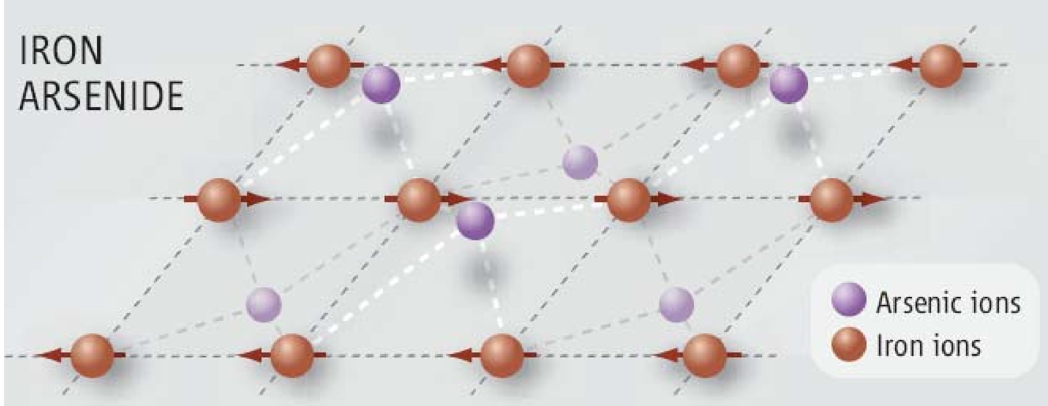
Magnetism and multi-orbital models in the iron-based superconductors

Dao-Xin Yao and Chun Loong

Sun Yat-sen University

Guangzhou

China



City of Guangzhou


Indiana

Guangzhou

Hong Kong

Sun Yat-sen University

Outline

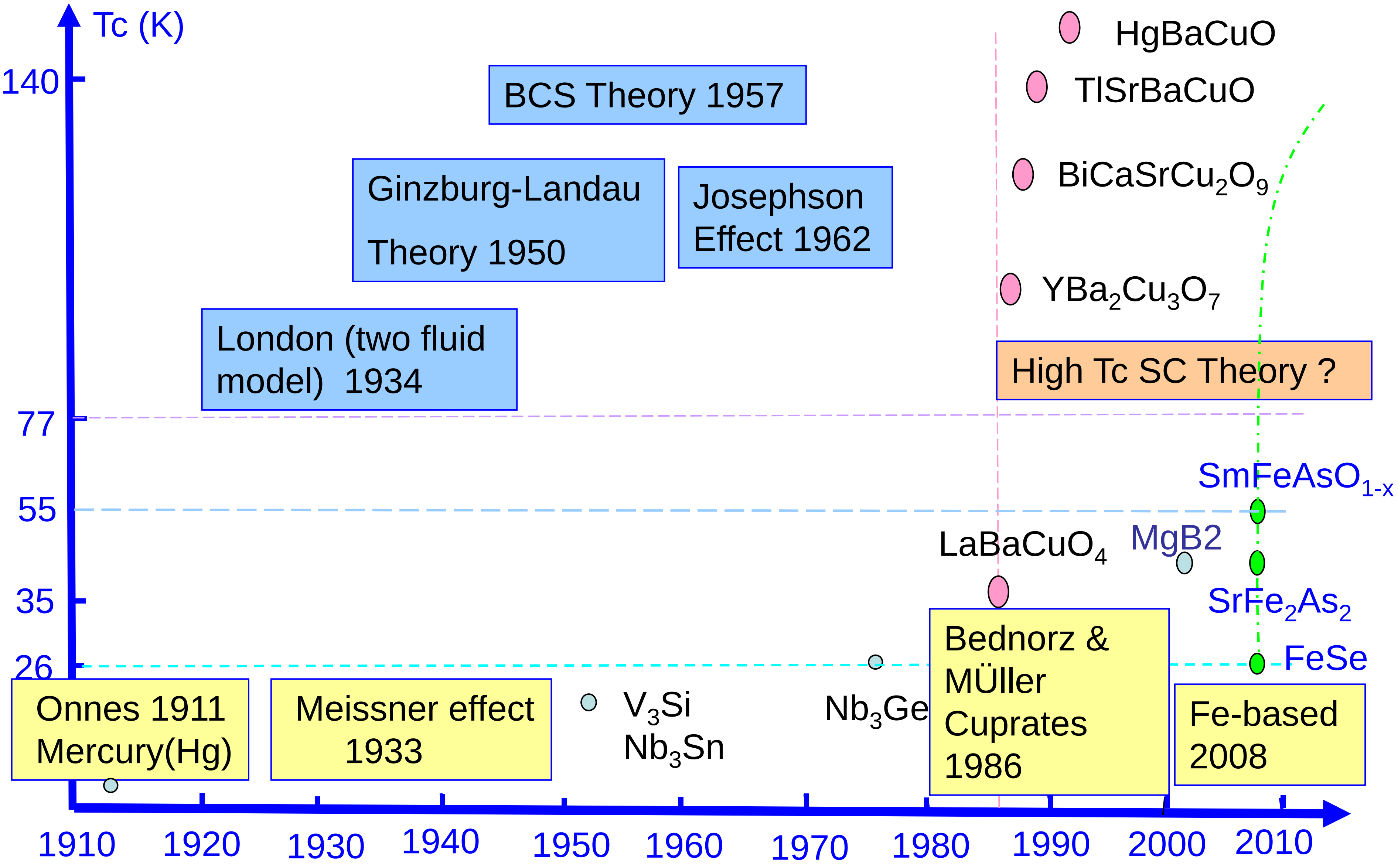
- Introduction
- Magnetism of parent compounds
- Two-, three-, five-orbital models
- Stripes
- Superconducting states
- New AFe2-ySe superconductors

Brief Review of Iron-based Superconductors

2011 is the100 anniversary of the discovery of superconductivity

Kamerlingh Onnes

History of Superconductivity



BCS Theory 1957

Ginzburg-Landau Theory 1950

Josephson Effect 1962

London (two fluid model) 1934

High Tc SC Theory ?

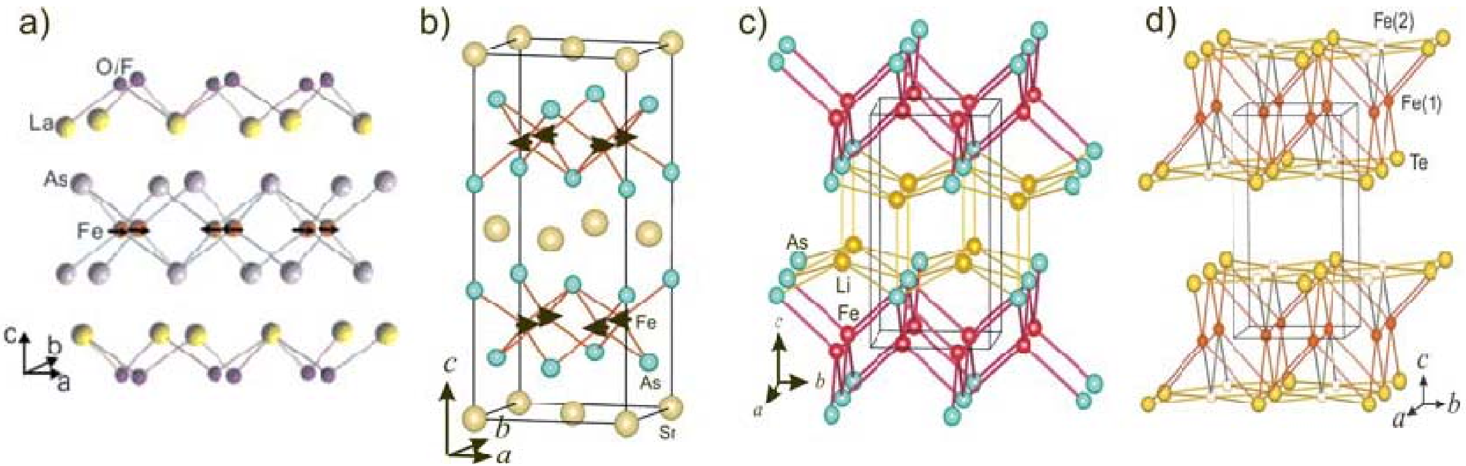
Onnes 1911 Mercury(Hg)

Meissner effect 1933

Bednorz & MÜller Cuprates 1986

Fe-based 2008

Fe-based Superconductors



- 1111 Series: LaOFeAs: 26K, 2008.02, Hideo Hosono Group
  CeO1-xFxFeAs: 41K SmO1-xFxFeAs: 55K
  PrO0.89F0.11FeAs: 52K （IOP, USTC, ZJU）, s± pairing

- 122 Series: 2008, BaFe2As2, 38K, SrFe2As2, Ca2Fe2As2, s±

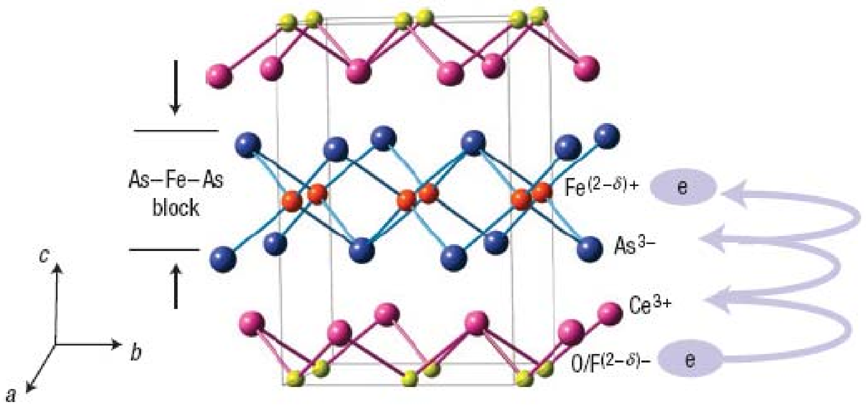
- 111 Series: 2008, Li$_x$FeAs，NaFeAs,16K, s±

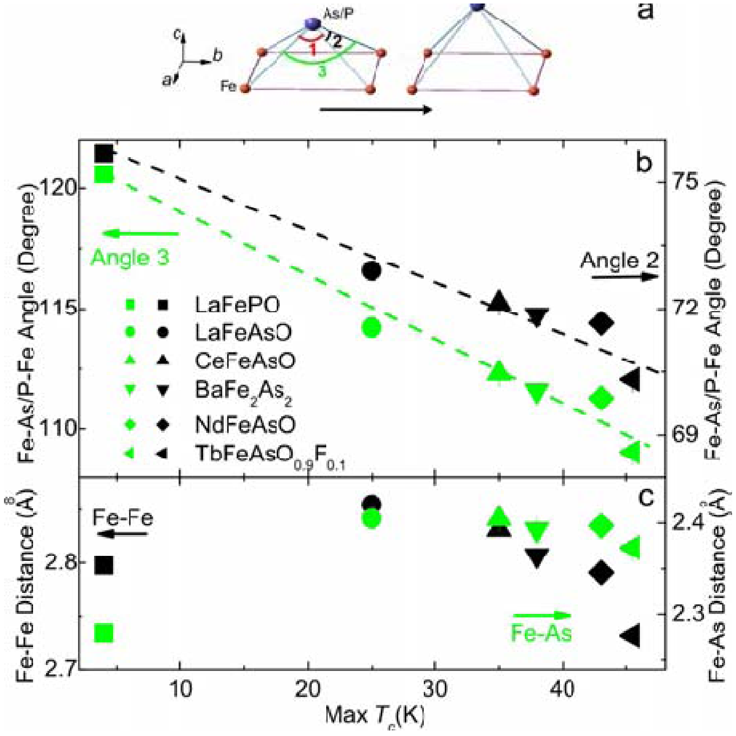
- 11 Series (Taiwan): 2008, FeTe，FeSe， 8K-26K with pressure.

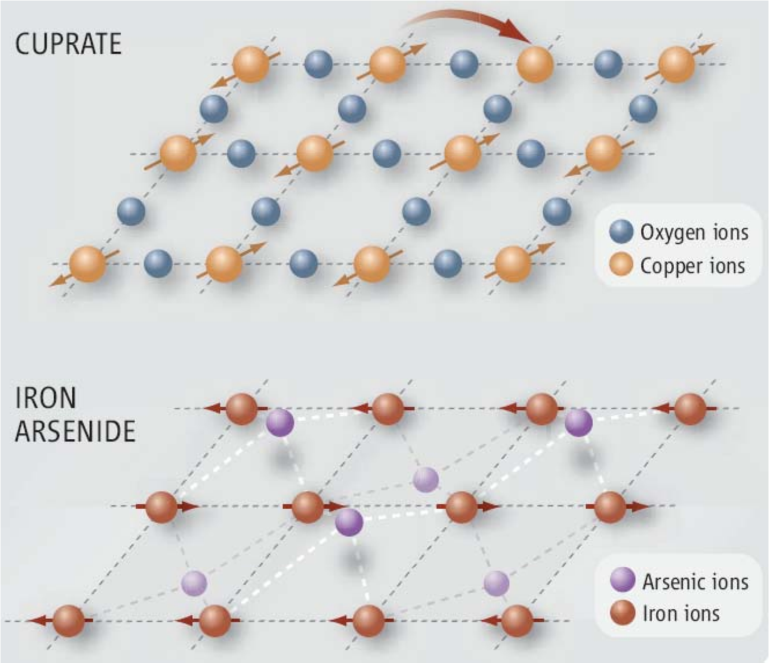
- New 122 Series: 2010.10, K0.8Fe1.6Se2, CsFe2-ySe2, RbFe2-ySe2, Tc~33K, different from all previous iron-based superconductors, close to cuprate superconductors, d-wave?

- …

Crystal Structure by Neutron Scattering





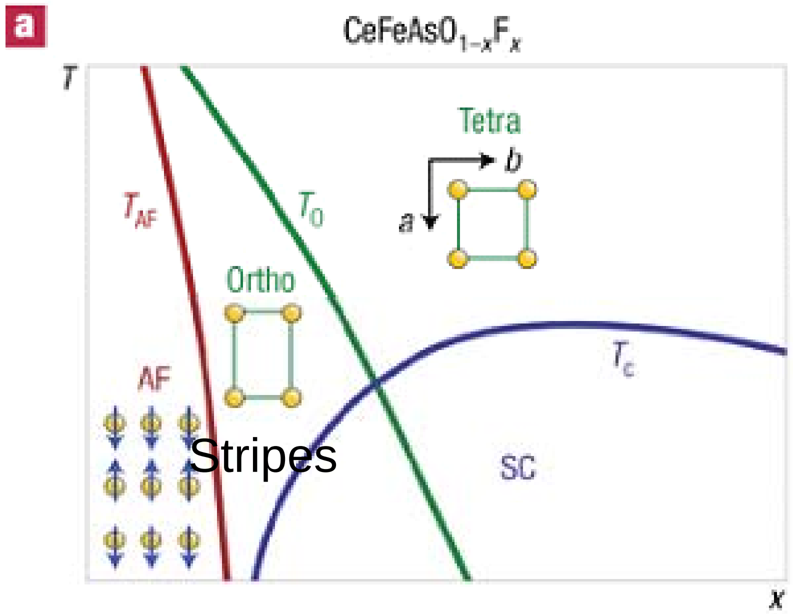


- 2D square lattice in tetragonal phase, T>Ts
  2D rectangular lattice in orthormbic phase, T<Ts
- Highest T_c approached when Fe-As-Fe angle is 109.47, which is perfect tetrahedron.
- Parent compounds show stripe-like collinear long range AF ordering.

J. Zhao *et al.*, Nature Materials 7, 953 (2008).

Phase Diagram

Iron-based superconductors



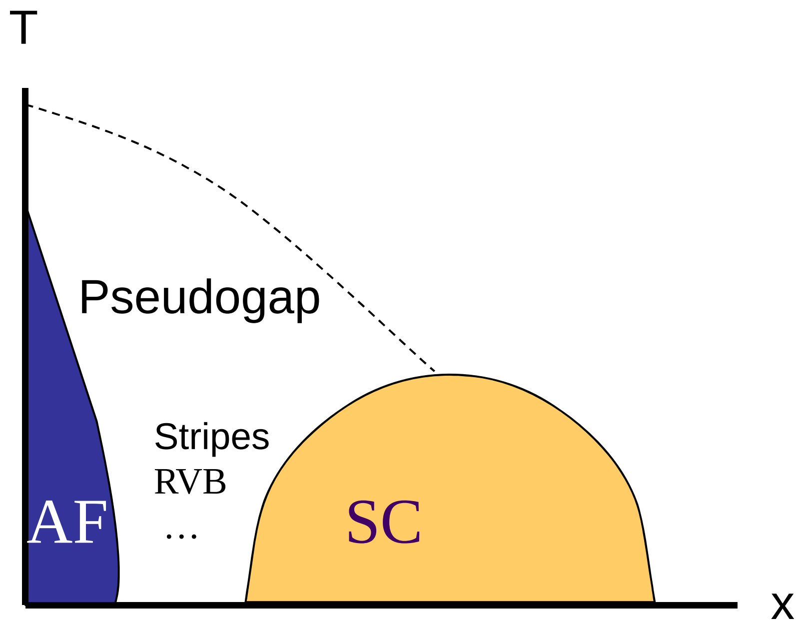
Stripes

Neutron Scattering

S. Kivelson *el al.* Nature Material, 7, 927 (2008)

J. Zhao *et al.*,Nature Materials 7, 953-959 (2008).

Cuprate superconductors



T

Pseudogap

Stripes
RVB
…

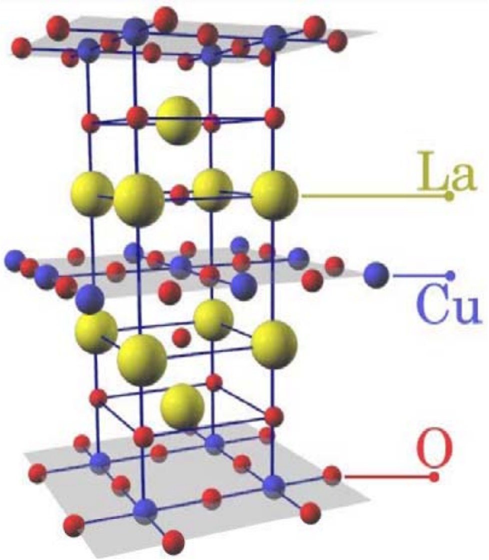
AF

SC

x

1111 materials: $T_O > T_{AF}$
122 materials: $T_O = T_{AF}$, first-order phase transition

Similarities of Cuprate and Fe-Superconductors



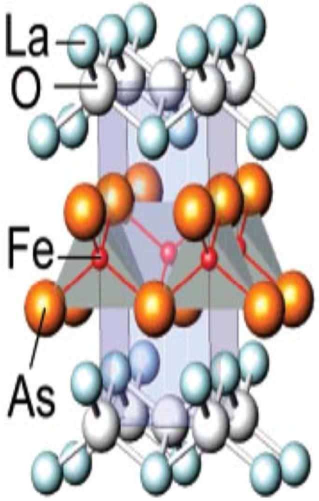
3d Transition Metal

Layered

Magnetically Ordered Parent

Doping Induces Superconductivity

Similar Phase Diagrams



Differences For Cuprate and FeAs Superconductors

Cuprates	**Iron Pnictides**
Spin 1/2	Spin ~ 1/2, 1, 3/2, …
Single *d*-orbital	Multiple *d*-orbitals
Parent is Mott Insulator	Parent is poor metal
Magnetism near (π, π)	Magnetism at (π,0)
d-wave (nodal quasiparticles)	s±

What's a Bad Metal?

Good metal: ρ increases with increasing Temperature
Mean Free Path > Fermi Wavelength
Energy > Lifetime (propagating quasiparticles)

Bad metal: ρ increases with increasing Temperature
Mean Free Path < Fermi Wavelength
Energy < Lifetime (overdamped)

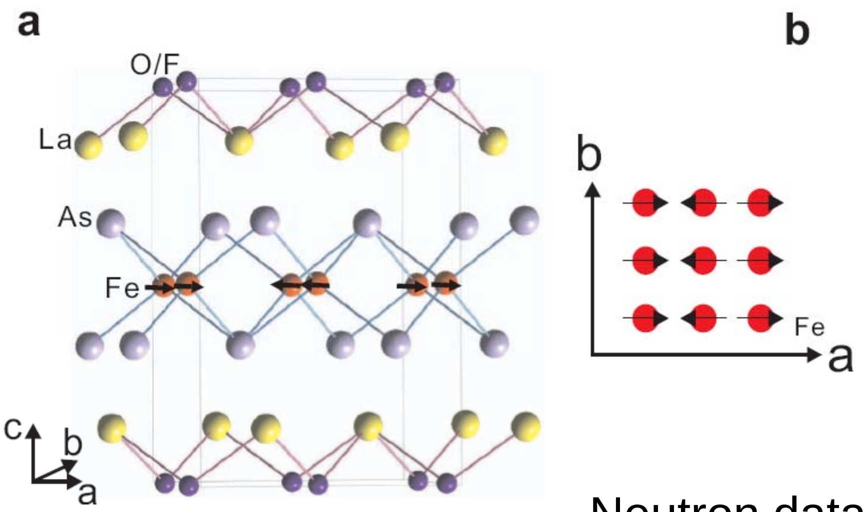
LaOFeAs: $\rho \sim 5$ mΩ-cm

$l \sim 0.08\, \lambda_F$

Si and Abrahams, PRL **101,** 076401 (2008)

Not a propagating quasiparticle

Magnetism of Parent Compounds



Long range collinear AF ordering with wave vector (π, 0)

Neutron Scattering Measurement,

C. de la Cruz et.al, Nature 453, 899 (2008).

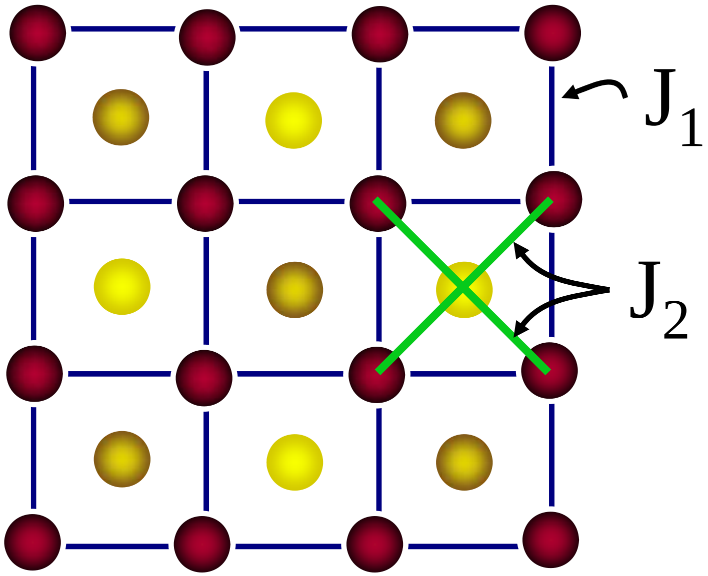
Neutron data

Material	T_S (K)	T_N(Fe) (K)	μ_{Fe} (μ_B)	q_{Fe}	Spin direction
LaOFeAs	155	137	0.36	101	likely *a*
CeOFeAs	158	140	0.8	100	*a*
PrOFeAs	153	127	0.48	100	*a*
NdOFeAs	150	141	0.25	101	likely *a*
$CaFe_2As_2$	173	173	0.80	101	*a*
$SrFe_2As_2$	220	220	0.94	101	*a*
$BaFe_2As_2$	142	143	0.87	101	*a*
$Fe_{1.068}Te$	67	67	2.25	100	*b*

J. Lynn and P. Dai, Physica C 2009

Why is μ not large?
Why does it vary so much?

Effective Spin Model :J1-J2 Model



● Fe

● As above plane

● As below plane

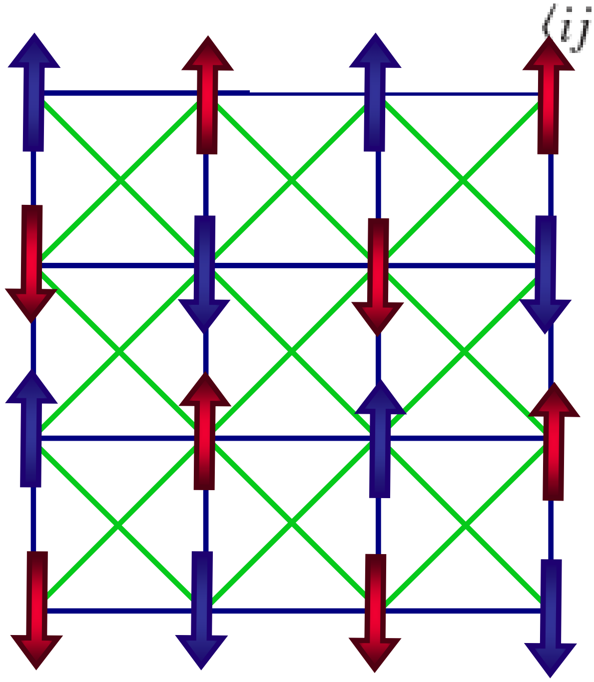
Frustration gives the spin stripe phase

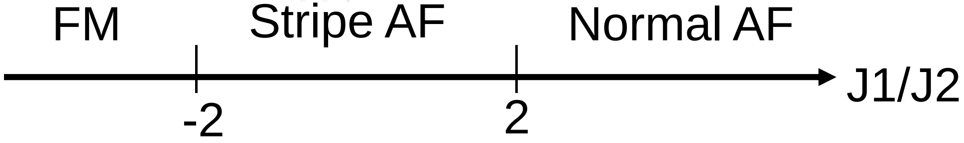
$$H = J_1 \sum_{\langle ij\rangle_{nn}} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle ij\rangle_{nnn}} \mathbf{S}_i \cdot \mathbf{S}_j$$

Q. Si and E. Abrahams, Phys. Rev. Lett. 101, 076401(2008).
D. X. Yao and E. W. Carlson, PRB **78,** 052507 (2008)
C. Fang et al. PRB 77, 224509 (2008).

Ground State of Effective Spin Model

$$H = J_1 \sum_{\langle ij\rangle_{nn}} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle ij\rangle_{nnn}} \mathbf{S}_i \cdot \mathbf{S}_j$$





FM | Stripe AF | Normal AF

-2 | 2 | J1/J2

For $J_2 > |J_1/2|$, classical ground state is two interpenetrating AF sublattices (Stripe AF).

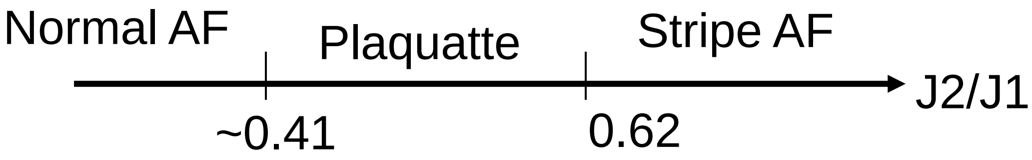
Quantum fluctuations lift degeneracy, leading to collinear AF order at $(\pi,0)$

P. Chandra *et al.*, PRB **38,** 9335 (1988)

P. Chandra *et al.*, PRL **64**, 88 (1990)

Ji-Feng Yu and Ying-Jer Kao

S=1/2



Normal AF | Plaquatte | Stripe AF

~0.41 | 0.62 | J2/J1

Two-orbital J1-J2 model ?

Sandvik, Liu, and Yao

Spin Wave Theory

Linear Spin Wave Theory (Holstein-Primakoff bosons):

$$H = E_{\mathrm{Cl}} + S\sum \left[A_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{\mathbf{k}} + \frac{1}{2}\left(B_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{-\mathbf{k}}^{+} + B_{-\mathbf{k}}^{*} a_{\mathbf{k}} a_{-\mathbf{k}}\right)\right]$$

$$E_{\mathrm{Cl}} = -2J_2 N S^2 \longrightarrow \text{J}_1 \text{ independent}$$

$$A_{\mathbf{k}} = (4J_2 + 2J_1 \cos k_x)$$

$$B_{\mathbf{k}} = (2J_1 \cos k_y + 4J_2 \cos k_x \cos k_y)$$

Diagonalize Hamiltonian:

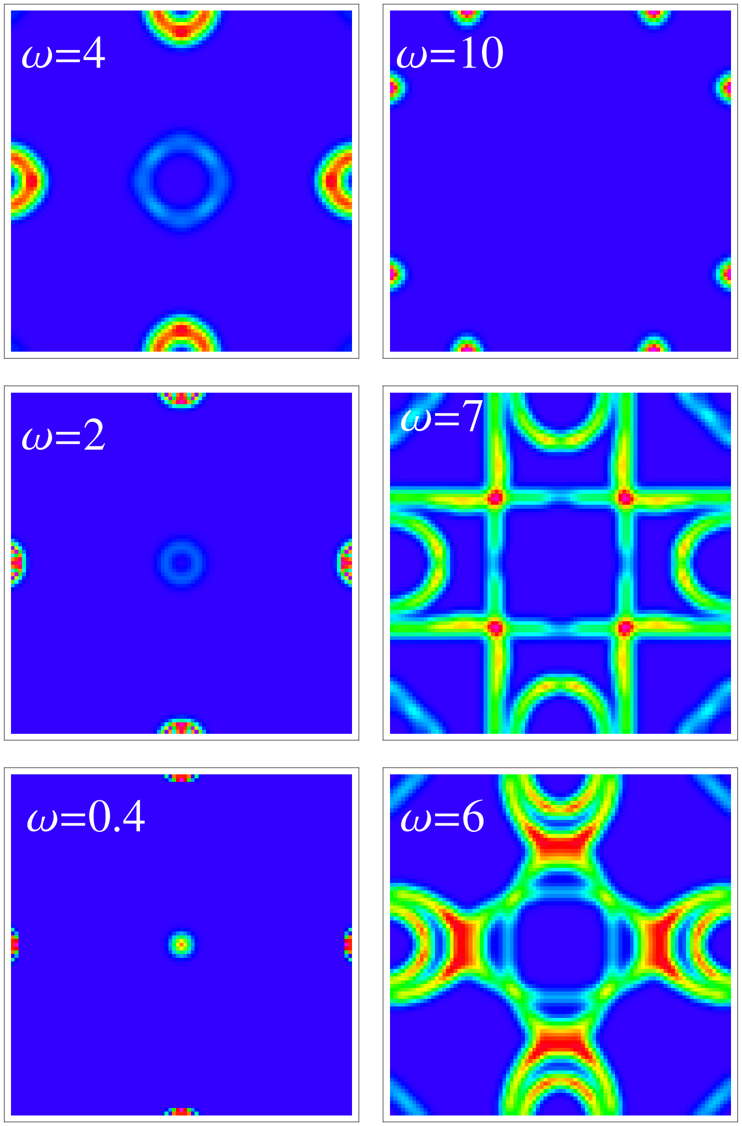
$$H = \sum_{\mathbf{k}} \omega(\mathbf{k}) b_{\mathbf{k}}^{+} b_{\mathbf{k}} + E_{\mathrm{Cl}} + E_0$$

where E_0 is the quantum zero-point energy correction

One Spin Wave Band:

$$\omega(\mathbf{k}) = S\sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}$$

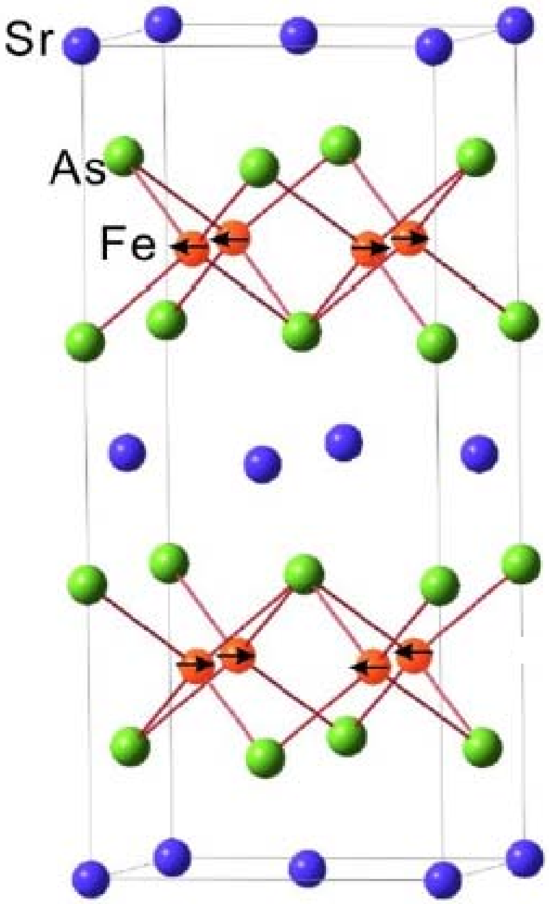
Expected Neutron Results from Spin wave theory



Constant Energy Cuts

D. X. Yao and E. W. Carlson, Phys. Rev. B 78, 052507 (2008)

Modeling of $SrFe_2As_2$

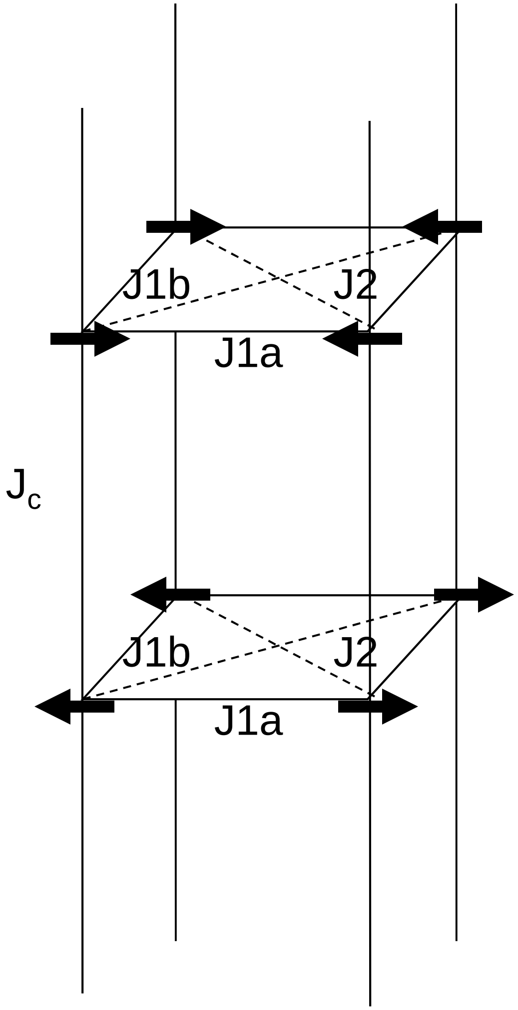


Model:

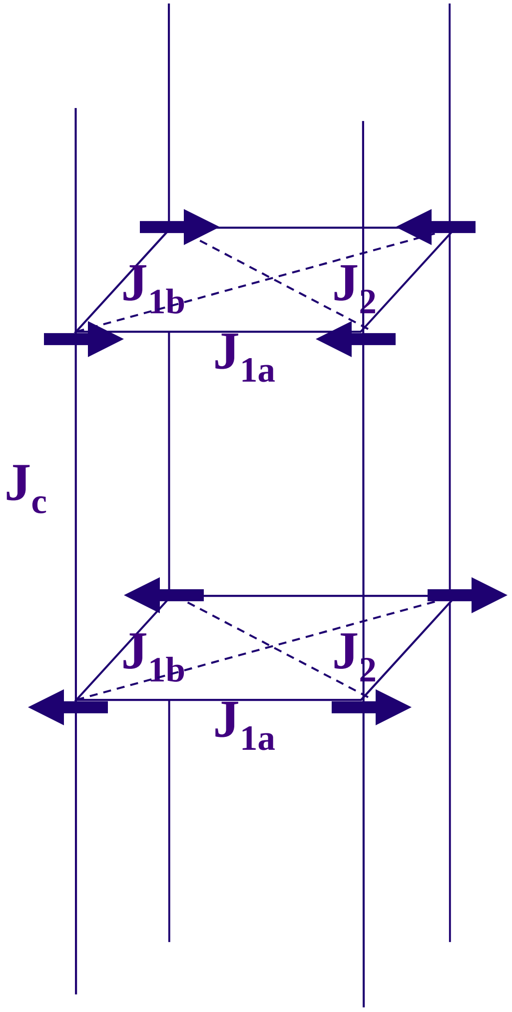
Antiferromagnetic between planes

Allow for lattice distortion, $J_{1a} \neq J_{1b}$

Allow single-ion anisotropy



3D Heisenberg model

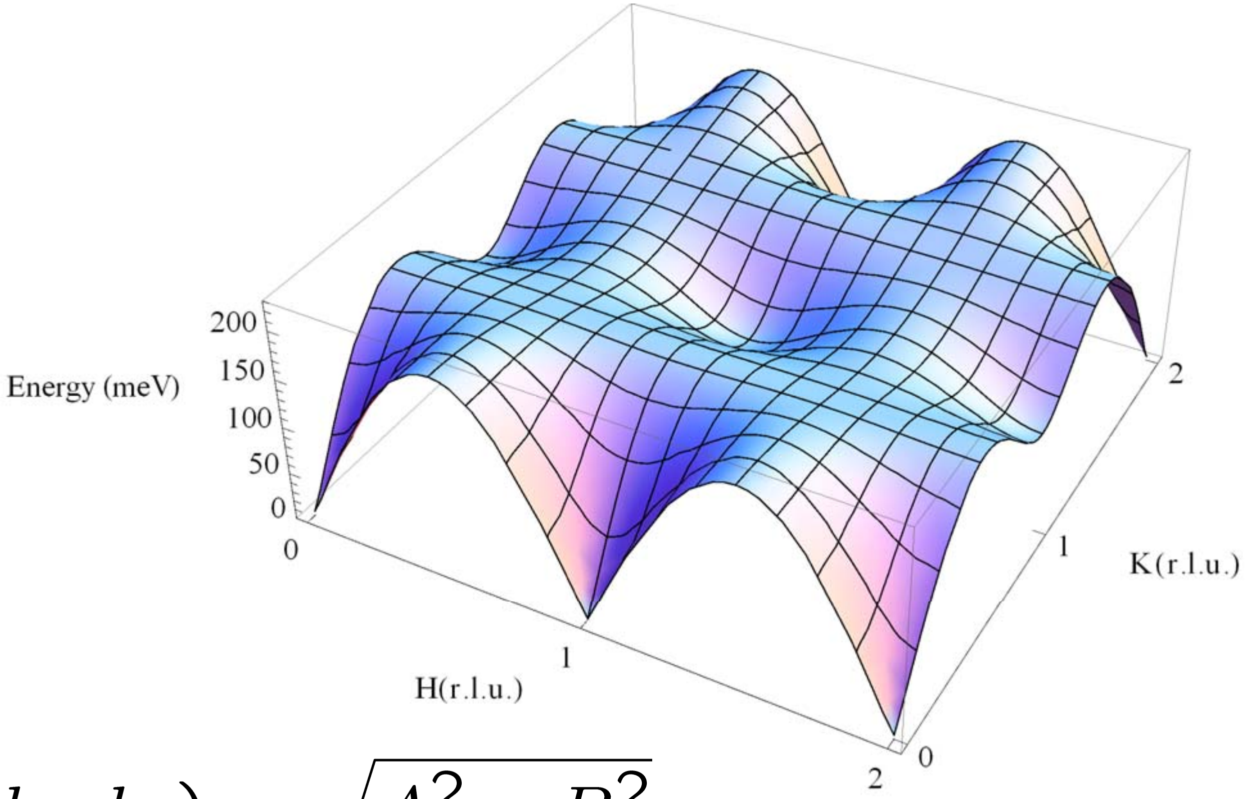


ab-Plane Anisotropy

$$H = J_{1a}\sum_{i,j}\mathbf{S}_i\cdot\mathbf{S}_j + J_{1b}\sum_{i,j}\mathbf{S}_i\cdot\mathbf{S}_j + J_2\sum_{i,j}\mathbf{S}_i\cdot\mathbf{S}_j$$
$$+J_c\mathbf{S}_i\cdot\mathbf{S}_j - J_s(S_i^z)^2,$$

Single-Ion Anisotropy

Spin Wave Spectrum

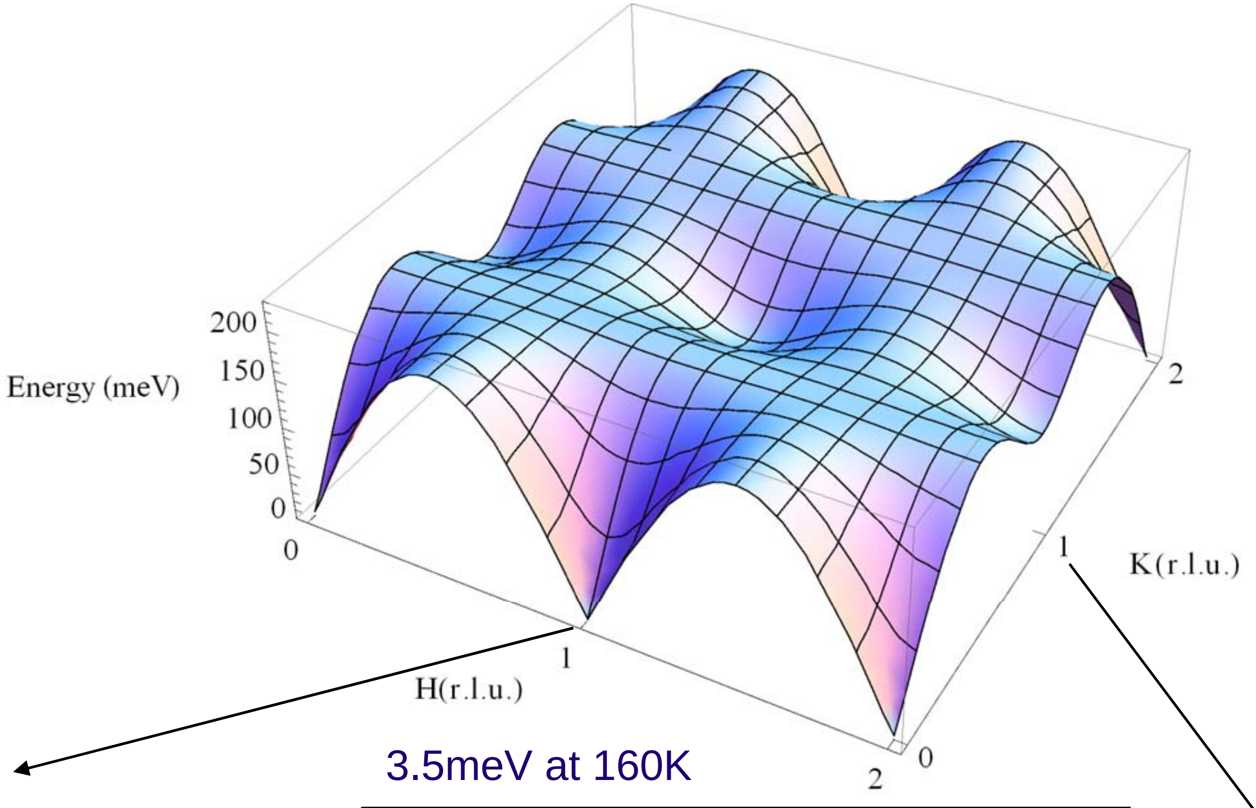


$$E(k_x, k_y, k_z) = \sqrt{A_k^2 - B_k^2}$$

$$A_k = 2[J_{1a} - J_{1b} + 2J_2 + J_s + J_c + J_{1b}\cos(k_y)]$$

$$B_k = 2\cos(k_x)(J_{1a} + 2J_2\cos(k_y)) + 2J_c\cos(k_z)$$

Spin Wave Spectrum



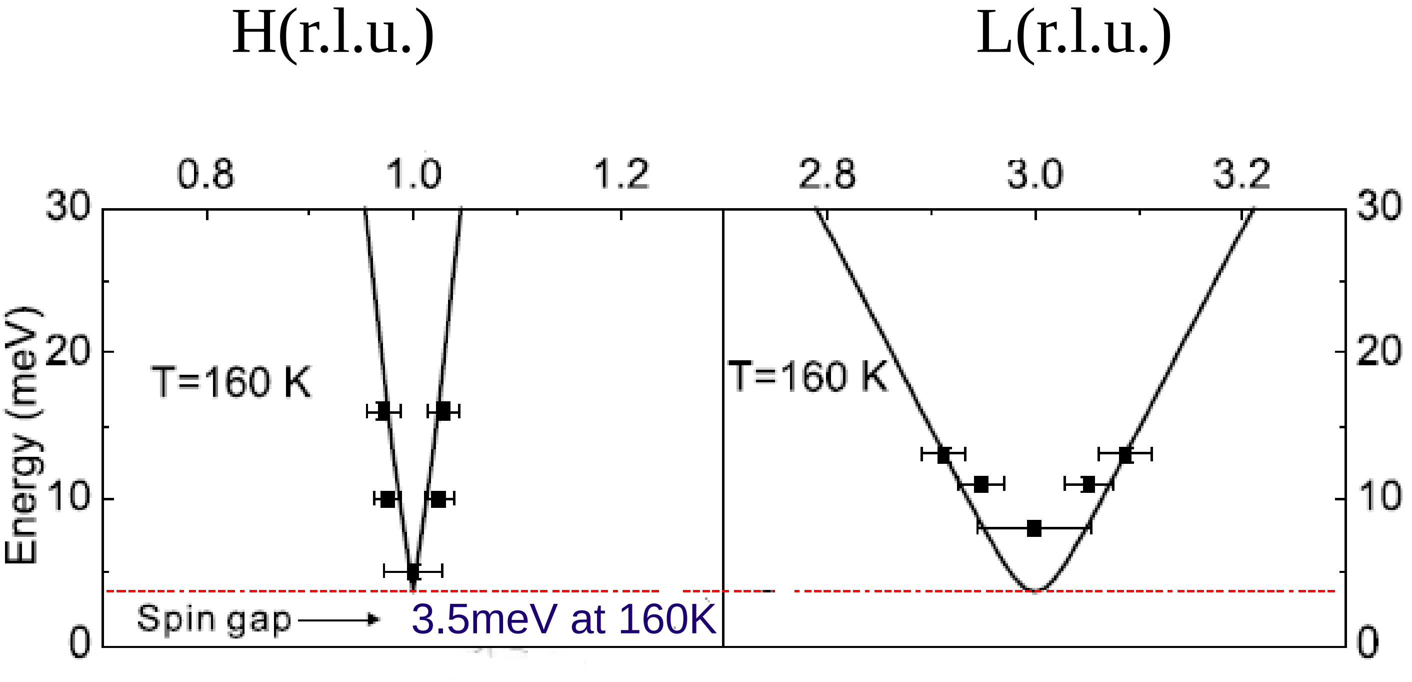
3.5meV at 160K

$$\Delta(1,0,1) = 2S\sqrt{J_s(2J_{1a} + 4J_2 + J_s + 2J_c)}$$

$$\Delta(0,1,1) = 2S\sqrt{(2J_{1a} - 2J_{1b} + J_s)(-2J_{1b} + 4J_2 + J_s + 2J_c)}$$

Values of gaps + shape of dispersion
can be used to set parameters

Fit to Inelastic Neutron Scattering Data



Fit to Data:

$J_{1a}+2J_2= 100 \pm 20$ meV

$J_c=5 \pm 1$ meV

$J_s=0.015 \pm 0.005$ meV

J. Zhao, D. X. Yao, …, PRL **101,** 167203 (2008)

Another Difference Between FeAs and Cuprates

Fit to Data:

$J_{1a}+2J_2= 100 \pm 20$ meV
$J_c=5 \pm 1$ meV
$J_s=0.015 \pm 0.005$ meV

For $J_{1a} \sim J_2/2$, then $J_{1a} = 20$meV and $J_2 = 40$meV.

$$\boxed{J_c/J_2 \sim 10^{-1}}$$

Spin gap at (101) is 3.5meV at 160K

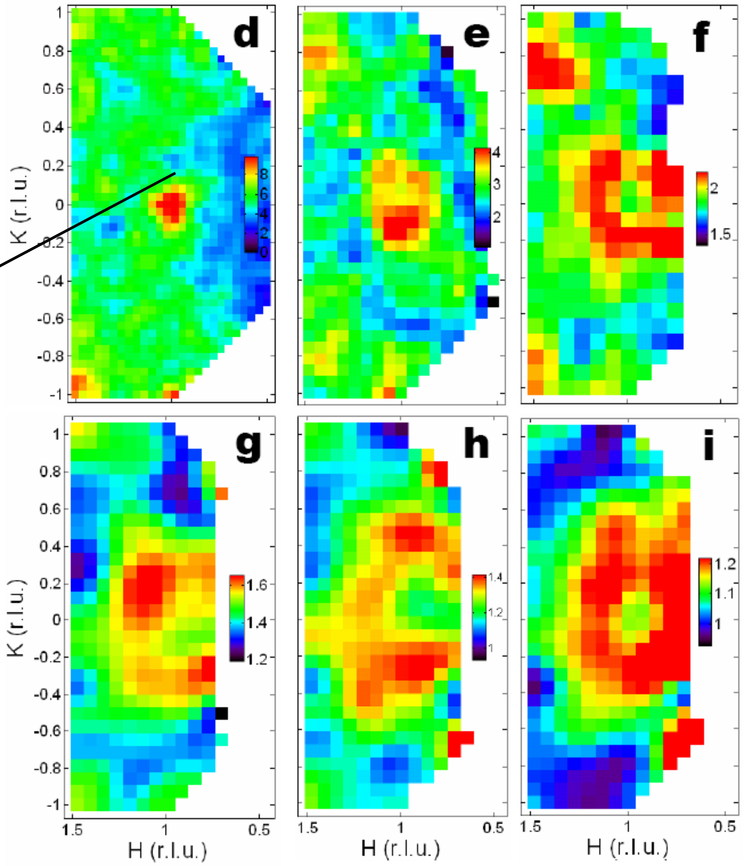
By contrast, $LaCuO_4$ has $J_c/J_{||} \sim 10^{-5}$!

J. Zhao, D. X. Yao et al, PRL **101,** 167203 (2008)

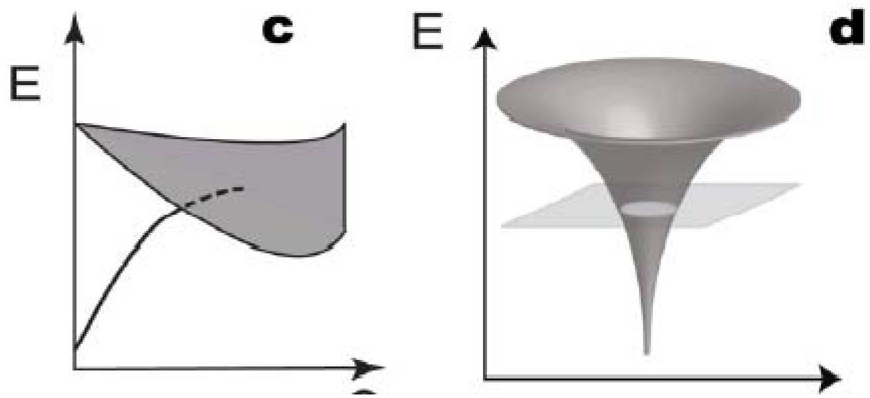
High Energy Neutron Scattering on CaFe2As2:

1. Spin wave cone (circular) found at extremely high energy (up to 200meV)
1. Only one spin gap (6-9meV) found at (101)
2. No signal found at (110) and (111)

T<<TN=170 K

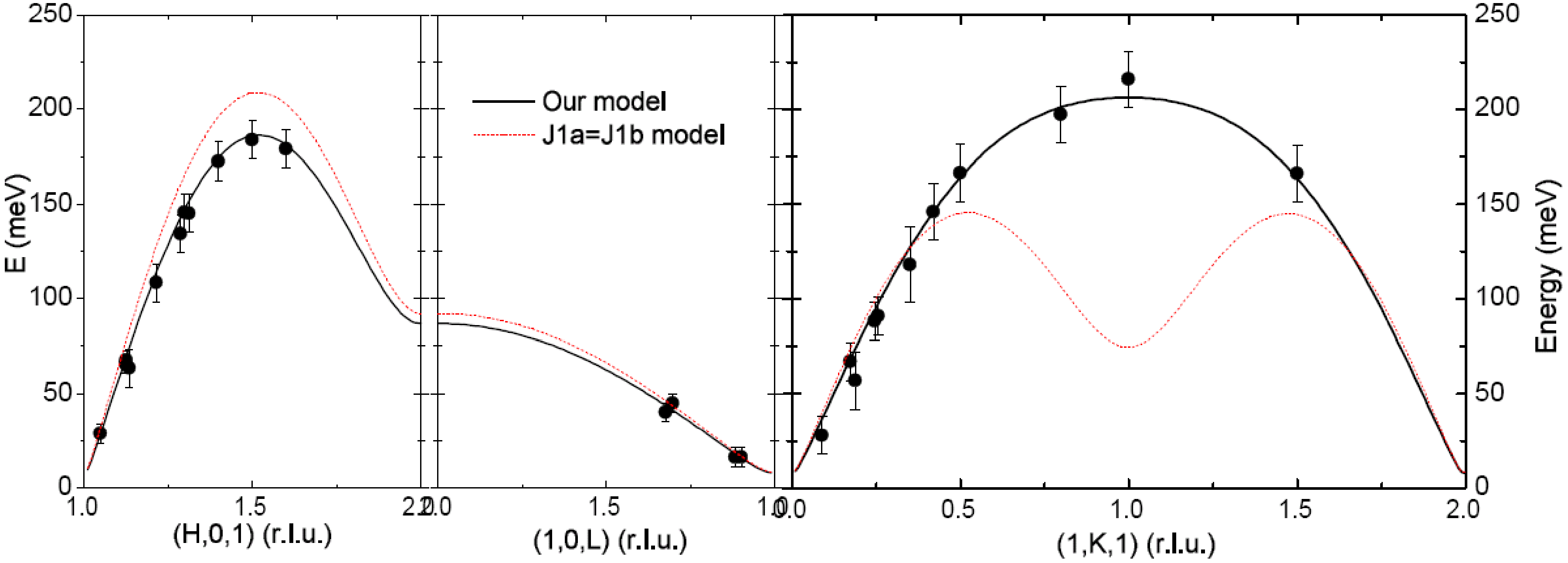


(101)



J. Zhao, **Dao-Xin Yao**, Pengcheng Dai et al, Nature Physics 5, 555 (2009).

Dispersions

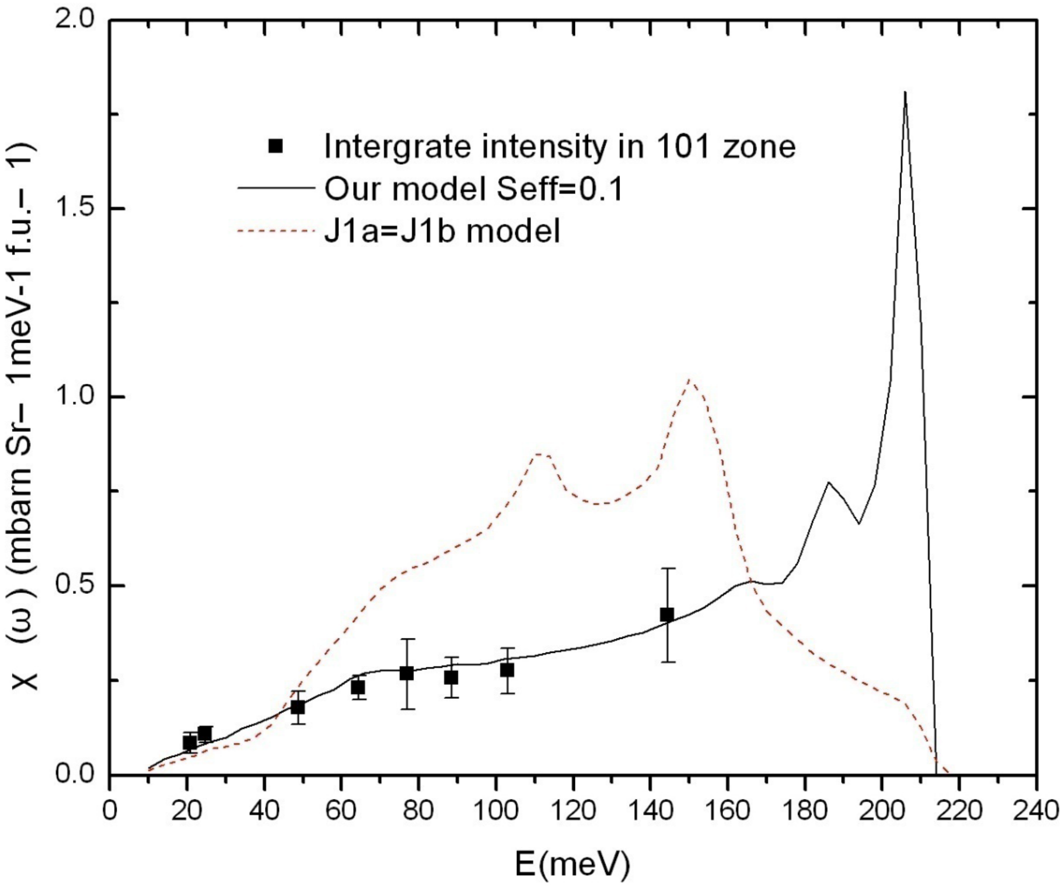


J1a=49.9, J1b=-5.7, J2=19, Jc=5.3, Js=0.084

No Frustration?

J. Zhao, **Dao-Xin Yao**，Pengcheng Dai et al, Nature Physics 5， 555 （2009）

Local Susceptibility



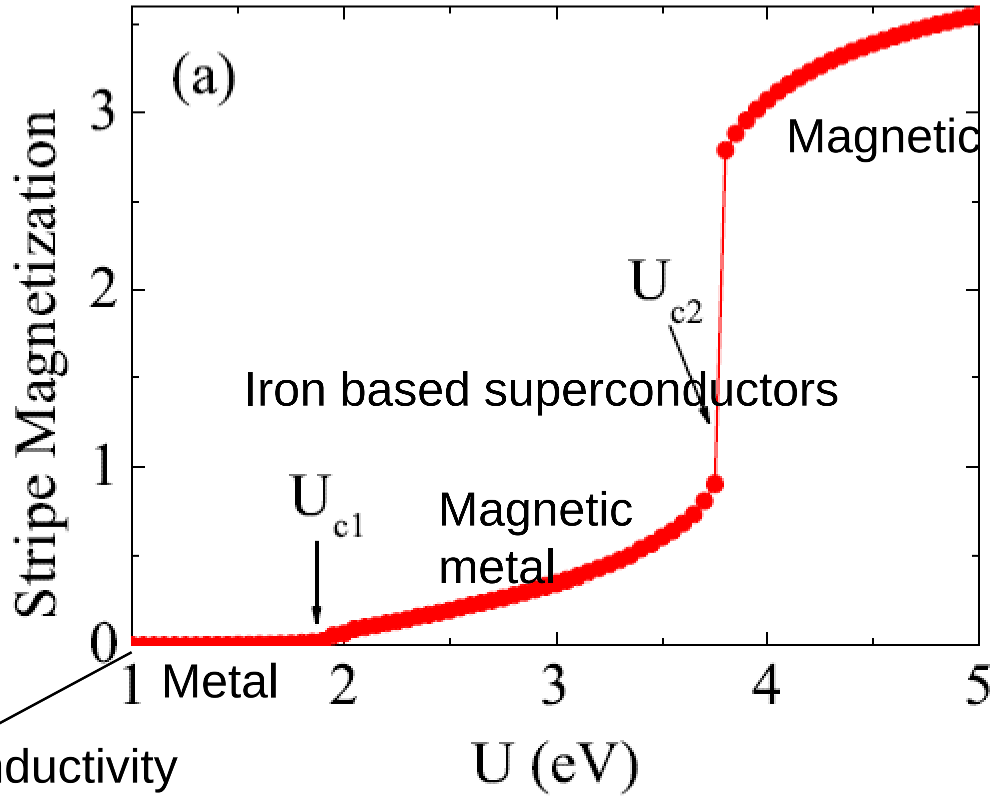
J1a=49.9, J1b=-5.7, J2=19, Jc=5.3, Js=0.084

J. Zhao, **Dao-Xin Yao**，Pengcheng Dai et al, Nature Physics 2009
Sublattice magnetization, magnetic moment，sum rule， etc
Dao-Xin Yao, E. W. Carlson, Frontiers of Physics in China (2010)

Hubbard Model

$$H = -t \sum_{<i,j>,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c.) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}.$$

Cuprate superconductor



Magnetic Insulator

Iron based superconductors

Magnetic metal

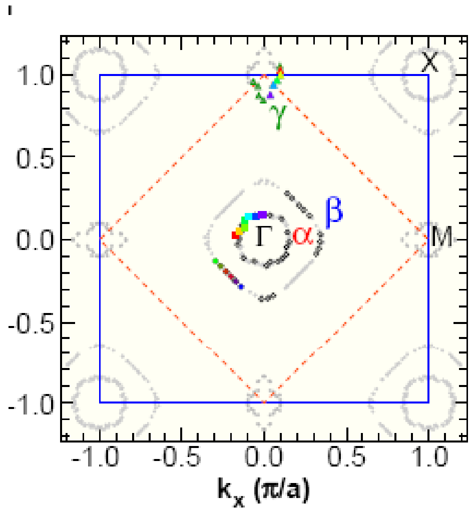
Metal

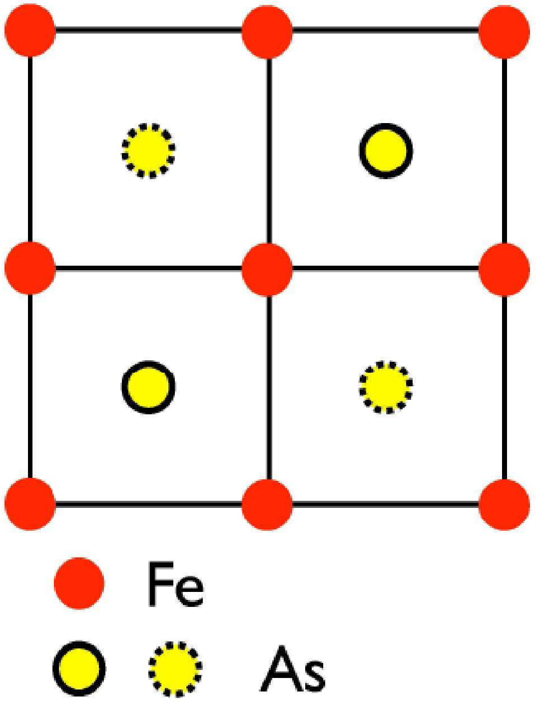
Superconductivity

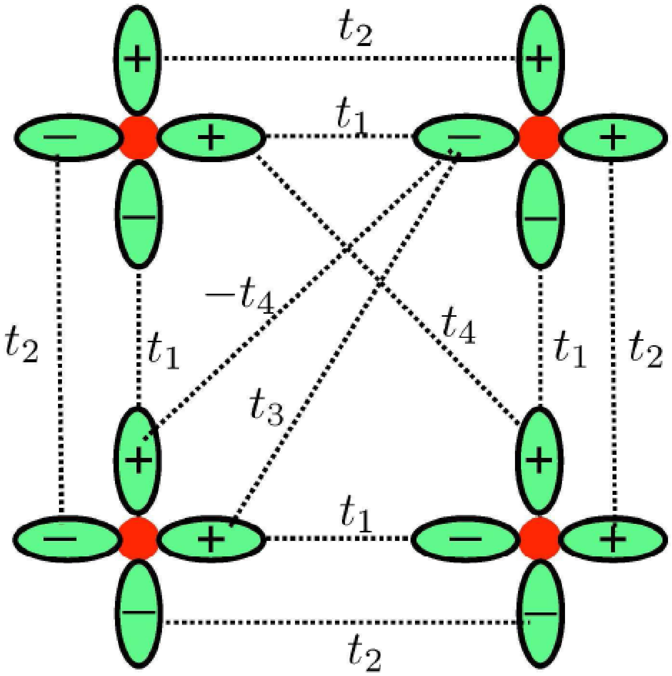
Doping x

Minimal Two-orbital Model
- dxz, dyz

Fermi surface

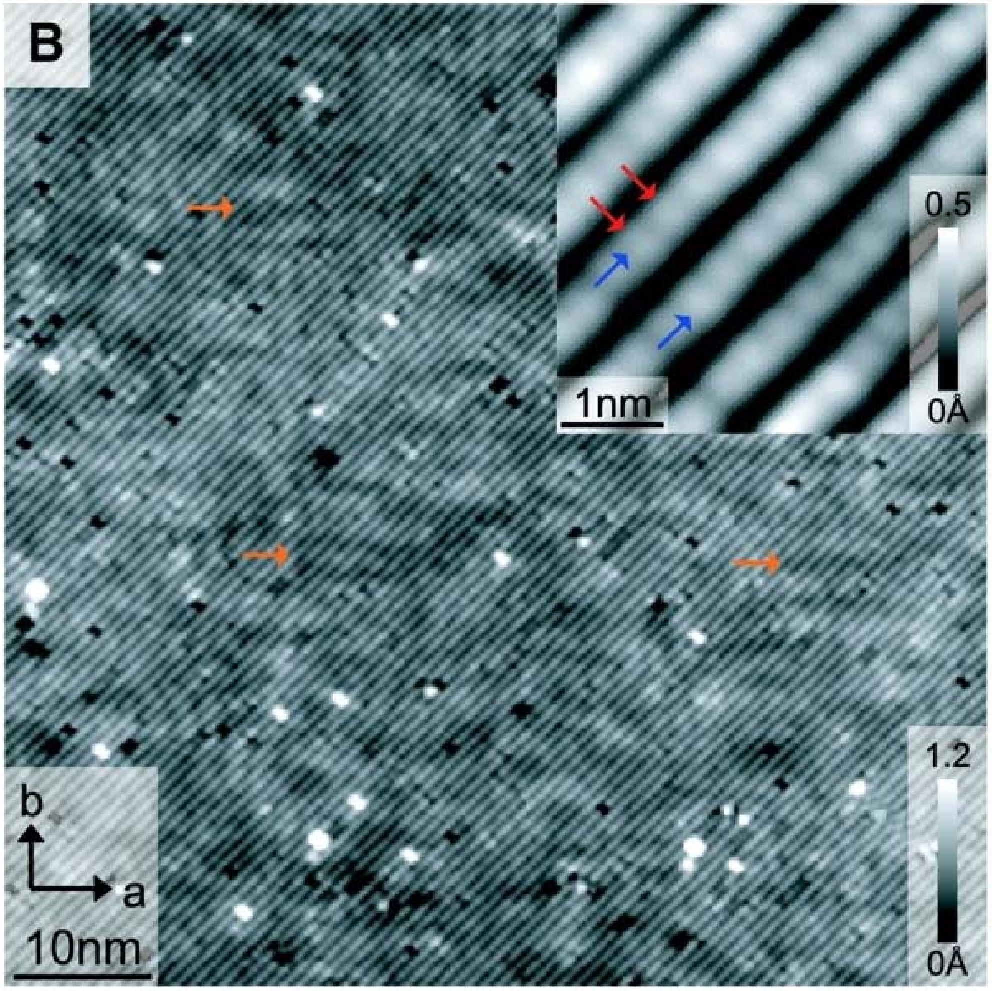






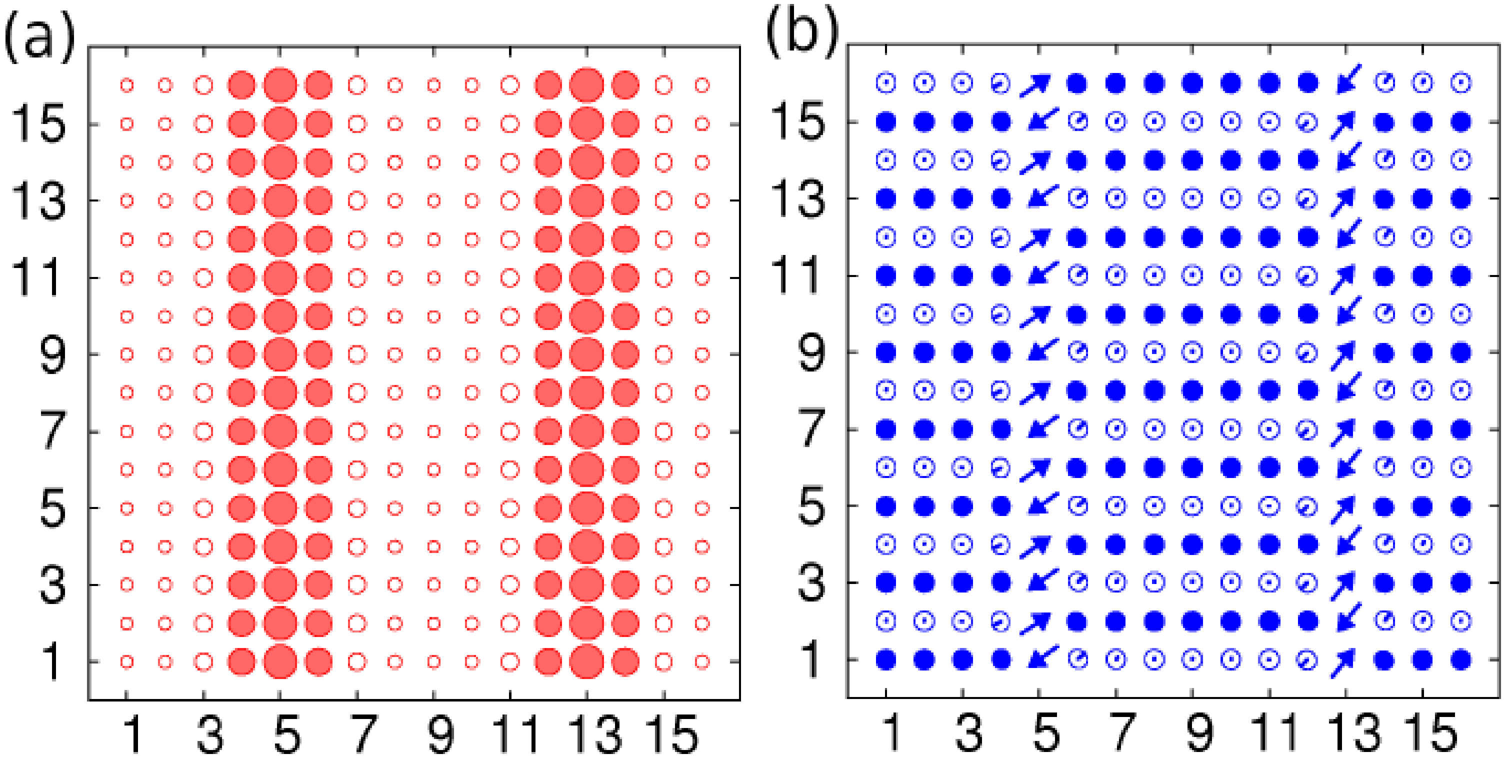
S. Raghu, S. C. Zhang et al, Phys.Rev.B 77 220503(R) (2008)

Nematic Electronic Nanostructure in Ca(Fe1–*x*Co*x*)2As2



J. C. Davis group, Science 327, 5962 (2010)

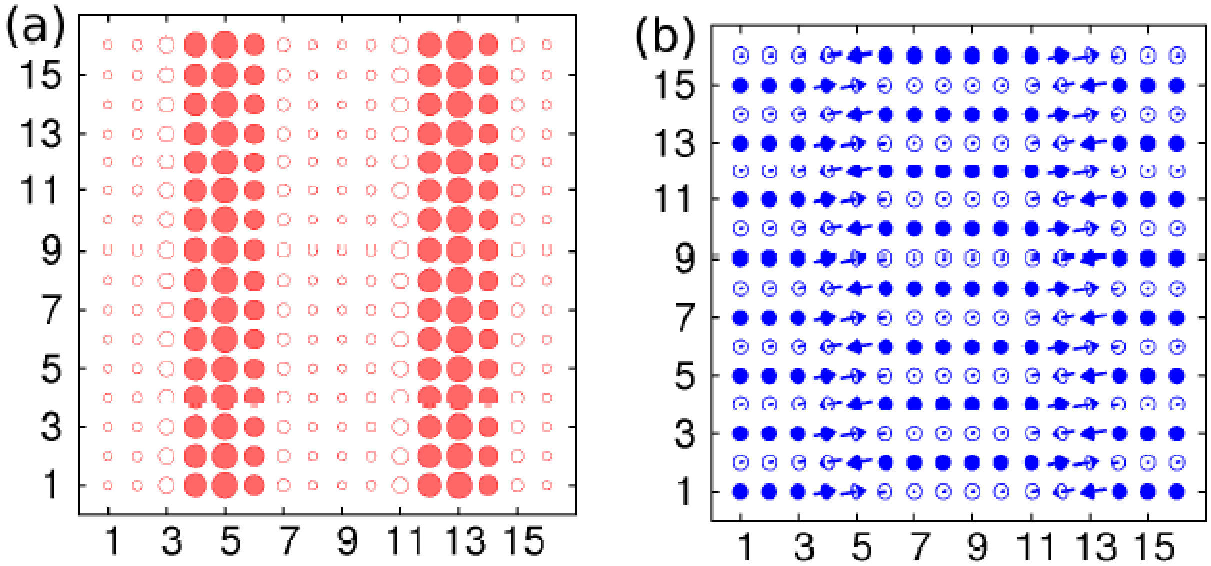
Charged Stripes
in the Two-Orbital Hubbard Model



- Real-space Hartree-Fock Mean-Field Approximation
- Spin Incommensurability (SI) at KFe2As2, FeSeTe, etc.
- n=2.313, U=0.5, Jh/U=0.25,

Luo, Yao, et al. Phys. Rev. B **83**, 174513 (2011)

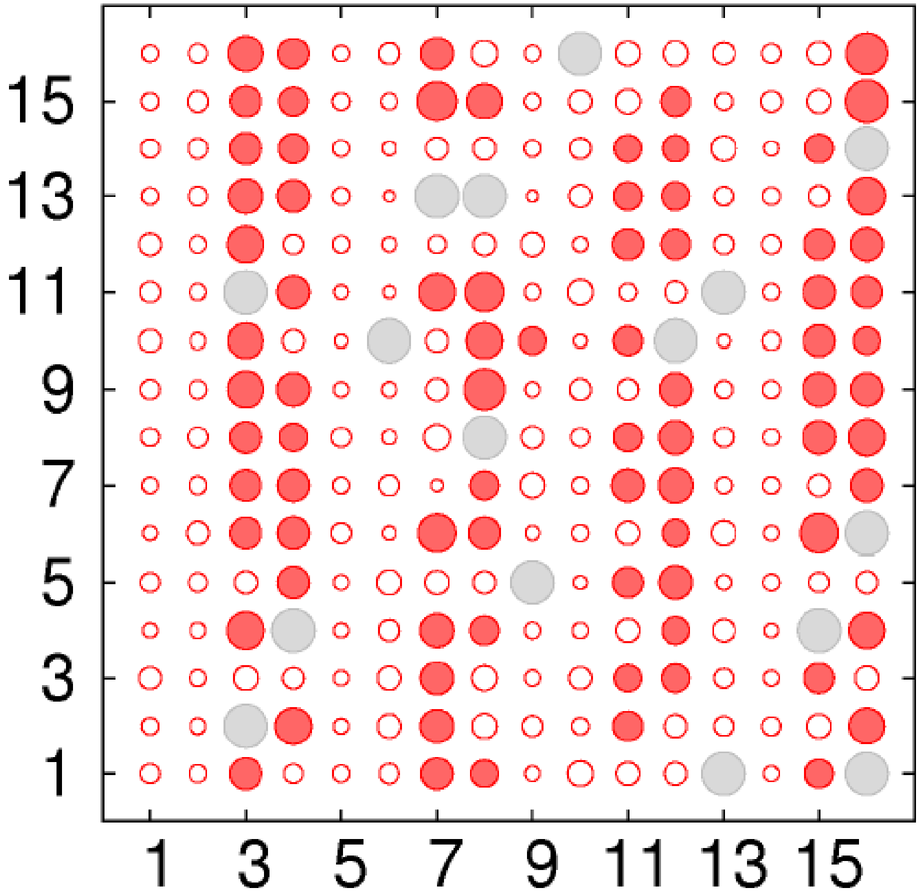
Properttties of Charge Striped State



(ii) HF striped state can produce spin incommensurability

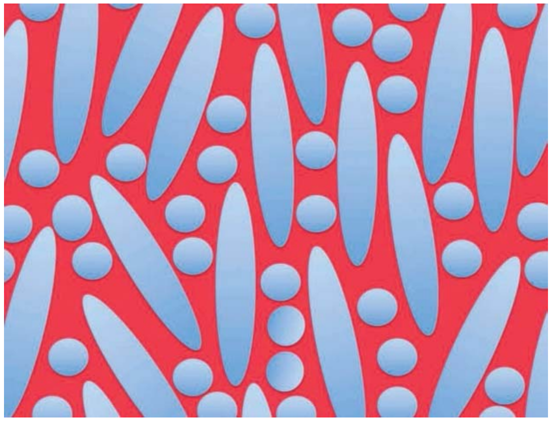
Luo, Yao, et al. Phys. Rev. B **83**, 174513 (2011)

Ground state with Quenched Disorder from the two-orbital Hubbard model



Luo, Yao, et al. **83**, 174513 (2011) .

Electron Nematic Phase

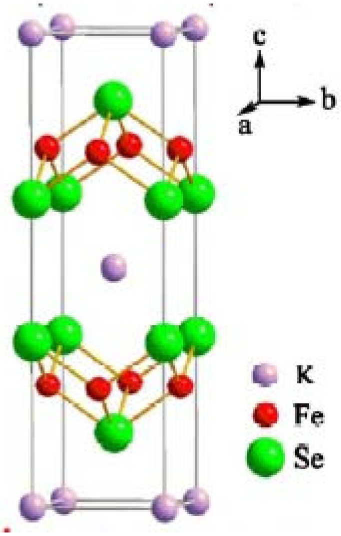


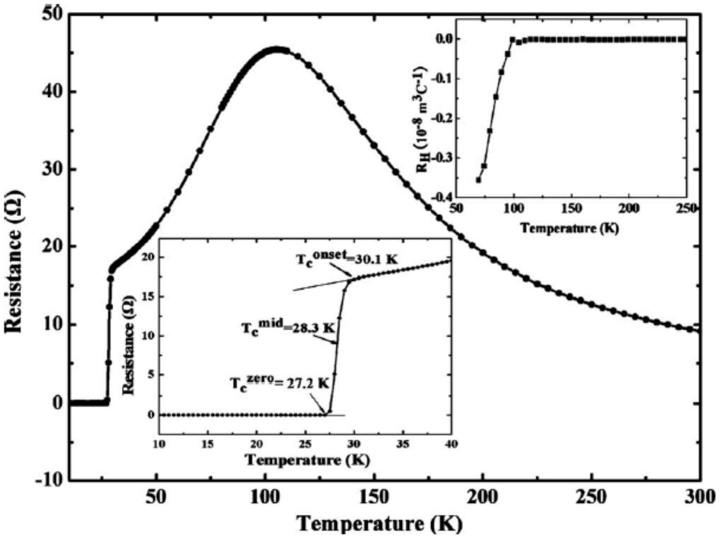
Fradkin and Kivelson
Science 2010

Need Neutron Scattering to detect

New iron selenide superconductors-

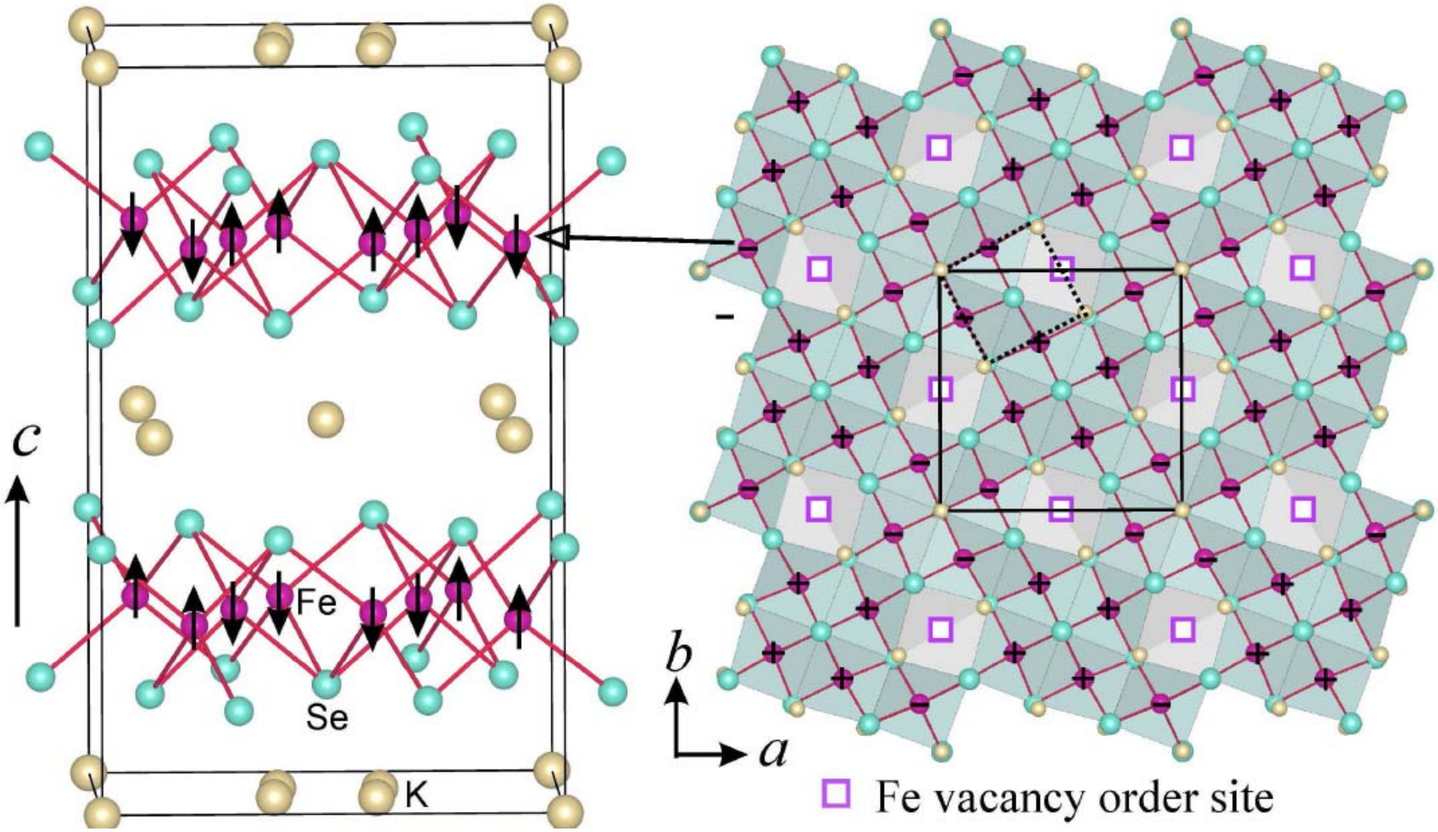
$K_xFe_{1.6+x}Se_2$, $Rb_xFe_{1.6+x}Se_2$, $Cs_xFe_{1.6+x}Se_2$, …





Jiangang Guo, Xiaolong Chen et al., Phys. Rev. B 82, 180520(R) (2010)
Institute of Physics in China

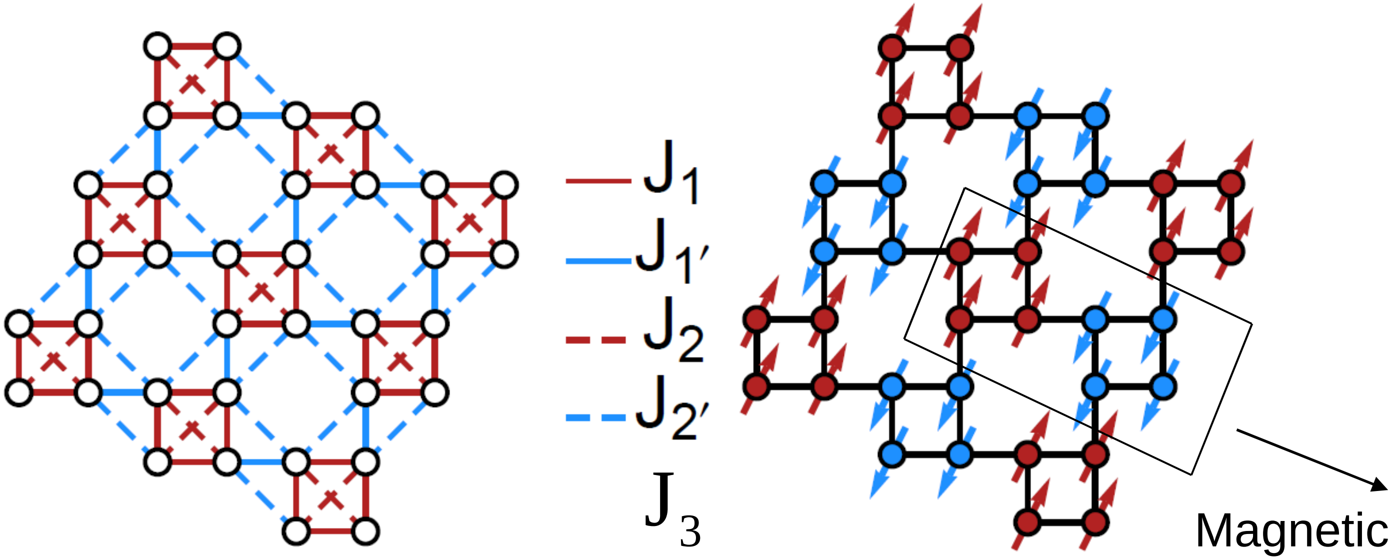
Magnetism of Iron Selenides from Elastic Neutron Scattering



Large magnetic moment: $M = 3.31\mu_B / Fe$

W. Bao et al., arXiv:1102.0830

Hamiltonian of ReFe(1.5)Se2



(a) (b)

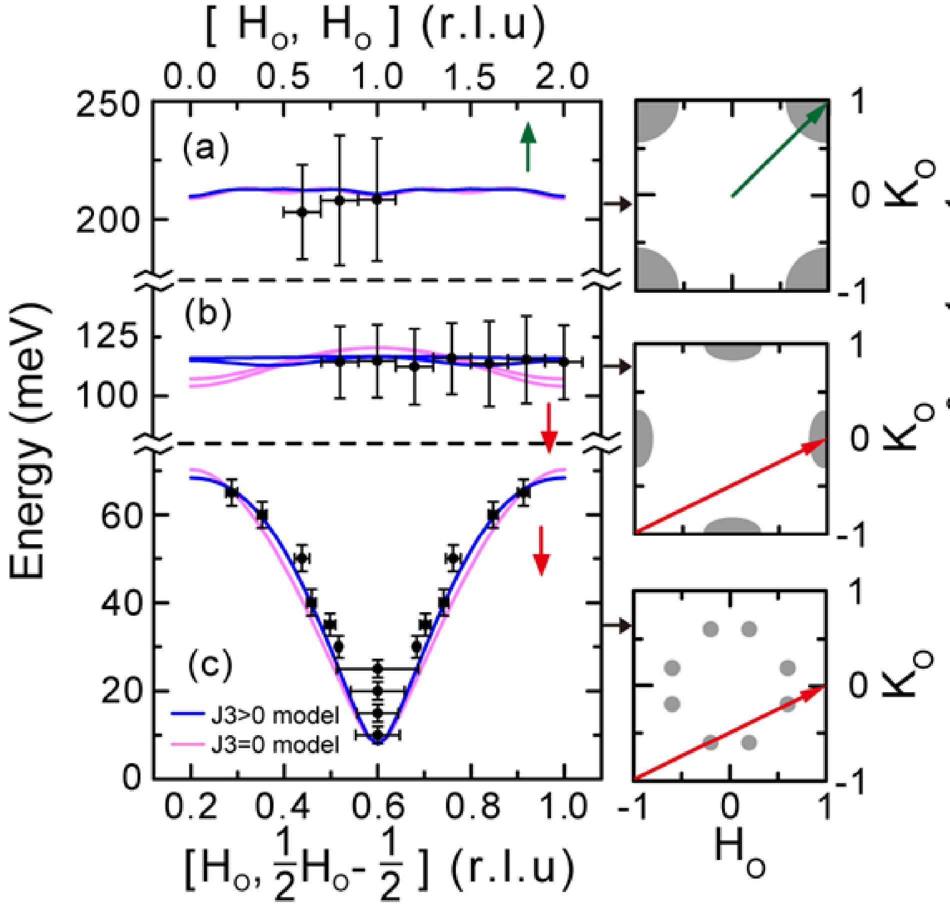
Magnetic unit cell
8 spins

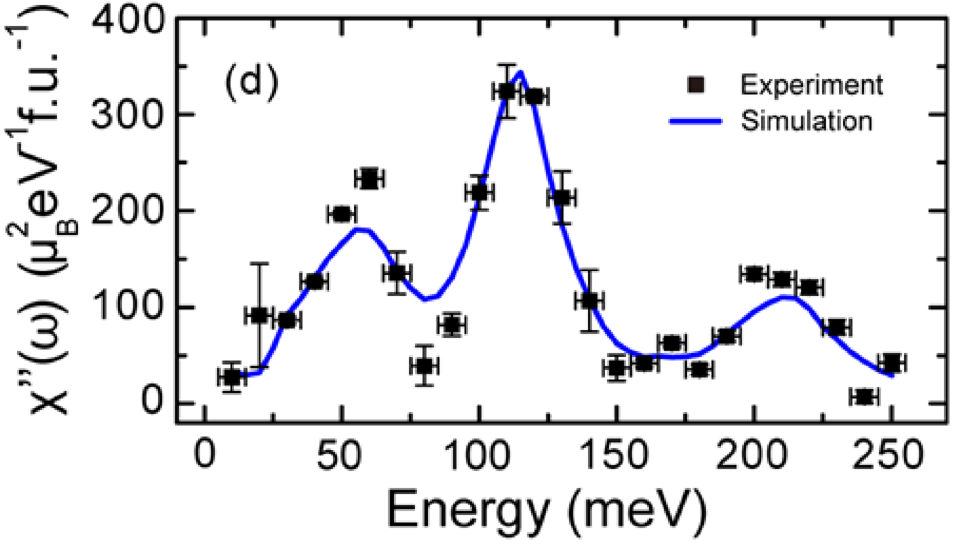
$$H = J_1 \sum_{<i,j>} S_i \cdot S_j + J_1^{'} \sum_{<i,j>} S_i \cdot S_j + J_2 \sum_{<i,j>} S_i \cdot S_j + J_2^{'} \sum_{<i,j>} S_i \cdot S_j + J_3 \sum_{<i,j>} S_i \cdot S_j + J_C \sum_{<i,j>} S_i \cdot S_j - J_S \sum_{i} (S_i^Z)^2$$

C-axis coupling

Yao, JP, et el.

Neutron Scattering Results with Theoretical calcualtions





$S = 2$

$J_1^{eff} = 17\text{meV}$

$$\mathrm{SJ}_1 = -36 \pm 2, \mathrm{SJ}_1' = 15 \pm 8, \mathrm{SJ}_2 = 12 \pm 2, \mathrm{SJ}_2' = 16 \pm 5, \mathrm{SJ}_3 = 9 \pm 5, \mathrm{SJ}_C = 1.4 \pm 0.2, \mathrm{SJ}_S = 0.44 \pm 0.1 meV$$

M. Wang, C. Fang, D. X. Yao, et al. arXiv:1105.4675

Conclusions

- **Fe-based superconductors have many similarities as Cu-based superconductors, including the superconducting mechanism. Magnetism plays an important role in these materials. Charge Stripes are found in the two-orbital Hubbard model**

- **Hund coupling is important in Fe-based superconductors**

- **Neutron Scattering is very important to detect Lattice structure, Magnetism, Superconductivity, Magnetic couplings, Phase Transitions.**

- **The field is booming!**

yaodaoxin@gmail.com

Thank you for your attention!