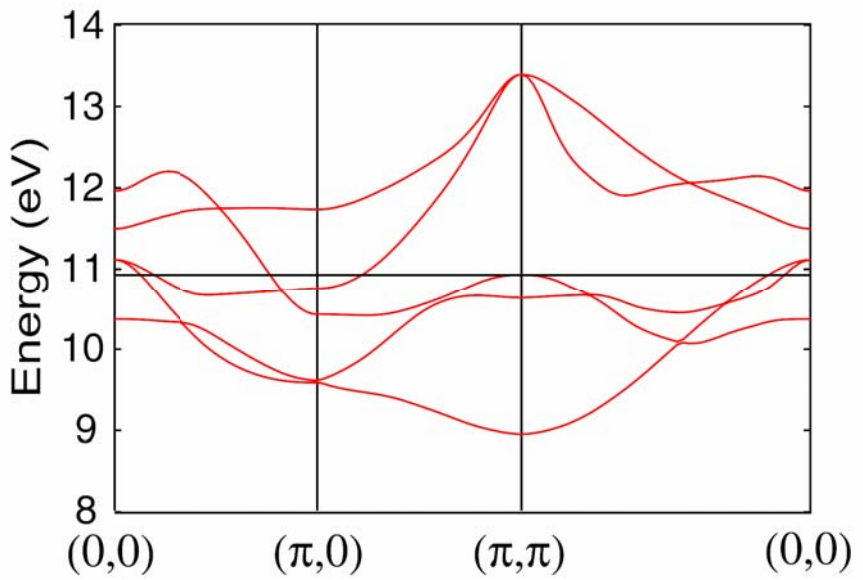
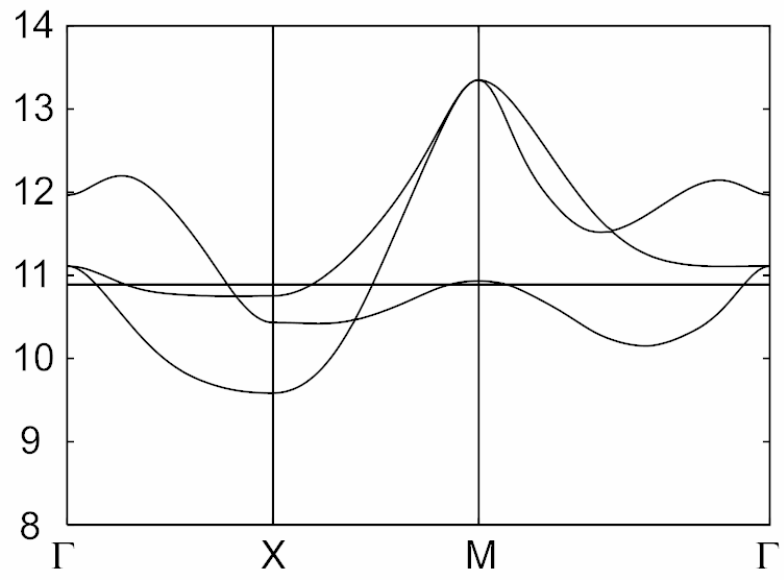
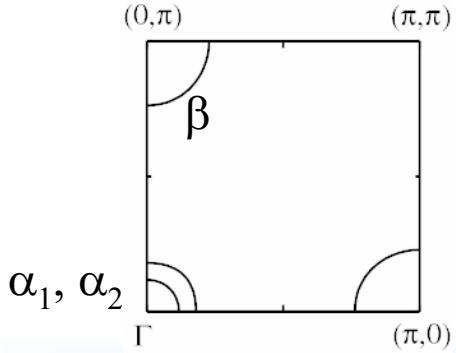
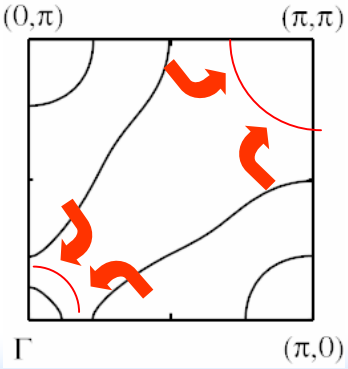








- ✘ α_2 absent
- ✘ γ ?
- ✓ Small β



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3 band model (d_{yz}+d_{xz}+d_{x2-y2})

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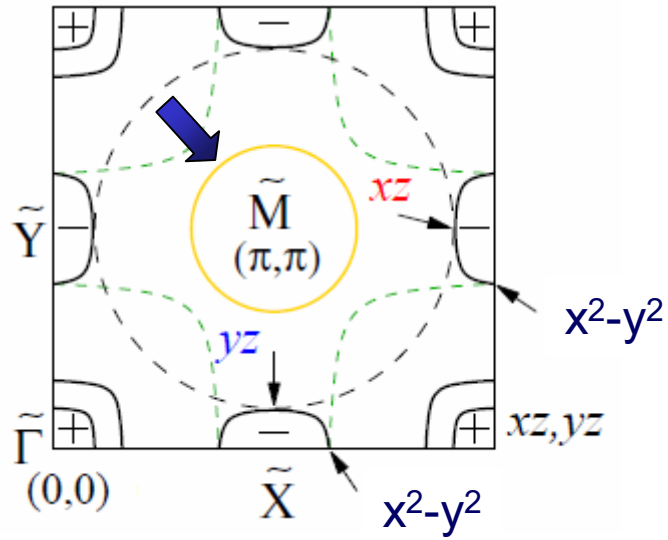
Lee & Wen, arXiv:0804.1739

To make α_1,α_2 around Γ and β around X, we have to consider d_{x2-y2}



d_{yz}+d_{xz} makes FS around M

4 band model (d_{yz}+d_{xz}+d_{x2-y2}+d_{xy})

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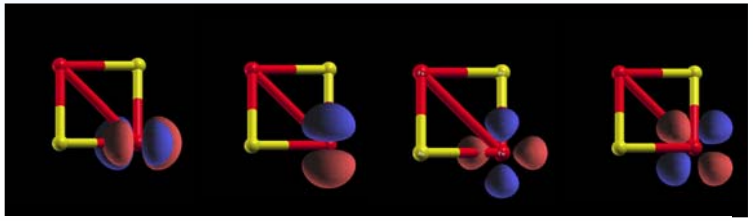
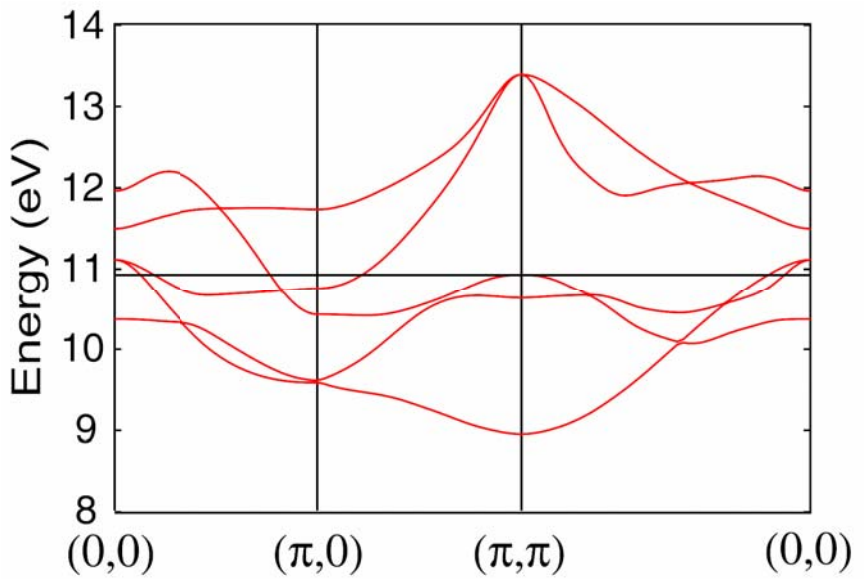
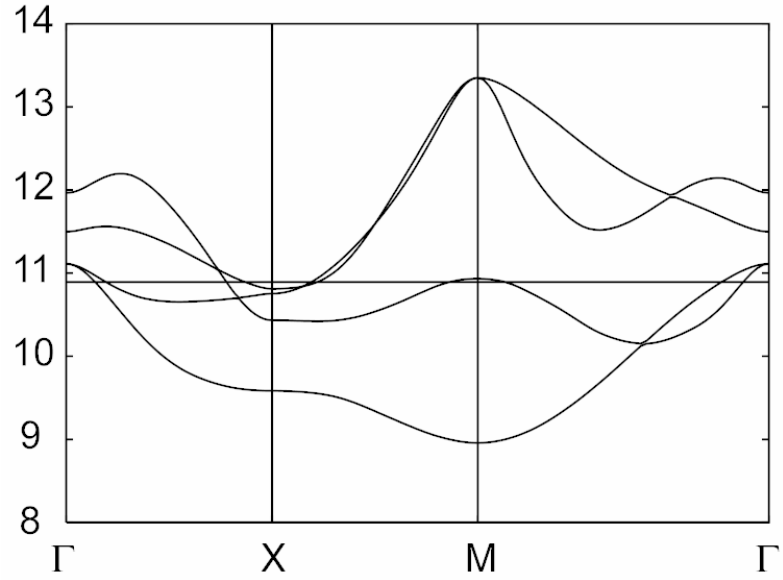
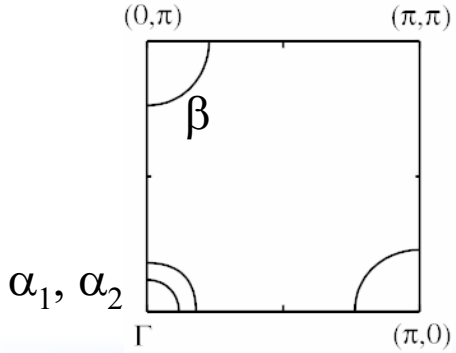






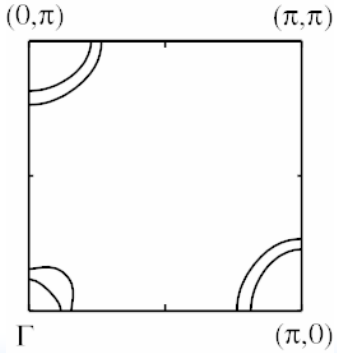


✘ β_2?

✓ small β

✓ No γ

✓ α_1 & α_2



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Character of the Fermi surface

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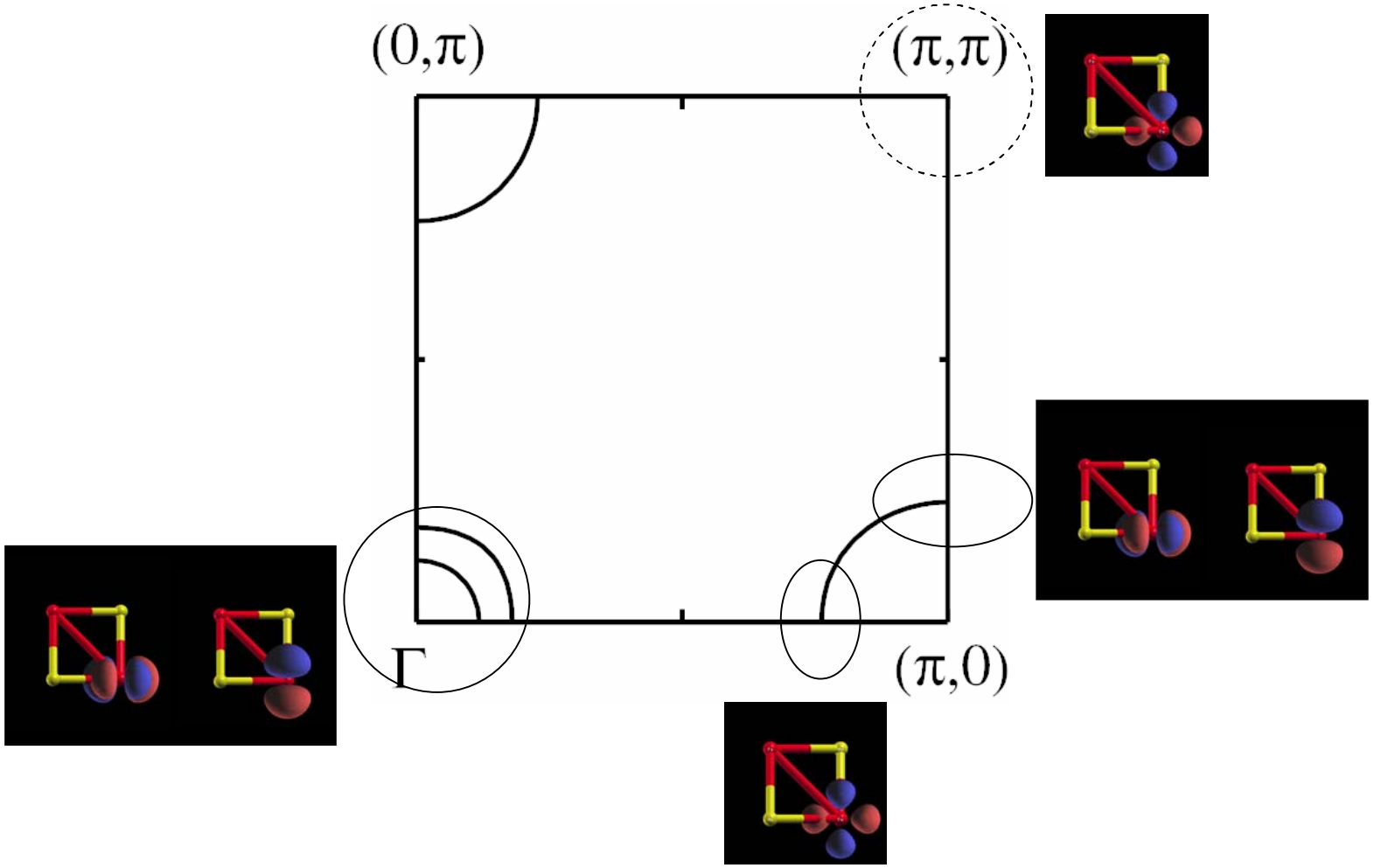
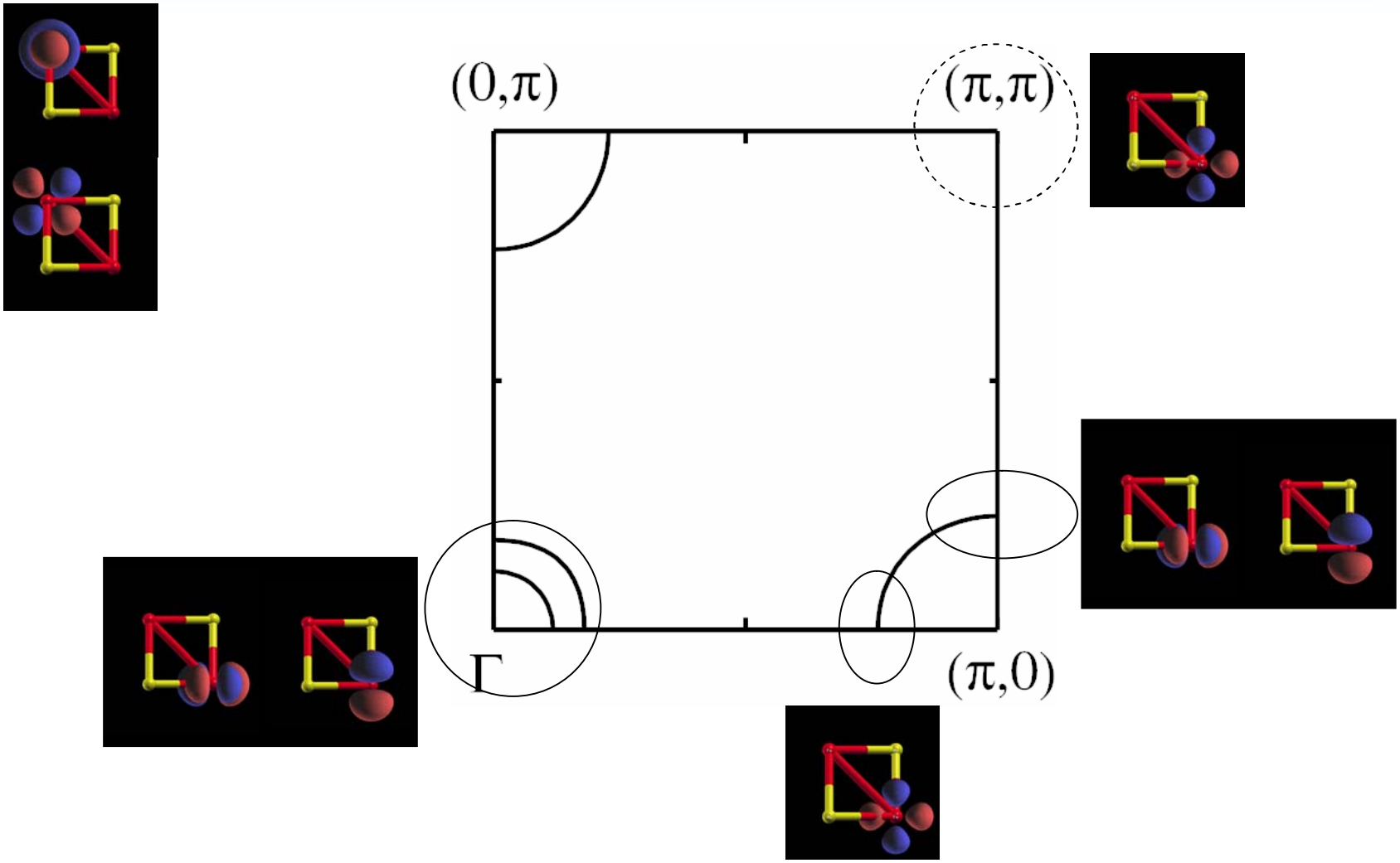


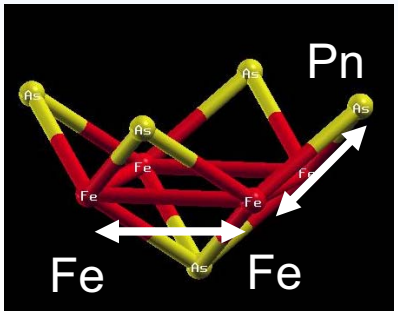
Character of the Fermi surface

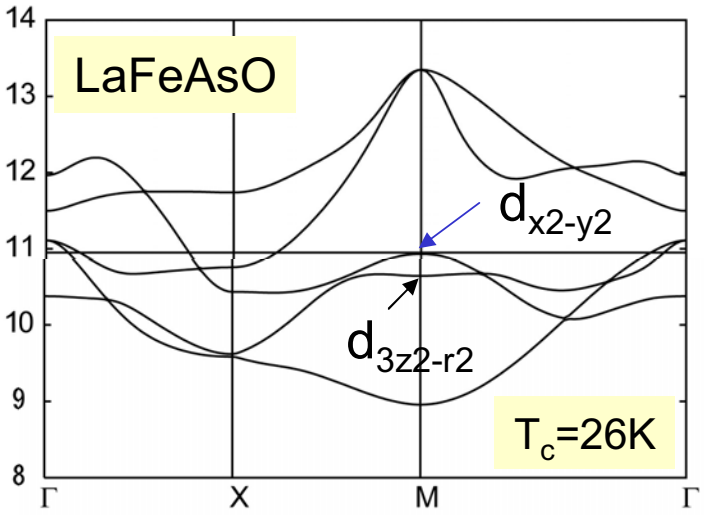


Effective model involves all five 3d orbitals

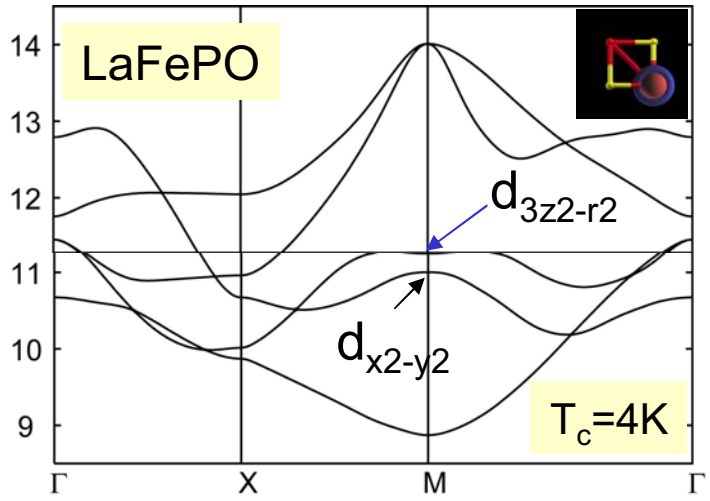
cf) Tesanovic et al, cond-mat/0804.4678

Material dependence

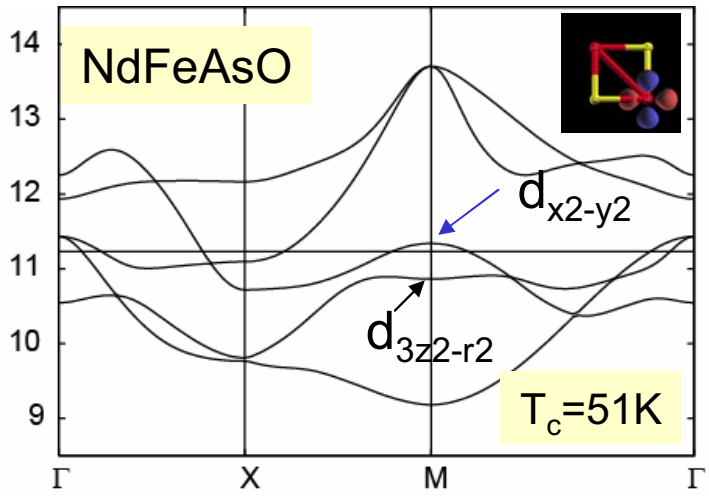




Fe-Fe: 4.04 Å
Fe-As: 2.41 Å



Fe-Fe: 3.96 Å
Fe-P: 2.29 Å



Fe-Fe: 3.95 Å
Fe-As: 2.40 Å

Ab initio construction of an effective model

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$$\mathcal{H}=\sum_{\sigma}\sum_{\boldsymbol{R}\boldsymbol{R}'}\sum_{nm} t_{m\mathbf{R}n\mathbf{R}'} a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'}$$

$$+\frac{1}{2}\sum_{\sigma\rho}\sum_{\boldsymbol{R}\boldsymbol{R}'}\sum_{nm}\Big\{ U_{m\mathbf{R}n\mathbf{R}'} a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{m\boldsymbol{R}'} a^{\rho}_{m\boldsymbol{R}'} a^{\sigma}_{n\boldsymbol{R}}$$

$$+J_{m\mathbf{R}n\mathbf{R}'}\left(a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{m\boldsymbol{R}'} a^{\rho}_{n\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'} + a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{n\boldsymbol{R}} a^{\rho}_{m\boldsymbol{R}'} a^{\sigma}_{m\boldsymbol{R}'}\right)\Big\}$$

Ab initio construction of an effective model

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$$\mathcal{H}=\sum_{\sigma}\sum_{\boldsymbol{R}\boldsymbol{R}'}\sum_{nm} t_{m\mathbf{R}n\mathbf{R}'} a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'}$$

$$+\frac{1}{2}\sum_{\sigma\rho}\sum_{\boldsymbol{R}\boldsymbol{R}'}\sum_{nm}\Big\{ U_{m\mathbf{R}n\mathbf{R}'} a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{m\boldsymbol{R}'} a^{\rho}_{m\boldsymbol{R}'} a^{\sigma}_{n\boldsymbol{R}}$$

$$+J_{m\mathbf{R}n\mathbf{R}'}\left(a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{m\boldsymbol{R}'} a^{\rho}_{n\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'} + a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{n\boldsymbol{R}} a^{\rho}_{m\boldsymbol{R}'} a^{\sigma}_{m\boldsymbol{R}'}\right)\Big\}$$

Constrained RPA

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

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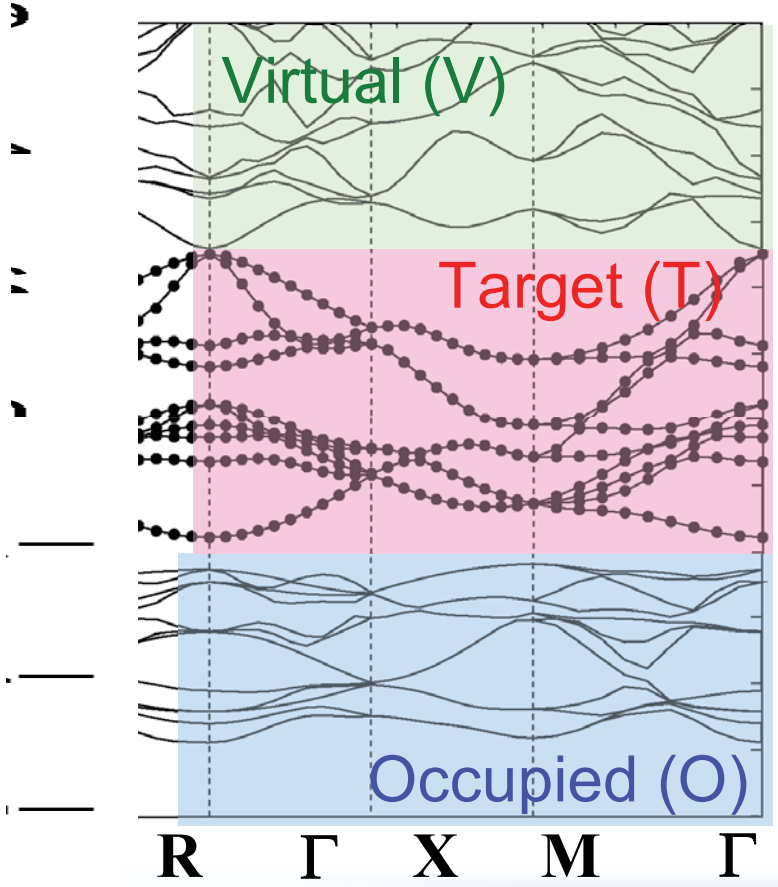
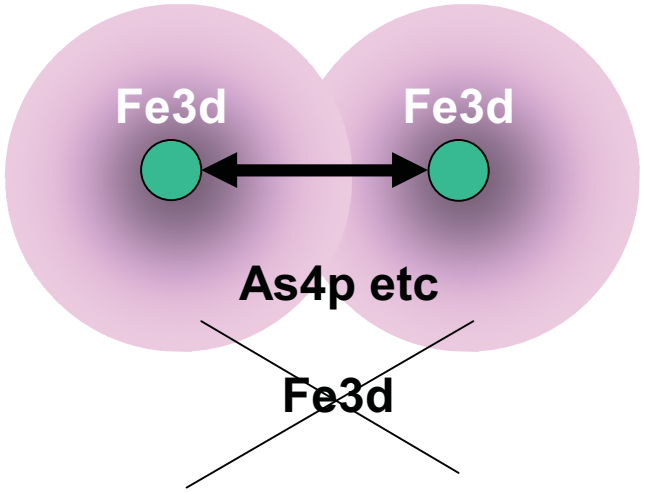
$$W = (1 - v\chi)^{-1} v$$

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

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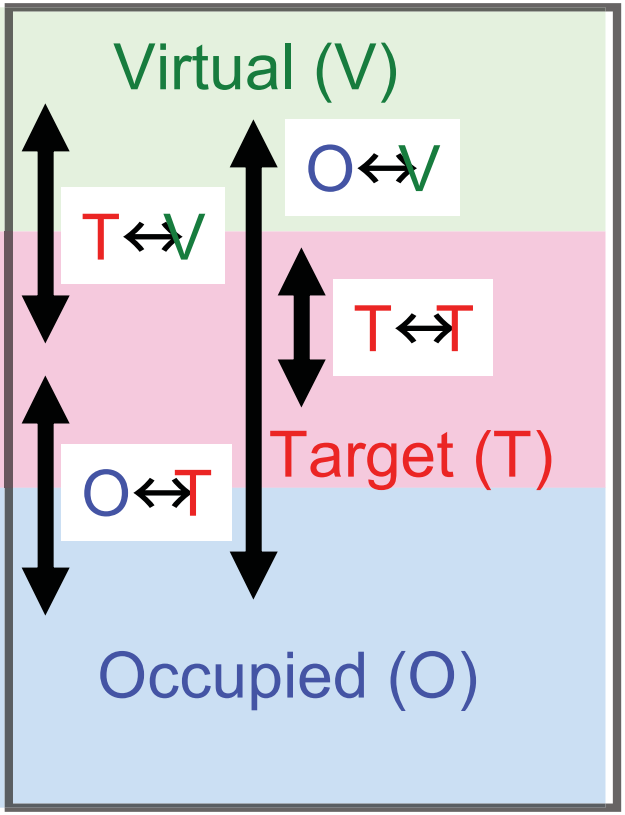
$$W = \left(1 - v\chi\right)^{-1} v$$



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

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

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

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

$$W = \frac{v}{1 - v\chi} = \frac{W_{eff}}{1 - W_{eff}\chi_d}$$

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

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Constrained RPA: Result

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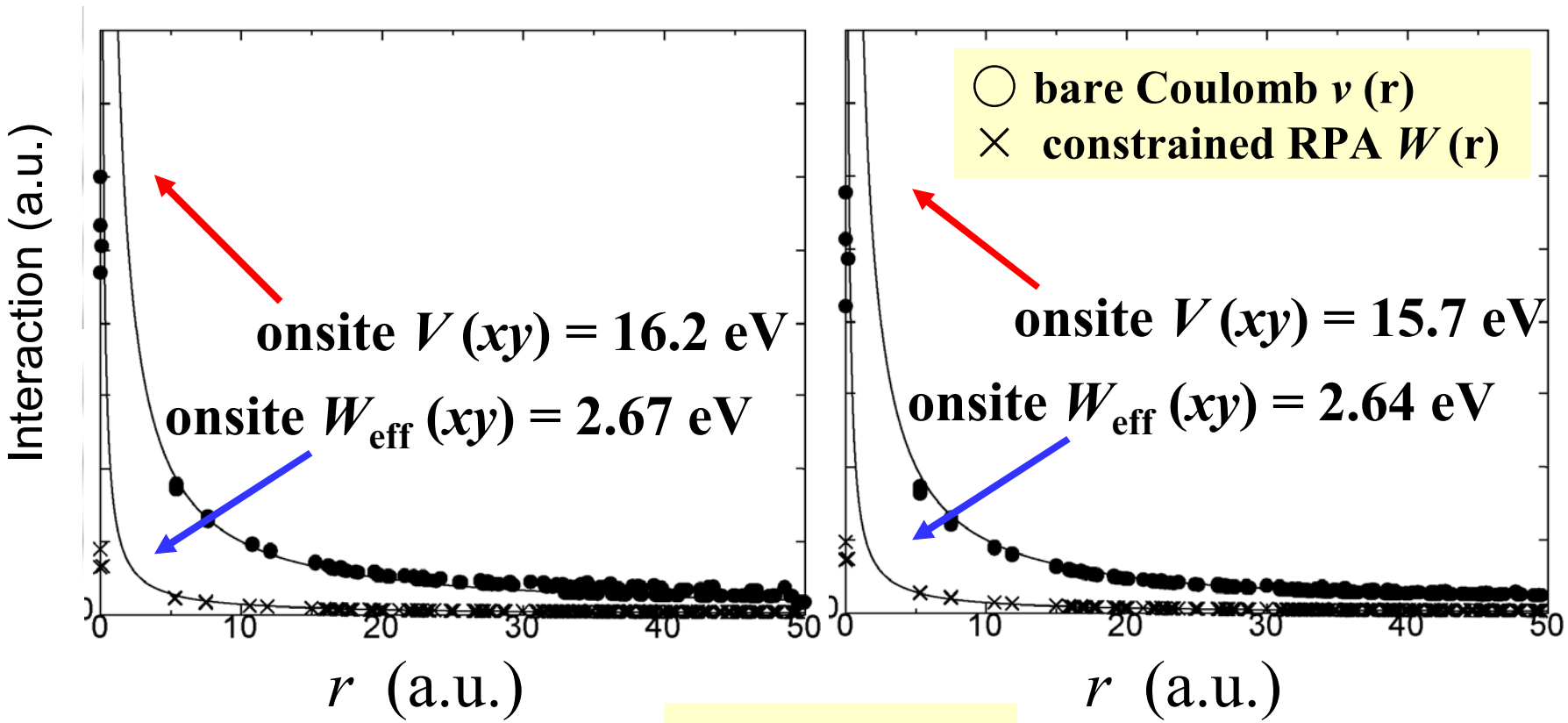

No big difference

Nakamura-RA-Imada, arxiv:0806.4750 to appear in JPSJ

cf) Sawatzky et al, arXiv:0808.1390

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cf) Sawatzky et al, arXiv:0808.1390

$$U = U_0 - 2E_p$$

$$E_p \sim \frac{1}{2}\sum_{i=1}^{4} \alpha_i E_i^2$$ α : polizability

$$E_i = e / R^2$$ R: Fe-Pn distance

Large atomic radius of Pn → large α → large screening

α (P) < α (As), but R(Fe-P) < R(Fe-As) → U(LaFePO)∼U(LaFeAsO)

Constrained RPA: Result

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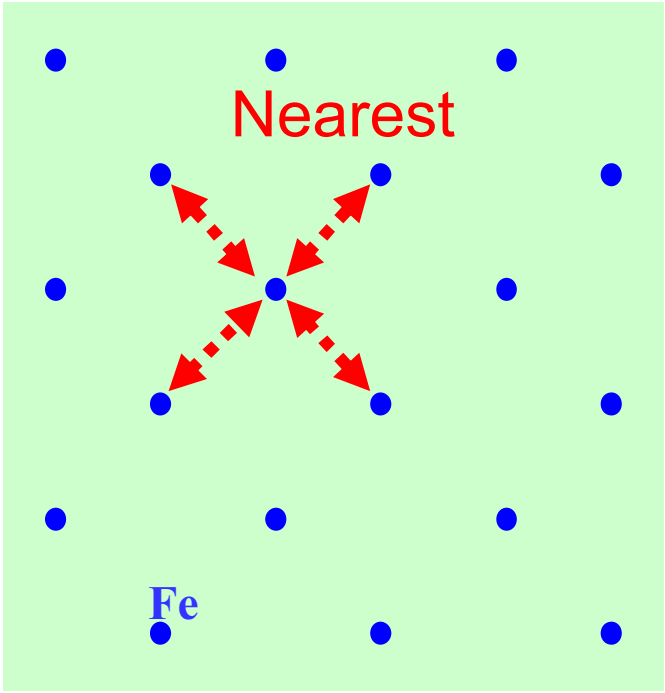
$$\langle w_i w_i | W_{eff} | w_j w_j \rangle$$



LaFeAsO

Onsite U

	xy	yz	z^2	zx	x^2-y^2
xy	2.66	2.00	1.98	2.00	2.11
yz	2.00	2.27	2.22	1.84	1.71
z^2	1.98	2.22	2.66	2.22	1.71
zx	2.00	1.84	2.22	2.27	1.71
x^2-y^2	2.10	1.71	1.71	1.71	1.83

Nearest neighbor V

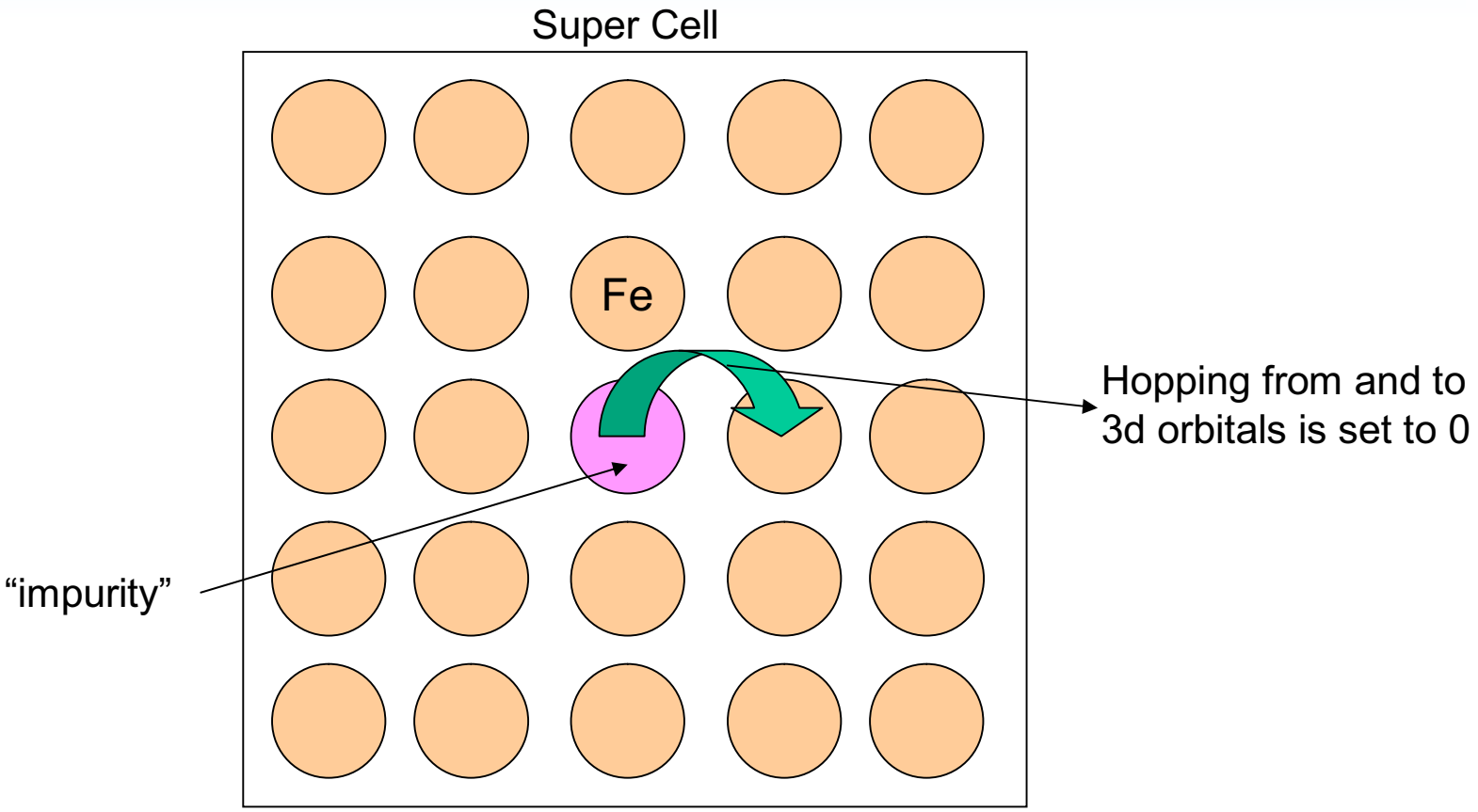
0.713	0.684	0.678	0.684	0.703
0.684	0.665	0.662	0.669	0.672
0.677	0.662	0.654	0.662	0.672
0.684	0.669	0.662	0.665	0.672
0.703	0.671	0.672	0.672	0.688

in eV

Nakamura-RA-Imada, arxiv:0806.4750 to appear in JPSJ

Constrained LDA

Anisimov et al. arXiv:0807.0547



Change the 3d charge on the impurity, keeping the system neutral,
do a self-consistent calculation
and calculate the change in the 3d energy level → U(3d).

$$U = \frac{\partial^2 E_{LDA}(n_d)}{\partial n_d^2}$$

$U' \sim 0.5eV,\ J \sim 0.5eV$

Multi-band RPA: which pairing symmetry is dominant ?

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$$\hat{H}_0 = \sum_{ijmm'\sigma} t_{ijmm'} c^{\dagger}_{im\sigma} c_{jm'\sigma} + h.c$$

$$\hat{H}_U \equiv U \sum_{im} n_{im\uparrow} n_{im\downarrow} + \sum_{i,m<m',\sigma} [U' n_{im\sigma} n_{im'-\sigma} + (U' - J) n_{im\sigma} n_{im'\sigma}]$$

$$\hat{H}_J \equiv J \sum_{i,m\neq m'} (c^{\dagger}_{im\uparrow} c^{\dagger}_{im'\downarrow} c_{im\downarrow} c_{im'\uparrow} + c^{\dagger}_{im\uparrow} c^{\dagger}_{im\downarrow} c_{im'\downarrow} c_{im'\uparrow})$$

Green's function:

$$G\ (k) = \frac{1}{i\omega_n + \mu - \epsilon^0(\boldsymbol{k})}$$

dispersion:

$$\epsilon^0_{\mu\nu}(\boldsymbol{k}) = \sum_{\boldsymbol{r}_i - \boldsymbol{r}_j} t^{\mu\nu}_{ij} e^{i(\boldsymbol{r}_i - \boldsymbol{r}_j)\cdot\boldsymbol{k}}$$

irreducible susceptibility: $\hat{\chi}^0_{l_1 l_2, l_3 l_4}(q) = -\frac{T}{N} \sum_k G_{l_1 l_3}(k+q) G_{l_4 l_2}(k)$

spin susceptibility:

$$\hat{\chi}^s(q) = \frac{\hat{\chi}^0(q)}{1 - \hat{S}^0 \hat{\chi}^0(q)}$$

charge (orbital) susceptibility:

$$\hat{\chi}^c(q) = \frac{\hat{\chi}^0(q)}{1 + \hat{C}^0 \hat{\chi}^0(q)}$$

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RPA result: spin susceptibility

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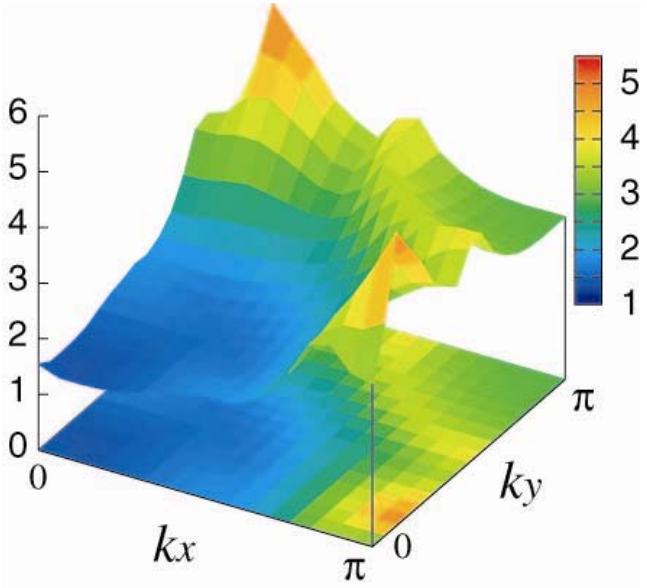
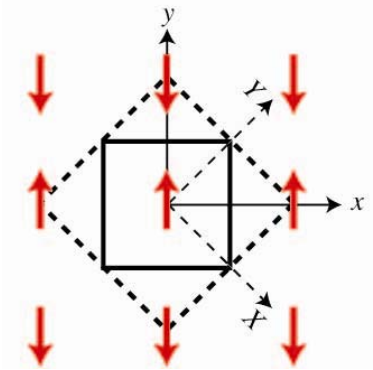
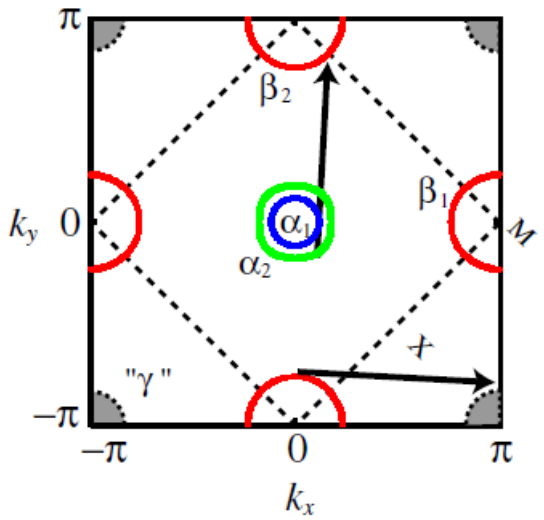
n=6.1 (10% dope)





$(\pi,0)_{\text{unfolded}} = (\pi,\pi)_{\text{folded}}$



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Linearized Eliashberg equation

effective interaction for singlet:

$$\hat{V}^s(q) = \frac{3}{2}\hat{S}^0\hat{\chi}^s(q)\hat{S}^0 - \frac{1}{2}\hat{C}^0\hat{\chi}^c(q)\hat{C}^0 + \frac{1}{2}(\hat{S}^0 + \hat{C}^0)$$

effective interaction for triplet:

$$\hat{V}^t(q) = -\frac{1}{2}\hat{S}^0\hat{\chi}^s(q)\hat{S}^0 - \frac{1}{2}\hat{C}^0\hat{\chi}^c(q)\hat{C}^0 + \frac{1}{2}(-\hat{S}^0 + \hat{C}^0)$$

linerized Eliashberg eq. :

$$\lambda\Delta_{l_1 l_4}(k) = -\frac{T}{N}\sum_{q}\sum_{l_2 l_3 l_5 l_6}\hat{V}^{s(t)}_{l_1 l_2, l_3 l_4}(q)G_{l_2 l_5}(k-q)\Delta_{l_5 l_6}(k-q)G_{l_3 l_6}(q-k)$$

$T=T_c$ when $\lambda=1$

RPA result: gap function

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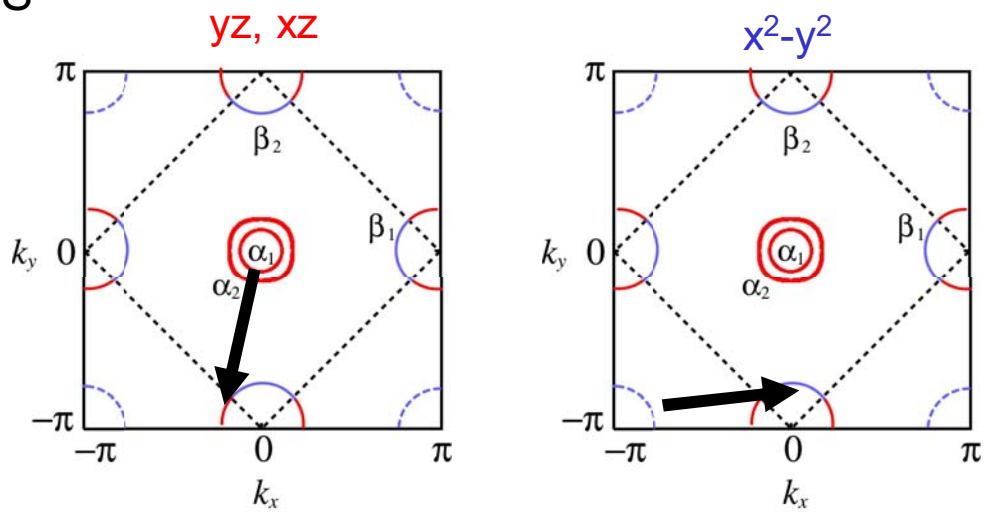
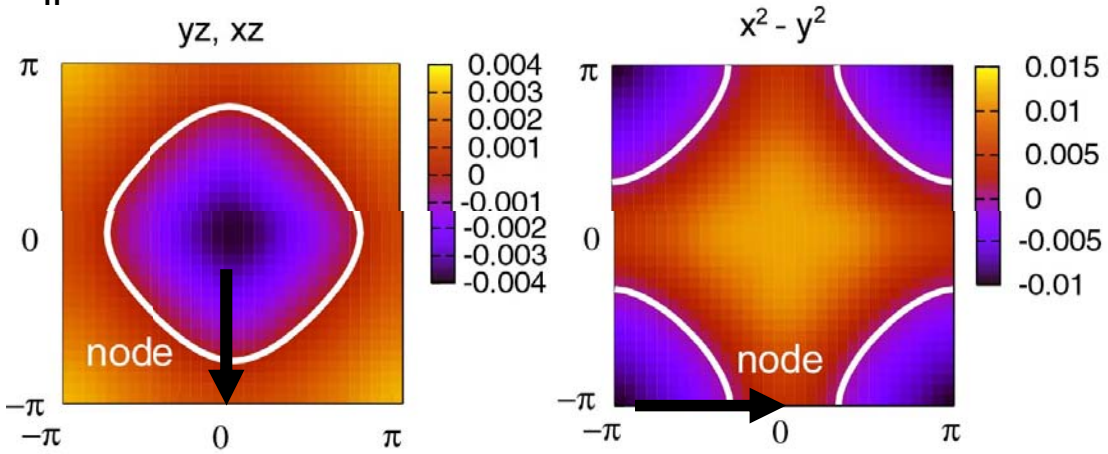
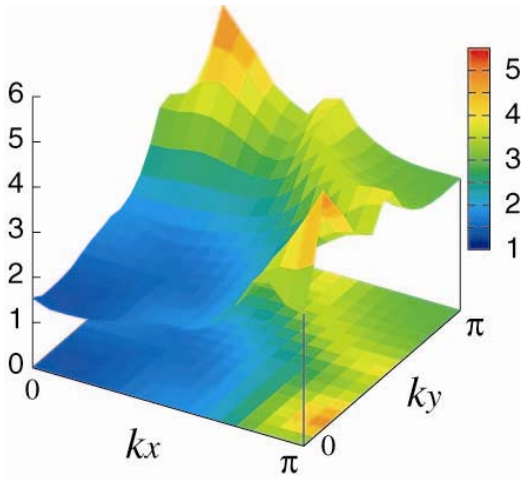


Δ_{ii}





Kuroki, RA et al, arXiv:0803.3325
to appear in PRL

LaFeAsO vs LaFePO

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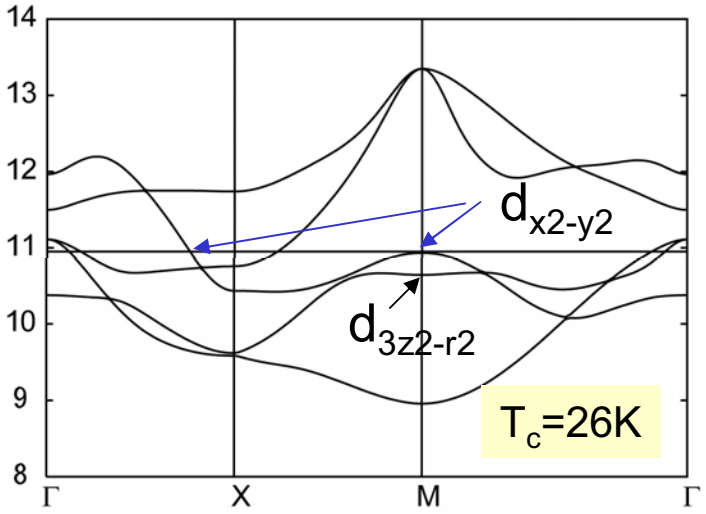
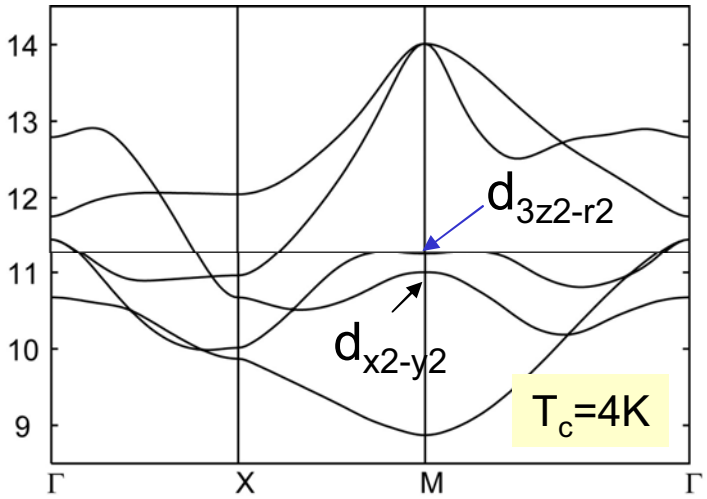
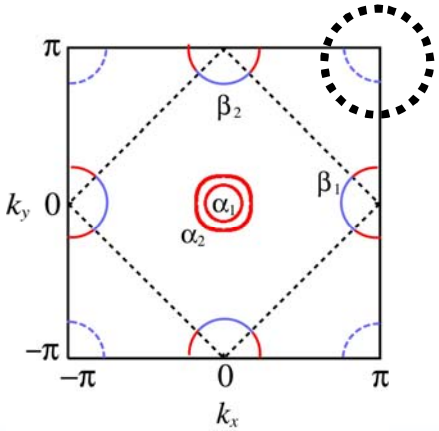
LaFeAsO



LaFePO





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Possibility of unconventional superconductivity

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- ARPES e.g. H. Ding et al, EPL 83 47001 (2008)
- Andreev reflection e.g. Y.Y. Chen et al, Nature 453, 1224 (2008)
- Micro wave Penetration depth e.g. K. Hashimoto et al, arXiv:0806.3149

} Nodeless SC ?

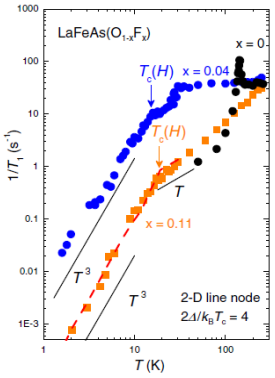
Possibility of extended-s: e.g. Mazin et al., arXiv:0803.2740, Kuroki et al., arXiv:0803.3325, Korshunov et al.,arXiv:0804.1793, Chubukov et al.,arXiv:0807.3735, Parker et al.,arXiv:0807.3729, Sknepnek et al., arXiv:0807.4566, Parish et al., arXiv:0807.4572 …..

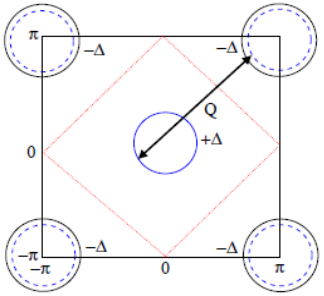
Possibility of s: Wang et al., arXiv:0807.0498

- Nuclear Magnetic Resonance
  - Absence of coherence peak
  - $1/T_1 \sim T^3$

} nodes intersect FS?

Nakai et al, JPSJ 77 073701(2008)
Matano et al, arXiv:0806.0249
Grafe et al, PRL101 047003 (2008)





Chubukov et al.: arXiv:0807.3735
Parker et al.:arXiv:0807.3729
Parish et al.:arXiv:0807.4572

"sign change in Δ + unitary impurity scattering"

- Weak Co-doping effect on T_c Kawabata et al, arXiv:0807.3480

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Conclusions

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- Model construction based on ab-initio downfolding
  - Effective model seems to involve all five 3d orbitals
  - moderately correlated (U/W~1/2)
- Possibility of extended-s SC
  - d_{x2-y2}, d_{yz}, d_{xz} orbital must be considered