KITP MiniProgram 2011 1.13

Spin fluctuation mediated pairing and lattice structure sensitivity of iron-based superconductors

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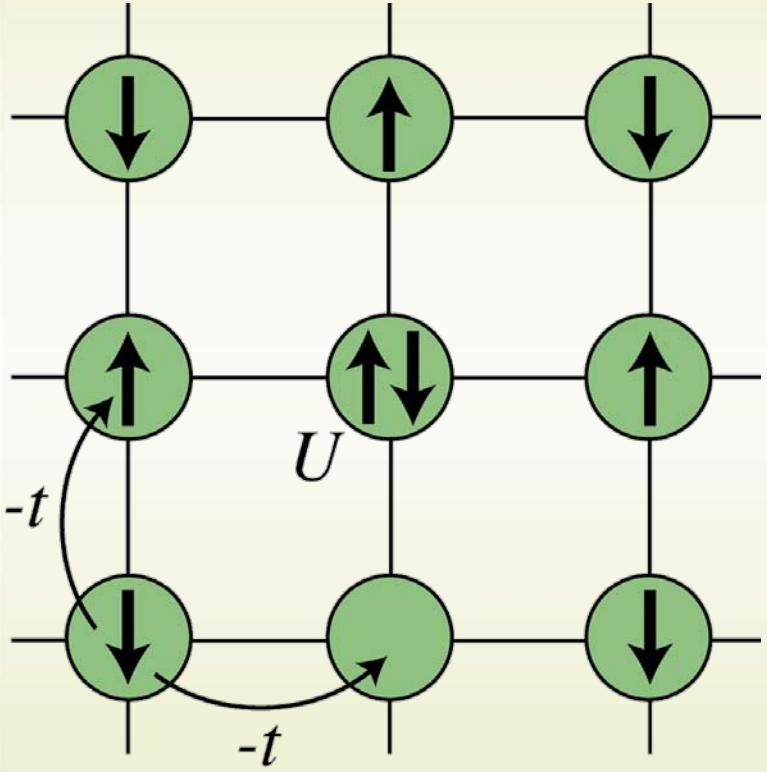
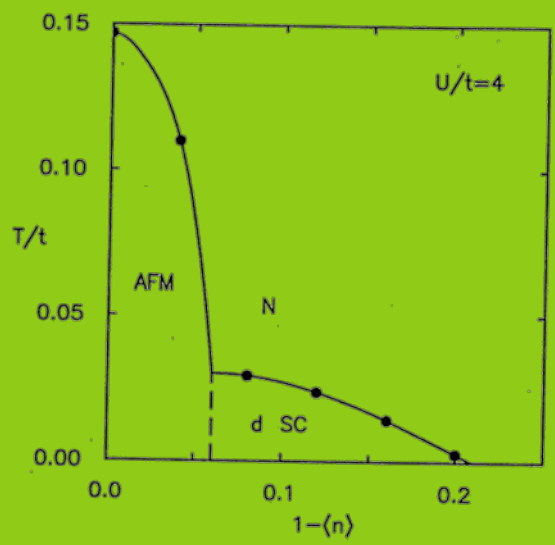
Acknowledgment T. Miyake (AIST)

d-wave SC in the Hubbard model on square lattice





Bickers et al, PRB **43** (1991) 8044

Fluctuation Exchange study
d_{x2-y2}-wave SC $T_c \sim O(0.01t)$

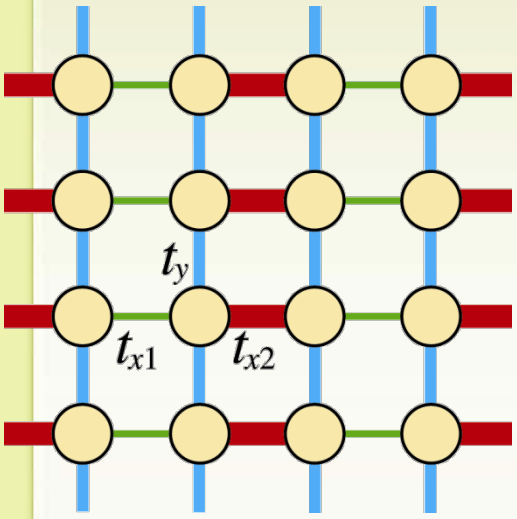
Problems regarding Tc…

- t’ (or Fermi surface shape) dependence of Tc as a model for cuprates ?

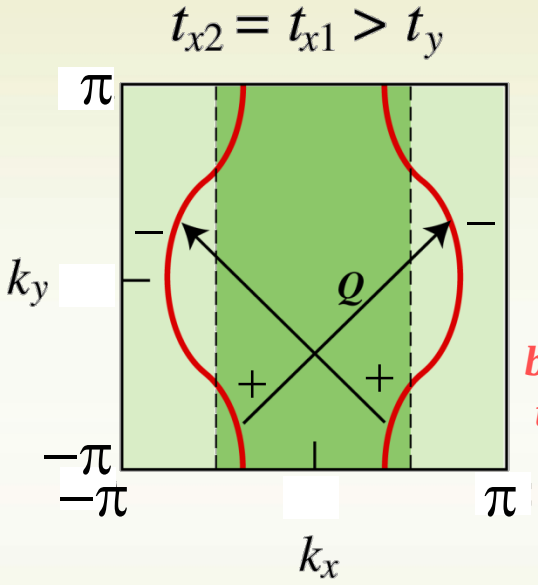
- can we *raise* Tc by modulating the Fermi surface ?

Can we raise Tc ? Nested Fermi Pockets

— an example —

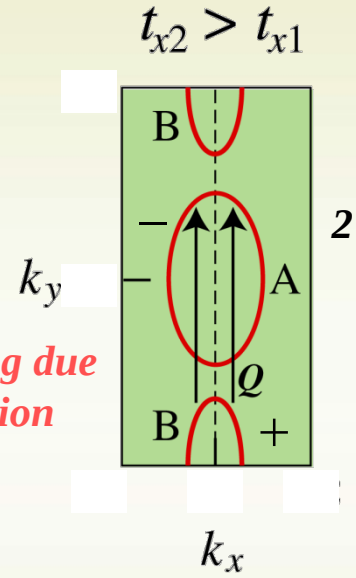


near half-filling



Q: nesting vector

band folding due to modulation



Q bridges A and B

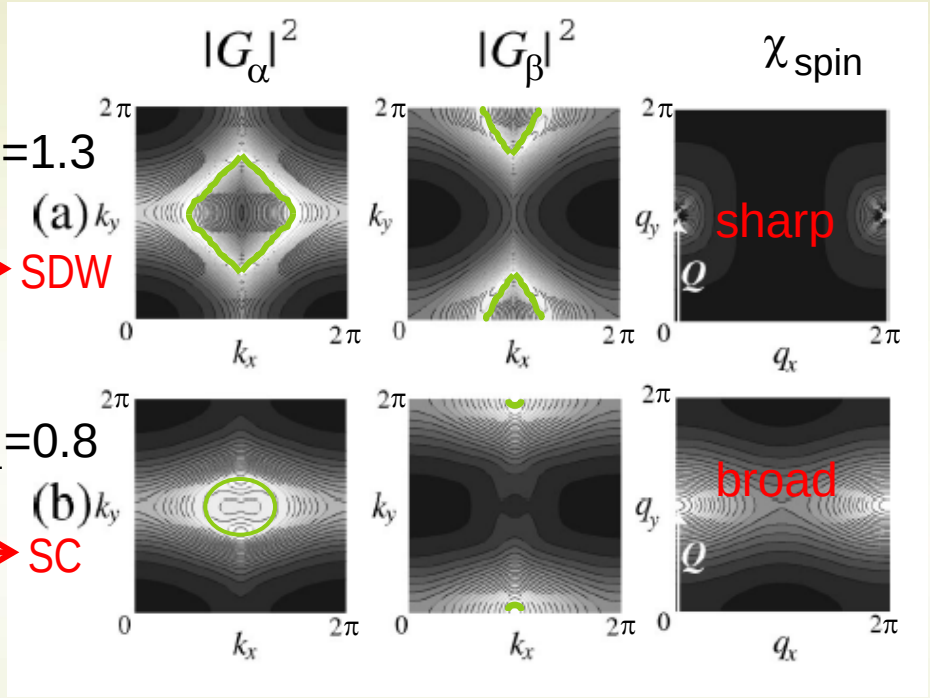
2 band system with FS in each band

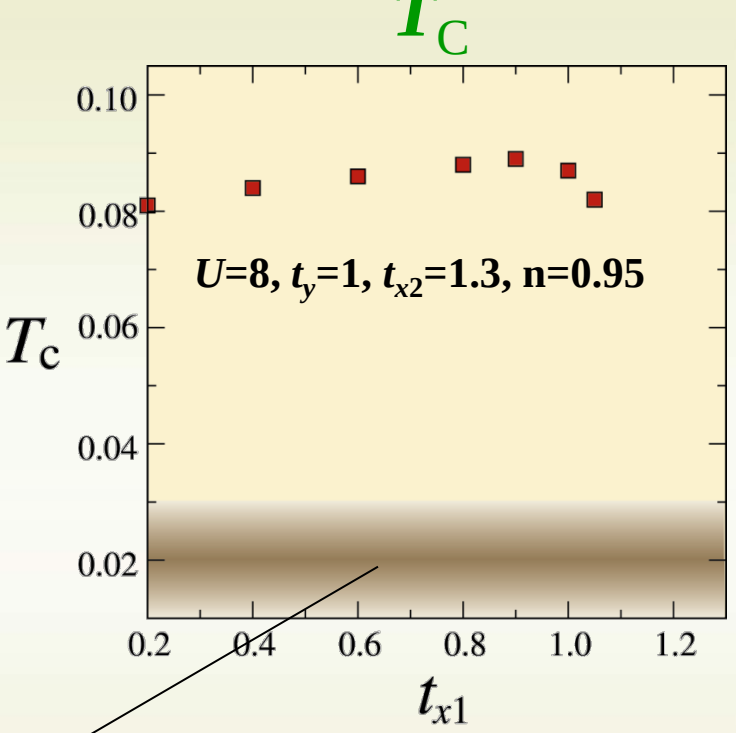
gap function should change sign *between* the Fermi surfaces→s+−

KK& Arita, PRB 64, 024501 (2000)

also, QMC by Bulut et al, PRB 45, 5557 (1992)

FLEX Calculation

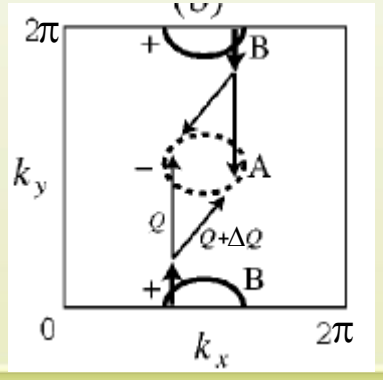


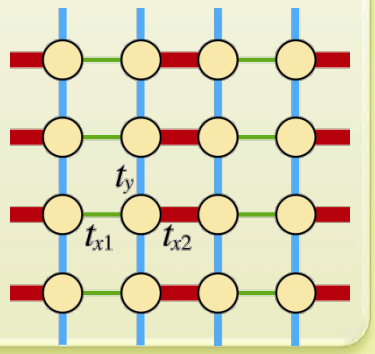


typical T_C on the square lattice

KK&Arita '01

electron&hole FS with volume $\lesssim \Delta Q$
is favorable for s+- superconductivity
moderate electron-hole assymetry→
moderate ΔQ





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Iron-Based Layered Superconductor La[$O_{1-x}F_x$]FeAs ($x = 0.05-0.12$) with $T_c = 26$ K

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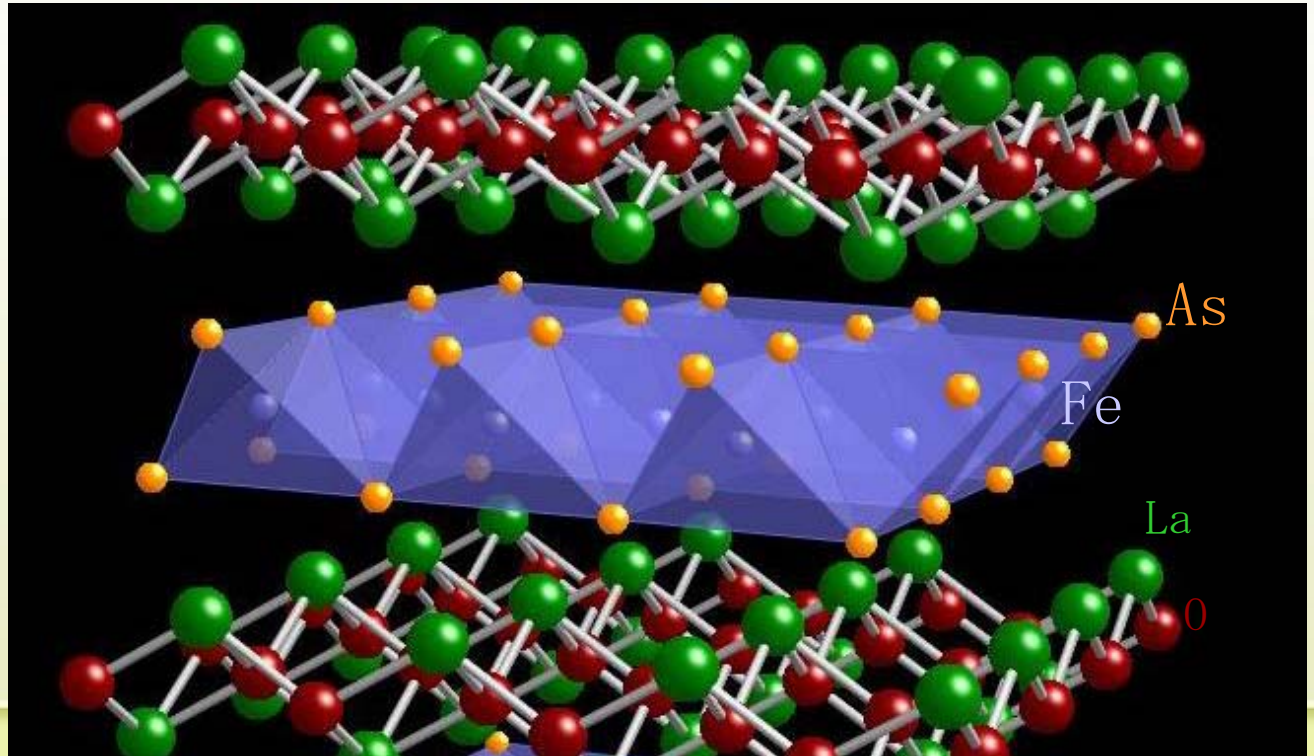
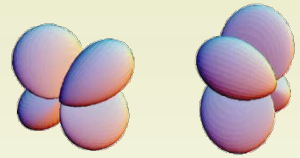
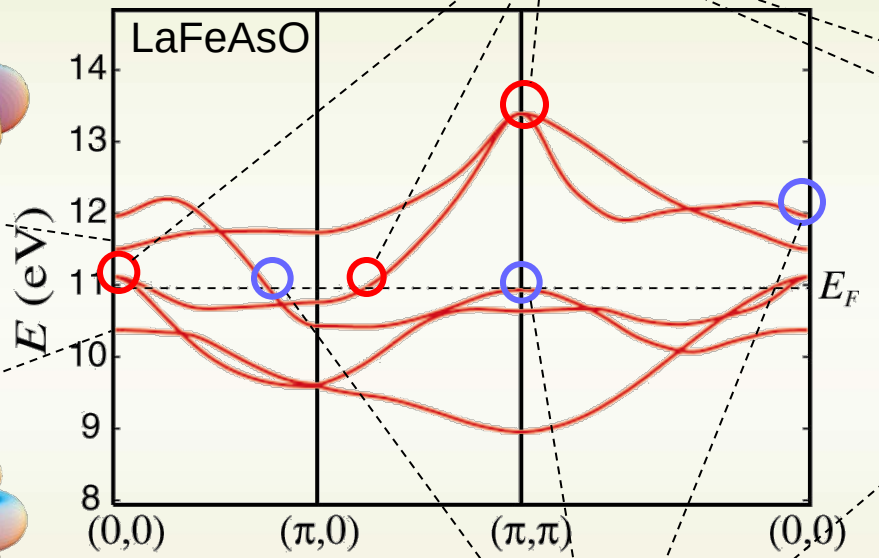


Character of the bands and Fermi surface



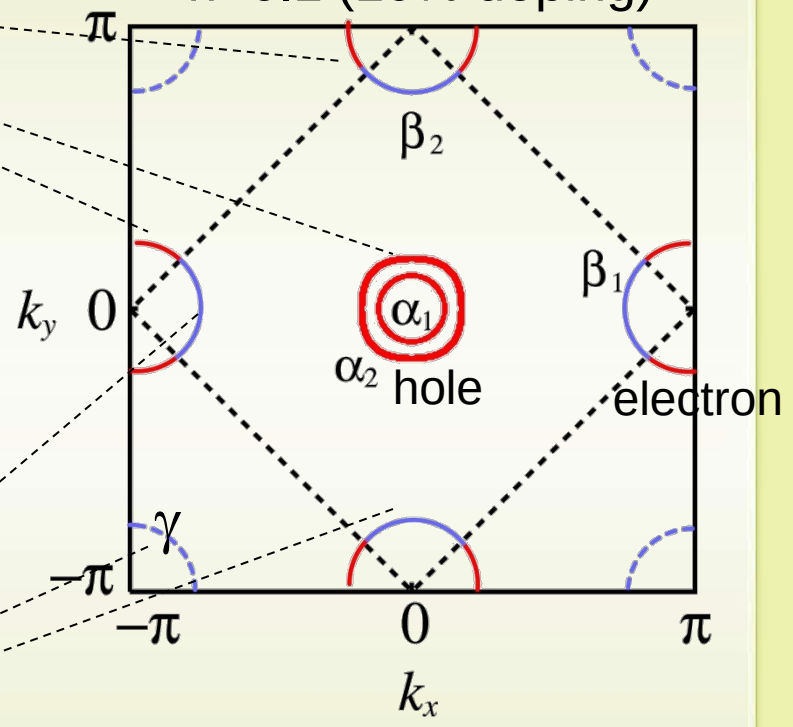
mainly XZ, YZ

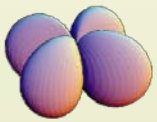
XY



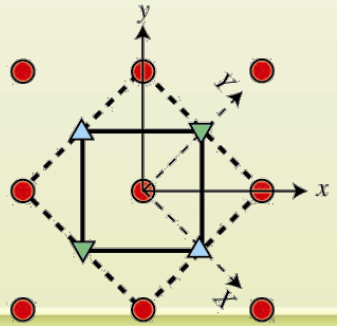
Z^2

n=6.1 (10% doping)



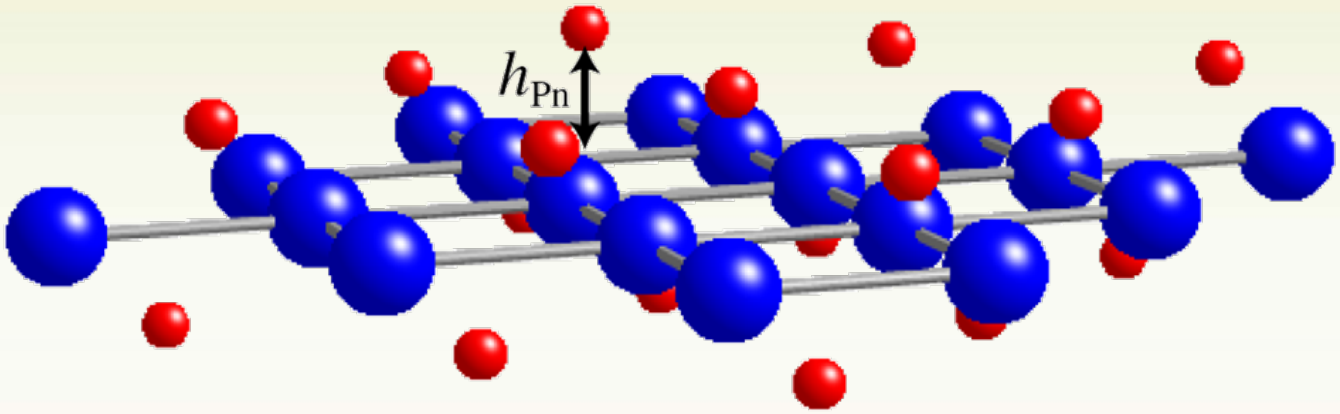


mainly X^2-Y^2= *xy*



heavily entangled !

Pnictogen “height”



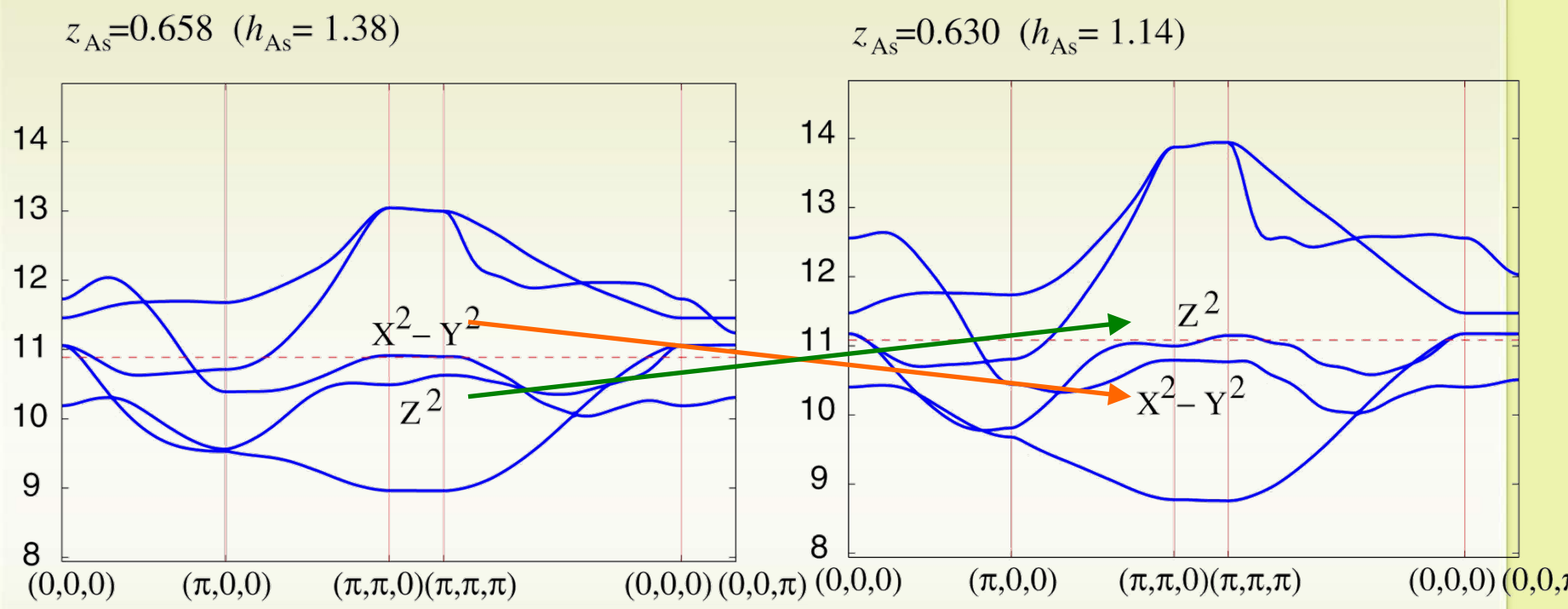
LaFePO(~ 5K) h_P = 1.14 Å

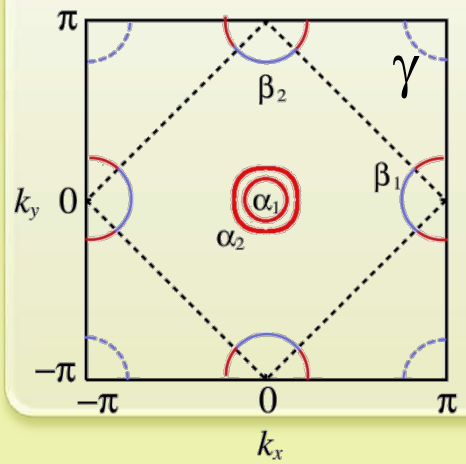
LaFeAsO(~26K) h_{As} = 1.32 Å

NdFeAsO(~50K) h_{As} = 1.38 Å

high

low





KK et al., PRB **79** (2009) 224511

also by Singh&Du, Vildosola et al, others

Effective Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

$$\mathcal{H}_0 = \sum_{ij} \sum_{\mu\nu} \sum_{\sigma} t_{ij}^{\mu\nu} c_{i\mu\sigma}^{\dagger} c_{j\nu\sigma} + \sum_{i\mu\sigma} \epsilon_{\mu} n_{i\mu\sigma}$$

i, j: site、μ, ν: orbitals

$$\mathcal{H}_1 = \sum_i \left[U \sum_{\mu} n_{i\mu\uparrow} n_{i\mu\downarrow} + U' \sum_{\mu>\nu} n_{i\mu} n_{i\nu} + J \sum_{\mu\neq\nu} \boldsymbol{S}_{i\mu} \cdot \boldsymbol{S}_{i\nu} + J' \sum_{\mu\neq\nu} c_{i\mu\uparrow}^{\dagger} c_{i\mu\downarrow}^{\dagger} c_{i\nu\downarrow} c_{i\nu\uparrow} \right]$$

Multiorbital RPA

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

l_i : orbital indices

spin susceptibility:

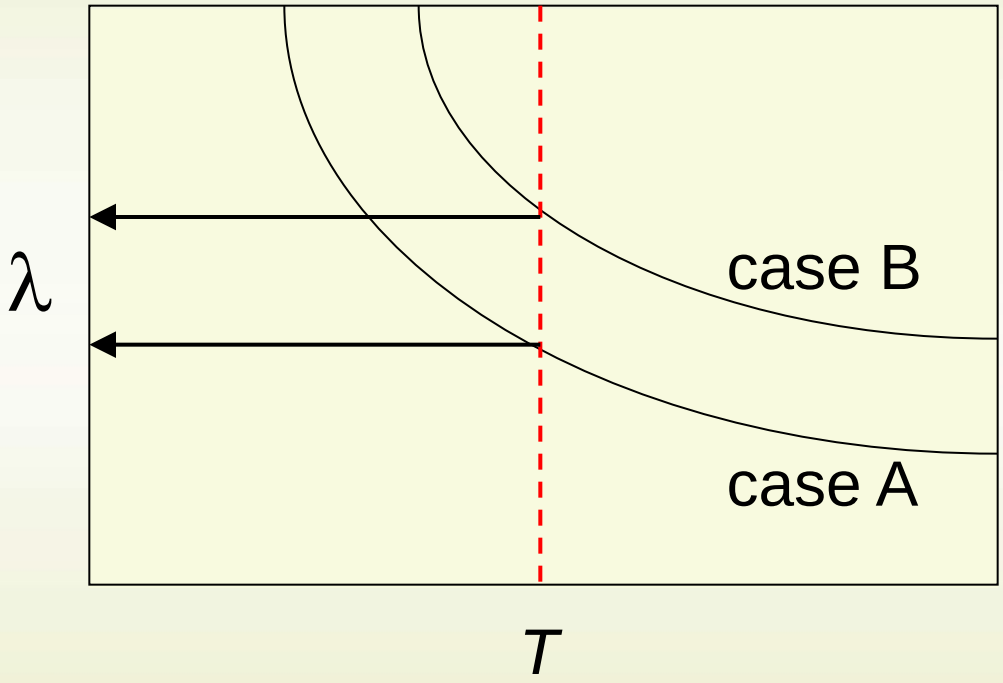
$$\hat{\chi}^s(q) = \frac{\hat{\chi}^0(q)}{1 - \hat{S}^0\hat{\chi}^0(q)}$$

charge (orbital) susceptibility:

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

3 dimensional calculation 32 x 32 x 4 k-point meshes, 512 Matsubara frequencies

Linearized Eliashberg equation

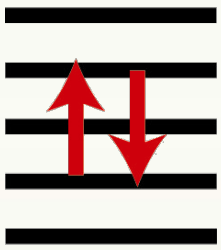


$$\lambda\Delta_{l_1 l_4}(k) = -\frac{T}{N}\sum_{q}\sum_{l_2 l_3 l_5 l_6}\hat{V}^{s(t)}_{l_1 l_2, l_3 l_4}(q)G_{l_2 l_5}(k-q)\Delta_{l_5 l_6}(k-q)G_{l_3 l_6}(q-k)$$

λ at a fixed *T* can used as a qualitative measure for Tc

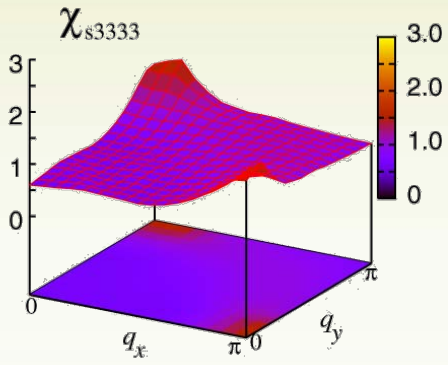
Intra-orbital interaction

LaFeAsO

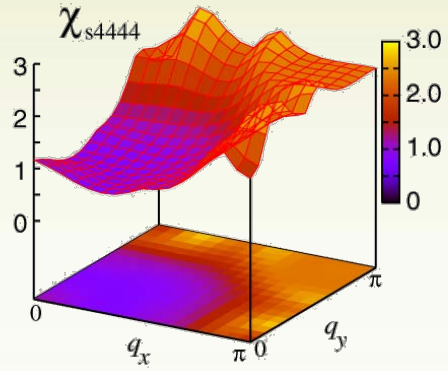


U

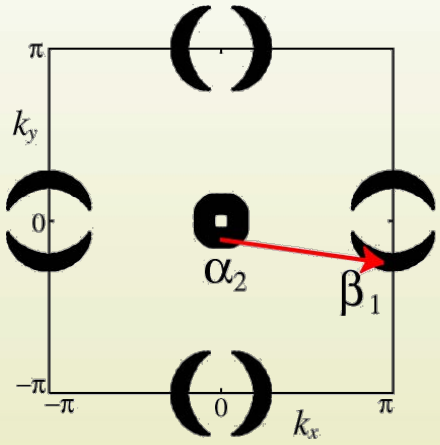
intra-orbital interaction

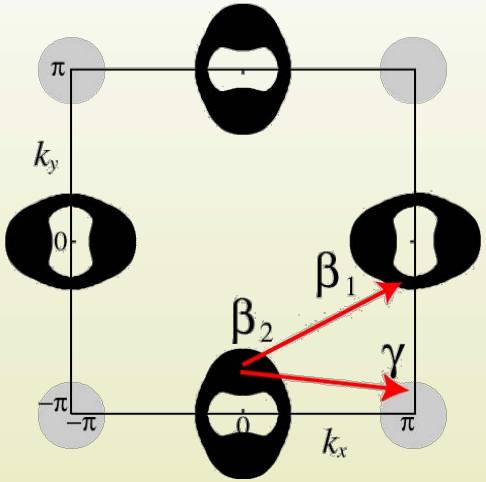


dXZ/ dYZ



$dX^2 - Y^2$





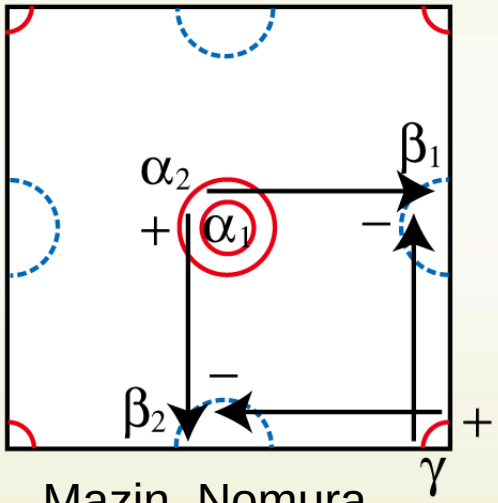
arrows : intra-orbital int.

Spin fluctuation mediated pairing

high

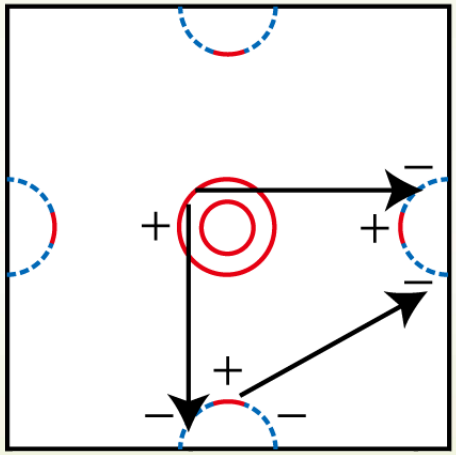
low

fully gapped $s\pm$wave



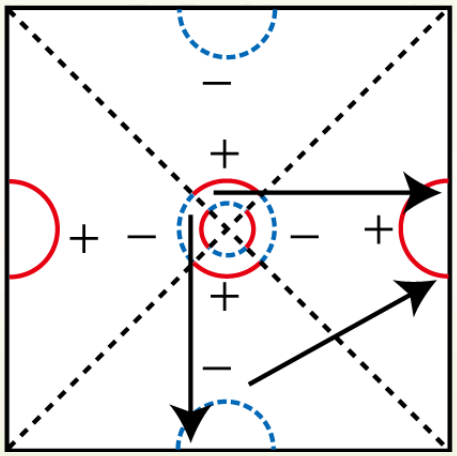
Mazin, Nomura, Ikeda, Wang, KK, Chubukov, Ji, Daghofer….

nodal $s\pm$wave



Graser et al.
Mishra et al.
KK et al.
Wang et al.
Thomale et al

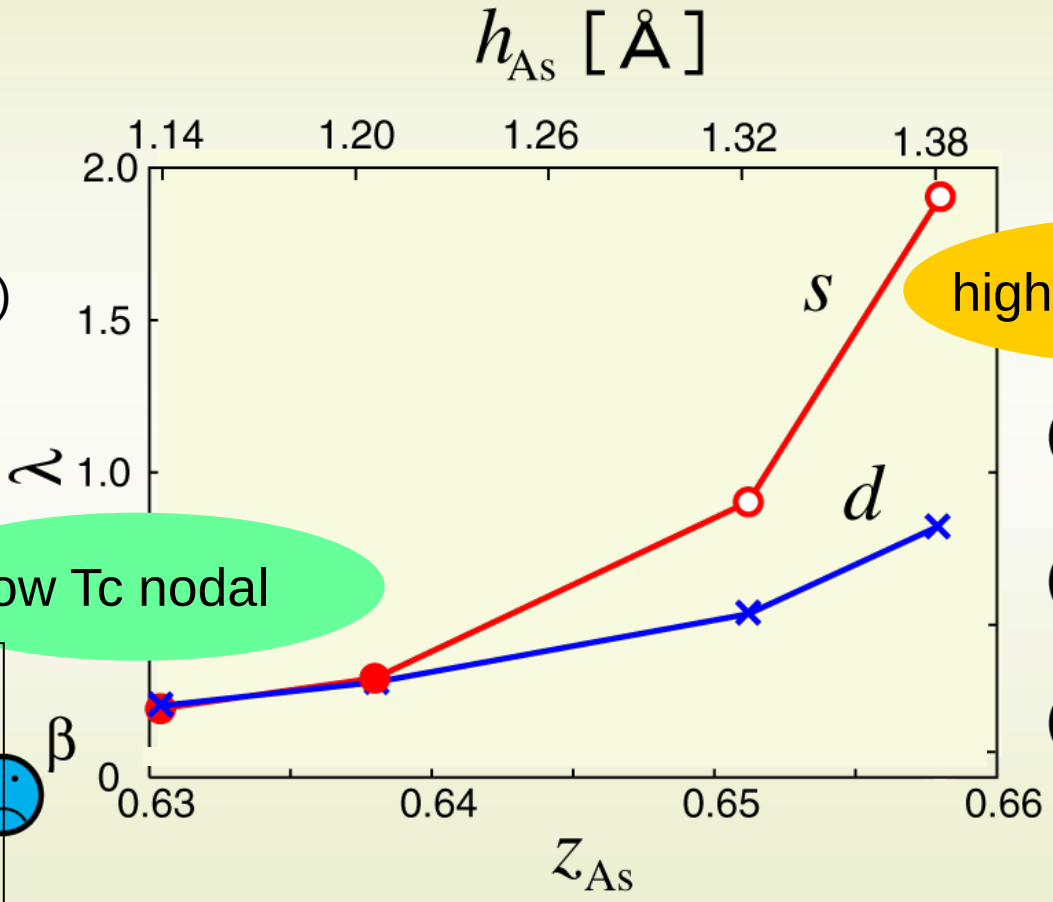
d-wave



KK et al.,
Graser et al,
Yanagi
Ikeda&Arita…

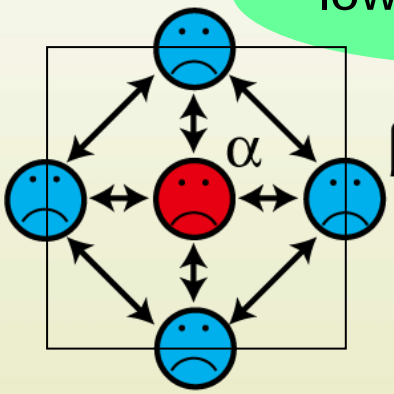
“Height” as a switch between high Tc nodeless and low Tc nodal pairings

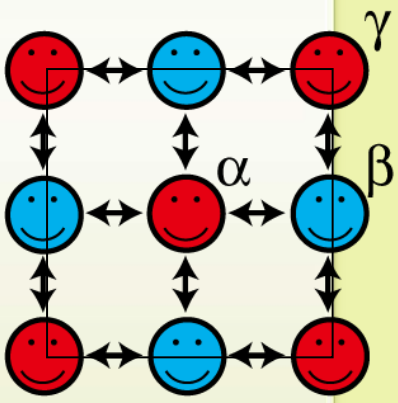
U=1.2, U’=0.9,
J=J’=0.15
n=6.1 (10% dope)
T=0.02 (eV)



high Tc nodeless

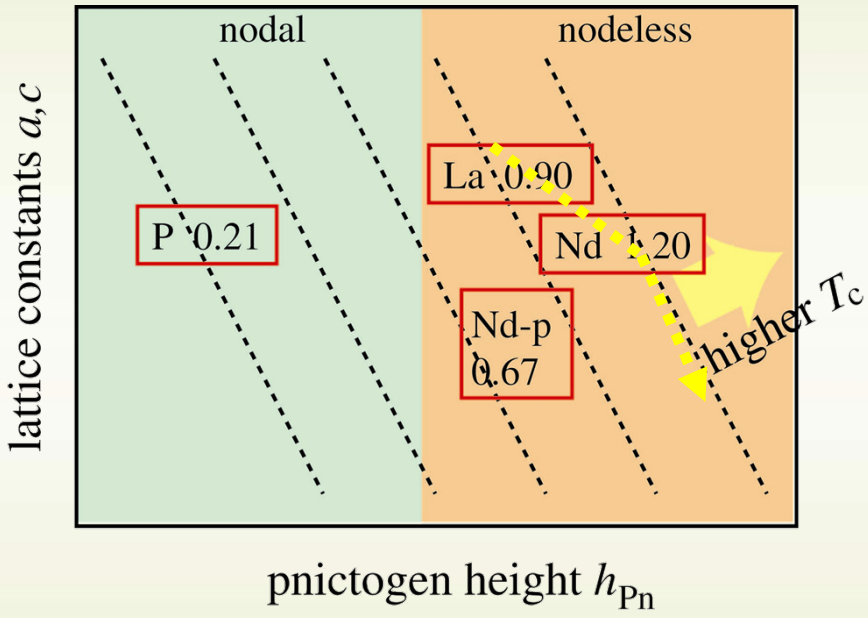
low Tc nodal





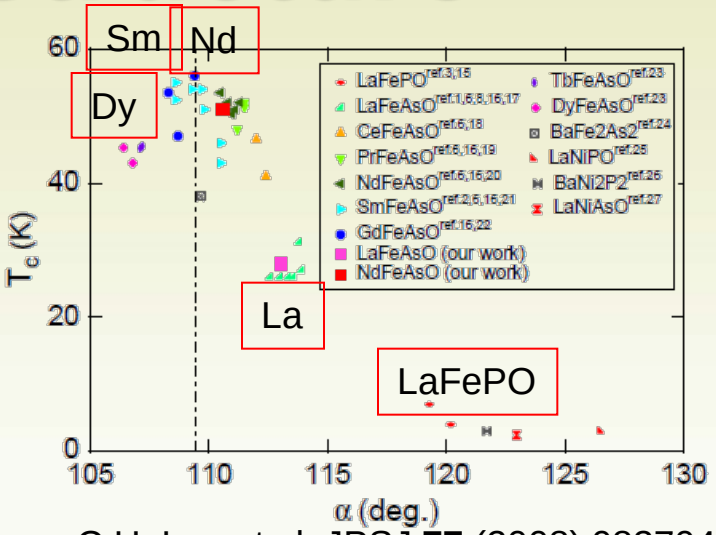
KK et al., PRB **79** (2009) 224511

Tc vs. lattice structure

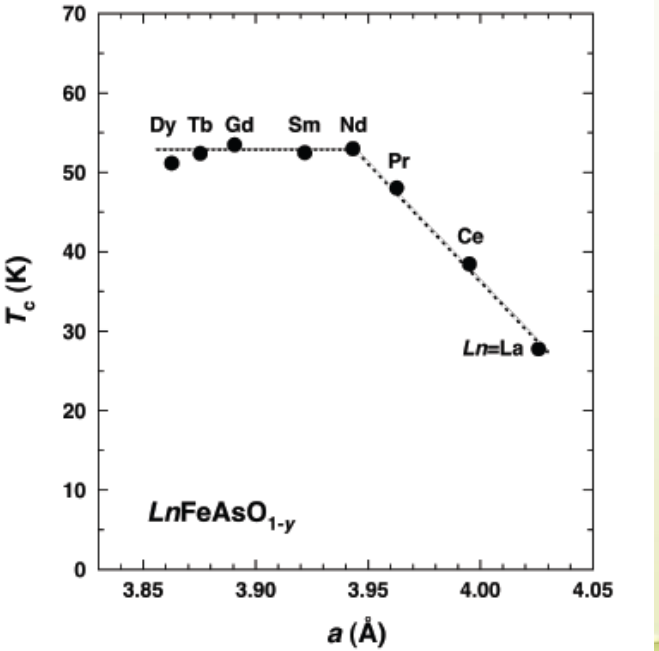


the numbers are the eigenvalue of the Eliashberg equation for T=0.02eV, n=6.1

KK et al., PRB **79** (2009) 224511

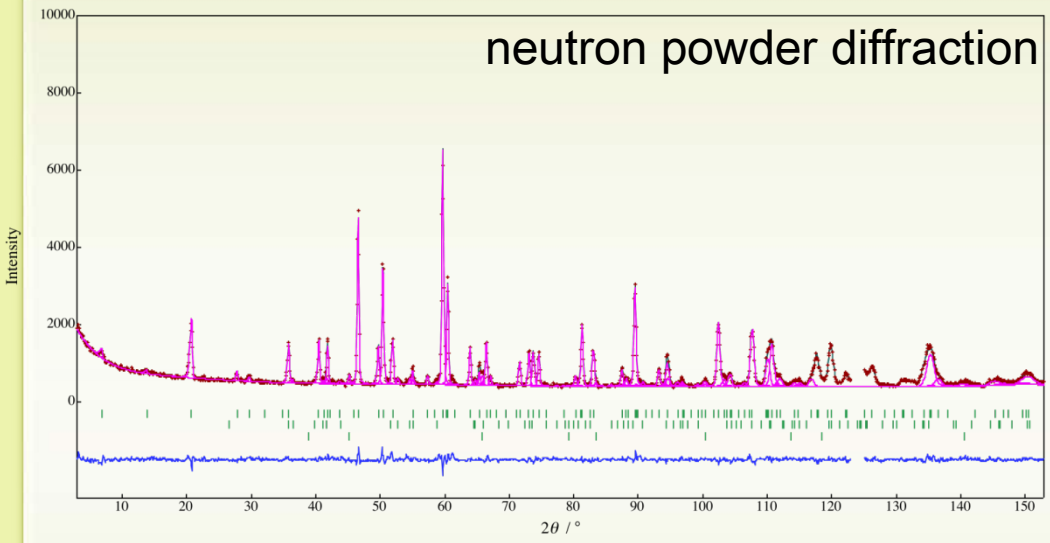


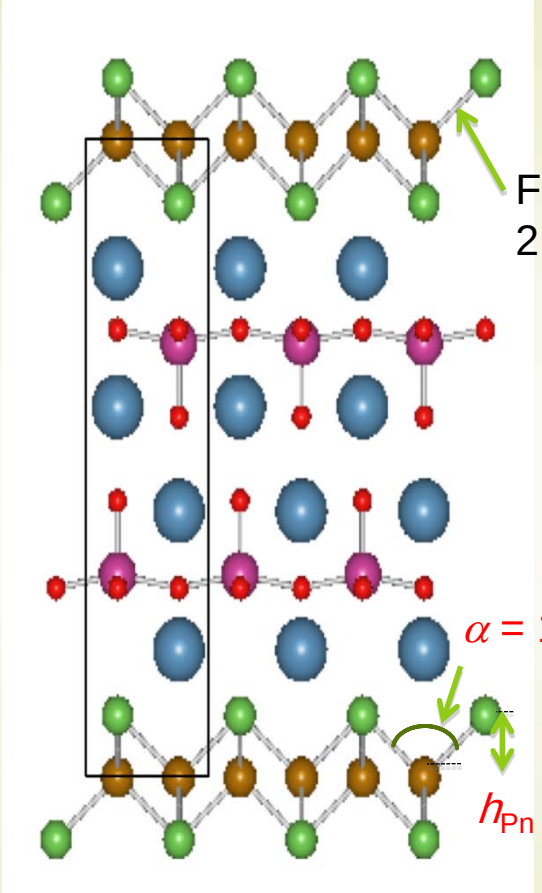
C.H. Lee et al, JPSJ **77** (2008) 083704



K. Miyazawa et al, JPSJ (2009)

Crystal structure of $(Ca_4Al_2O_6)(Fe_2As_2)$





a = 3.7133Å cf. a=4.005Å ($LaFeAsO_{1-y}$)

c = 15.404Å

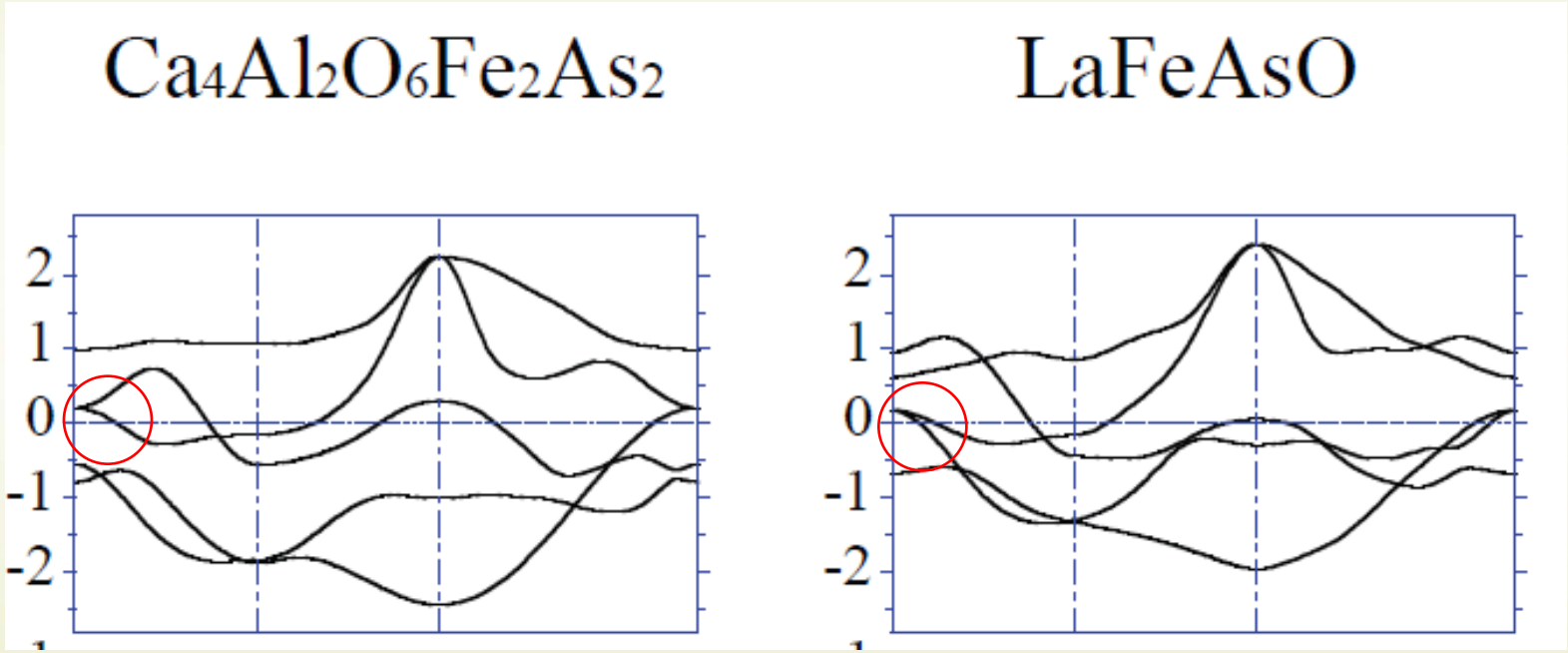
smallest α and highest h_{Pn} is realized!

Courtesy Eisaki

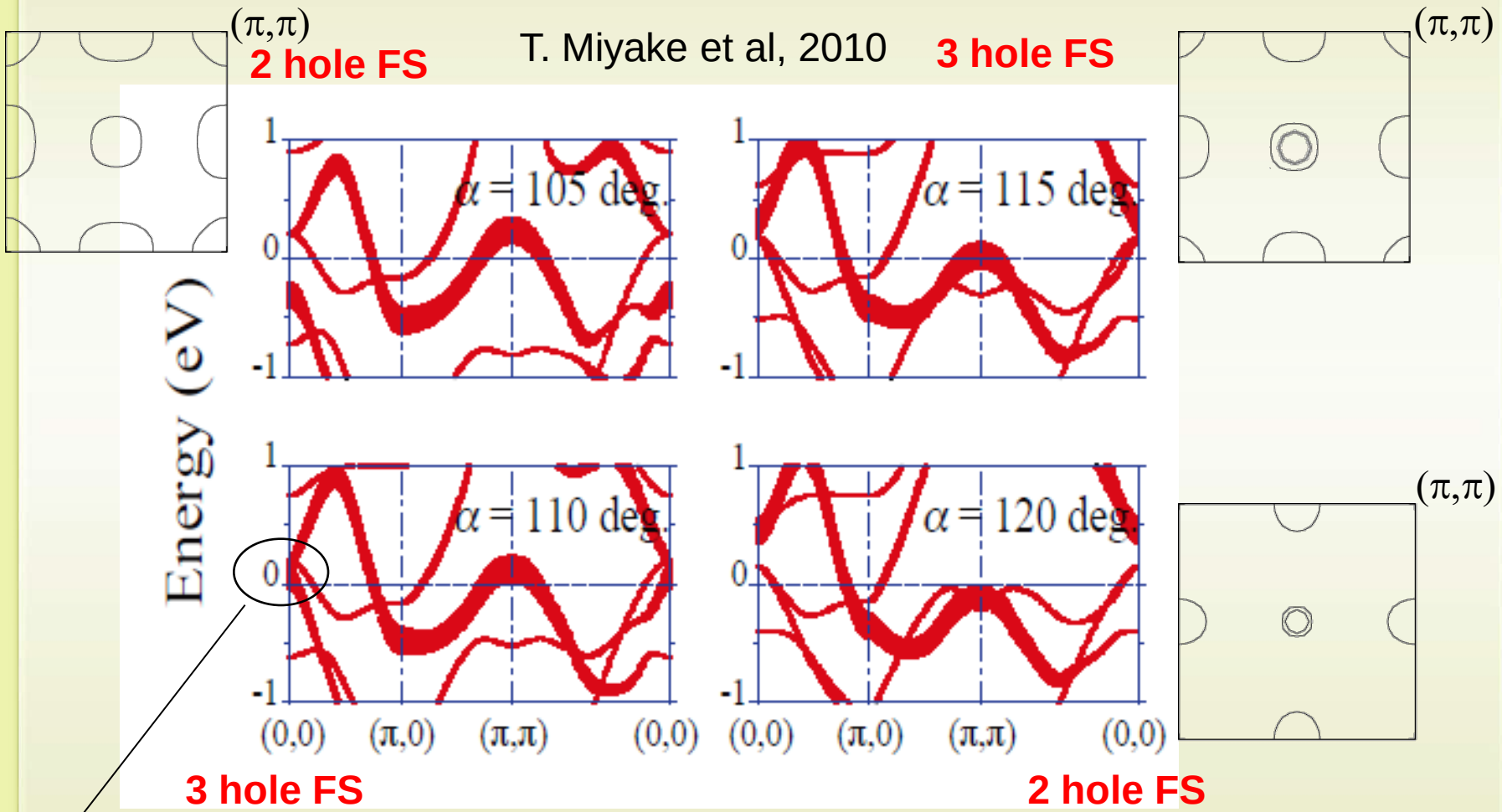
P.M.Shirage et al., Applied Physics Letters 97(2010)172506

Disappearance of α_1 hole Fermi surface

T. Miyake et al, arXiv:1009.5522, JPSJ (2011)



Bond angle dependence of Fermi surface

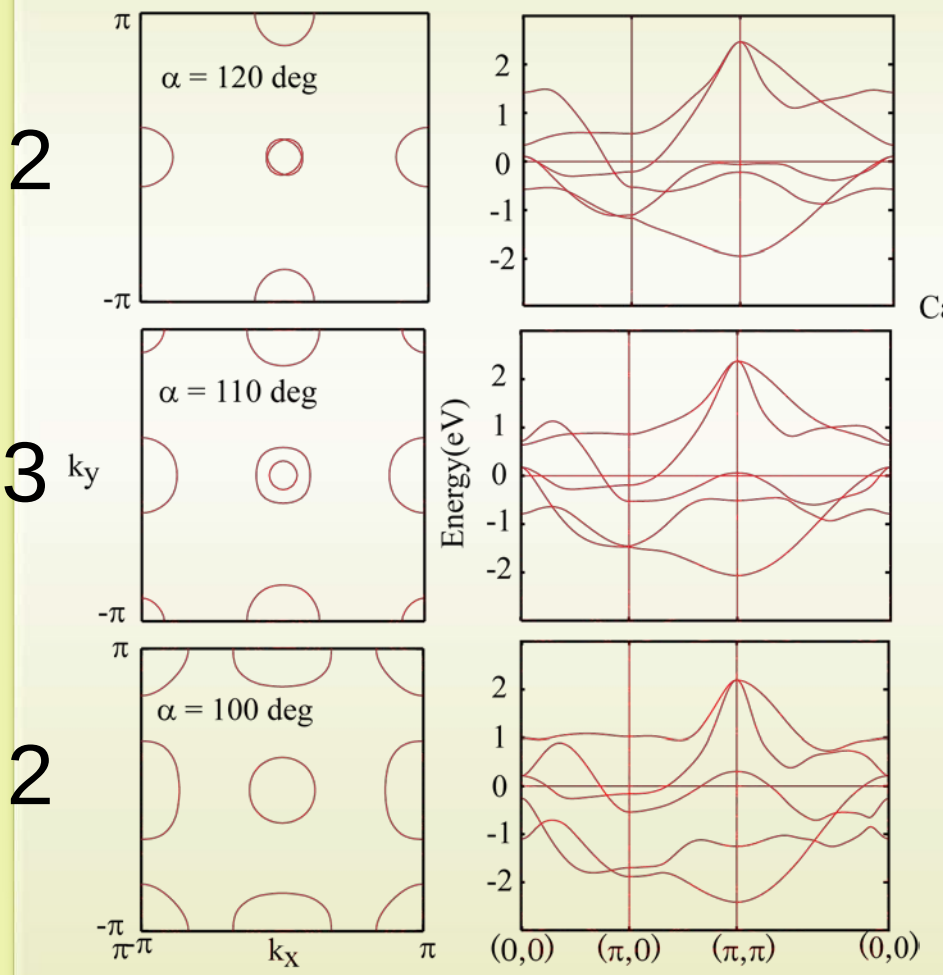


nearly degenerate

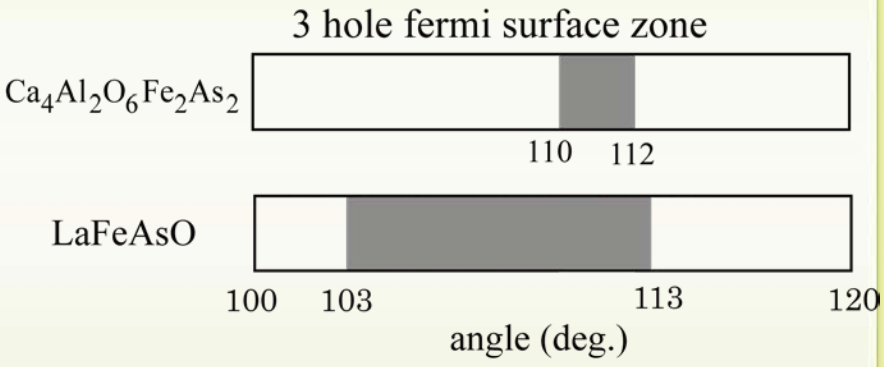
bond length = constant

Bond angle dependence of FS in 1111

FS for 10% doping



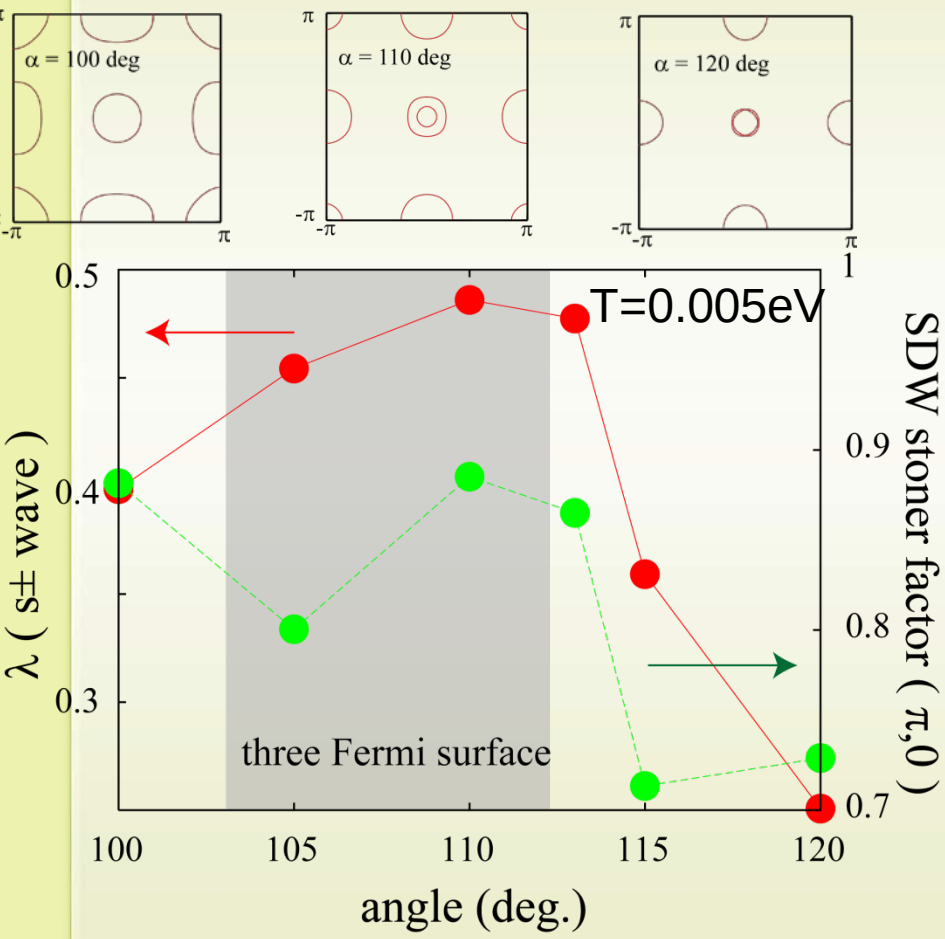
Fe-As bond length= fixed



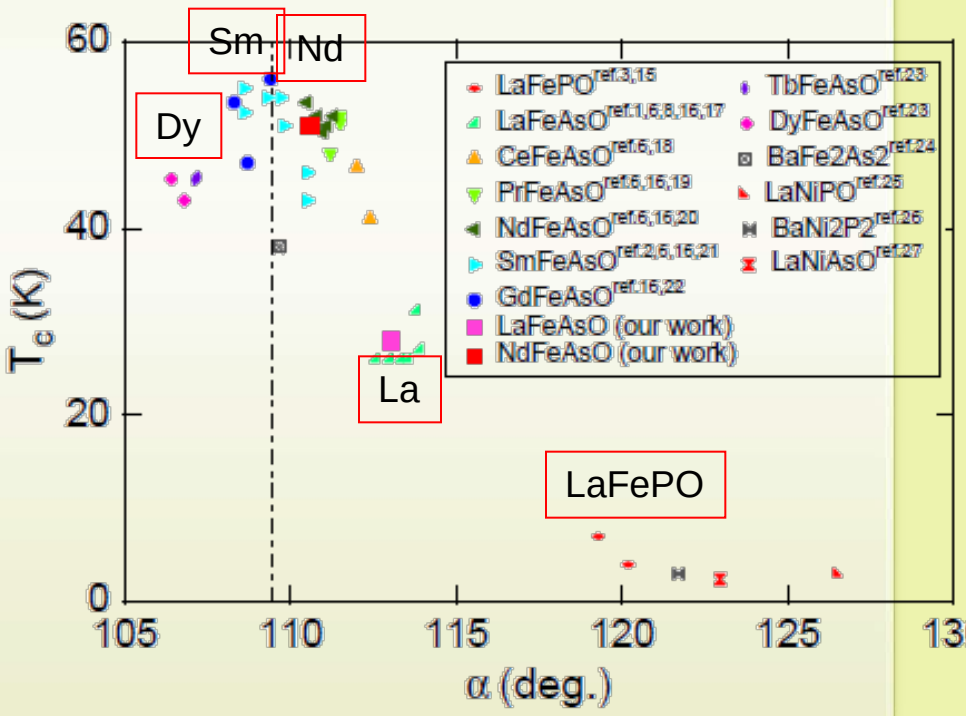
H. Usui and KK, in preparation

Bond angle dependence of SC in 1111

FLEX + linearized Eliashberg equation



H. Usui and KK, in preparation



C.H. Lee et al, JPSJ **77** (2008) 083704

Summary

- Lattice sensitivity of the bands
- number of hole FS changes as 2→3→2 as bond angle varies
- SC(s±) is maximized in the three FS hole regime
- correlation between SC and SDW stoner factor is complicated