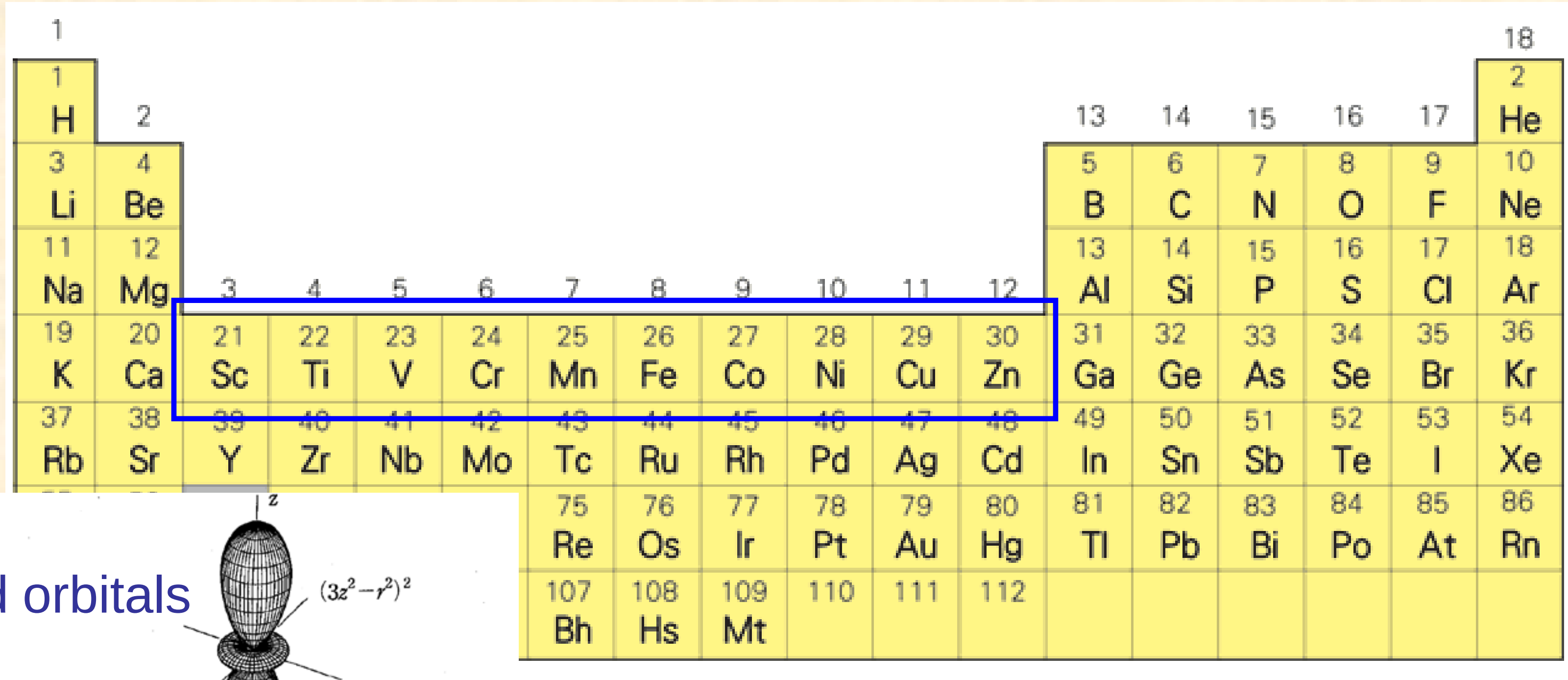
Behind the Scenes of High Temperature Superconductivity: Cuprates and Iron Pnictides

Yukawa Institute for Theoretical Physics

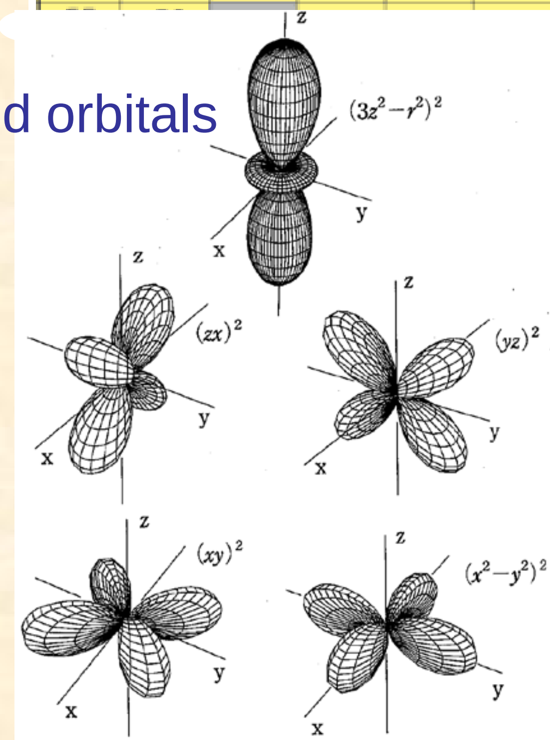
Takami Tohyama
Eiji Kaneshita
Takao Morinari

YITP
YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

3d transition-metal compounds



3d orbitals

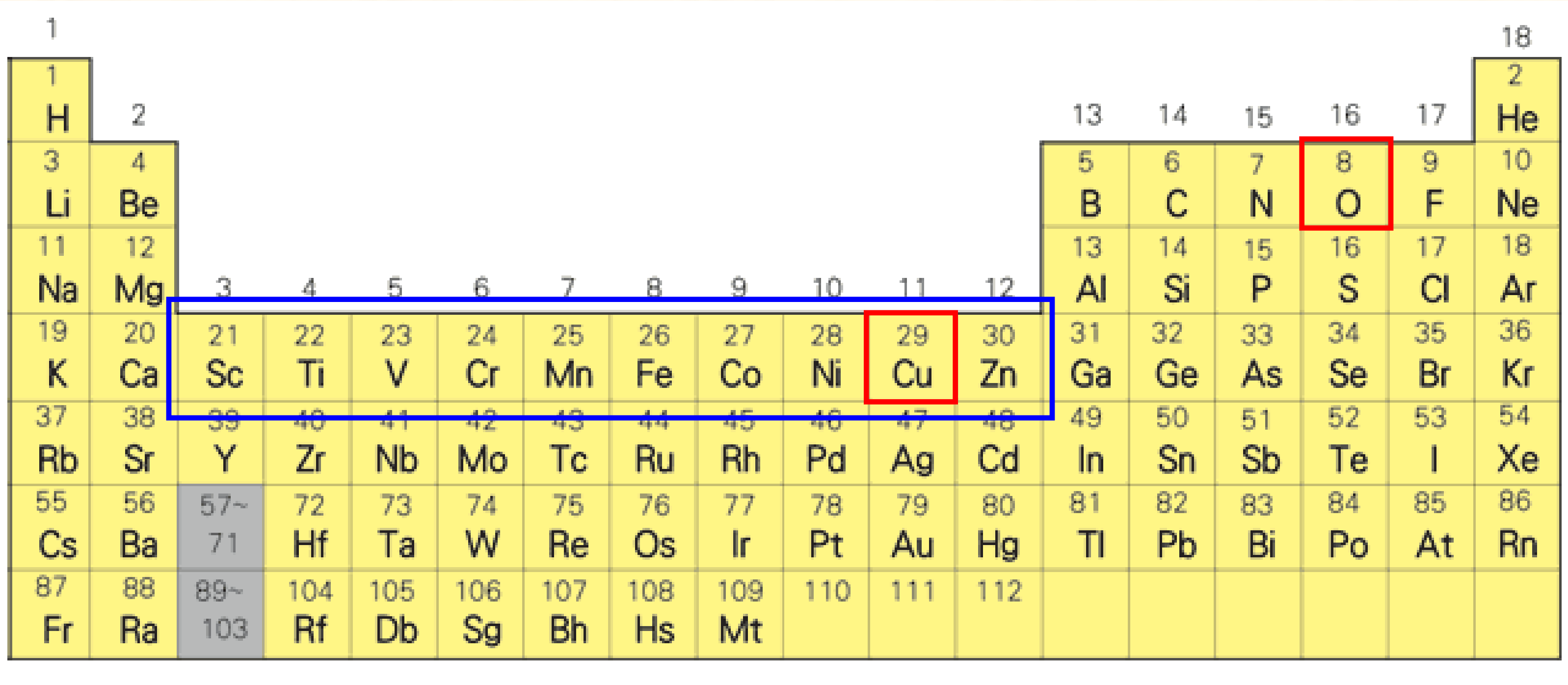


Localized and itinerant natures compete.

⇩

Complicated interactions among the internal degrees of freedom of electrons: charge, spin, orbital

Cuprate superconductors

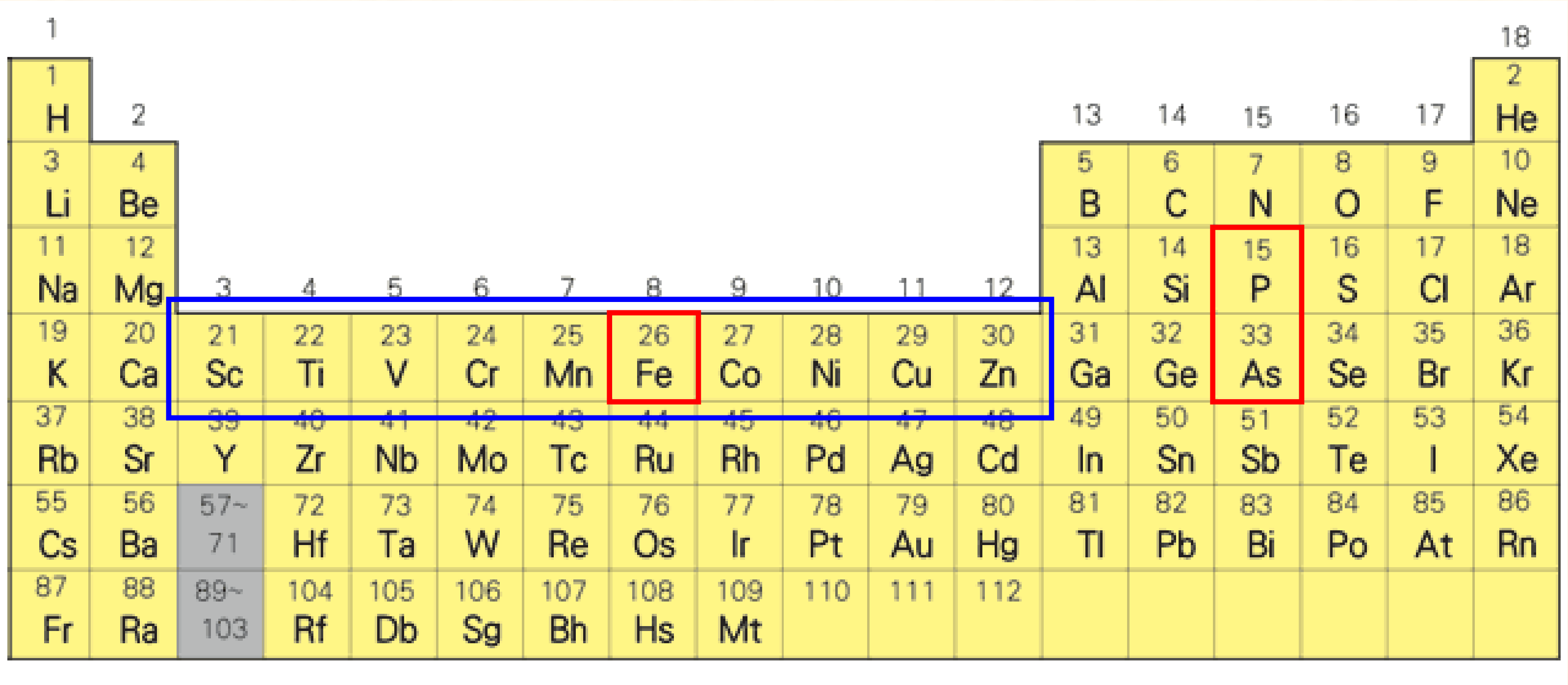


1986 High-temperature superconductivity

T_c ~ 160K under pressure

Oxides, two-dimensionality → superconductivity

Iron-pnictide superconductors



2008 Hosono's Group at TIT

$T_c \sim 55K$

Fe: typical magnetic metal → superconductivity

OUTLINE

Motivation

Similarity and difference between cuprate and iron-pnictide superconductors

Cuprates

- Ionic material
- doped Mott insulator

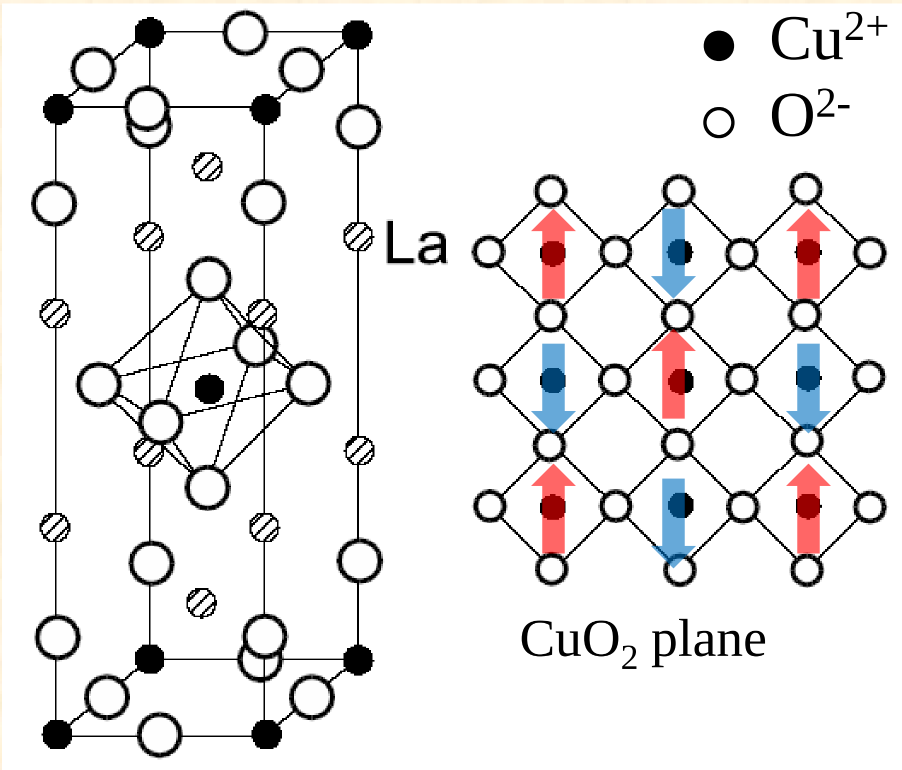
Iron pnictides

- band material
- spin-density wave (SDW)

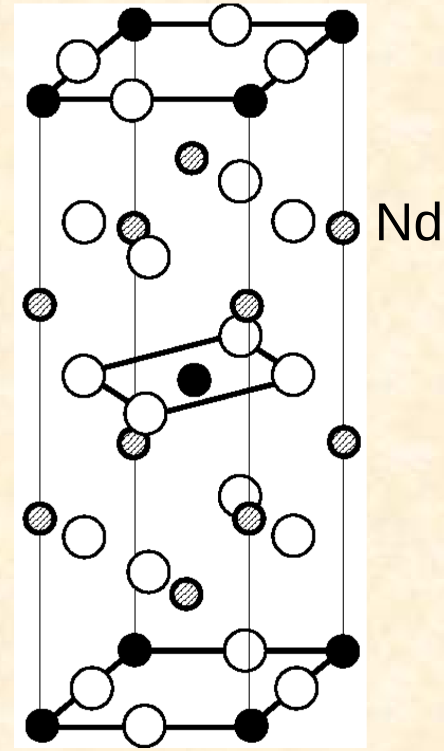
Summary and perspectives

Crystal structure of high T_c cuprates

La_2CuO_4 (hole-doping)



Nd_2CuO_4 (electron-doping)



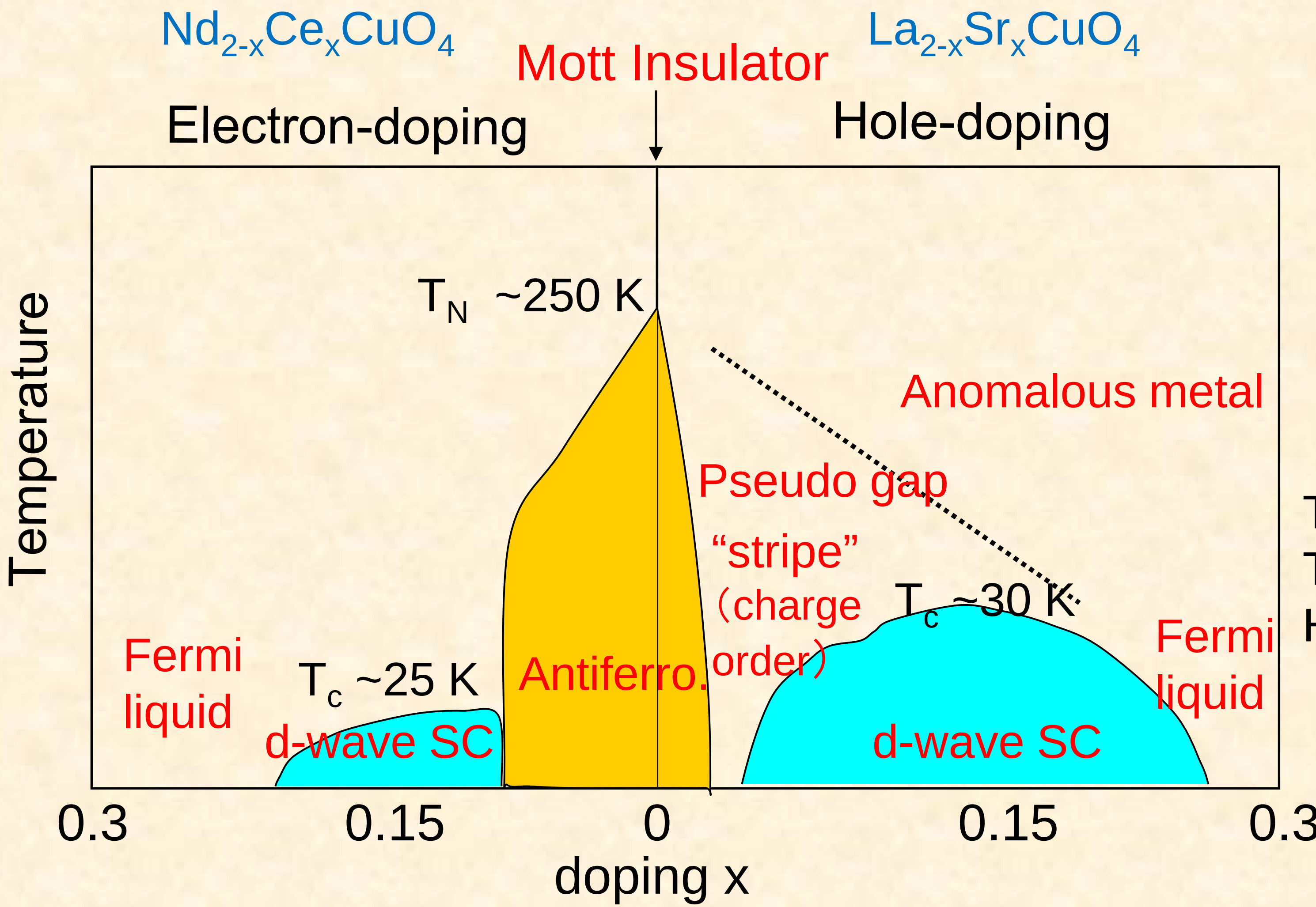
Cu^{2+} $3d^9$ S=1/2 hole on each x^2-y^2 orbital

Strong local Coulomb interaction → Mott insulator

localized spin → antiferromagnetic exchange interaction

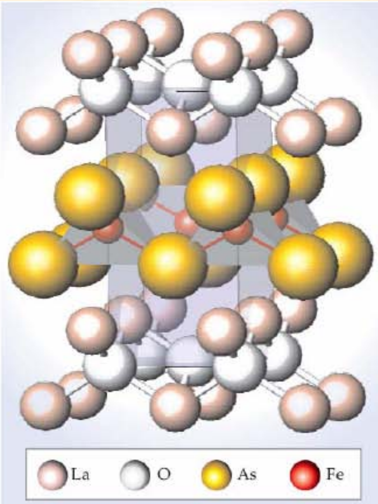
J~1400K

Phase diagrams



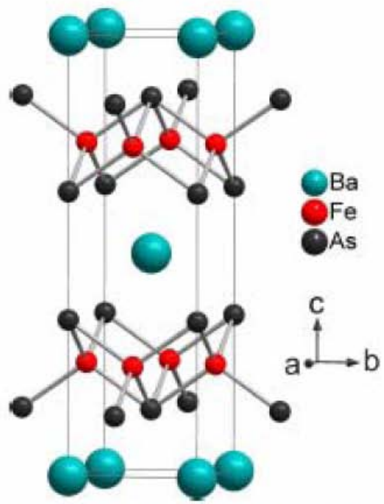
The highest T_c ~135 K for Hg system

Crystal structure of high T_c iron pnictides



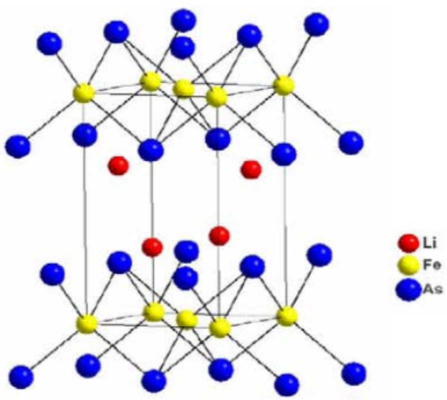
LnFeAsO (1111)

$T_c \sim 55$ K



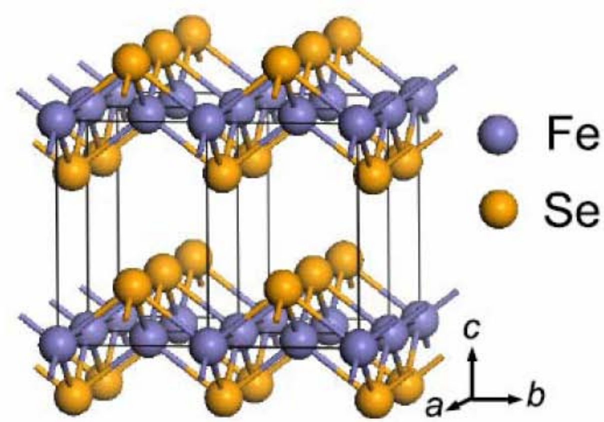
BaFe2As2 (122)

$T_c \sim 37$ K



LixFeAs (111)

$T_c \sim 33$ K



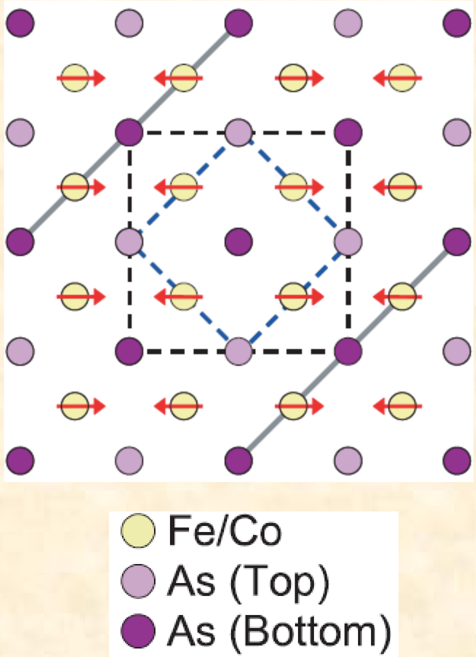
FeSe (11)

$T_c \sim 37$ K (under press.)

Layered structures

Fe-As layer

Quasi-2D system



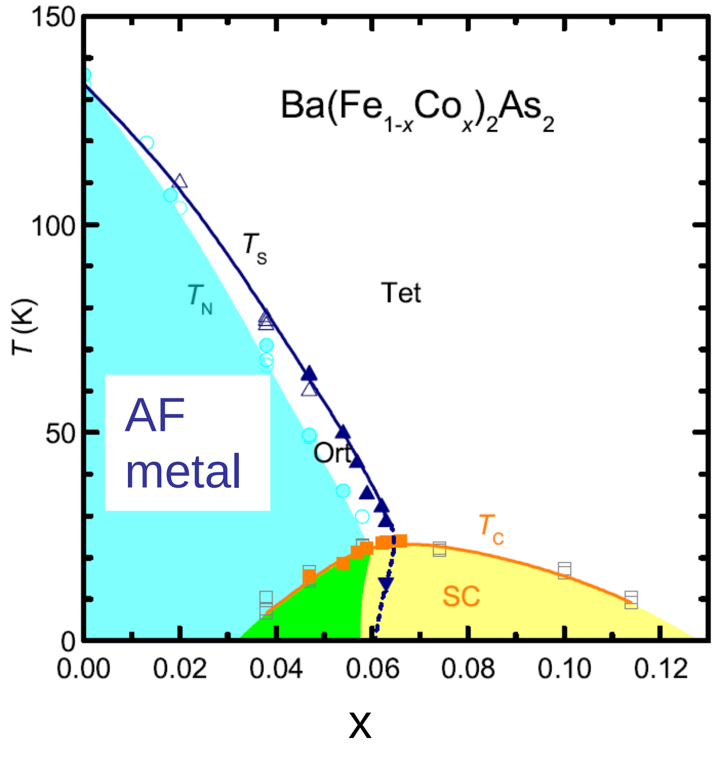
Q=$(\pi,0)$

"Stripe" order

Phase diagram of high-T_c iron pnictides

$Ba(Fe_{1-x}Co_x)_2As_2$

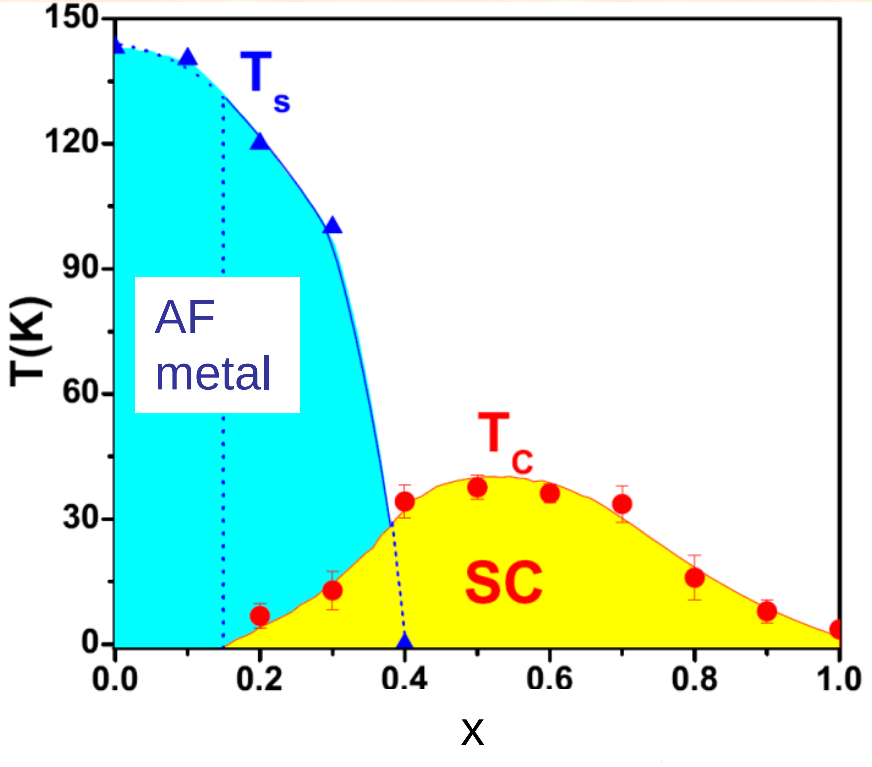
Electron "doping"



S. Nandi *et al*., PRL **104**, 057006 (2010)

$Ba_{1-x}K_xFe_2As_2$

Hole "doping"



H. Chen *et al*., Europhys. Lett. **85**, 17006 (2009)

Cuprates and iron pnictides

Similarity — Superconductivity next to magnetism

Difference	cuprates	iron pnictides
electronic structure	crystal-field, $3d^9$ single band (x^2-y^2)	hybridization, $3d^6$ multi band (five orbitals)
magnetism	Antiferro. insulator	Antiferro. metal
super-conductivity	carrier doping	carrier doping pressure
super-conductivity	d_{x2-y2} symmetry	sign-reversed or preserved s anisotropic s, d ??

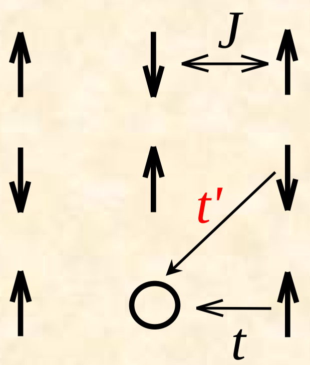
approaches from ionic picture and doped Mott insulator

approaches from band picture and spin-density wave

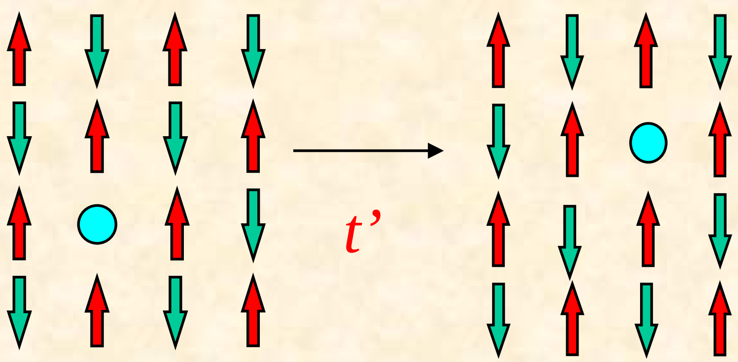
Origin of the electron-hole asymmetry in cuprates

- low-energy effective model: *t-J* model
- Introduction of the second nearest-neighbour hopping *t'*

$$H_{tJ} = -t \sum_{<i,j>_1,\sigma} \tilde{c}^{+}_{i,\sigma}\tilde{c}_{j,\sigma} + J\sum_{i\delta} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} - t' \sum_{<i,j>_2,\sigma} \tilde{c}^{+}_{i,\sigma}\tilde{c}_{j,\sigma}$$



hole carrier	electron carrier	
$t' = -0.4$	$t' = +0.4$	$(t = 1)$



No change of spin configuration by *t'*

The magnitude of the self-energy of this configuration is dependent of the sign of *t'*

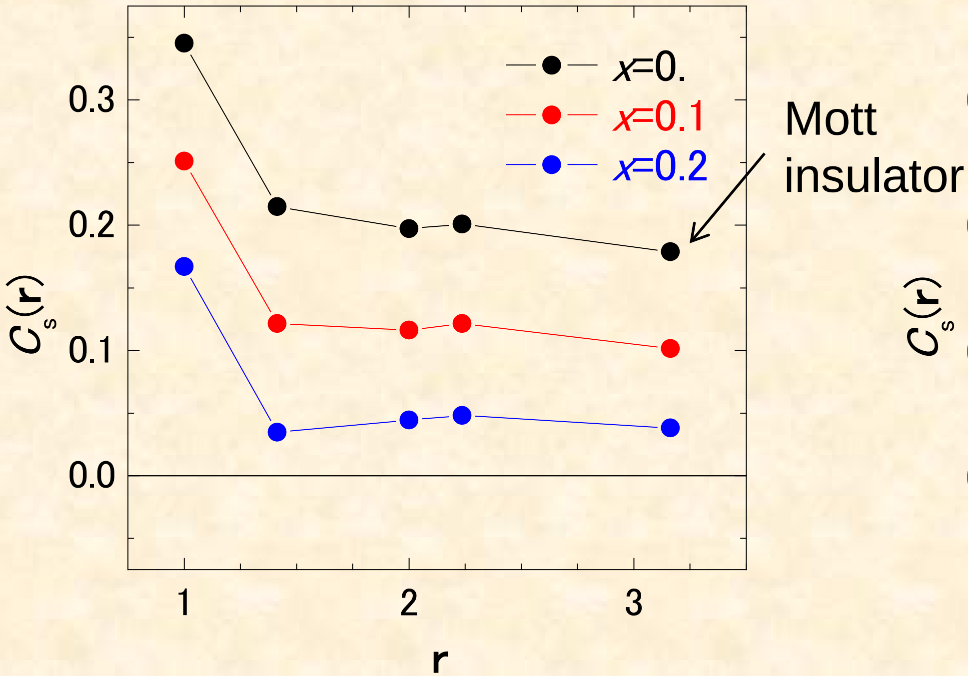
Asymmetry of spin-spin correlation function

distance r

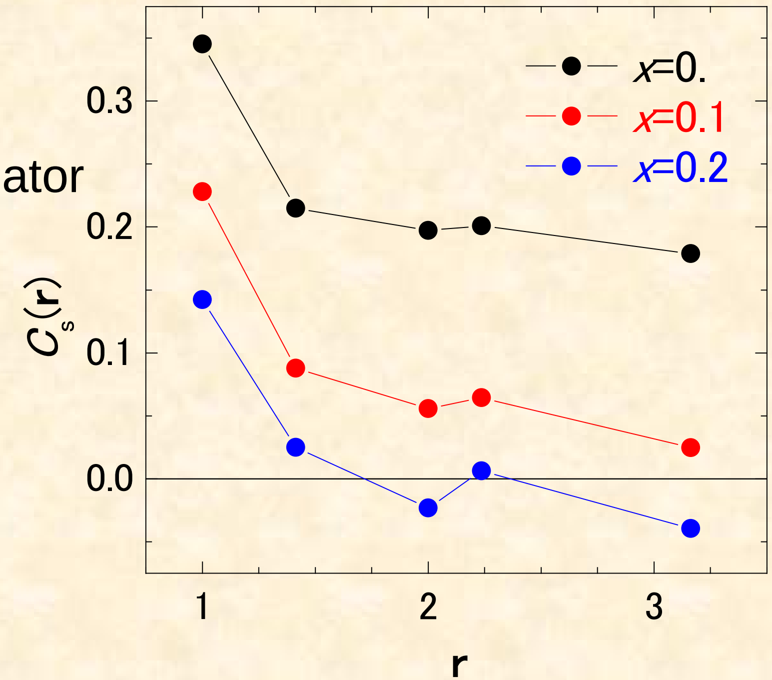
Exact results for a
20-site t-t'-J model

x : carrier density

Electron carrier



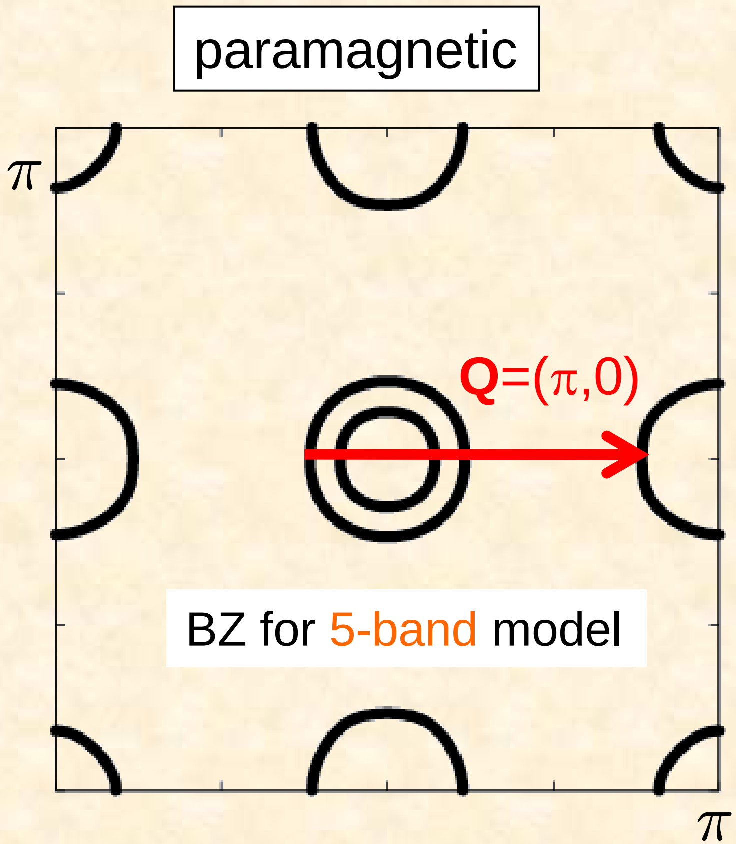
Hole carrier



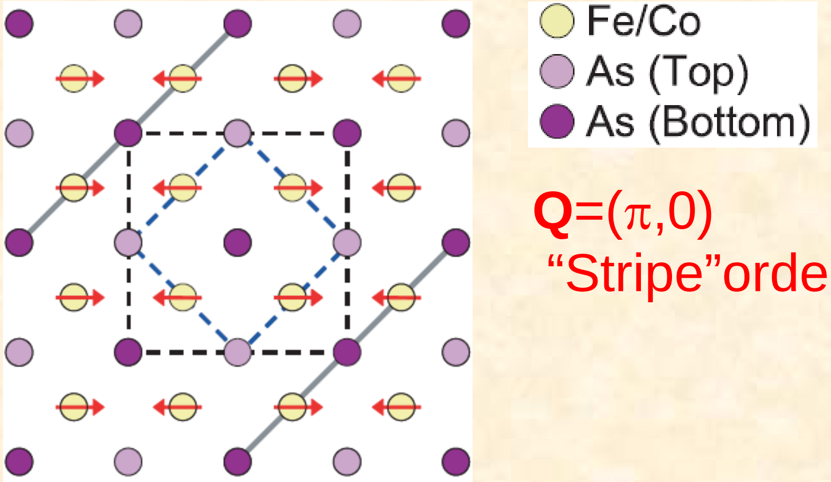
Antiferromagnetic correlation survives for the electron carrier.

T. T., PRB **70**, 174517 (2004)

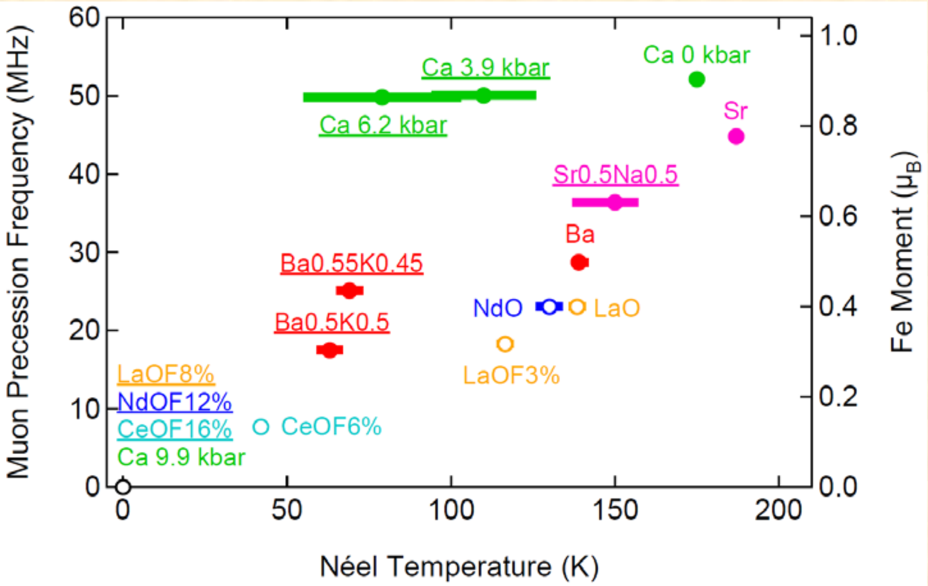
Antiferromagnetic phase of iron pnictides



5-band tight-binding model
[K. Kuroki *et al*., PRL **101**, 087004 (2008)]



Q=(π,0)
"Stripe" order



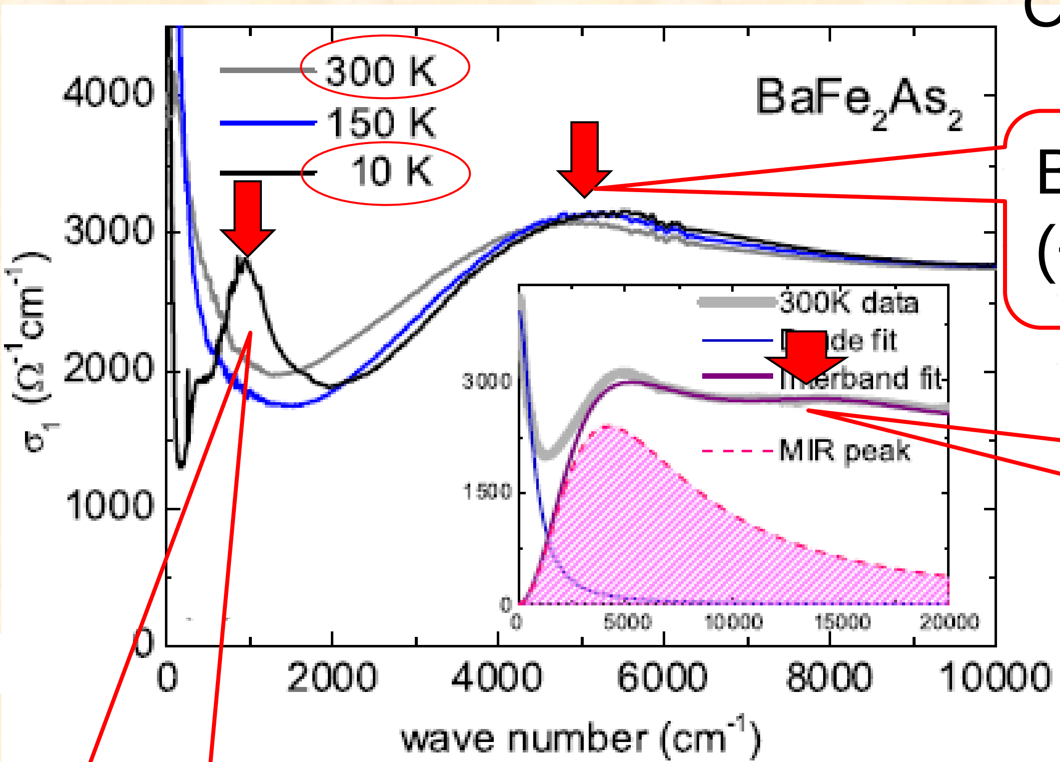
T. Goko *et al*., PRB 80, 024508 (2009); arXiv:0808.1425

spin-density wave (SDW) ?

Characteristics of optical conductivity

grey black

Compare PM and AF data



Broad excitation structure (~0.5eV) slightly shifted

Unchanged in high energies

AF gap (~0.1eV)

W. Z. Hu *et al*., PRL **10**, 257005 (2008)

Mean-field calculation of the stripe AF state

Five-band model for the Fe square lattice

$$H = H_0 + H_I$$

$$H_0 = \sum_{\mathbf{k},\mu,\nu,\sigma} \left[\sum_{\Delta} t(\Delta_x, \Delta_y; \mu, \nu) \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\Delta} + \epsilon_\mu \delta_{\mu,\nu} \right] c^\dagger_{\mathbf{k}\mu\sigma} c_{\mathbf{k}\nu\sigma}$$

K. Kuroki *et al*., Phys. Rev. Lett. **101**, 087004 (2008)

$$H_I = U \sum_{i,\mu} n_{i\mu\uparrow} n_{i\mu\downarrow} + \frac{2U-5J}{4} \sum_{i,\mu\neq\nu,\sigma,\sigma'} n_{i\mu\sigma} n_{i\nu\sigma'}$$

$$+ J \sum_{i,\mu\neq\nu} (c^\dagger_{i\mu\uparrow} c_{i\nu\uparrow} c^\dagger_{i\mu\downarrow} c_{i\nu\downarrow} - \mathbf{S}_{i\mu} \cdot \mathbf{S}_{i\nu})$$

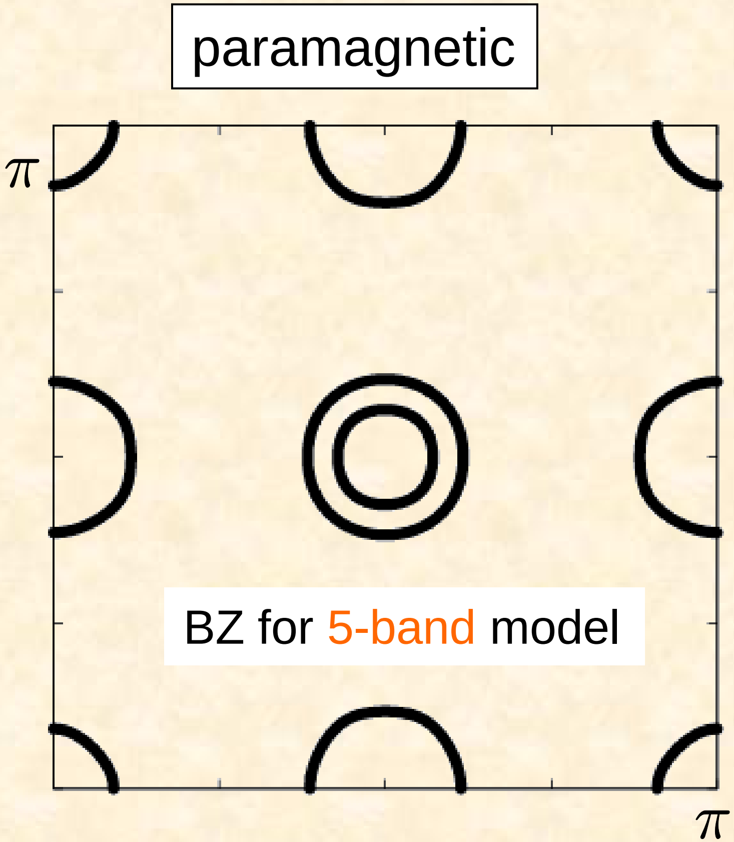
Striped AF order

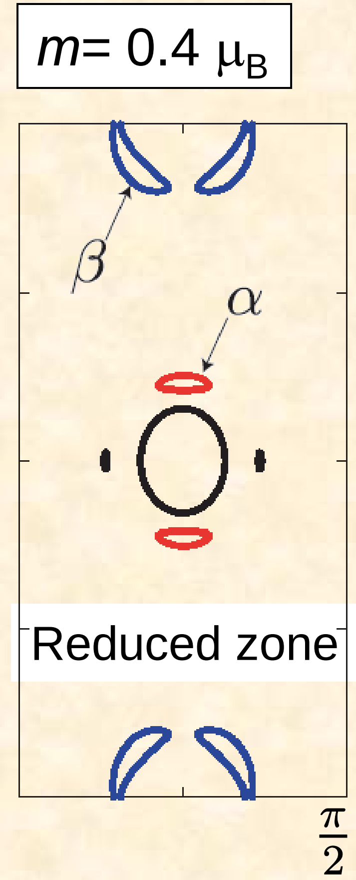
Order parameter

$$\langle n_{\mathbf{Q}\,\mu\nu\sigma} \rangle = \frac{1}{N} \sum_{\mathbf{k}} \langle c^\dagger_{\mathbf{k}+\mathbf{Q}\,\mu\sigma} c_{\mathbf{k}\,\nu\sigma} \rangle$$

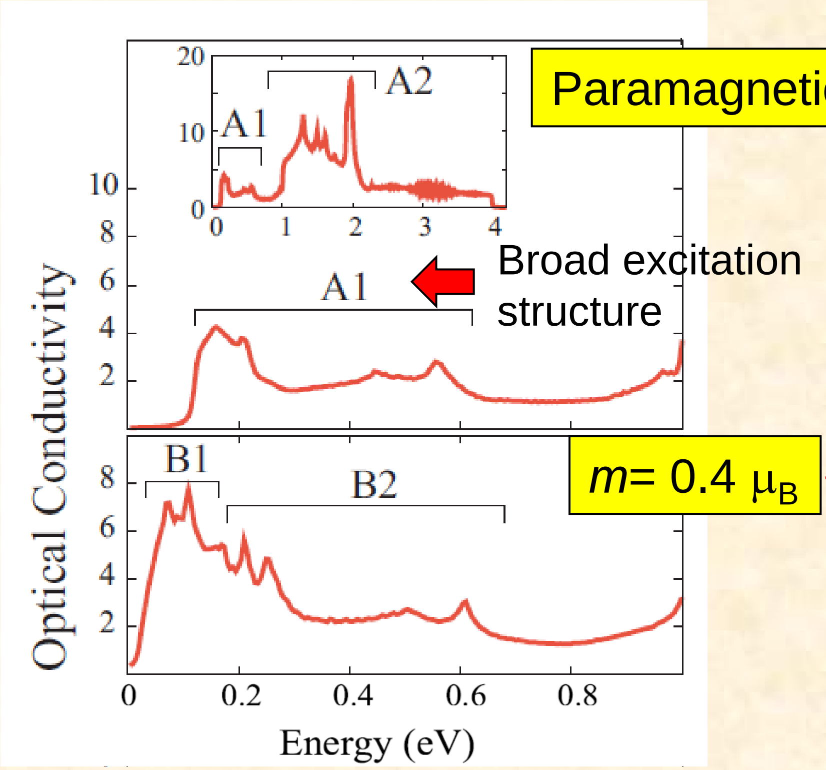
$m = 0.4\ \mu_B$

Fermi surfaces





Calculated optical conductivity (Interband transitions)



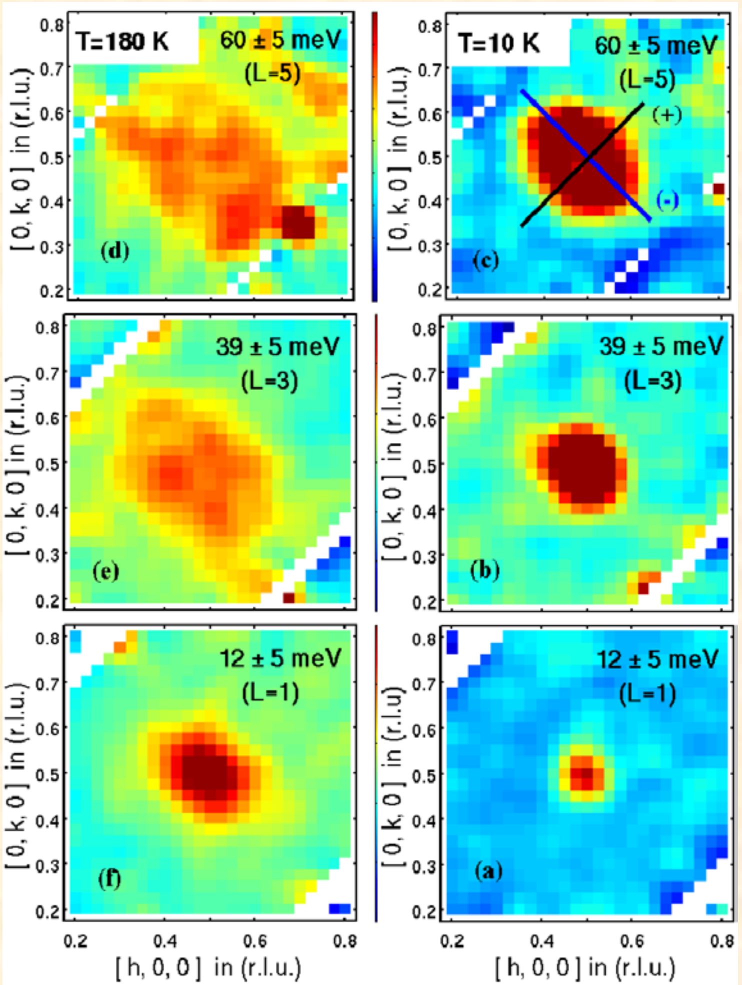
#1: SDW gap state (~0.1eV) (B1)
#2: Small shift of broad structure (A1→B2)
#3: No change in high energy > 0.5eV (Similar DOS)

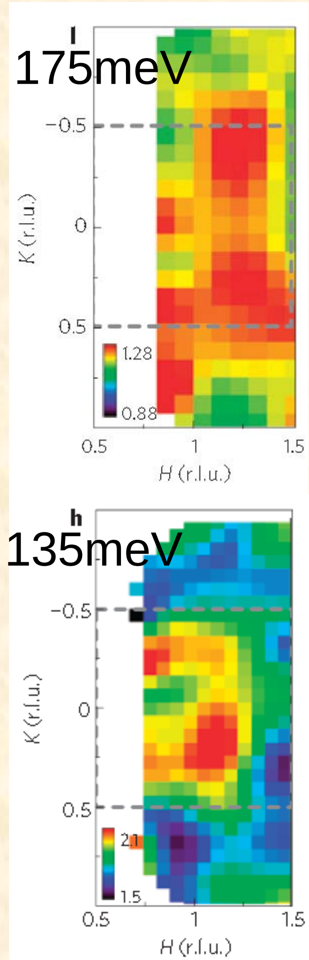
The AF state exhibits optical conductivity consistent with experiments.

E. Kaneshita, T. Morinari, T.T., PRL **103**, 224519 (2009)

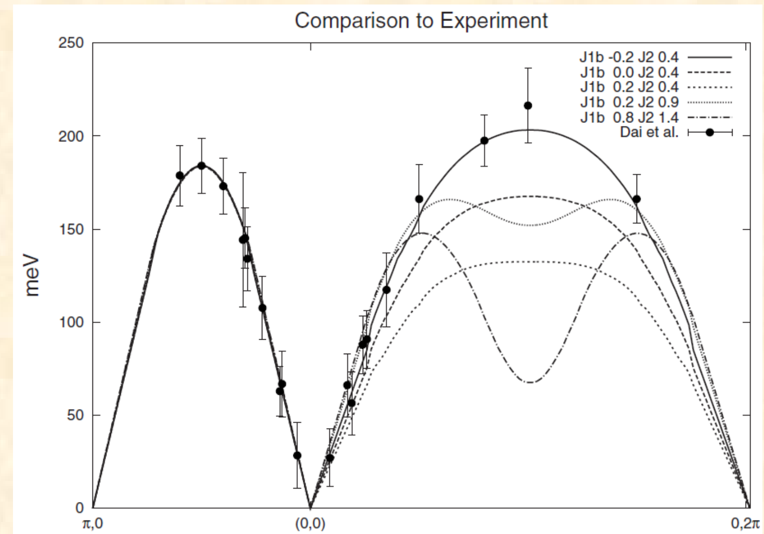
Spin excitation of $CaFe_2As_2$ Experiment

Para. AFM





dispersion



J. Zhao *et al*., Nat. Phys. **5**, 555 (2009)

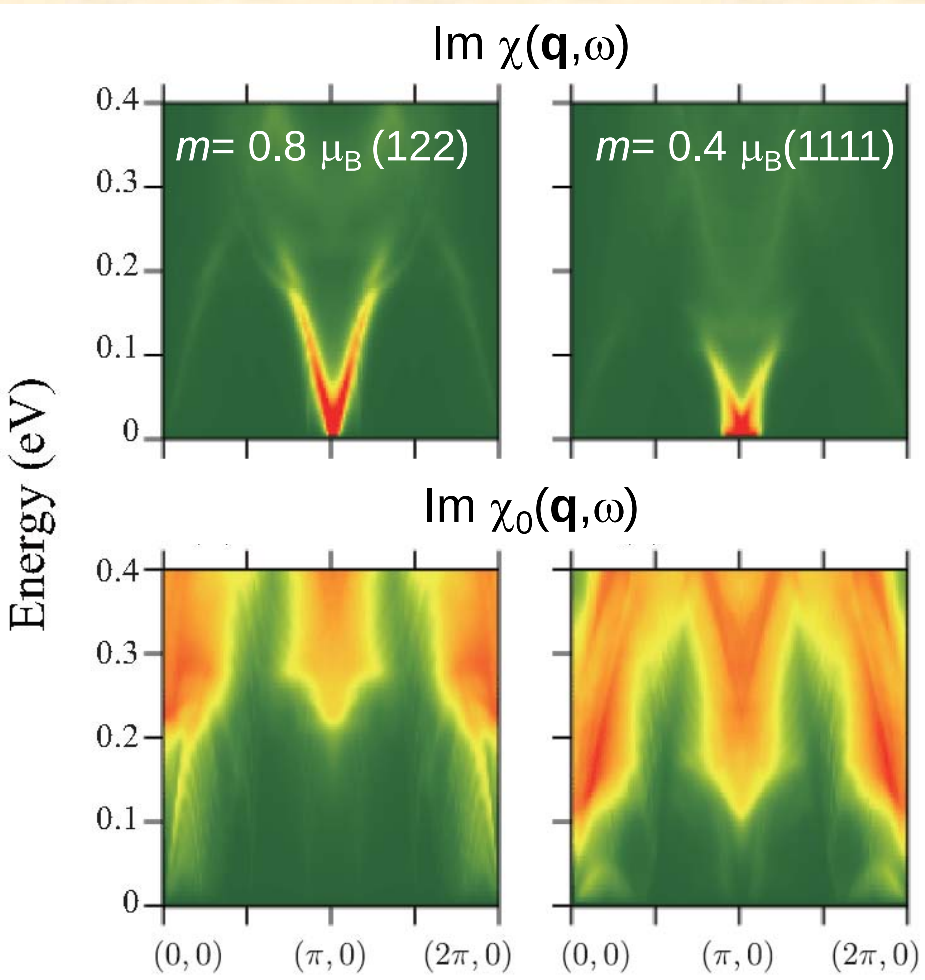
Localized spin model

C. Lester *et al*., arXiv:0912.4134

Spin excitation for AF metal Theory

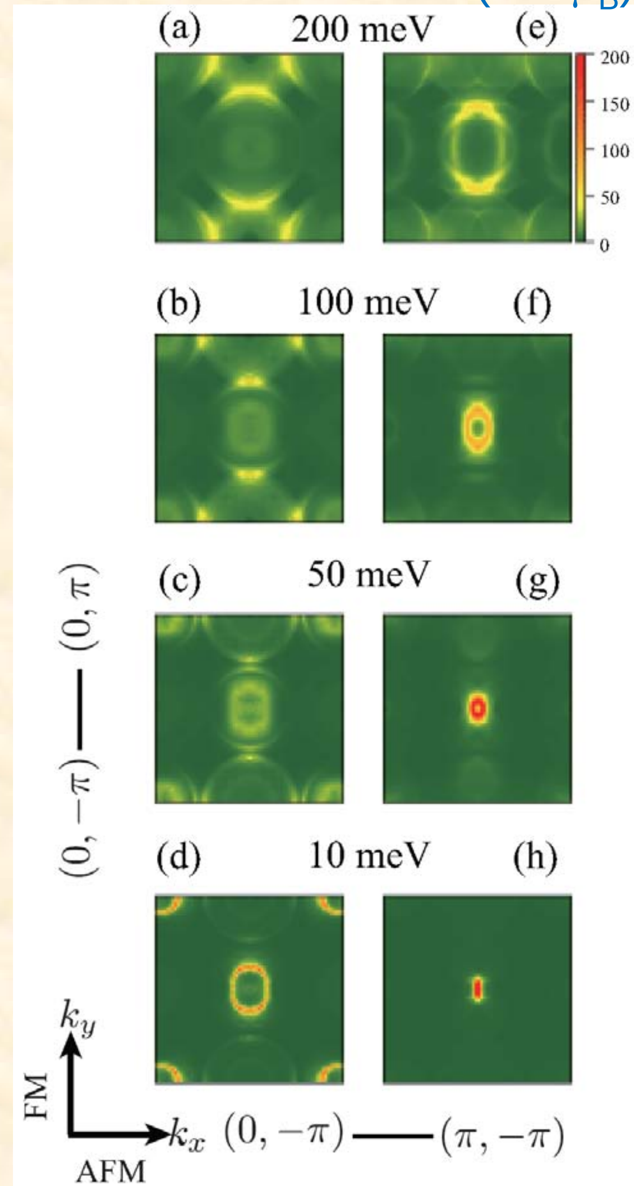
E. Kaneshita and T.T., arXiv:1002.2701

Five band + mean-field **Q**=(π,0) “Stripe”order
Random phase approximation



Im χ(**q**,ω)

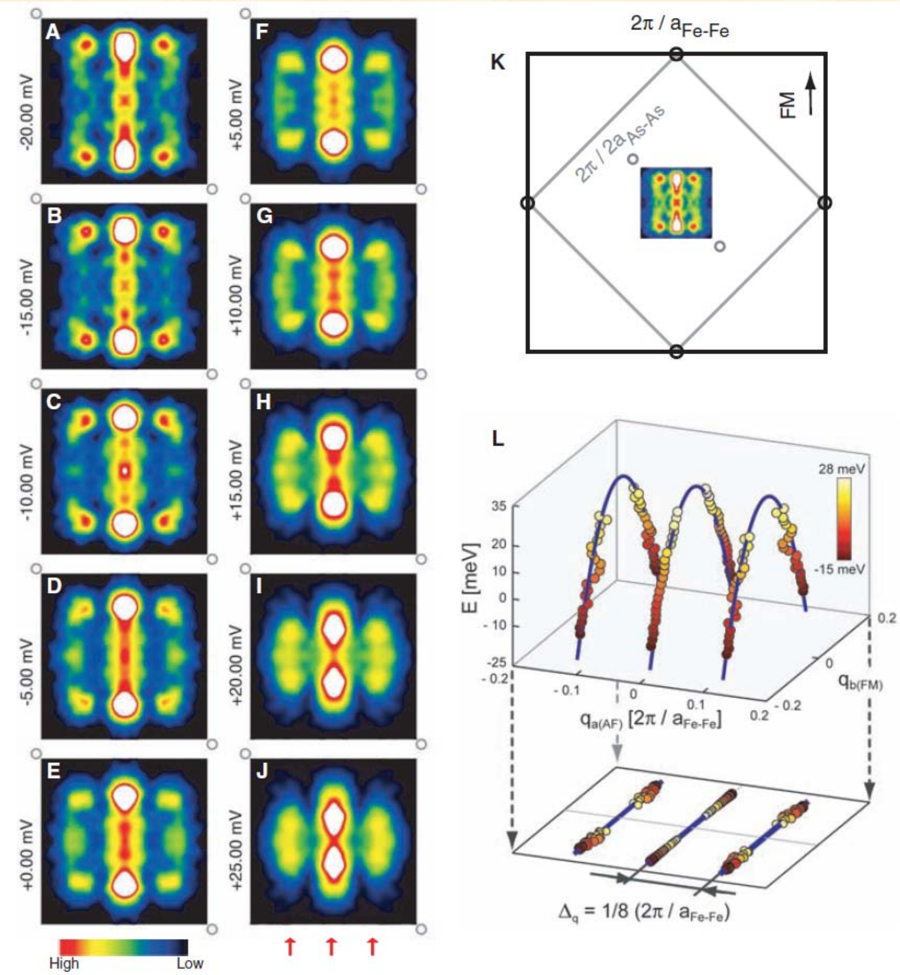
Para. AFM(0.8 μ_B)



"Nematic" electronic nanostructure seen in AF metal

STM for $CaFe_{1.94}Co_{0.06}As_2$

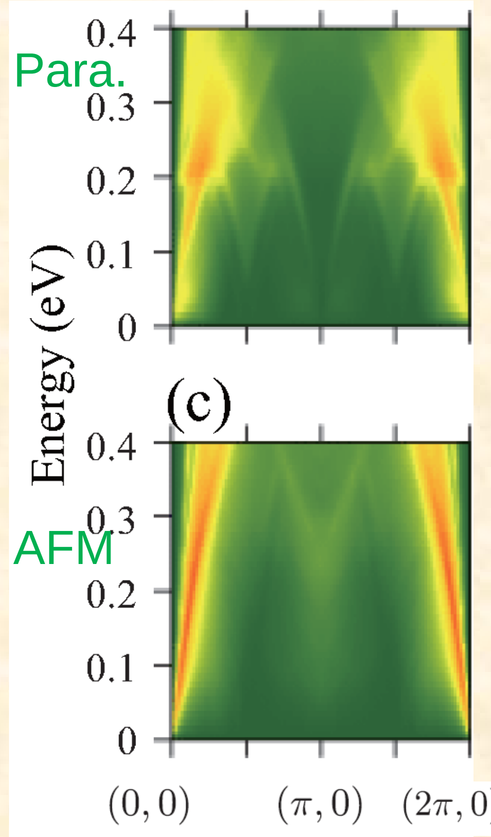
T.-M. Chuang *et al.*, Science **327**, 181 (2010)



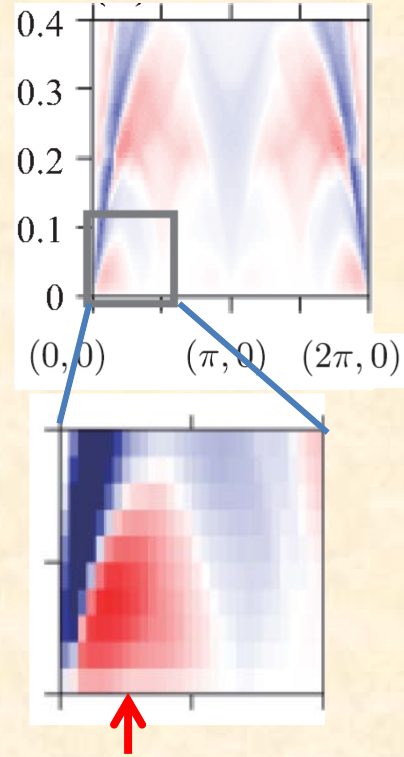
charge modulation with 8 Fe-Fe distance

Charge response function

E. Kaneshita and T.T., arXiv:1002.2701



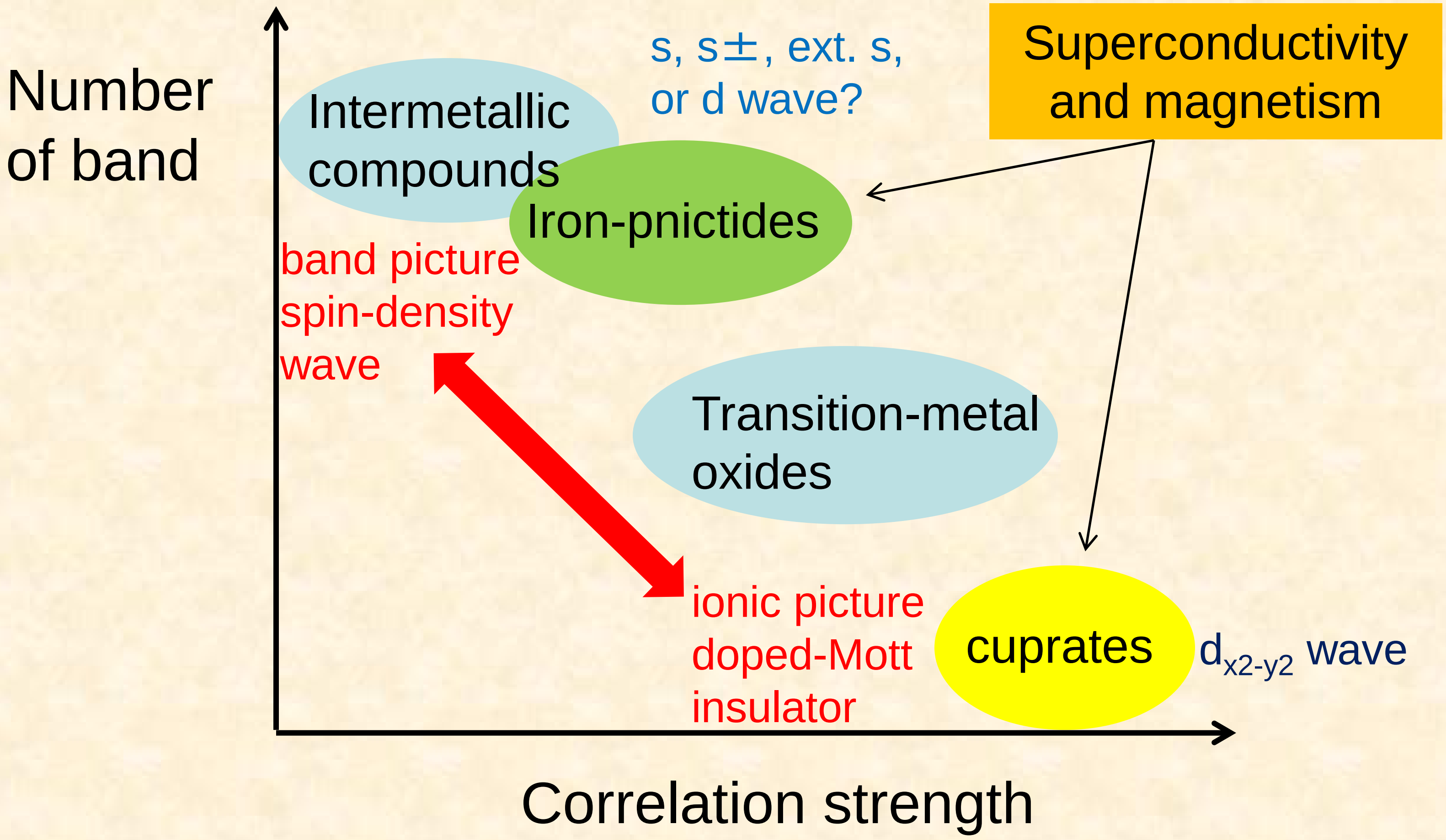
difference



q=(2π/8,0)

Charge fluctuations from residual Fermi surfaces

Summary

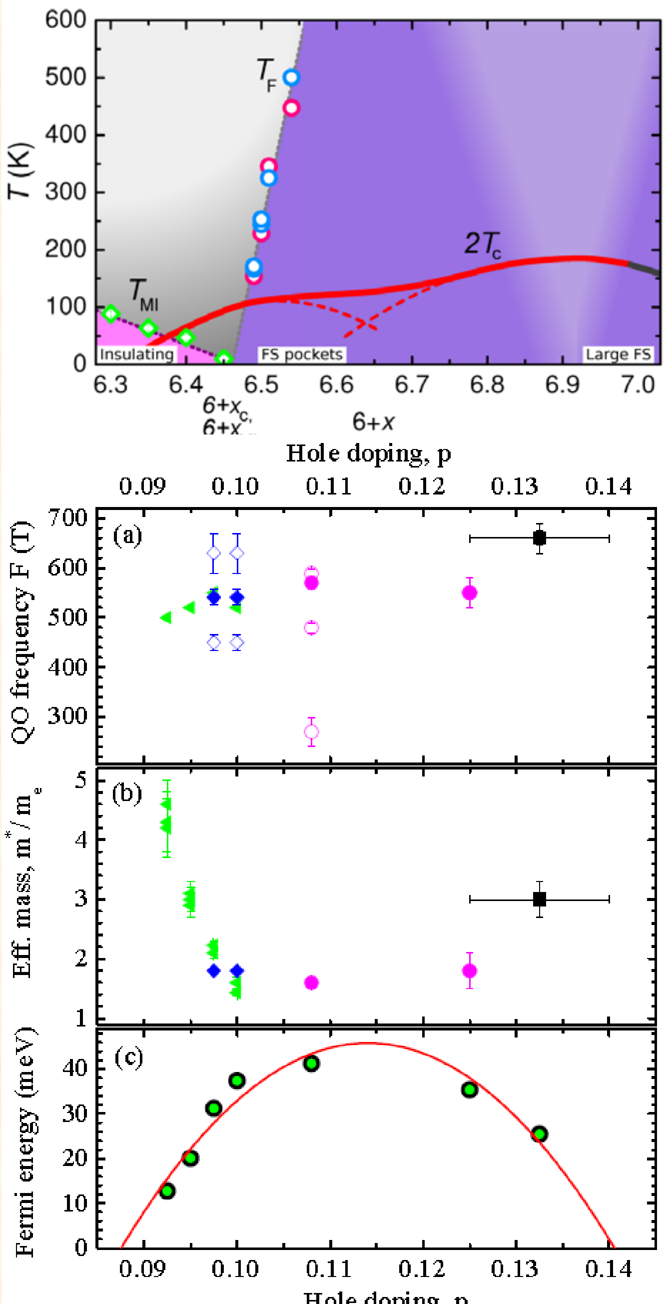


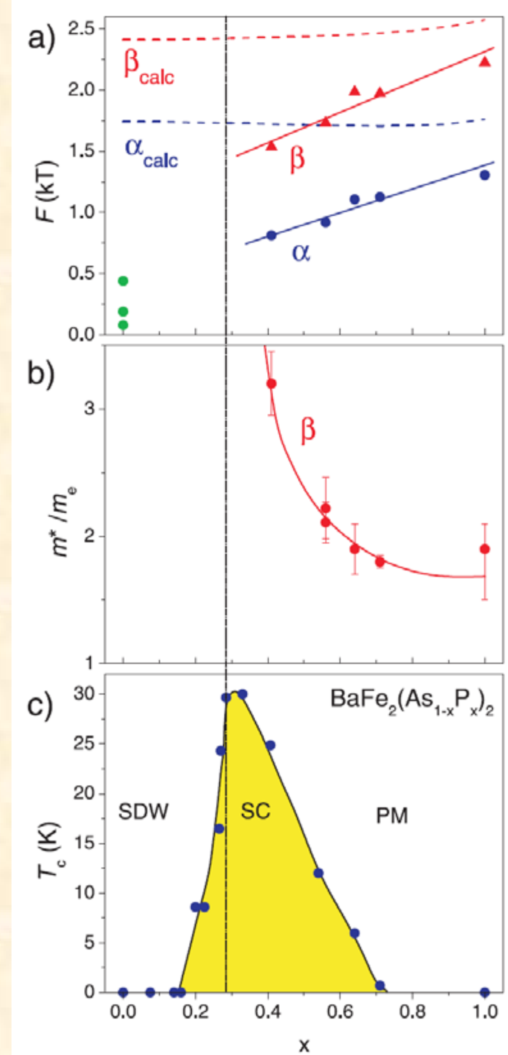
Number of band
Intermetallic compounds
s, s±, ext. s, or d wave?
Superconductivity and magnetism
Iron-pnictides
band picture spin-density wave
Transition-metal oxides
ionic picture doped-Mott insulator
cuprates
d_{x2-y2} wave
Correlation strength

$YBa_2Cu_3O_{6+x}$

Perspective: Quantum oscillations

$BaFe_2(As_{1-x}P_x)_2$





H. Shishido *et al.*, PRL **104**, 057008 (2010)

- Multiple Fermi surfaces
- Divergence of the effective mass

Similar to iron-pnictides?

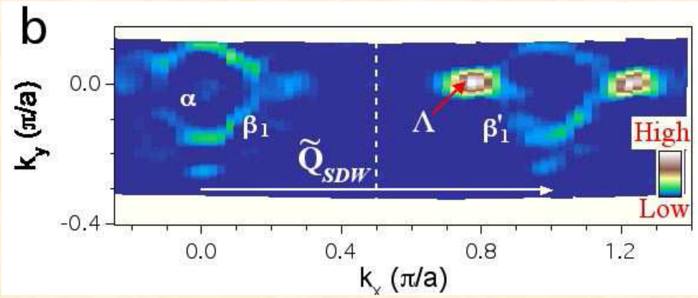
S. E. Sebastian *et al.*, arXiv:0910.2359

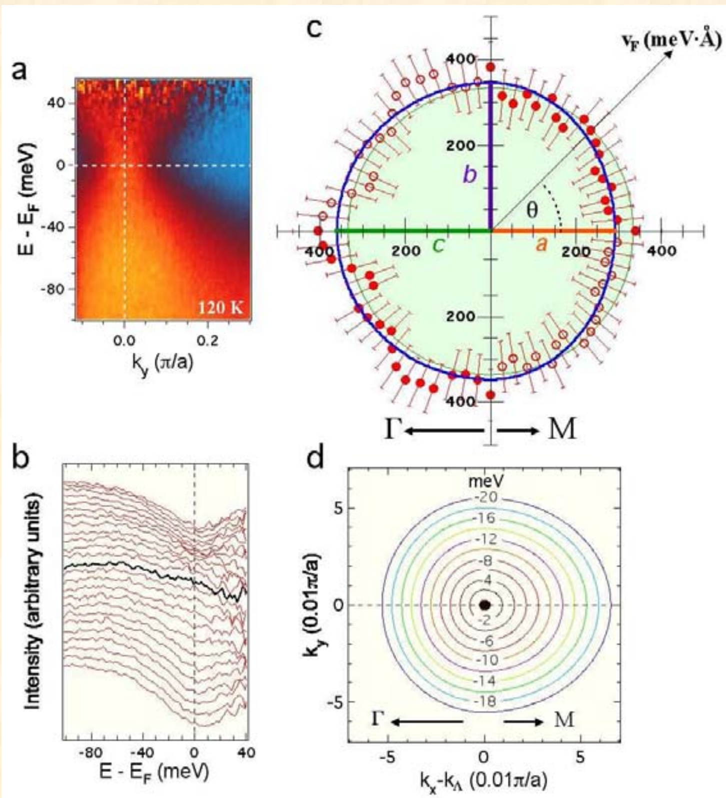
J. Singleton *et al.*, arXiv:0911.2745

Perspective for iron-pnictides

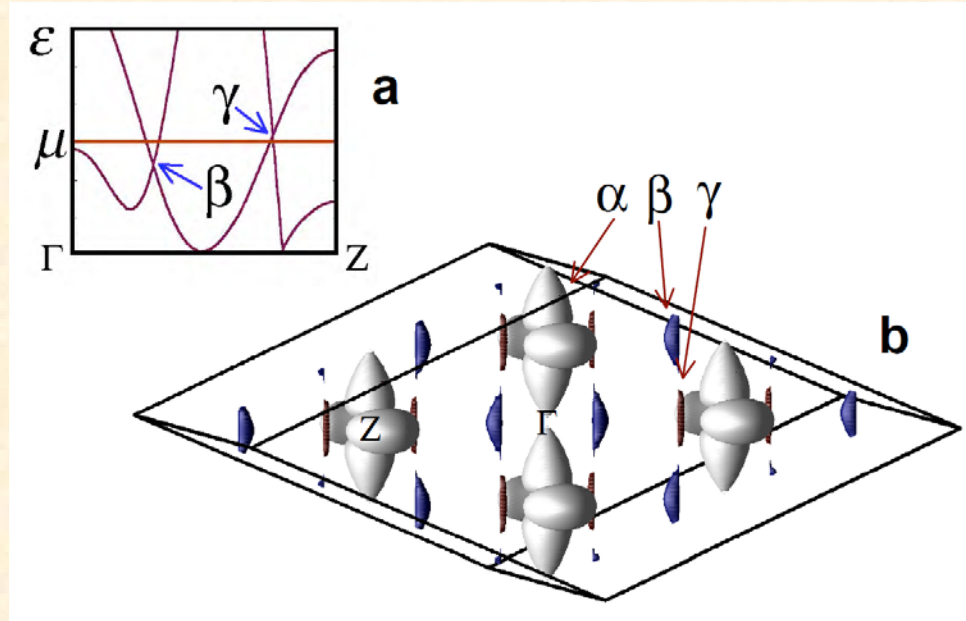
Dirac particles in band dispersions of AFM $BaFe_2As_2$

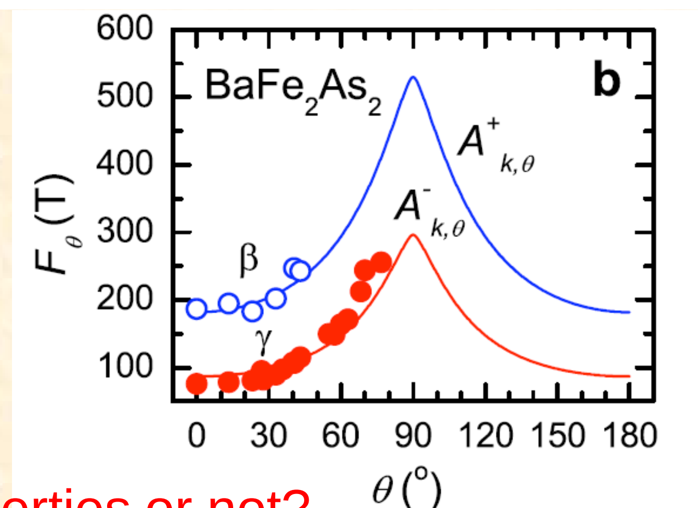
P. Richard *et al*., arXiv:0909.0574





N. Harrison and S. E. Sebastian, arXiv:0910.4199





Real effect on transport properties or not?