Magnetism, Structure and Pairing in the Iron Based High Tc Superconductors

Ashvin Vishwanath

UC Berkeley, LBNL

Ari Turner
Pouyan Ghaemi
D.H. Lee

Fa Wang
Ying Ran
Hui Zhai

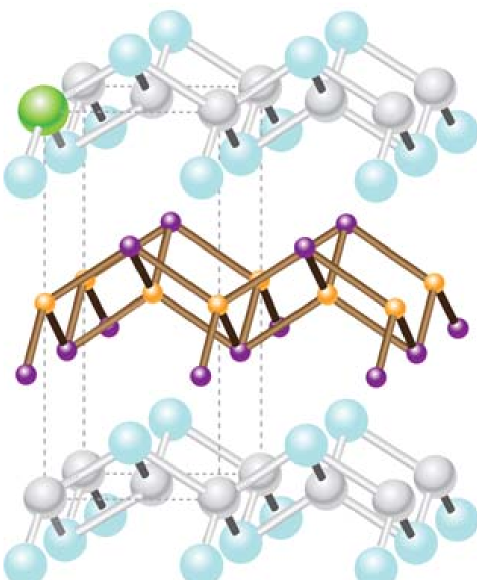
References:
Y. Ran, et al. PRB, 79, 014505 (2009)
Ari Turner, F. Wang, AV; arXiv: 0905.3782
P. Ghaemi, F. Wang AV PRL 102, 157002 (2009)

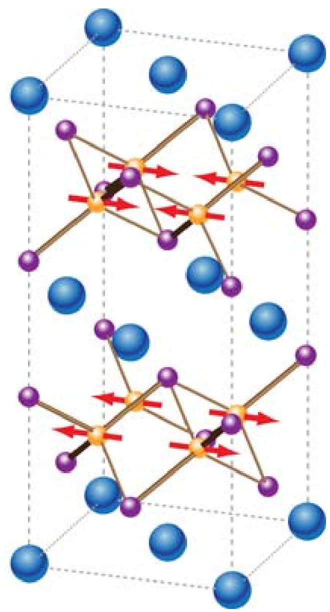
J|A|C|S
COMMUNICATIONS

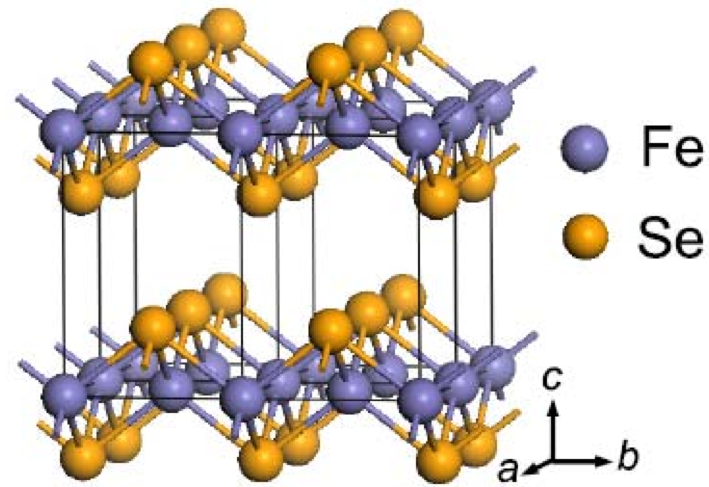
Published on Web 02/23/2008

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

Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§





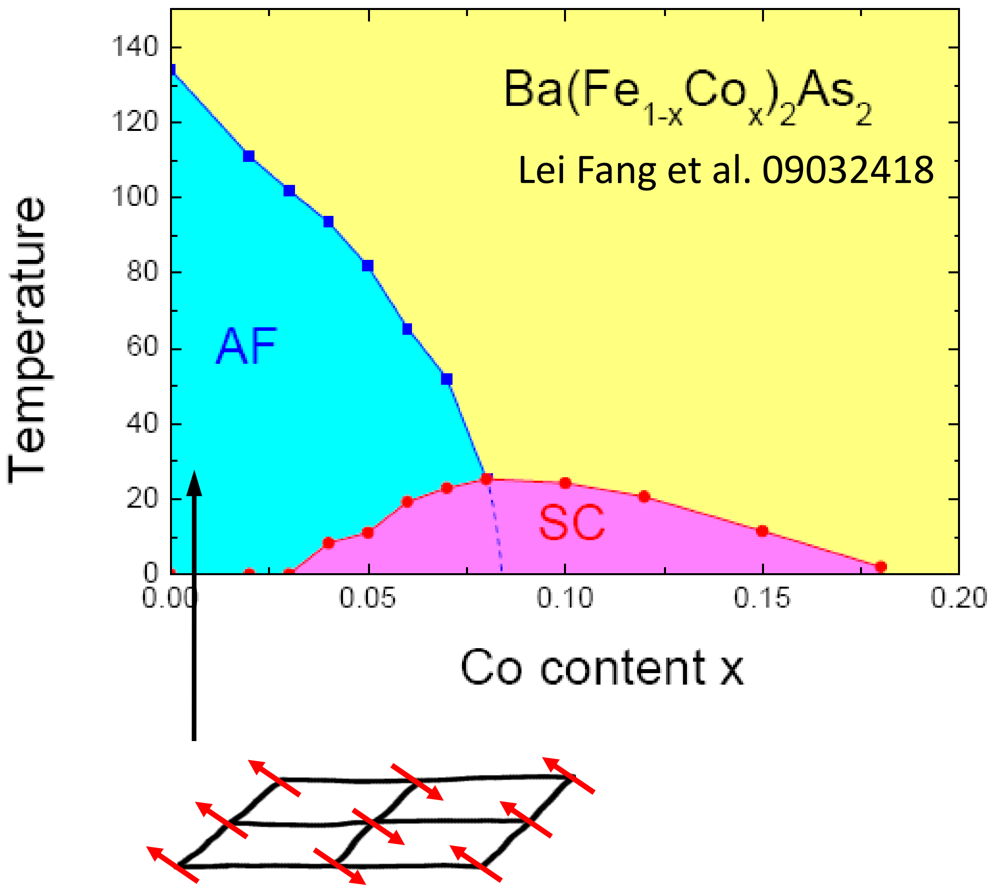


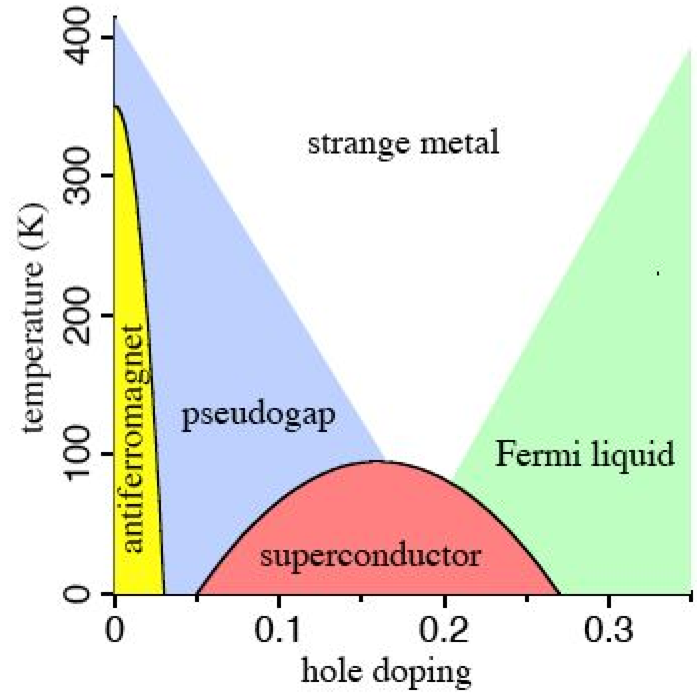
LaOFe$As_{1-x}F_x$ [1111]
Tc=56K in Sm compound.
No copper

BaFe_2As_2 (more 3D) [122]
Tc=38K in with K doping
No oxygen

FeTe/FeSe – superconductor
Tc=8K; =27K under 2GPa
No pnictide

Comparison with Cuprates

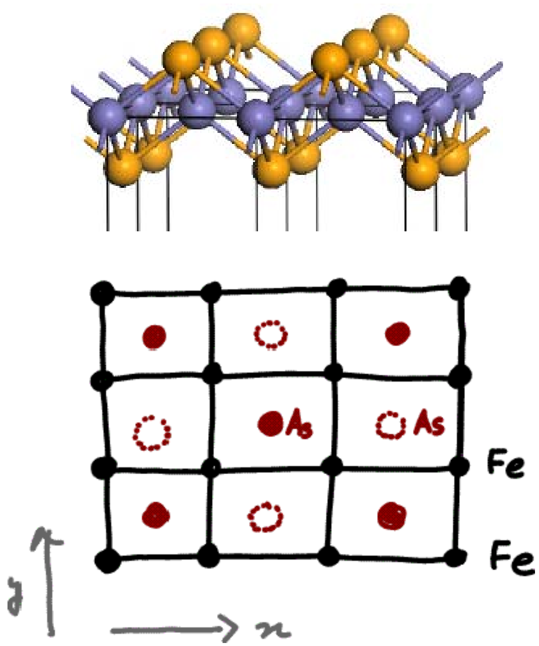


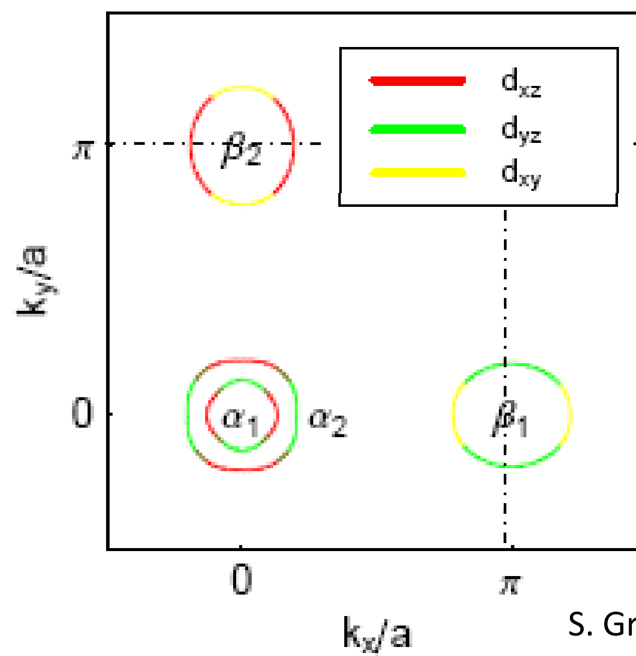


1. Undoped state is a **metallic** magnet. **Multi orbital system**.
2. **Structural Distortion** – connection to magnetism?
3. Pairing symmetry

LDA Band Structures

- Effective 2D tight binding model: all 5 d-orbitals.
- Fermi surface in xtended zone (2 hole pockets at Γ, electron pockets on BZ edge) composed of d orbitals. Nested for (π,0) SDW.





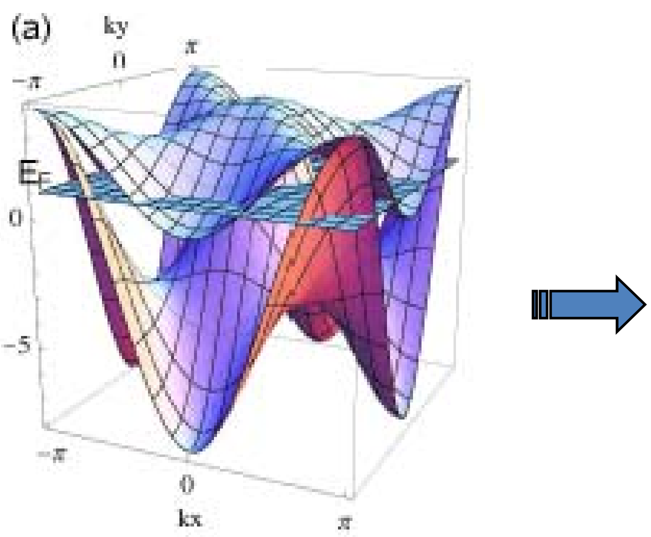
S. Graser et al.

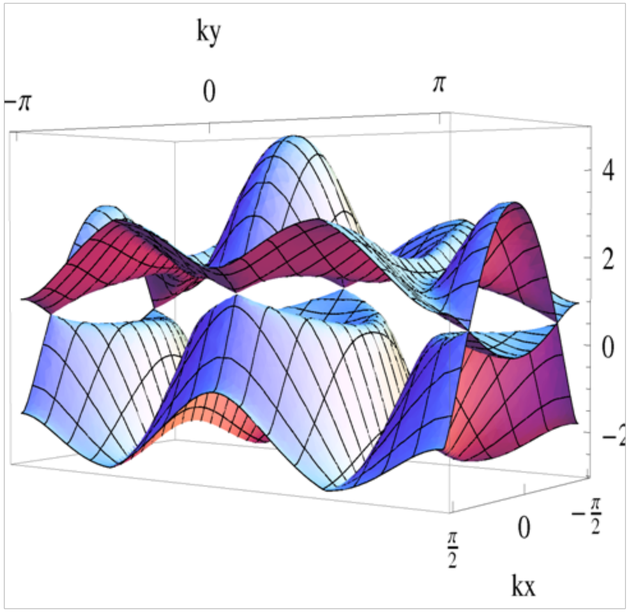
Popular 2-band model, (d_{yz} and d_{xz}) has a hole pocket at wrong position.

‘Nodal’ Spin Density Wave

Multi-orbital nature –consequences for SDW.

- Simplified Two Band Model – d_{xz} and d_{yz} orbitals
- At x=0, perfect electron-hole nesting at [π,0] if $t'_1=0$. Expect *fully gapped* SDW.





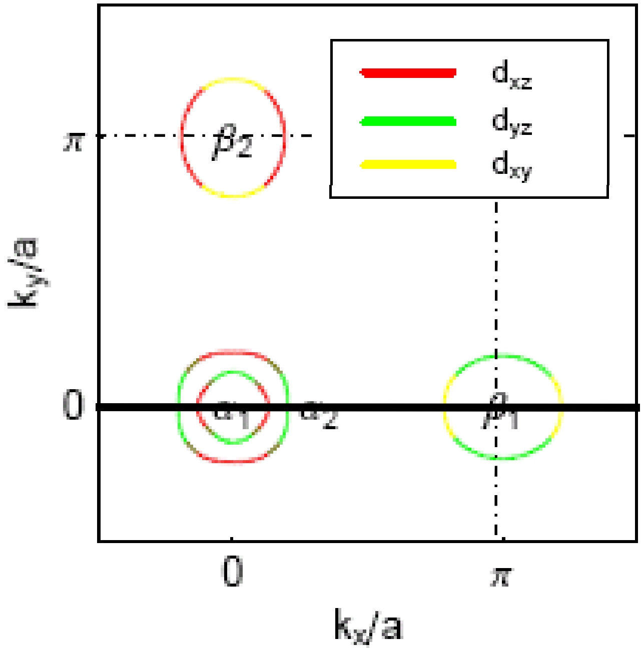
But – Anisotropic gap with Dirac points instead.

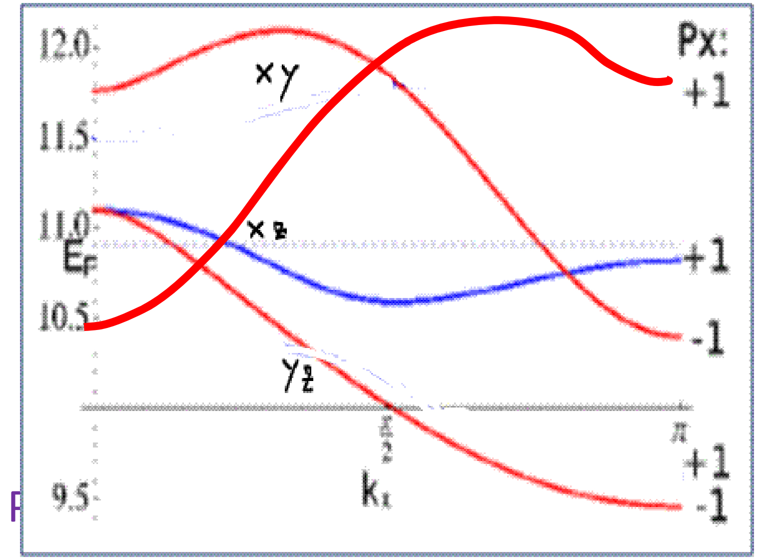
Y. Ran, et al. PRB, 79, 014505 (2009)

Nodal SDW in FeAs

- More realistic band structure: 5 band tight binding model with LDA parameters.
  - `Nodal' SDW:

Weak coupling picture: utilize reflection symmetry:

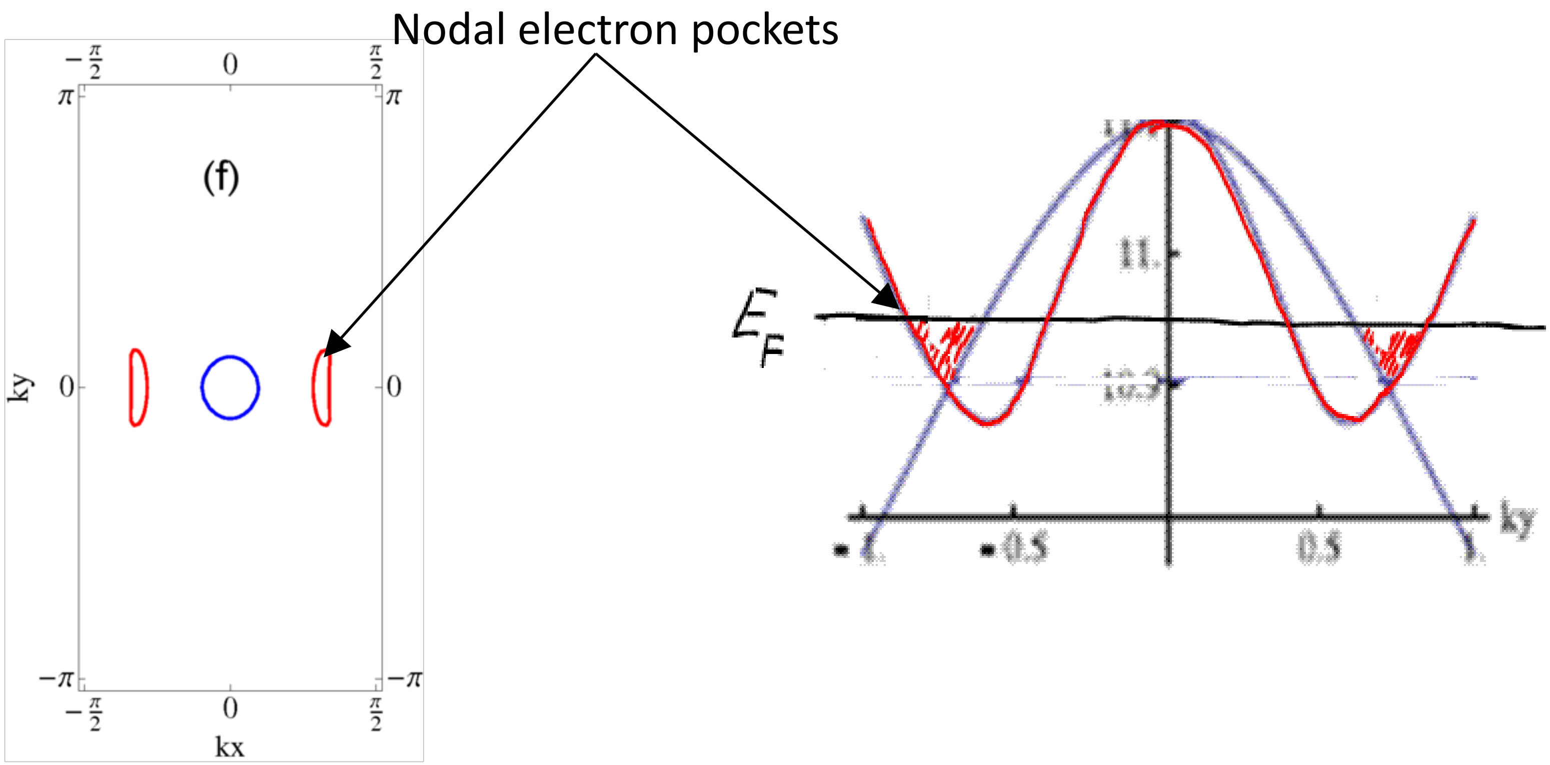




Y. Ran, et al. PRB, 79, 014505 (2009)

Nodal SDW in FeAs

- 5 band tight binding model with LDA parameters.
  - `Nodal' SDW: electron pockets with nodal dispersion in SDW along high symmetry axis. Metallic even at large U.



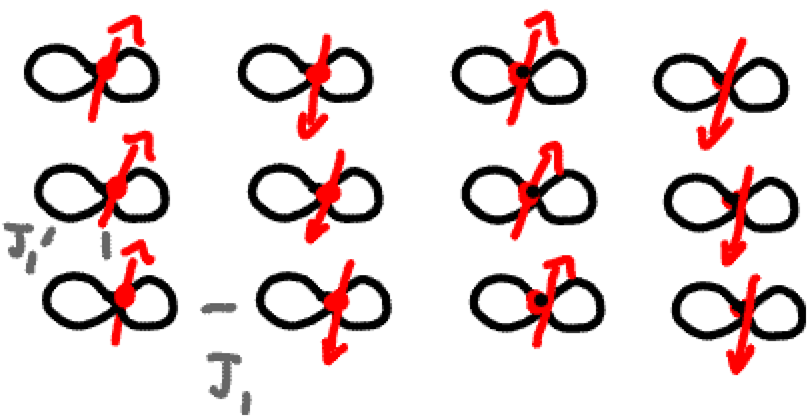
U=1.6eV; $\langle \mathbf{S} \rangle = 2.3\mu_\mathbf{B}$

Y. Ran, et al. PRB, 79, 014505 (2009)

(consistent with LDA calculations: Kuroki et al., Yin et al. And quantum oscillation measurements Sebastian et al.)

Orbital order in FeAs?

- A different theory of magnetic order and structural transition: (Kruger et al., Philips et al., R. Singh)
  - Assume structural transition driven by orbital ordering.
  - Structure drives magnetism.
  - More natural explanation for spin wave spectrum (R.Singh)

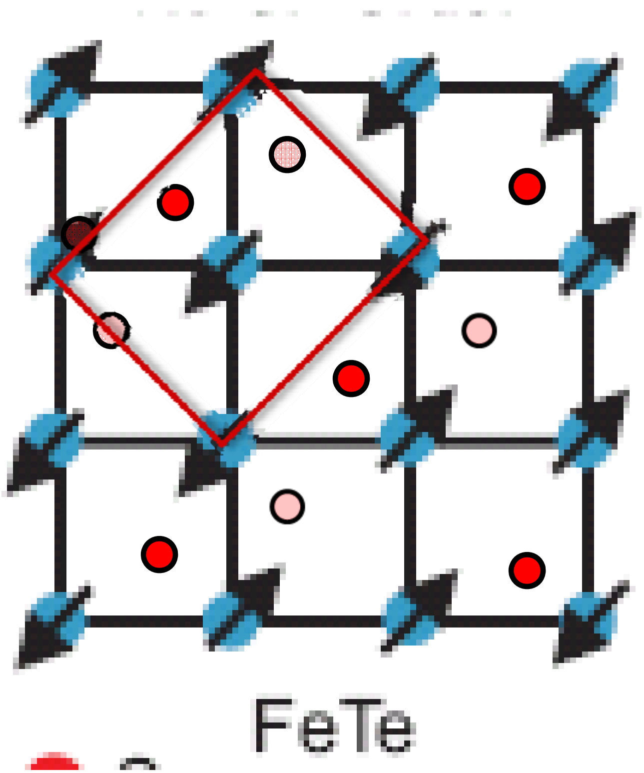


BUT:

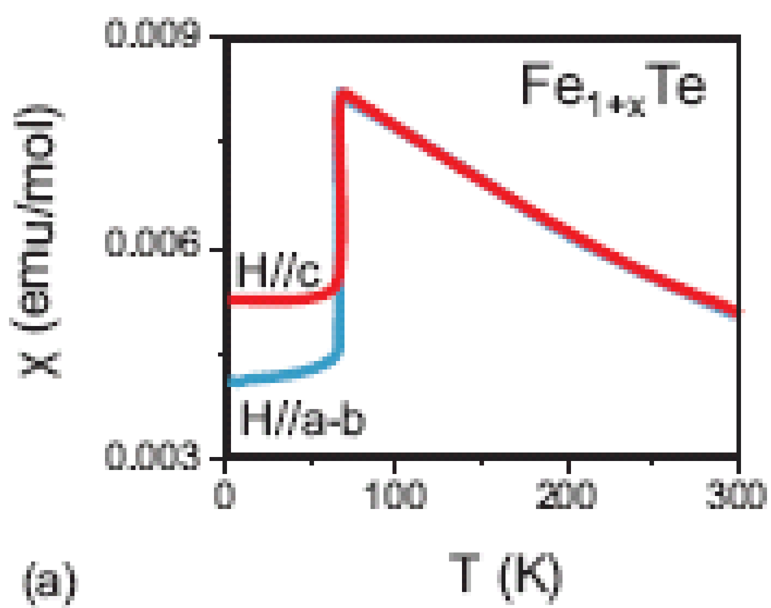
1. Not clear if a local electronic picture is valid for FeAs
2. Competing explanation – SDW order even in weak coupling from nesting.

Orbital order in FeTe

- Novel magnetism in FeTe. (same structure and Fe electron count as FeAs layers. Same Fermi surface predicted.)
  - Different wave-vector: (π/2, π/2). Monoclinic distortion



W. Bao et al, arXiv:0809.2058



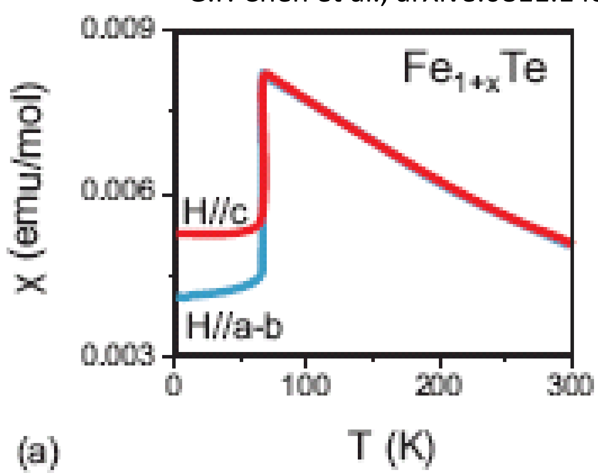
First order magnetic –structural transition at T~ 80K

FeTe - a strongly correlated system?

- Unusual wavevector [no nesting (Hasan et al.)]
  - {recent LDA based explanations Johannes &Mazin, Savrasov et al.}

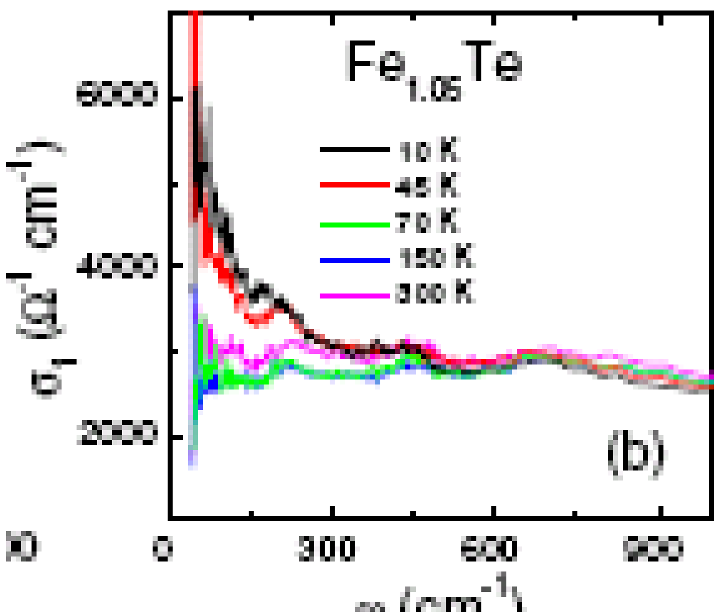
FeTe	FeAs
1. Large ordered moment (~2.0μ_B)	0.3μ_B in LaOFeAs
2. Curie Weiss type susceptibility	2. non-Curie Weiss

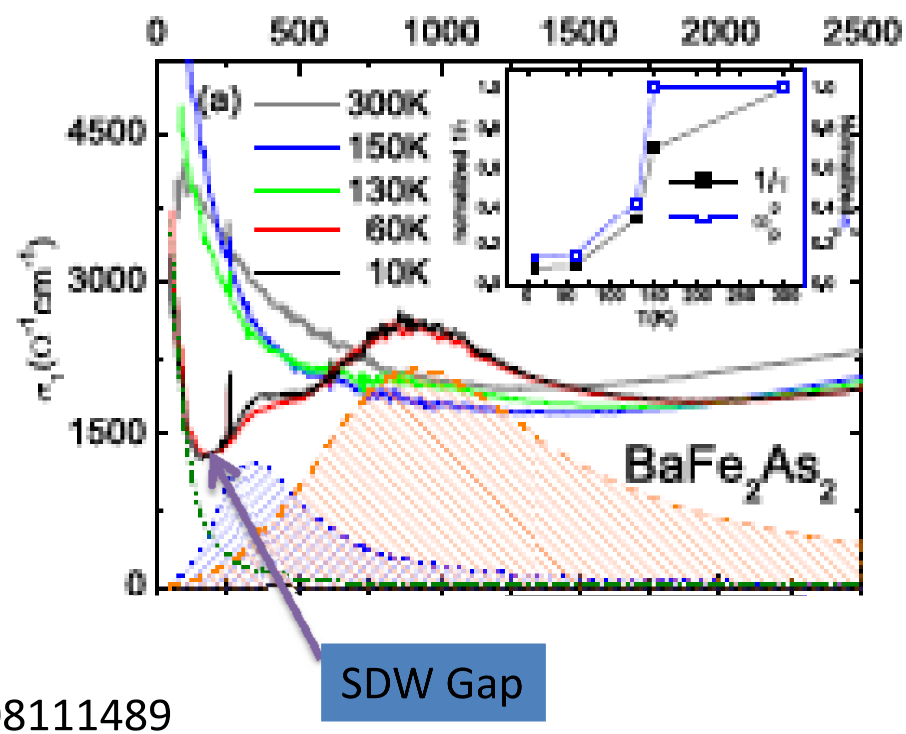
G.F. Chen et al., arXive:0811.1489



FeTe as a strongly correlated system

3. No sign of SDW gap in optical conductivity. Drastic change in longitudinal, Hall conductivity.

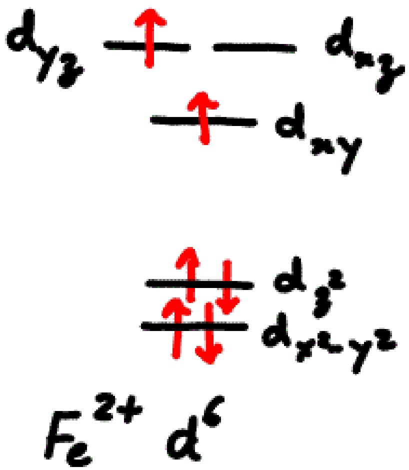


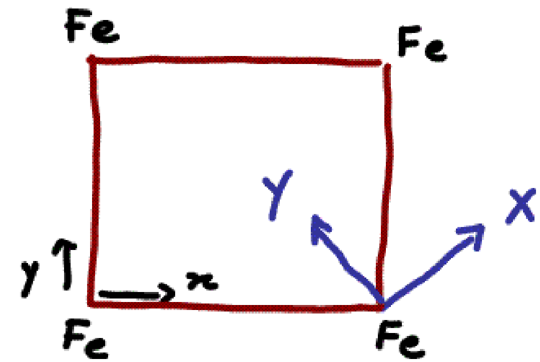


Chen et al. arxiv:08111489

Assumptions: Microscopic Model

- Assume "close" to a S=1 insulator with orbital degeneracy. (metallic due to small density of electrons/holes).





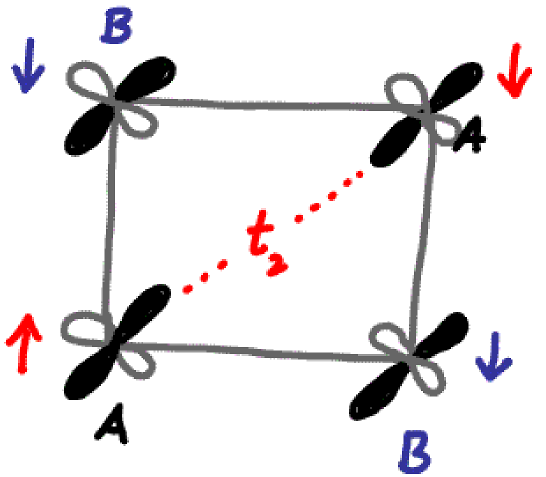
Example: Consistent with the (elongated) tetrahedral coordination of FeTe

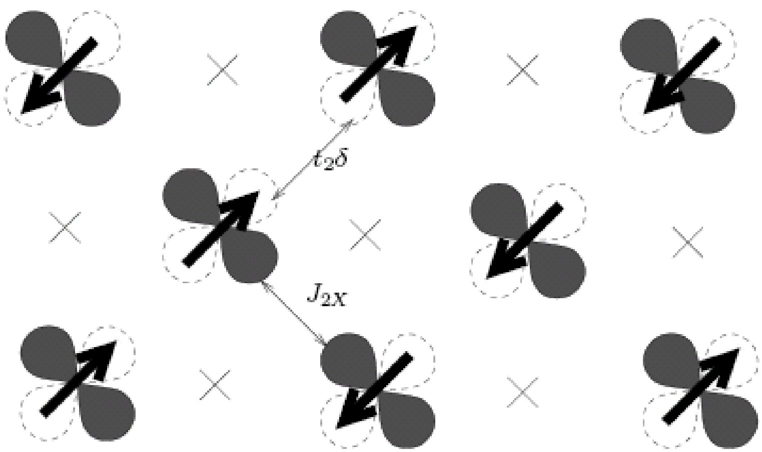
- Orbital degeneracy resolved by Jahn Teller effect. *Assume*, ordering along the diagonals.

Ari Turner, F. Wang, AV; arXiv: 0905.3782

Magnetism From Orbital Order

- Dominant hopping t_2 (along diagonals).
- Generates AF Exchange along orbital order.
- Small excess density of electrons generates ferromagnetic super-exchange perp.





Leads to wave-vector (π/2, π/2) on each sublattice

Ortho-rhombic lattice distortion attributed to orbital order

for coupling sublattices and doping induced incommensuration see: **Ari Turner, F. Wang, AV; arXiv: 0905.3782**

Coupling the sublattices

- Sublattices coupled antiferromagnetically (J1).
  - Need spin-phonon coupling for commensurate order to lock in.

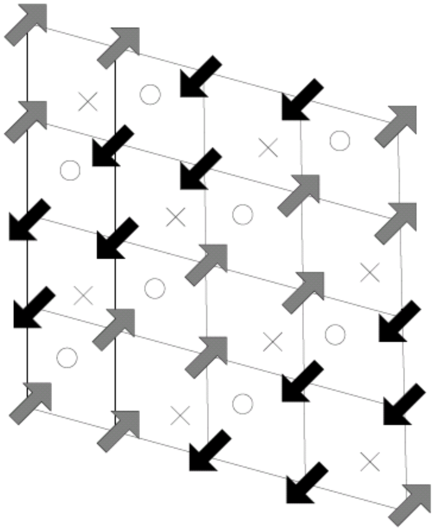
$$J_{2X} = t_2^2/U$$
$$J_{2Y} = -2|t_2|\delta$$
$$J_1 > 0$$

$$H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - K \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2$$

Relatively small K $K \gtrsim J_1^2 / J_{2X}$

= commensurate, colinear state.

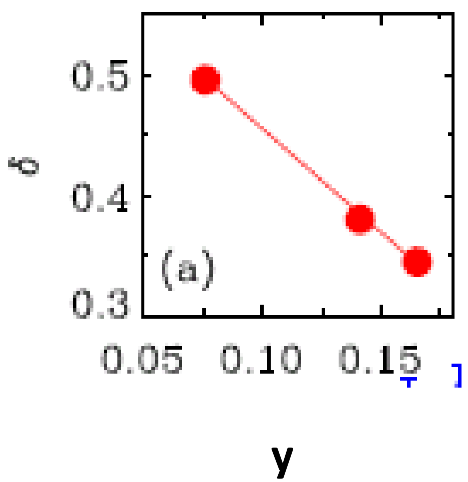
: (π/2, π/2)

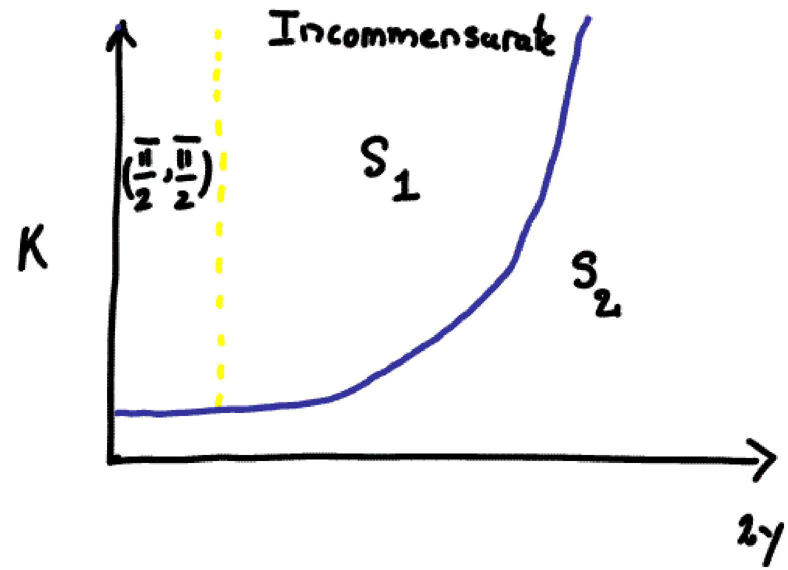


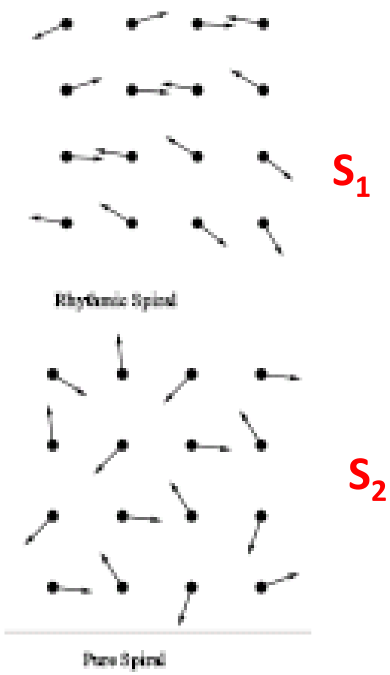
Ari Turner, F. Wang, AV; arXiv: 0905.3782

Incommensuration from Doping

- Experimentally, excess iron: $Fe_{1+y}Te$. Wavevector : : $\pi(\delta, \delta)$ $[\delta \sim y]$





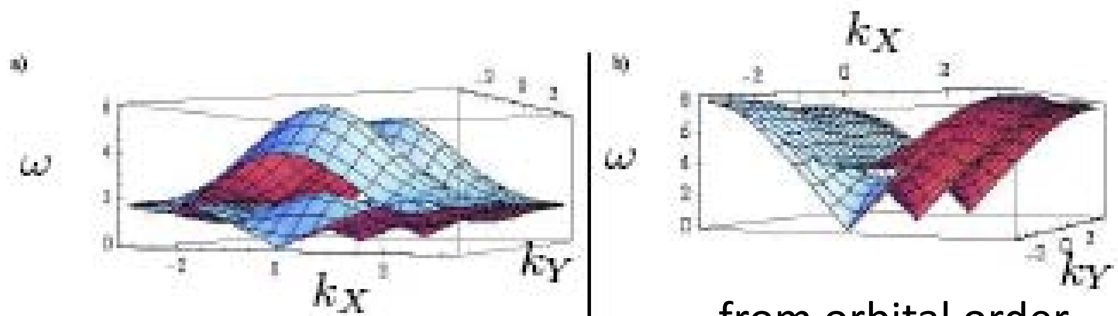


Excess iron -> electron doping.
Leads to incommensuration from Kinetic energy.
Wave-vector proportional to doping .

Ari Turner, F. Wang, AV; arXiv: 0905.3782

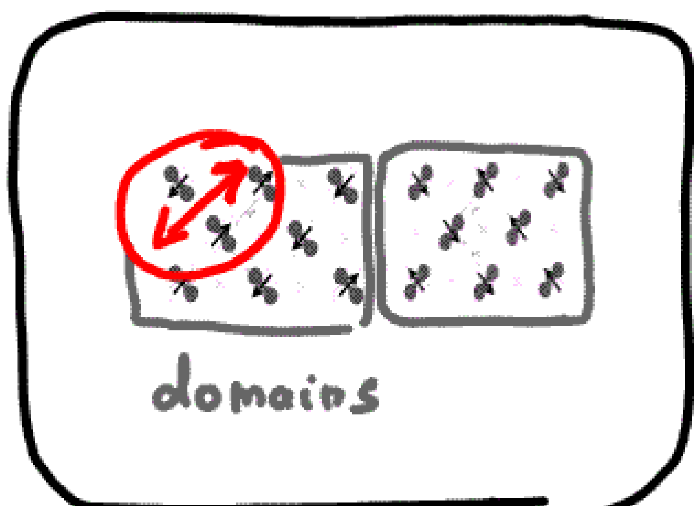
Predictions for experiments

- Spin wave spectrum:



J1-J2-J3 model | from orbital order

- Orbital order: resonant X-rays
- Strongly anisotropic conductivity:
  - Optical conductivity on single domains. Large conductivity along ferromagnetic diagonals
  - Quasi 1D features in ARPES.



Ari Turner, F. Wang, AV; arXive: 0905.3782

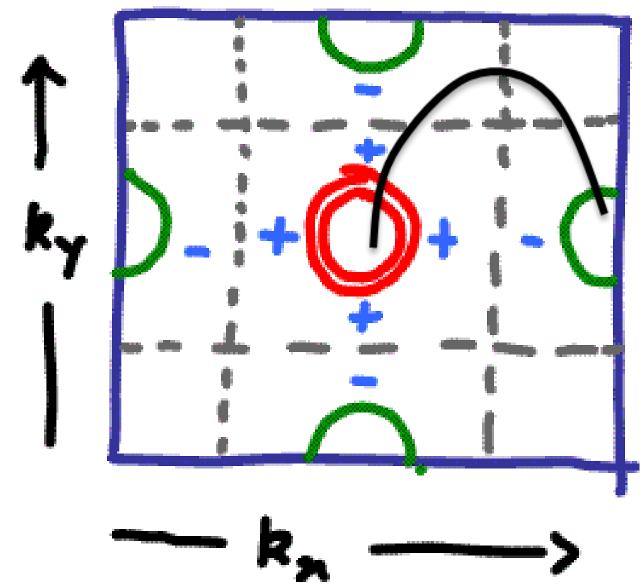
Superconductivity

- Probably non-phononic in origin.
- Many theories predict a spin-singlet extended s-wave ($s_{\pm}$) symmetry, that can be fully gapped.
- Near nesting of electron-hole Fermi pockets believed to be important.

RPA:
Mazin et. al., Kuroki et al., Scalapino et al.

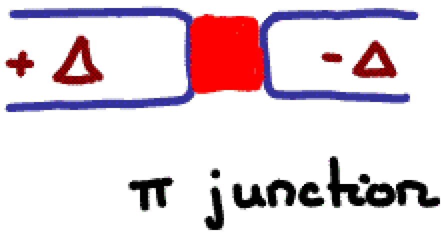
Renormalization Group:
Numerical (FNRG):
F. Wang et al. arXiv:080305.3535; PRL 102, 47005 (2009).
Analytical RG:
A. Chubukov et al.

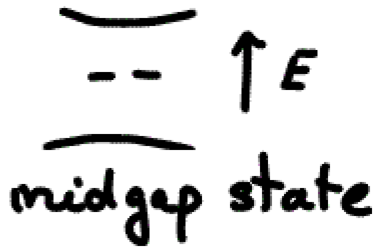
Strong Coupling Treatment:
Seo, Bernevig, Hu

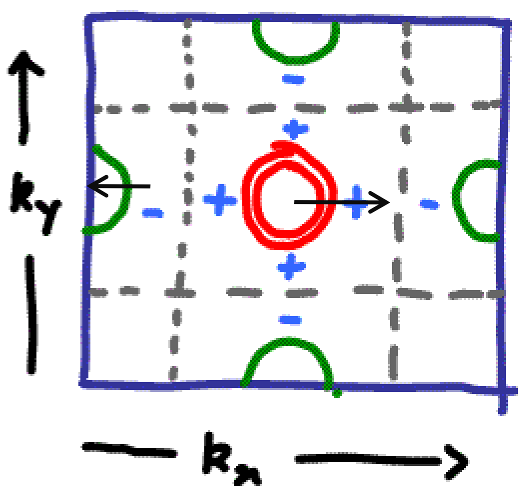


Phase sensitive measurement?

Surface Andreev Bound States

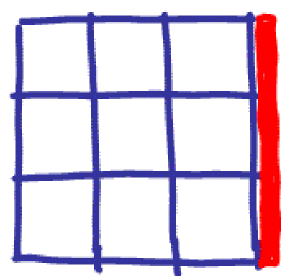


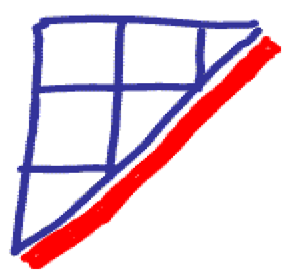




Pouyan Ghaemi, Fa Wang, AV
PRL 102, 157002 (2009)

(100) edge

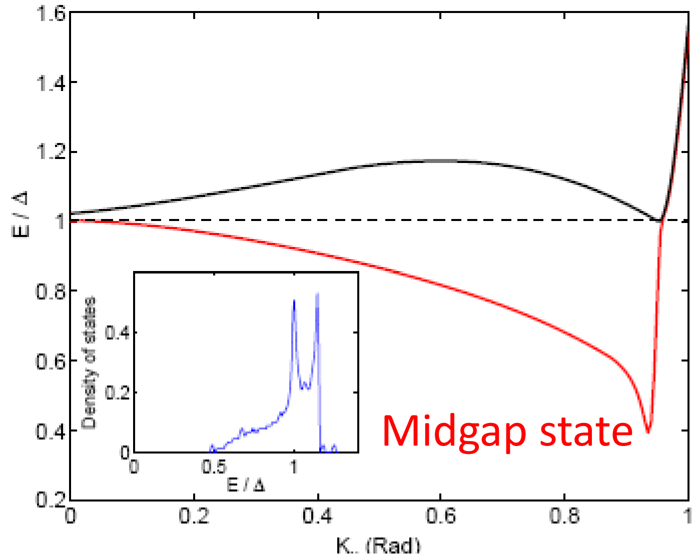




diagonal edge

- Low energy states expected at the edge for certain boundary orientations.
- Midgap states expected for 100 edge, but not for diagonal.
- Complicated by multi-orbital nature.

Surface Andreev Bound States

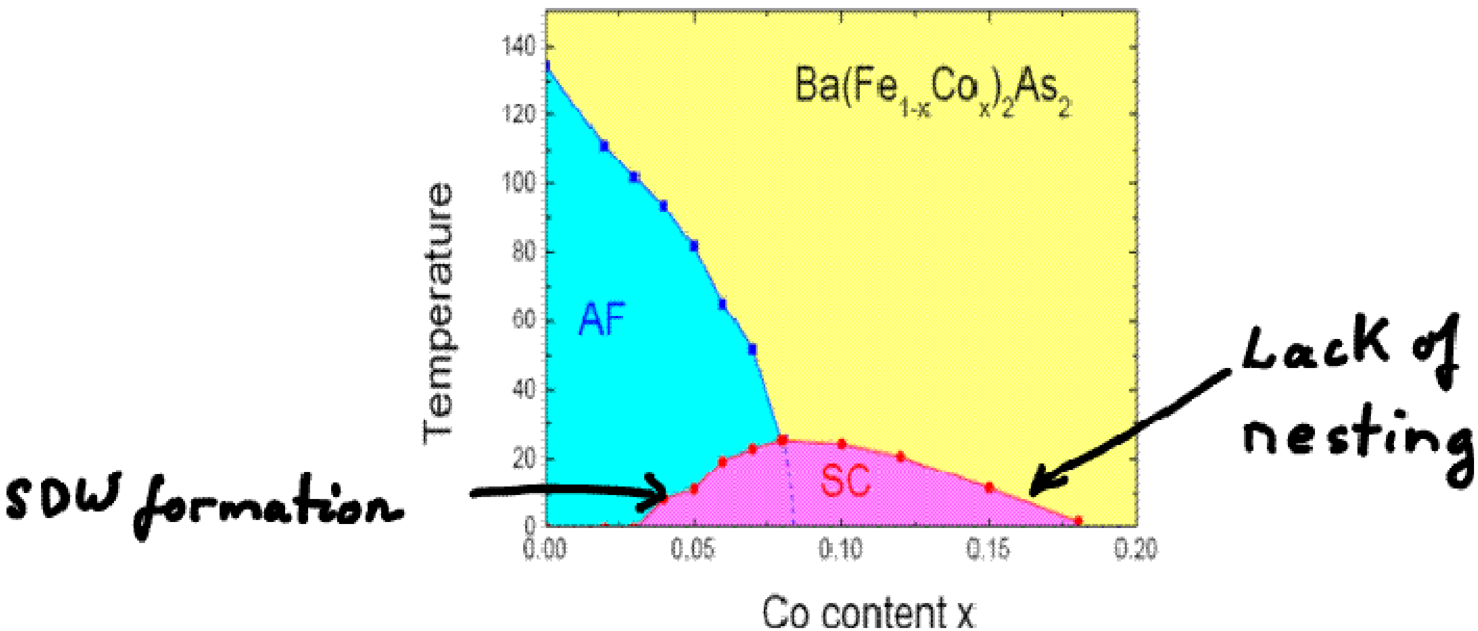


- Midgap states for (100) edge but not (110).
- Only occurs with $s_{\pm}$
- Not at zero energy. Accessible to tunneling measurements.

Pouyan Ghaemi, Fa Wang, AV
PRL 102, 157002 (2009) (among many others refs…)

Chairman's Question: How to raise T_c?

- What destroys superconductivity?



- Frustrate magnetic order (and structural transition) – good nesting but no SDW, leads to higher Tc?
  - Crystalline defects in $SrFe_2As_2$ lead to Sc without doping. Disappears on annealing (Paglione et al.)

Open Questions and Directions

- How important are correlations?
- Relation between structure and magnetism?
- Anomalous phases (like the psuedogap and strange metal) in Fe based high Tc
- Phase coexistence of magnetism and superconductivity.
- New tests and effects resulting from $s_{\pm}$ pairing symmetry.