Arsenic and Old Lace:
A Tale of Two Electrons in iron-based superconductors

F. Kruger

Antonio

W. Lv

Jiansheng Wu (not shown)

What are the pnictides Really?

manganites

Cuprates

What are the pnictides Really?

~~Cuprates~~

manganites

What are the pnictides Really?

manganites

multi-orbitals,
orbital order,
lattice distortions
magnetism, local/
itinerant electrons

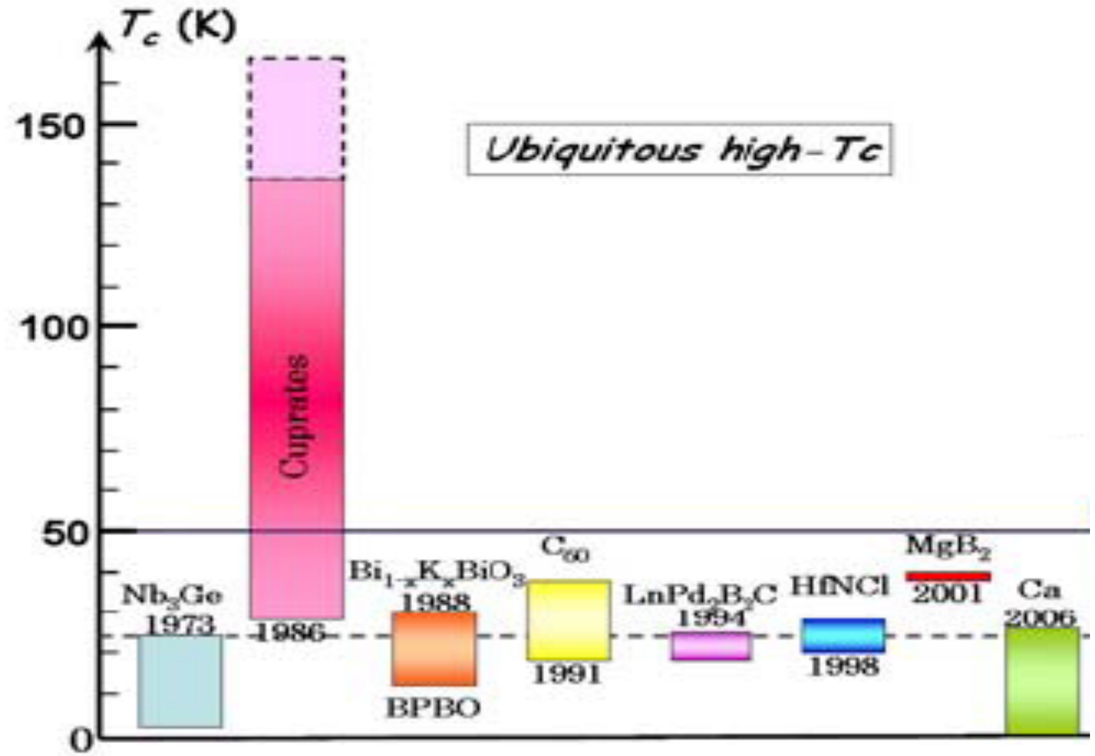
What are the pnictides Really?

manganites

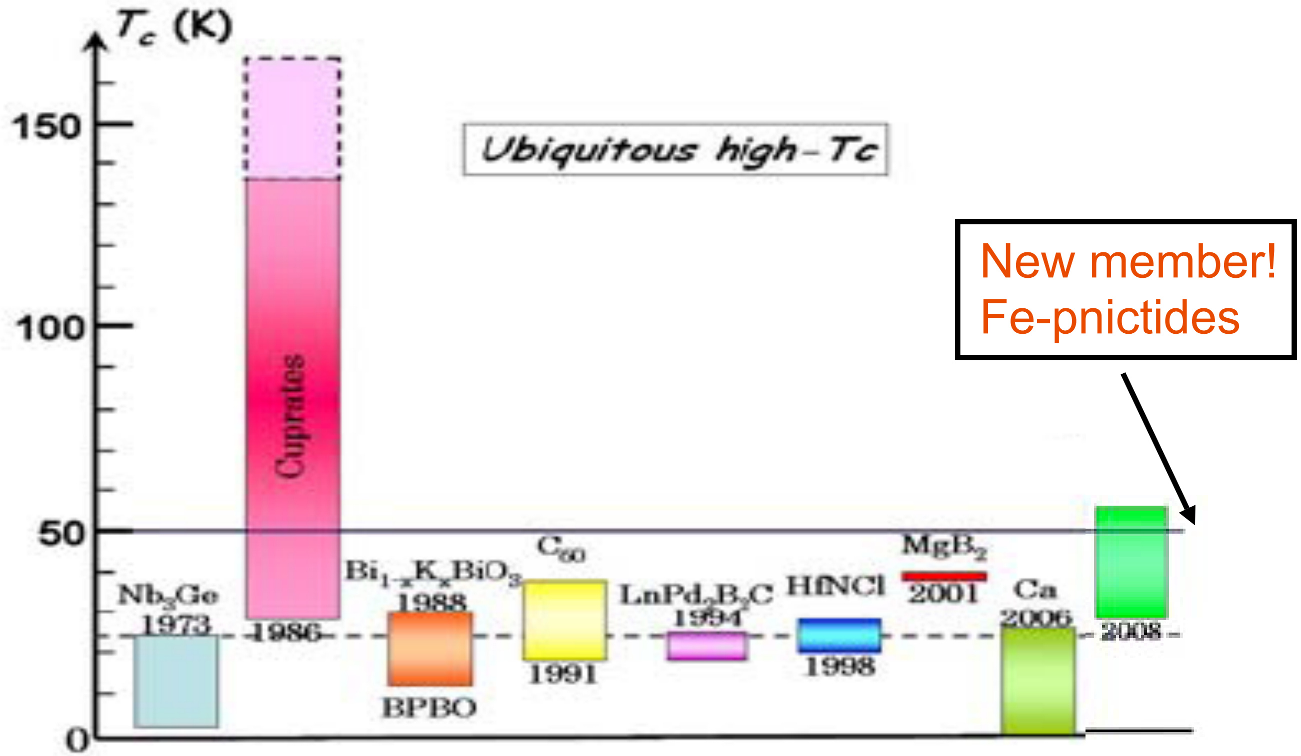
multi-orbitals,
orbital order,
lattice distortions
magnetism, local/
itinerant electrons

$$J_H S_c \ll \infty$$

Search for high T_c



Search for high T_c



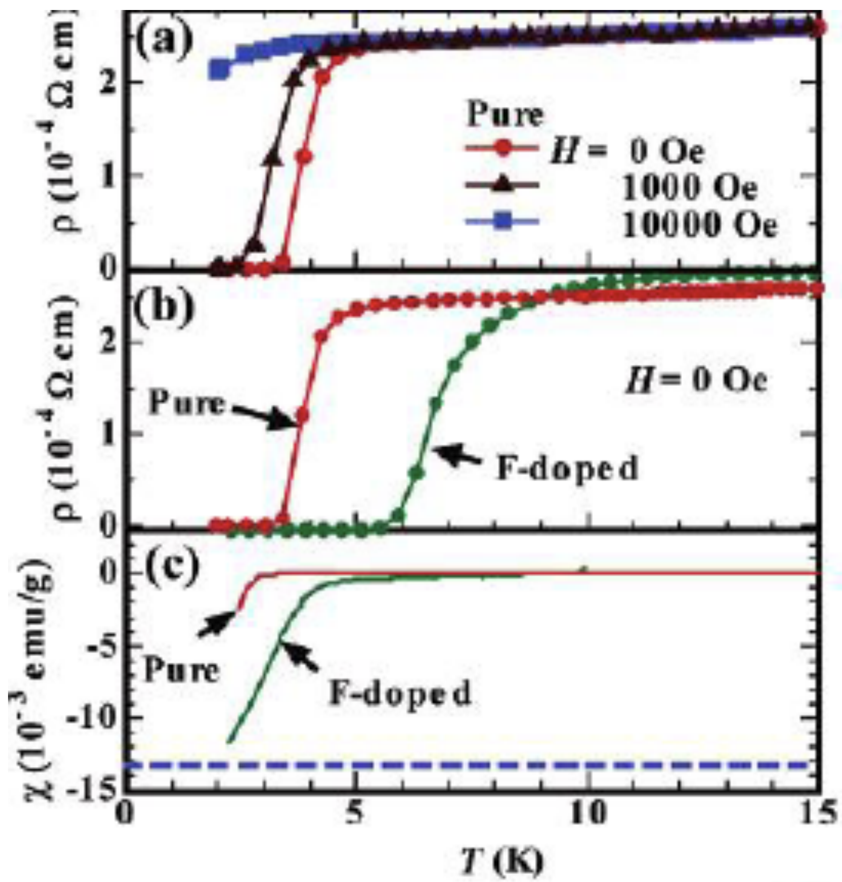
J|A|C|S
COMMUNICATIONS

Published on Web 07/15/2006

Iron-Based Layered Superconductor: LaOFeP

Yoichi Kamihara,† Hidenori Hiramatsu,† Masahiro Hirano,†,‡ Ryuto Kawamura,§ Hiroshi Yanagi,§ Toshio Kamiya,†,§ and Hideo Hosono*,†,‡

ERATO-SORST, JST, Frontier Collaborative Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan, Frontier Collaborative Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan, and Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-4, 4259 Nagatsuta, Yokohama 226-8503, Japan



T_C = 4 K,
7 K (F doping)

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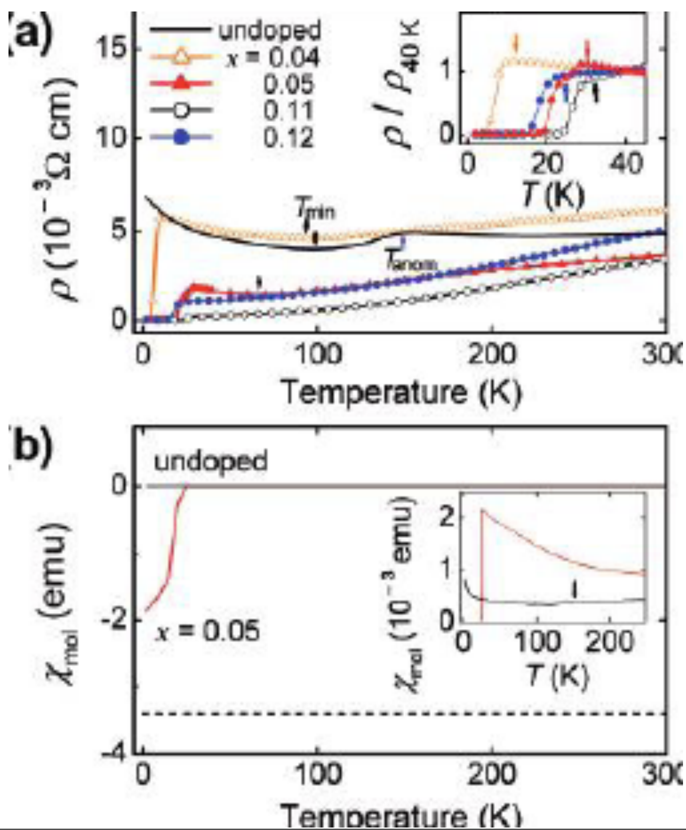
COMMUNICATIONS

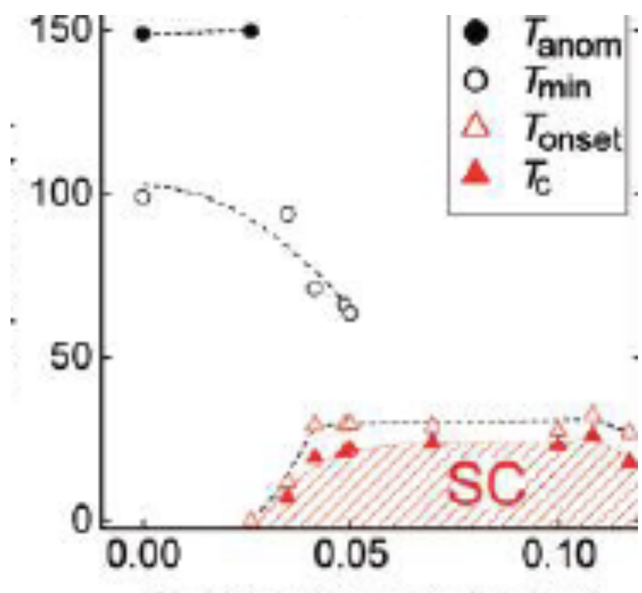
Published on Web 02/23/2008

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

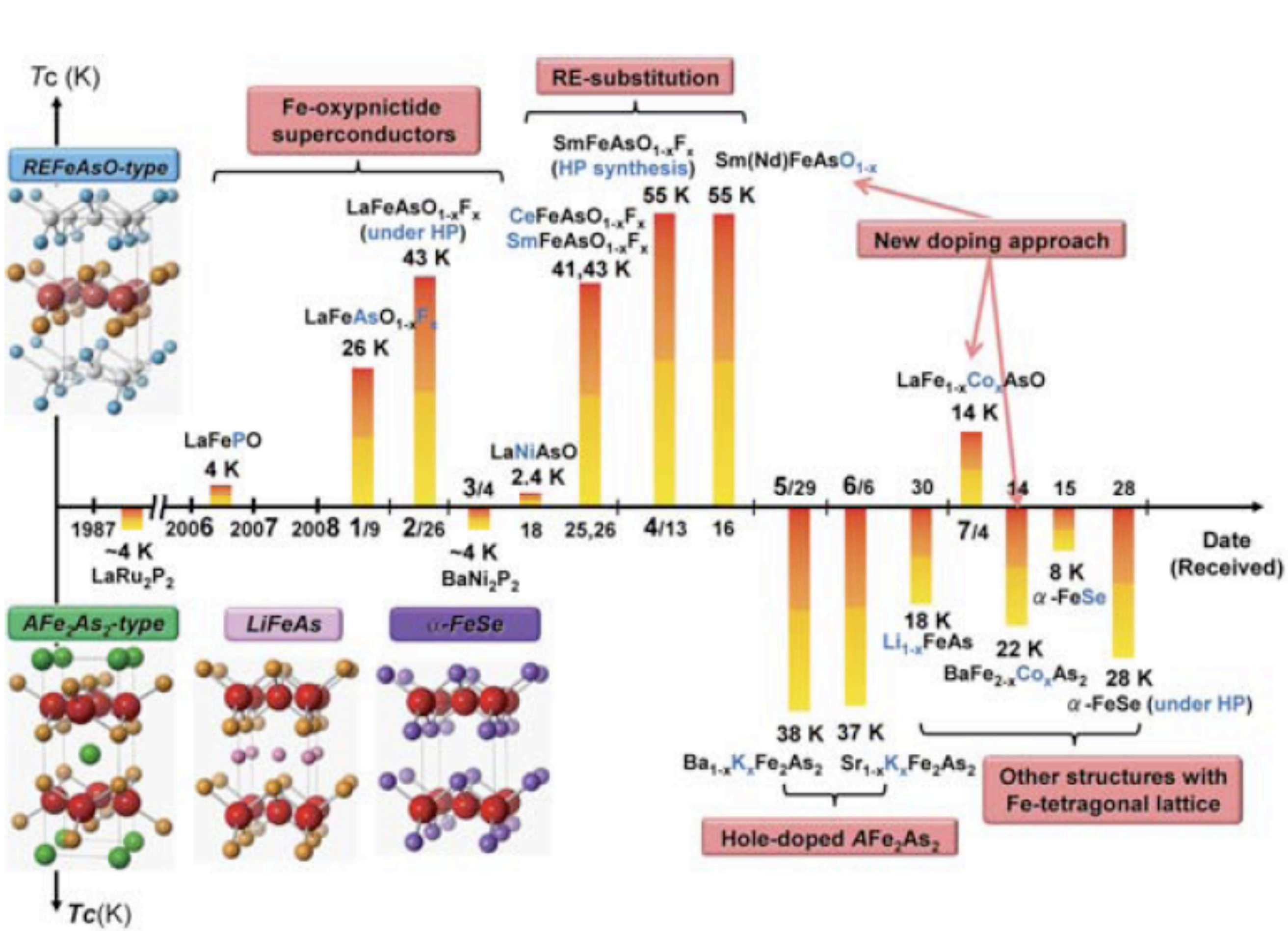
Yoichi Kamihara,*[†] Takumi Watanabe,[‡] Masahiro Hirano,[†,§] and Hideo Hosono[†,‡,§]

ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan





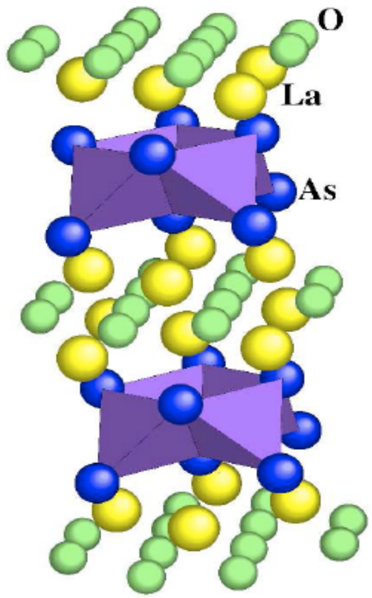
Many iron-based superconductors with T_c up to 56K



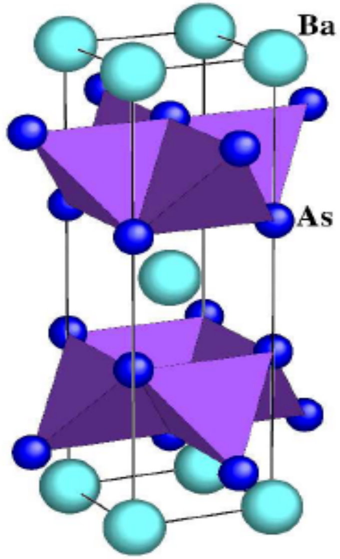
Tour of iron village

Taxonomy

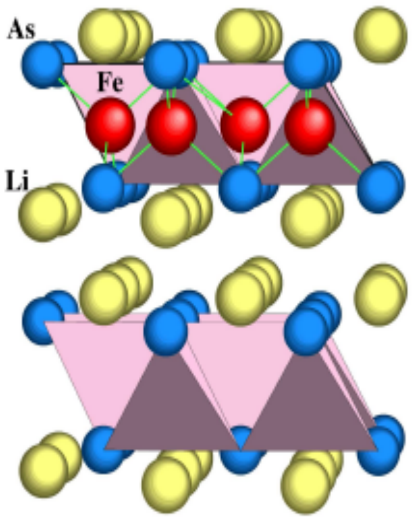
- 1111-family
- 122-family
- 111-family



LaOFeAs



$BaFe_2As_2$

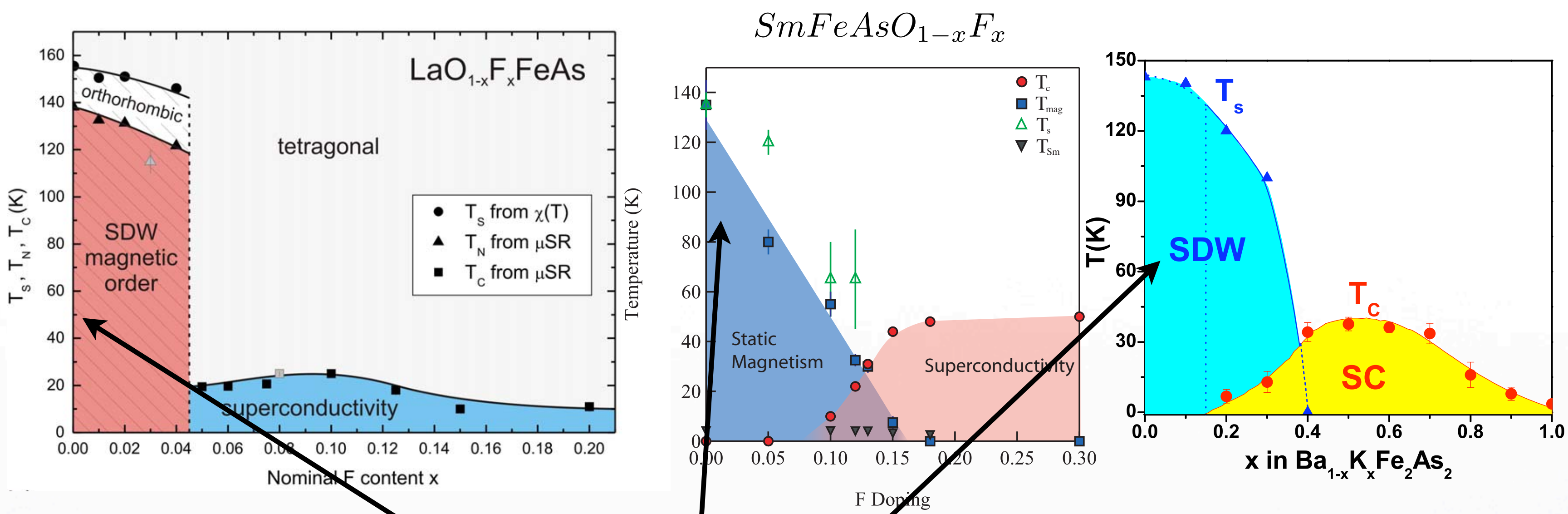


LiFeAs

11-family FeSe, 32522-family $(Sr_3Sc_2O_5)Fe_2As_2$ and many

4 As: tetrahedron

Key Structure:
Fe As-trilayers



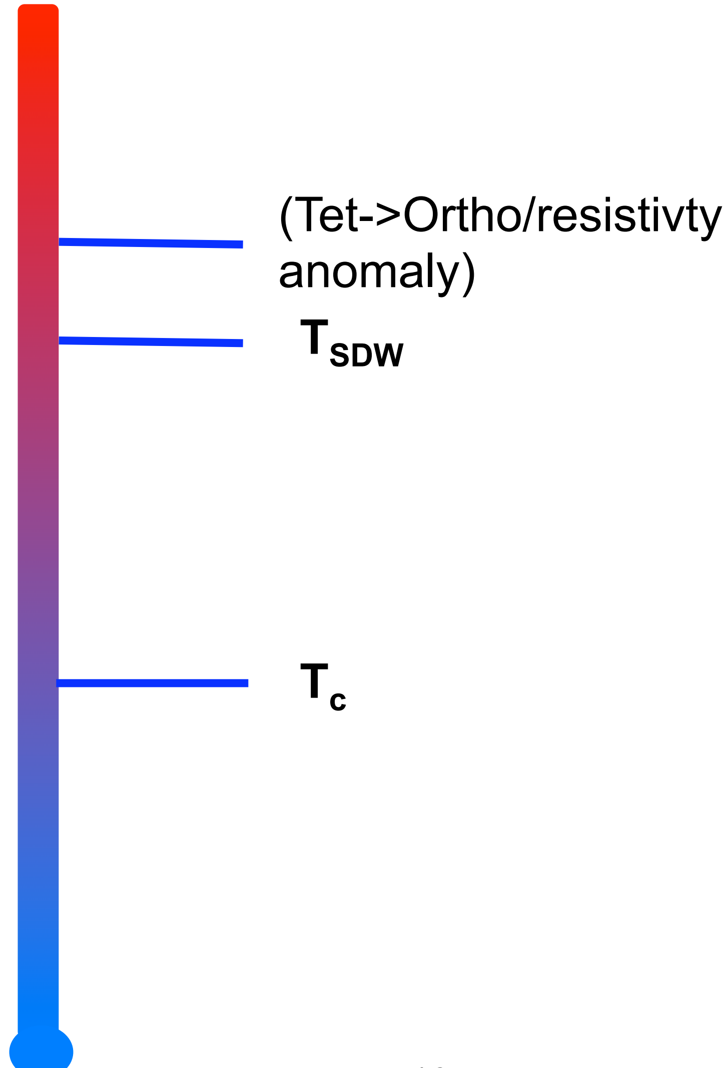
LaO1-xFxFeAs
orthorhombic
tetragonal
SDW magnetic order
superconductivity
Ts from χ(T)
TN from μSR
TC from μSR
Ts, TN, TC (K)
Nominal F content x
SmFeAsO1-xFx
Temperature (K)
Static Magnetism
Superconductivity
Tc
Tmag
Ts
TSm
F Doping
Ts
SDW
TC
SC
T(K)
x in Ba1-xKxFe2As2

1111

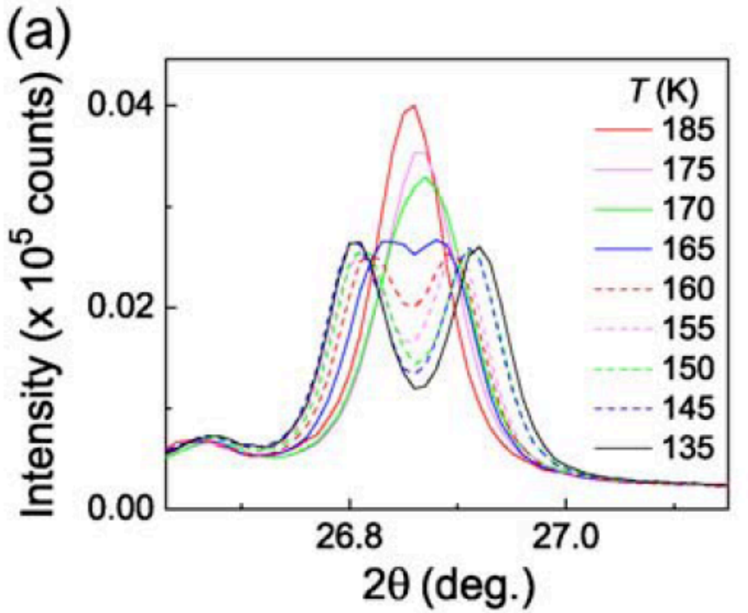
122

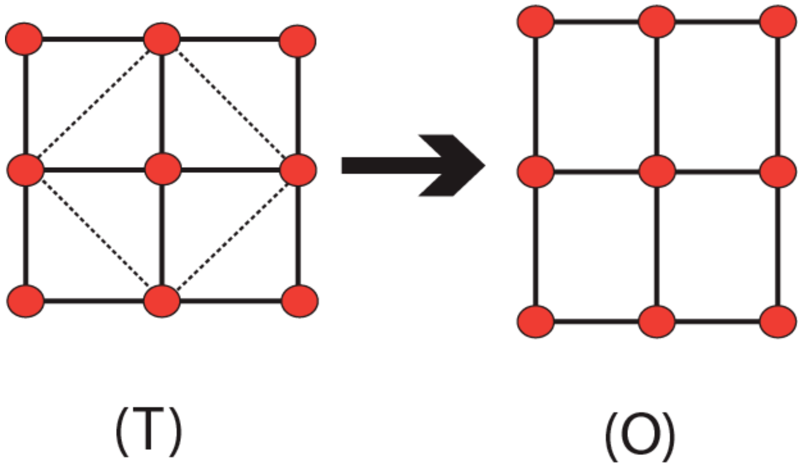
Why?

To explain??



Structural Phase Transition





$T_{\mathrm{SPT}} = 150$ K

Fe-Fe Bond Length:

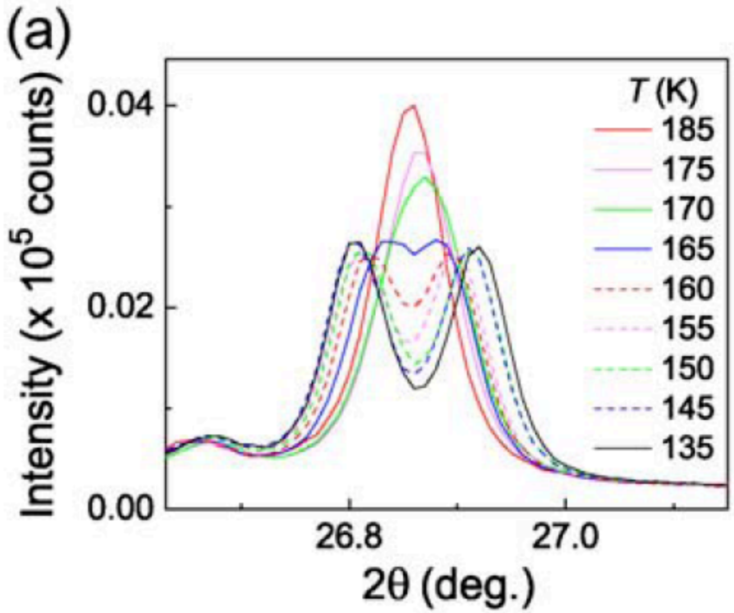
$a = b = 2.85$ Å (**T**)

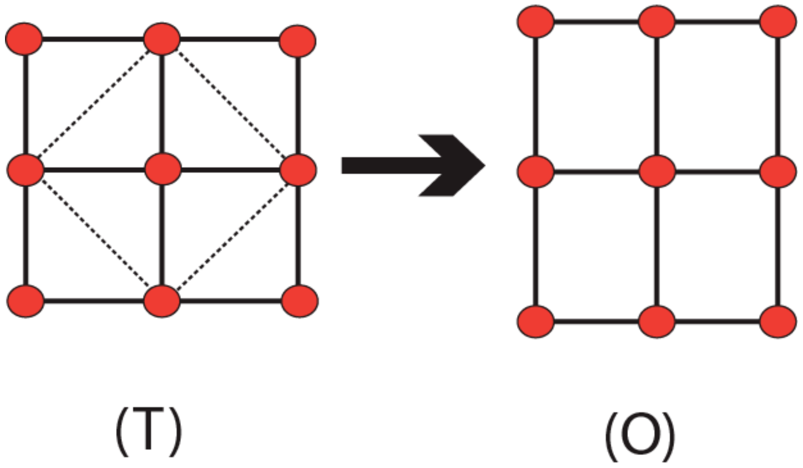
$a = 2.84$ Å

$b = 2.86$ Å (**O**)

$\delta = 0.01$ Å

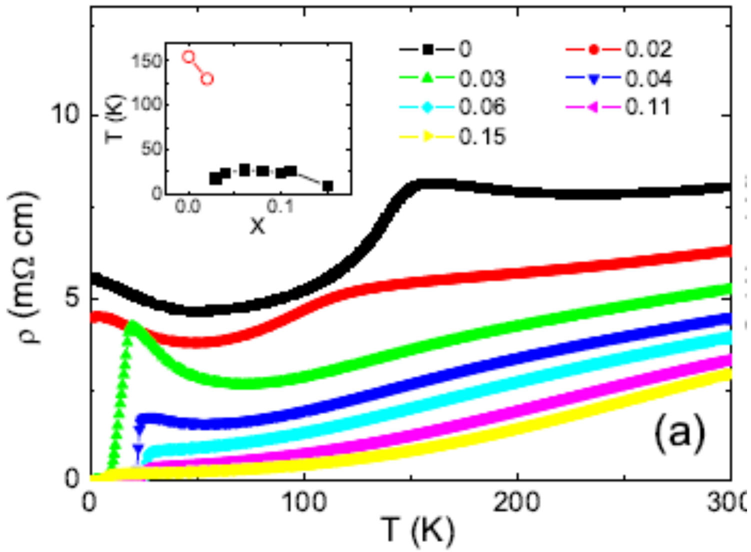
Structural Phase Transition





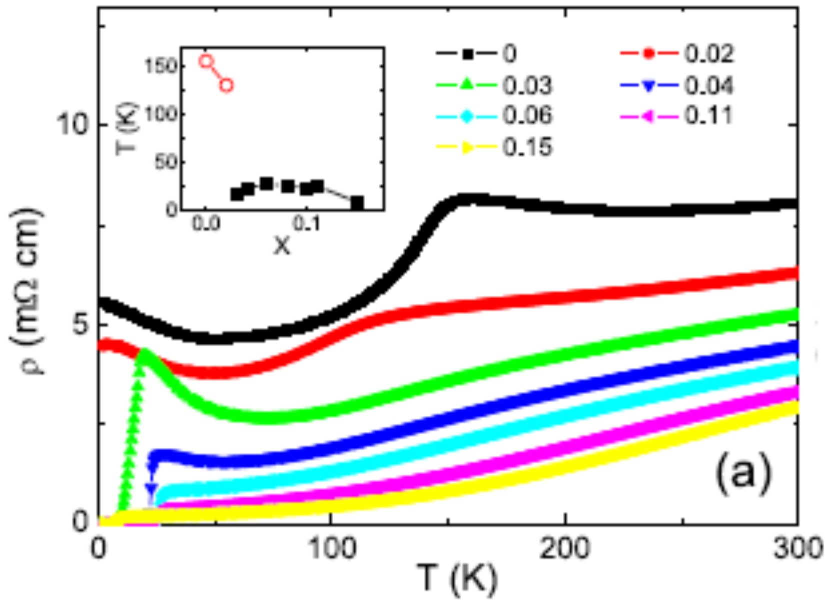
- **Resistivity Anomaly** $T_{\mathrm{RA}} = T_{\mathrm{SPT}}$

$T_{\mathrm{SPT}} = 150$ K
Fe-Fe Bond Length:
$a = b = 2.85$ Å (T)
$a = 2.84$ Å
$b = 2.86$ Å (O)
$\delta = 0.01$ Å



arXiv:0803.3426

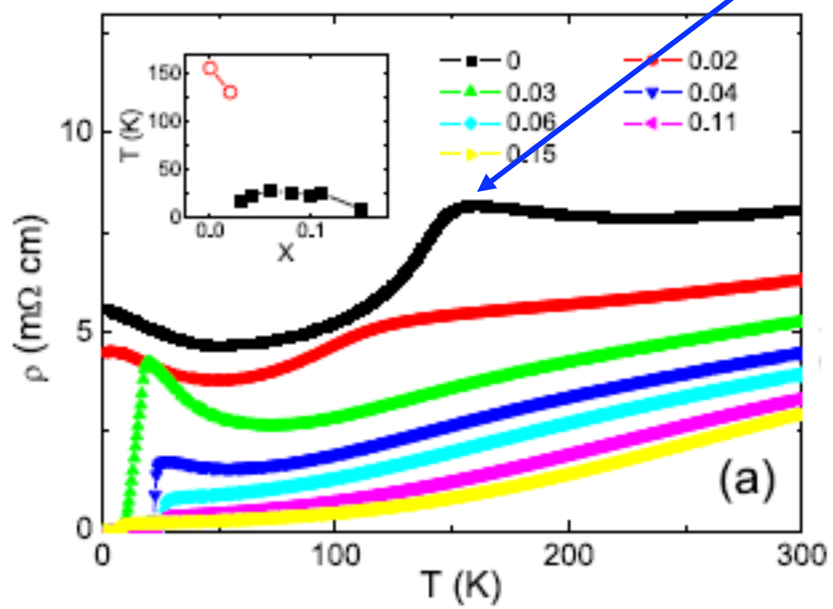
$LaO_{1-x}F_x$ Fe As



arXiv:0803.3426

Structural phase transition (1)
And Resistivity Anomaly(150K)

$LaO_{1-x}F_x$ Fe As



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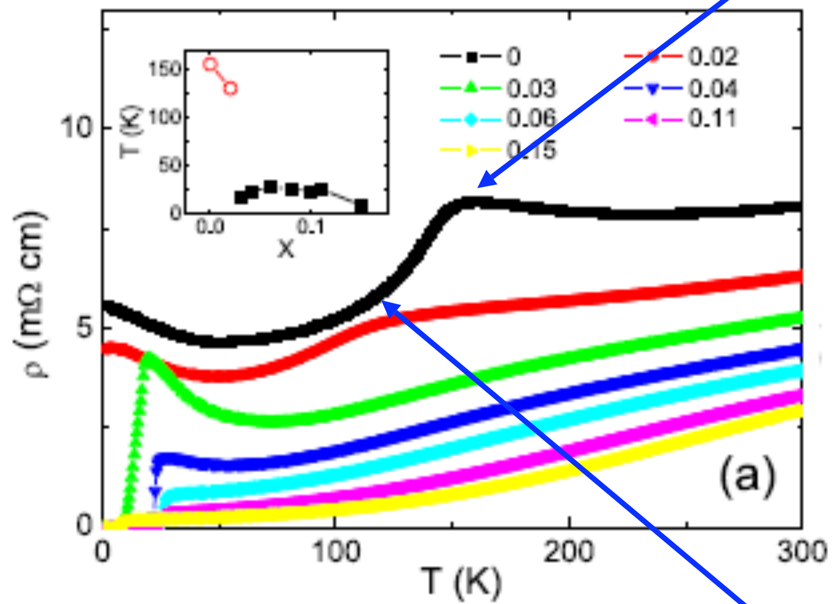
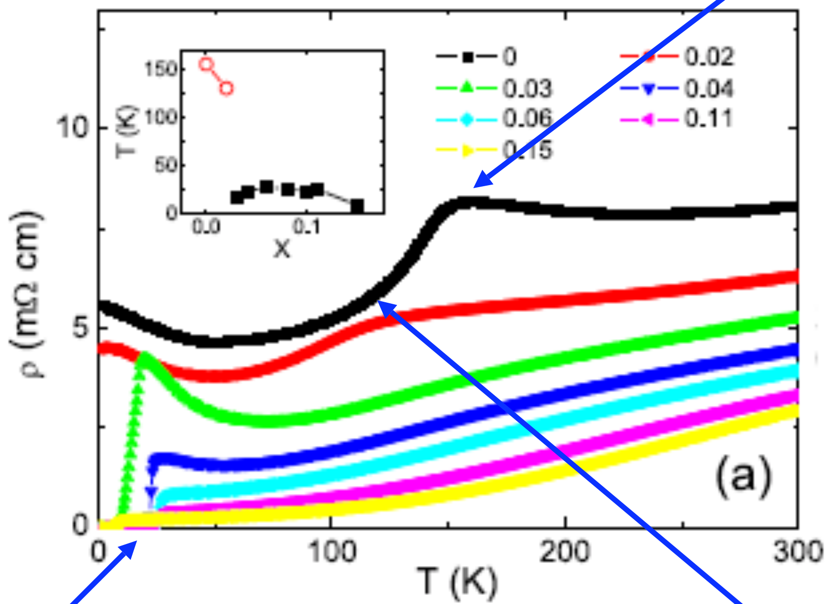


Spin-density-wave
Transition (137K) (2)

arXiv:0803.3426

Structural phase transition (1)
And Resistivity Anomaly(150K)

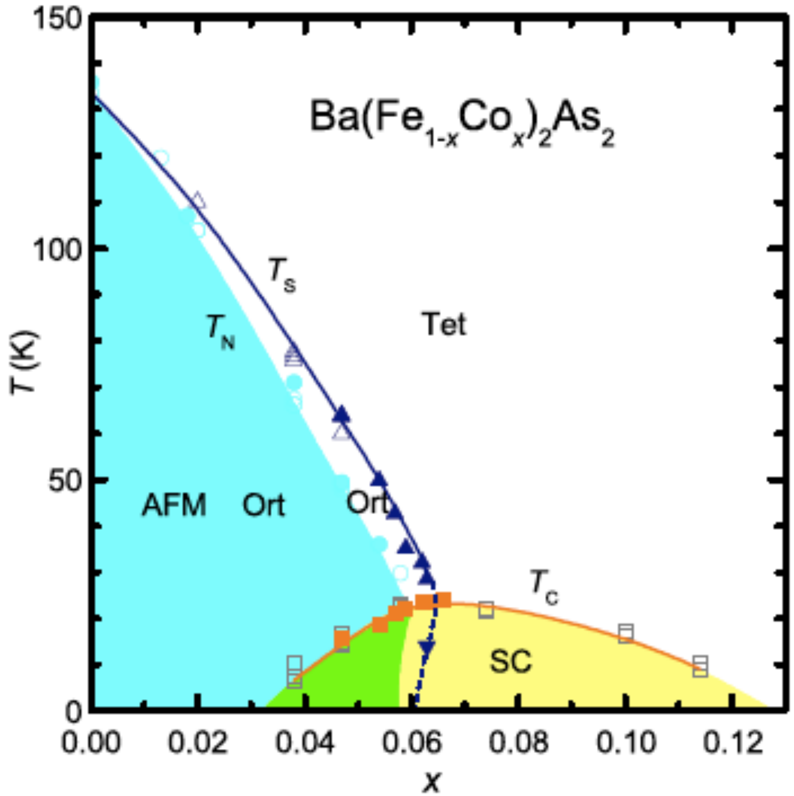
$LaO_{1-x}F_x$ Fe
As



T_c=26 K
Superconductivity (3)

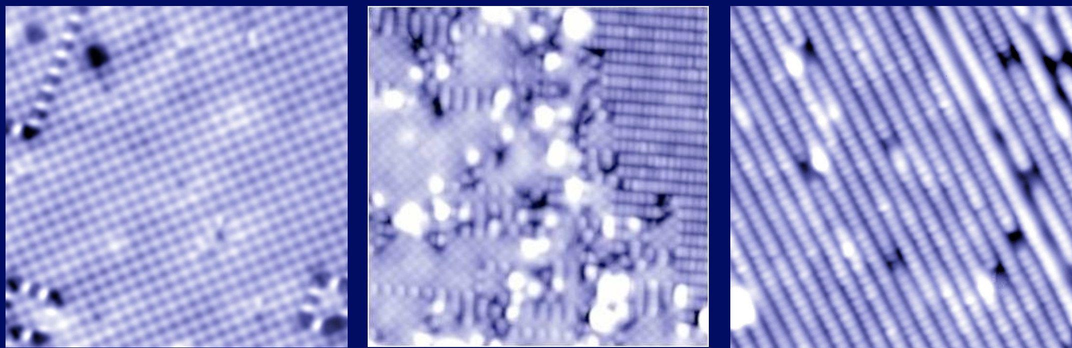
Spin-density-wave
Transition (137K) (2)

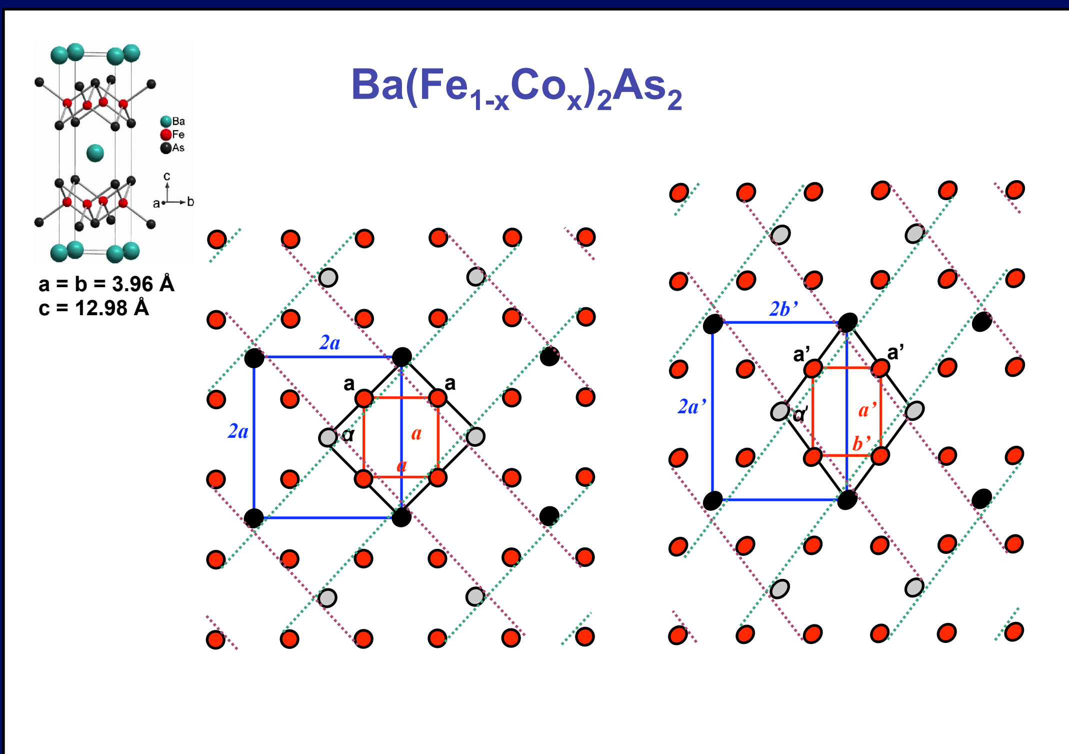
Where does the stuctural transition end?

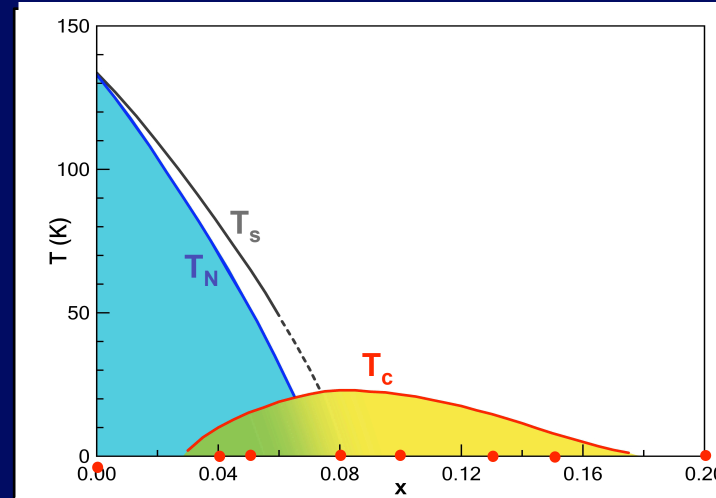


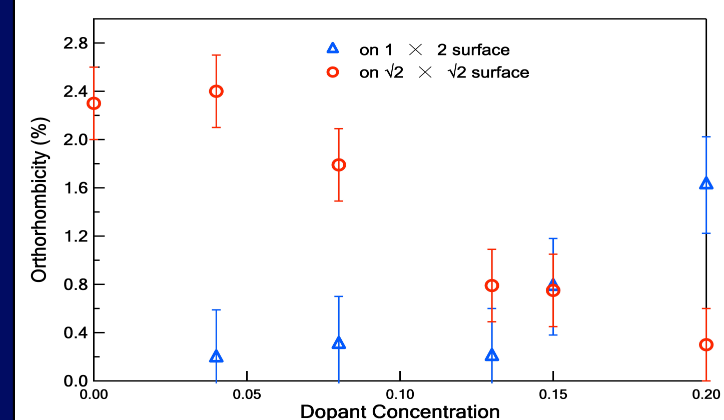
Phys. Rev. Lett. 104, 057006 (2010)

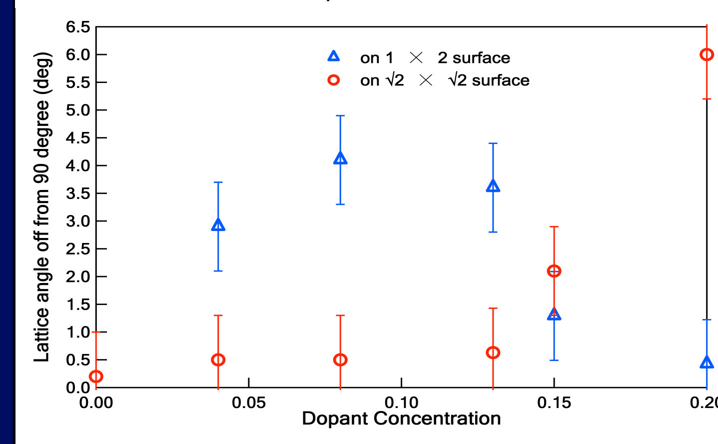
Doping Dependence *of* Lattice Orthorhombicity



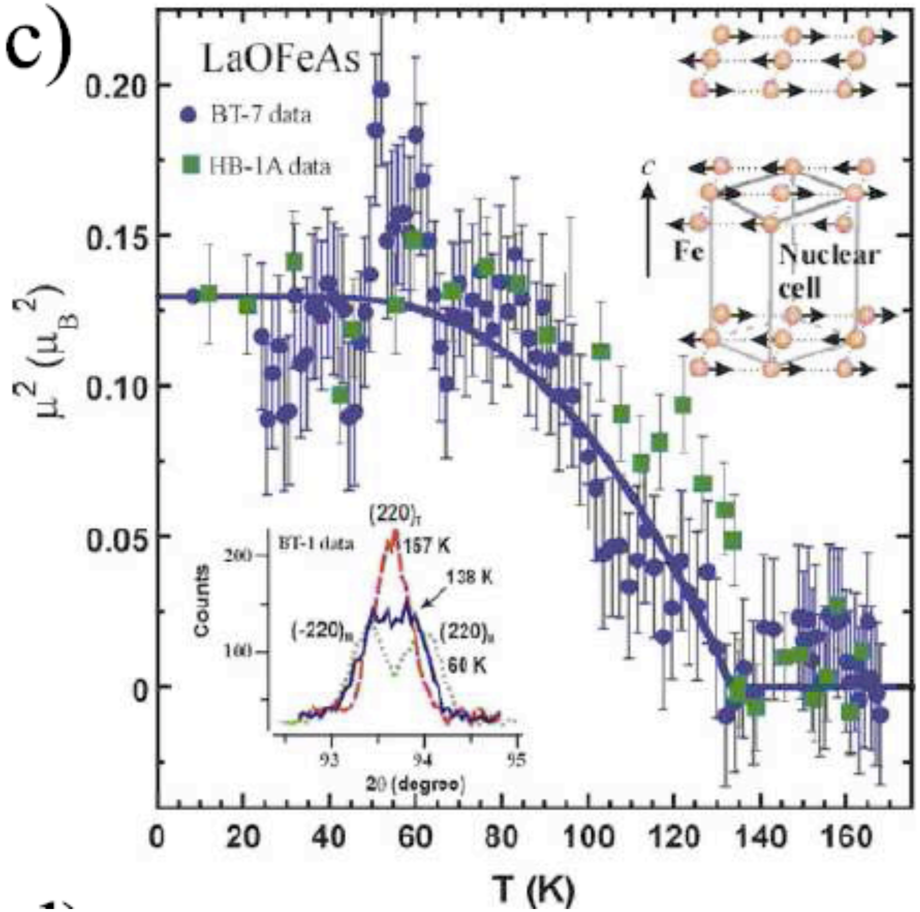




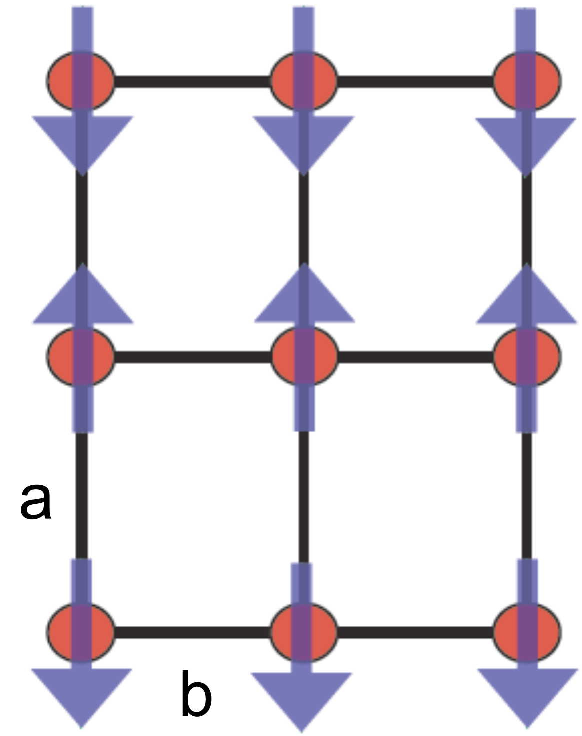




Collinear Anti-ferromagnetism (SDW)



C. de la Cruz, Nature



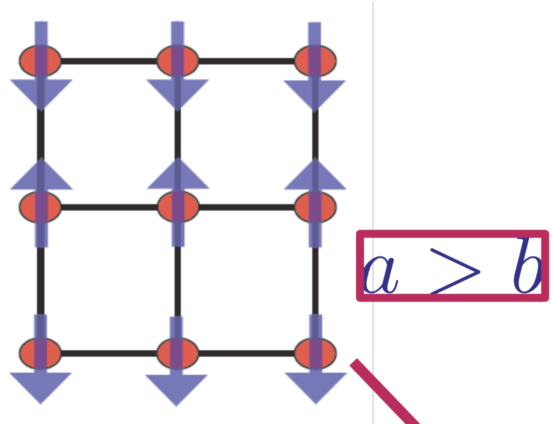
1111 family:

$T_{\mathrm{SDW}} < T_{\mathrm{SPT}}$

122 family:

$T_{\mathrm{SDW}} = T_{\mathrm{SPT}}$

Magnetism



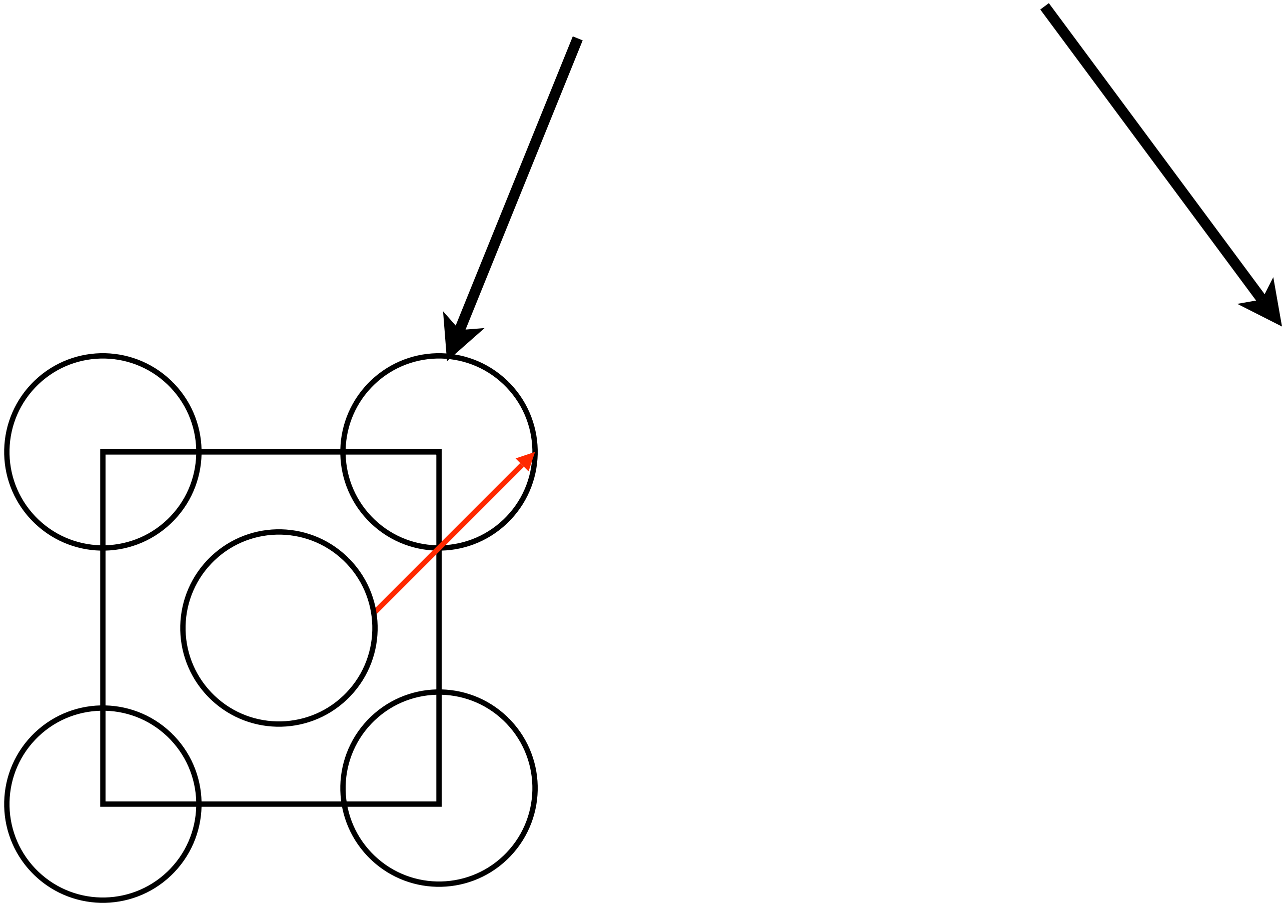
- 1111 (LaOFeAs)
- 2 second-order phase transitions

T_S=157, T_M=137K

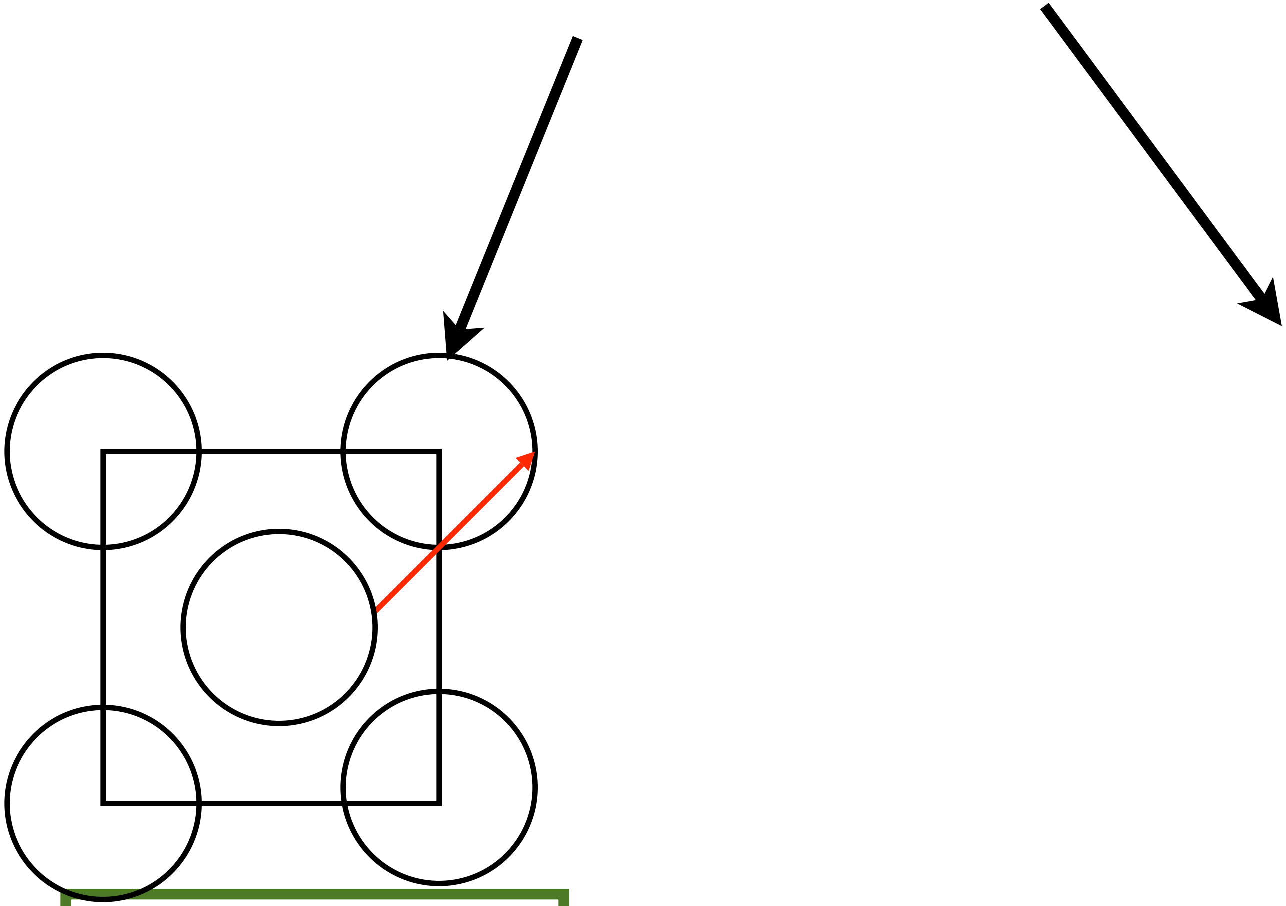
- 122 (LaOFeAs)
- 1 first-order transition

T_S=T_M=144K

Simple Model for Magnetism

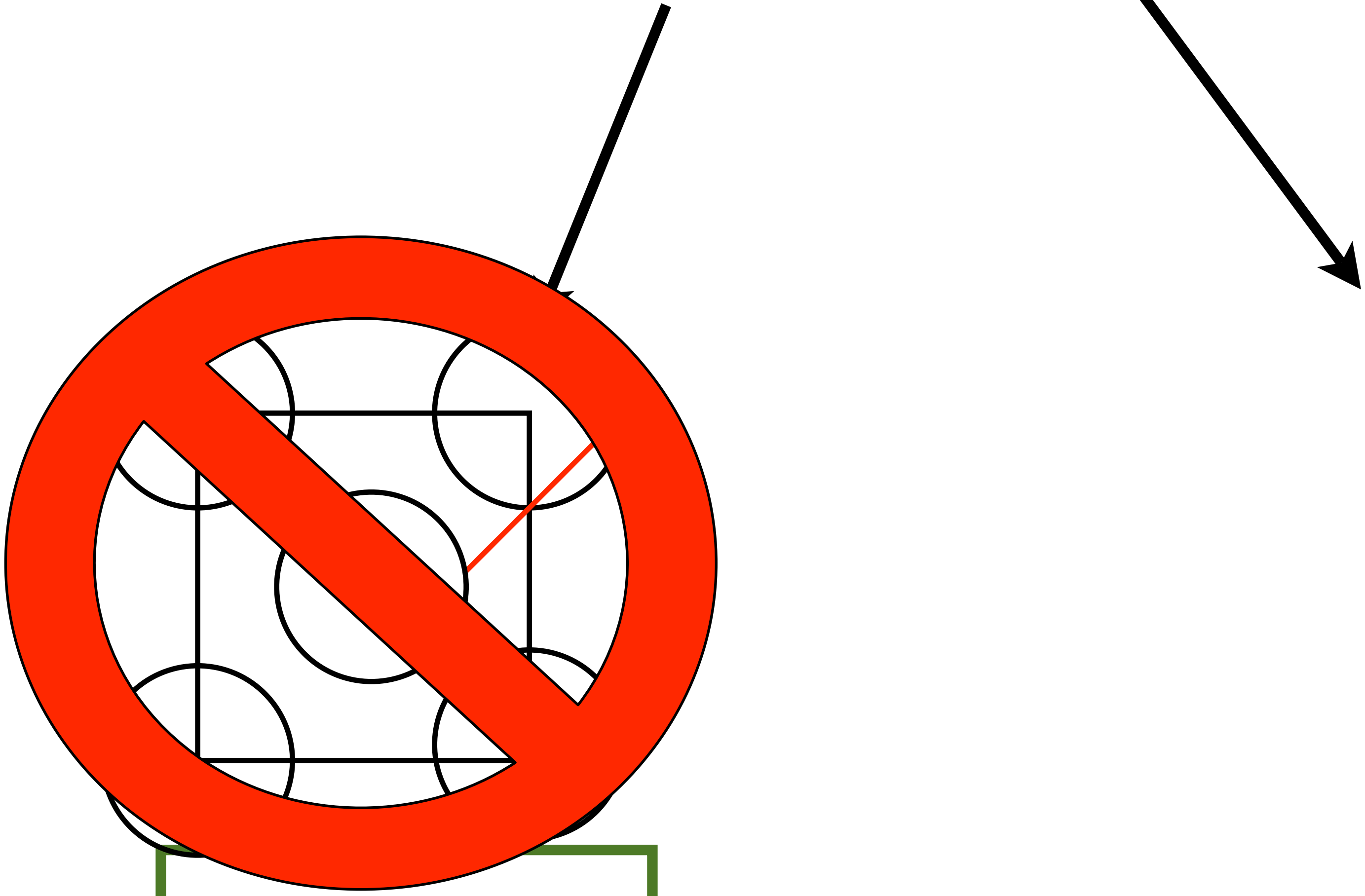


Simple Model for Magnetism



monoclinic distortion

Simple Model for Magnetism



monoclinic distortion

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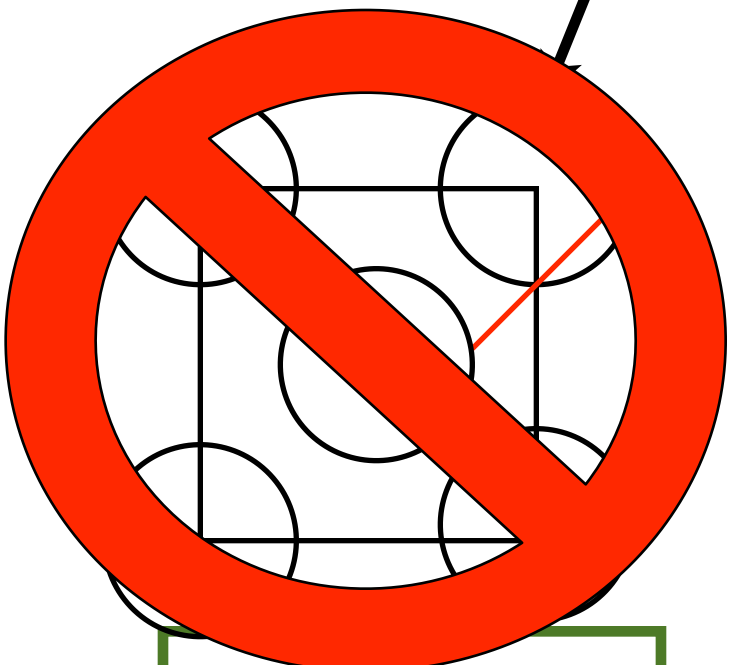
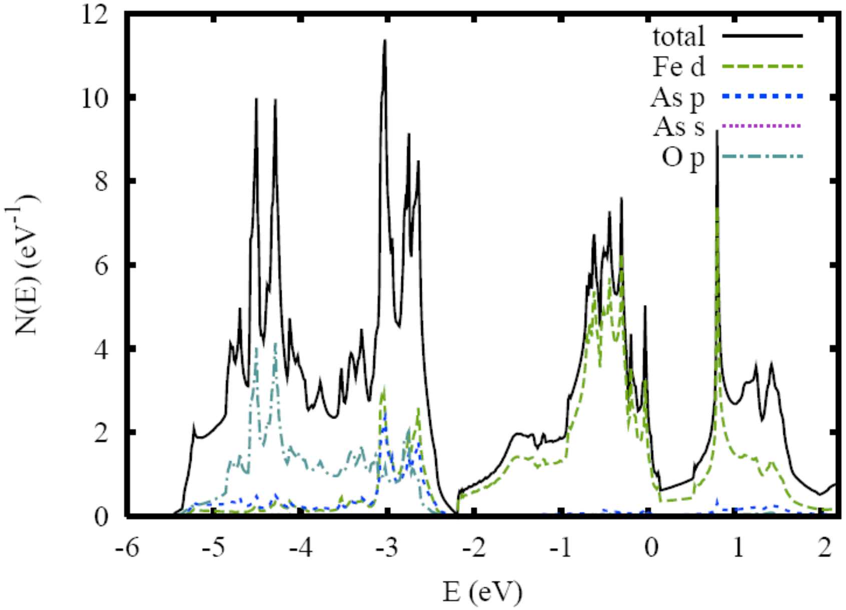


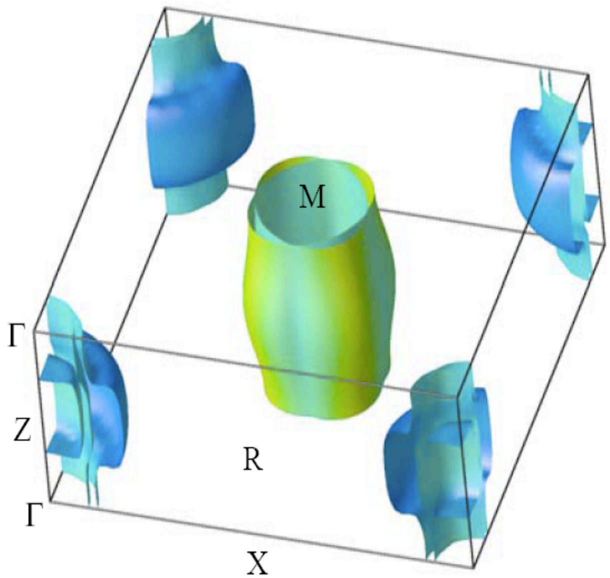
monoclinic distortion

local moments

Are the pnictides strongly correlated?

Multibands





PRL **100**, 237003 (2008) PHYSICAL REVIEW LETTERS week ending 13 JUNE 2008

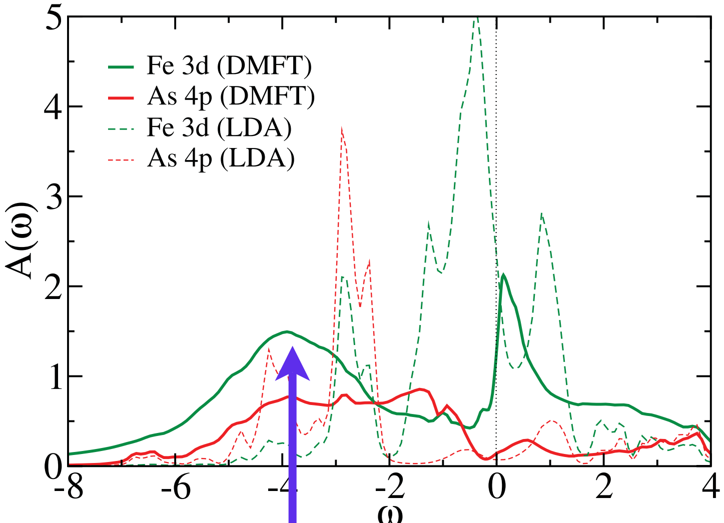
Density Functional Study of LaFeAs$O_{1-x}F_x$: A Low Carrier Density Superconductor Near Itinerant Magnetism

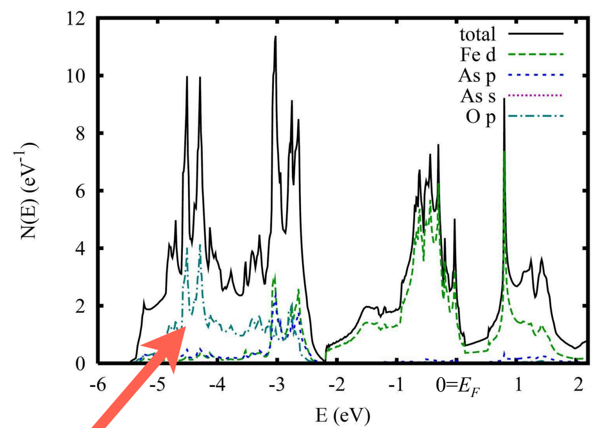
D. J. Singh and M.-H. Du

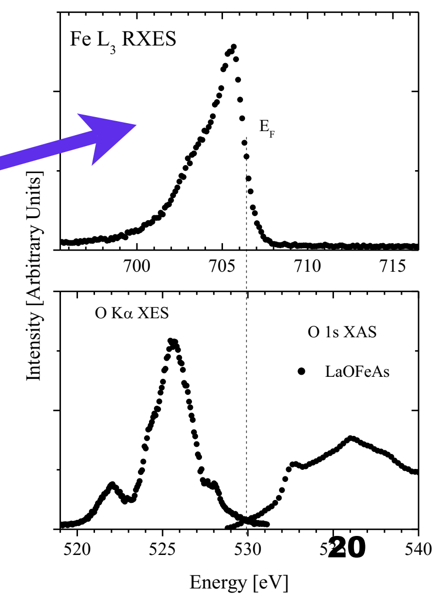
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114, USA

(Received 4 March 2008; published 12 June 2008)

Are the pnictides strongly correlated?





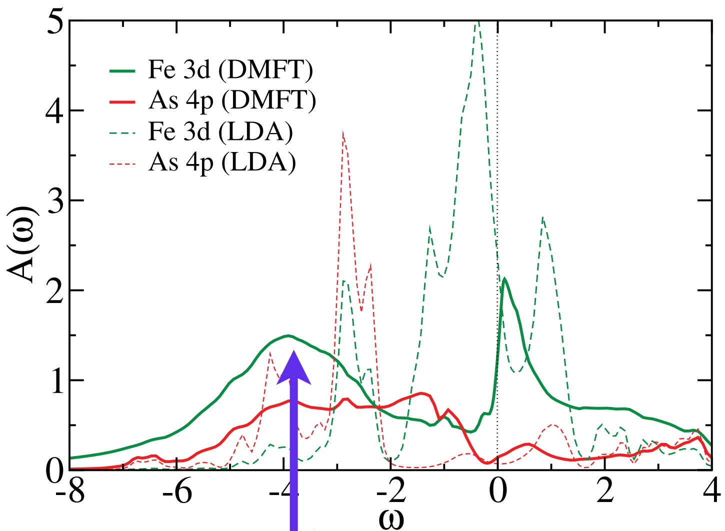


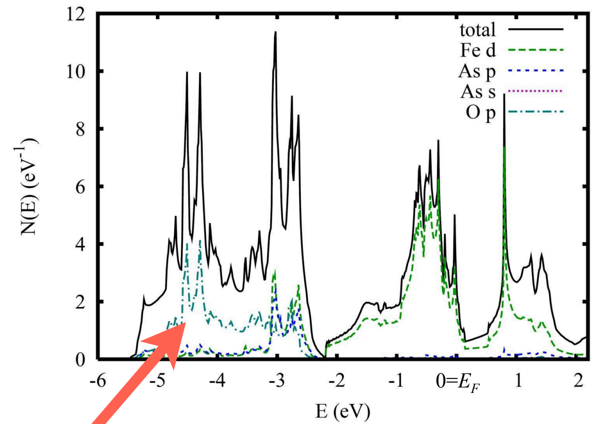
Fe 3d peak at 4eV below E_F:
Lower Hubbard band

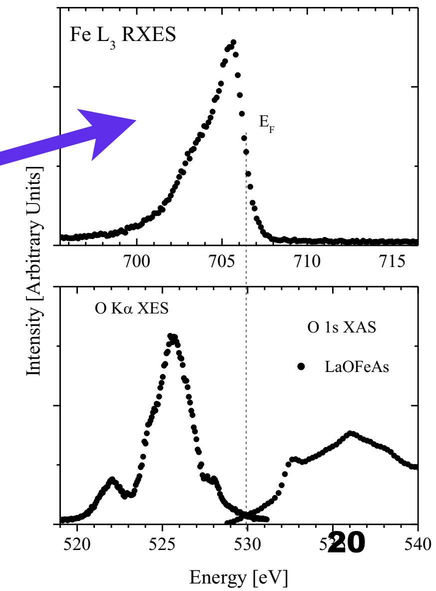
LDA and Experiment show no Fe 3d lower Hubbard band

Are the pnictides strongly correlated?

Where's Mott?





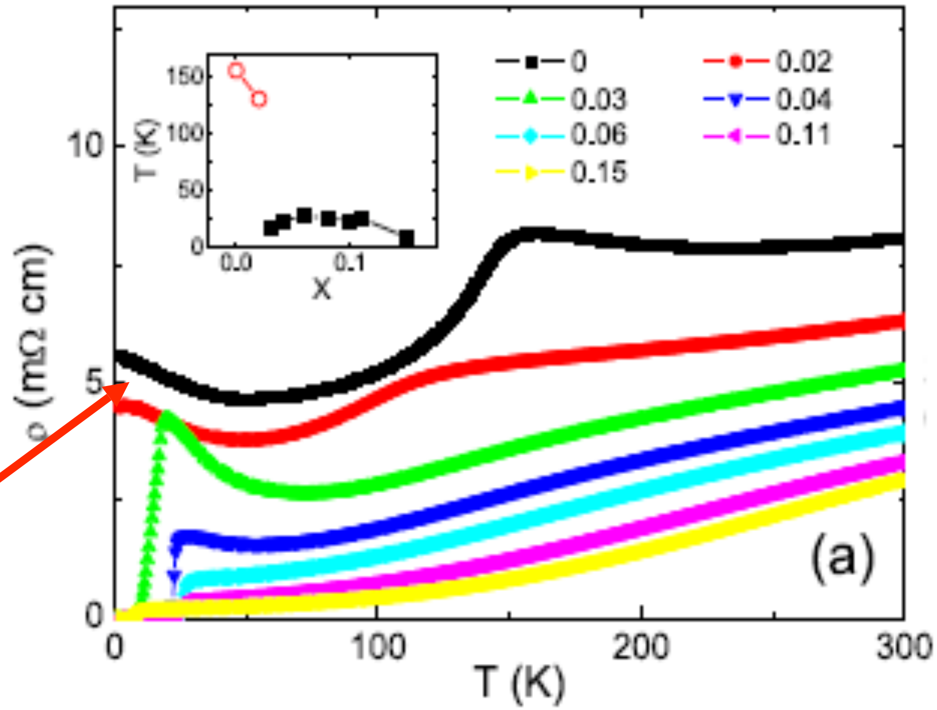


Fe 3d peak at 4eV below E_F:
Lower Hubbard band

LDA and Experiment show no Fe 3d lower Hubbard band

$\boxed{\text{No}}$

Intermediate Coupling

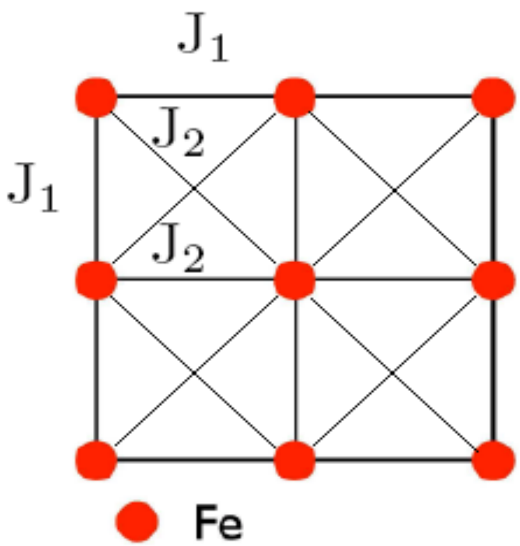


Fe-pnictides

Parent compound:

Bad metal

how far can one get with local moments?



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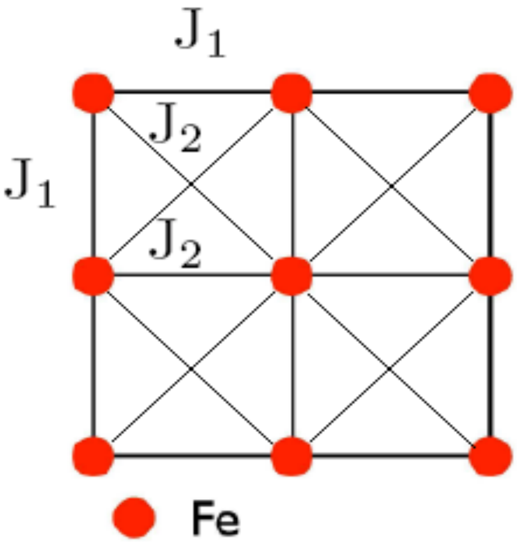
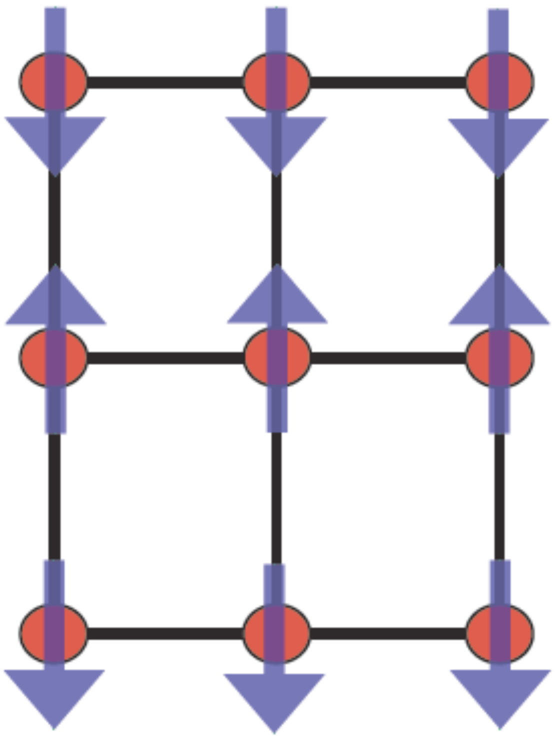
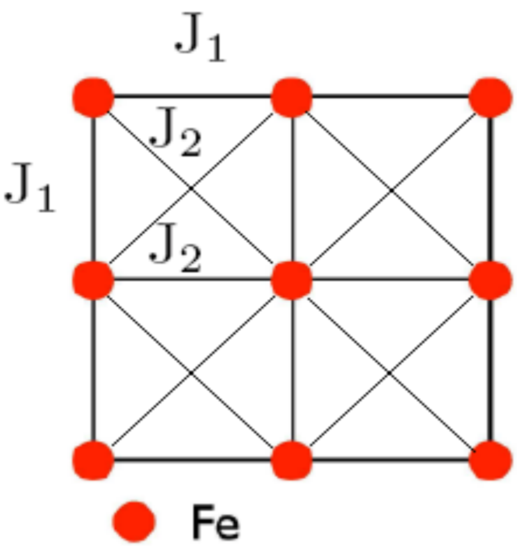


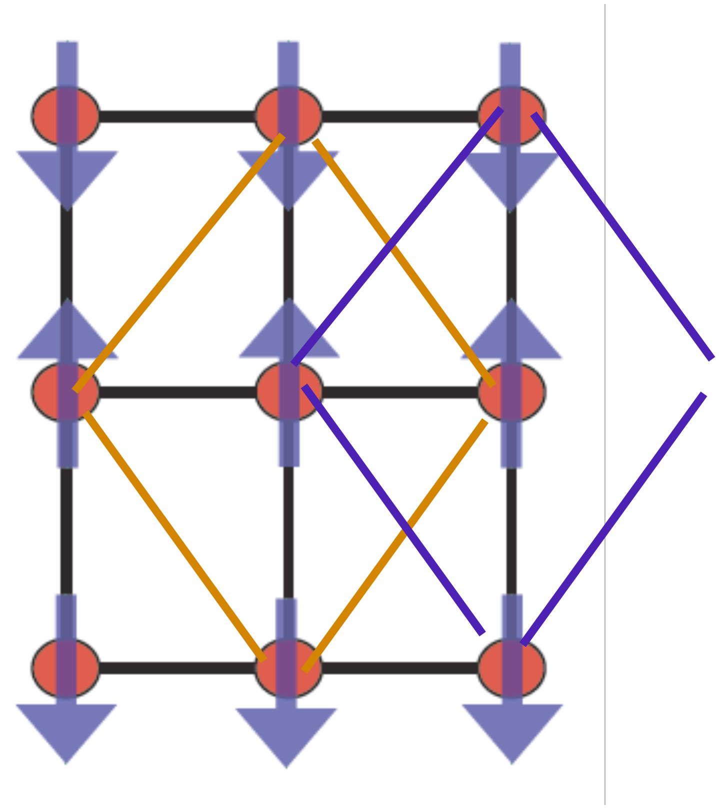
$$J_2 > J_1/2$$



how far can one get with local moments?

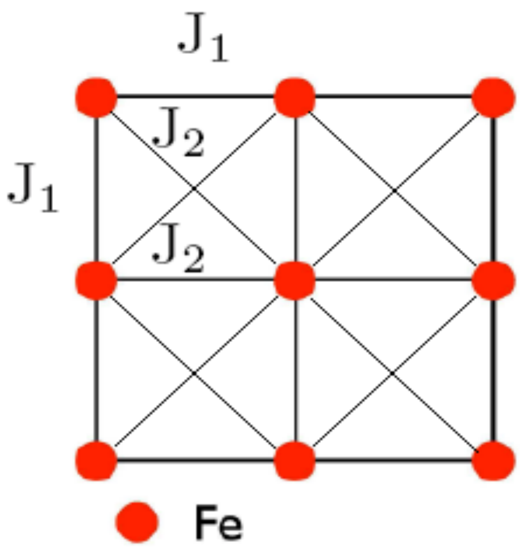


$$J_2 > J_1/2$$



Two interpenetrating AF sublattices

how far can one get with local moments?

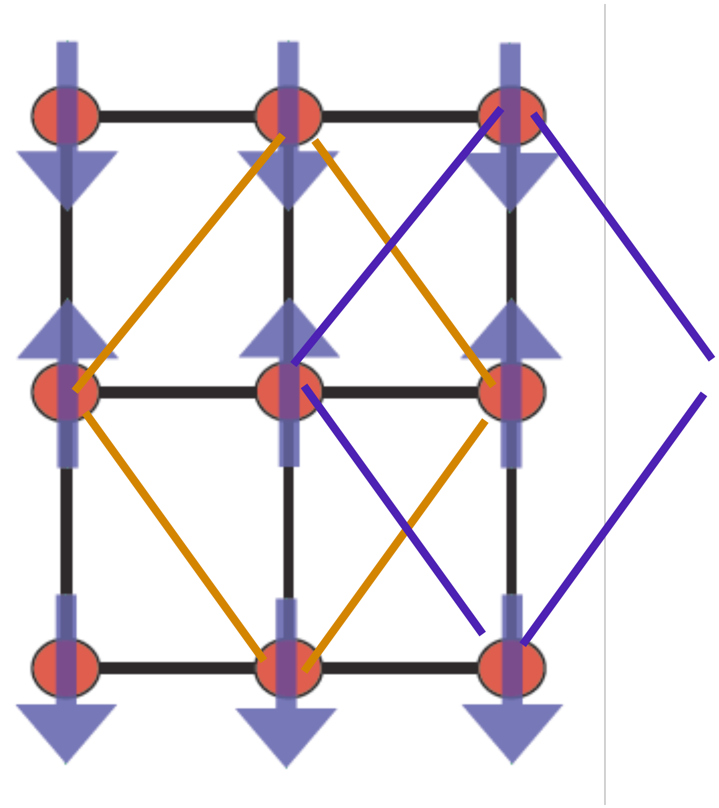


$$J_2 > J_1/2$$

$$\varphi = \hat{n}_1 \cdot \hat{n}_2$$

$$\langle \varphi \rangle \neq 0$$

$$\langle n_1 \rangle = \langle n_2 \rangle \neq 0$$



Two interpenetrating AF sublattices

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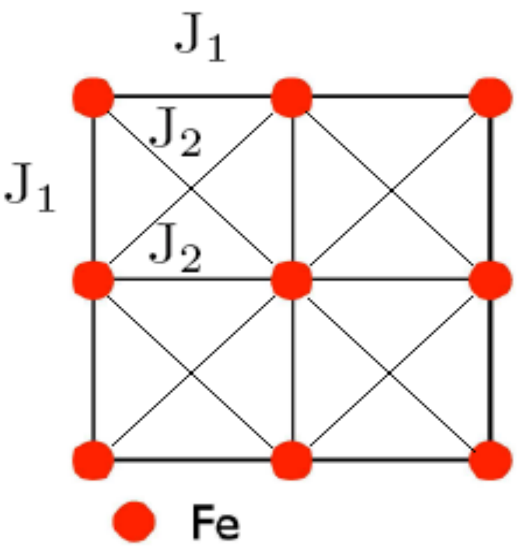

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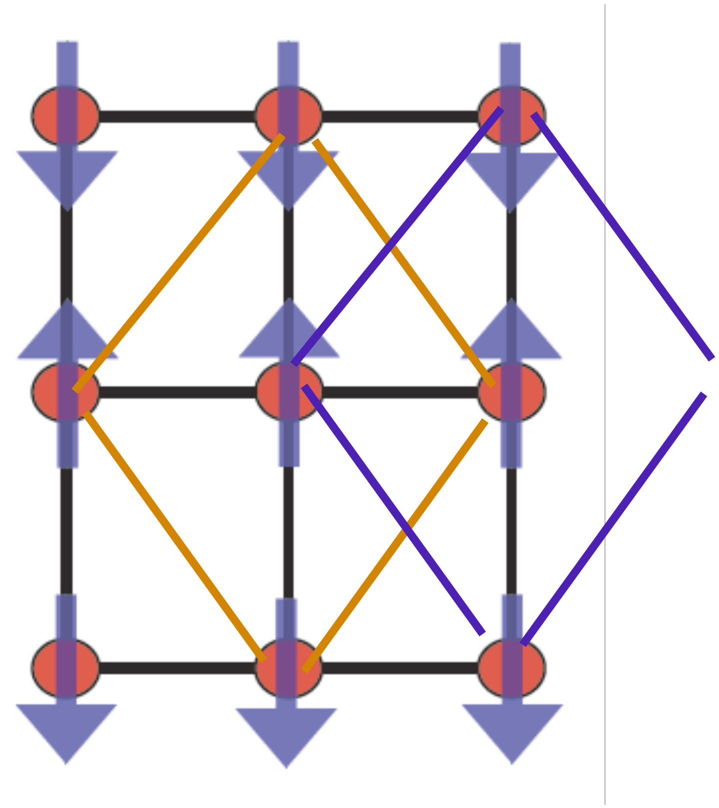
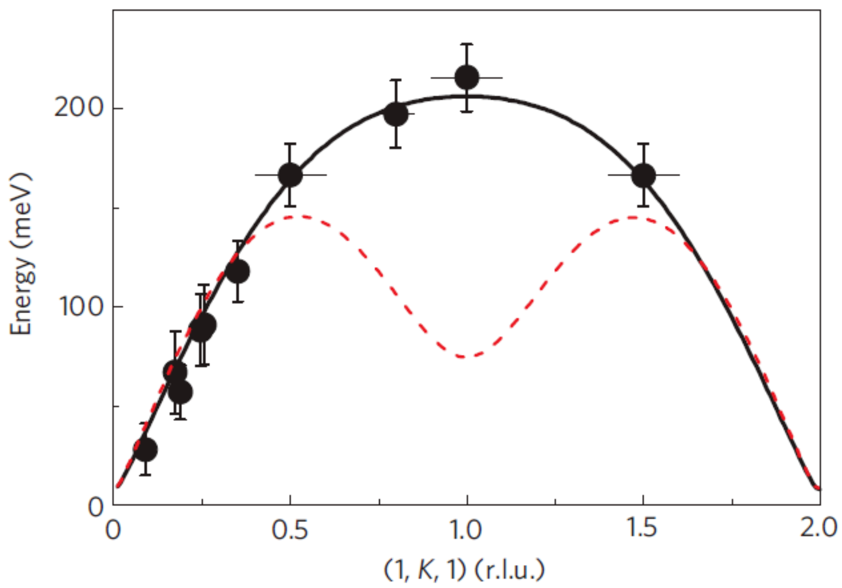


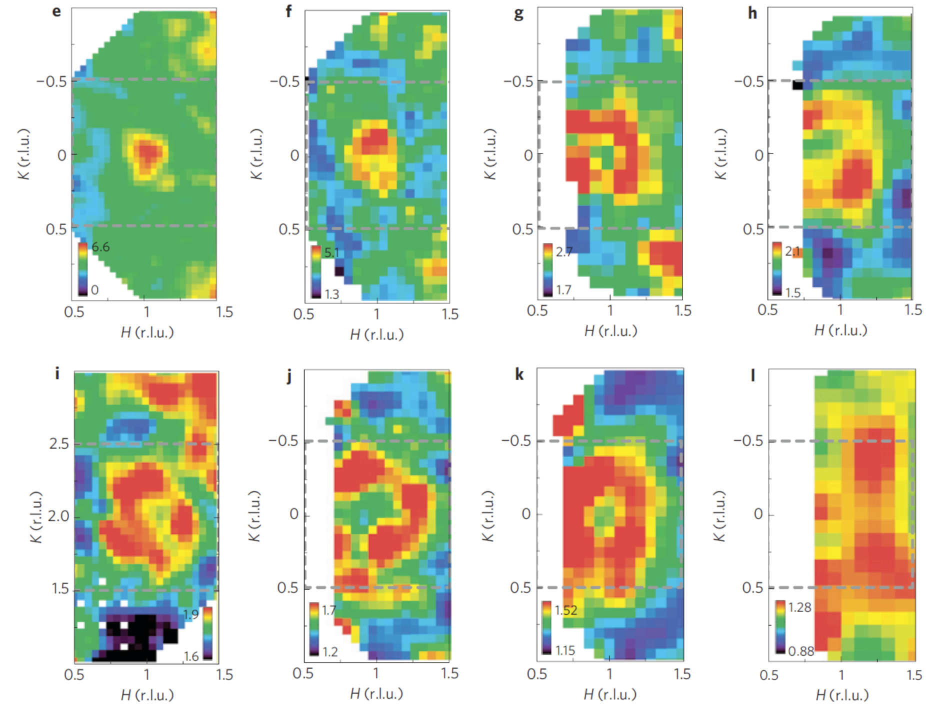
Two interpenetrating AF sublattices

$\boxed{\text{`nematic'}}$ $\langle \varphi \rangle \neq 0$

$$\langle n_1 \rangle = \langle n_2 \rangle = 0$$

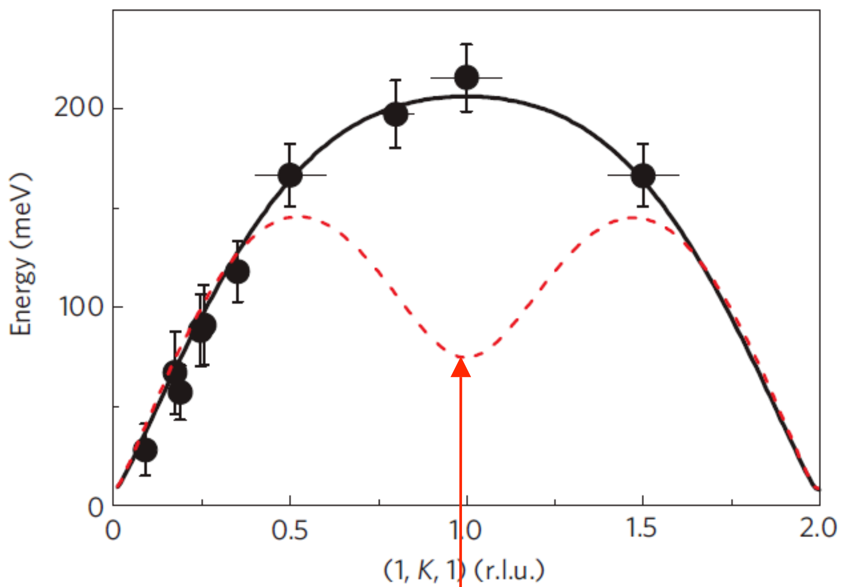
• *Inelastic neutron scattering*





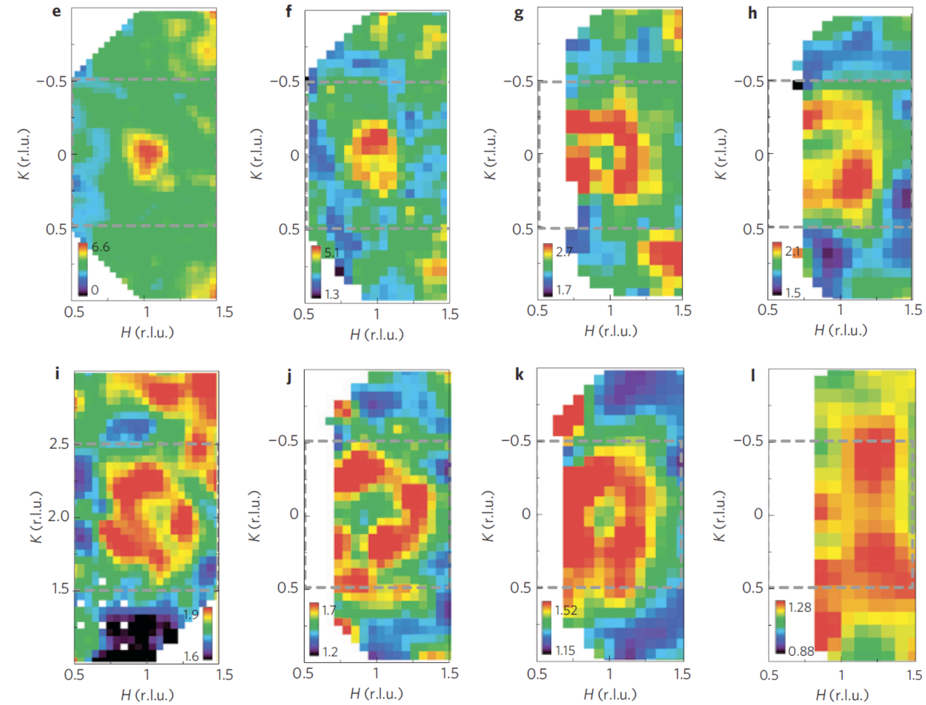
J. Zhao, *et al.* Nature Physics (2009)

- *Inelastic neutron scattering*



Isotropic $J_{1a} \simeq J_{1b}$

$$SJ_1^a = 27\,\mathrm{meV}$$
$$SJ_1^b = 25\,\mathrm{meV}$$
$$SJ_2 = 36\,\mathrm{meV}$$



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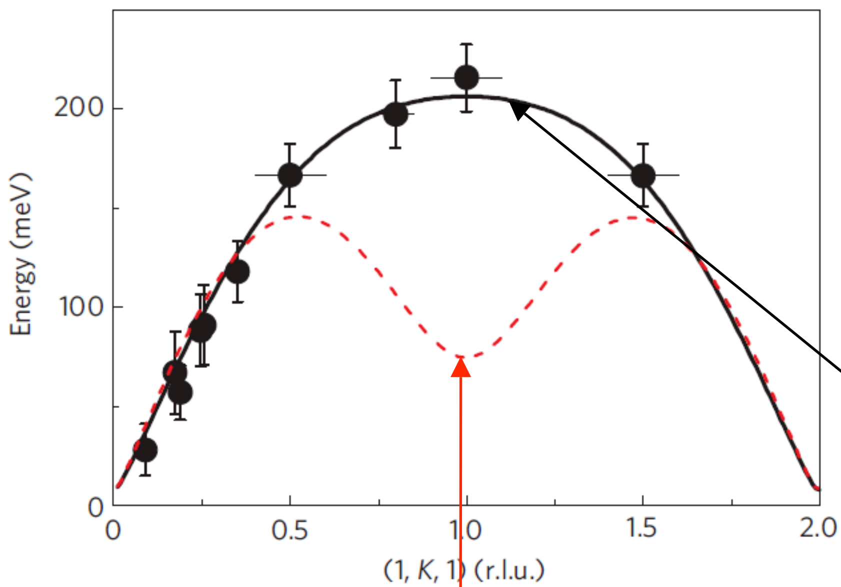

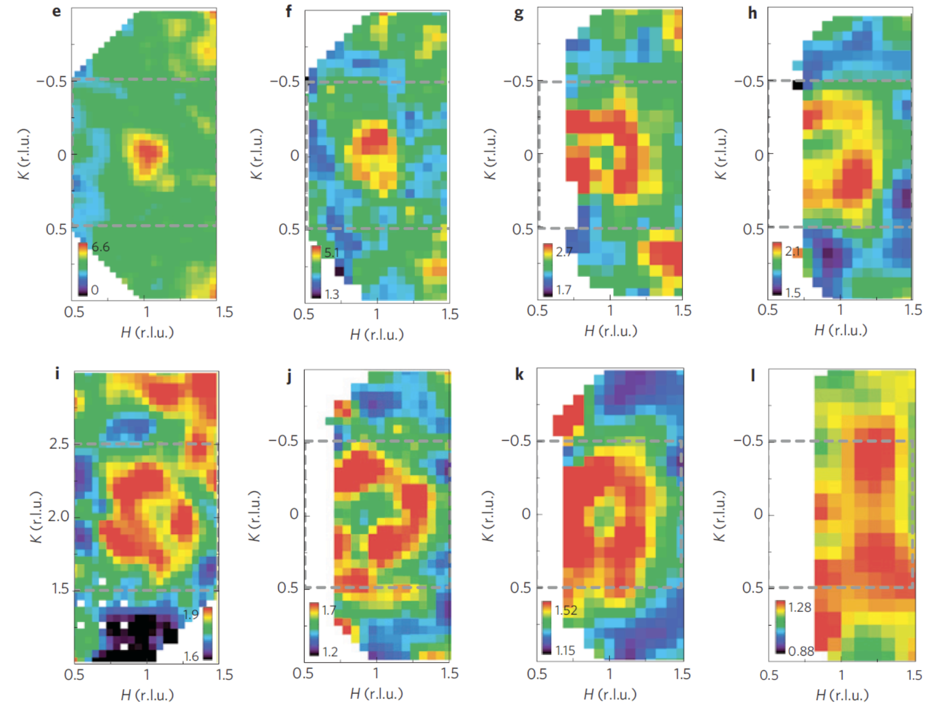

J. Zhao, *et al.* Nature Physics (2009)

Isotropic $J_{1a} \simeq J_{1b}$

$$SJ_1^a = 27\,\mathrm{meV}$$
$$SJ_1^b = 25\,\mathrm{meV}$$
$$SJ_2 = 36\,\mathrm{meV}$$

Anisotropic $J_{1a} \gg J_{1b}$

$$SJ_1^a = 49.9 \pm 9.9\,\mathrm{meV}$$
$$SJ_1^b = -5.7 \pm 4.5\,\mathrm{meV}$$
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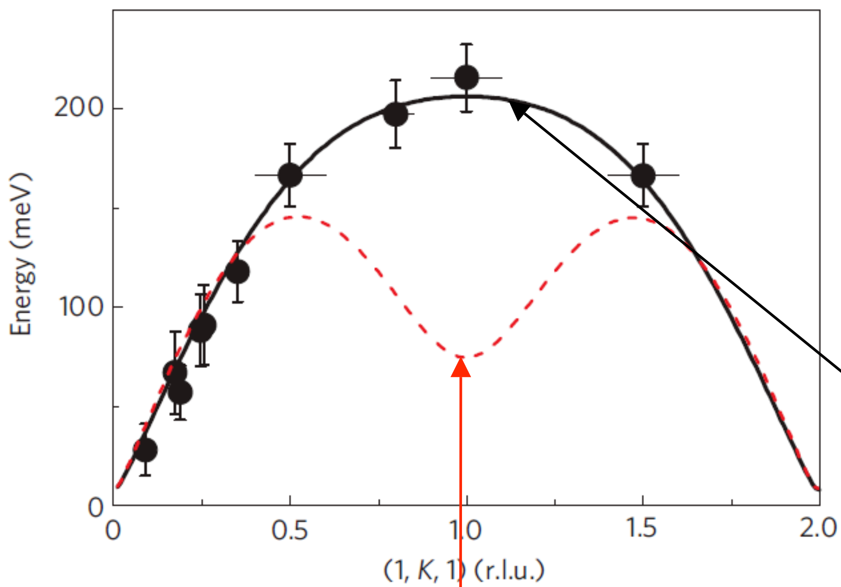
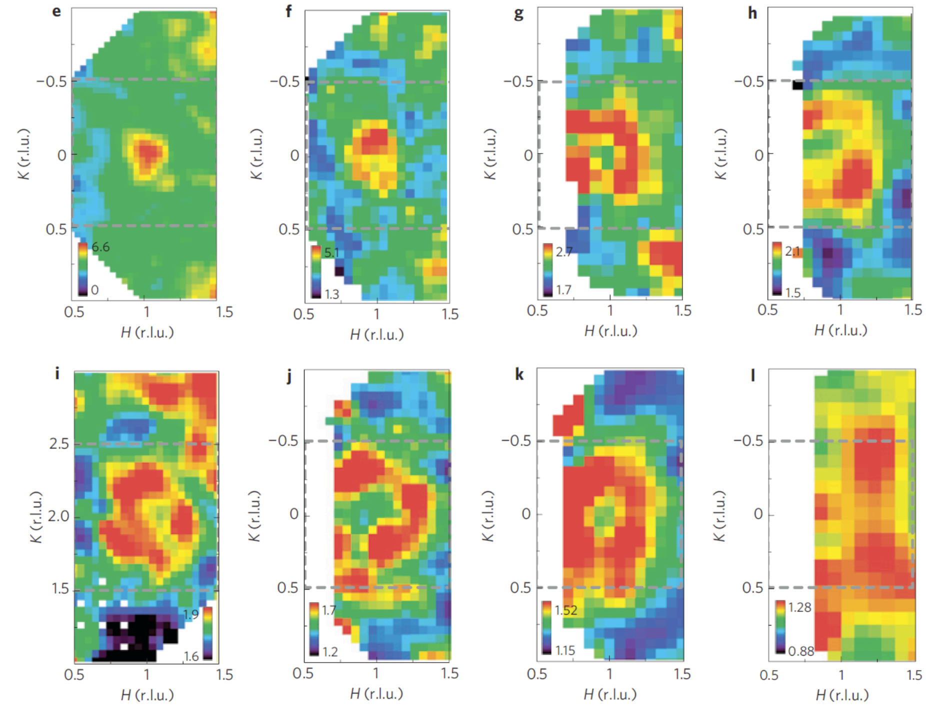
- *Inelastic neutron scattering*





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Problem?

itinerant model

local picture (different signs of J along x and y axes???)

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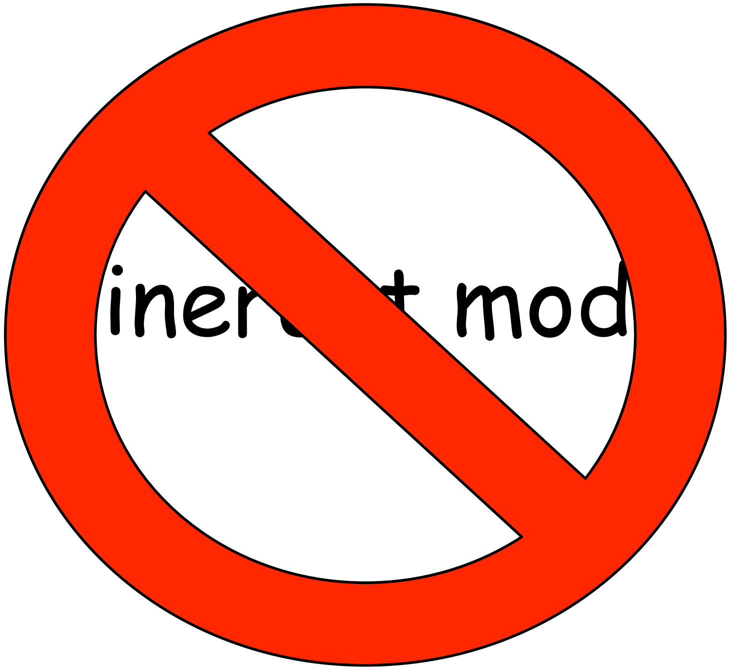
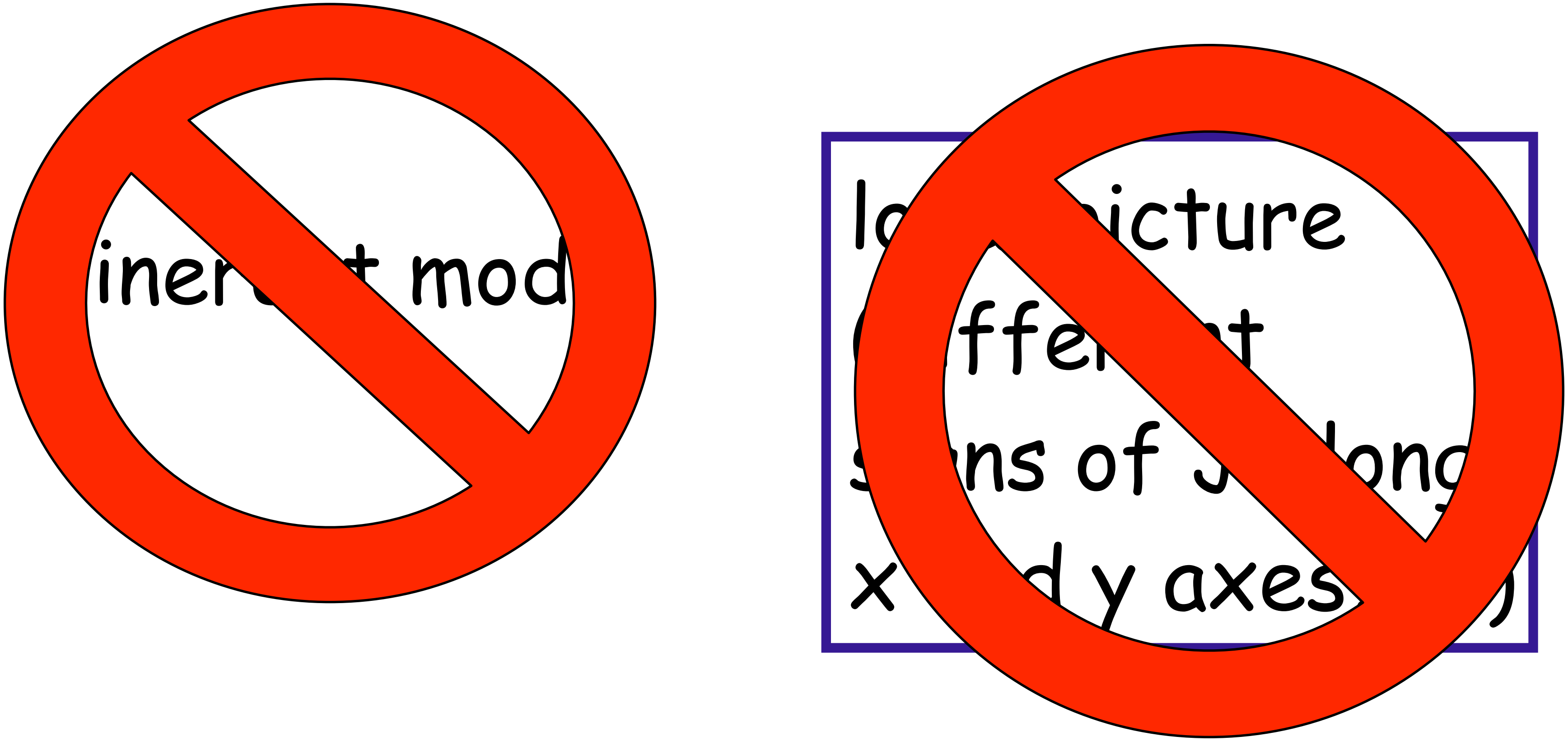


local picture (different signs of J along x and y axes???)

Problem?



Is there a simple model that captures this physics?

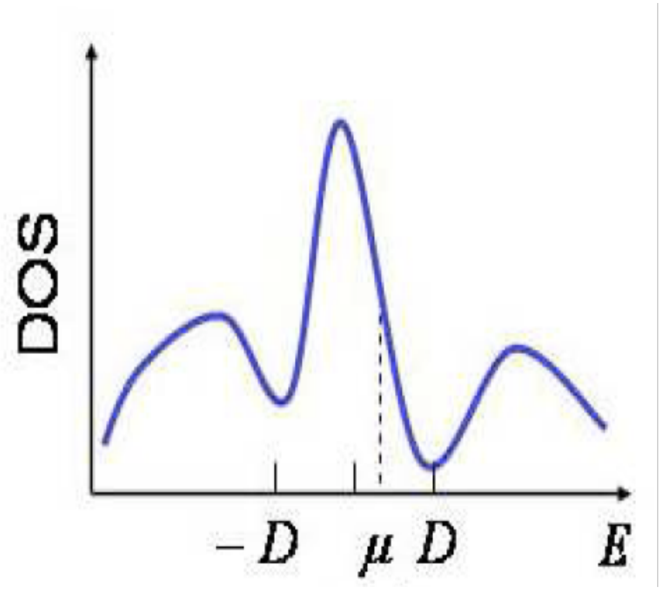
localized/extended electrons+Hund's coupling

orbital ordering

unfrustrated magnetism, SPT, RA

A new scenario: itinerant-localized dichotomy

J. Wu, P. Phillips, A. Castro-Neto, PRL(2008);
Z.-Y. Weng et.al., arXiv:0811.4111,
Q. Si, et.al. arXiv: 0901.4112.
J. Dai. et.al., arXiv: 0901.2787



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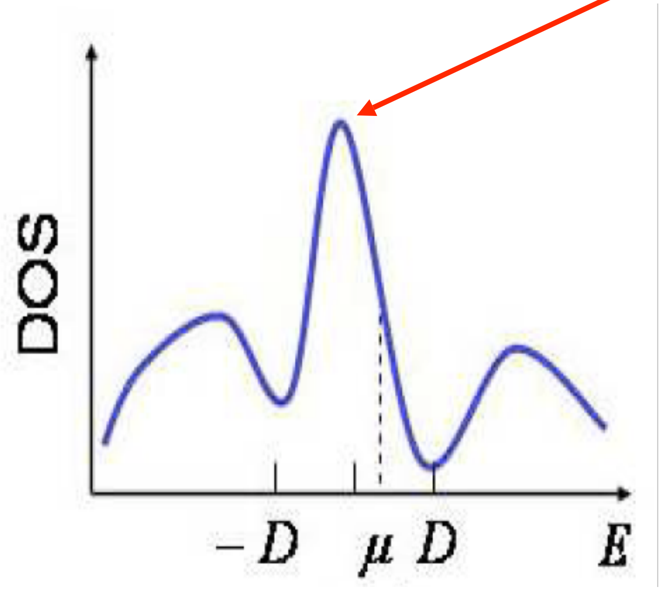

Itinerant electrons (coherent, ungapped) Metallic state

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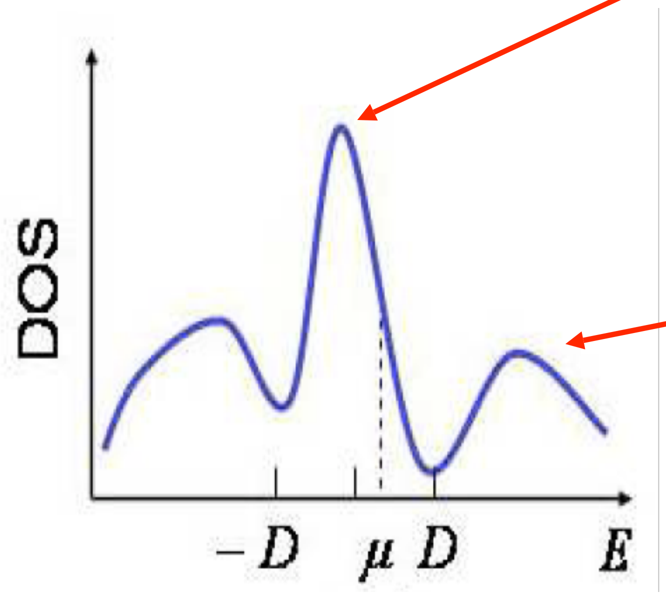

Localized electrons (incoherent, gapped) magnetic order

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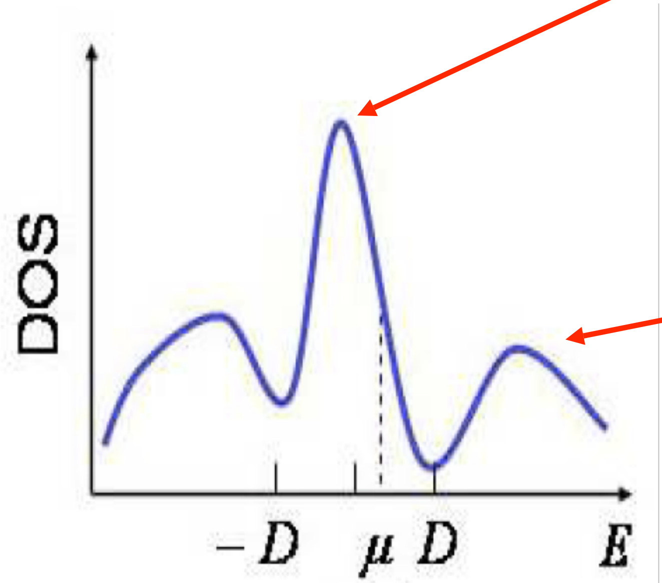


Itinerant electrons (coherent, ungapped) Metallic state

Localized electrons (incoherent, gapped) magnetic order

But how ?

1.) Why magnetic moments are so small?

J. Wu, P. Phillips, A. Castro-Neto, Phys. Rev. Lett. 101,126401(2008)

Antiferromagnetic magnetic Order

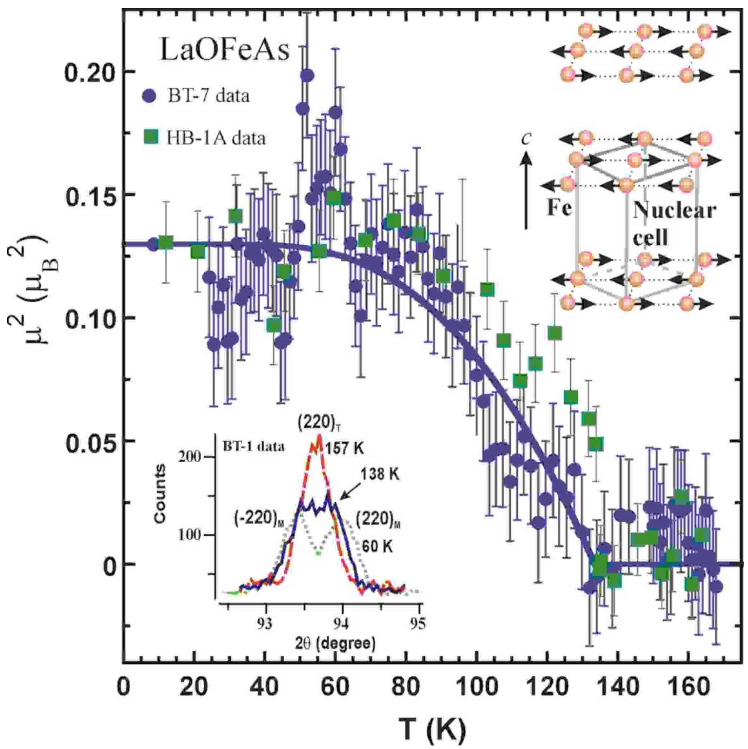


Figure 4 Temperature dependence of the order parameter at Q = 1.53 Å^{-1} obtained on BT-7/HB-1A and our determined magnetic structure for LaOFeAs. The solid blue circles are data obtained on BT-7 and solid green squares are data taken on HB-1A. The solid line is a simple fit to mean field theory which gives T_N = 134(1) K. The lower

$$.25\mu_B - .4\mu_B$$

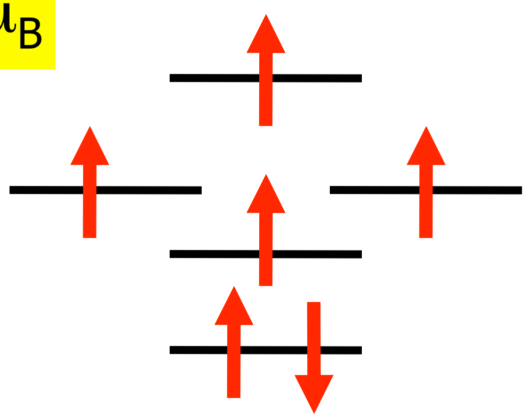
Why?

Why small magnetic moments are so striking?

No way to get $0.36\mu_B$ given Hund's rules: Fe^{2+} 6 electrons on 5 orbitals (local moments)

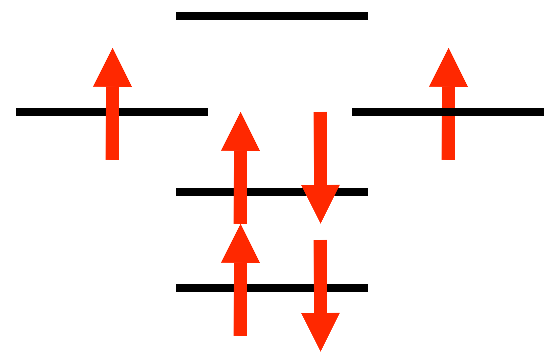
High spin configuration

$4\mu_B$

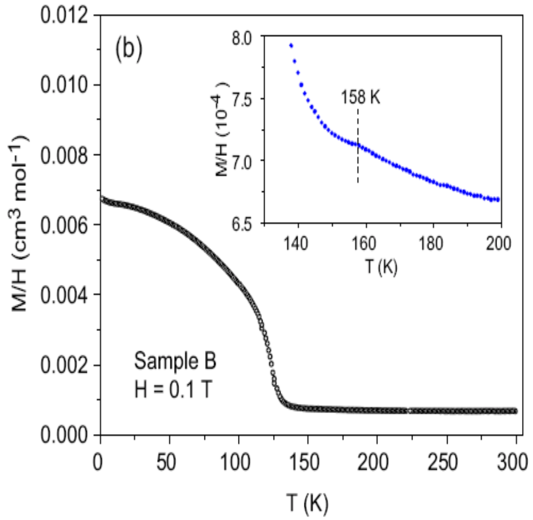


Low spin configuration

$2\mu_B$

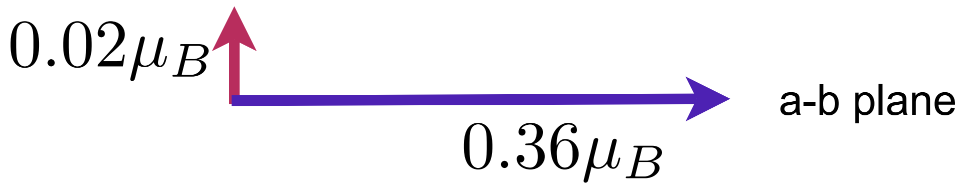


Origin of residual moment along z-axis??



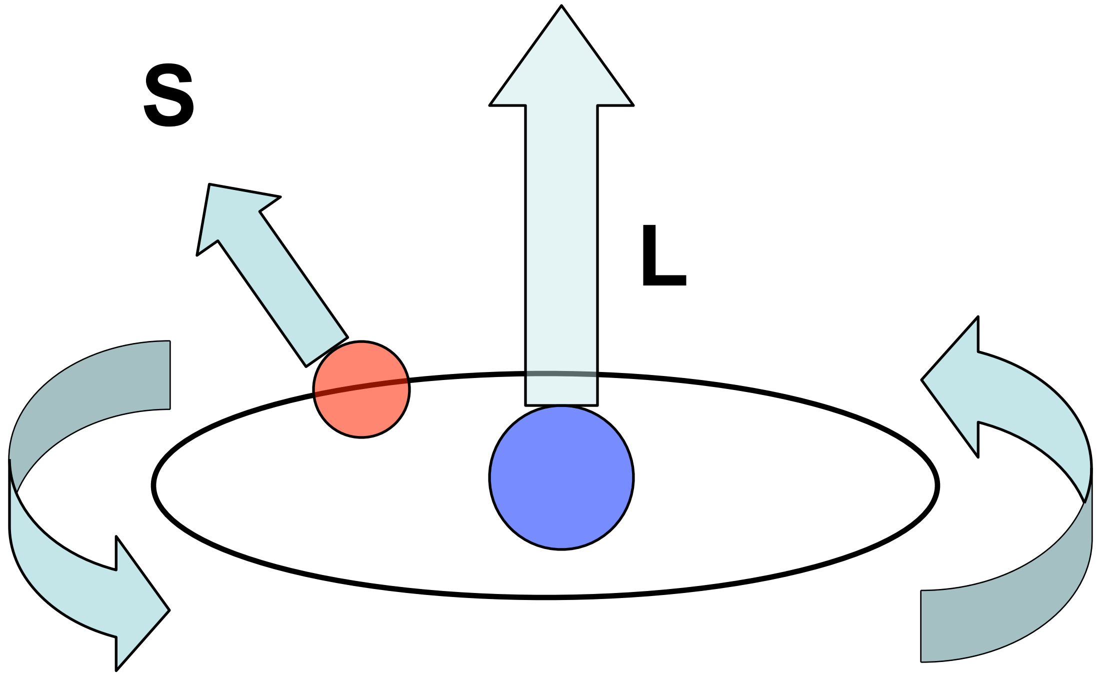
PRB, vol. 78, 094517 (2008).

Why?



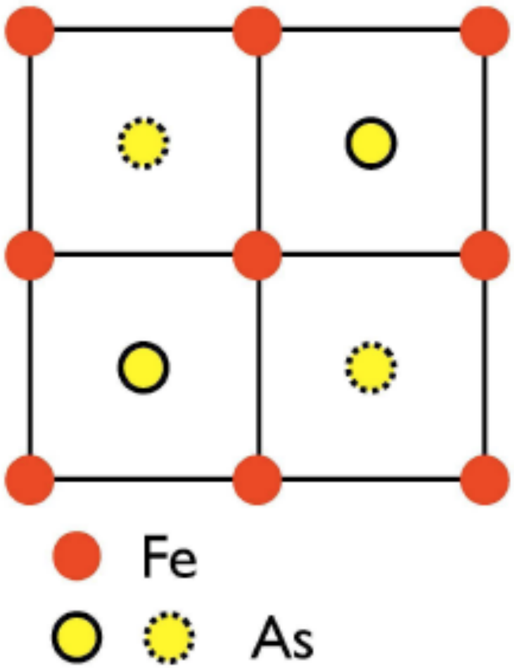
122, 1111(La)

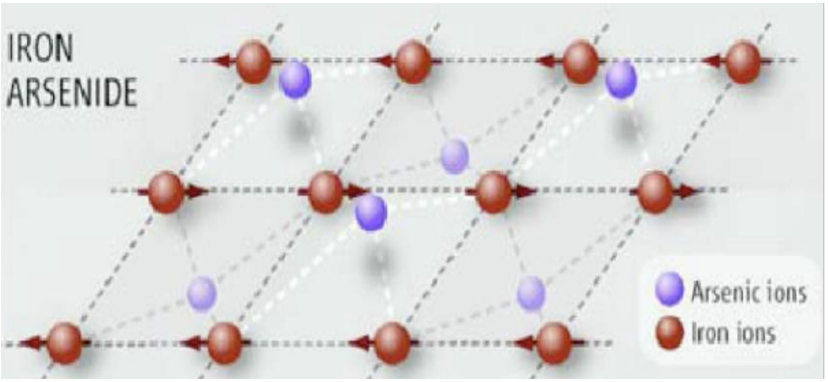
Spin-Orbit interaction



As: $V_{spin\text{-}orbit}$=0.4 eV

Key structure: Fe-As plane





arXiv: 0812.0302

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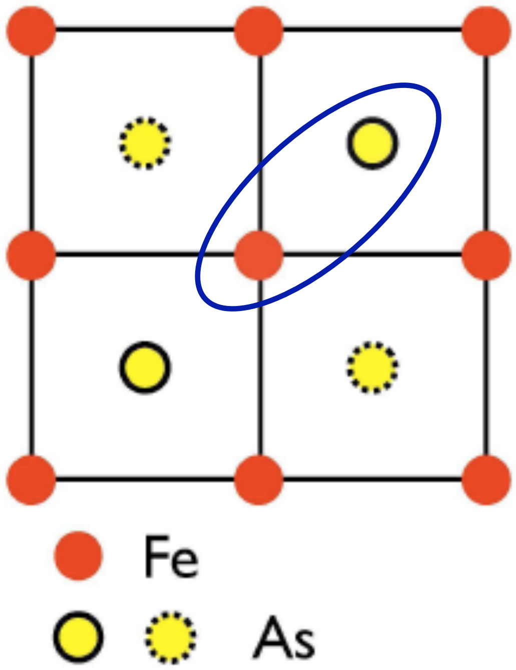

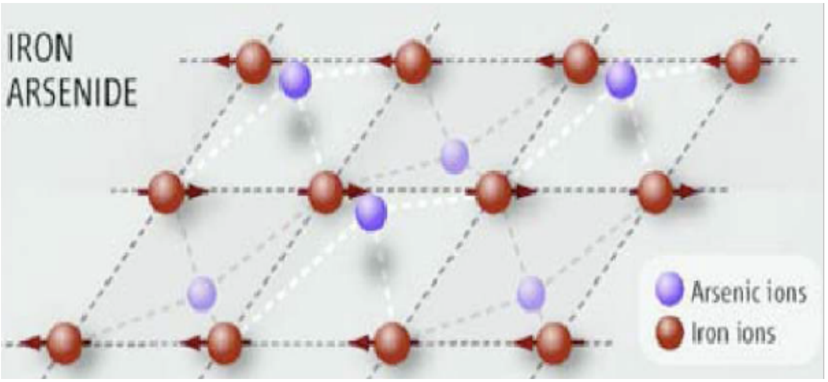

arXiv: 0812.0302

A hint

PHYSICAL REVIEW B **67**, 155421 (2003)

First-principles calculations of Fe on GaAs(100)

S. Mirbt, B. Sanyal, C. Isheden, and B. Johansson
Department of Physics, Uppsala University, Uppsala, Sweden
(Received 10 December 2002; published 30 April 2003)

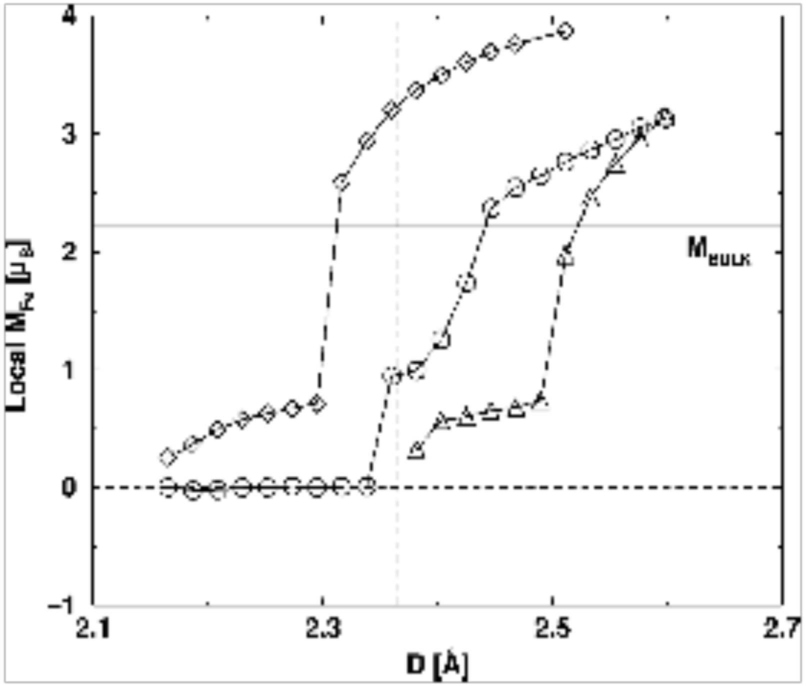

FIG. 8. Bulk magnetic moment per Fe atom for zinc-blende FeAs (circles), zinc-blende FeSe (diamonds), and zinc-blende FeTe (triangles) as a function of the Fe-anion distance *D*. The dashed vertical line is the same as in Fig. 7 shown here for comparison.

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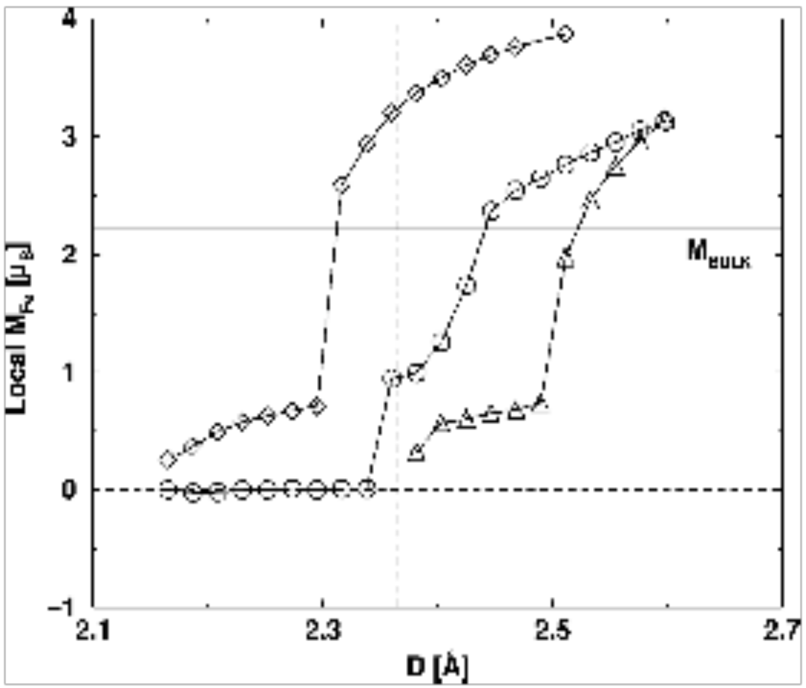

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As 4p-Fe 3d hybridisation is crucial

PHYSICAL REVIEW B VOLUME 30, NUMBER 10 15 NOVEMBER 1984

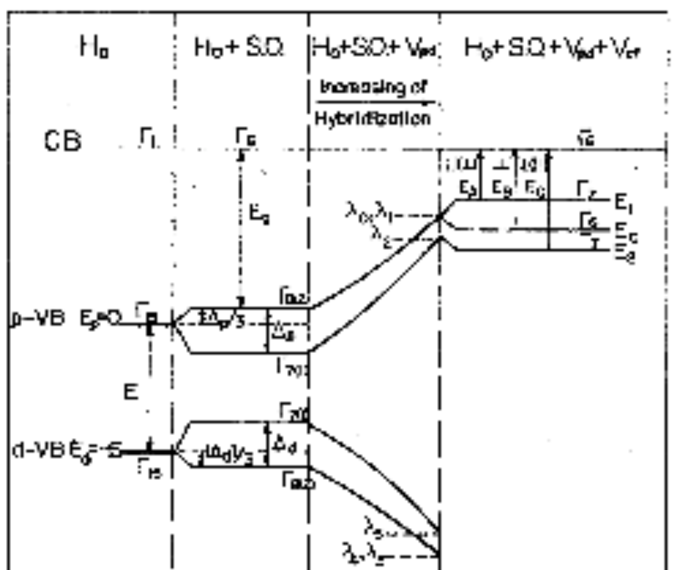
Effects of *p-d* hybridization on the valence band of I-III-VI$_2$ chalcopyrite semiconductors

Kajornyod Yoodee[a] and John C. Woolley
Physics Department, University of Ottawa, Ottawa, Ontario, Canada K1N 6N5

Virulh Sa-yakanit
Physics Department, Chulalongkorn University, Bangkok 10500, Thailand

(Received 15 June 1984)

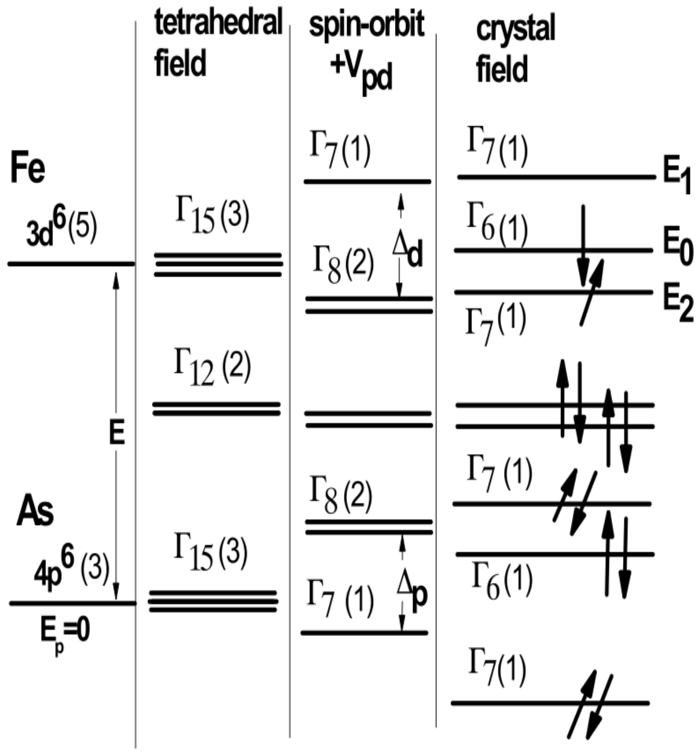
The electronic structure of the valence band at the Brillouin-zone center of the I-III-VI$_2$ chalcopyrite compounds has been calculated using a model developed by adding the effects of p-d hybridization and the crystal field to the Hamiltonian of the Kane model. Two important parameters in the model are the energy separation E between the p and d levels and the interaction M between these levels. It is shown that three previous models (Tell and Bridenbaugh, Kildal, and the linear hybridization model) can be derived as special cases of the present model. The model has been used to analyze the available data on some 13 compounds. It is shown that the dimensionless parameters M/E and $\Delta E_g/E$, where ΔE_g is the band-gap anomaly, show a smooth variation with the fractional d character of the valence band and appear to be characteristic of the structure. Values of the deformation potentials b_p and b_d averaged over all of the compounds have been determined and found to be $b_p = (-0.8 \pm 0.2)$ eV and $b_d = (-4.3 \pm 1.5)$ eV.



spin-orbit+
pd hybridization+
crystal field

New way to arrange electrons in As-Fe band:

(by diagonalizing the above Hamiltonian)



Sketch of the energy levels of the Fe 3p and As 4p hybridized levels after the inclusion of spin-orbit coupling, p-d hybridization, and the monoclinic crystal field distortion.

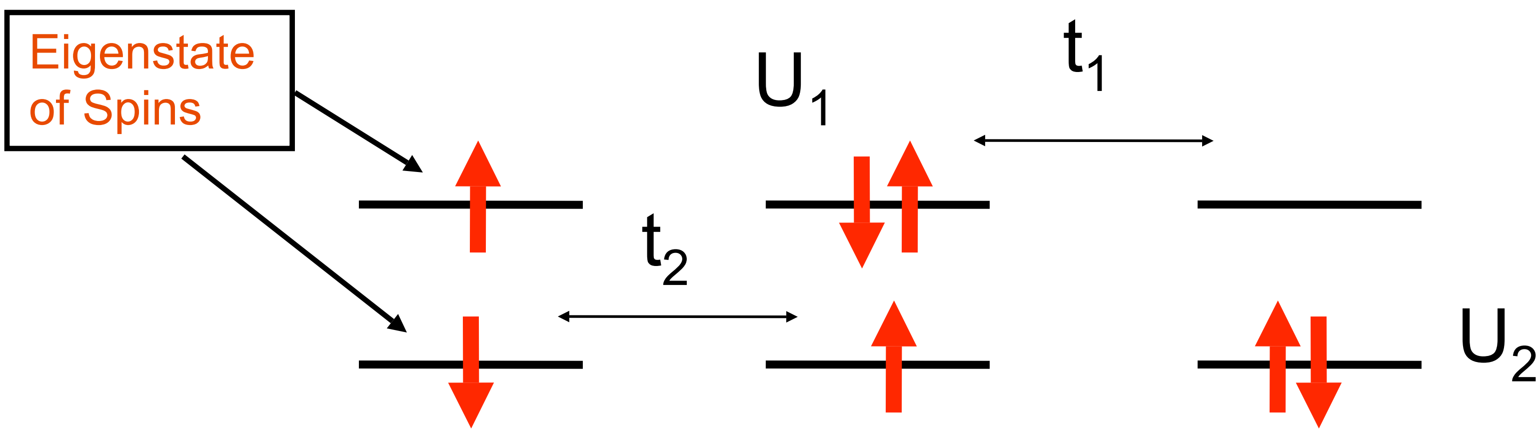
Only the Γ_{15} p-levels of Fe hybridize with the As 4p levels. The Γ_{12} levels remain non bonding.

Each of the hybridized levels is doubly degenerate, though not an eigenstate of S_z. The only hybridized level which is an eigenstate of S_z is E_0. The lowest-energy configuration of the spins in E_0 and E_2 is indicated. As a result, only the x-y component produces a non-zero moment.

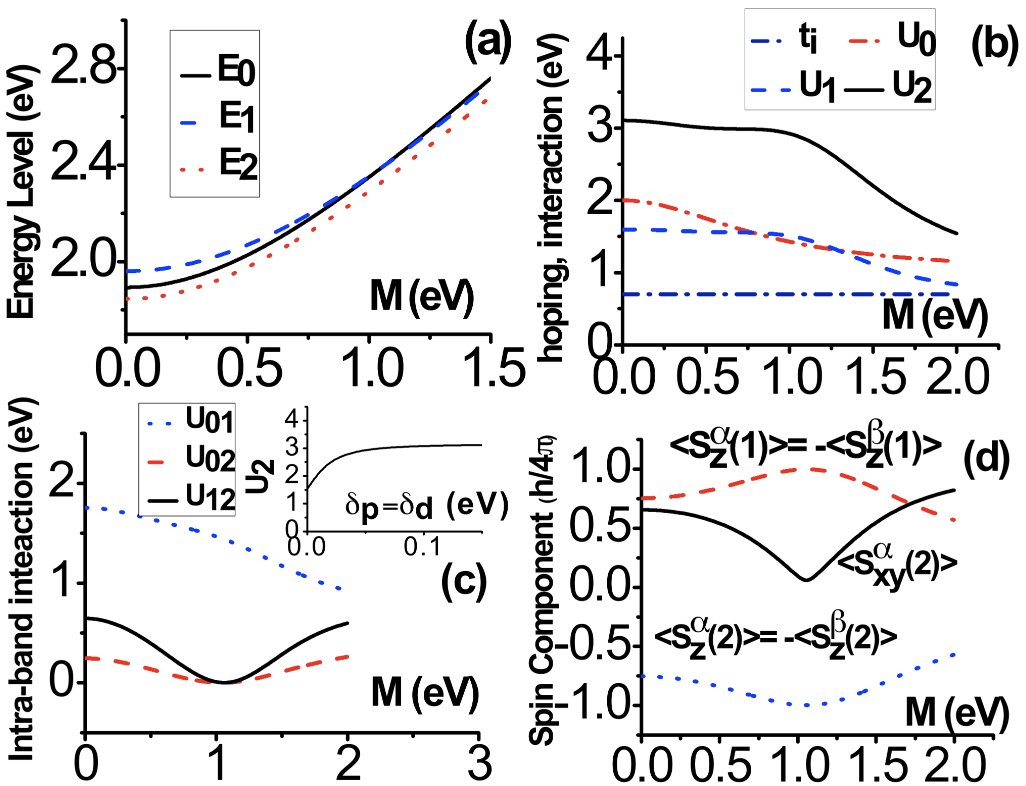
Hamiltonian in orbital basis:

$$H = \sum_{\mathbf{a},\mathbf{i}} E_{\mathbf{a}} c^{\dagger}_{\mathbf{a},\mathbf{i}}(\sigma) c_{\mathbf{a},\mathbf{i}}(\sigma) - \sum_{\mathbf{a},\langle \mathbf{i},\mathbf{j}\rangle} t_{\mathbf{a}} c^{\dagger}_{\mathbf{a},\mathbf{i}}(\sigma) c_{\mathbf{a},\mathbf{j}}(\sigma) + \text{h.c.}$$

$$+ \sum_{\mathbf{a}} U_{\mathbf{a}} n_{\mathbf{i},\mathbf{a}\uparrow} n_{\mathbf{i},\mathbf{a}\downarrow} ,$$



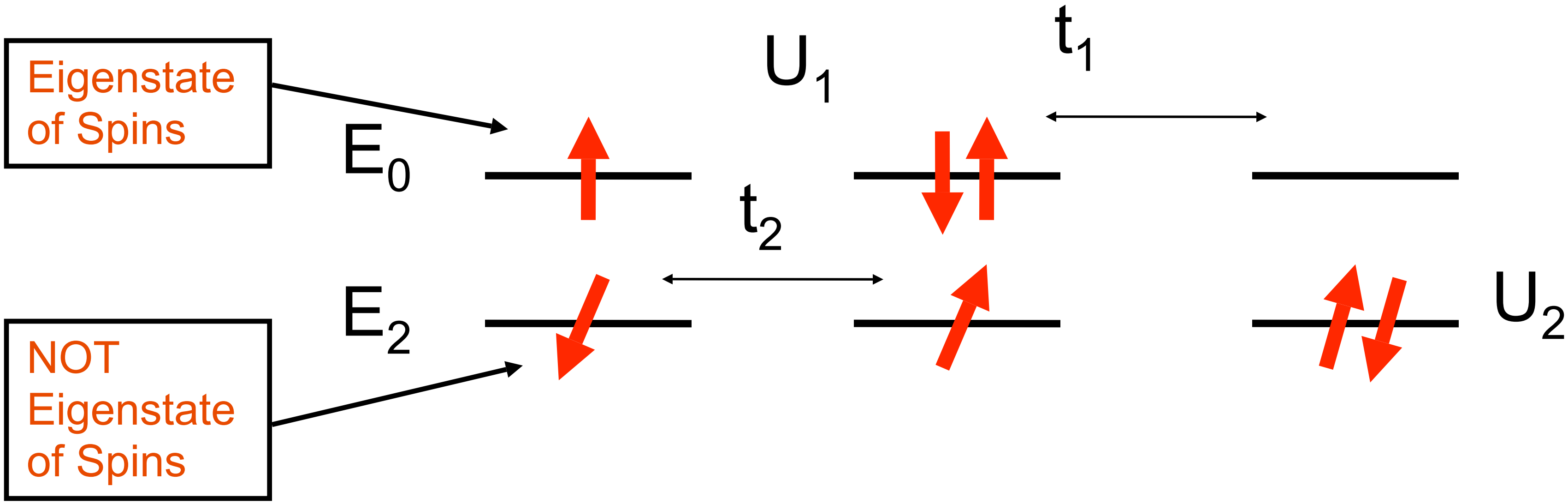
Magnitude of parameters



(a) Energy levels, (b) hopping matrix elements, on-site interactions, (c) intra-band interaction and (d) spin components as a function of hybridization M. Shown in the inset of (c) is the on-site interaction U_2 as a function of the crystal field (monoclinic distortion).

Hamiltonian in new basis

$$\mathbf{H} = \sum_{\mathbf{a},\mathbf{i}} E_{\mathbf{a}} c^{\dagger}_{\mathbf{a},\mathbf{i}}(\mu) c_{\mathbf{a},\mathbf{i}}(\mu) - \sum_{\mathbf{a},\mathbf{b},\langle \mathbf{i},\mathbf{j}\rangle} t_{\mathbf{a},\mathbf{b}}(\mu,\nu) c^{\dagger}_{\mathbf{a},\mathbf{i}}(\mu) c_{\mathbf{b},\mathbf{j}}(\nu) + \text{h.c.}$$
$$+ \sum_{\mathbf{a},\mathbf{b},\mathbf{i}} U_{\mathbf{ab}}(\mu\nu) n_{\mathbf{ia}}(\mu) n_{\mathbf{ib}}(\nu)\,,$$



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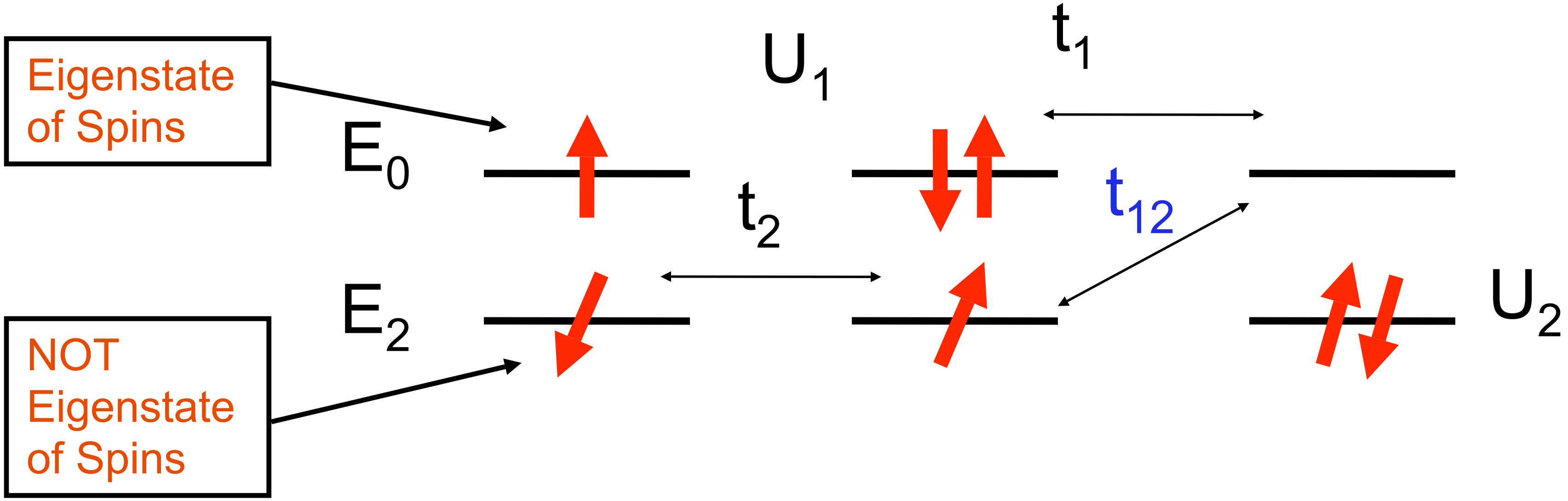

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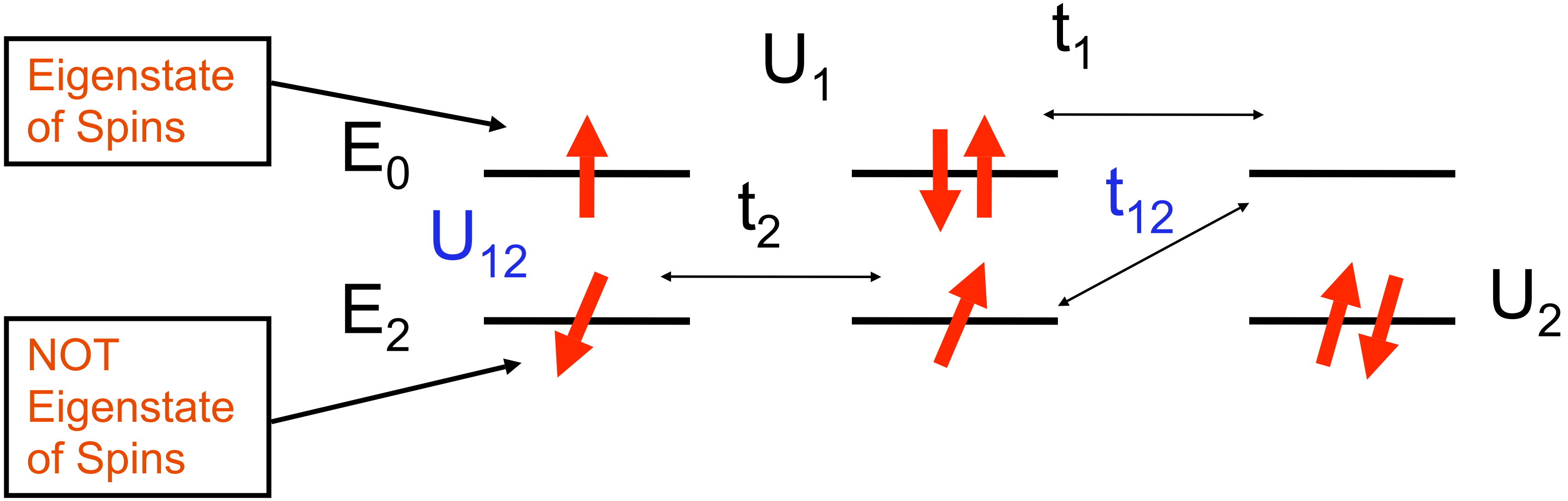

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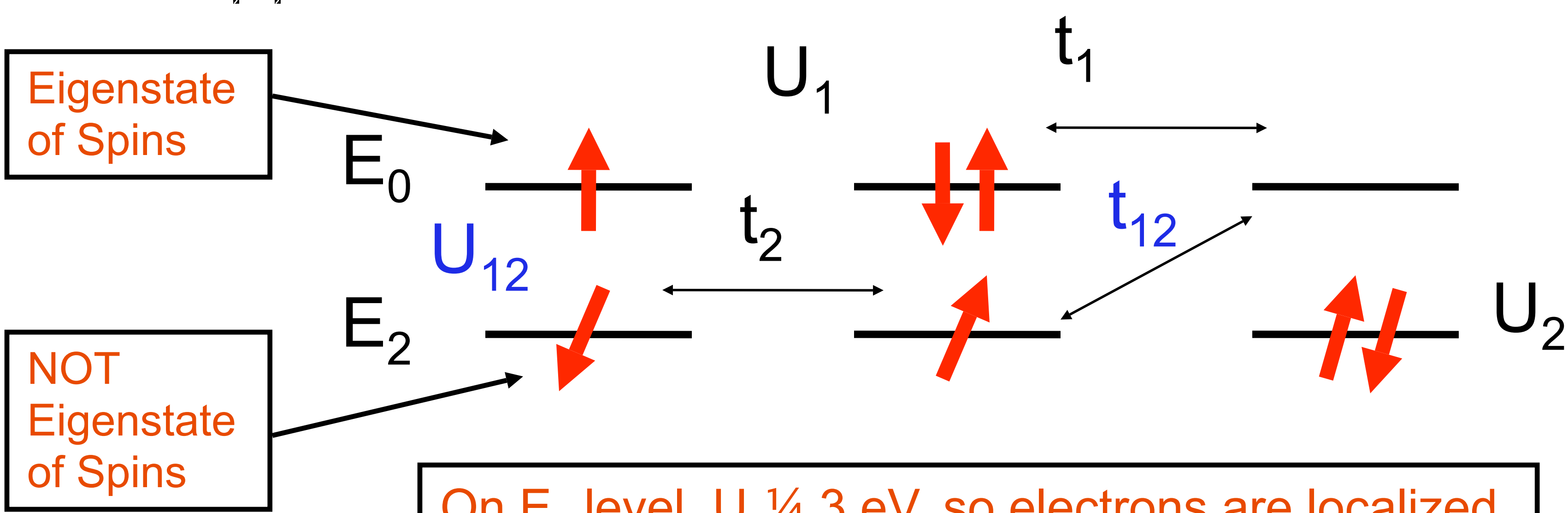
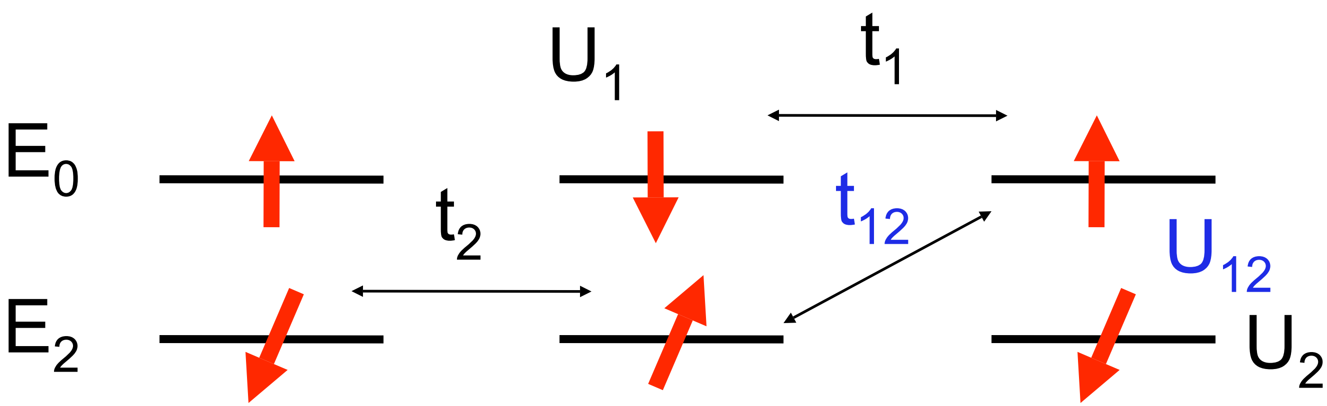
$$\begin{aligned}\mathbf{H} &= \sum_{\mathbf{a},\mathbf{i}} E_{\mathbf{a}} c^{\dagger}_{\mathbf{a},\mathbf{i}}(\mu) c_{\mathbf{a},\mathbf{i}}(\mu) - \sum_{\mathbf{a},\mathbf{b},\langle \mathbf{i},\mathbf{j}\rangle} t_{\mathbf{a},\mathbf{b}}(\mu,\nu) c^{\dagger}_{\mathbf{a},\mathbf{i}}(\mu) c_{\mathbf{b},\mathbf{j}}(\nu) + \text{h.c.} \\ &+ \sum_{\mathbf{a},\mathbf{b},\mathbf{i}} U_{\mathbf{ab}}(\mu\nu) n_{\mathbf{ia}}(\mu) n_{\mathbf{ib}}(\nu)\,,\end{aligned}$$

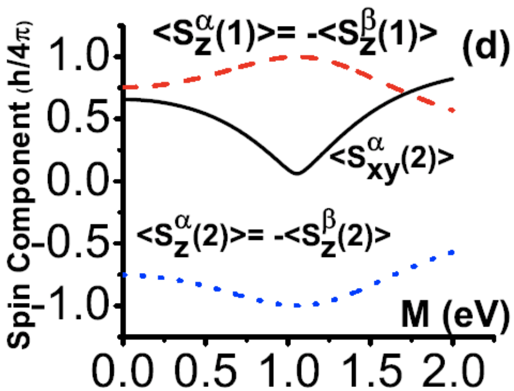


On E_2 level, U_2¼ 3 eV, so electrons are localized
On E_0 level, U_1¼ 0.5 eV, so electrons are itinerant

Why the magnetic moments are so small?

$\mu_z = 0.06\mu_B$ $\mu_{xy} = 0.25\mu_B$ agree with experiments





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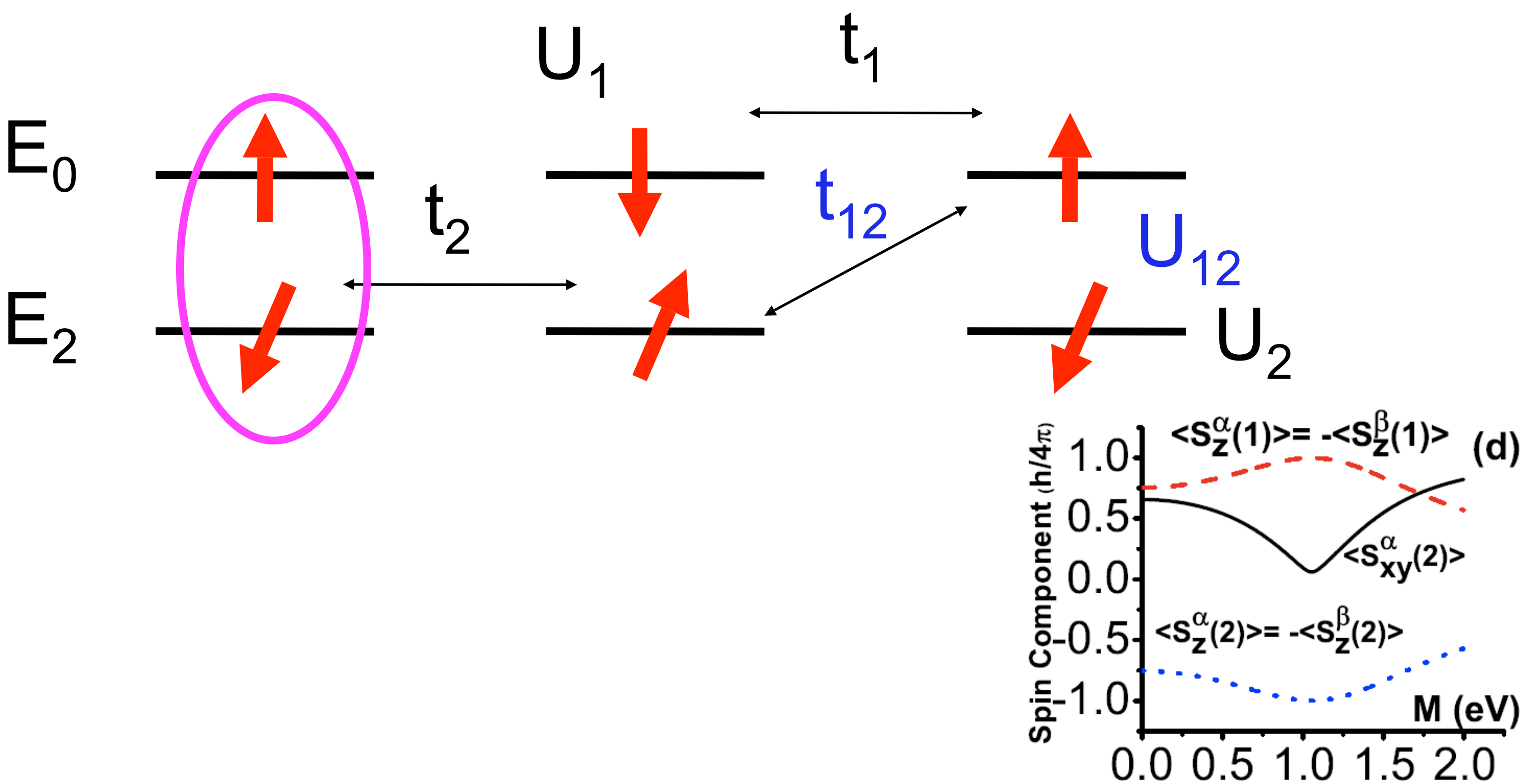

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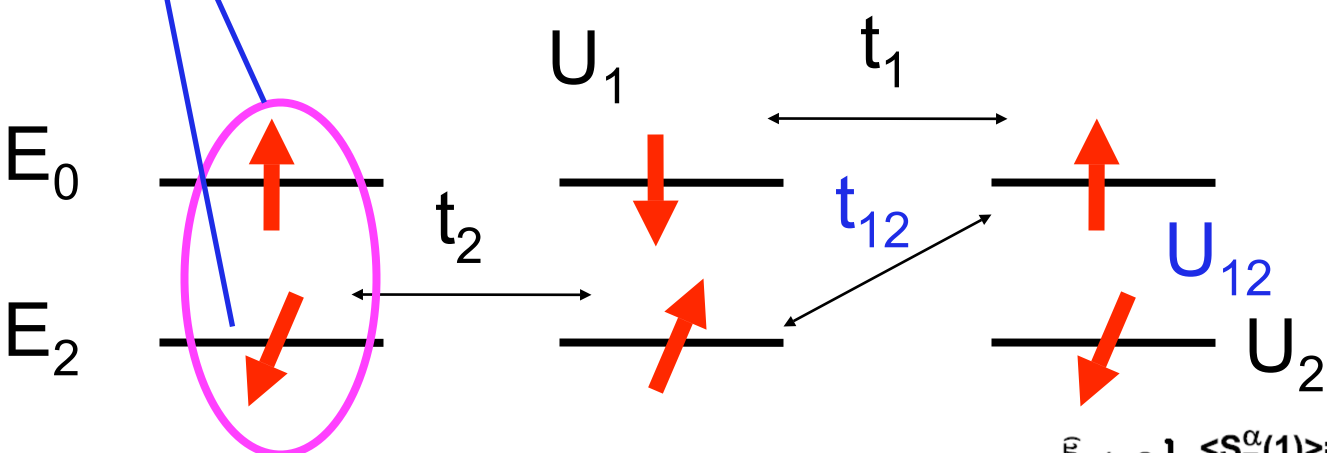

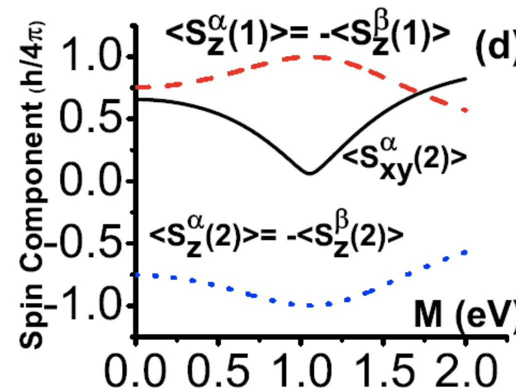

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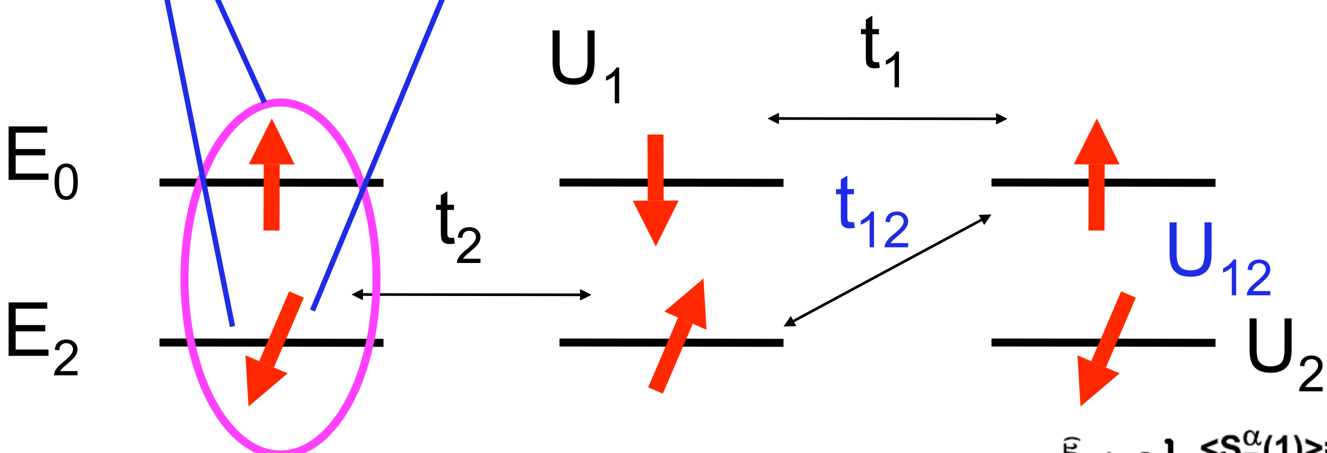
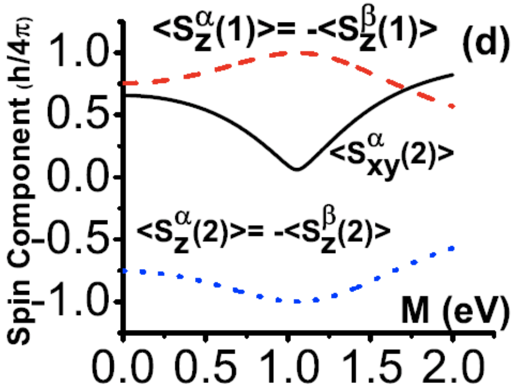




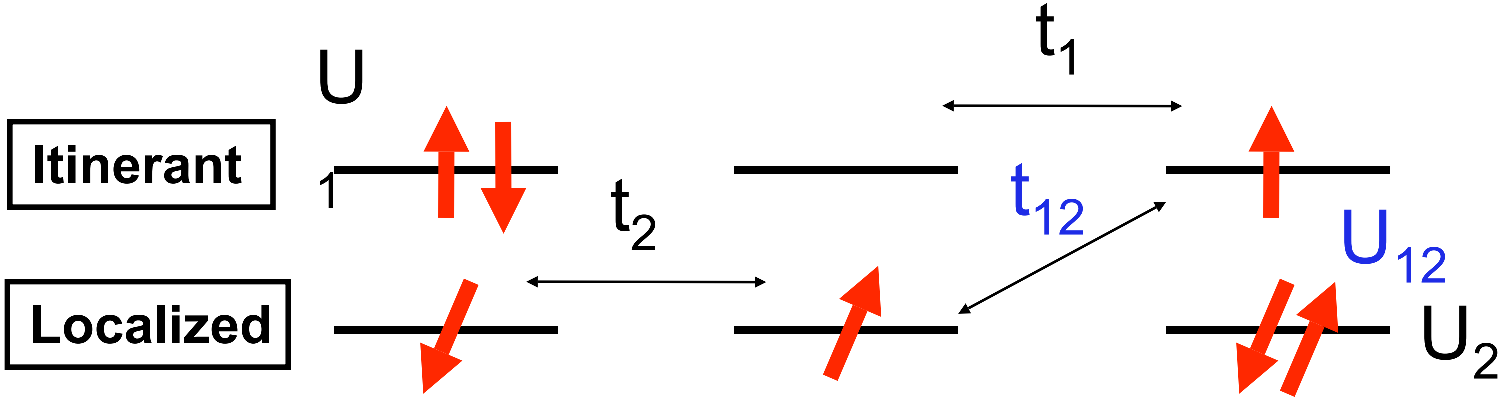
Why the magnetic moments are so small?

Localized magnetic moments are screened by the itinerant electrons

Why the magnetic moments are so small?

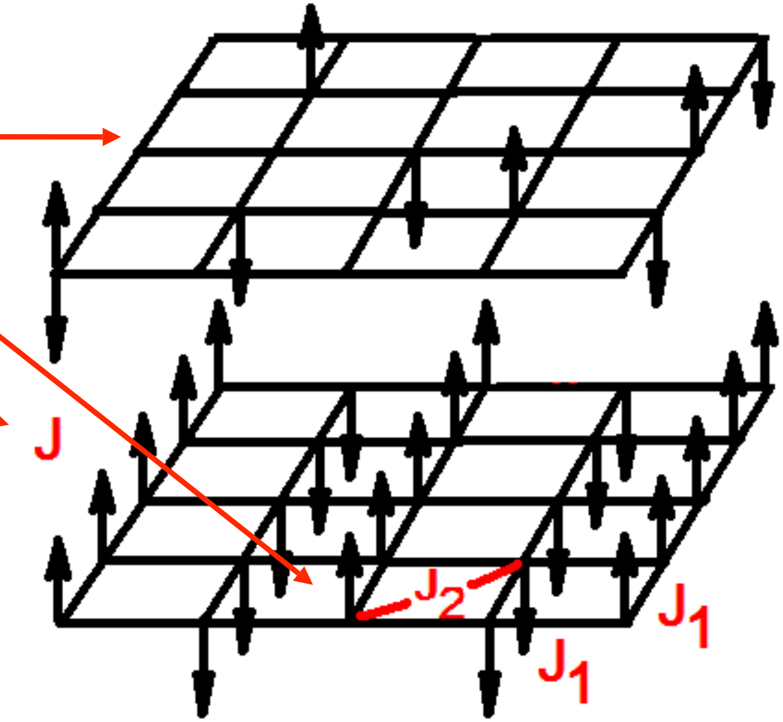
Localized magnetic moments are screened by the itinerant electrons

We also get the minimal model:
Itinerant-localized dichotomy



Itinerant-localized dichotomy

$$
\begin{aligned}
H &= H_{\rm e} + H_{\rm s} + H_{\rm sf} \\
H_{\rm e} &= \sum \epsilon_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \\
H_{\rm s} &= J_1 \sum_{n.n} \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{j}} + J_2 \sum_{n.n.n} \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{j}} \\
H_{\rm sf} &= J \sum c^{\dagger}_{\mathbf{i},\alpha} \sigma_{\alpha\beta} c_{\mathbf{i},\beta} \cdot \mathbf{S}_{\mathbf{i}}.
\end{aligned}
$$



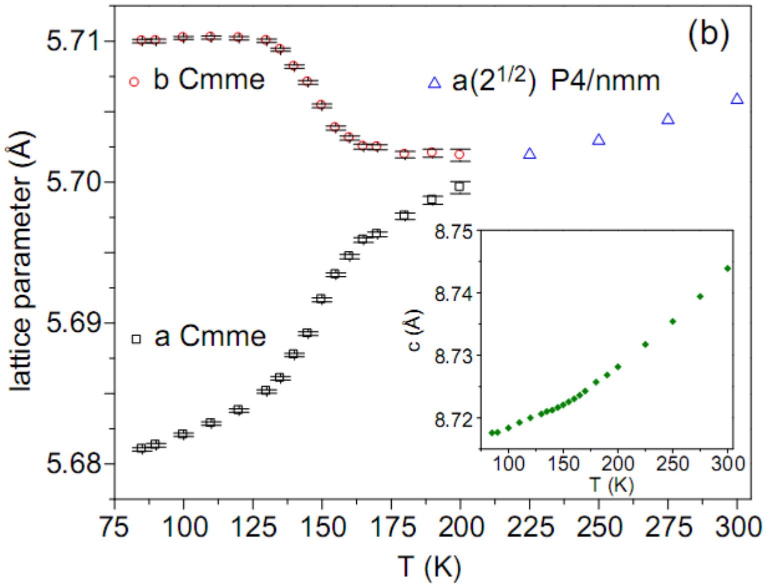
Kondo coupling

Itinerant electrons interact
with each other by propagating magnons in localized level

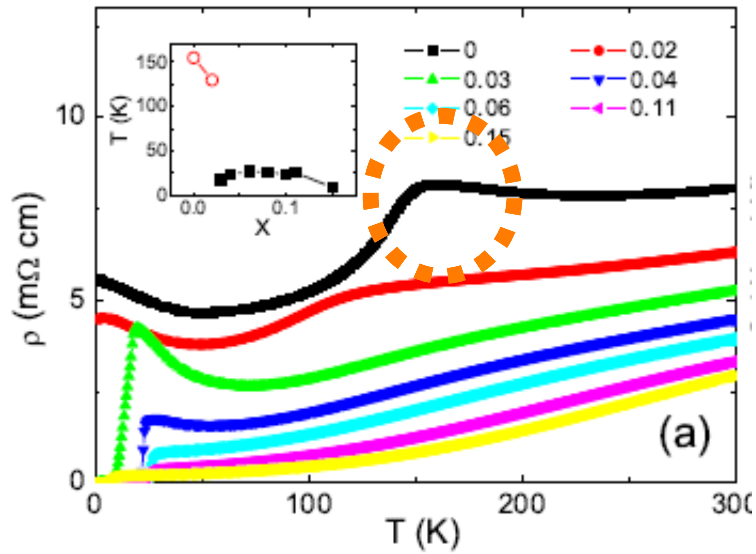
2.) What causes the structural phase transition and resistivity anomaly?

W. Lv, J. Wu, P. Phillips, PRB, 80, 224506 (2009)

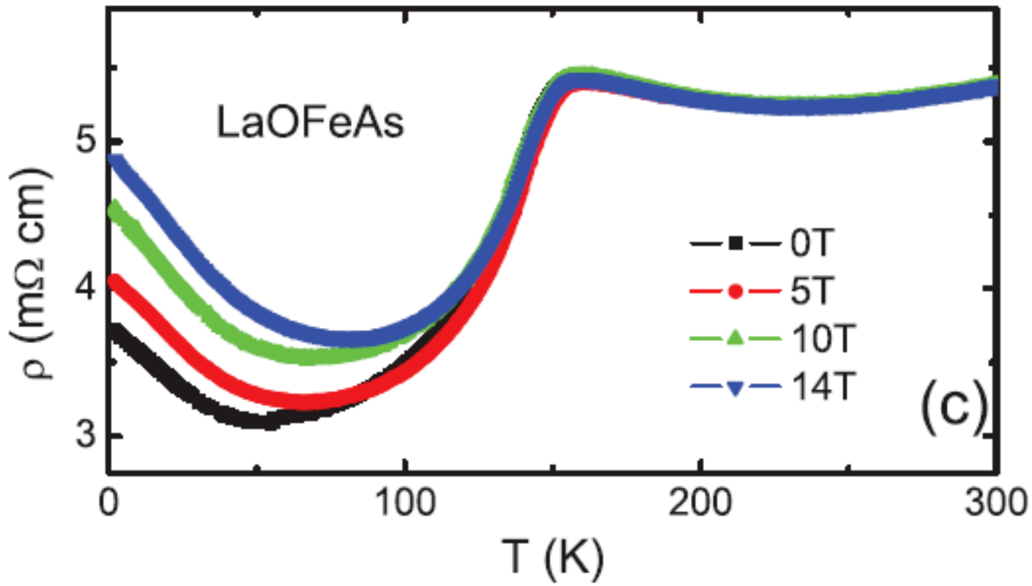
- **Structural Phase Transition**



- **Resistivity Anomaly** $T_{\mathrm{RA}} = T_{\mathrm{SPT}}$



SPT is insensitive to external magnetic field



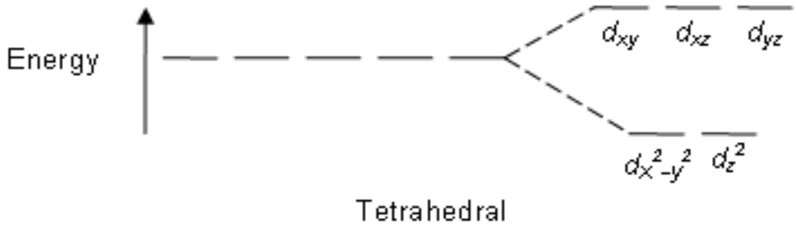
What breaks symmetry in x-y plane?

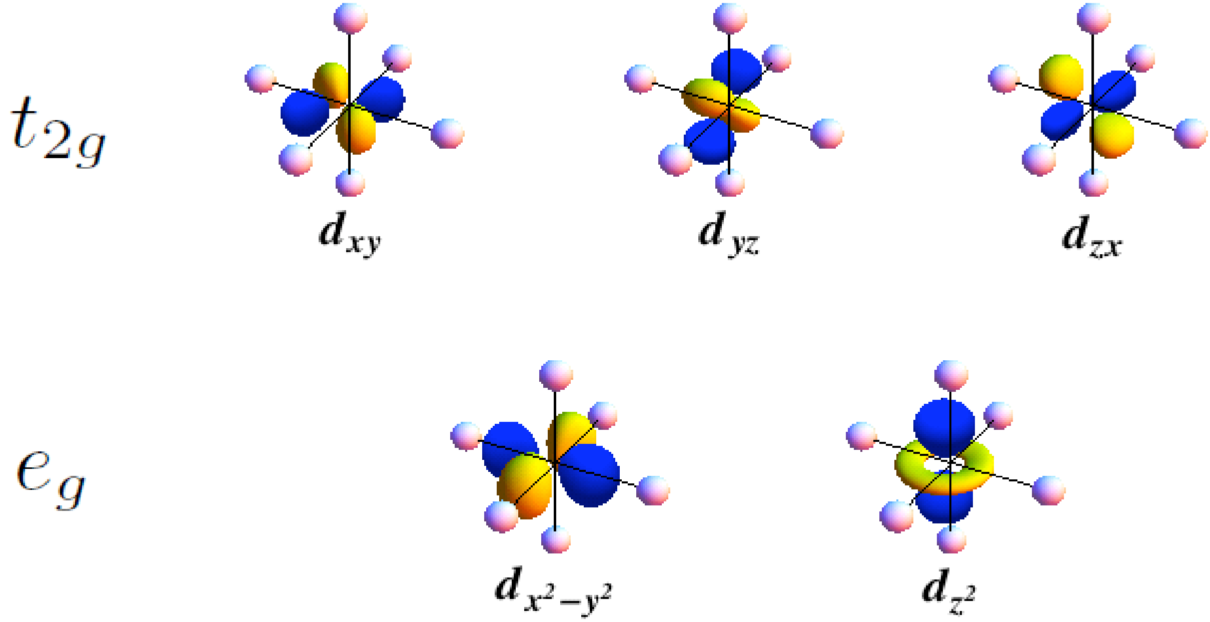
What breaks symmetry in x-y plane?

orbital ordering

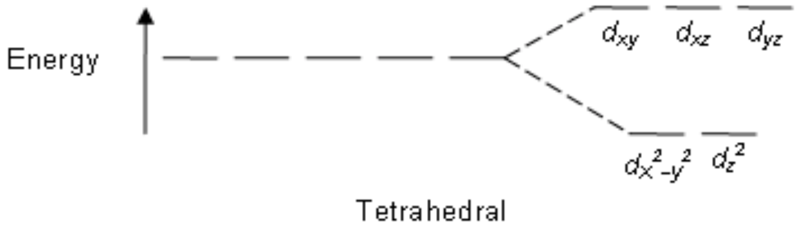
F. Krüger, *et al.* PRB (2009)
R.R.P. Singh, arXiv:0903.4408
W. Lv, *et al.* PRB (2009)
A.M. Turner, *et al.* PRB (2009)
C.-C. Lee, *et al.* PRL (2009)
……

Orbital ordering (multi-bands)

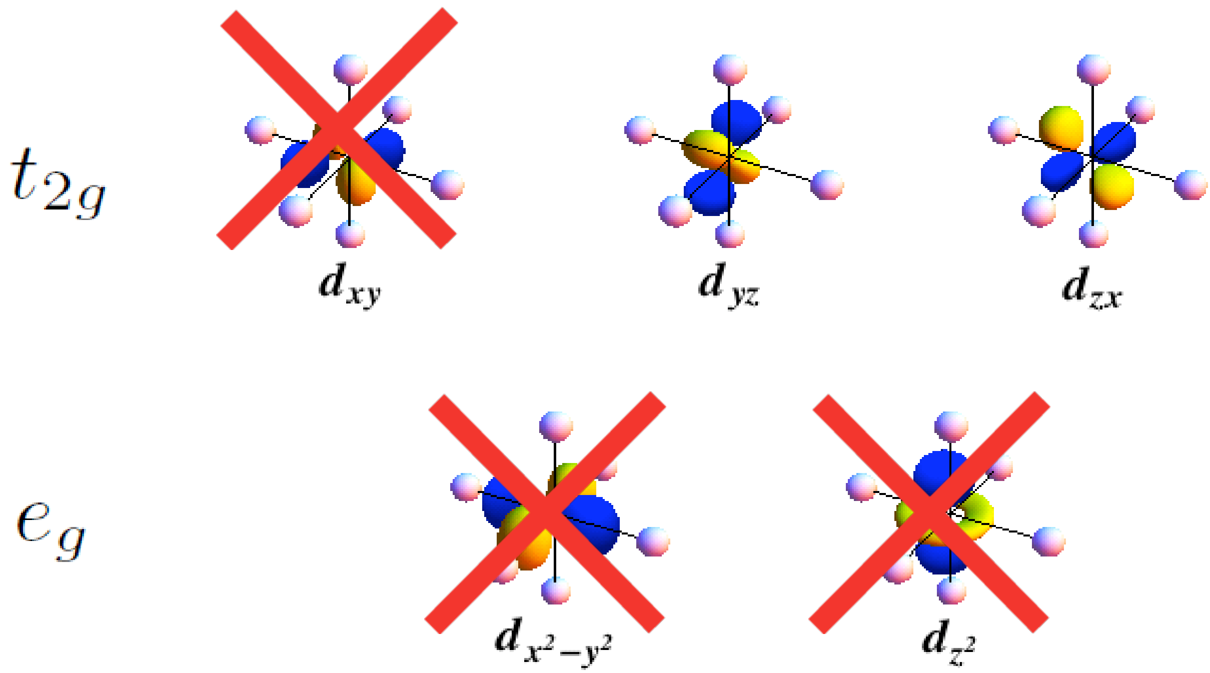




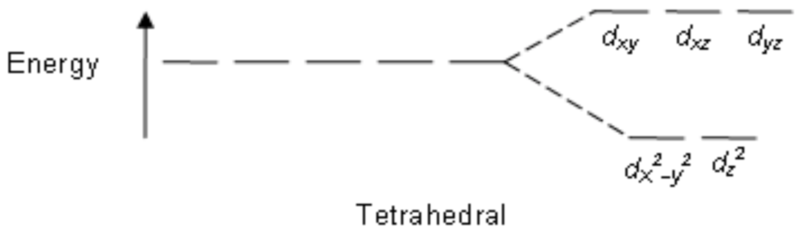
Orbital ordering (multi-bands)



$d_{x^2-y^2}$, d_{z^2}, d_{xy}, with the rotational symmetry in *xy*-plane, will not contribute to SPT.



Orbital ordering (multi-bands)



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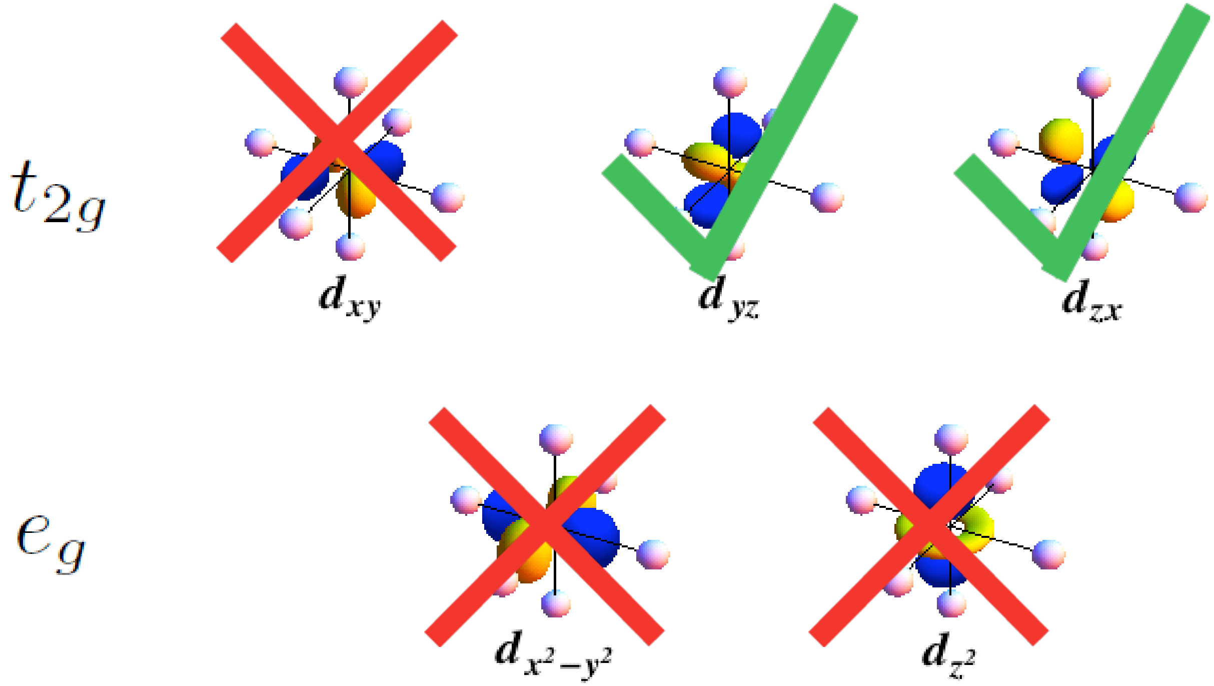
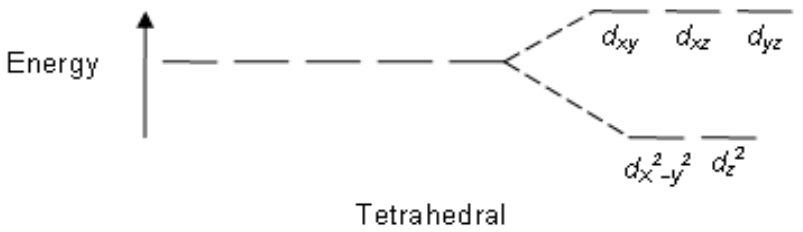


Orbital ordering (multi-bands)



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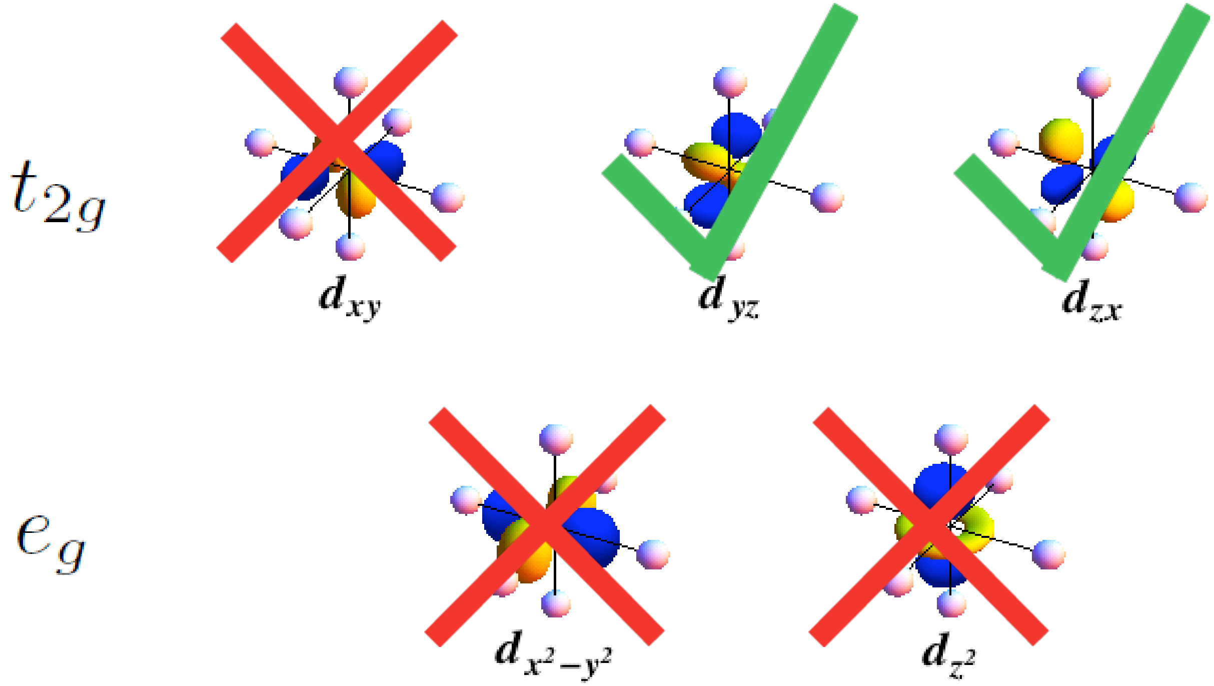
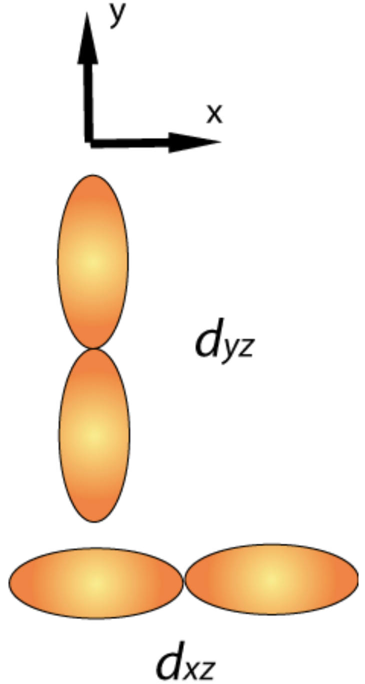
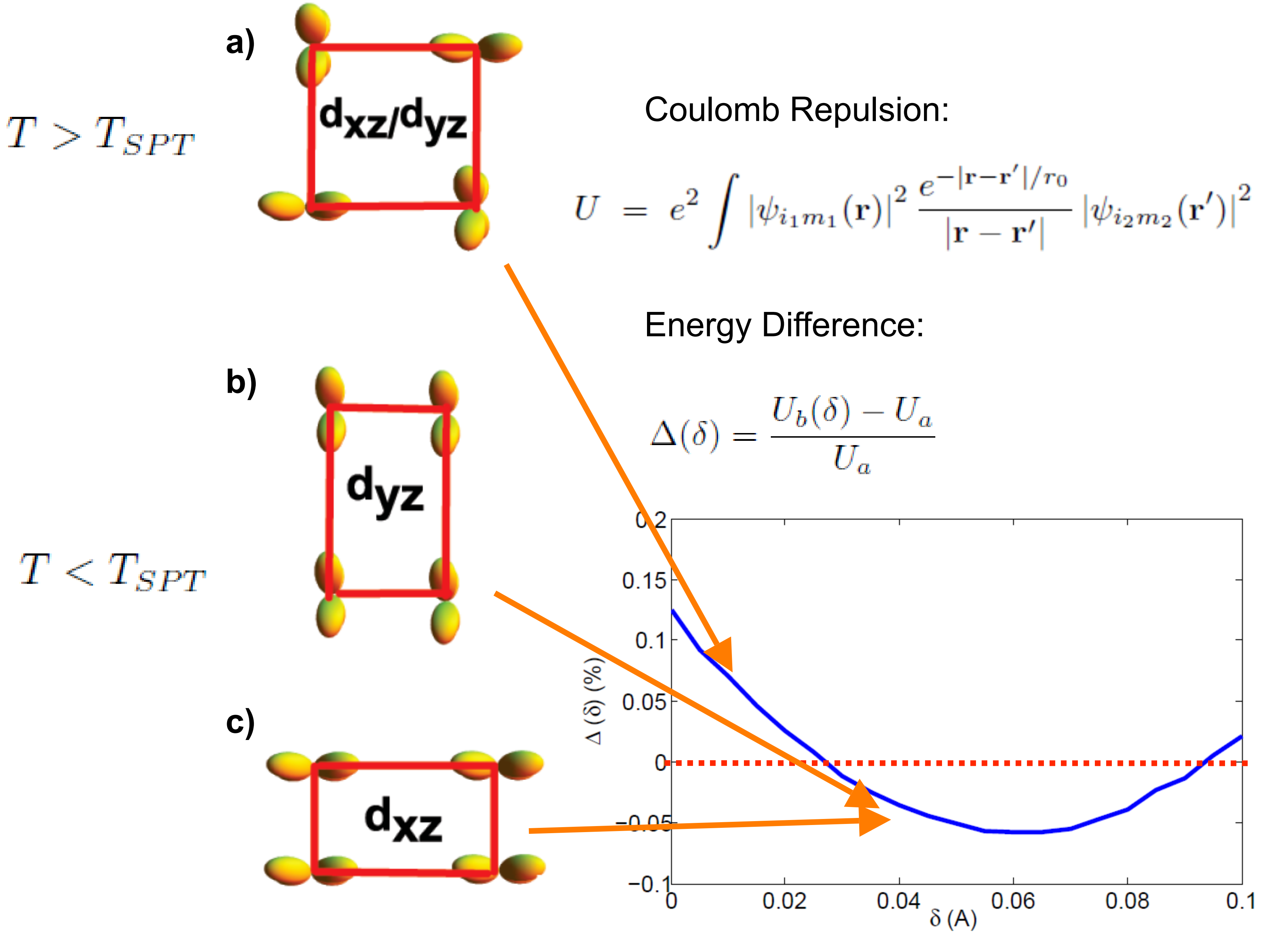





a)
d_{xz}/d_{yz}
$T > T_{SPT}$
Coulomb Repulsion:
$U = e^2 \int |\psi_{i_1 m_1}(\mathbf{r})|^2 \frac{e^{-|\mathbf{r}-\mathbf{r}'|/r_0}}{|\mathbf{r}-\mathbf{r}'|} |\psi_{i_2 m_2}(\mathbf{r}')|^2$
Energy Difference:
$\Delta(\delta) = \frac{U_b(\delta) - U_a}{U_a}$
b)
d_{yz}
$T < T_{SPT}$
c)
d_{xz}
0.2
0.15
0.1
0.05
0
−0.05
−0.1
Δ (δ) (%)
0
0.02
0.04
0.06
0.08
0.1
δ (A)

SPT in Ising Universality Class

$$H_{\mathrm{SPT}} = -J_{\mathrm{SPT}} \sum_{\langle i,j \rangle} M_i M_j$$

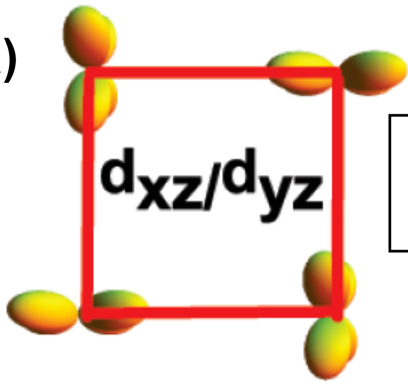
$$M_i = \pm 1, i = d_{yz}, d_{xz}$$

SPT-induced Collinear AF

SPT-induced Collinear AF

$T > T_{SPT}$

a)

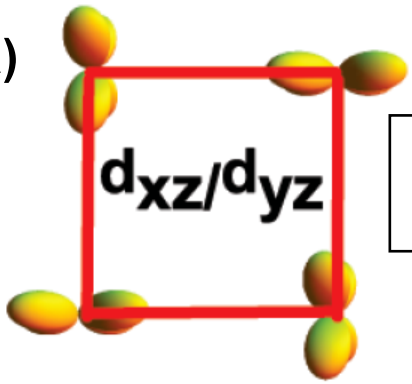


spin disordered

SPT-induced Collinear AF

$T > T_{SPT}$

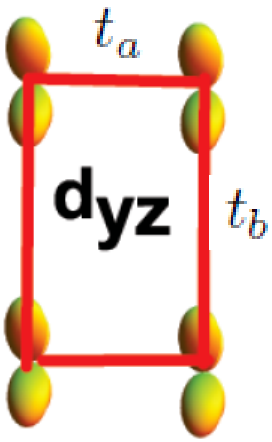
a)



spin
disordered

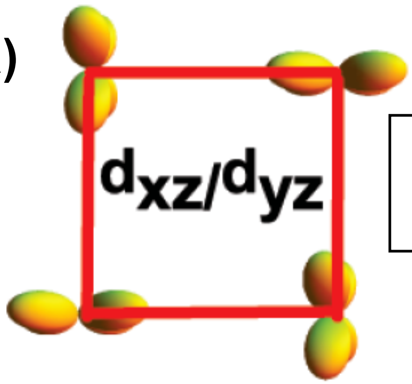
$T < T_{SPT}$

b)



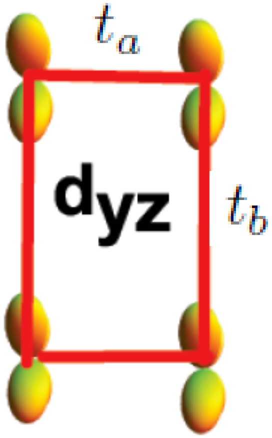
SPT-induced Collinear AF

$T > T_{SPT}$

a) 

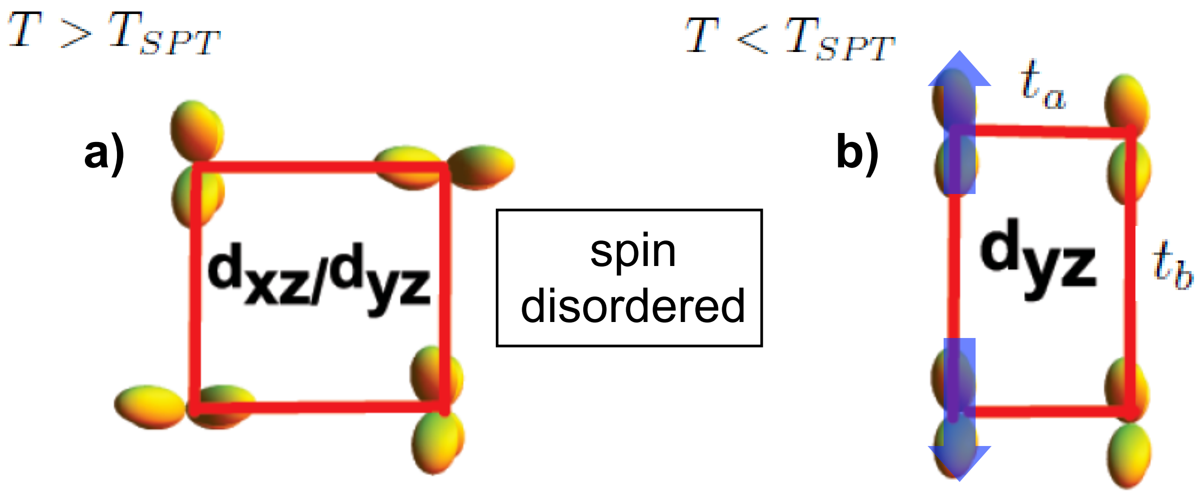
spin
disordered

$T < T_{SPT}$

b) 

$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$

SPT-induced Collinear AF



spin disordered

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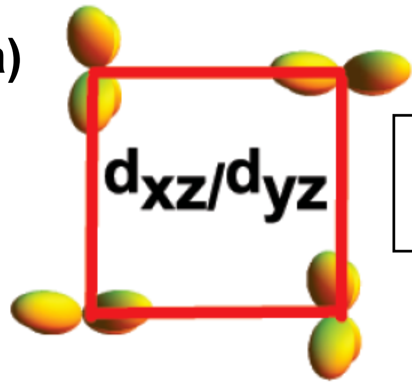
$$J_b > J_a$$

SPT-induced Collinear AF

$T > T_{SPT}$

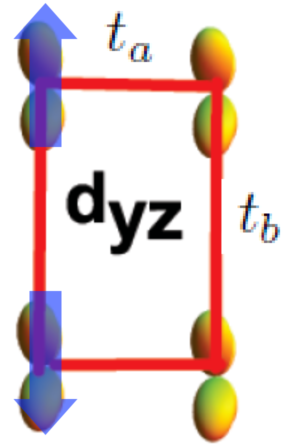
a)



spin disordered

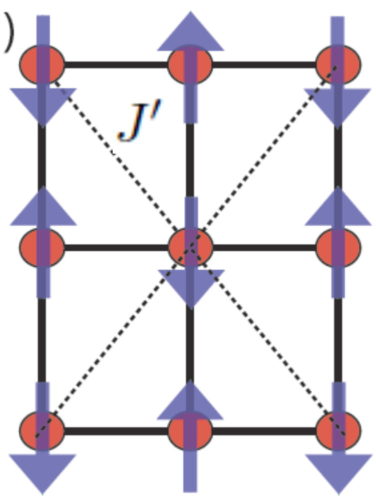
$T < T_{SPT}$

b)



$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$

AF1)

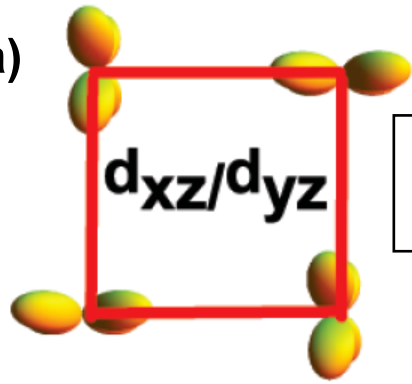


$$E_1 = -2J_a + 4J'$$

SPT-induced Collinear AF

$T > T_{SPT}$

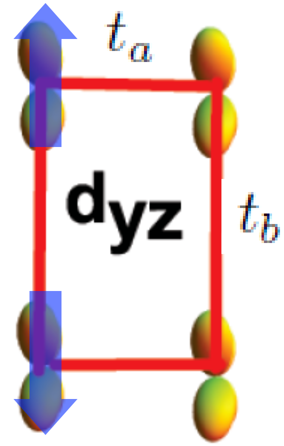
a)



spin
disordered

$T < T_{SPT}$

b)



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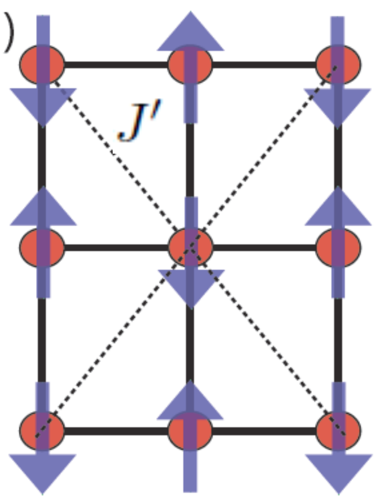
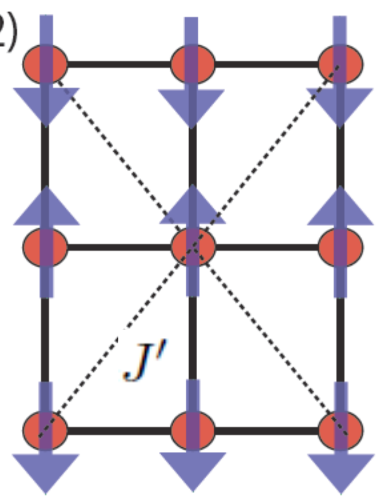
AF1)



AF2)



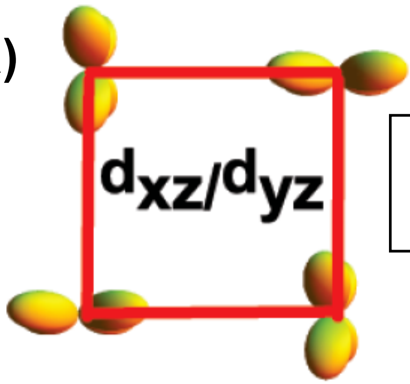
$$E_1 = -2J_a + 4J'$$

$$E_2 = +2J_a - 4J'$$

SPT-induced Collinear AF

$T > T_{SPT}$

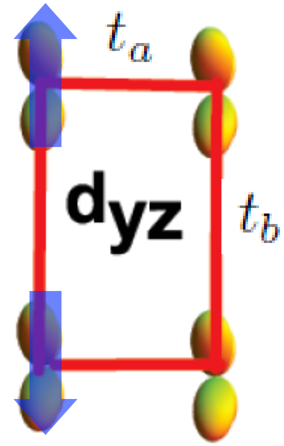
a)



spin disordered

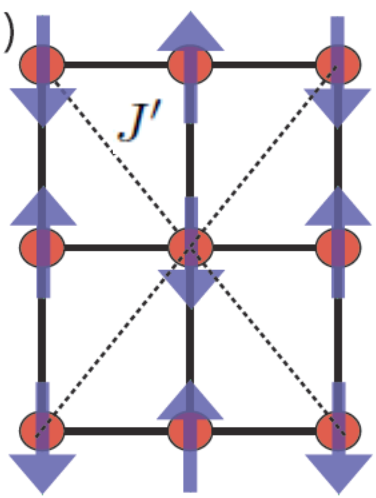
$T < T_{SPT}$

b)

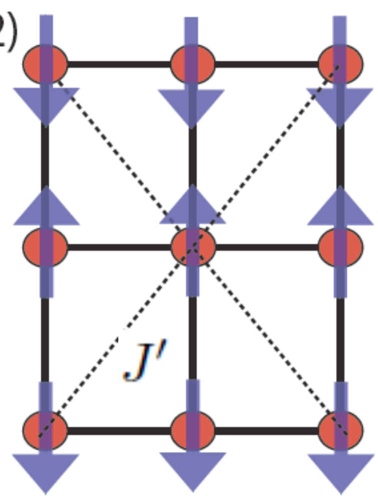


$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$

AF1)



AF2)



$$J' > \frac{J_a}{2}$$

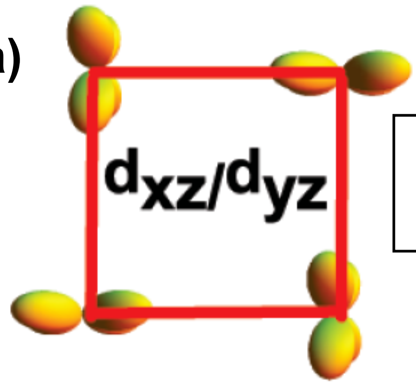
$$E_1 = -2J_a + 4J'$$

$$E_2 = +2J_a - 4J'$$

SPT-induced Collinear AF

$T > T_{SPT}$

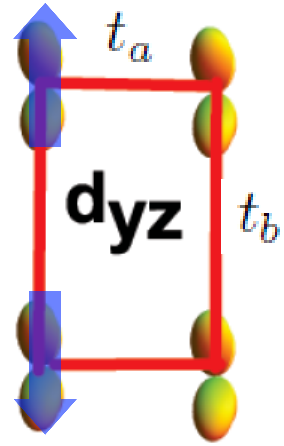
a)



spin disordered

$T < T_{SPT}$

b)



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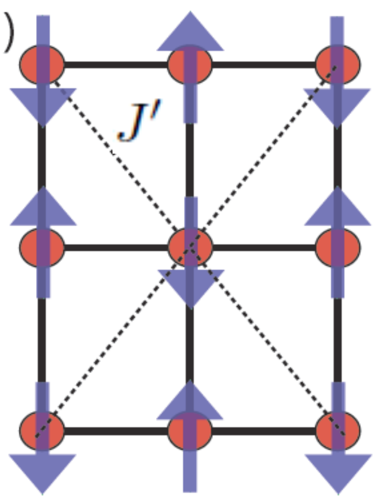
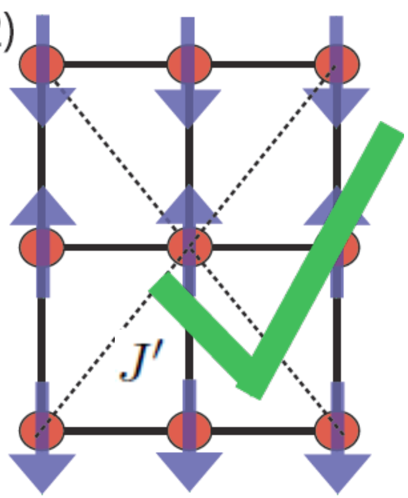
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$

AF1)



AF2)



$$J' > \frac{J_a}{2}$$

$$E_1 = -2J_a + 4J'$$

$$E_2 = +2J_a - 4J'$$

SPT-induced magnetism

$$
\begin{aligned}
H_{\mathrm{SO}} &= J_{\mathrm{SPT}} \sum_{\langle i,j \rangle} M_i M_j + \sum_{\langle\langle i,j \rangle\rangle} J_2\left(M_i, M_j\right) \mathbf{S}_i \cdot \mathbf{S_j} \\
&+ \sum_i J_{1x}\left(M_i, M_{i+\hat{x}}\right) \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}} \\
&+ \sum_i J_{1y}\left(M_i, M_{i+\hat{y}}\right) \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}}
\end{aligned}
$$

$$
\begin{aligned}
J_{1x}\left(M_i, M_j\right) &= \delta_{M_i,M_j}\left(J_{1b}\delta_{M_i,1} + J_{1a}\delta_{M_i,-1}\right) \\
J_{1y}\left(M_i, M_j\right) &= \delta_{M_i,M_j}\left(J_{1a}\delta_{M_i,1} + J_{1b}\delta_{M_i,-1}\right) \\
J_2\left(M_i, M_j\right) &= \delta_{M_i,M_j} J_2
\end{aligned}
$$

122 Fe-Fe is shorter: J_{1b} is enhanced

orbital ordering

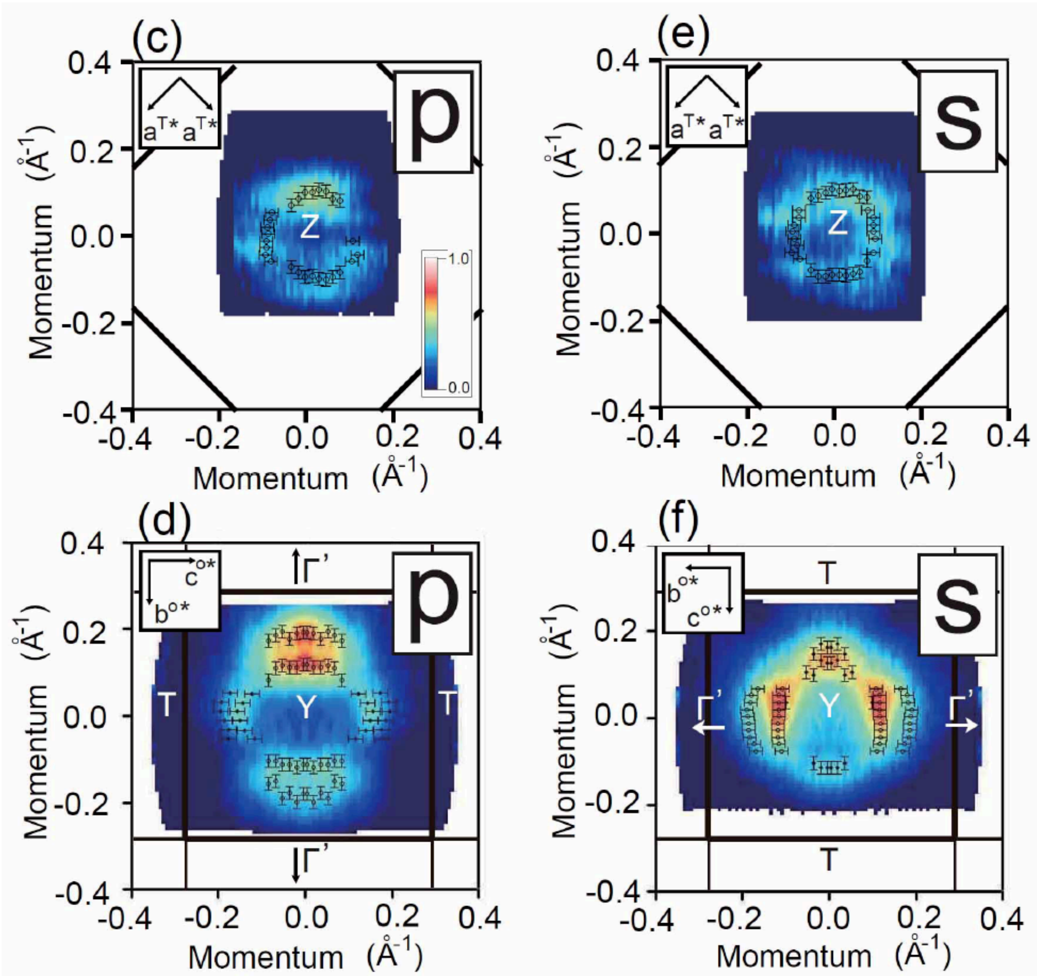
$\Downarrow$

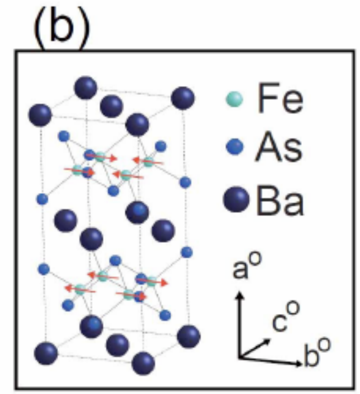
transport anisotropies

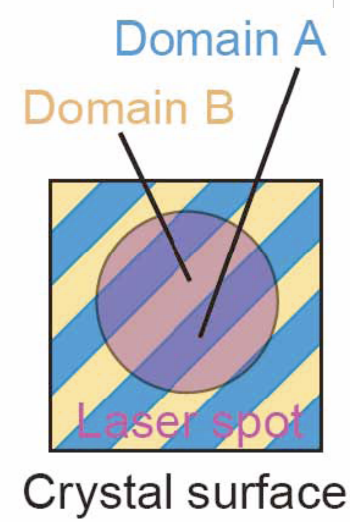
Orbital-polarized Fermi surface in antiferromagnetic state of $BaFe_2As_2$

Shimojima, et al.
arXiv:0904.1632

- **Polarized ARPES**







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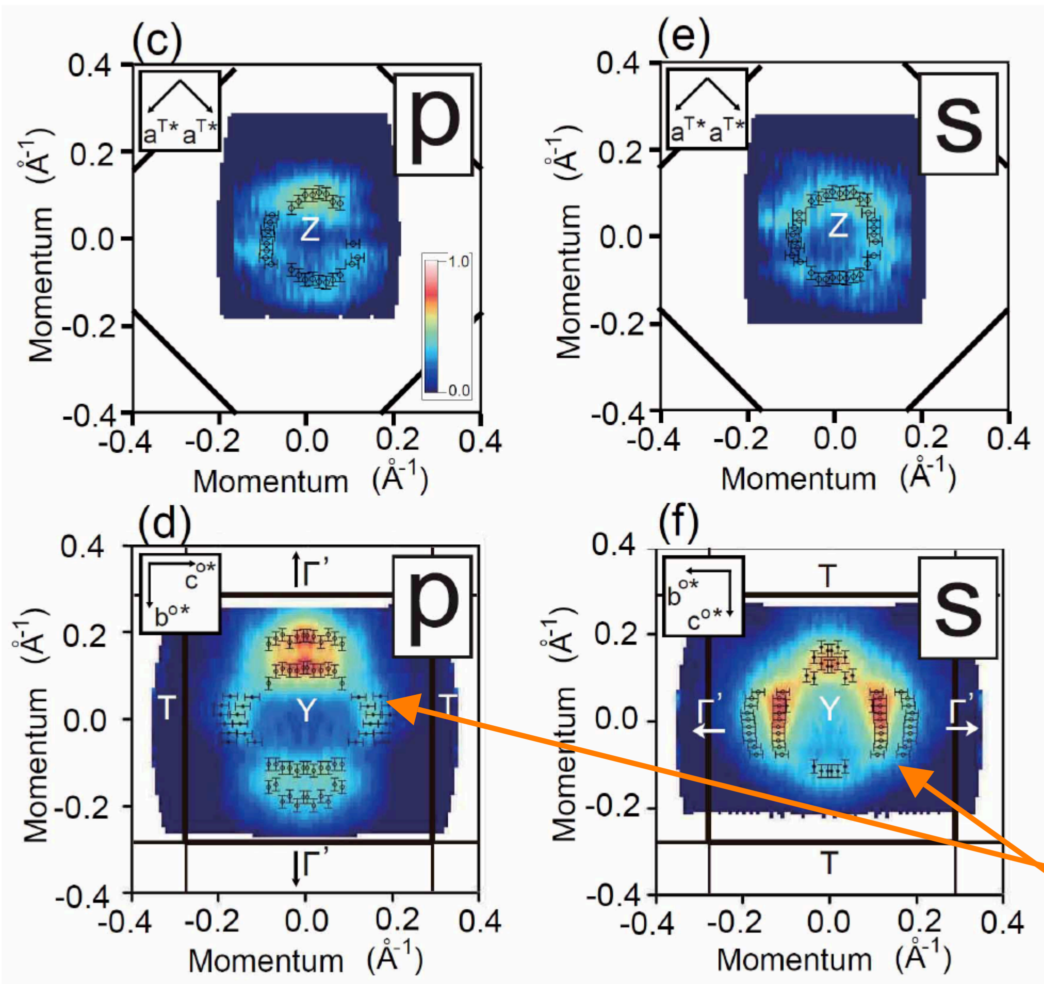
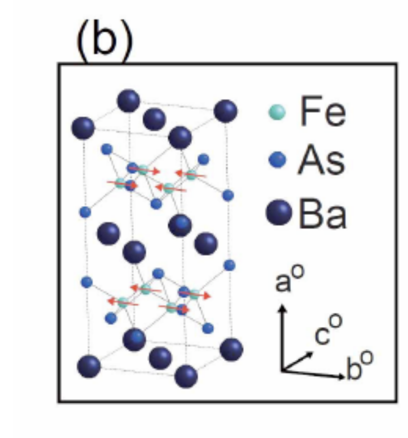
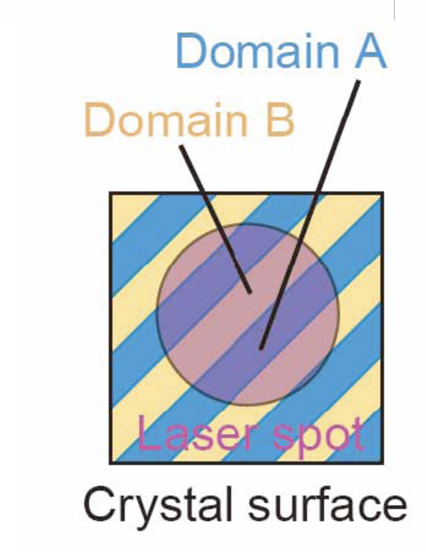
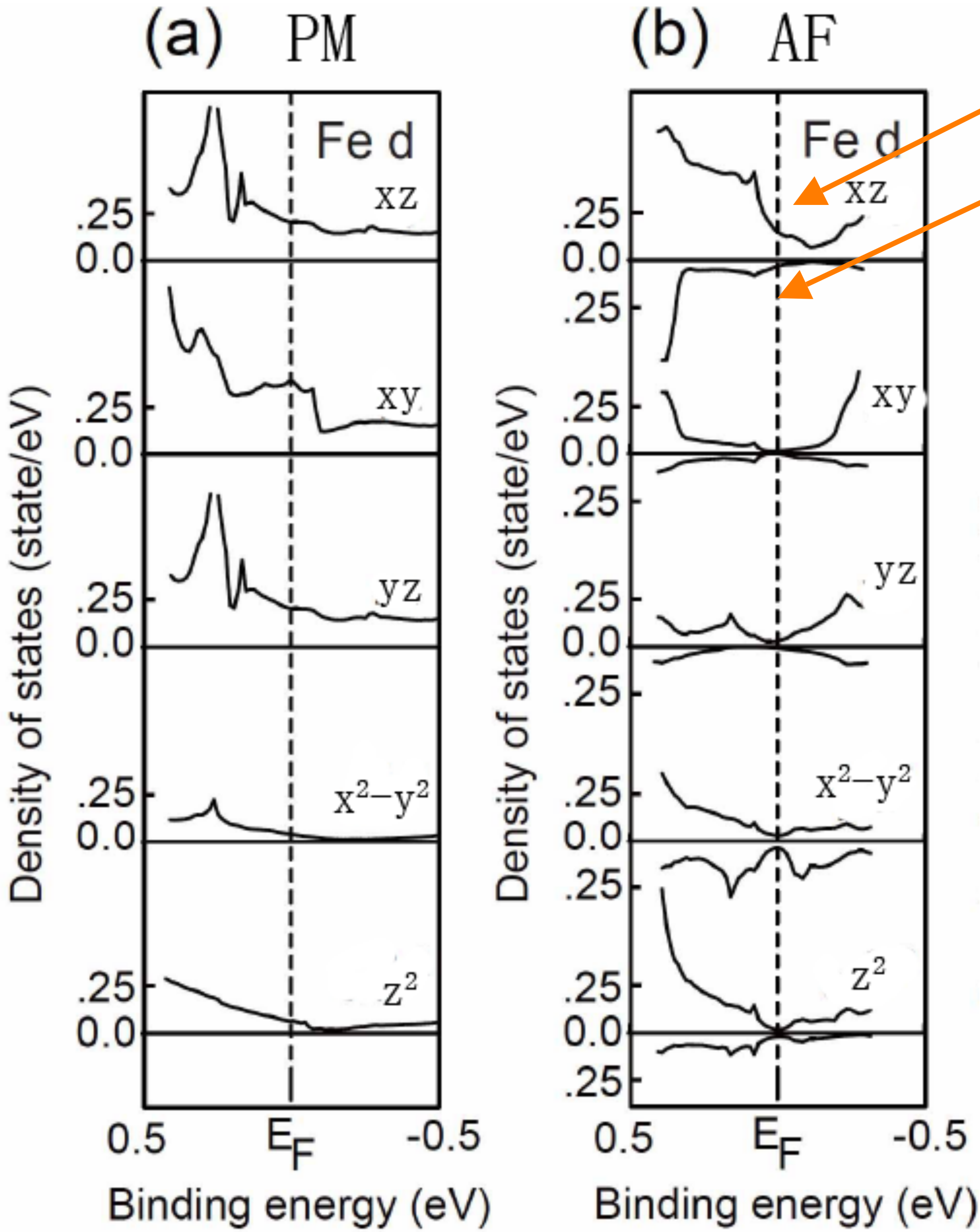






d_{xz} **in domain A**

d_{xz} **in domain B**



(a) PM state:

1. d_{xz}, d_{yz} degenerate
2. Fermi surface is composed by multiple orbitals

(b) AF state:

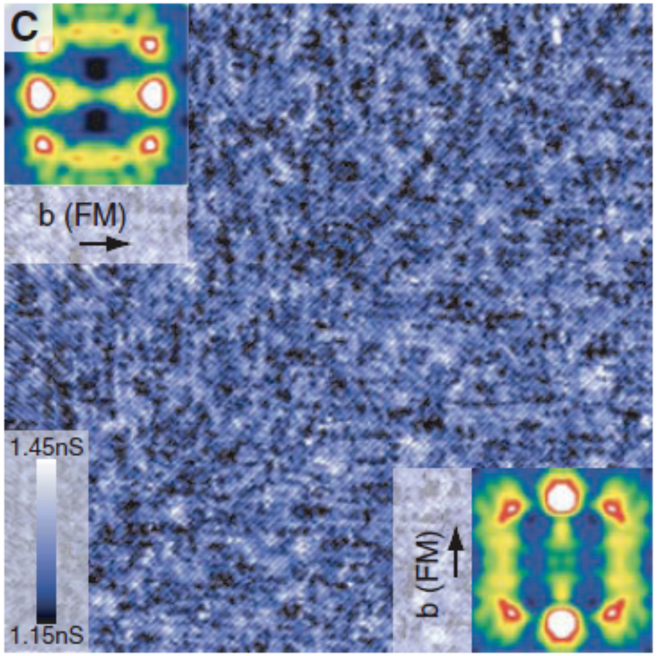
1. Localized moment is formed by d_{xz}
2. Fermi surface is orbital-polarized

OO-induced anisotropies

OO-induced anisotropies

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

FM easy axis!



OO-induced anisotropies

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

- *STM*

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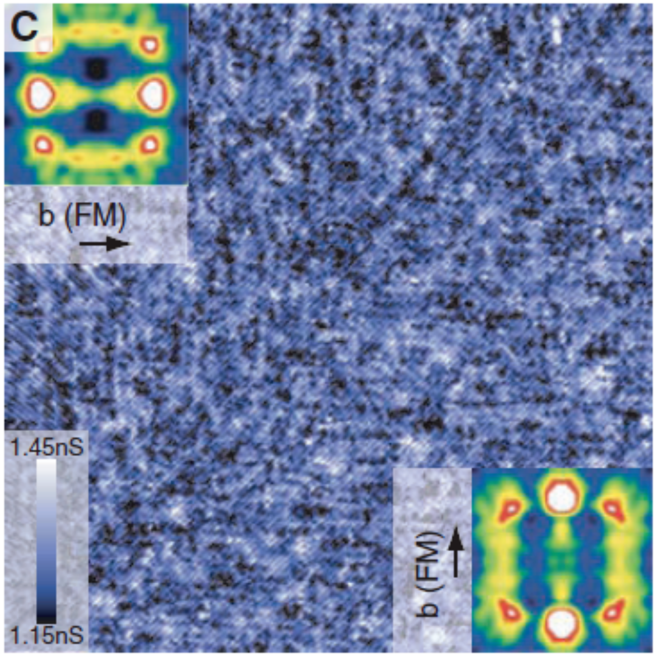

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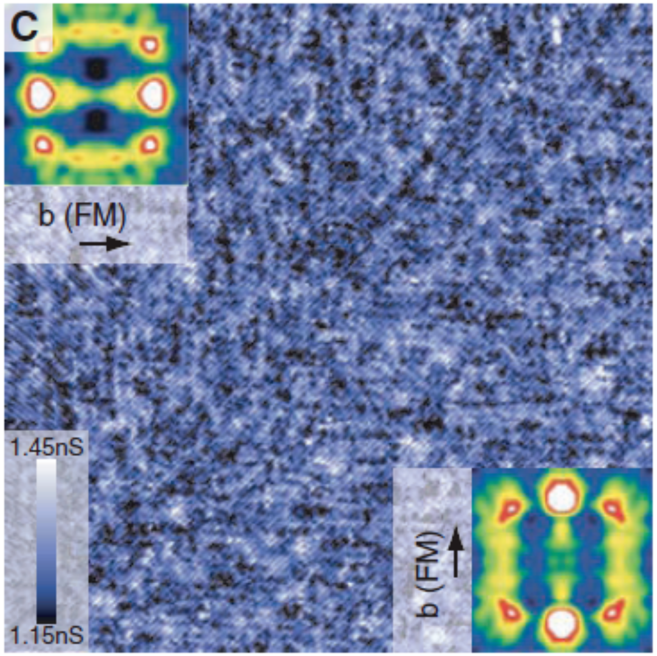
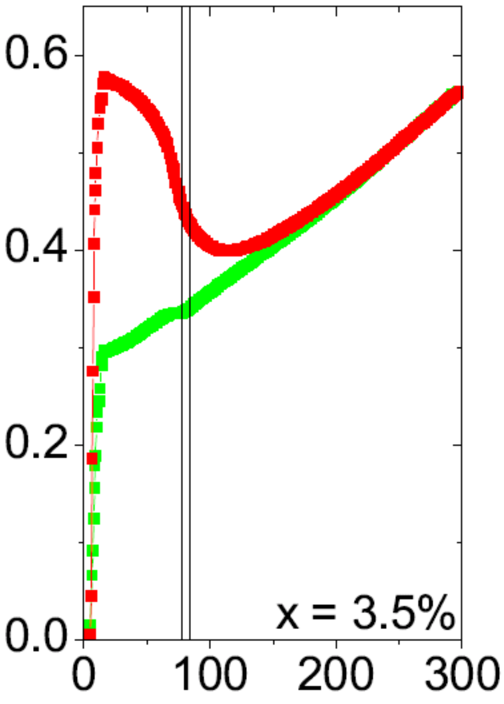


AF is easy axis!

- *Resistivity*

J.-H. Chu, *et al.*
arXiv:1002.3364



Tetragonal : Even occupancy of two degenerate orbitals d_{xz} and d_{yz}

Jahn-Teller Effect (orbital ordering)

Orthorhombic : Break the degeneracy of two orbitals d_{xz} and d_{yz} , occupy only one orbital

A gap open between d_{xz} and d_{yz}

Resistivity Anomaly

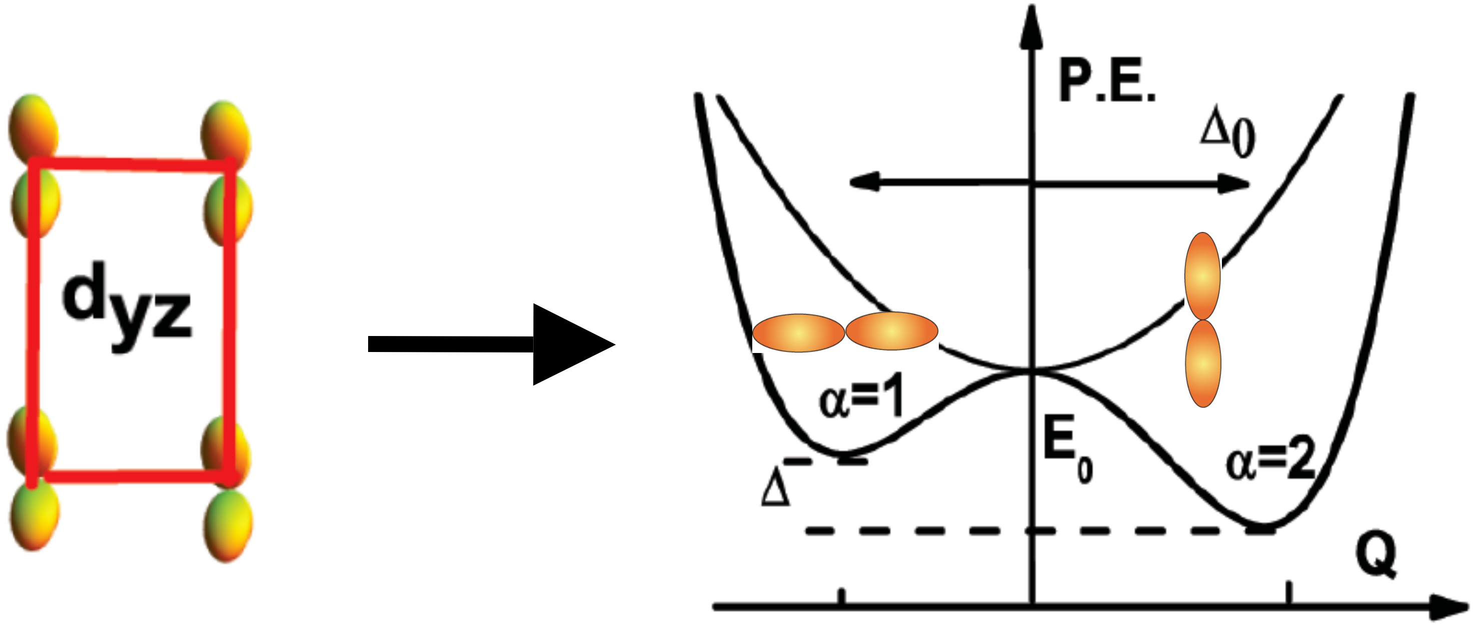
$$T > T_{SPT}$$

d_{xz}

d_{yz}

two-level system:
Kondo-like problem

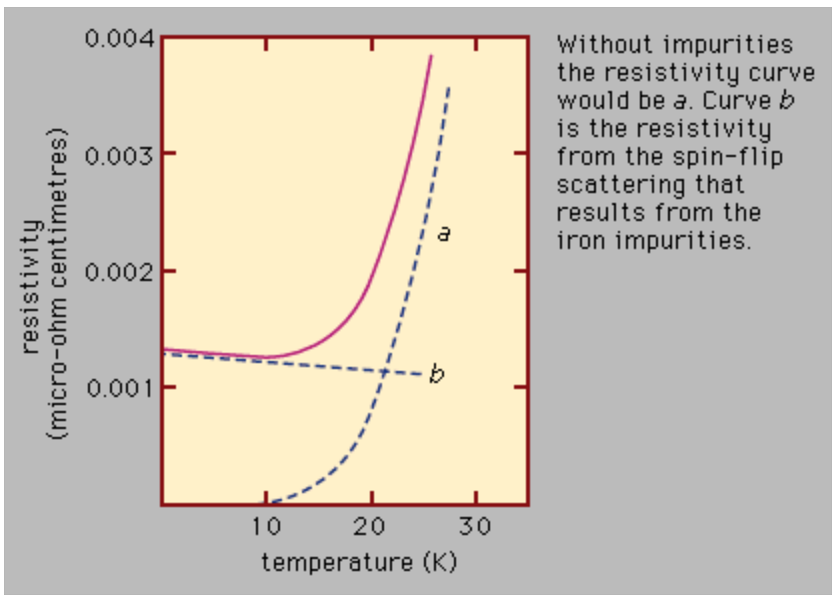
A Two-level System

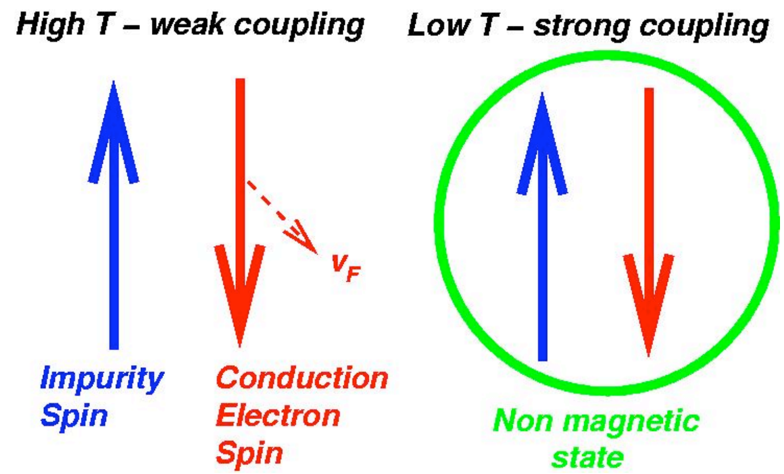


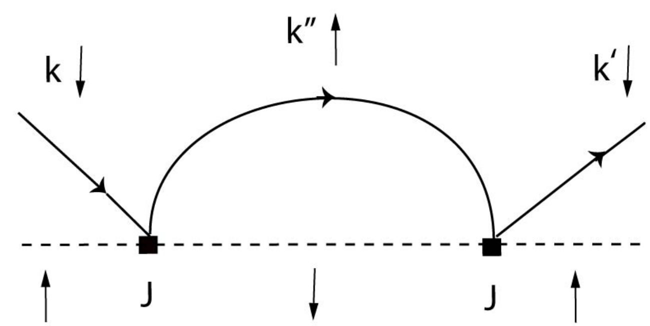
$$H_{\rm TLS} = \lambda_{ps} \sum_{\alpha} a_\alpha^\dagger a_\alpha + \frac{1}{2}\Delta \sum_{\alpha\beta} a_\alpha^\dagger \sigma^z_{\alpha\beta} a_\beta + \frac{1}{2}\Delta_0 \sum_{\alpha\beta} a_\alpha^\dagger \sigma^x_{\alpha\beta} a_\beta$$

$$E = \sqrt{\Delta_0^2 + \Delta^2}$$

Kondo effect

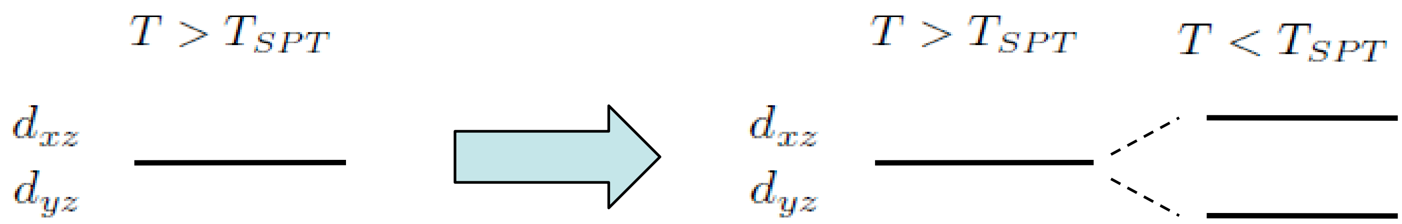




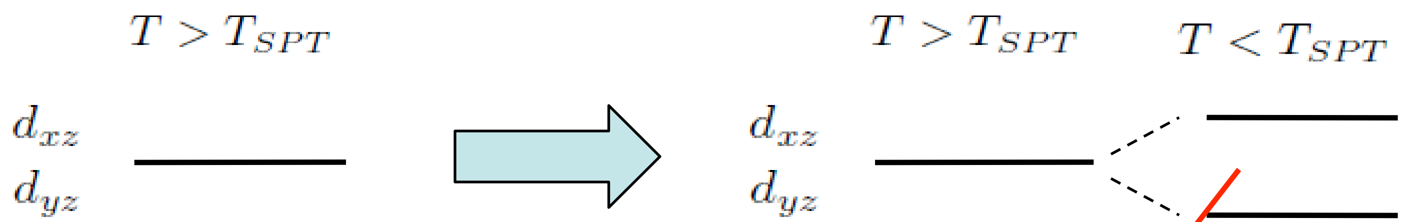


Resistivity anomaly

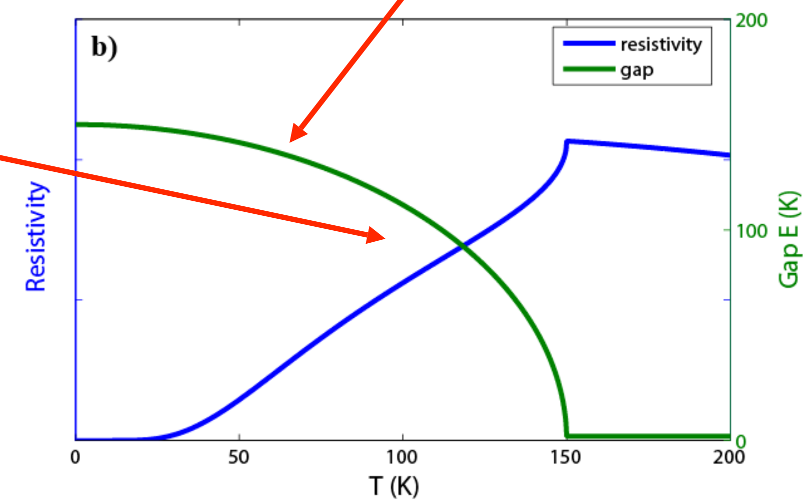
Resistivity anomaly



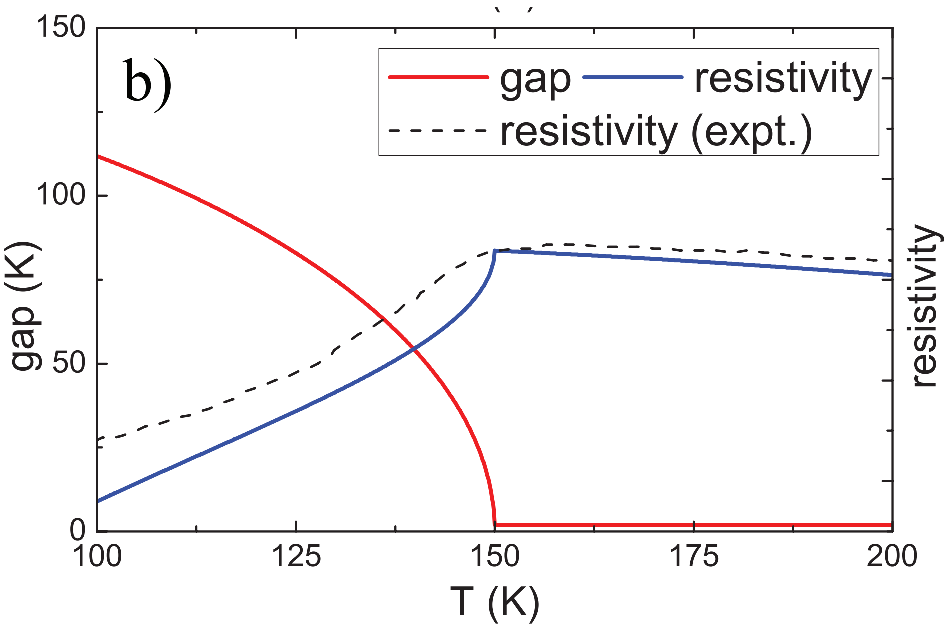
Resistivity anomaly



Opening of the gap makes scattering difficult; Resistivity decreases



Resistivity Anomaly



Conclusion I:

Orbital-ordering

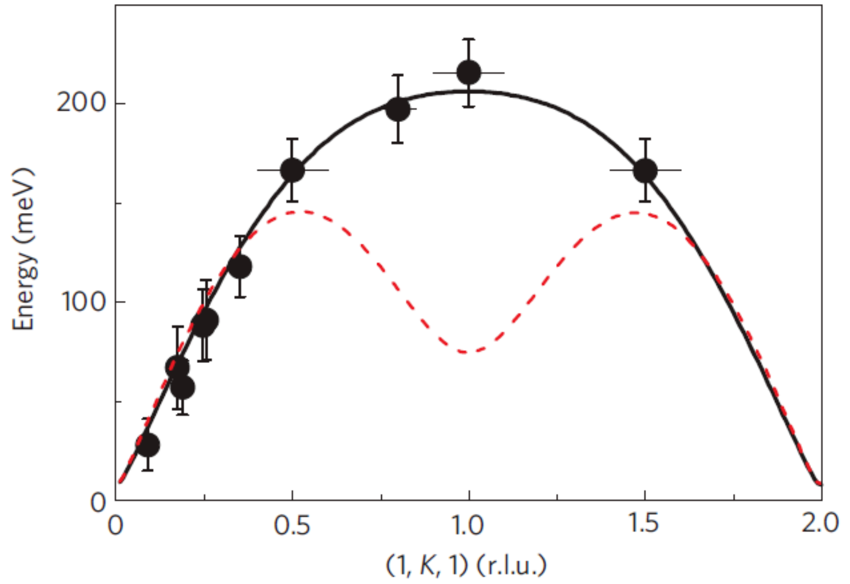
$\Downarrow$

Structural Phase Transition

$\Downarrow$

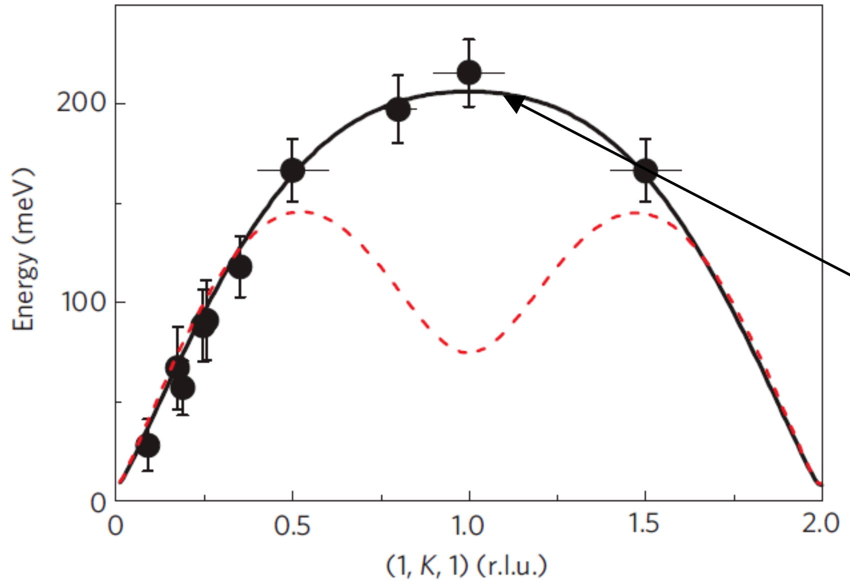
Resistivity anomaly

spin-wave spectrum



origin of ferromagnetic coupling?

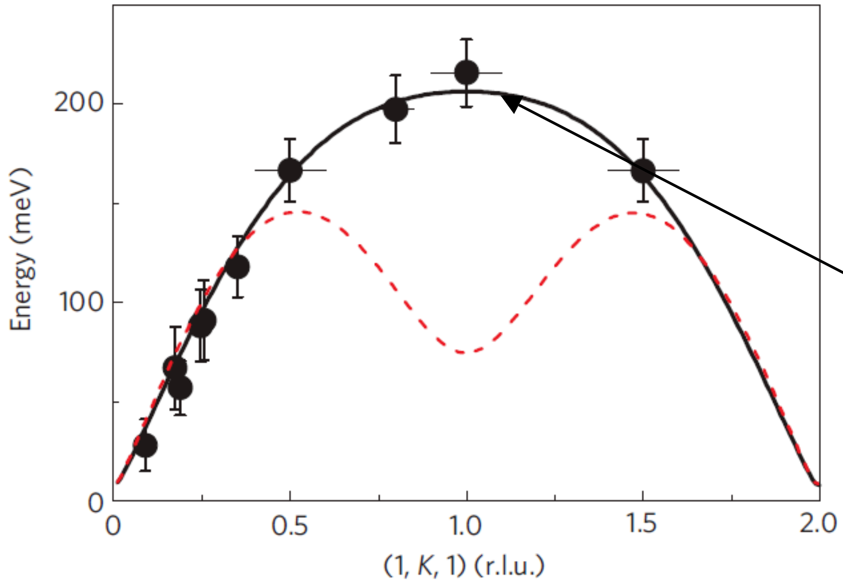
spin-wave spectrum



$$
\begin{aligned}
SJ_1^a &= 49.9 \pm 9.9\,\mathrm{meV} \\
SJ_1^b &= -5.7 \pm 4.5\,\mathrm{meV} \\
SJ_2 &= 18.9 \pm 3.4\,\mathrm{meV}
\end{aligned}
$$

origin of ferromagnetic coupling?

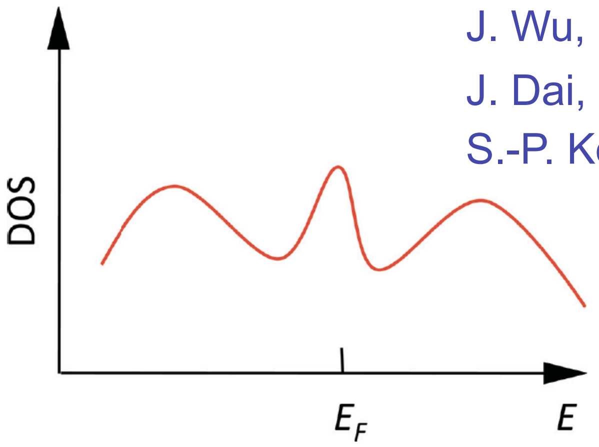
spin-wave spectrum



$$SJ_1^a = 49.9 \pm 9.9\,\mathrm{meV}$$
$$\boxed{SJ_1^b = -5.7 \pm 4.5\,\mathrm{meV}}$$
$$SJ_2 = 18.9 \pm 3.4\,\mathrm{meV}$$

origin of ferromagnetic coupling?

- *A local-itinerant model*



J. Wu, *et al.* PRL (2008)

J. Dai, *et al.* PNAS (2009)

S.-P. Kou, *et al.* EPL (2009)

- *A local-itinerant model*

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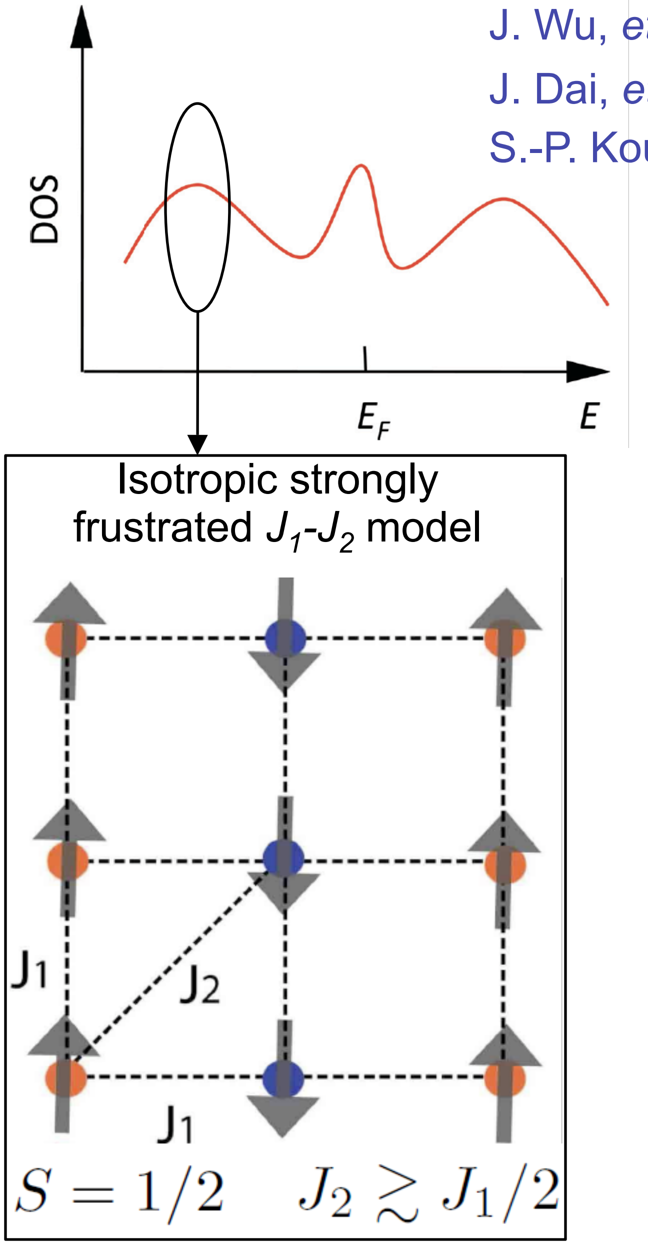

- *A local-itinerant model*

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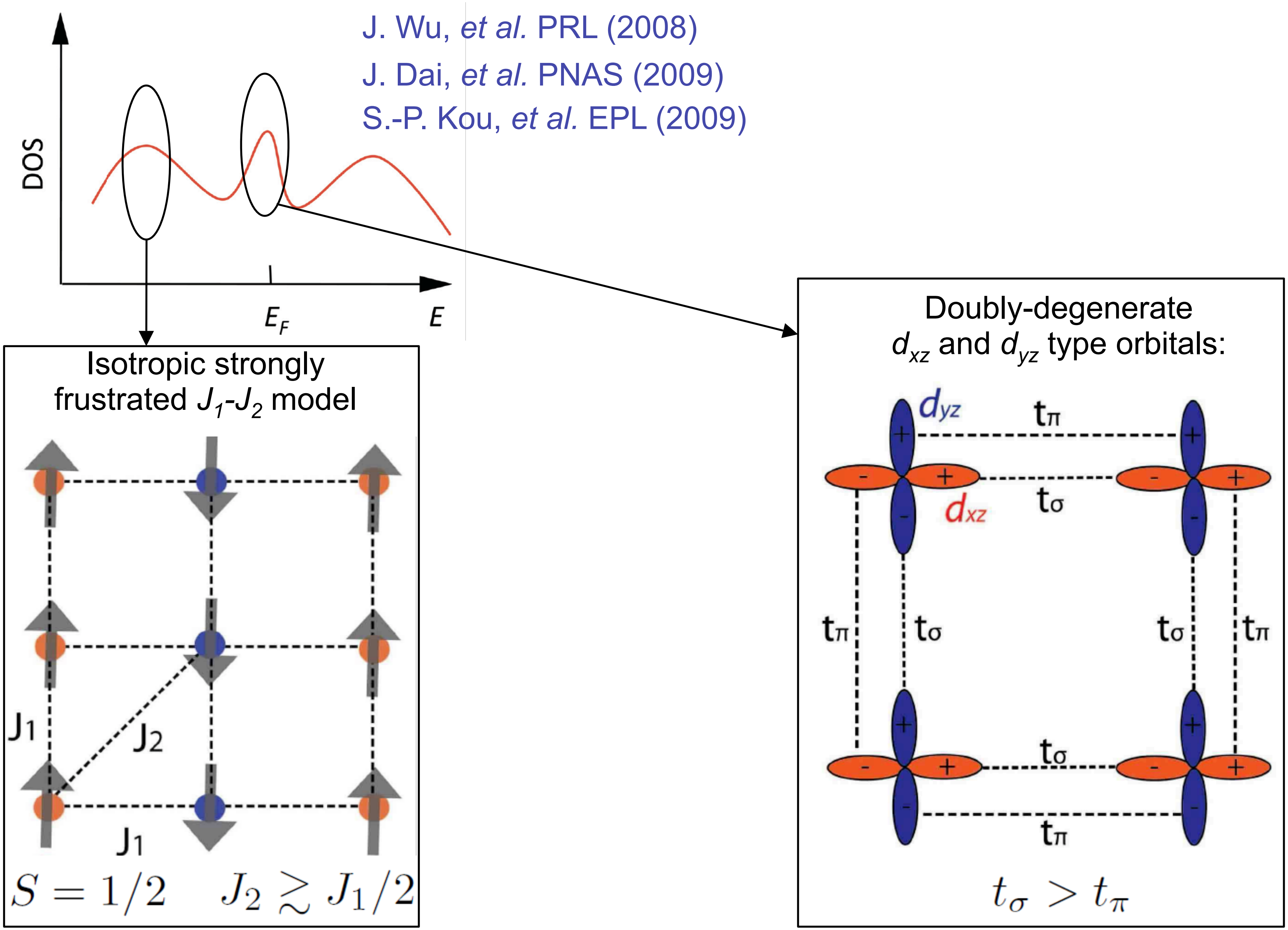

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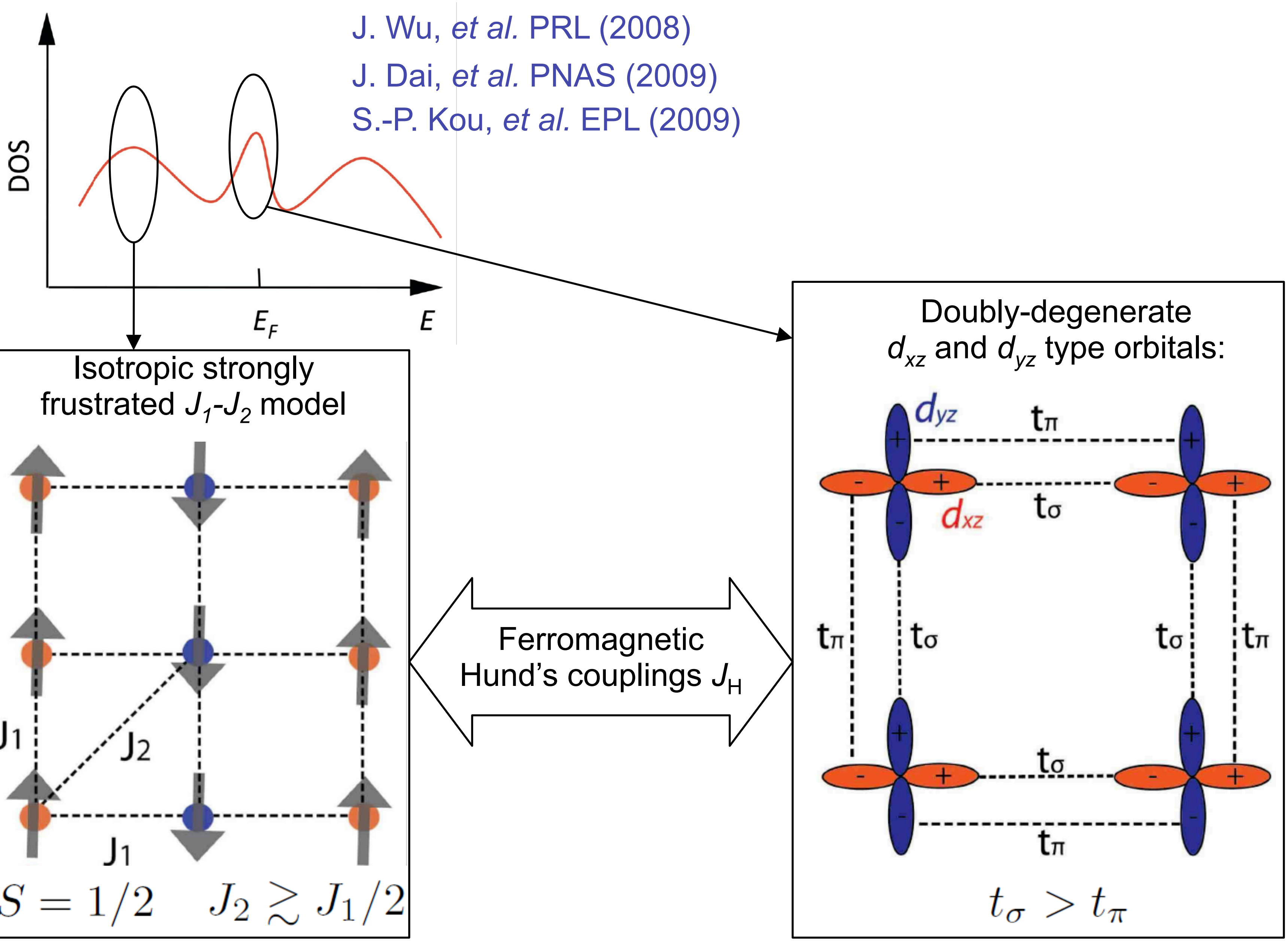

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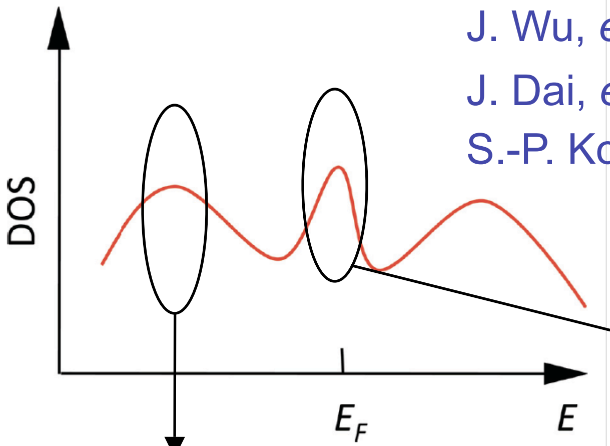
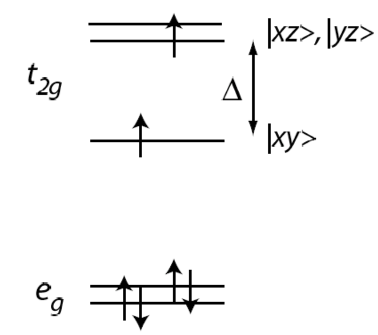
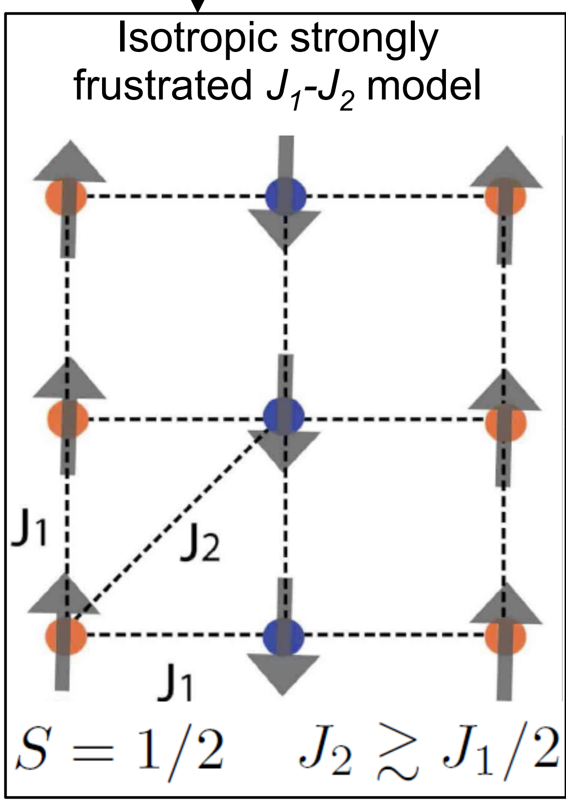
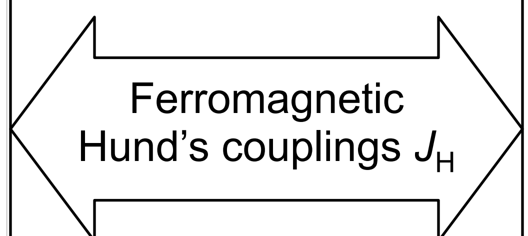
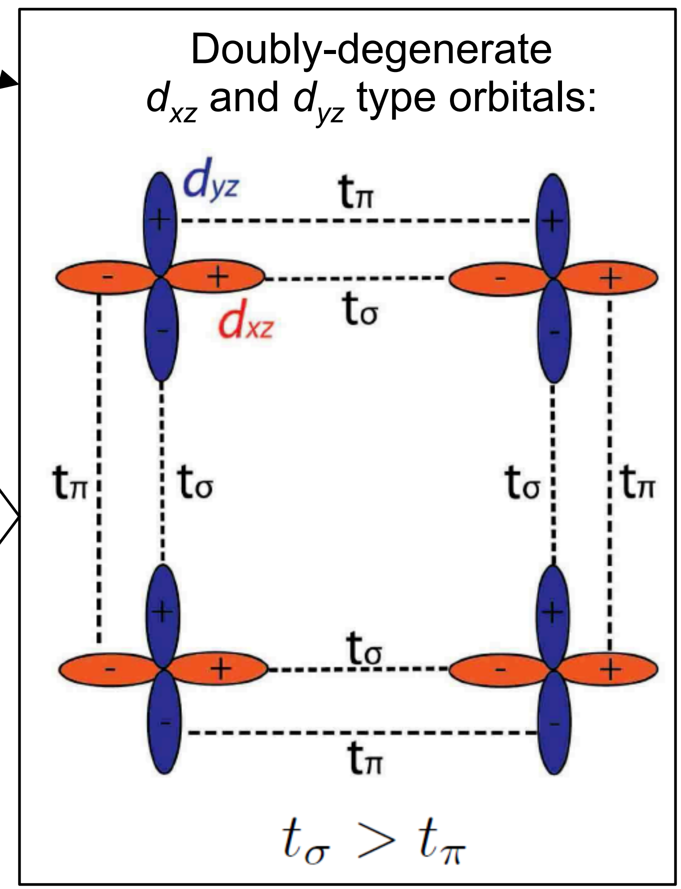


consistent with the local multiplet structure:









Double-Exchange Model

$$\mathcal{H}_{\text{loc}} = \frac{J_1}{S^2} \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \frac{J_2}{S^2} \sum_{\langle\langle i,j \rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

unlike manganites

$$\nu J_H \ll \infty$$

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$$\mathcal{H}_{\rm it} = - \sum_{ij,\alpha\beta,\nu} t_{ij}^{\alpha\beta} c^{\dagger}_{i\alpha\nu} c_{j\beta\nu} + \frac{V}{2} \sum_{i,\alpha\neq\beta,\nu\nu'} \hat{n}_{i\alpha\nu} \hat{n}_{i\beta\nu'}$$

$$\mathcal{H}_{\rm H}^{(0)} = -\frac{J_{\rm H}}{2} \sum_{k,\alpha,\nu} \nu \tilde{c}^{\dagger}_{k\alpha\nu} \tilde{c}_{k\alpha\nu}$$

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• *local moments*:

$$\boxed{\mathcal{H}_{\mathrm{loc}} = \frac{J_1}{S^2} \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \frac{J_2}{S^2} \sum_{\langle\langle i,j \rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j}$$

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sublattice rotations ⬇ Holstein-Primakoff bosons

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sublattice rotations Holstein-Primakoff bosons

$$\mathcal{H}^{\rm sw}_{\rm loc} = \sum_q \left[A_0(q)\left(a^\dagger_q a_q + a_{-q} a^\dagger_{-q}\right) + B_0(q)\left(a^\dagger_q a^\dagger_{-q} + a_{-q} a_q\right)\right]$$

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sublattice rotations $\quad\Downarrow\quad$ Holstein-Primakoff bosons

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sublattice rotations | Holstein-Primakoff bosons

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sublattice rotations | mean-field decoupling

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sublattice rotations

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sublattice rotations

mean-field decoupling

$$\mathcal{H}^{(0)}_{\mathrm{H}} = -\frac{J_{\mathrm{H}}}{2} \sum_{k,\alpha,\nu} \nu \tilde{c}^\dagger_{k\alpha\nu} \tilde{c}_{k\alpha\nu}$$

$$\begin{aligned} \mathcal{H}_{\mathrm{e}} &= \mathcal{H}^{\mathrm{mf}}_{\mathrm{it}} + \mathcal{H}^{(0)}_{\mathrm{H}} \\ &= \sum_{k,\alpha,\nu} \left[\left(\varepsilon^\alpha_1(k) - \nu \frac{J_{\mathrm{H}}}{2} + V \rho_{\bar{\alpha}} \right) \tilde{c}^\dagger_{k\alpha\nu} \tilde{c}_{k\alpha\nu} + \varepsilon^\alpha_2(k)\, \tilde{c}^\dagger_{k\alpha\nu} \tilde{c}_{k\alpha\bar{\nu}} \right] \end{aligned}$$

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sublattice rotations Holstein-Primakoff bosons

$$\mathcal{H}_{\text{loc}}^{\text{sw}} = \sum_q \left[A_0(q) \left(a_q^\dagger a_q + a_{-q} a_{-q}^\dagger \right) + B_0(q) \left(a_q^\dagger a_{-q}^\dagger + a_{-q} a_q \right) \right]$$

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sublattice rotations mean-field decoupling

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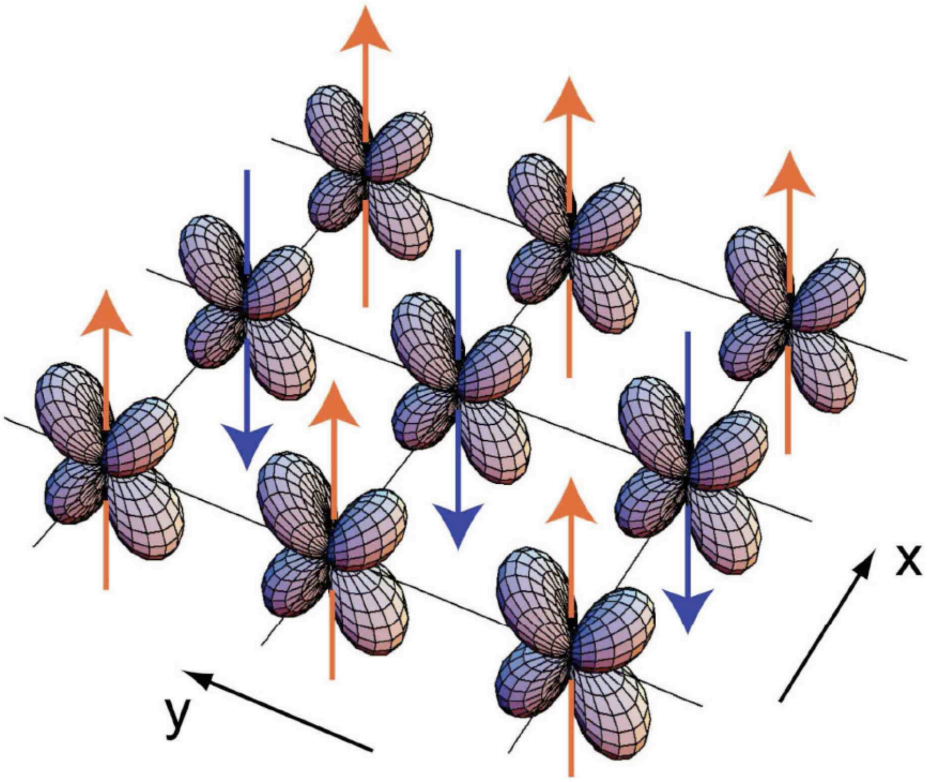
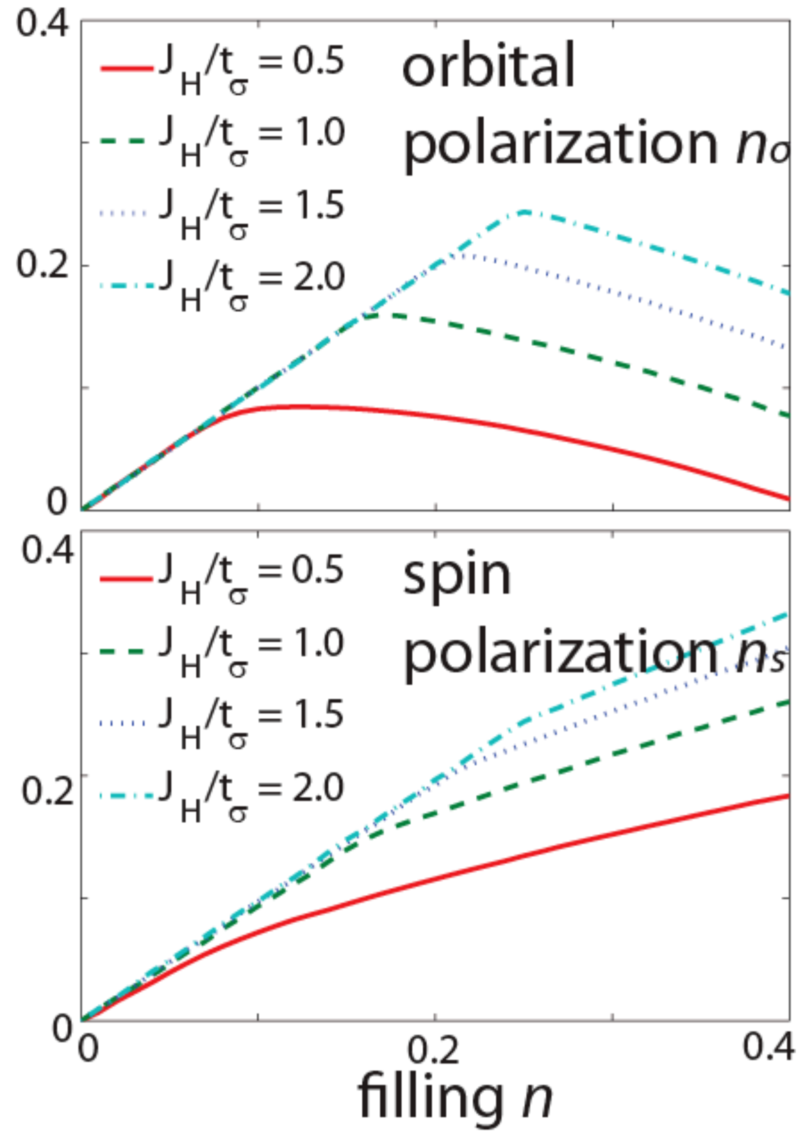
- *Orbital ordering*

$$n_o = \sum_\nu (\rho_{yz,\nu} - \rho_{xz,\nu})$$

$$n_s = \sum_\alpha (\rho_{\alpha,\uparrow} - \rho_{\alpha,\downarrow})$$





$t_\pi = 0.1 t_\sigma$

- *Spin-wave dispersion with both super- and double-exchange*

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  - *Hund's coupling*: $\mathcal{H}_{\mathrm{H}} = \mathcal{H}_{\mathrm{H}}^{(0)} + \mathcal{H}_{\mathrm{H}}^{(1)} + \mathcal{H}_{\mathrm{H}}^{(2)}$

$$\mathcal{H}_{\mathrm{H}}^{(1)} = -\frac{J_{\mathrm{H}}}{\sqrt{2S}} \sum_{kq,\alpha} \left(a_q \tilde{c}^{\dagger}_{k+q,\alpha\downarrow} \tilde{c}_{k\alpha\uparrow} + \mathrm{h.c.} \right)$$

$$\mathcal{H}_{\mathrm{H}}^{(2)} = \frac{J_{\mathrm{H}}}{2S} \sum_{k,qq',\alpha\nu} \nu a^{\dagger}_q a_{q'} \tilde{c}^{\dagger}_{k-q,\alpha\nu} \tilde{c}_{k-q',\alpha\nu}$$

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    Eliminating terms linear in a_q*, we require:* $[\Delta, \mathcal{H}_{\rm e}] + \mathcal{H}_{\rm H}^{(1)} = 0$

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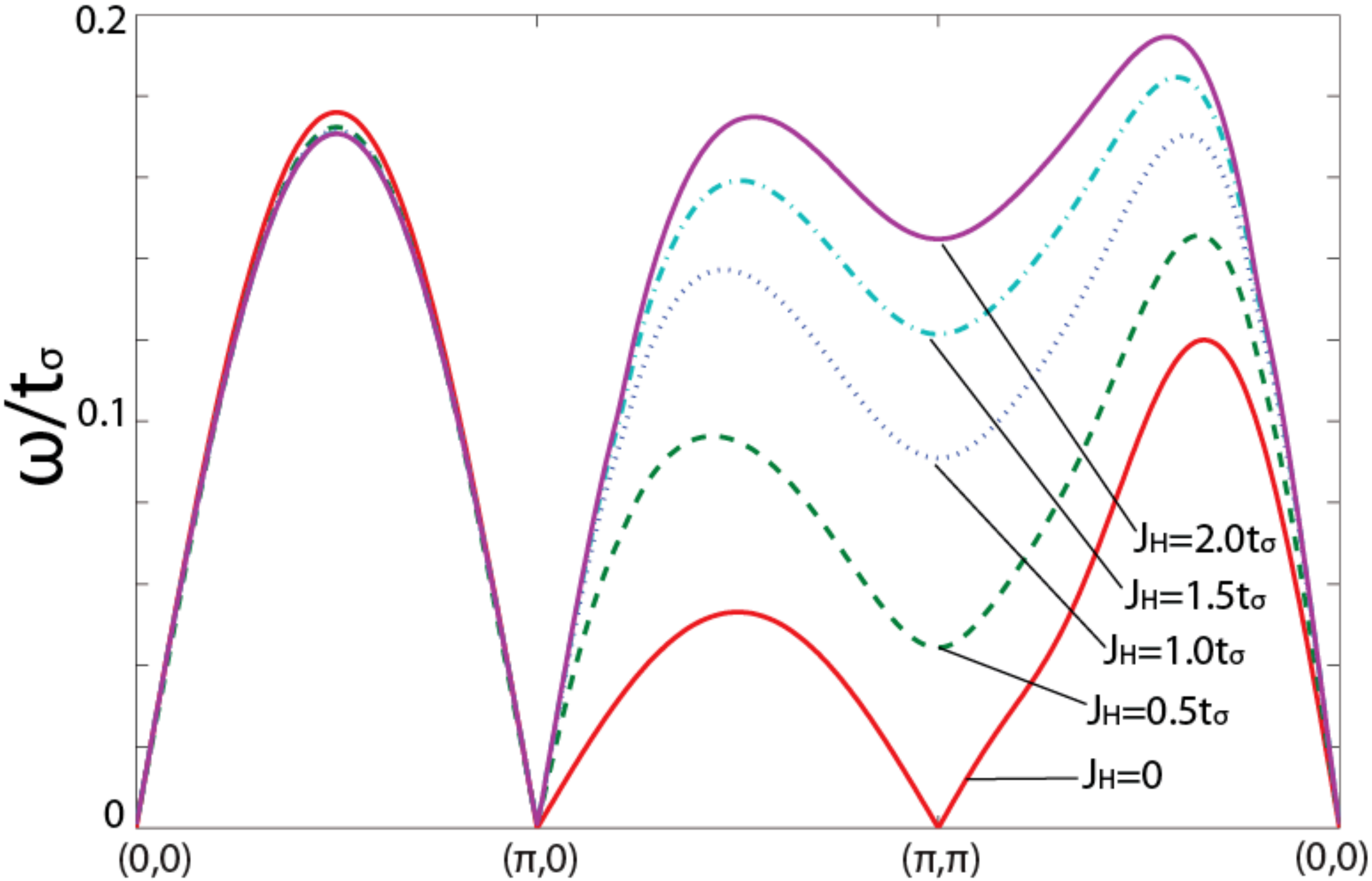
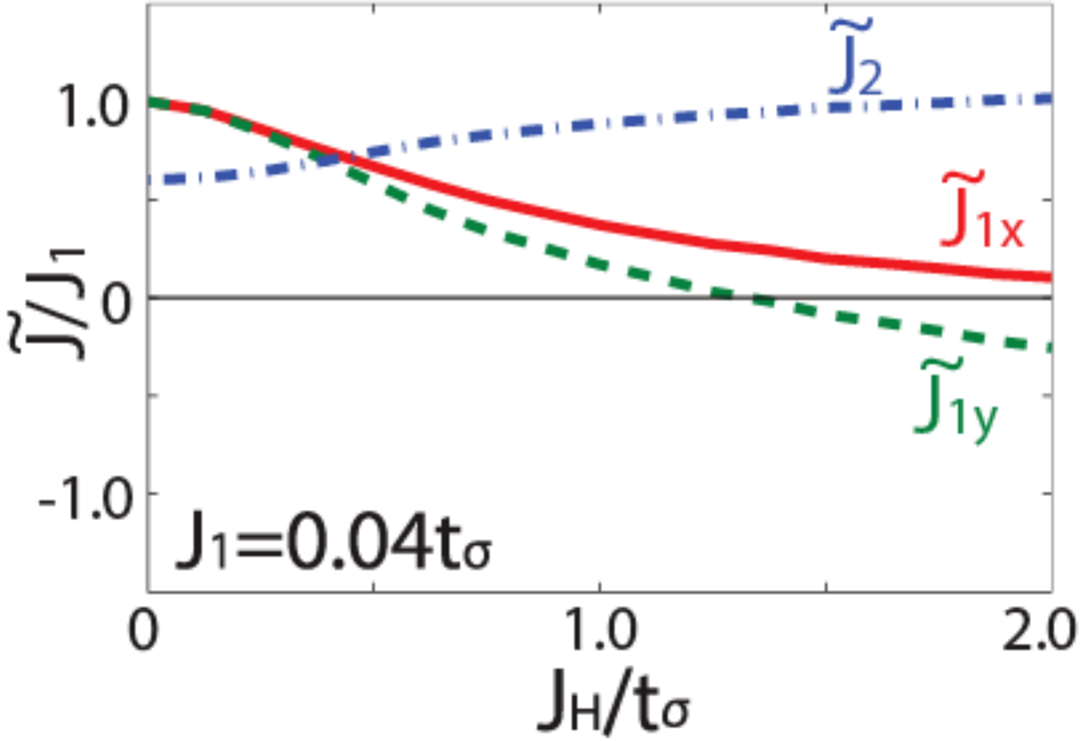
Spin-wave dispersions: $\omega(q) = \sqrt{A^2(q) - B^2(q)}$

- *Spin-wave dispersion with both super- and double-exchange*



$J_1 = 0.04t_\sigma,\ J_2 = 0.6J_1$ $\qquad n = 0.1,\ t_\pi = 0.1t_\sigma$

• *Fitting to an anisotropic Heisenberg model*:



emergent ferro-orbital order

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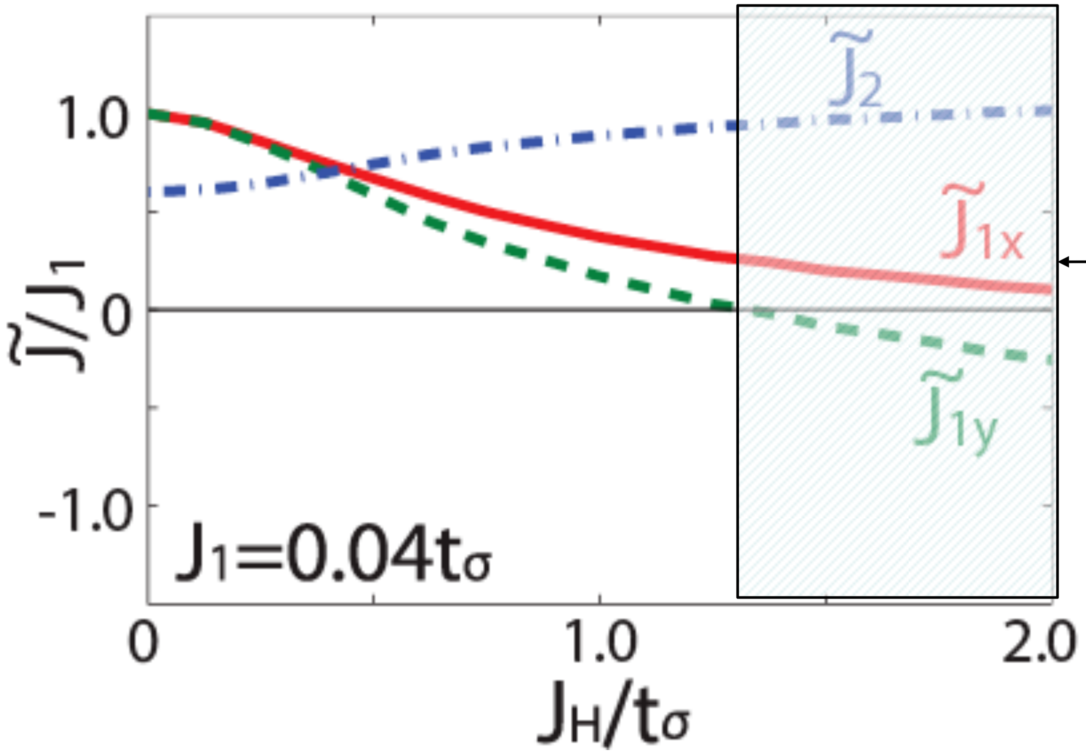

For large J_H, magnetism is unfrustrated!

emergent ferro-orbital order

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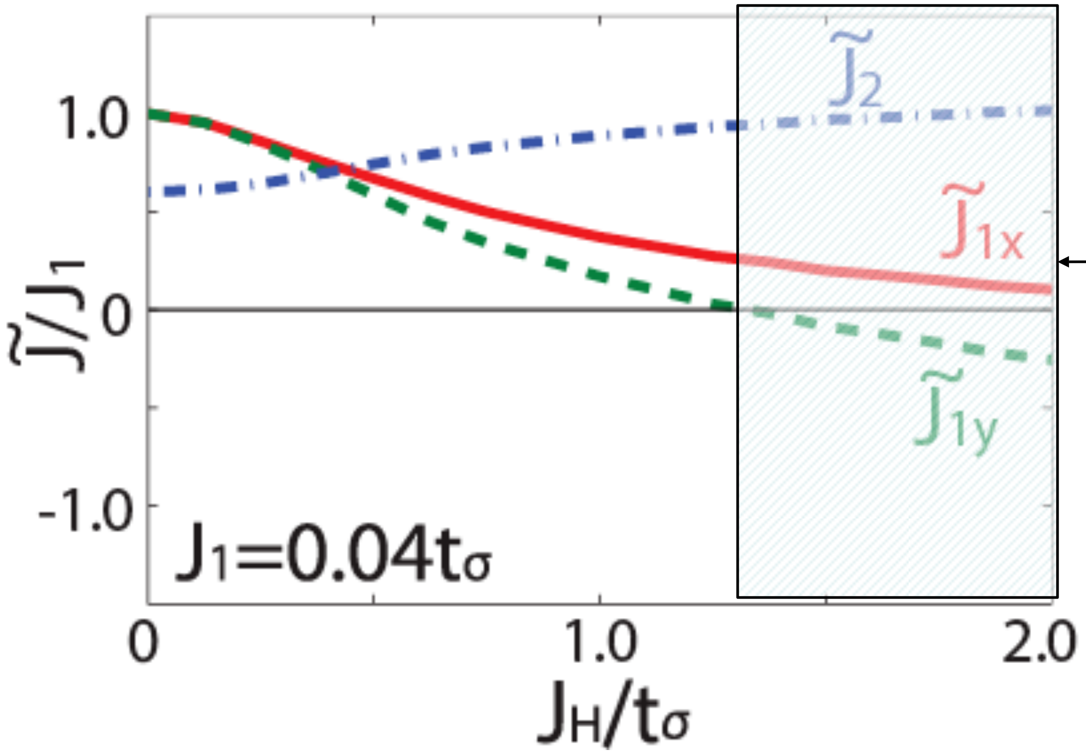


For large J_H, magnetism is unfrustrated!

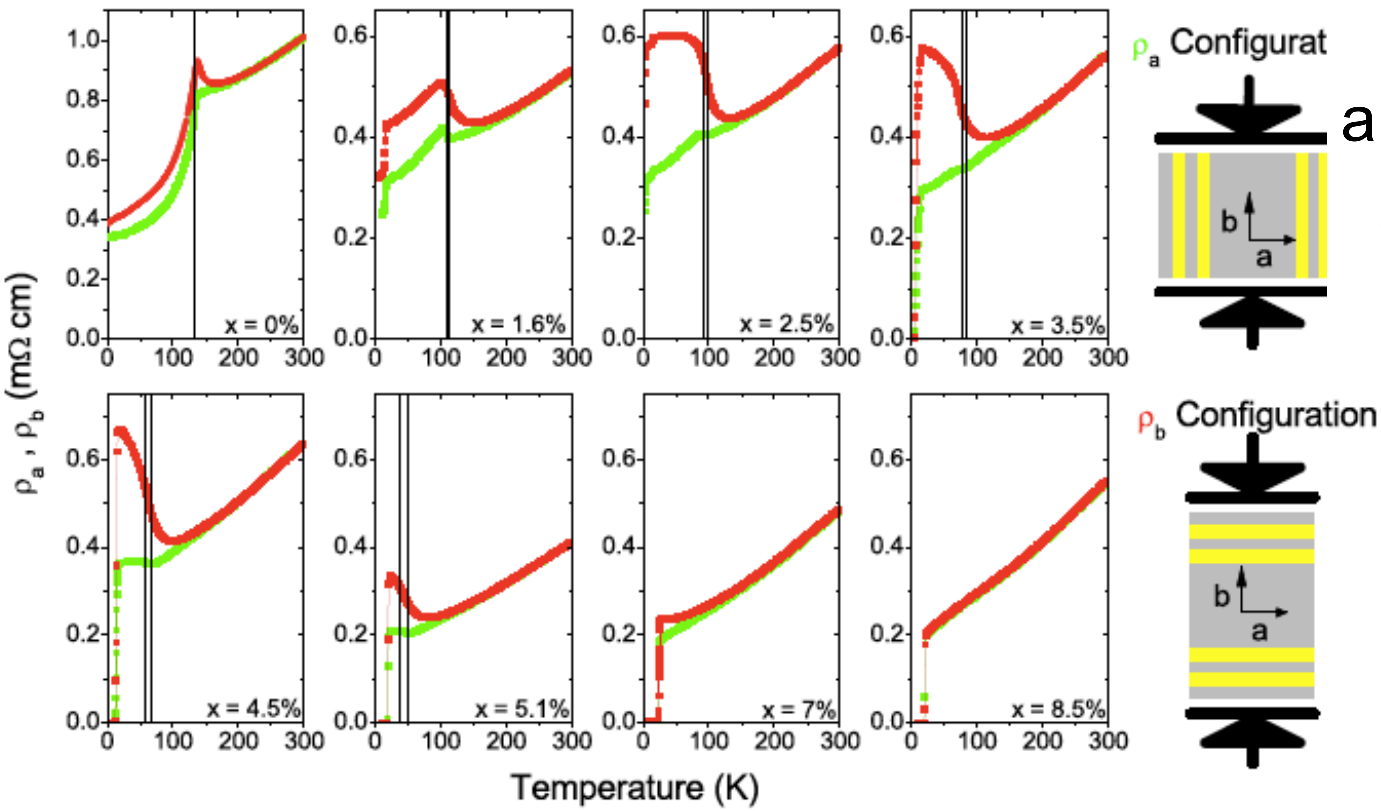
• *Comparison with experiments*:

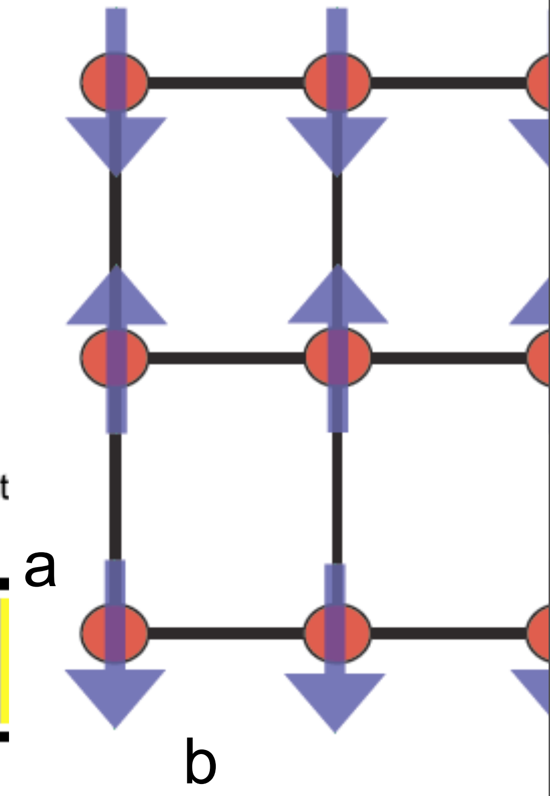
$$J_{\rm H} \sim t_\sigma \sim 1\,{\rm eV} \quad \tilde{J} \sim 0.01\,t_\sigma \sim 10\,{\rm meV}$$

emergent ferro-orbital order

Remaining issues

1.) Expt. AF direction is the easy axis



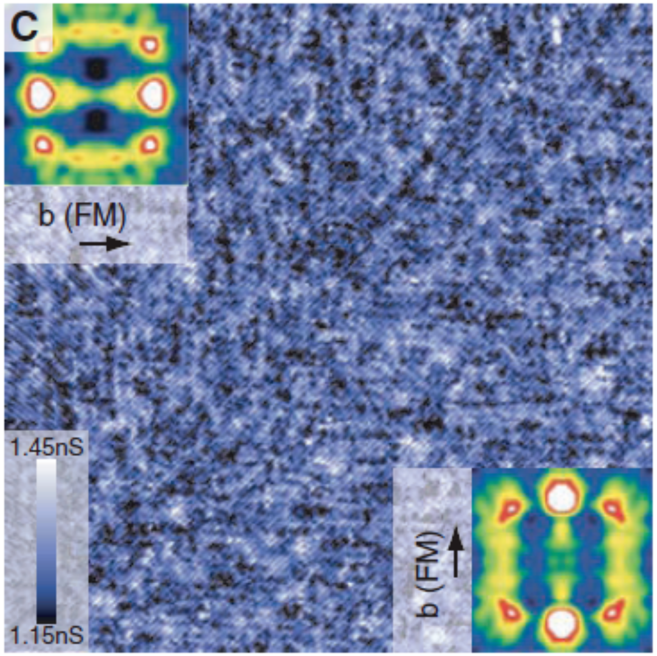


OO-induced anisotropies

OO-induced anisotropies

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

FM easy axis!

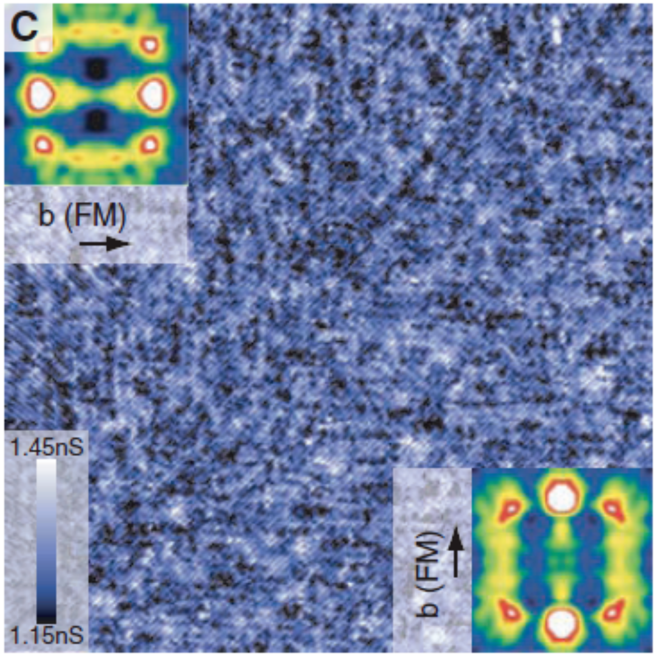


OO-induced anisotropies

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

- *STM*

FM easy axis!



OO-induced anisotropies

AF is easy axis!

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

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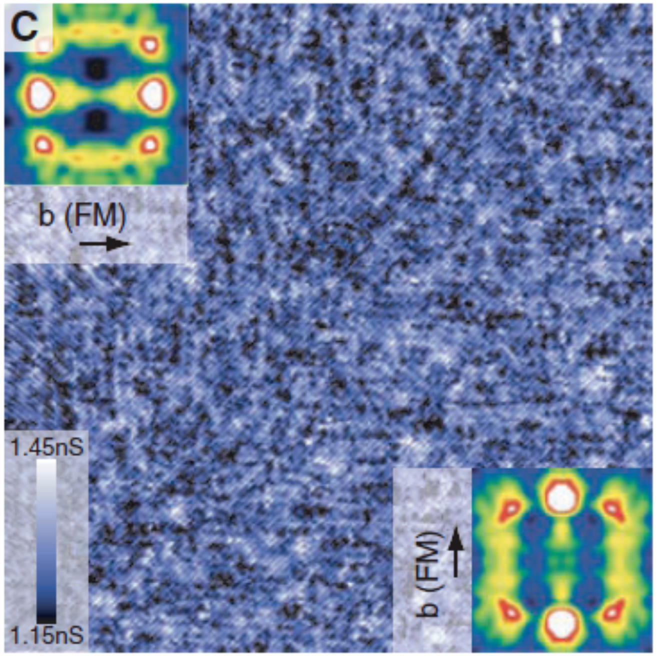
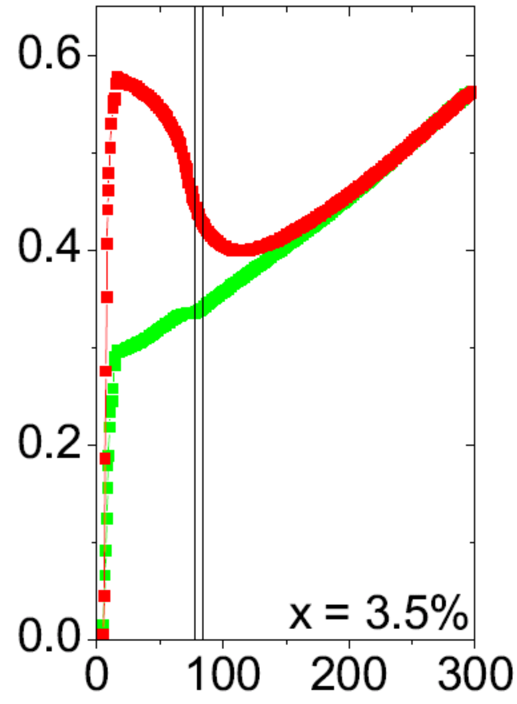
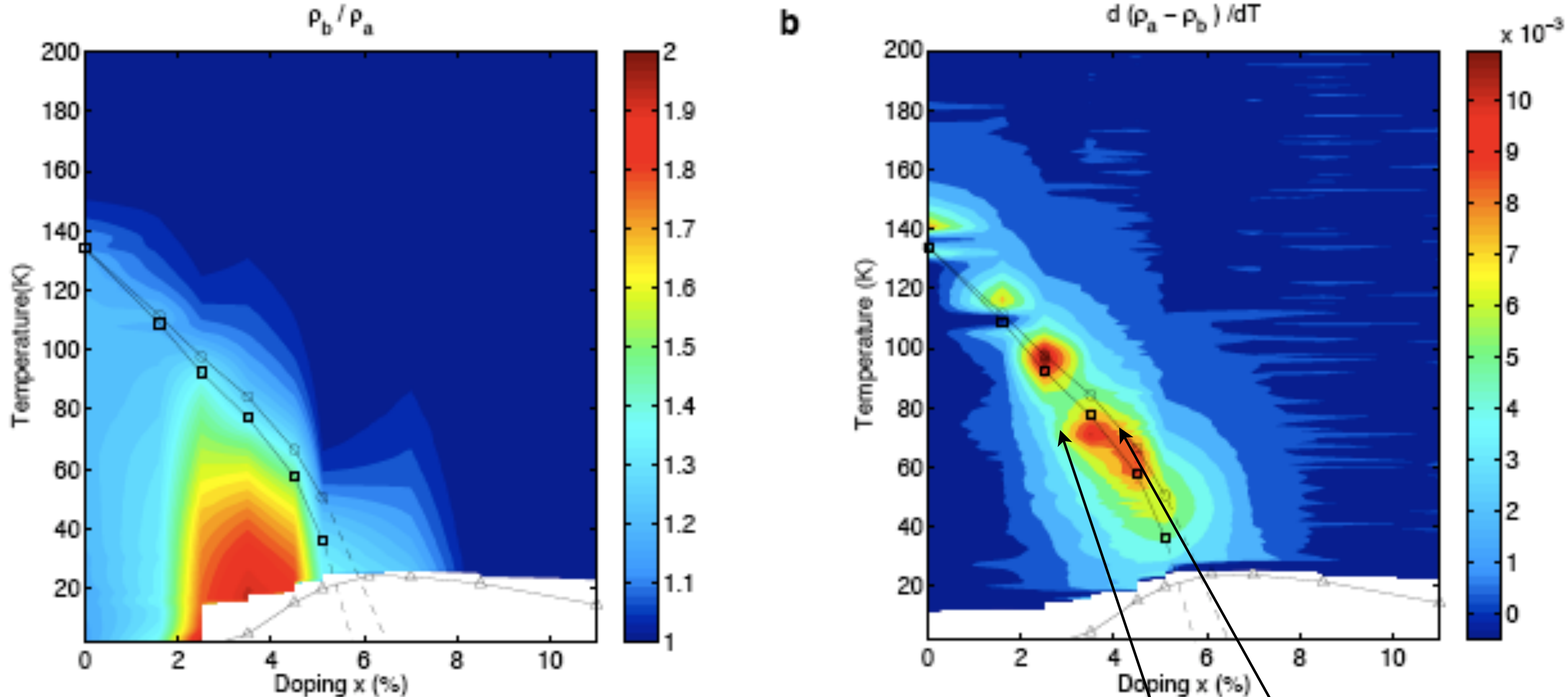


- *Resistivity*

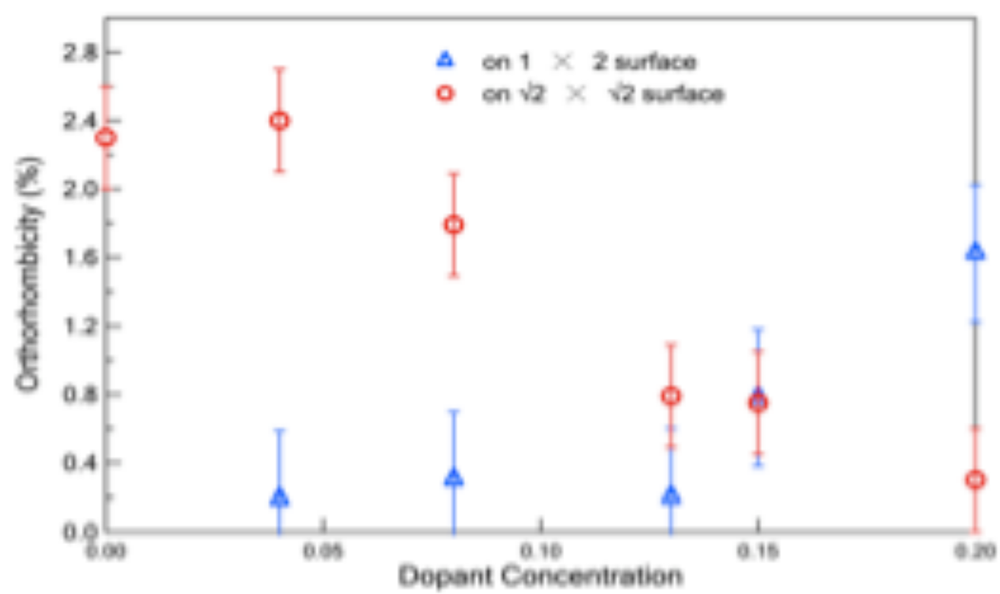
J.-H. Chu, *et al.*
arXiv:1002.3364





nematic

not nematic

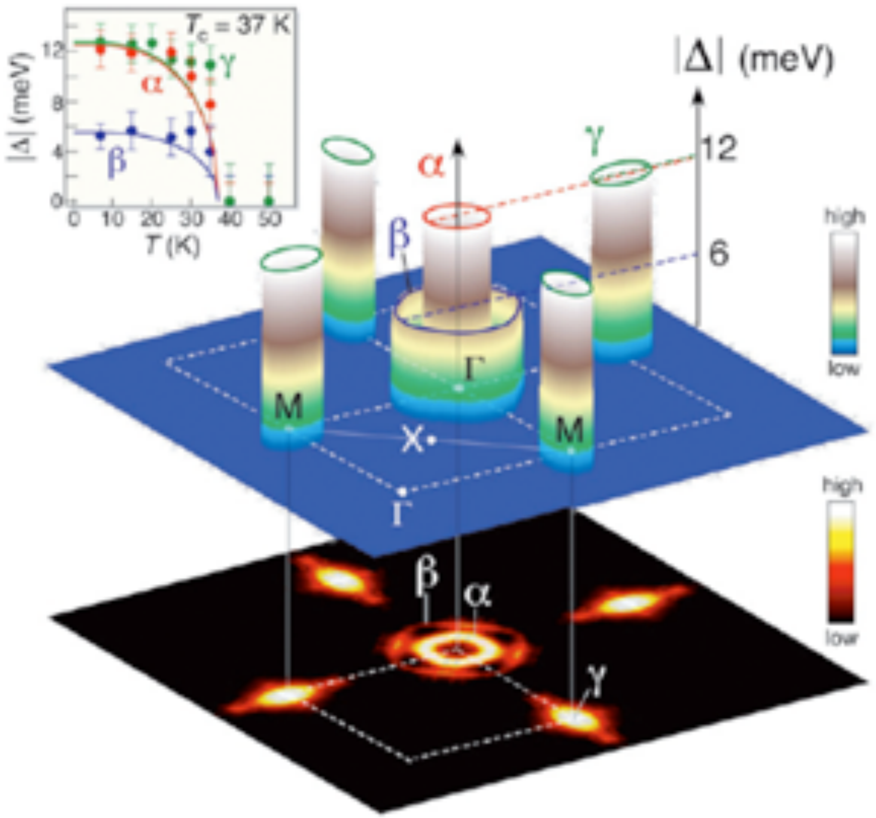


Pairing Mechanism?

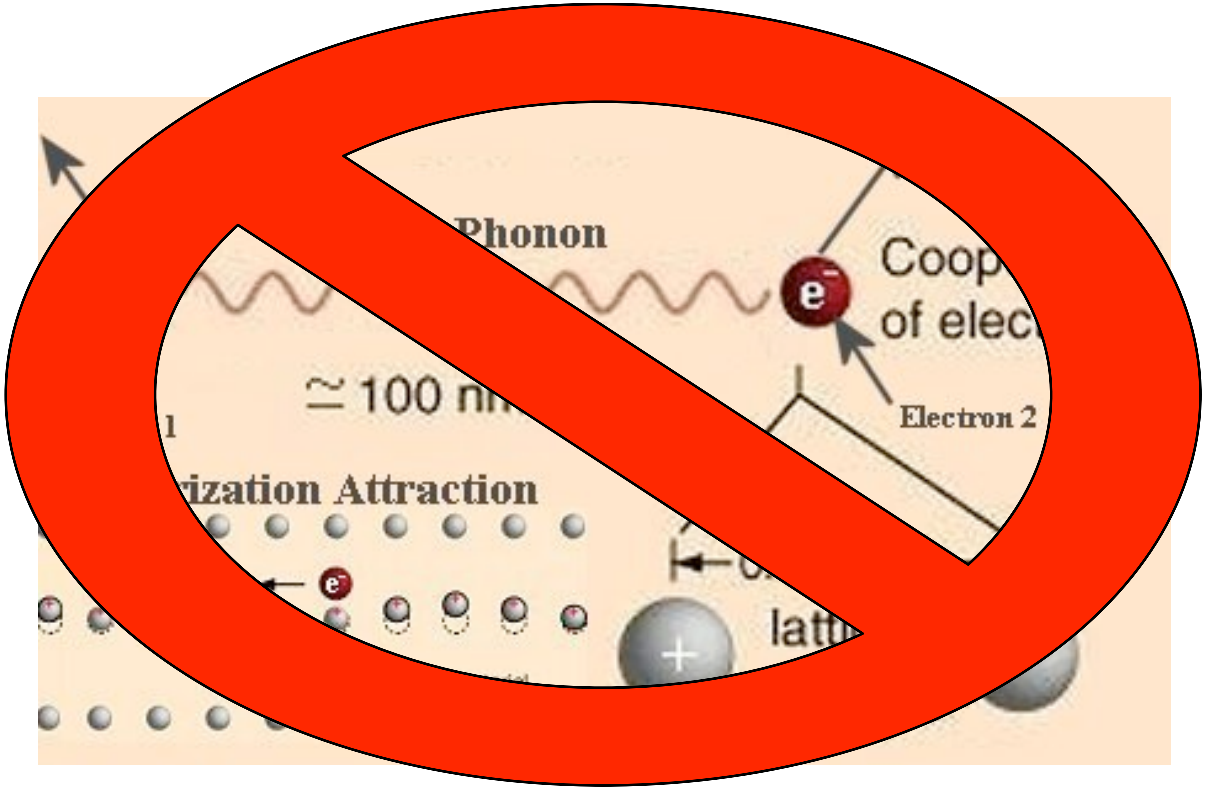
What is the pairing mechanism?

J. Wu, P. Phillips, arXiv:0901.3538

Fermi surface sheets



Pairing Mechanism?

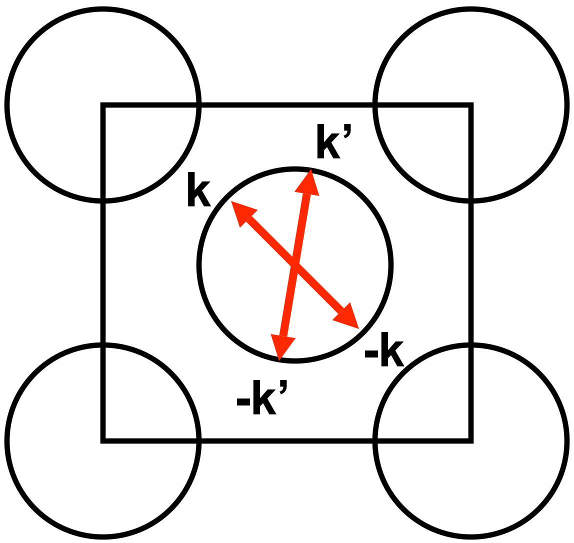


magnons not phonons

Magnon-induced interaction

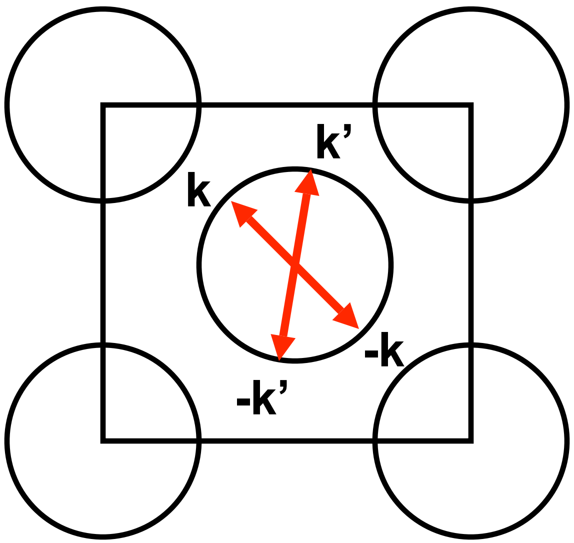
Magnon-induced interaction

Intra-band interaction

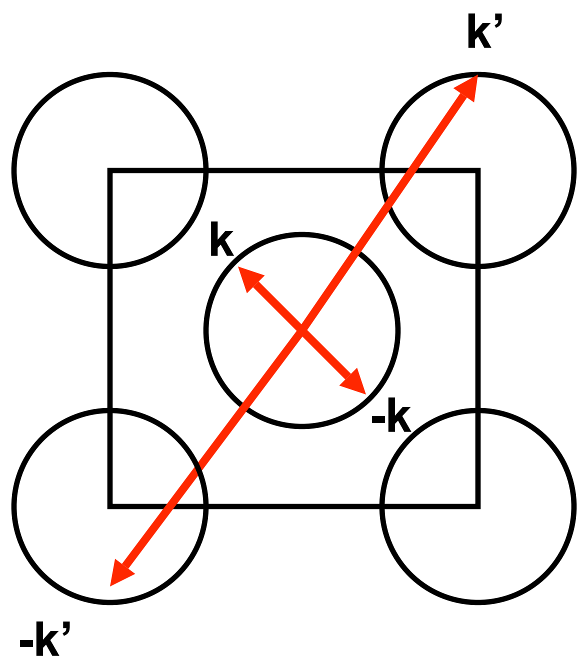


Magnon-induced interaction

Intra-band interaction

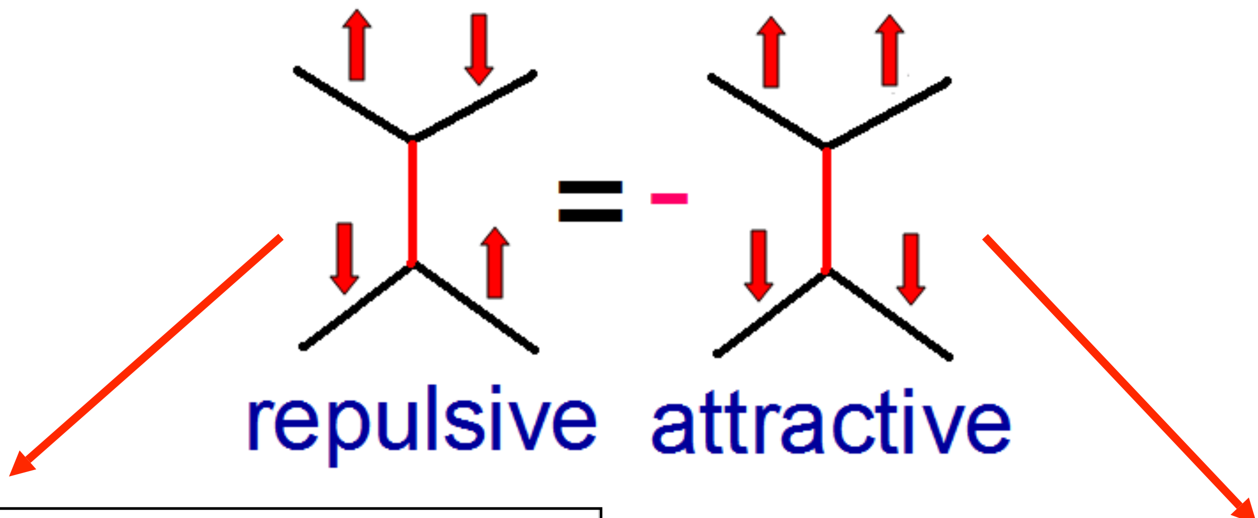


Inter-band interaction



Properties of magnon-mediated interaction

1) Both repulsive (due to spin-flip);



$$\boxed{\begin{aligned} & V(\mathbf{q})\;\; a^{\dagger}_{\mathbf{k_1+q},\uparrow} a^{\dagger}_{\mathbf{k_2-q},\downarrow} a_{\mathbf{k_1},\downarrow} a_{\mathbf{k_2}\uparrow} \\ = - \;\; & V(\mathbf{q})\;\; a^{\dagger}_{\mathbf{k_1+q},\uparrow} a^{\dagger}_{\mathbf{k_2-q},\downarrow} a_{\mathbf{k_2},\uparrow} a_{\mathbf{k_1}\downarrow} \end{aligned}}$$

$$\boxed{V(\mathbf{q}) a^{\dagger}_{\mathbf{k_1+q},\uparrow} a^{\dagger}_{\mathbf{k_2-q},\downarrow} a_{\mathbf{k_1},\uparrow} a_{\mathbf{k_2}\downarrow}}$$

Interpretation I: pairing from repulsive interaction

1) 2 inter-band scattering bring attractive interaction for each band;

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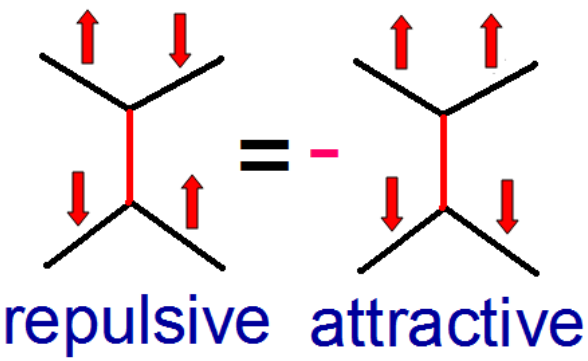
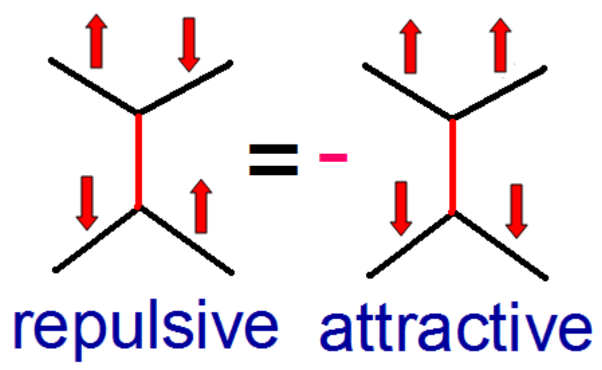
Propagating one magnon



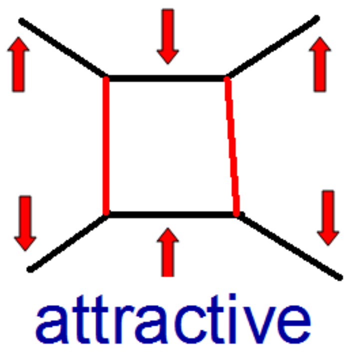
Interpretation I: pairing from repulsive interaction

1) 2 inter-band scattering bring attractive interaction for each band;

Propagating one magnon



Propagating two magnons



J. Appel and A. W. Overhauser
Physica B 199 & 200, 310(1994)

Properties of magnon-mediated interaction

2) Inter-band>>intra-band

$$V_{\mathrm{ii}}(\mathbf{k},\mathbf{k}') = \frac{(J^2)|f_{\nu,\nu'}(\mathbf{k},\mathbf{k}')|^2}{qF(\alpha)} \qquad V_{\mathrm{eh}}(\mathbf{k},\mathbf{k}') = \frac{(J^2)|f_{\nu,\nu'}(\mathbf{k},\mathbf{k}')|^2}{qG(\alpha)}$$

Intra-band

transferred momentum

Inter-band

q

Q+q

Why S±-pairing symmetry?

- From gap equation:

$$\lambda \begin{pmatrix} \Delta^h_{\mathbf{k}} \\ \Delta^e_{\mathbf{k}} \end{pmatrix} = -\sum_{\mathbf{k}'} \left\langle \begin{pmatrix} V_{\mathrm{hh}} & V_{\mathrm{eh}} \\ V_{\mathrm{eh}} & V_{\mathrm{ee}} \end{pmatrix} (\mathbf{k}, \mathbf{k}') \begin{pmatrix} \Delta^h_{\mathbf{k}'} \\ \Delta^e_{\mathbf{k}'} \end{pmatrix} \right\rangle$$

- Eigenvalue:

$$\lambda_{\mathrm{e}} = V_{\mathrm{ee}} N_{\mathrm{e}}(E_{\mathrm{F}}) \quad \lambda_{\mathrm{h}} = V_{\mathrm{hh}} N_{\mathrm{h}}(E_{\mathrm{F}})$$

$$\lambda_{\mathrm{eh}} = V_{\mathrm{eh}} \sqrt{N_{\mathrm{e}}(E_{\mathrm{F}}) N_{\mathrm{h}}(E_{\mathrm{F}})}$$

$$\lambda = -\left(\lambda_{\mathrm{h}} + \lambda_{\mathrm{e}}\right)/2 + \sqrt{\left(\lambda_{\mathrm{h}} - \lambda_{\mathrm{e}}\right)^2/4 + \lambda_{\mathrm{eh}}^2}$$

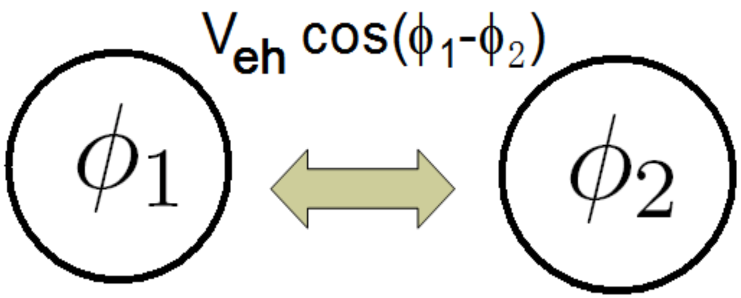
- Order parameters:

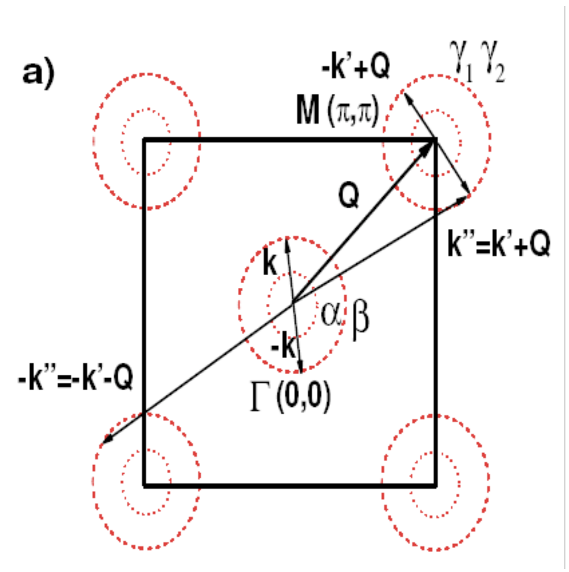
$$\left(\Delta^h_{\mathbf{k}}, \Delta^e_{\mathbf{k}}\right)^{\mathrm{T}} \quad \propto \quad \left(\lambda_{\mathrm{eh}}, -\left(\lambda + \lambda_{\mathrm{h}}\right)\right)^{\mathrm{T}}$$

Interpretation II: Invert sign

2) phase-shift for different bands

depends on the sign of inter-band hopping



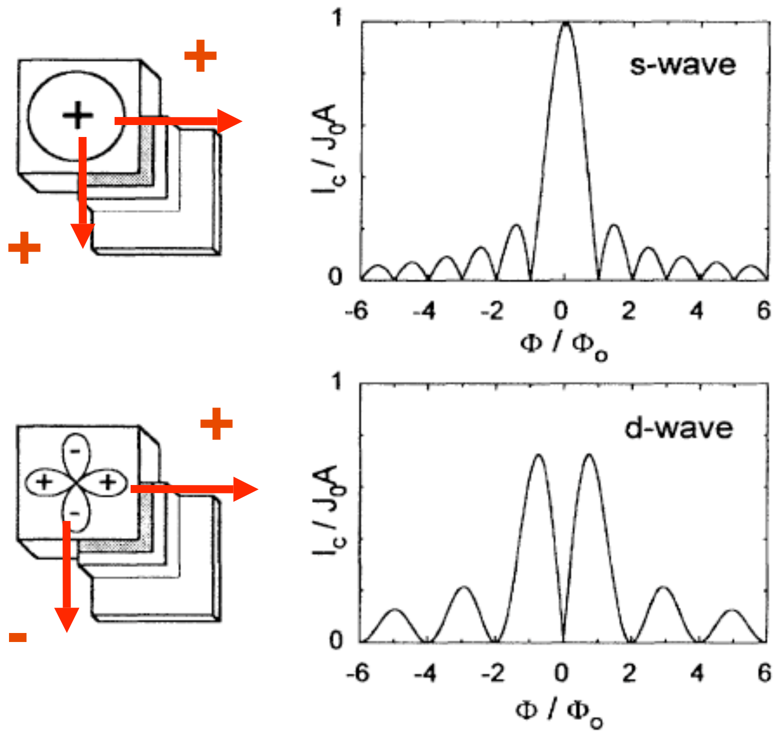


How to detect S±-pairing symmetry ?

J. Wu, P. Phillips,

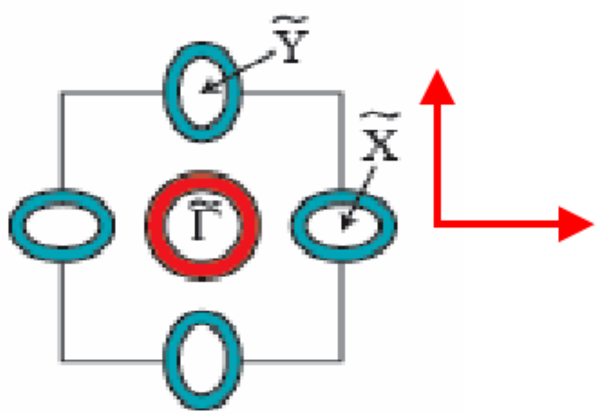
Phys. Rev. B 79, 092502 (2009)

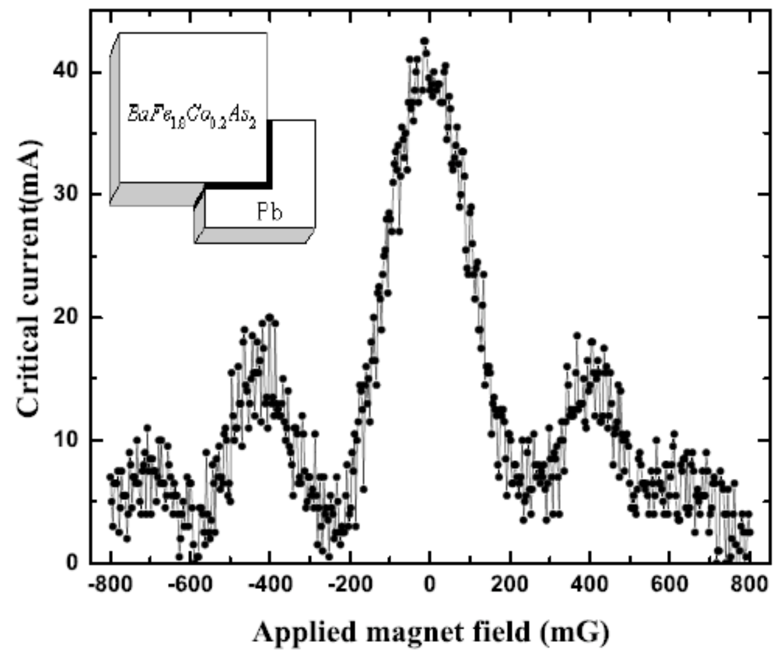
Phase sensitive measurement



D.J. Van Harlingen, PRL,1995

Ordinary corner Josephson junction cannot tell the inverse sign (still A_{1g} symmetry)

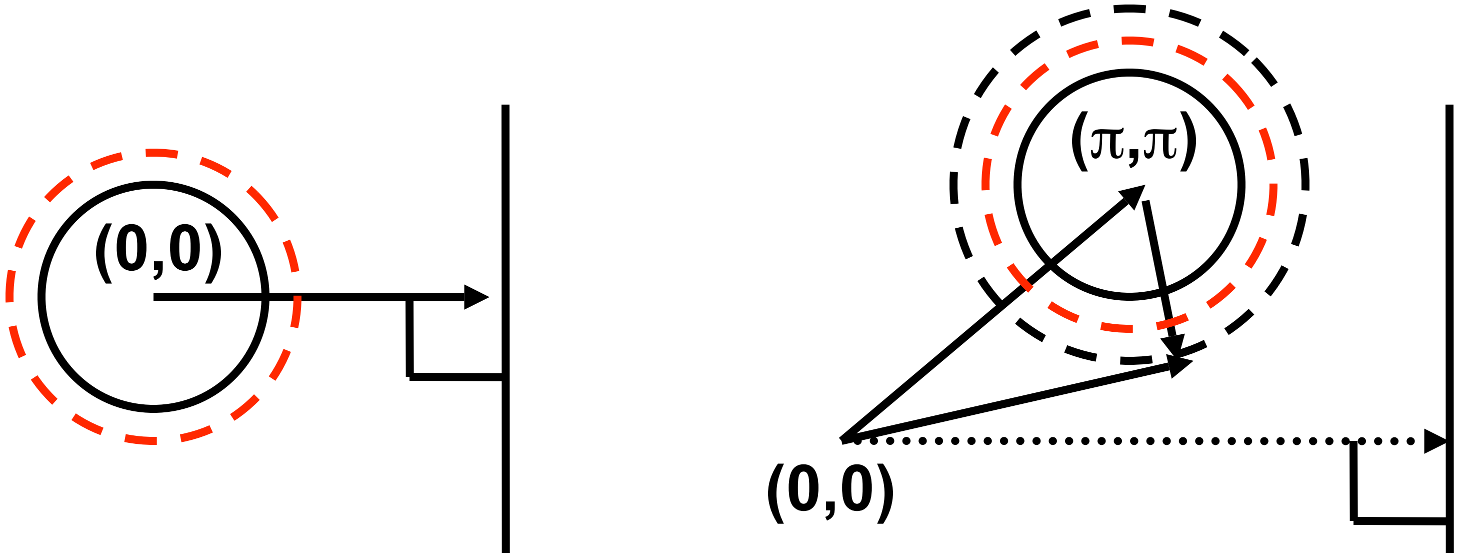




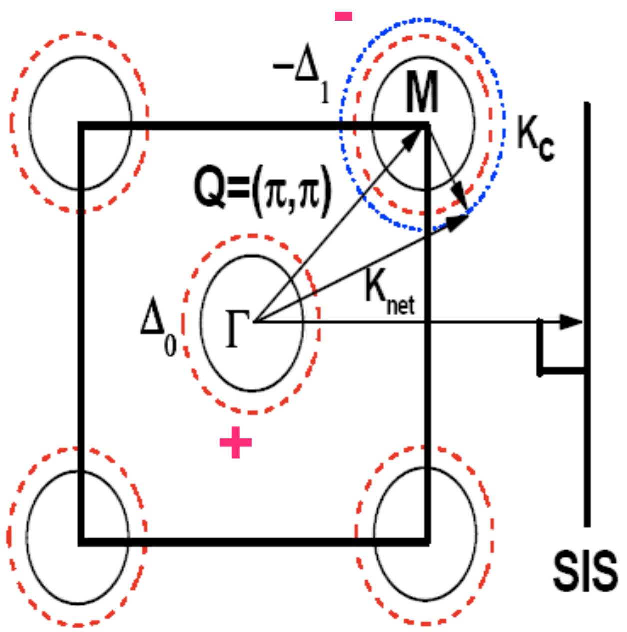
arXiv: 0812.3295

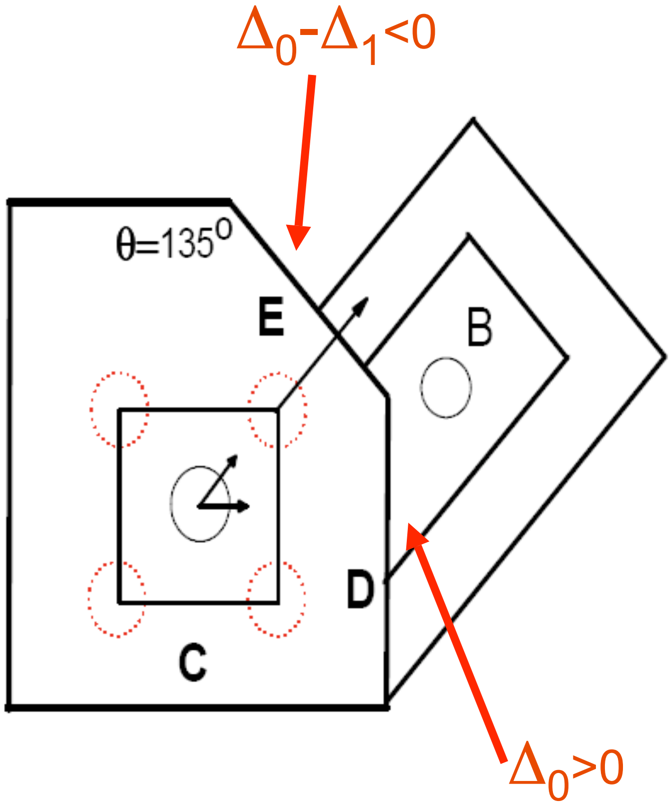
Principle of SIS junction

Supercondutor-Insulator-Superconductor(SIS) Junction can only measure order parameters perpendicular to the surface of the junction.



Modified corner Josephson junction





How to test?

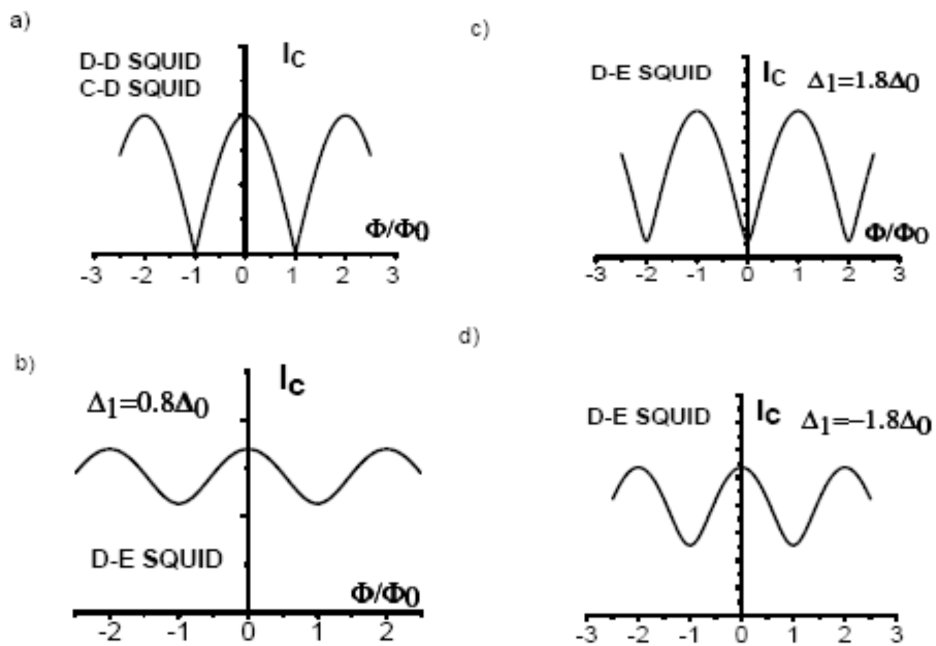
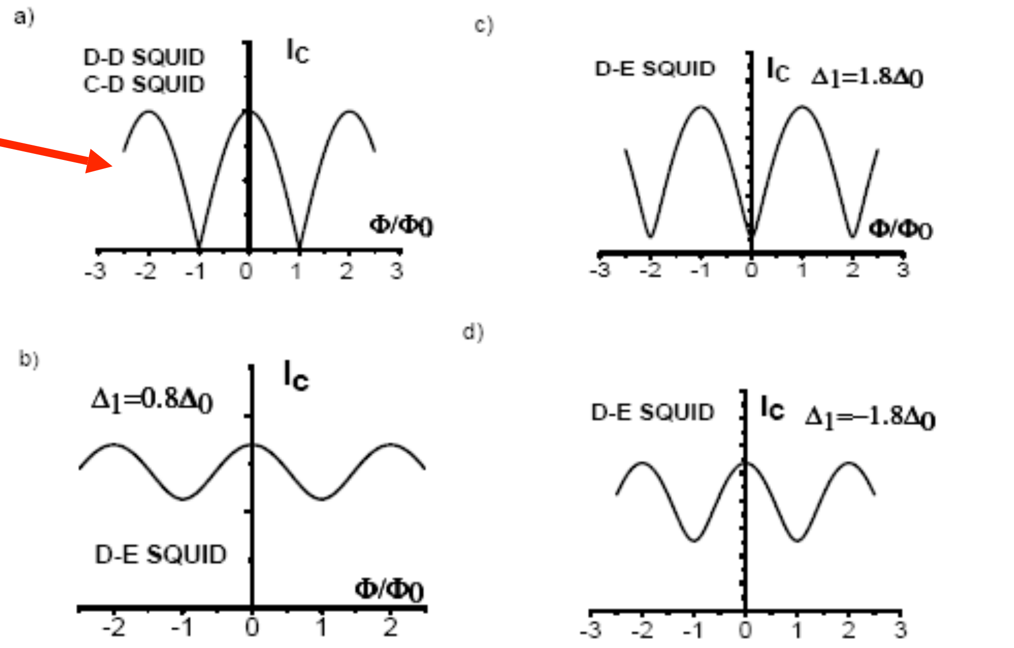


FIG. 2: All possible interference pattern for different x values where x is defined as $\Delta_1 = -x\Delta_0$. a) For junction connecting D-D or C-D faces; b) c) d) are all junction connecting D-E faces. b) $x \in [0, 1]$; c) $x \in [1, \infty)$; d) $x \in (-\infty, 0]$.

How to test?

Ordinary 90^0 JJ



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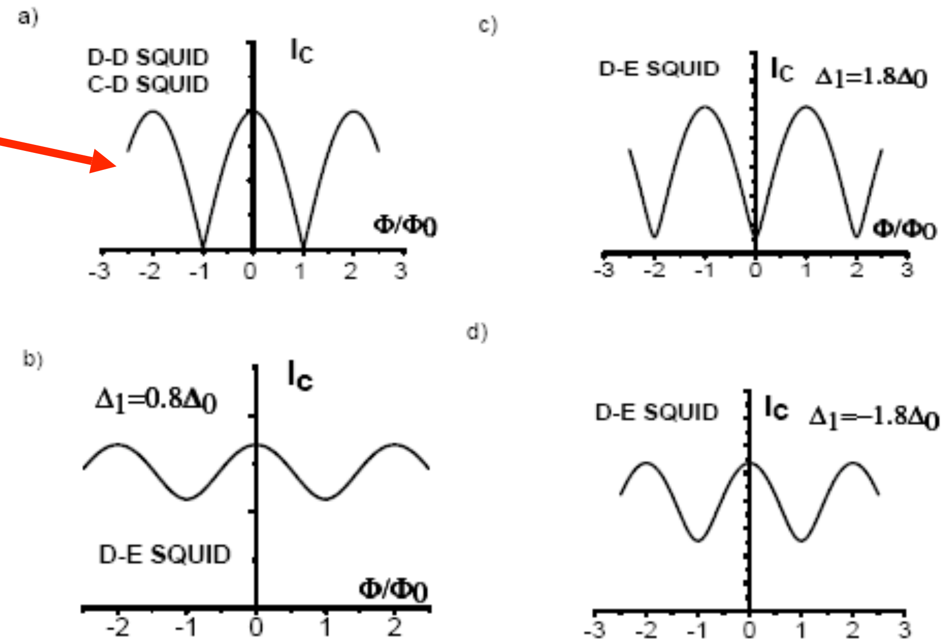

modified 135^0 JJ

FIG. 2: All possible interference pattern for different x values where x is defined as $\Delta_1 = -x\Delta_0$. a) For junction connecting D-D or C-D faces; b) c) d) are all junction connecting D-E faces. b) $x \in [0, 1]$; c) $x \in [1, \infty)$; d) $x \in (-\infty, 0]$.

Summary

Key properties for Iron-pnictides:

(1) Fe-As trilayers

(2) Multi-bands

(3) Intermediate
coupling

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Orbital Ordering

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Key properties for Iron-pnictides:

(1) Fe-As trilayers

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Orbital Ordering

Itinerant-localized dichotomy

What are the pnictides Really?

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Itinerant electrons

What are the pnictides Really?

Itinerant electrons

Localized electrons

What are the pnictides Really?

Arsenic and Old Lace

Itinerant electrons

Localized electrons

What are the pnictides Really?

Arsenic and Old Lace

Itinerant electrons

"I'm not a Brewster, I'm a son of a sea cook!"[

Localized electrons

What are the pnictides Really?

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What are the pnictides Really?

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?

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Are the pnictides important?

manganites
multi-orbital
high-moment
no T_c

Cuprates,
single-orbital
Mott-system,
low-moment,
high T_c

pnictides
multi-orbital
low-moment
moderate
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Cuprates,
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Mott-system,
low-moment,
high T_c

Multi-orbital
Mott system,
low-moment
??? T_c
EFRC Center

pnictides
multi-orbital
low-moment
moderate
T_c