Multi-Orbital Physics in the Oxypnictides: Are they important?

F. Kruger

D. Argyriou

W. Lv

J. Wu, W. C. Lee (not shown)

What are the pnictides Really?

manganites

Cuprates

What are the pnictides Really?

manganites

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manganites

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

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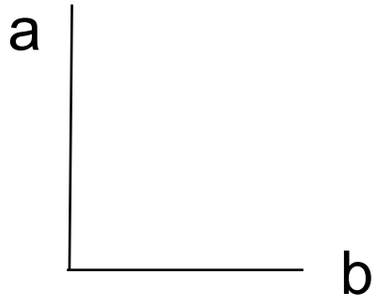
$$J_H S_c \ll \infty$$

To explain??



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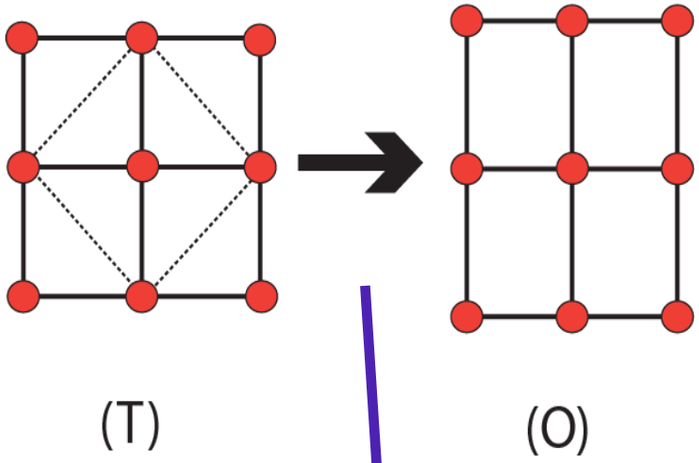
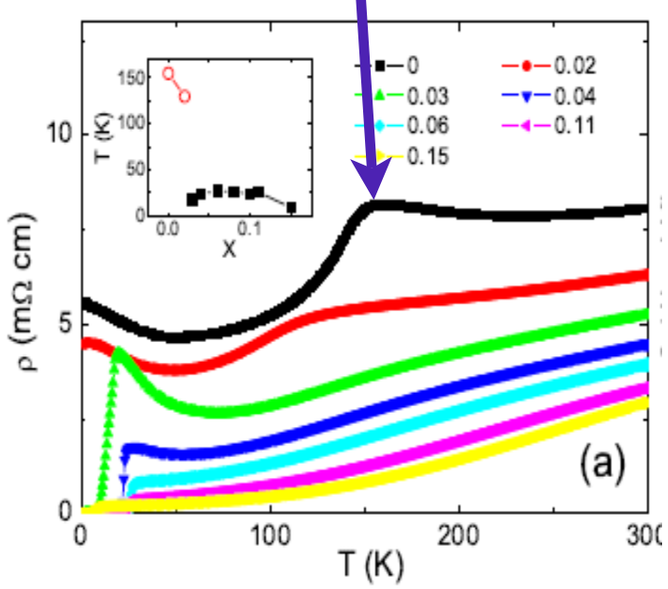
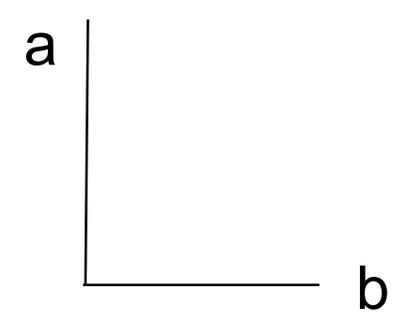


(Tet->Ortho/resistivty anomaly)

- **Resistivity**

$T_{RA} = T_{SPT}$





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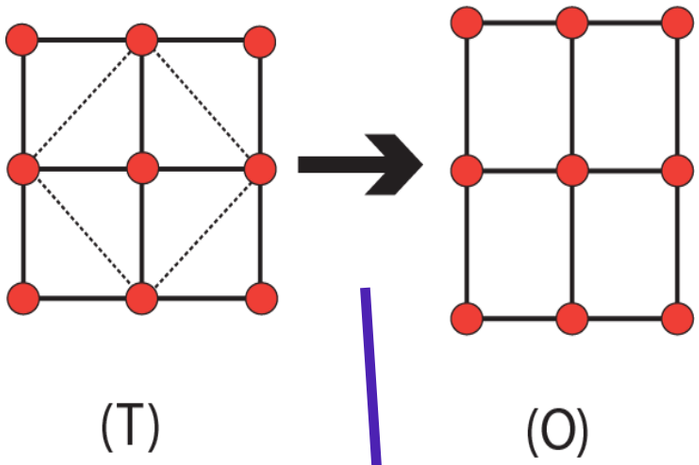

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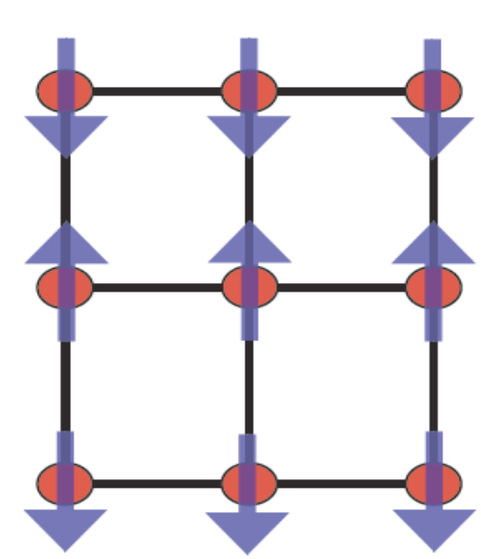
T_{SDW}



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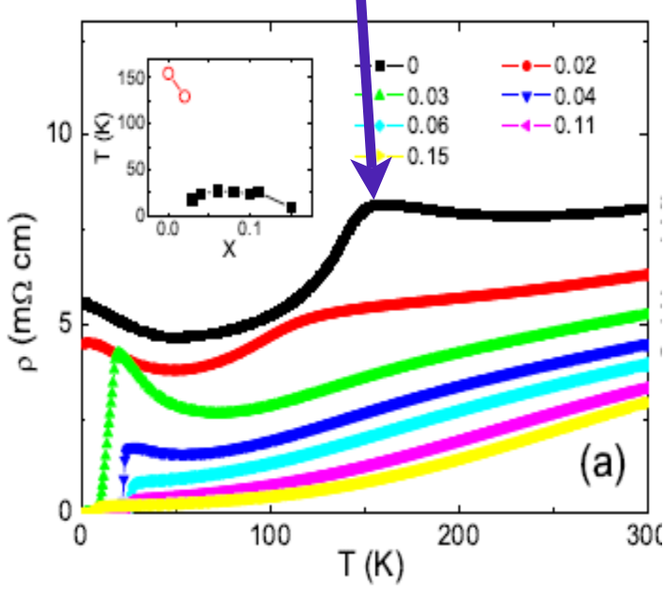

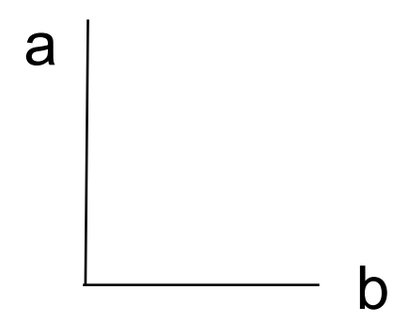

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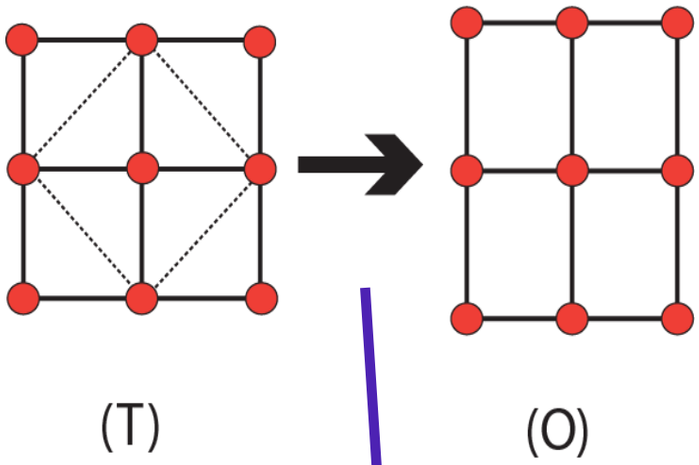

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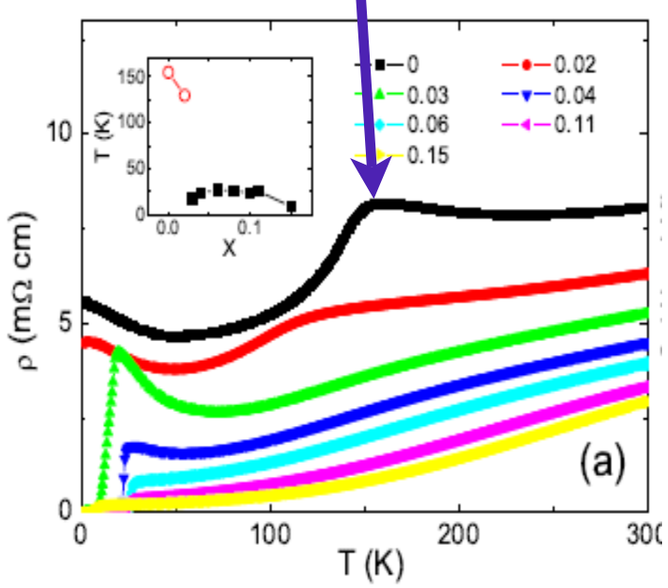
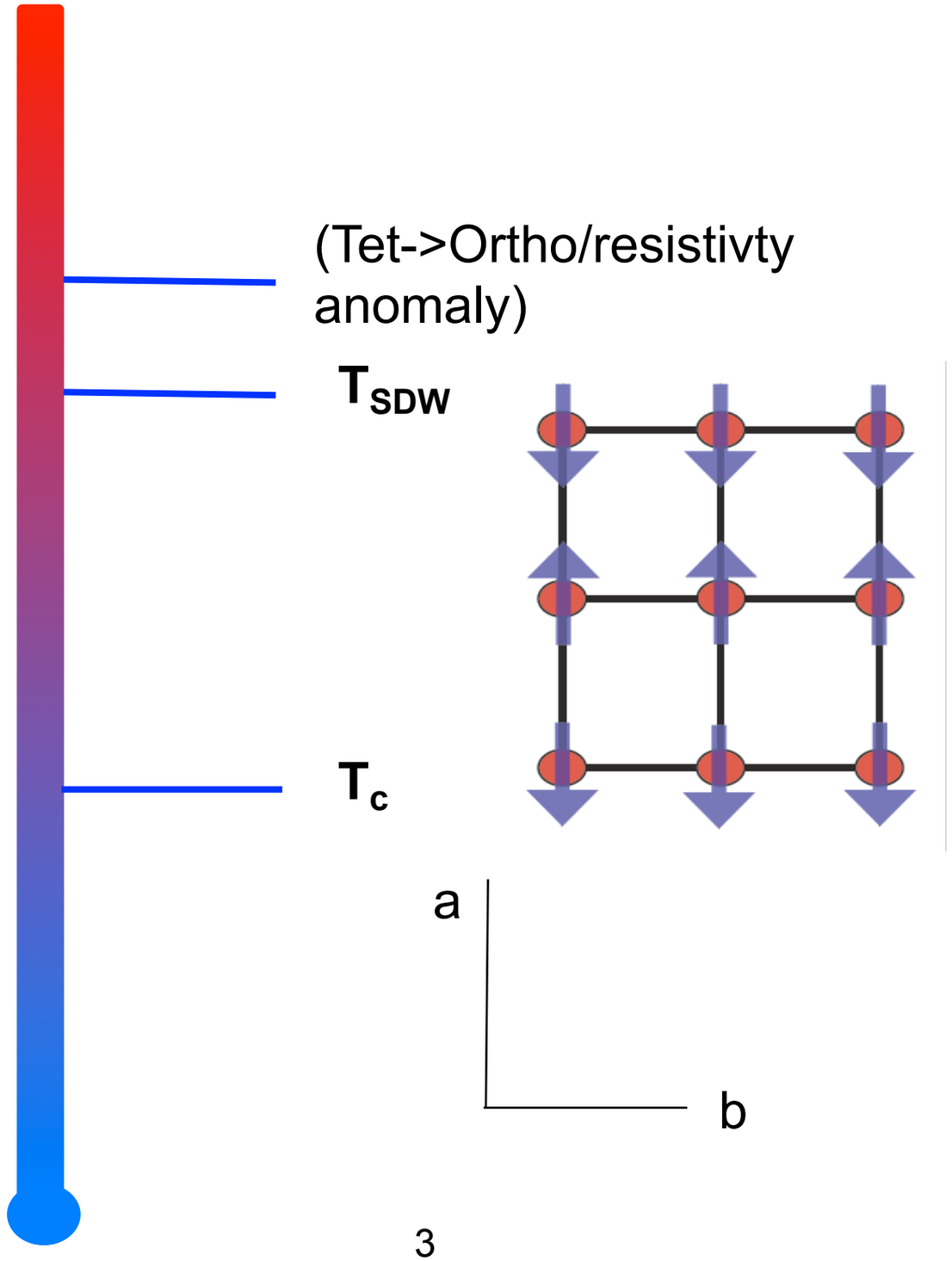
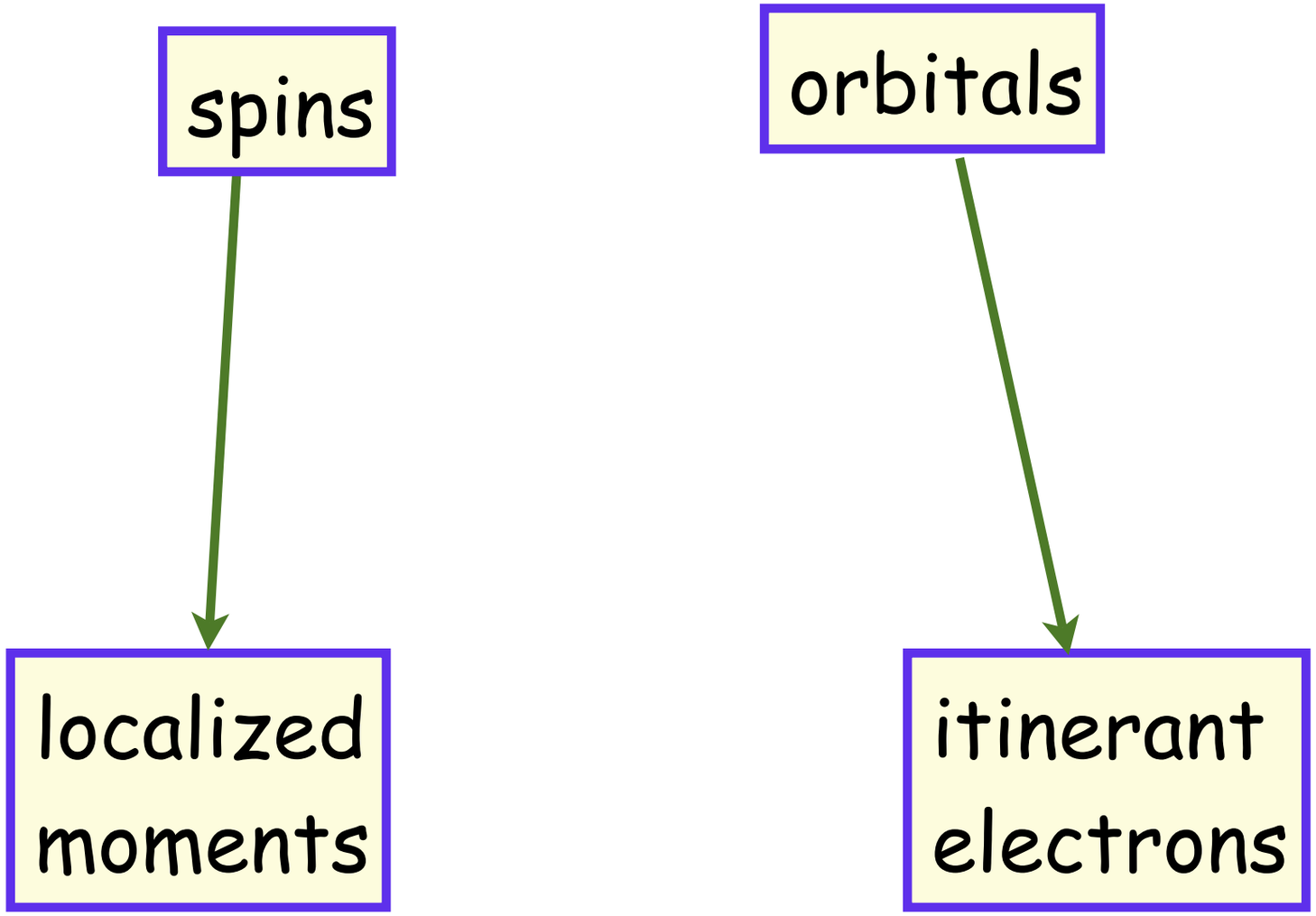
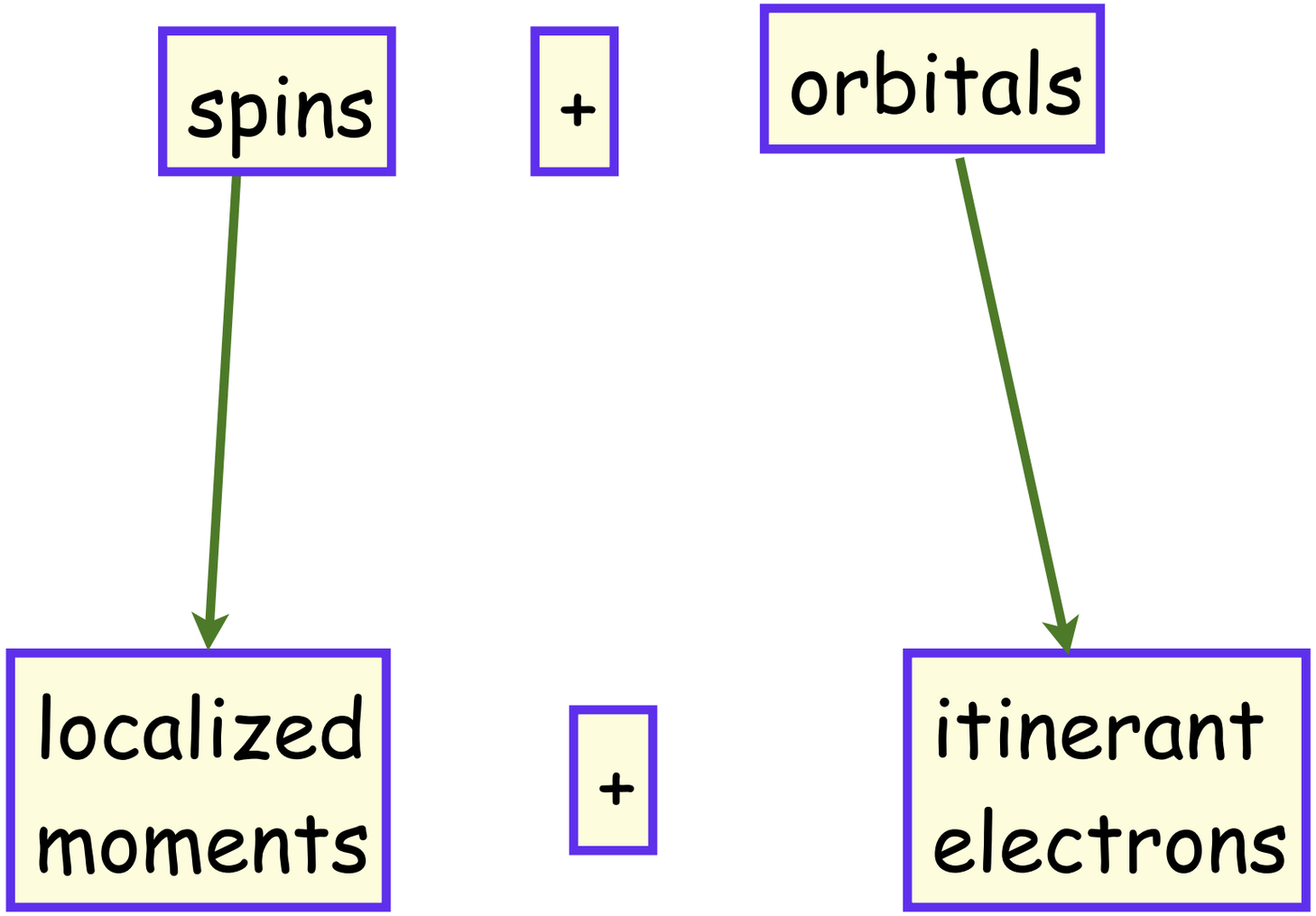





spins
orbitals
localized moments
itinerant electrons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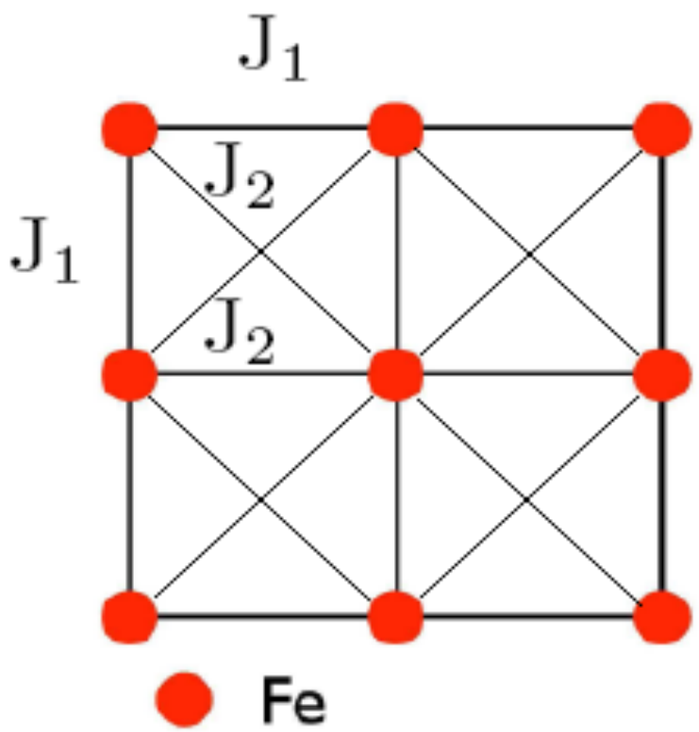
how far can one get with local moments?



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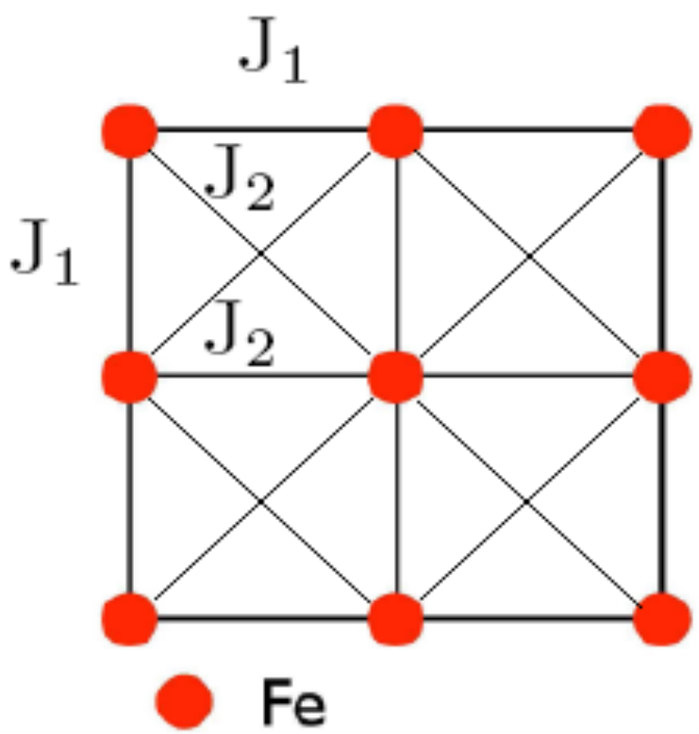
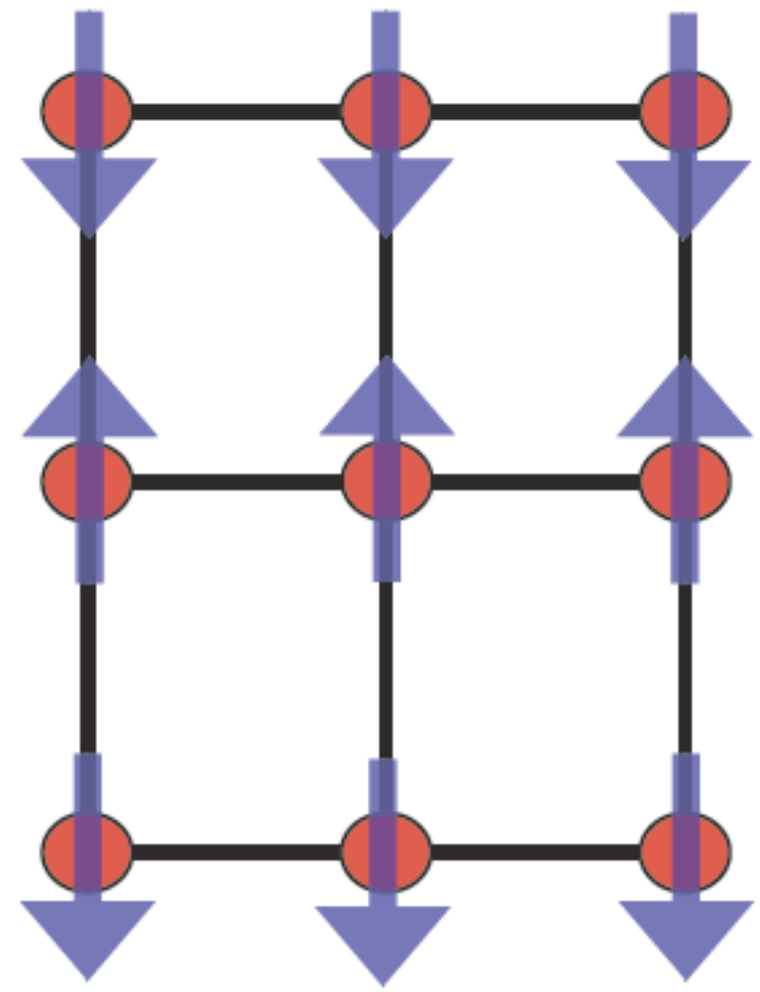


$J_2 > J_1/2$



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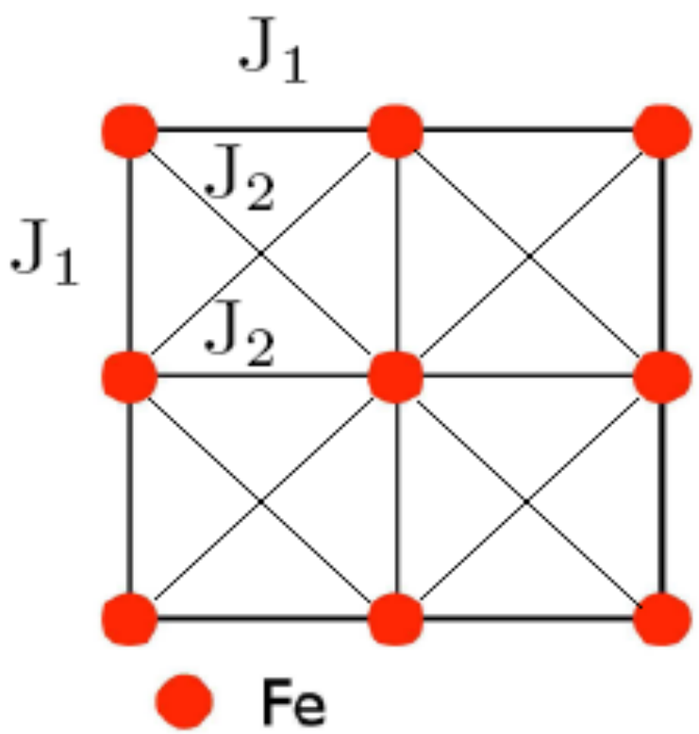

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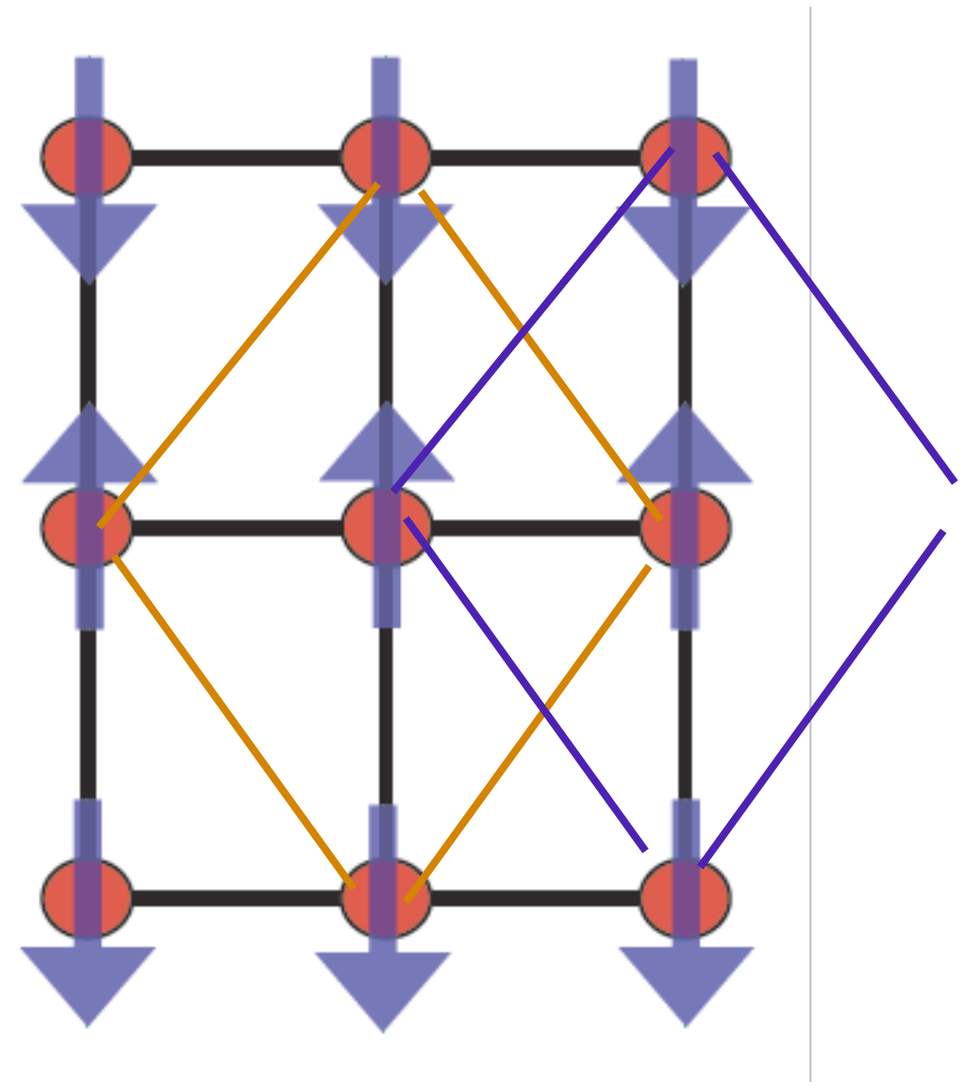

Two interpenetrating AF sublattices

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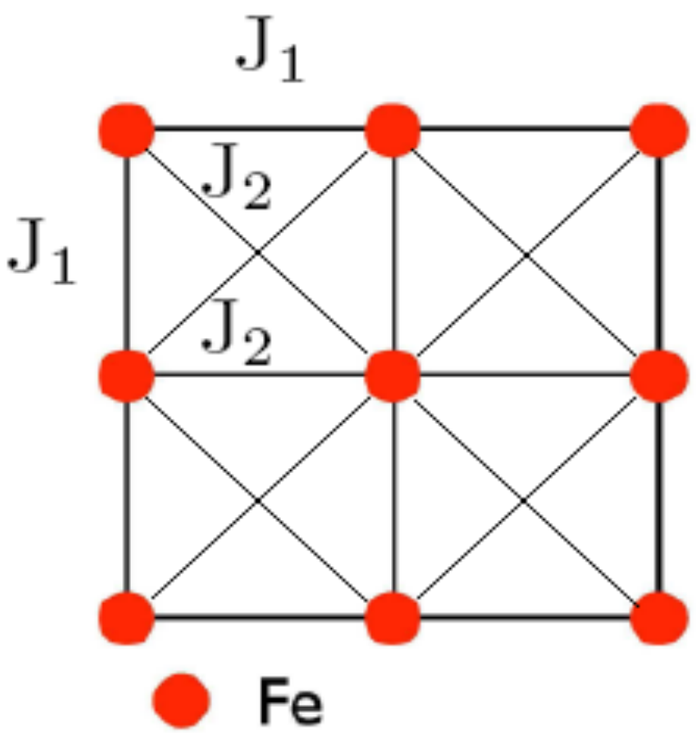

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$$\varphi = \hat{n}_1 \cdot \hat{n}_2$$

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

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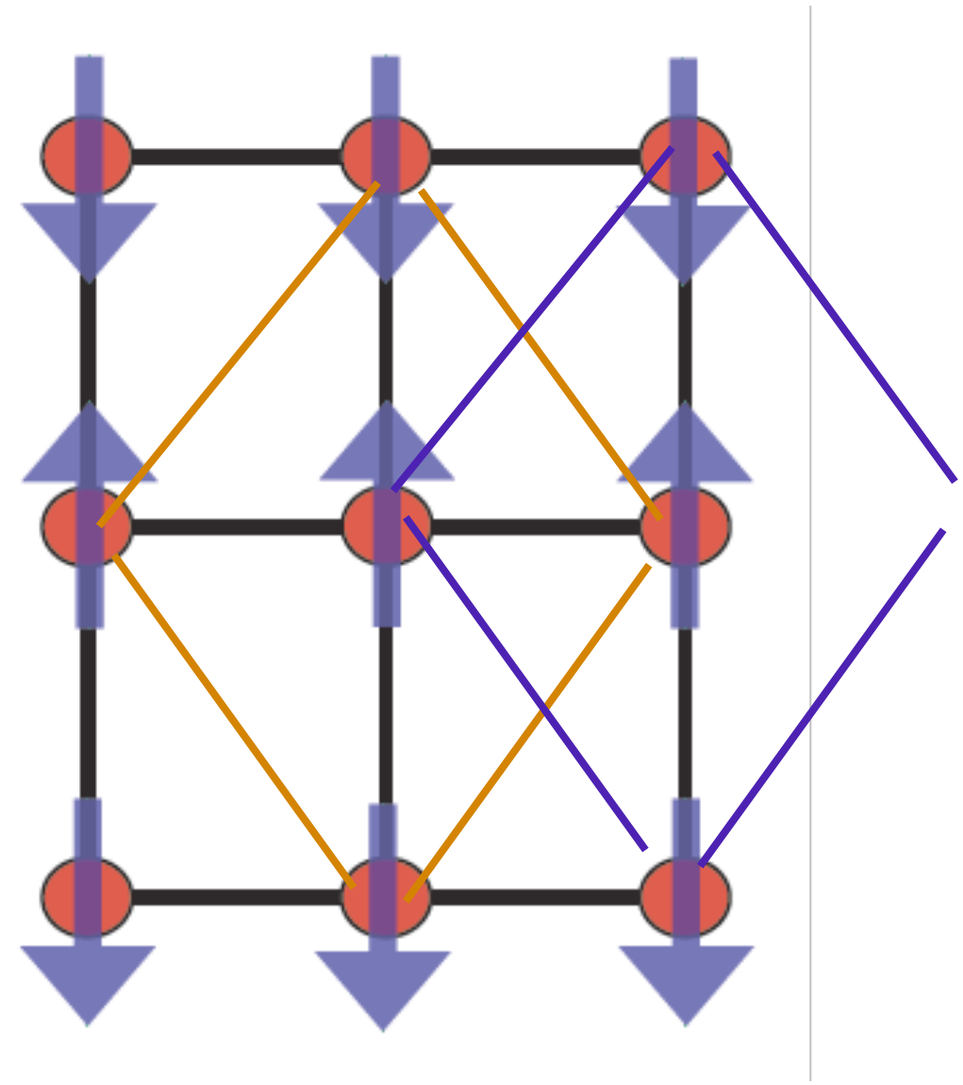

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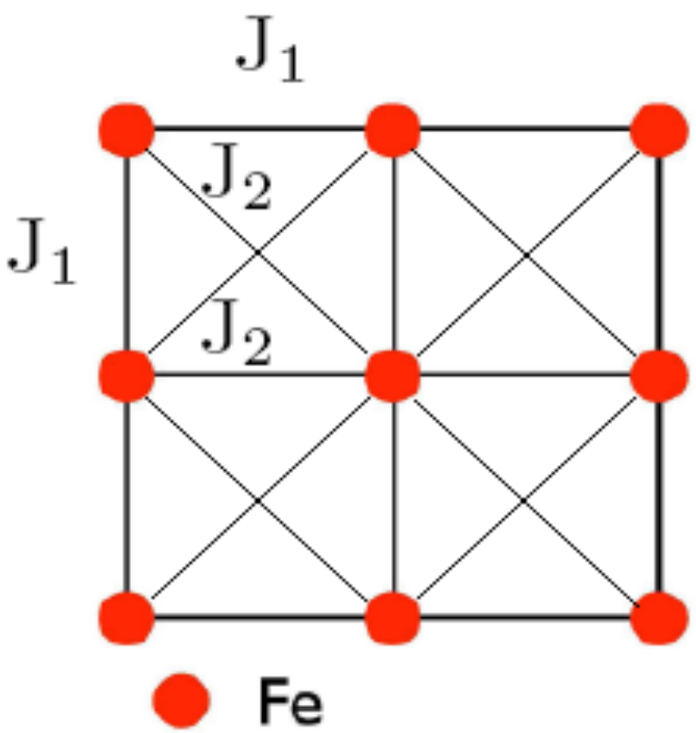

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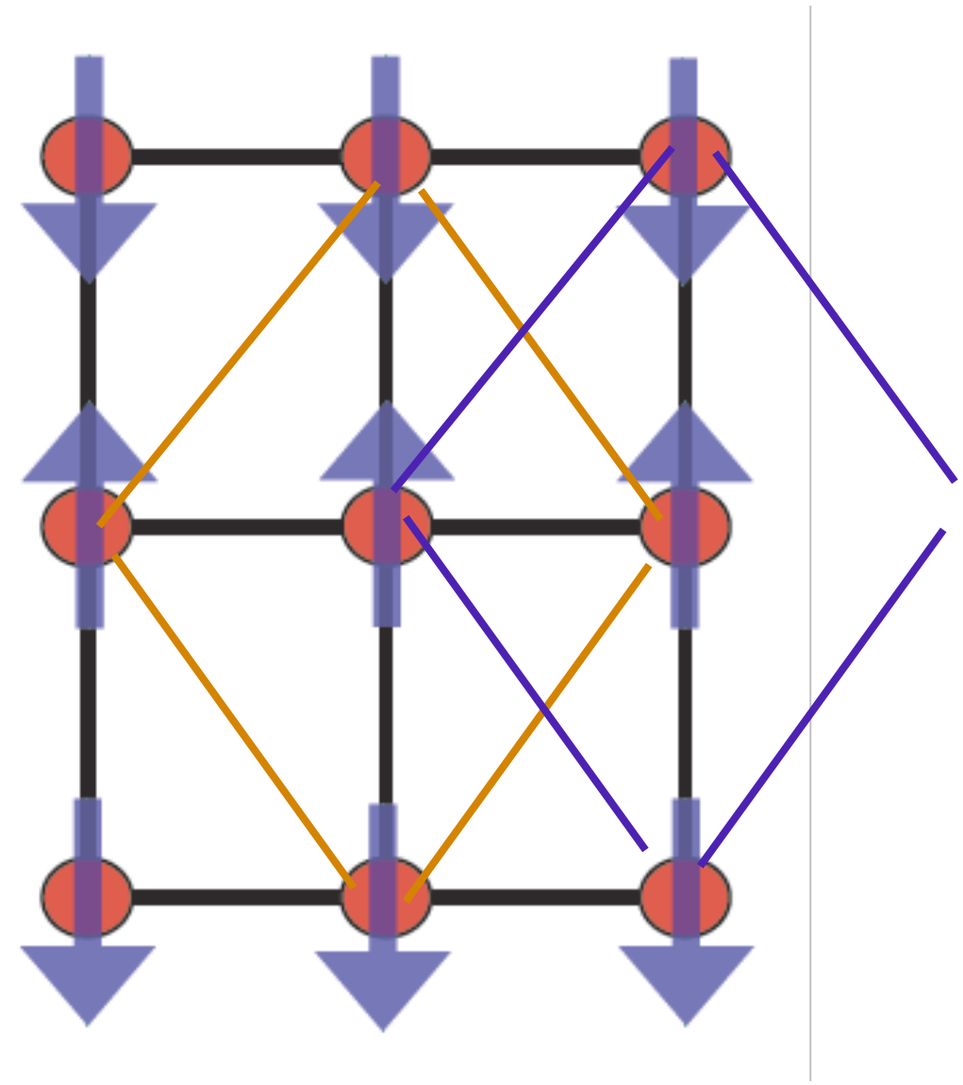

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`nematic'

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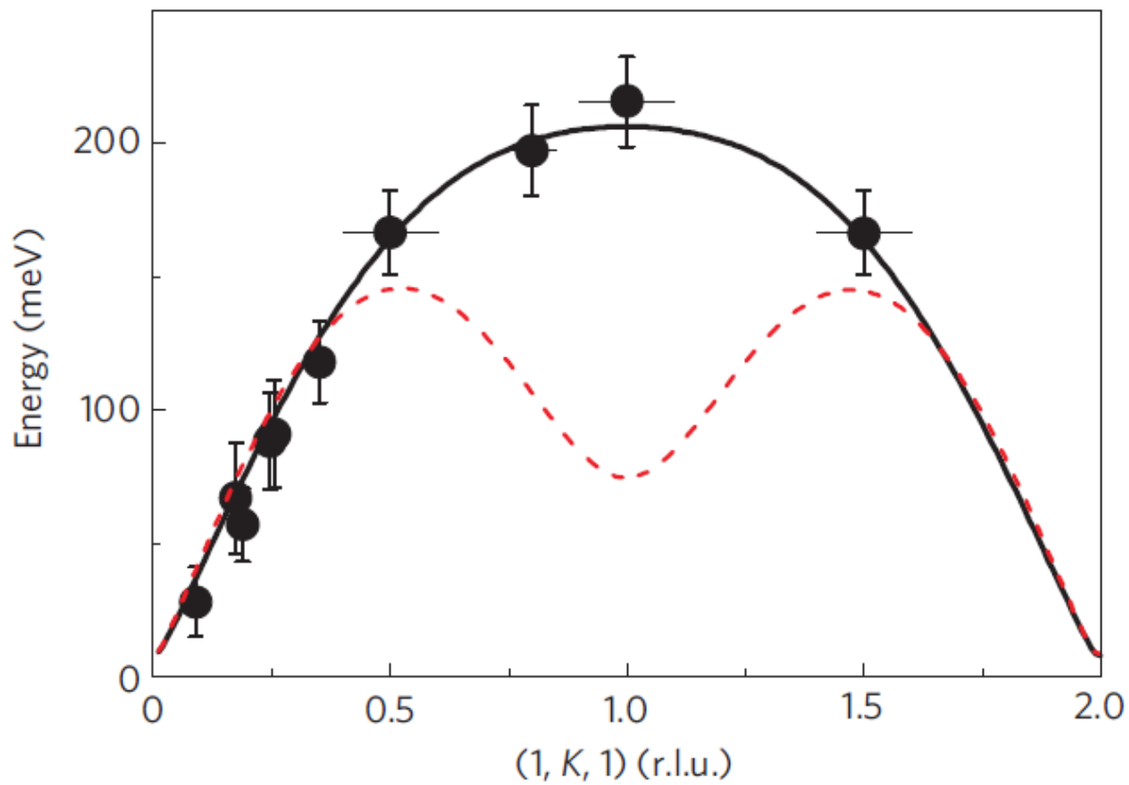
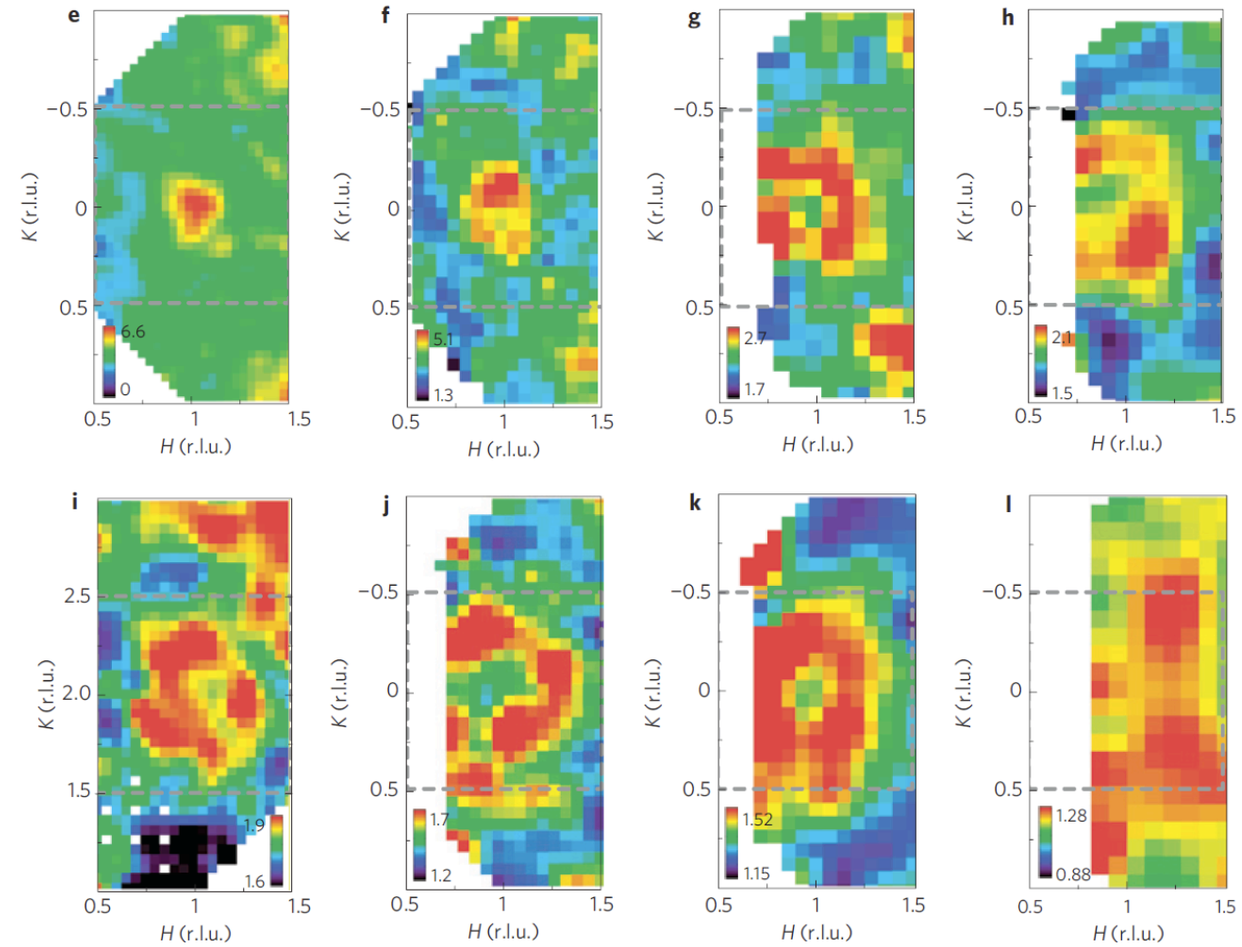
- *Inelastic neutron scattering*





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

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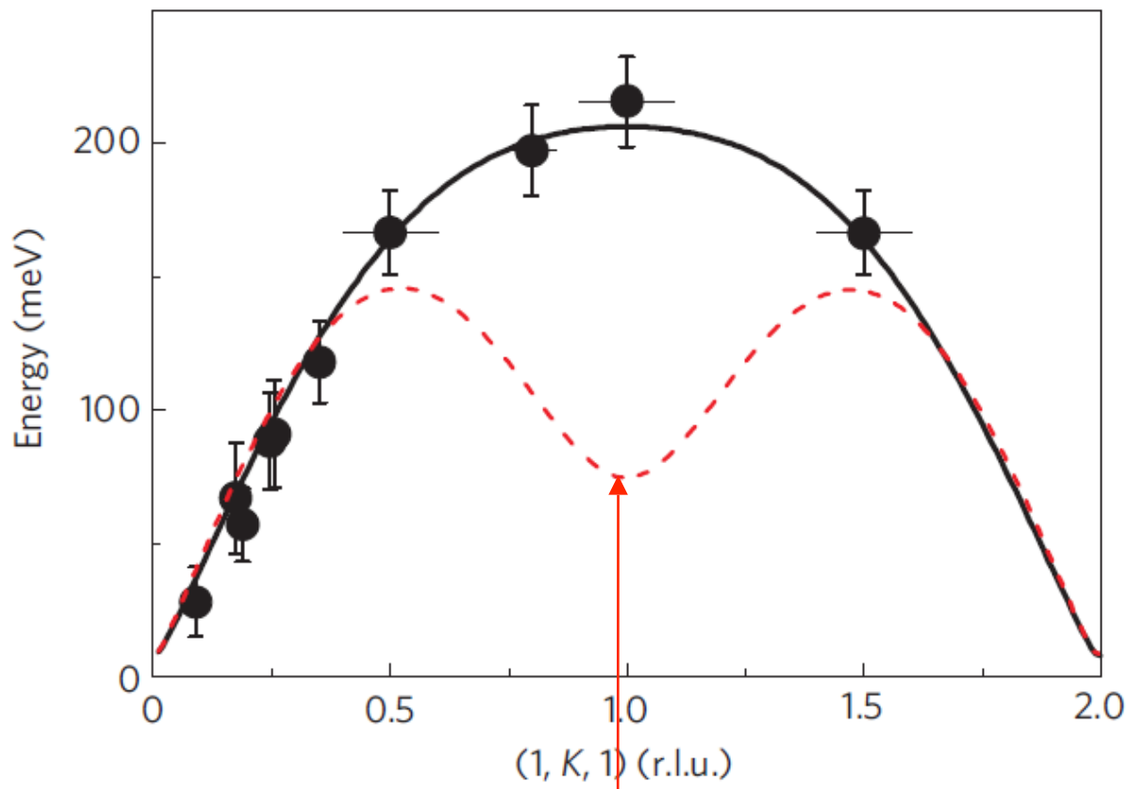

Isotropic $J_{1a} \simeq J_{1b}$

$$SJ_1^a = 27\,\mathrm{meV}$$
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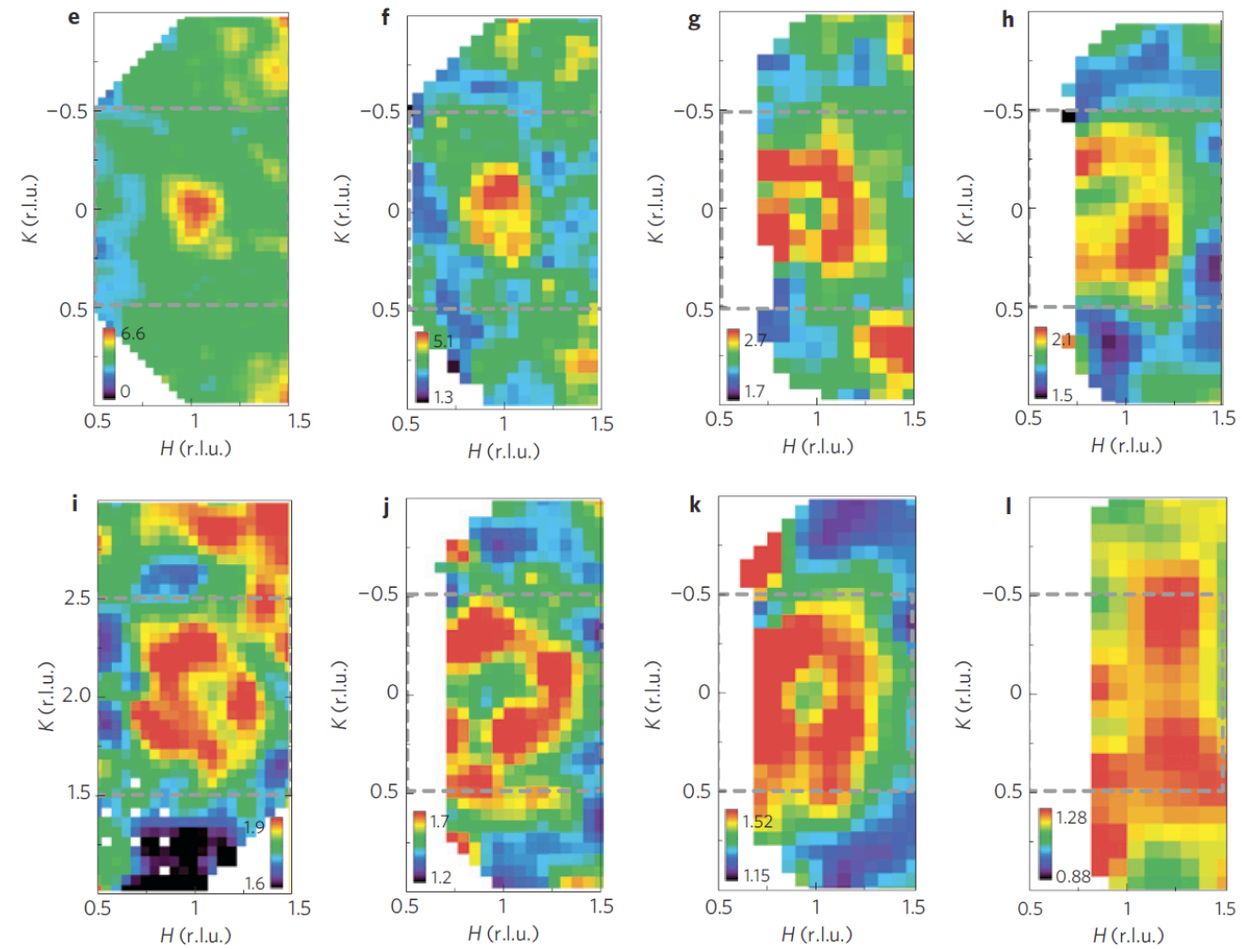

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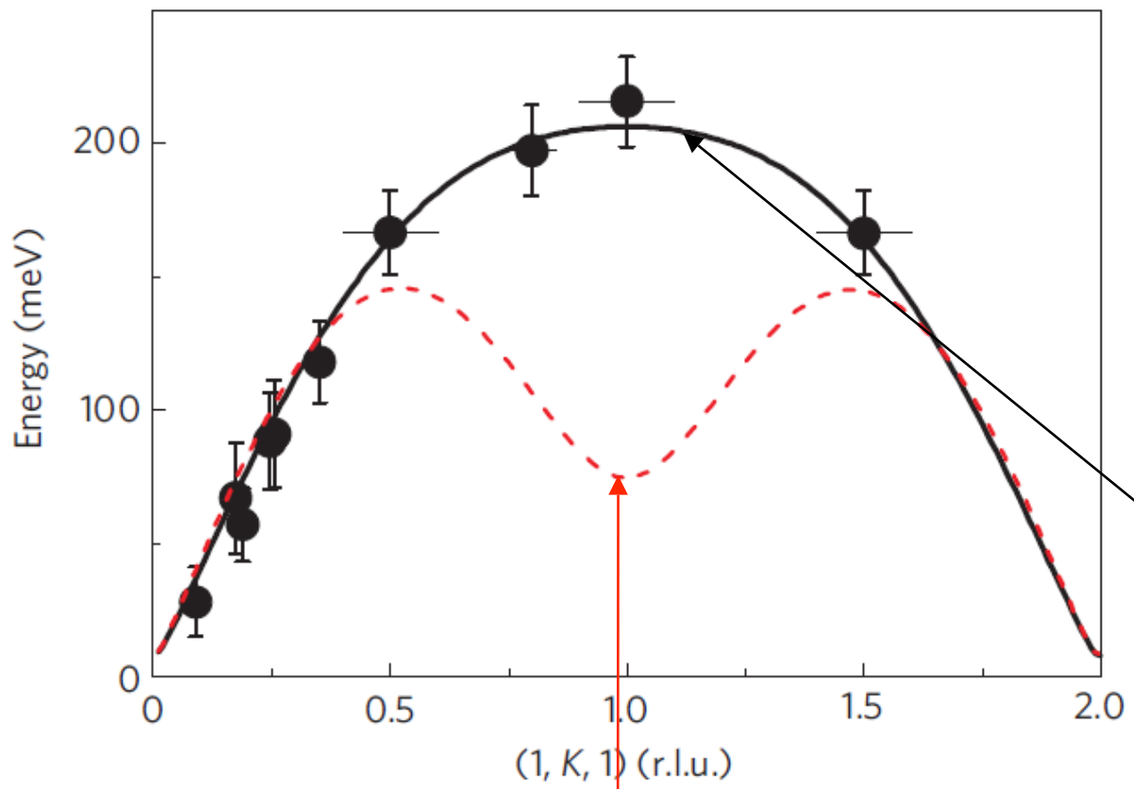

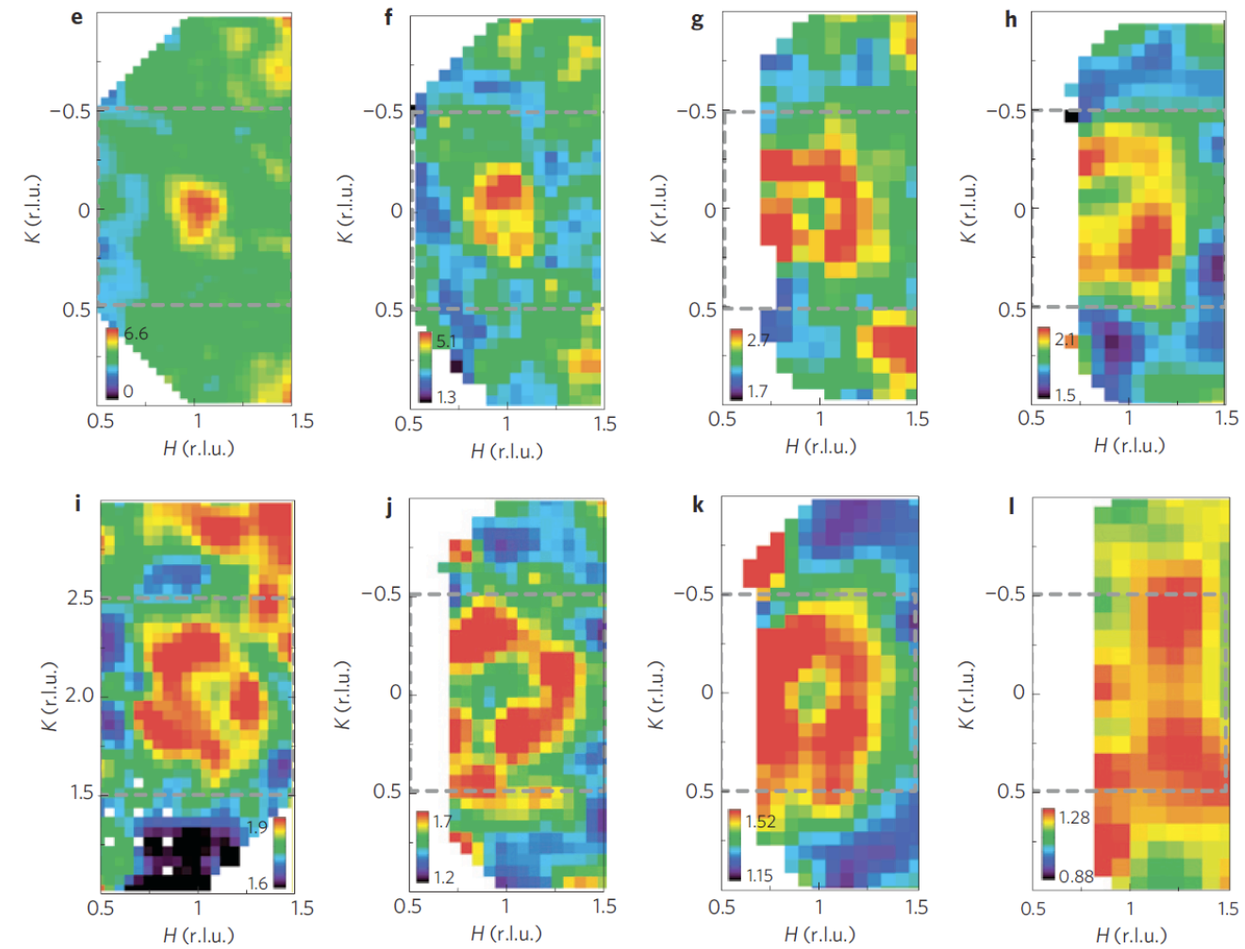

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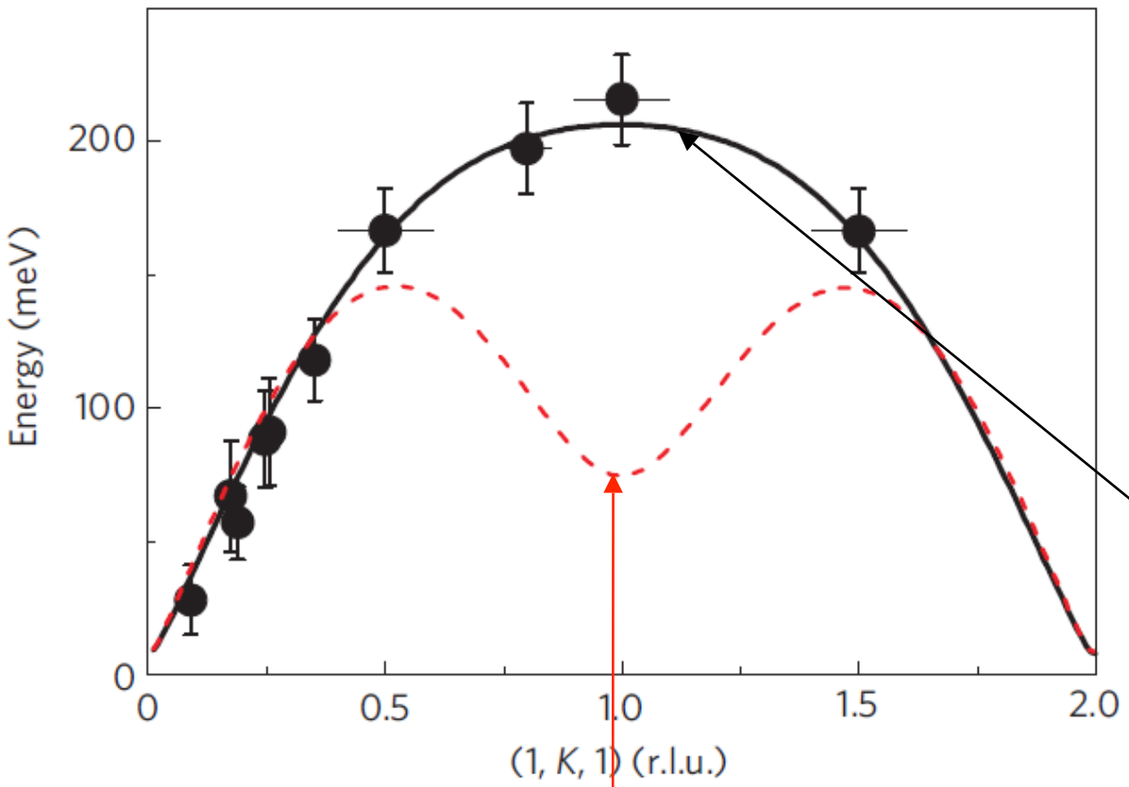

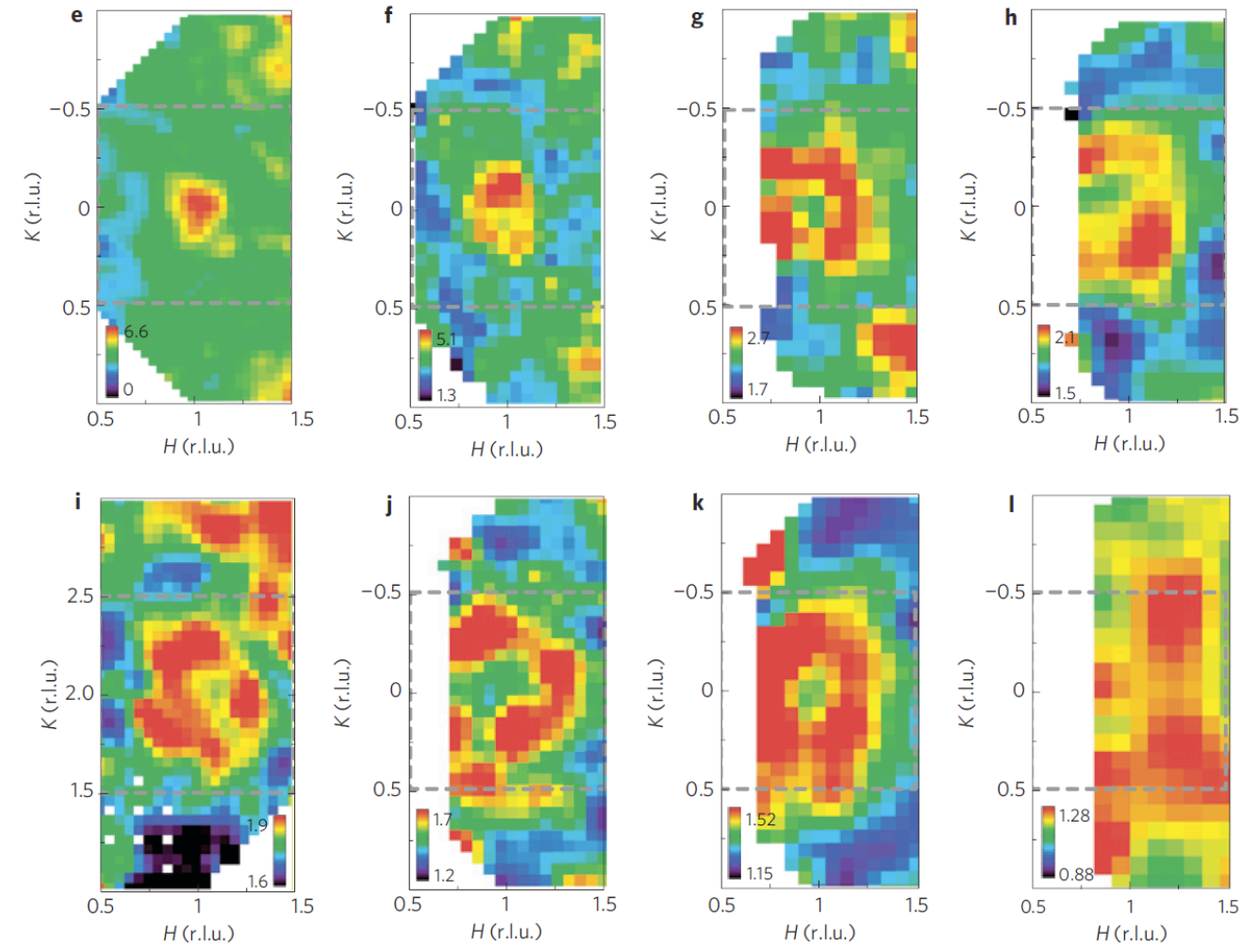

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Problem?

itinerant model

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

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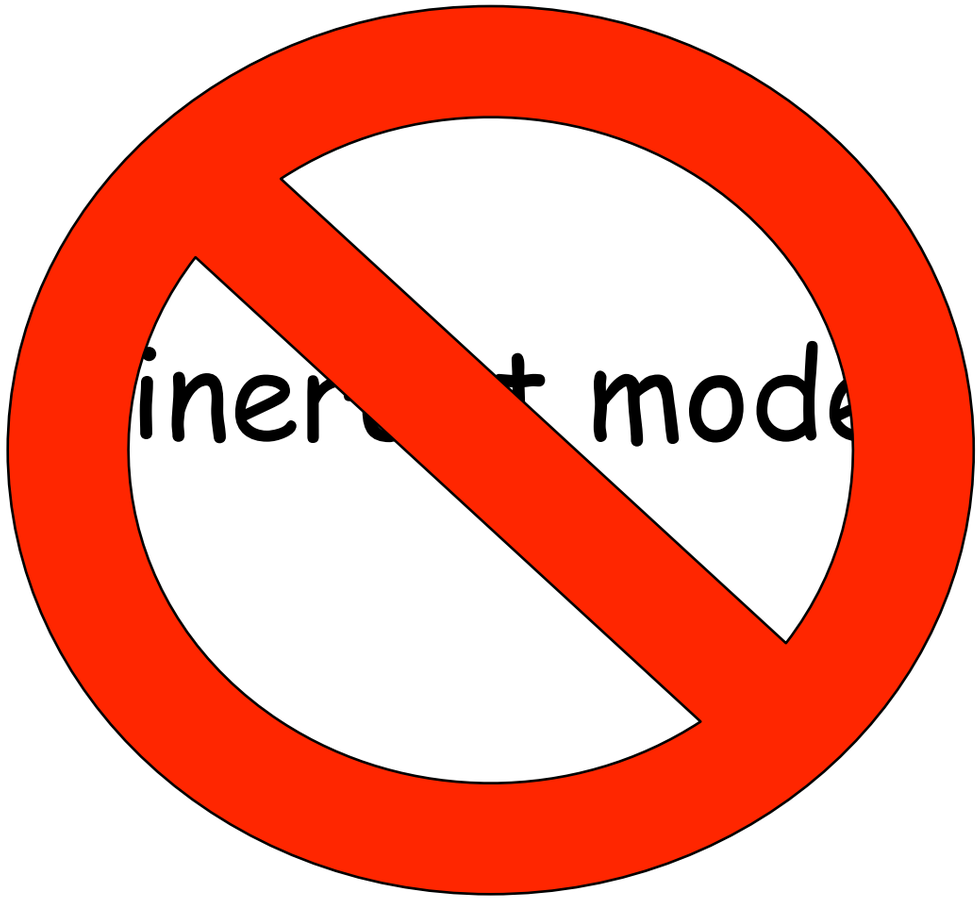

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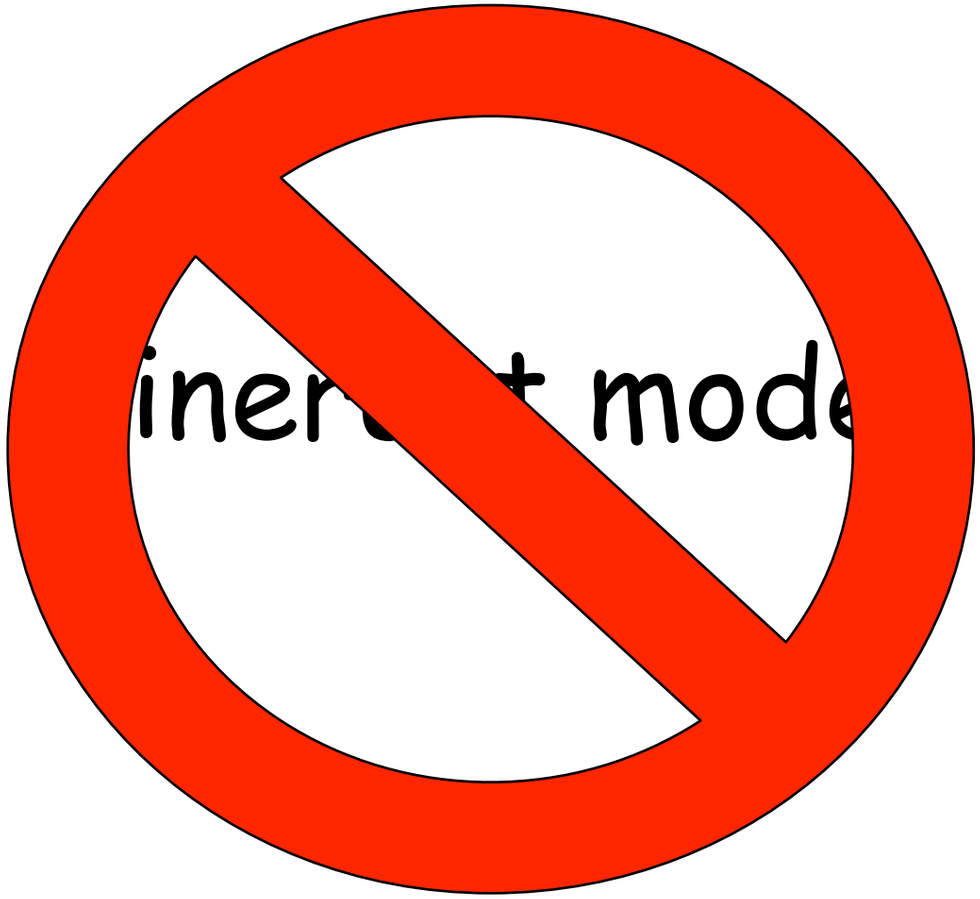
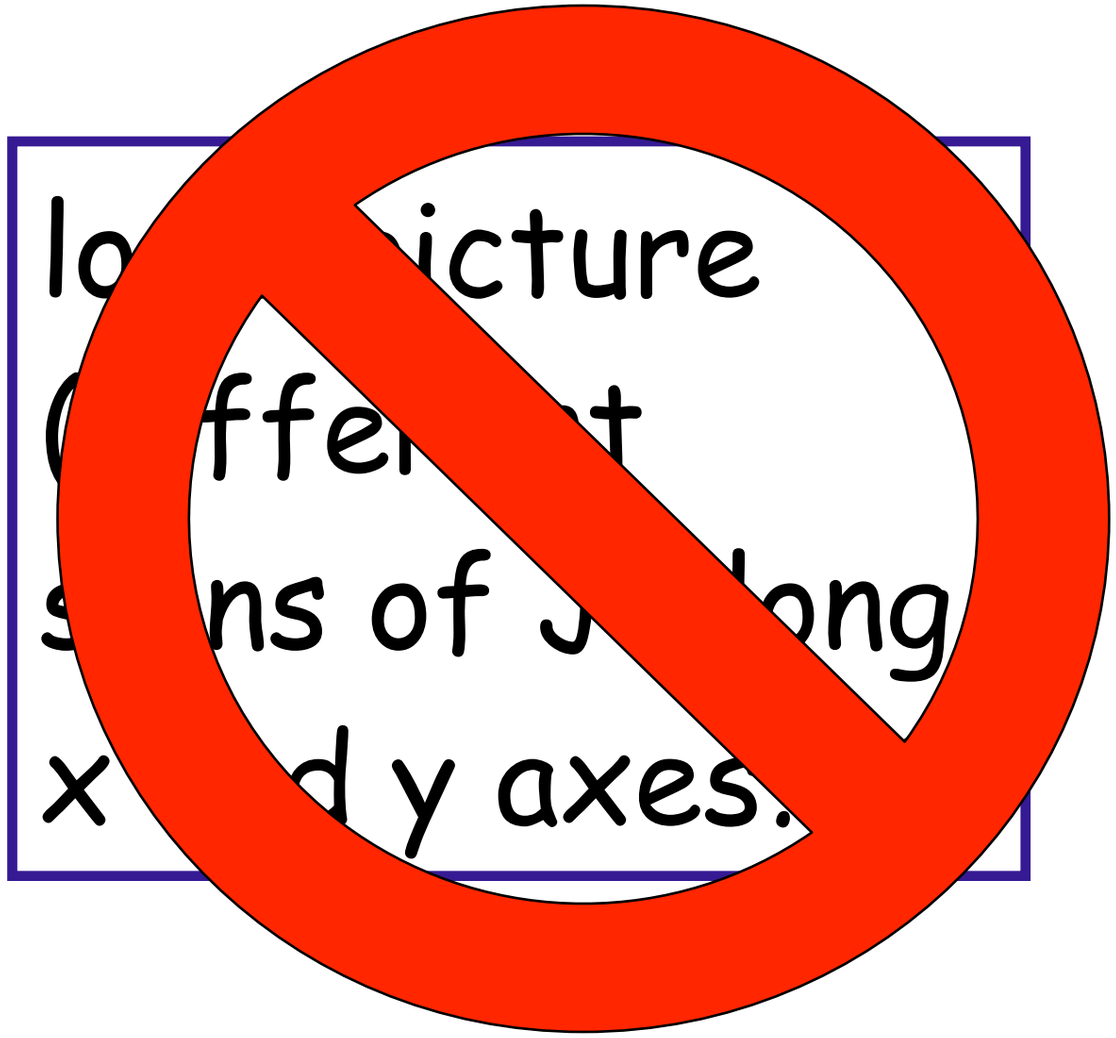




Is there a simple model that captures this physics?

localized/extended electrons+Hund's coupling

orbital ordering

unfrustrated magnetism, SPT, RA

$T > T_{SPT}$

a)

Coulomb Repulsion:

$$U = e^2 \int |\psi_{i_1 m_1}(\mathbf{r})|^2 \frac{e^{-|\mathbf{r}-\mathbf{r}'|/r_0}}{|\mathbf{r}-\mathbf{r}'|} |\psi_{i_2 m_2}(\mathbf{r}')|^2$$

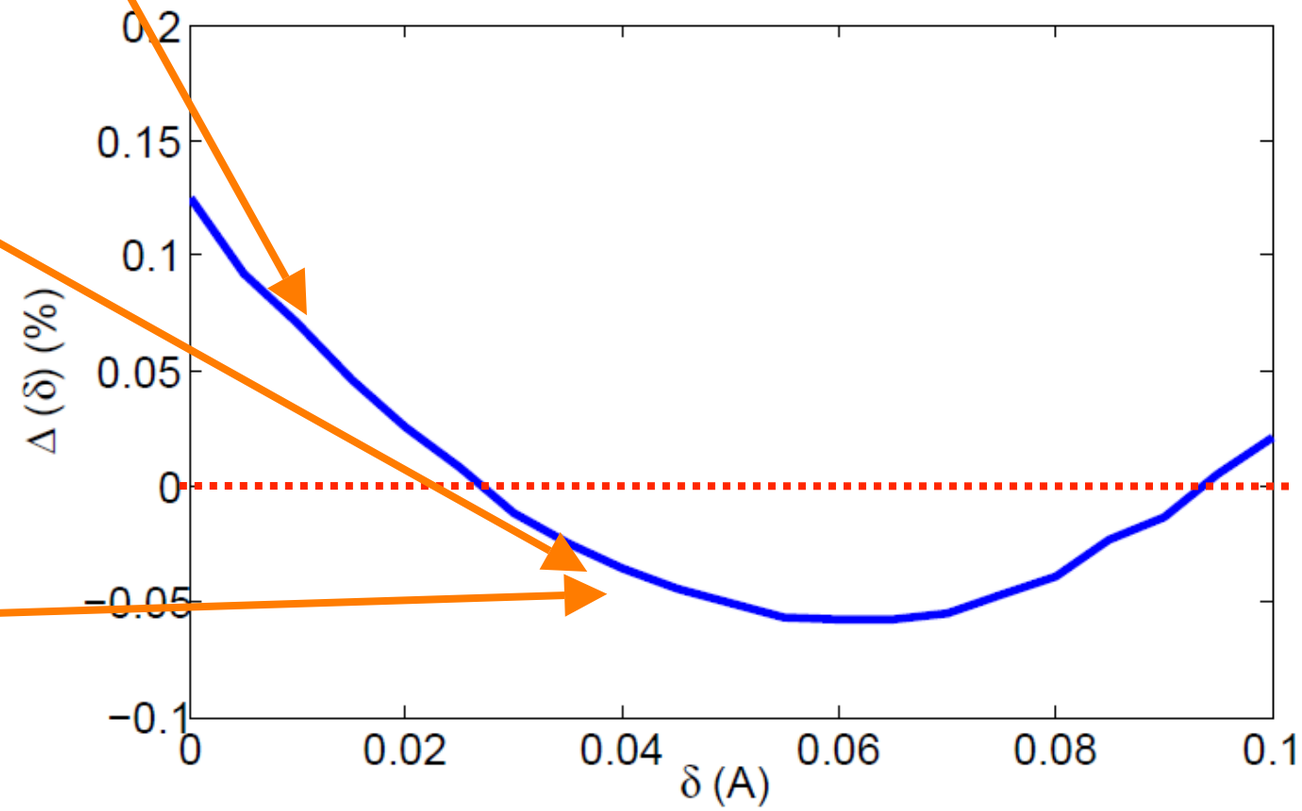
Energy Difference:

$$\Delta(\delta) = \frac{U_b(\delta) - U_a}{U_a}$$

b)

$T < T_{SPT}$

c)



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

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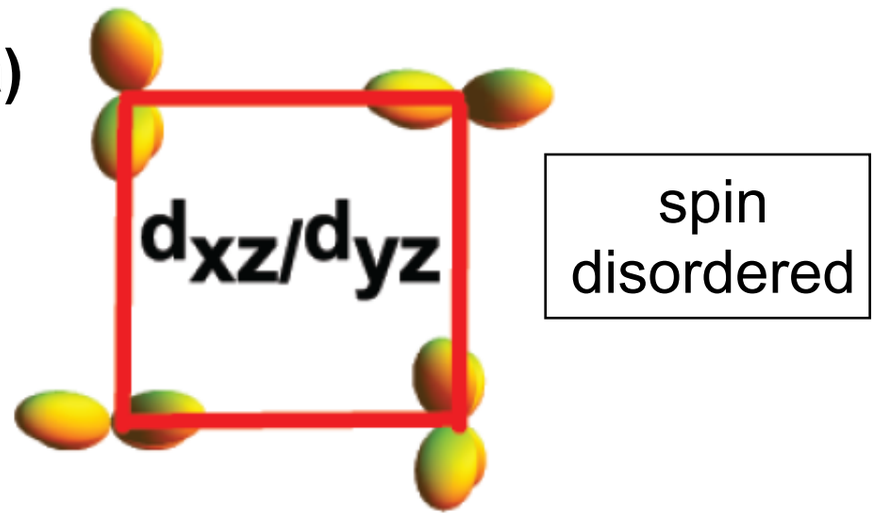

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spin disordered

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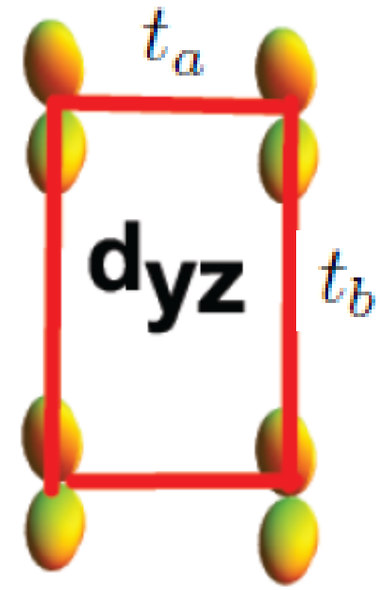

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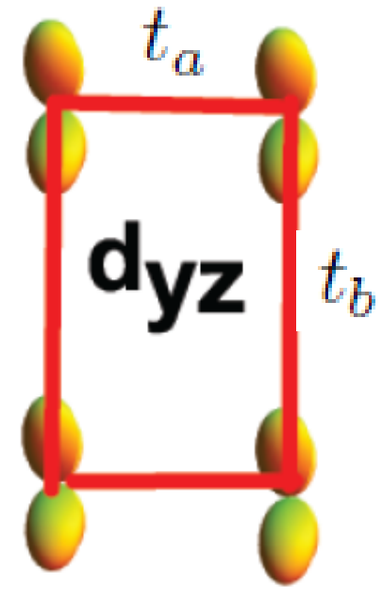

$$t_b > t_a$$

$$J \sim \frac{t^2}{U}$$

$$J_b > J_a$$

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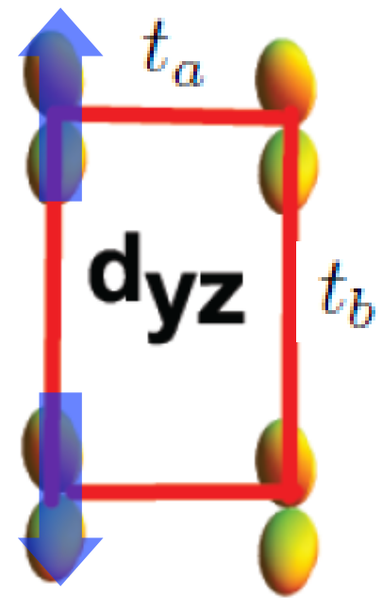

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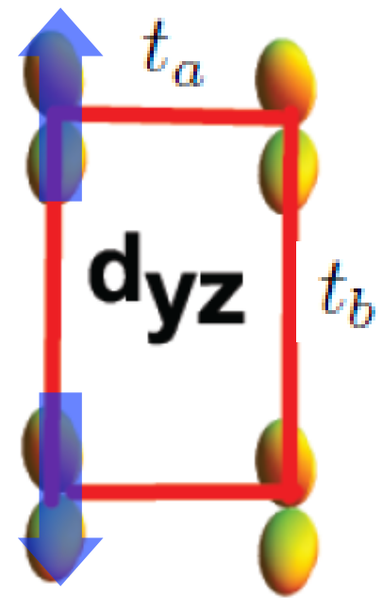

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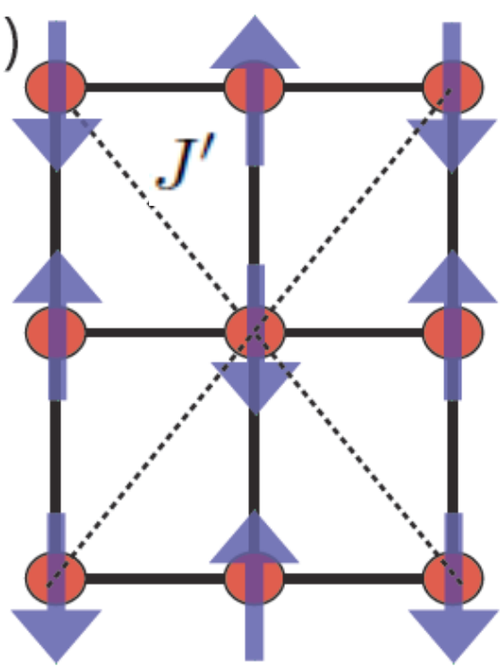

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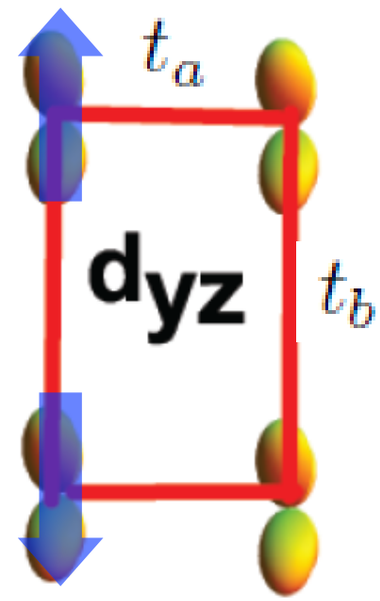

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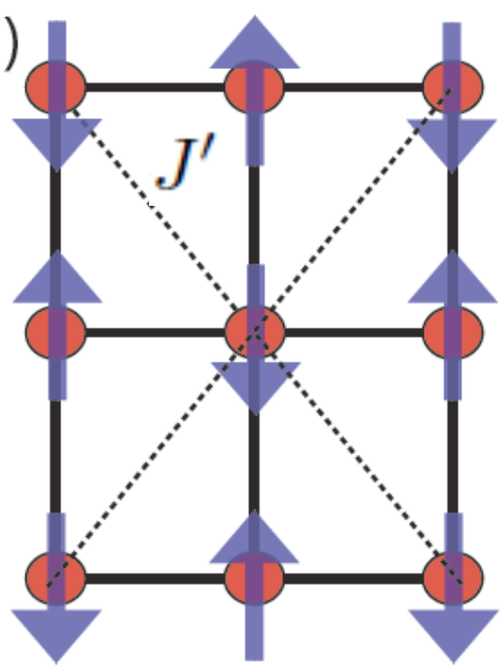

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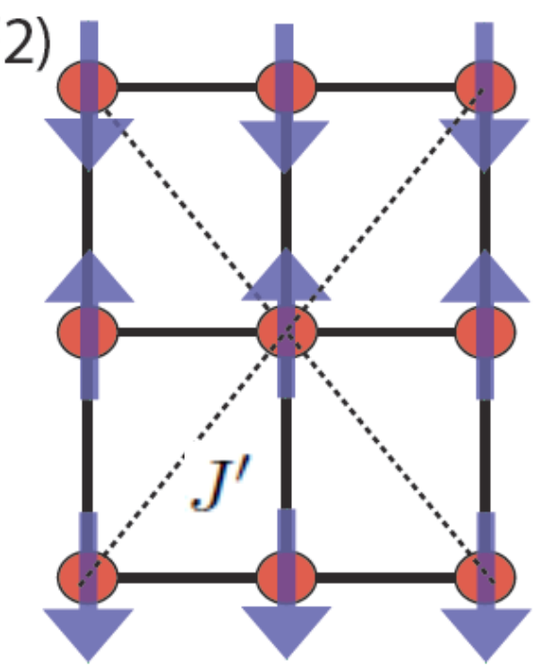

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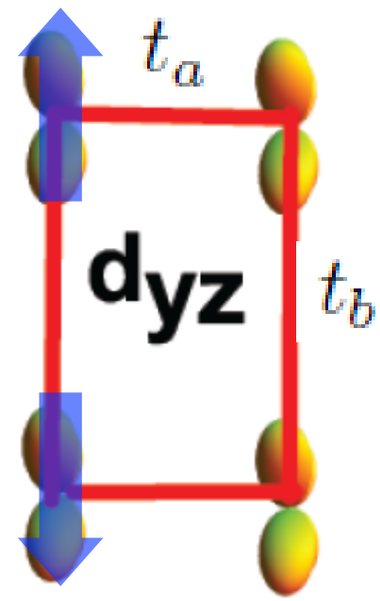

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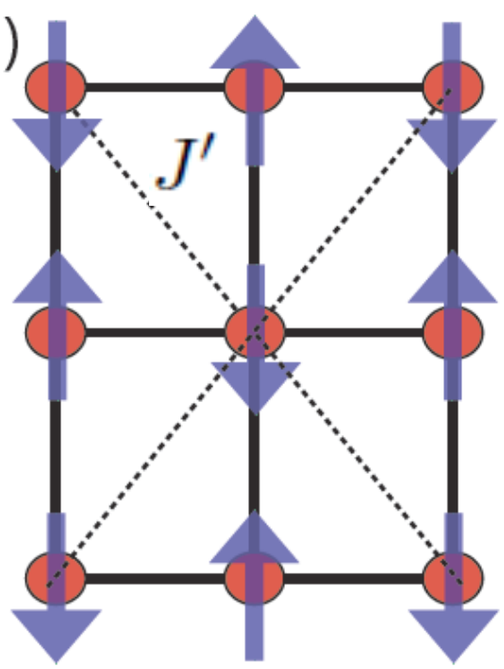

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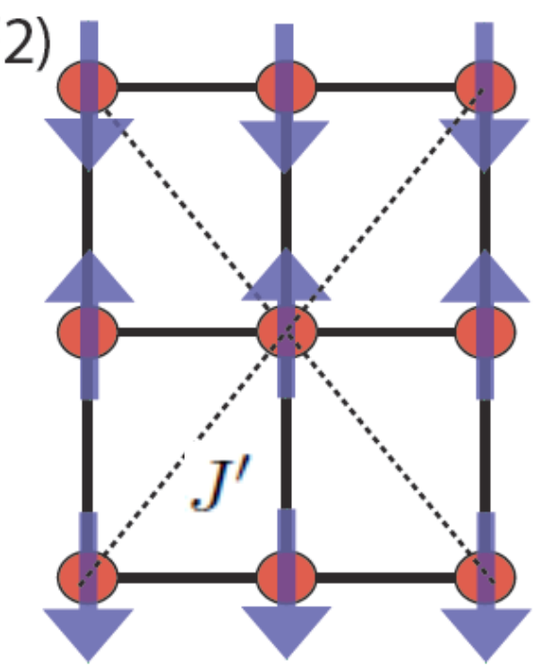

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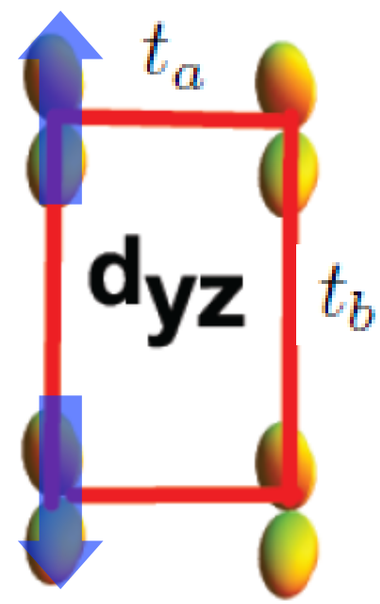

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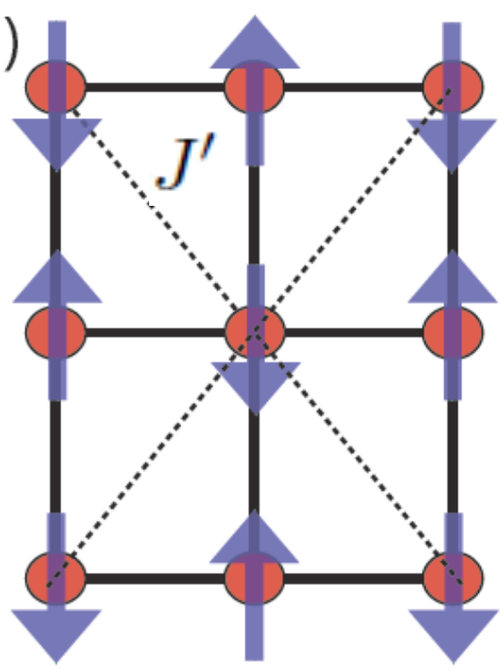
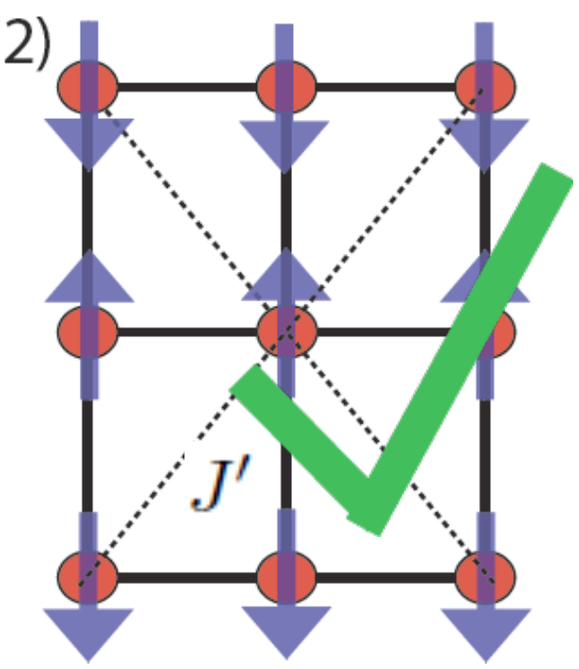
$$J_b > J_a$$

AF1)



AF2)



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

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

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

SPT-induced magnetism

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

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

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

orbital ordering

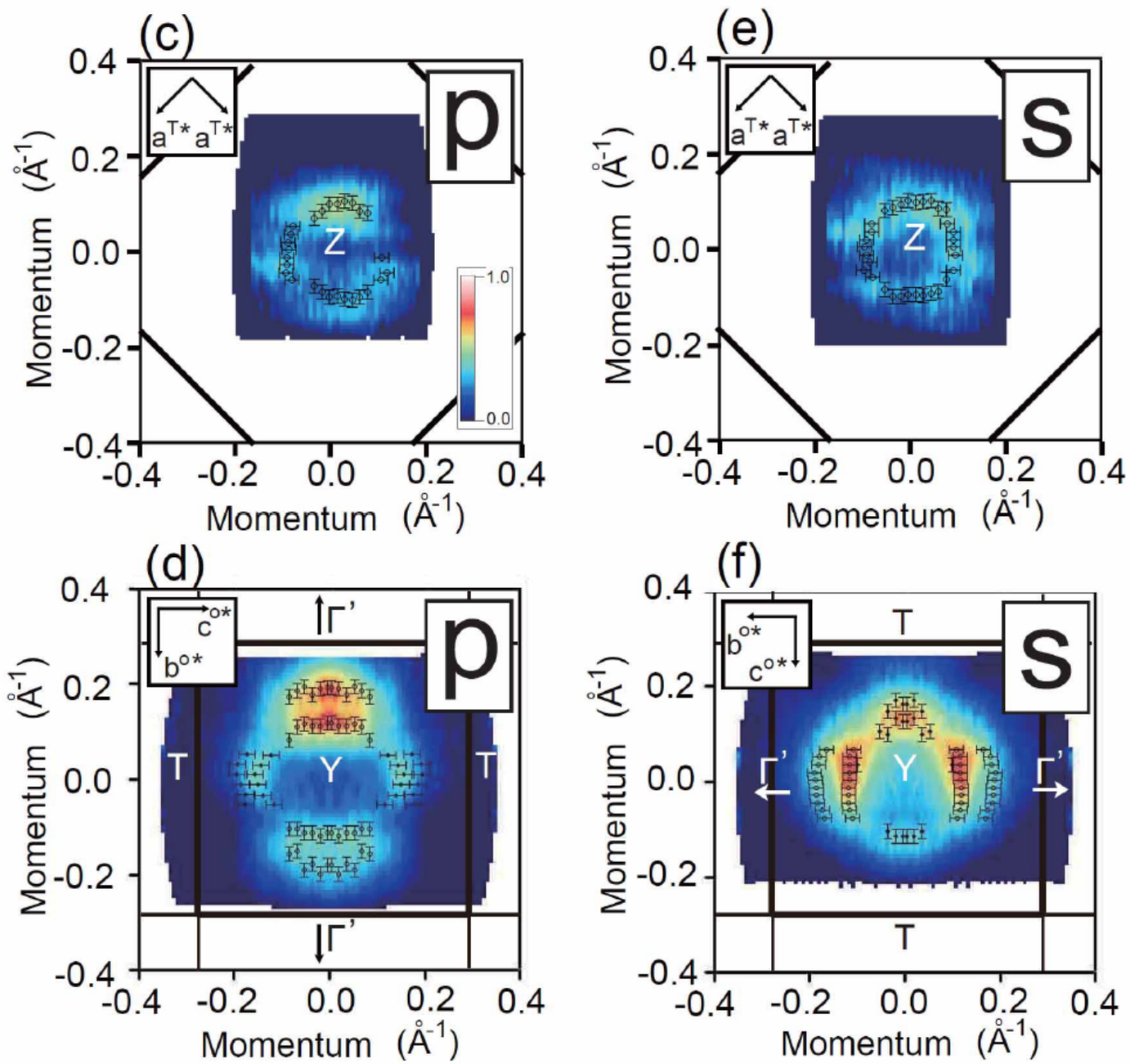
↓

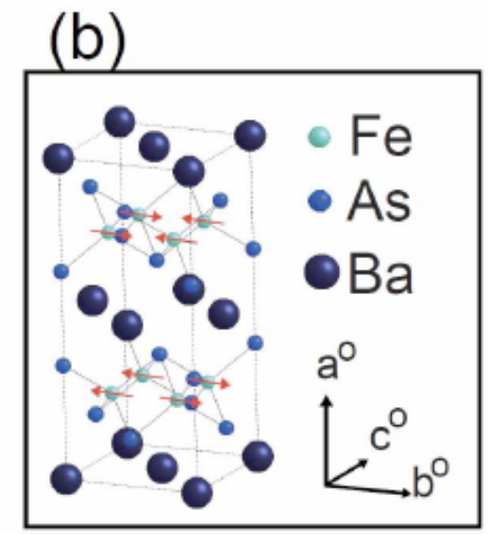
transport anisotropies

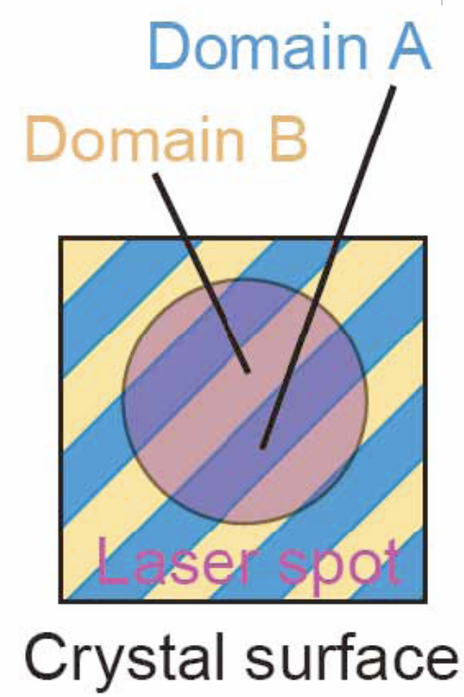
Orbital-polarized Fermi surface in antiferromagnetic state of $BaFe_2As_2$

Shimojima, et al.
arXiv:0904.1632

- **Polarized ARPES**







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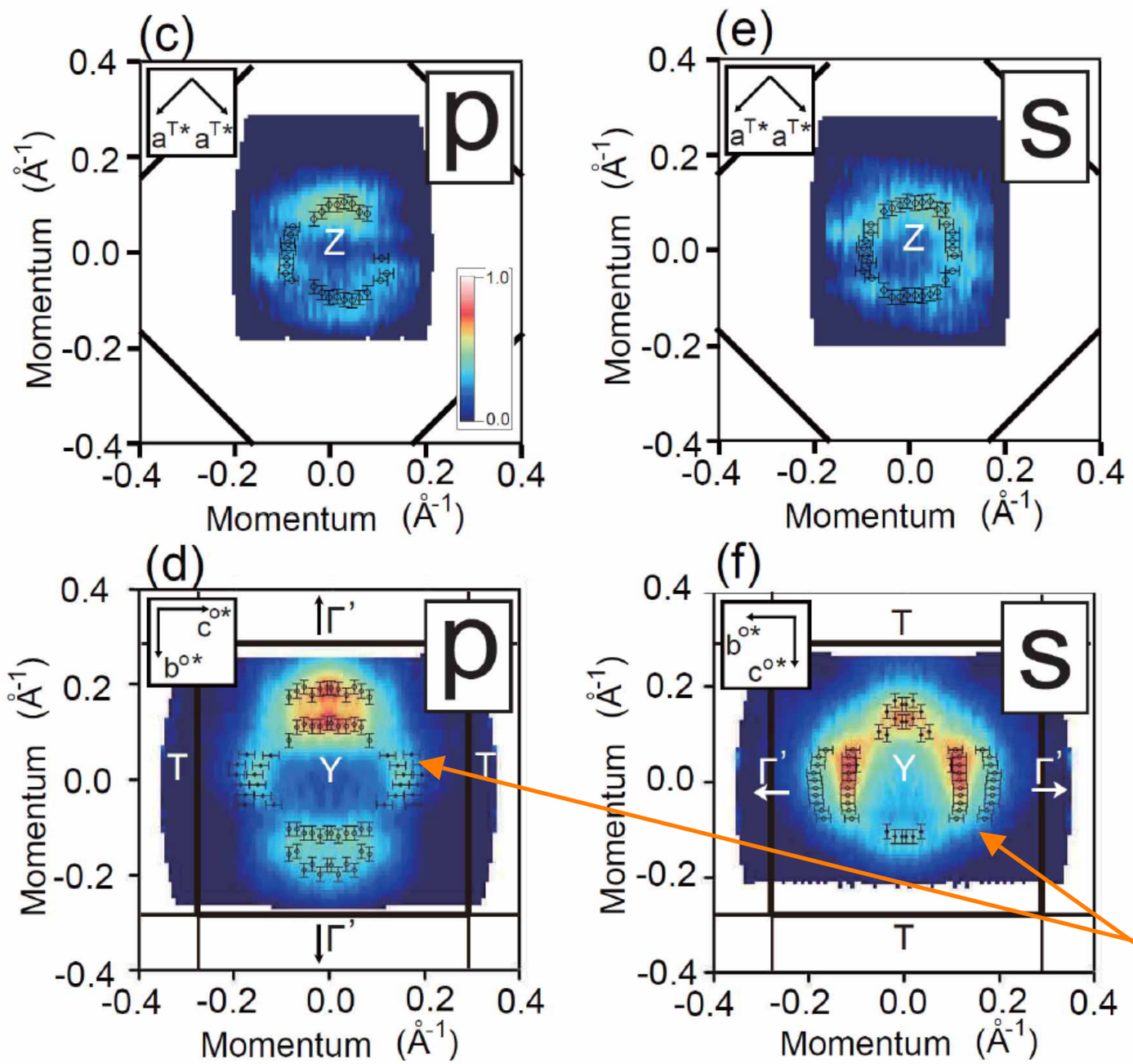
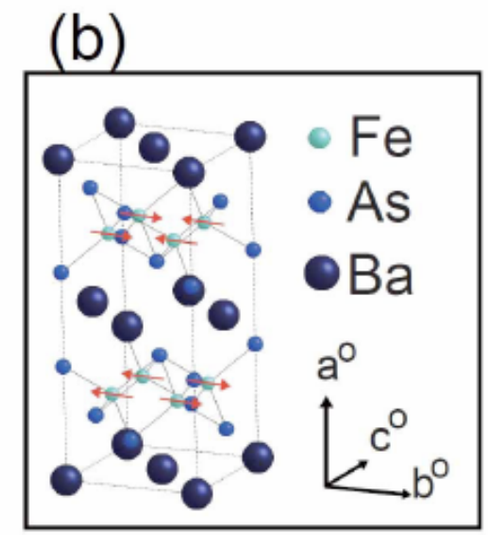
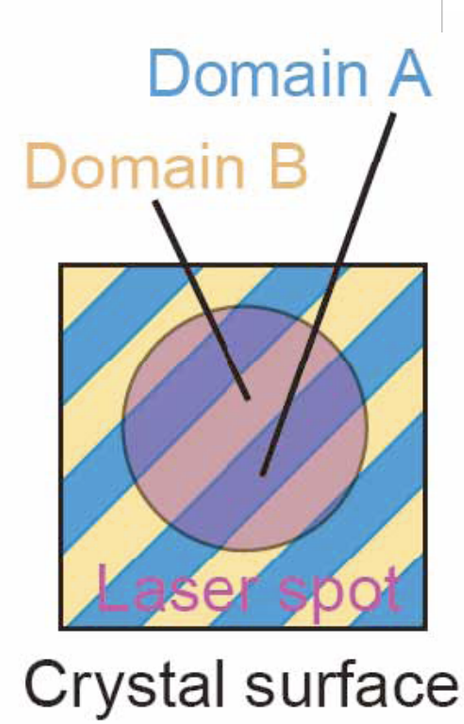
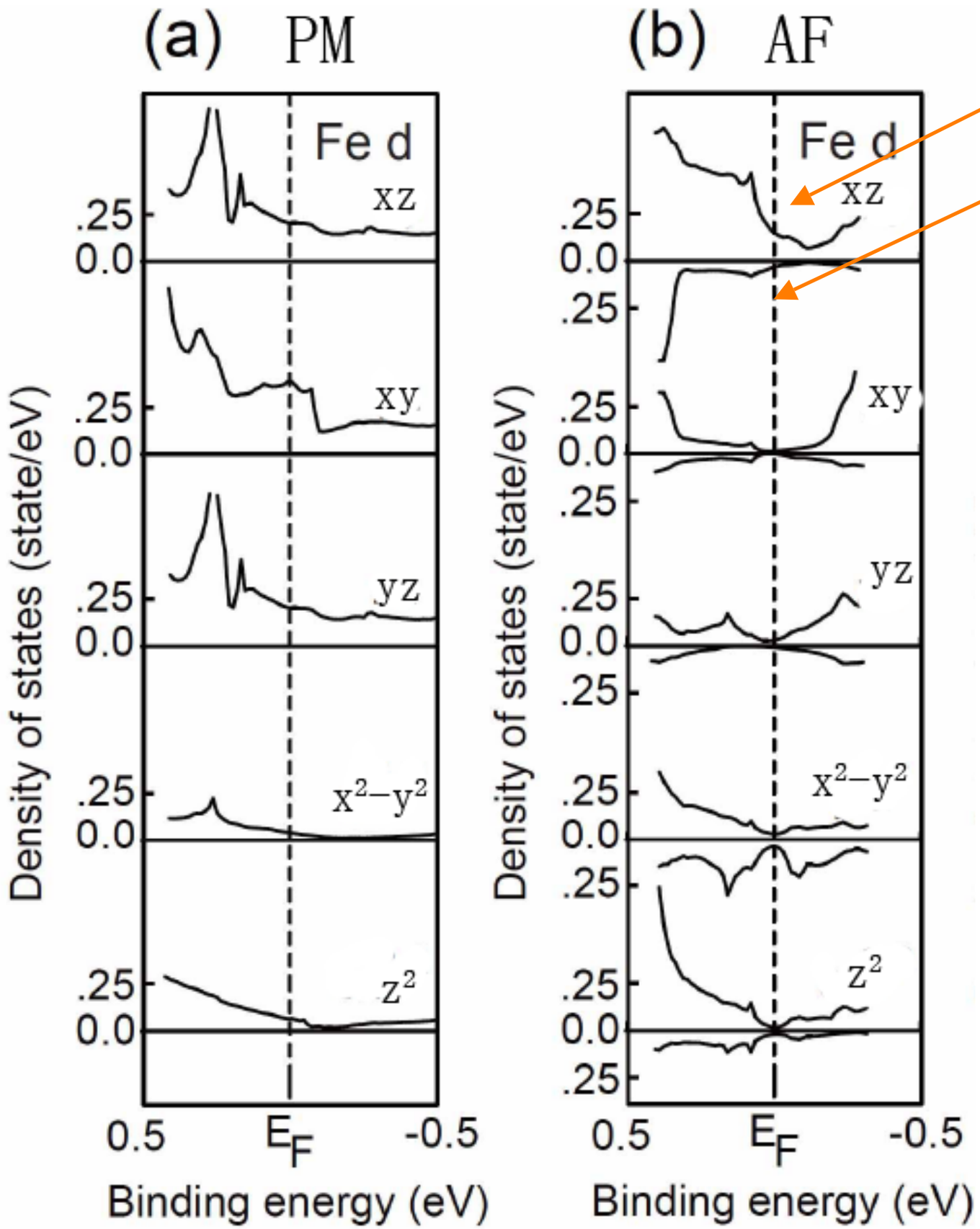






d_{xz} in domain A

d_{xz} in domain B



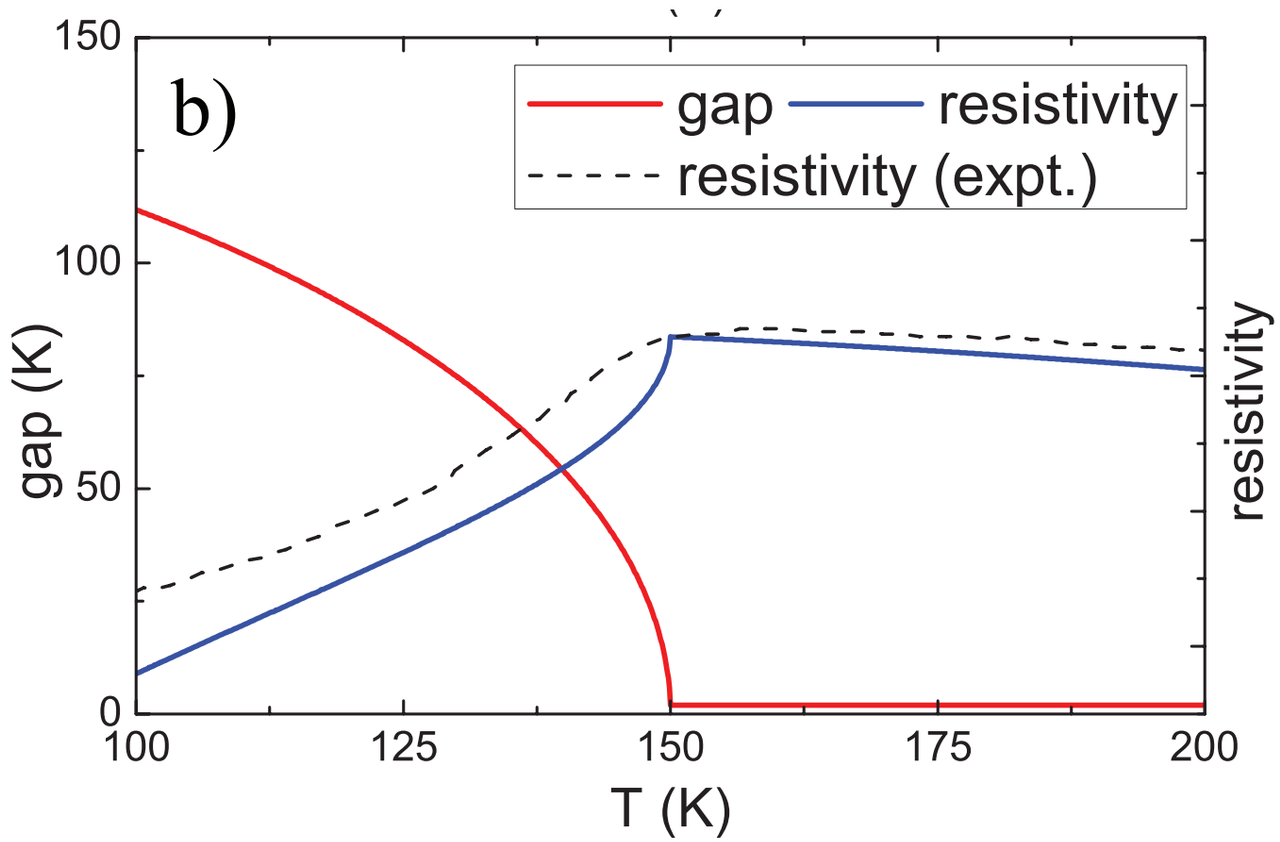
(a) PM state:

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

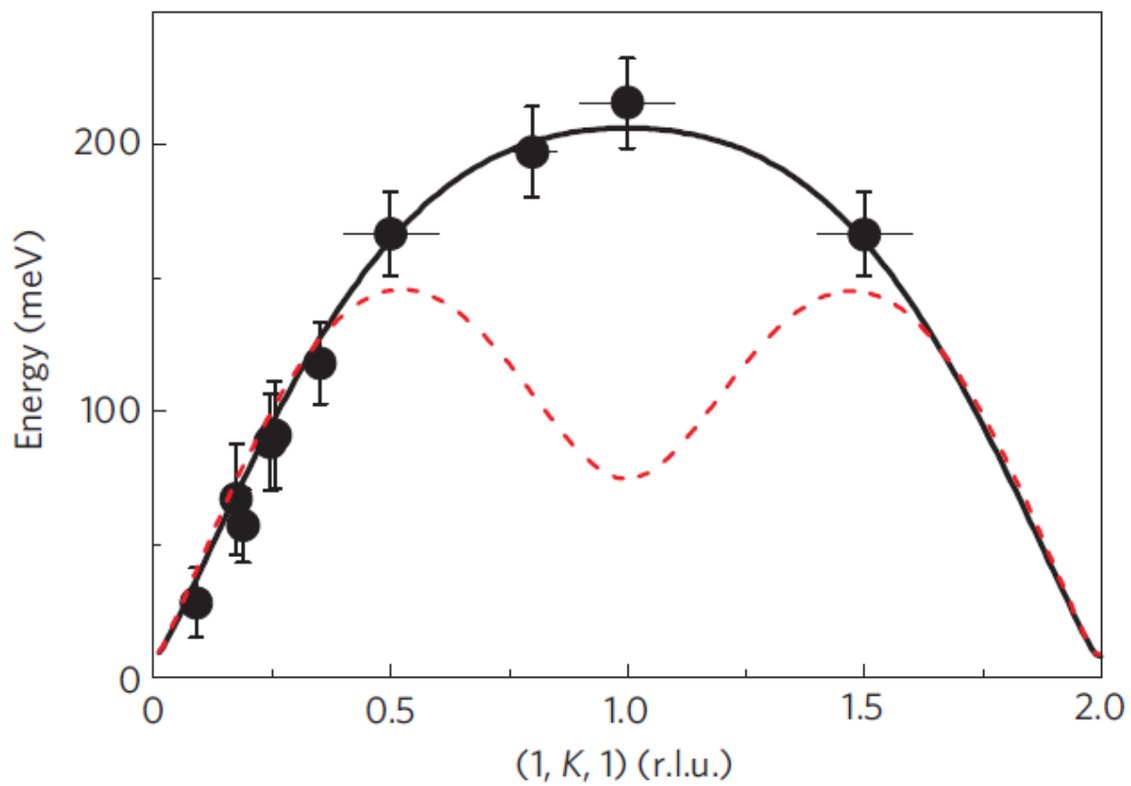
(b) AF state:

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

Resistivity Anomaly

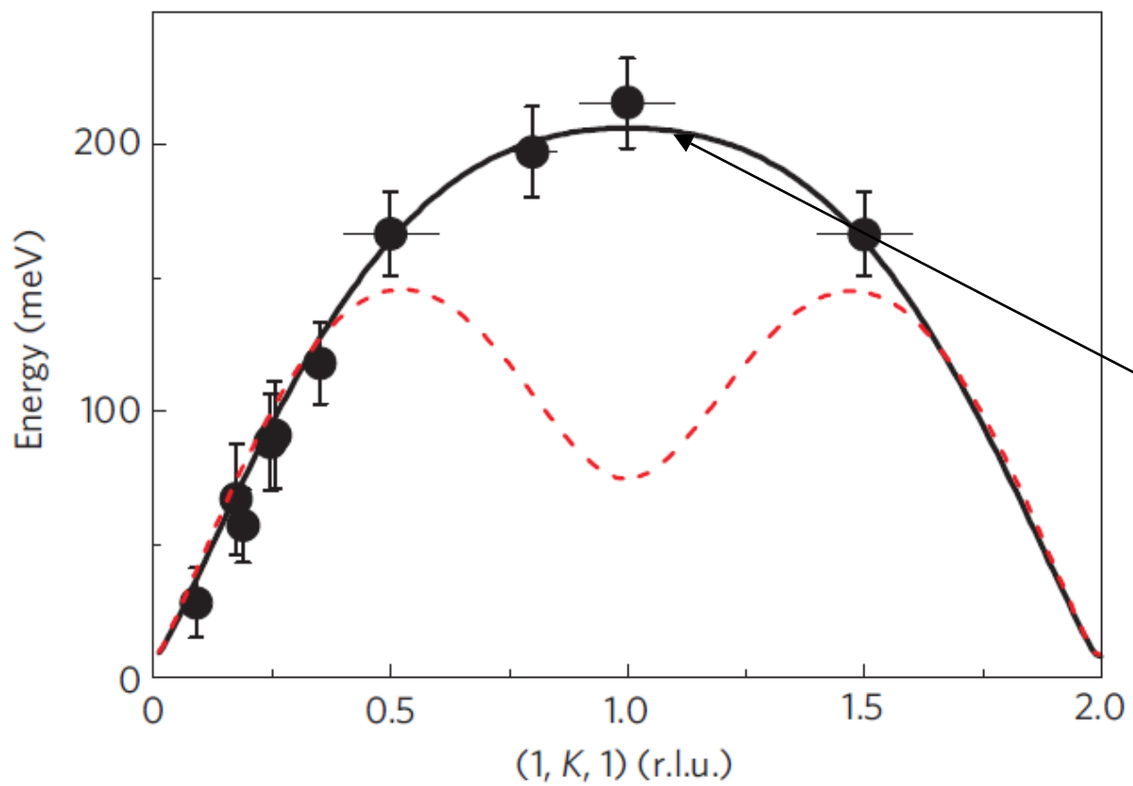


spin-wave spectrum



origin of ferromagnetic coupling?

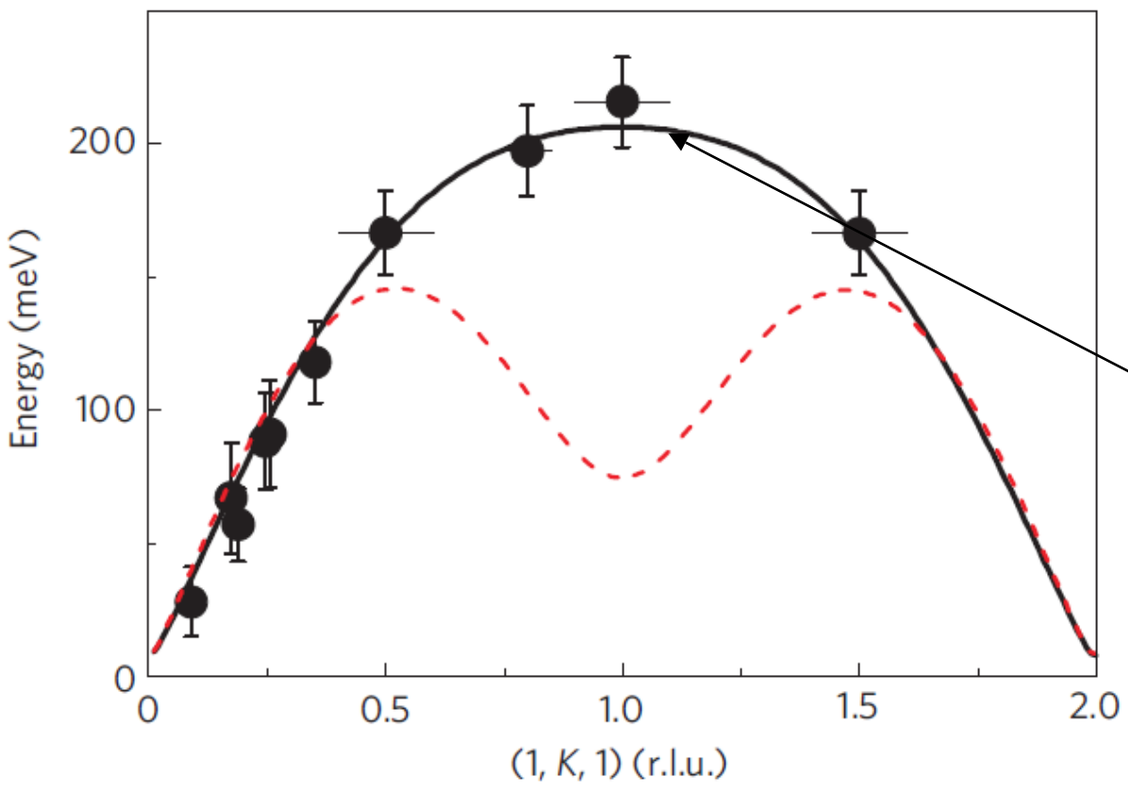
spin-wave spectrum



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

origin of ferromagnetic coupling?

spin-wave spectrum



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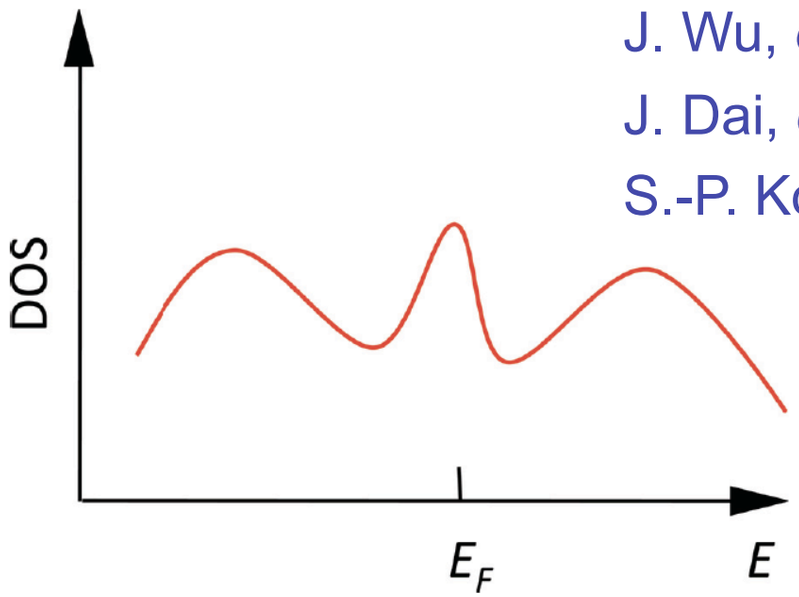
origin of ferromagnetic coupling?

- *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*

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

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

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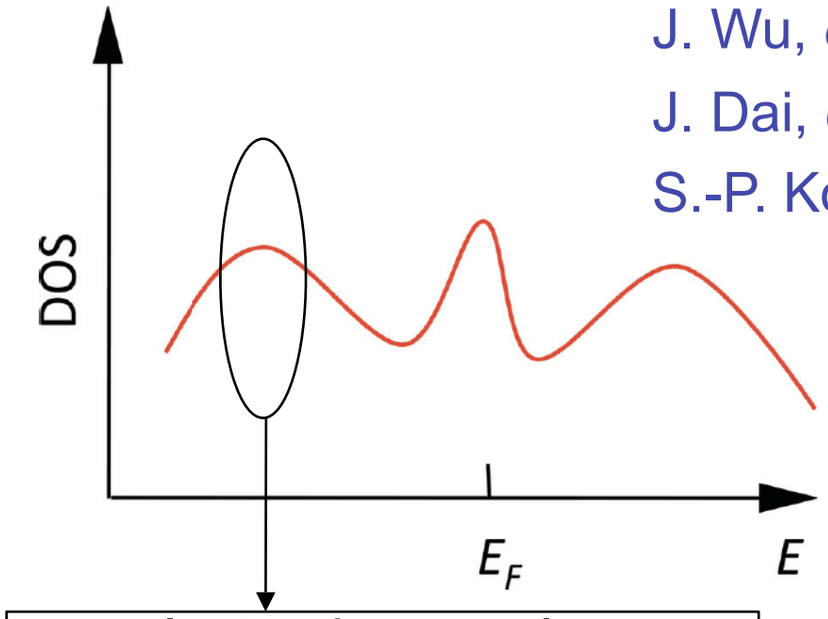
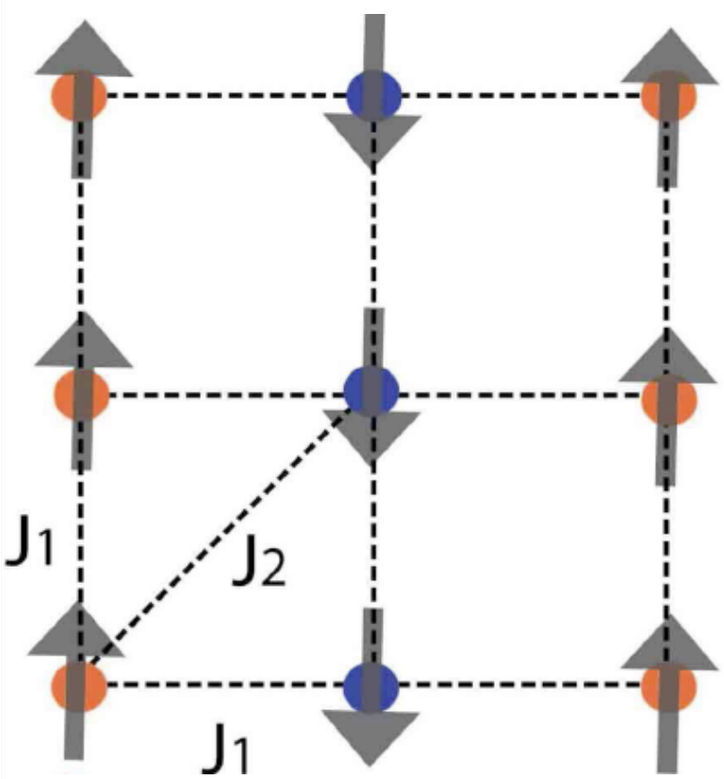


Isotropic strongly frustrated J_1-J_2 model



$S = 1/2 \quad J_2 \gtrsim J_1/2$

- *A local-itinerant model*

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

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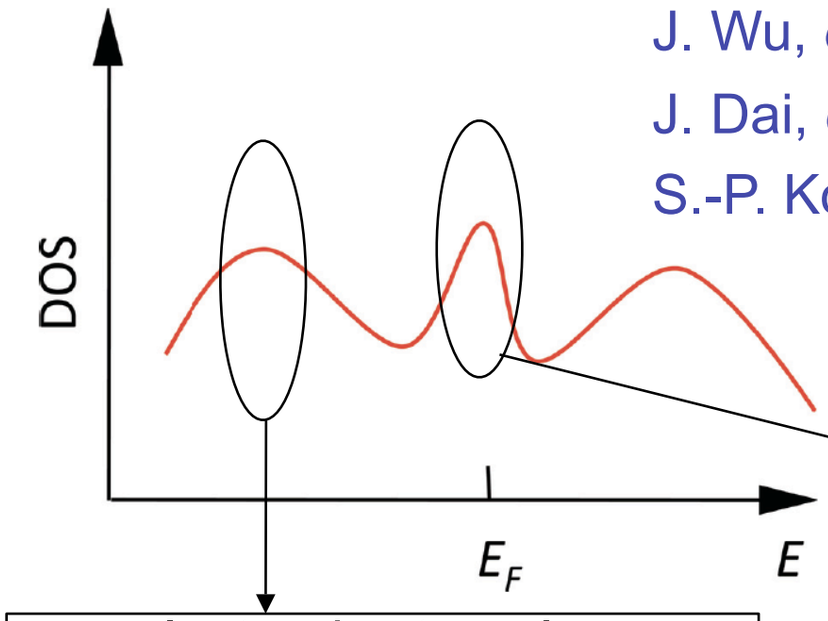

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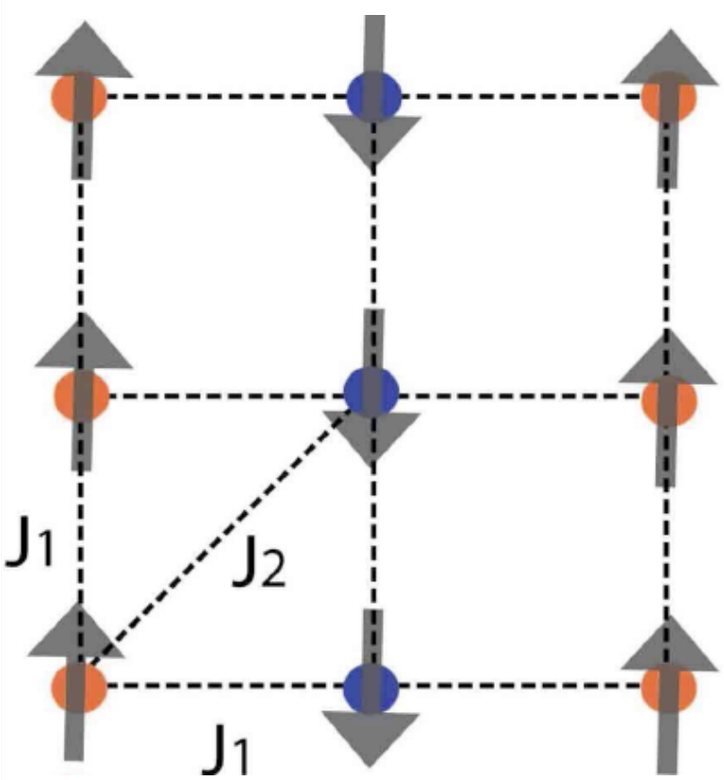
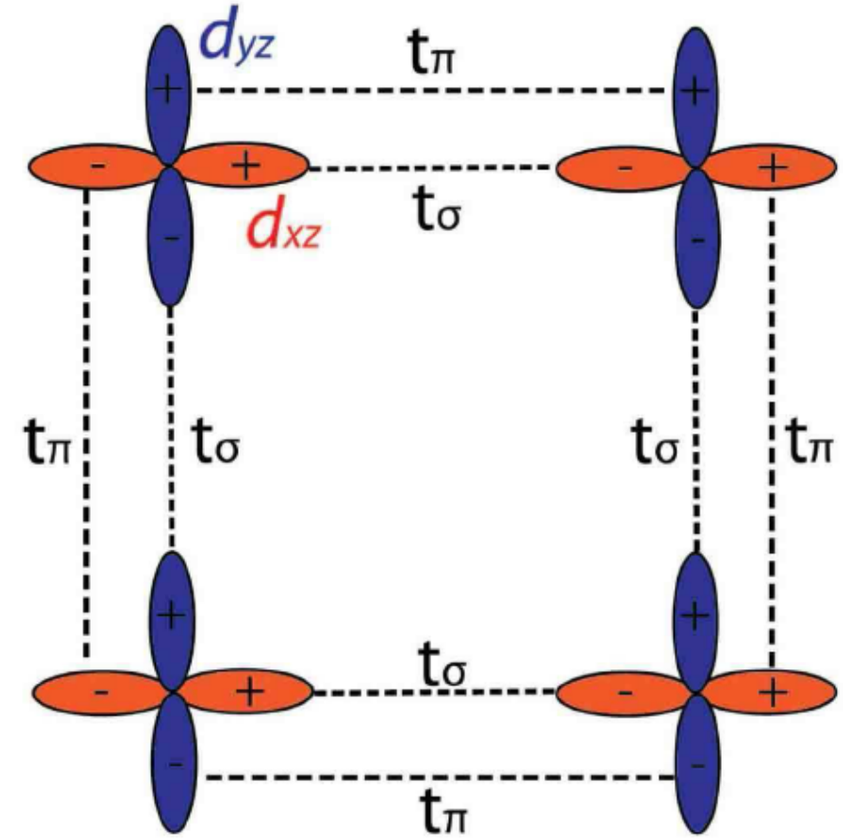


$S = 1/2 \quad J_2 \gtrsim J_1/2$

Doubly-degenerate d_{xz} and d_{yz} type orbitals:



$t_\sigma > t_\pi$

- *A local-itinerant model*

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

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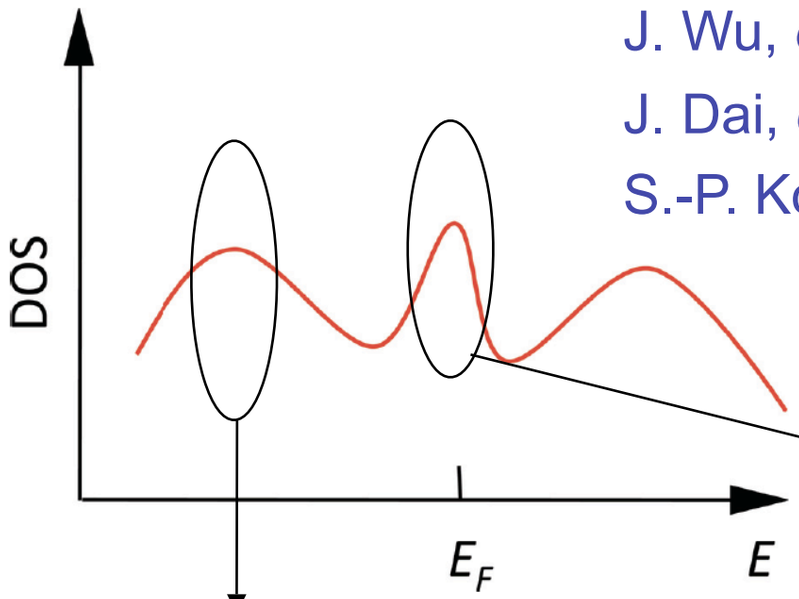
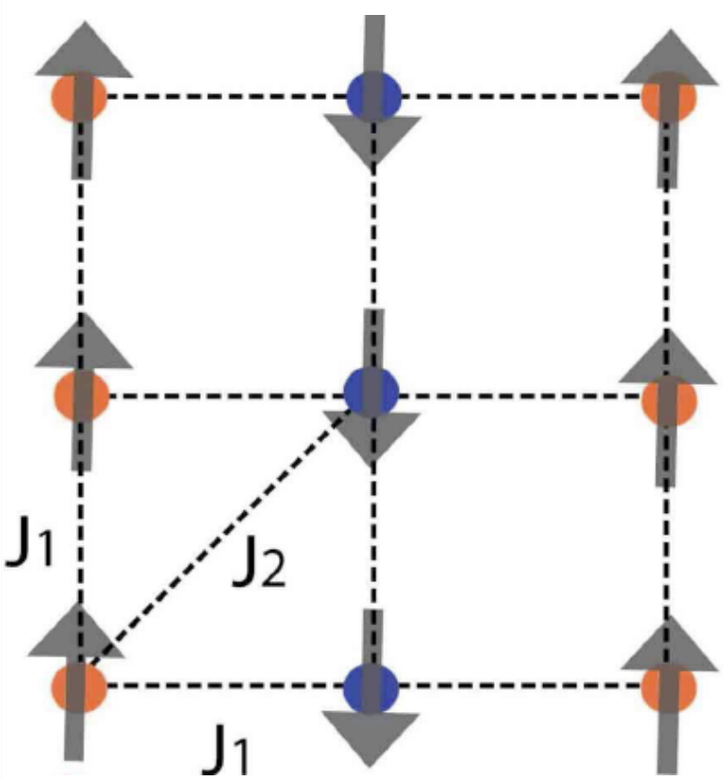


Isotropic strongly frustrated J_1-J_2 model



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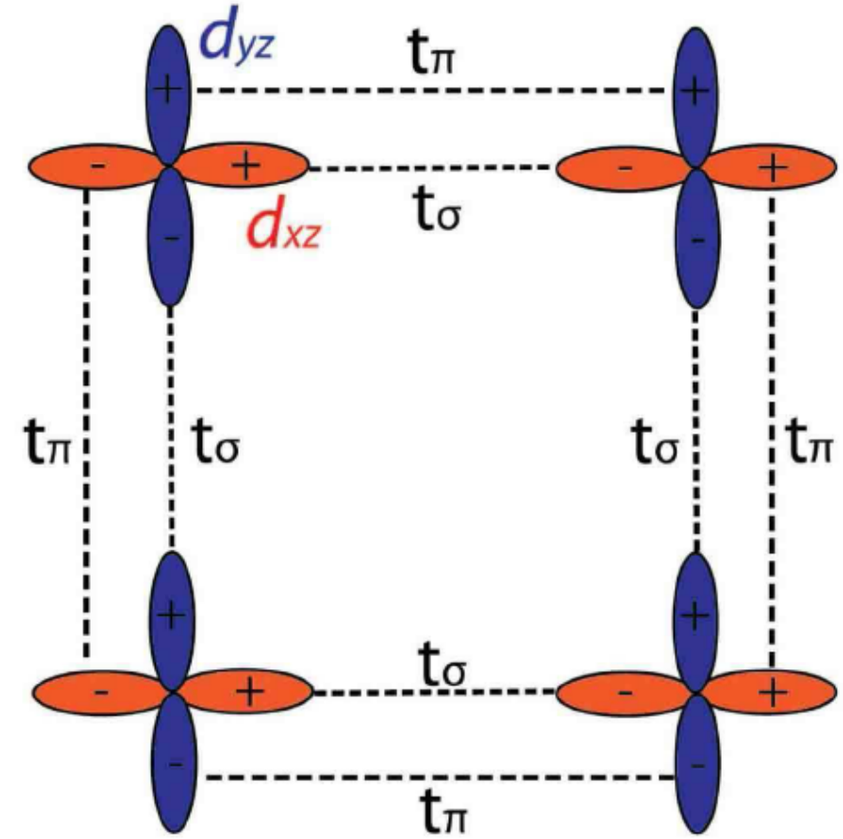
Ferromagnetic Hund's couplings J_H

Doubly-degenerate d_{xz} and d_{yz} type orbitals:



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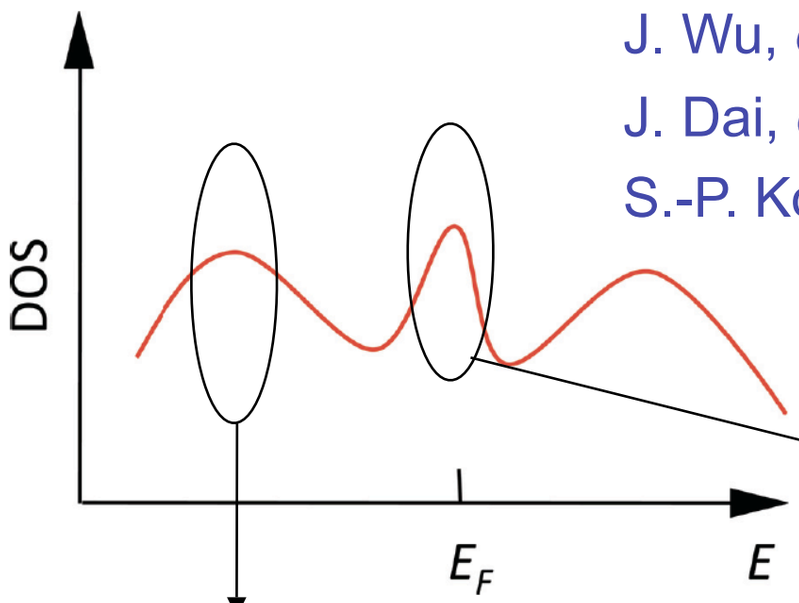
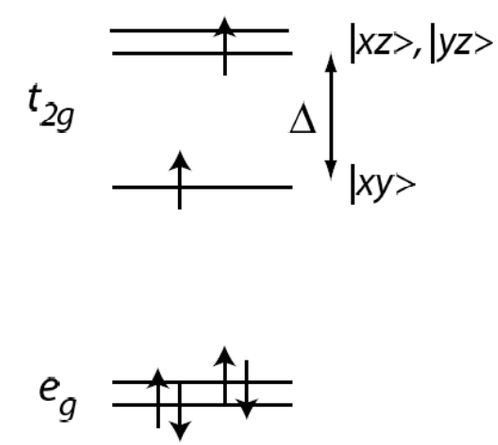
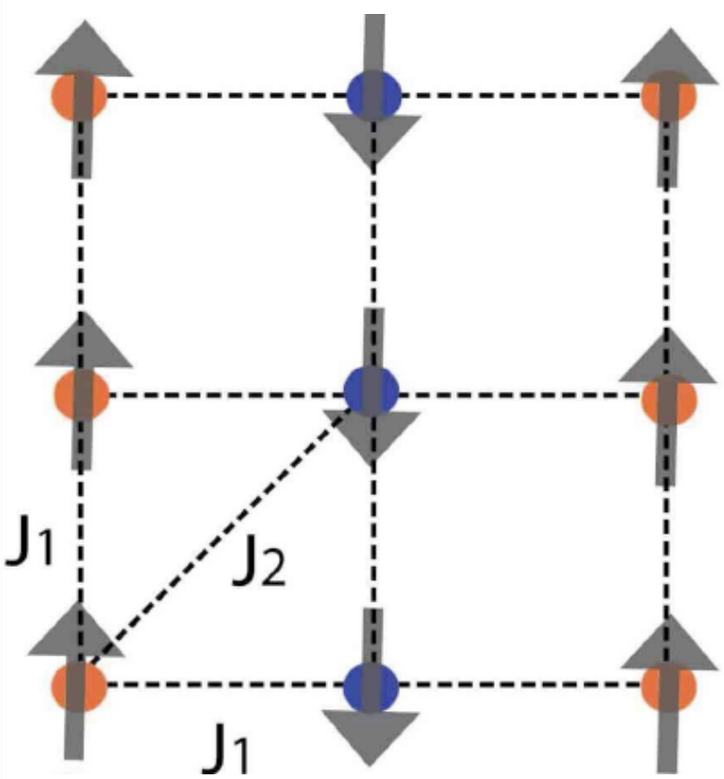


consistent with the local multiplet structure:



Isotropic strongly frustrated J_1-J_2 model



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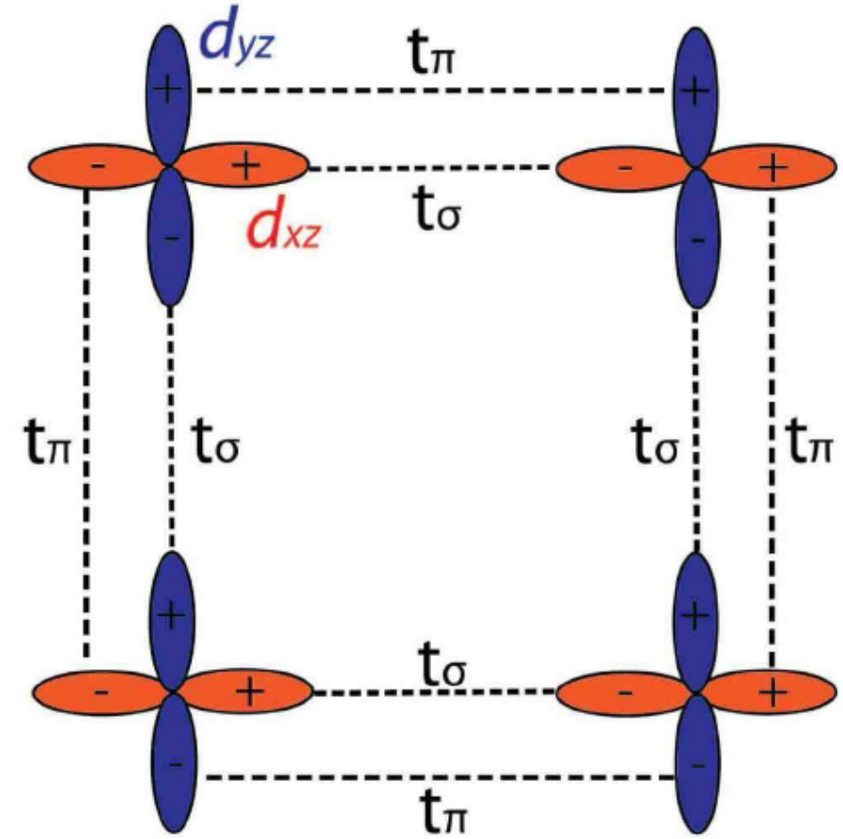
Ferromagnetic Hund's couplings J_H

Doubly-degenerate d_{xz} and d_{yz} type orbitals:



$t_\sigma > t_\pi$

Double-Exchange Model

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

unlike manganites

$$\nu J_H \ll \infty$$

Double-Exchange Model

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

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

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

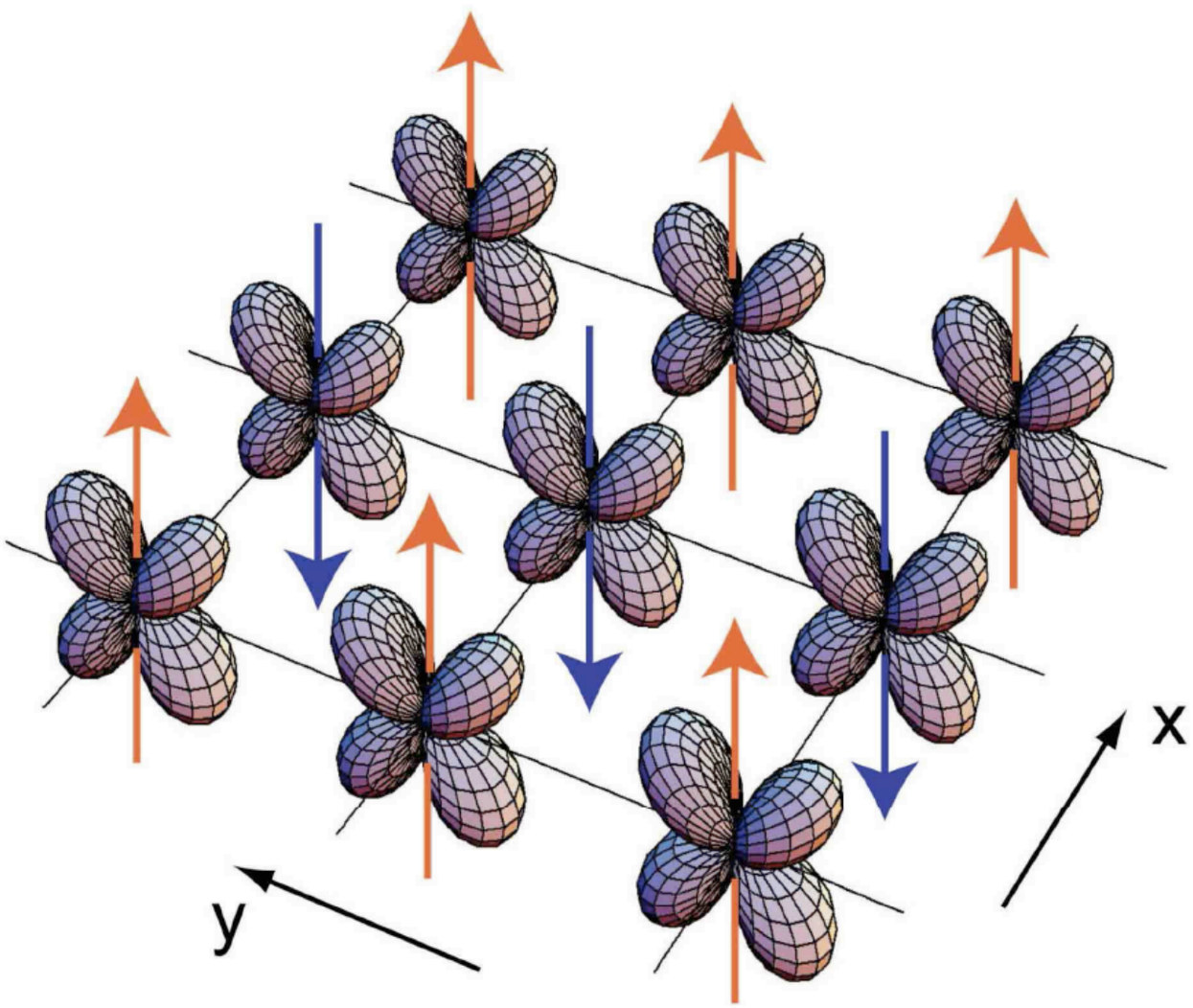
unlike manganites

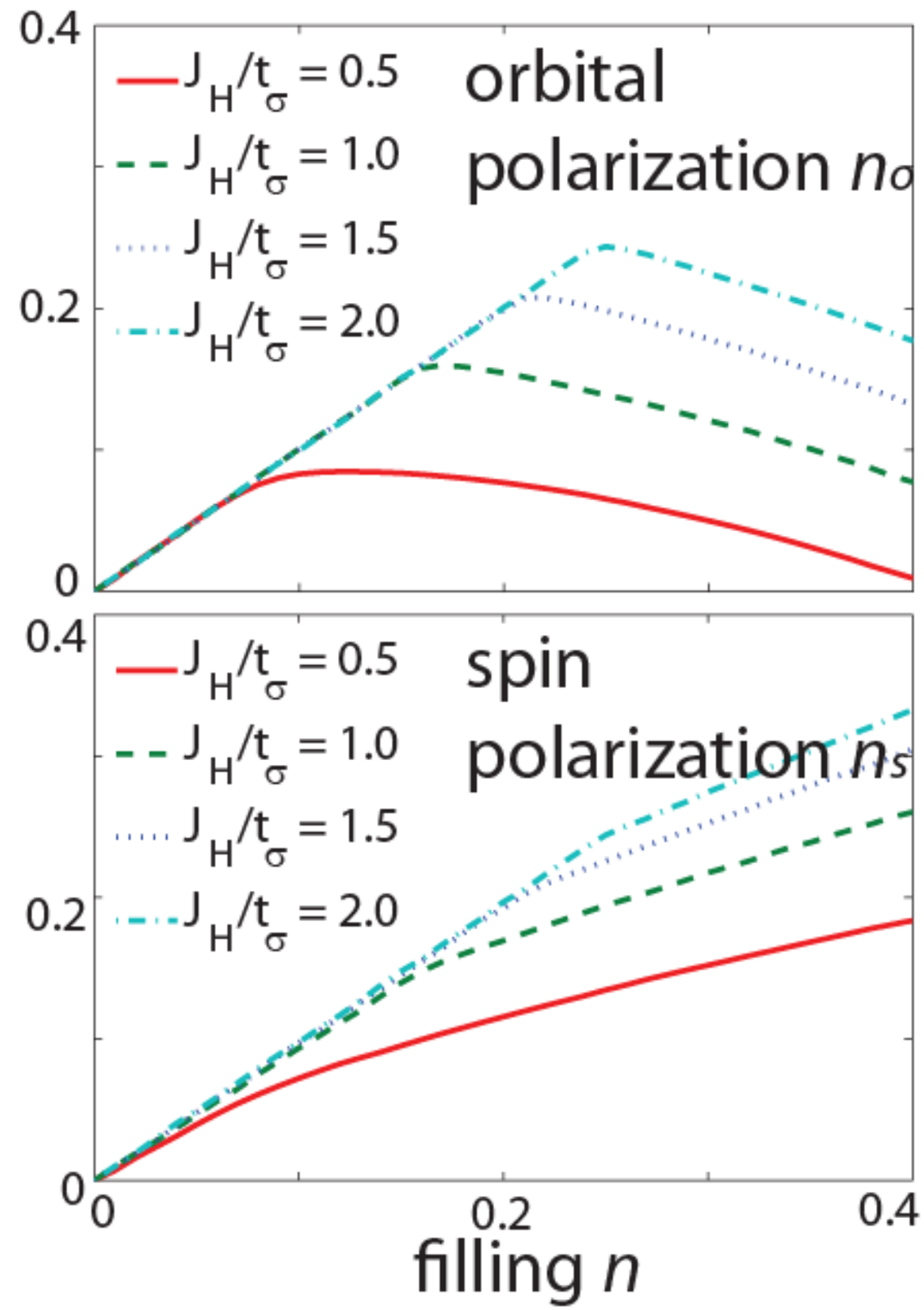
$$\nu J_H \ll \infty$$

- *Orbital ordering*

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

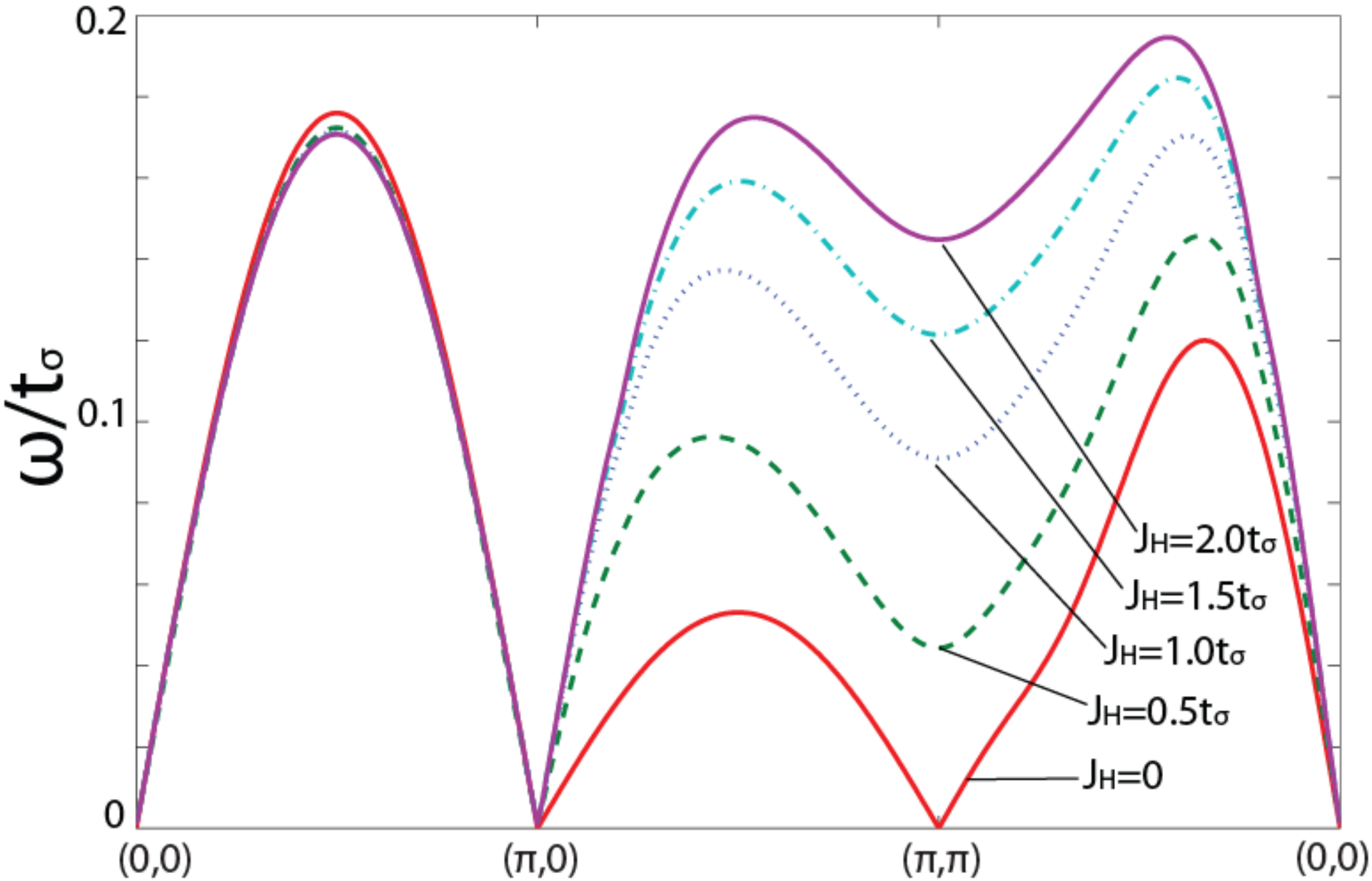
$$n_s = \sum_\alpha (\rho_{\alpha,\uparrow} - \rho_{\alpha,\downarrow})$$



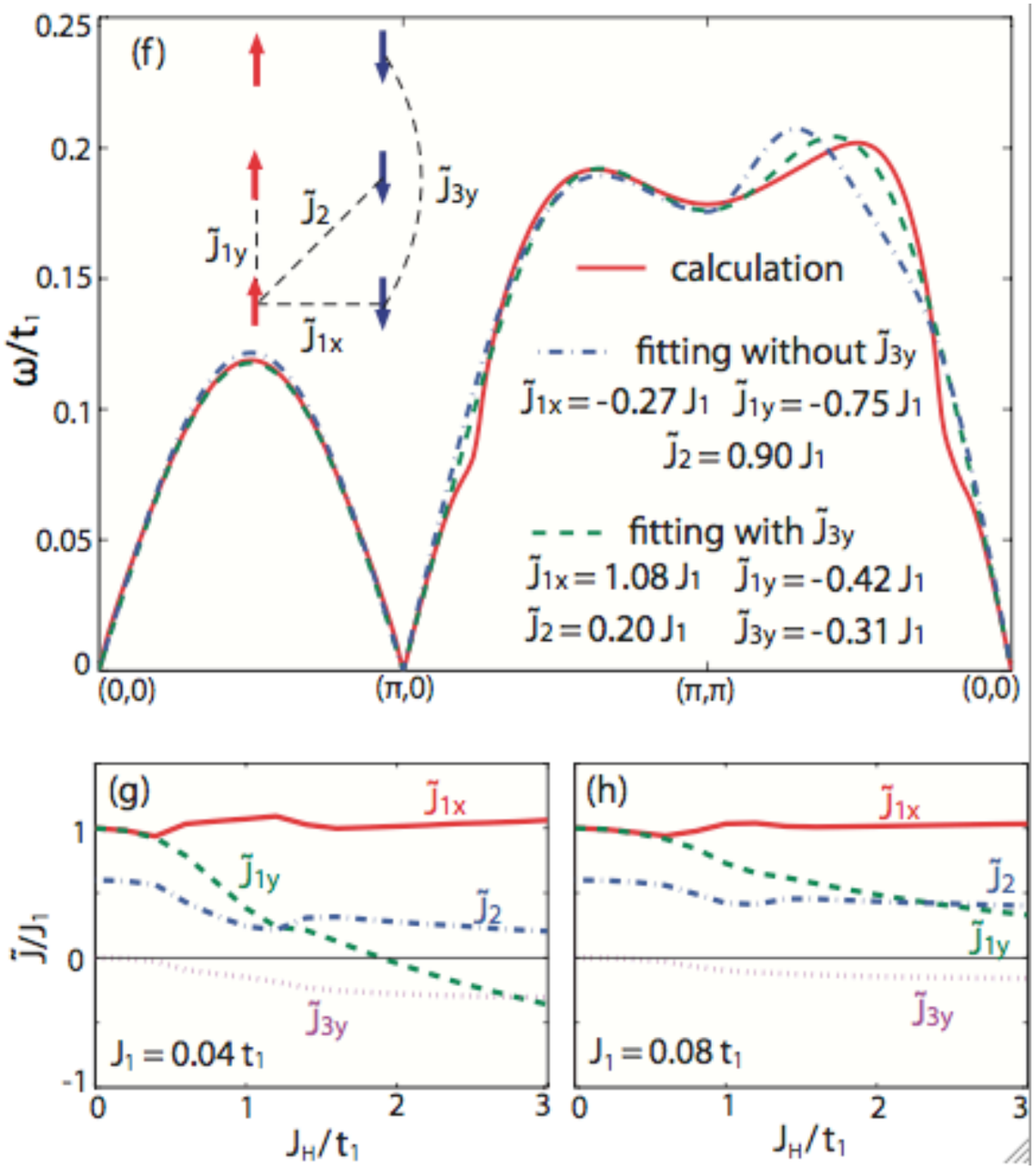


$$t_\pi = 0.1 t_\sigma$$

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



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



- *Comparison with experiments*:

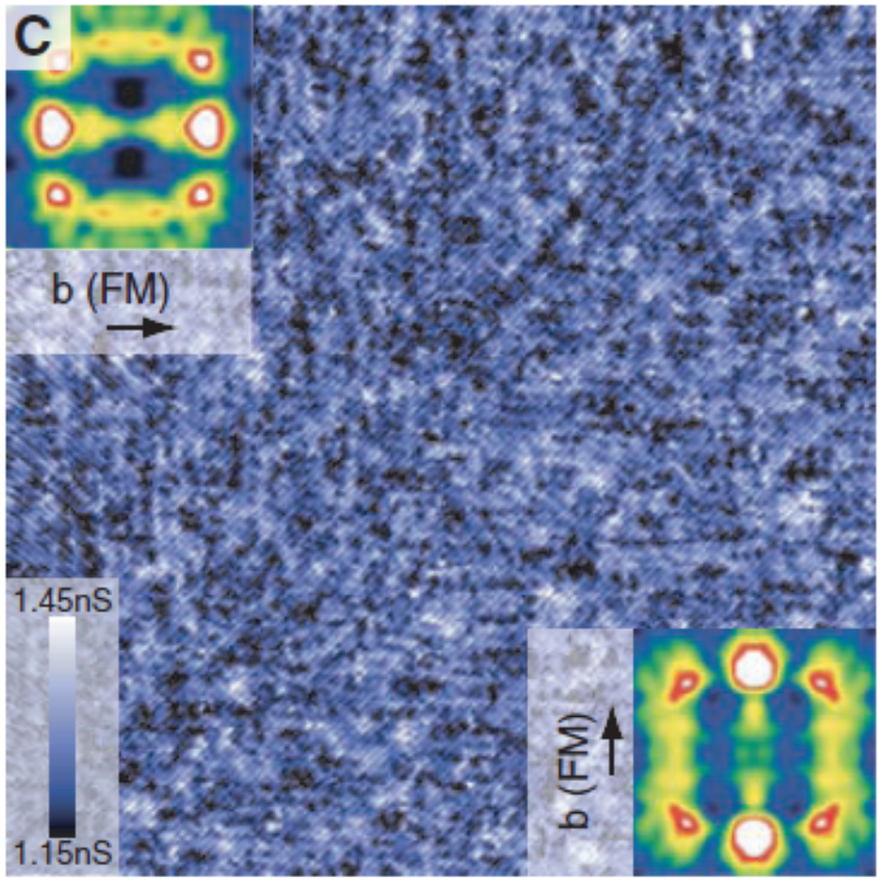
$$J_{\mathrm{H}} \sim t_\sigma \sim 1\,\mathrm{eV} \quad \tilde{J} \sim 0.01\, t_\sigma \sim 10\,\mathrm{meV}$$

emergent ferro-orbital order

OO-induced anisotropies

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

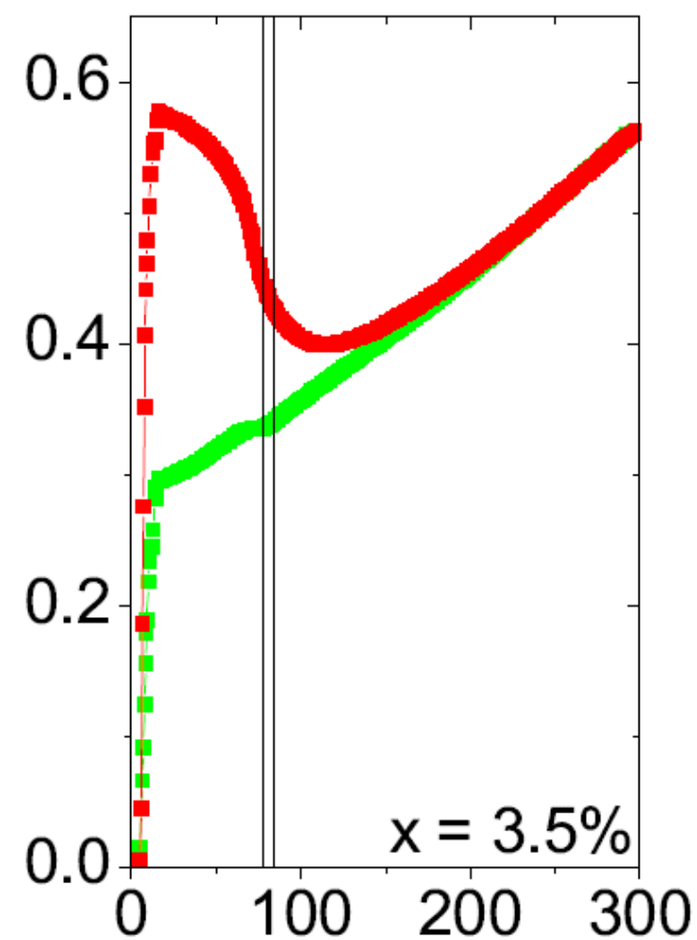
FM easy axis!



AF is easy axis!

- *Resistivity*

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



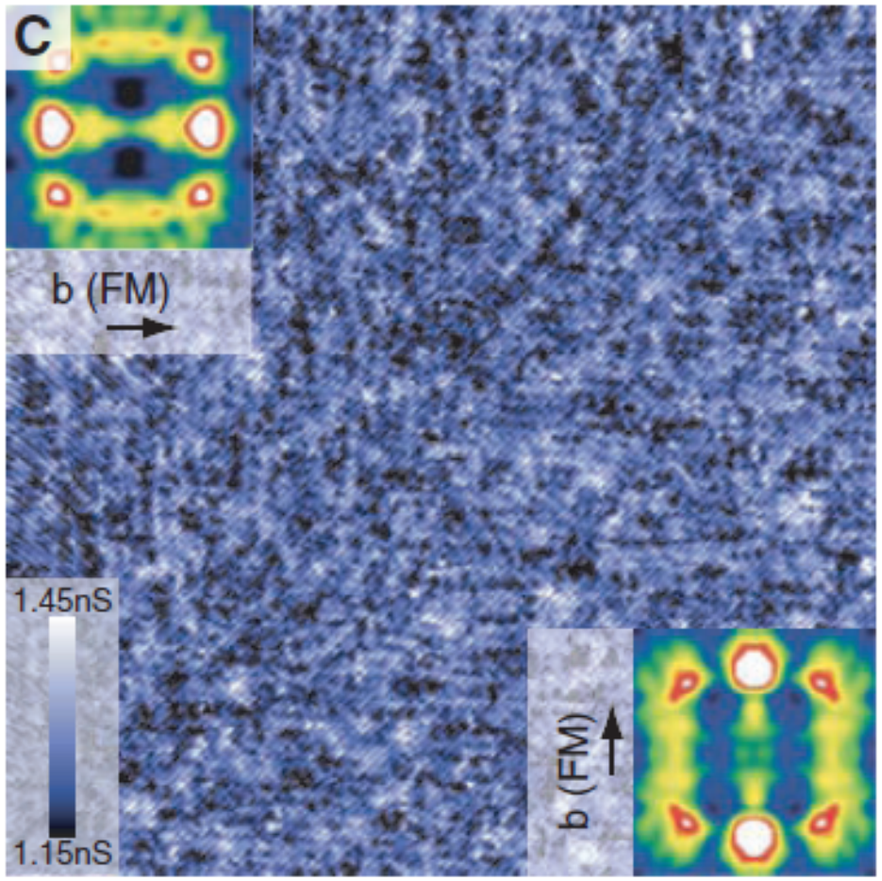
OO-induced anisotropies

AF is easy axis!

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

- *STM*

FM easy axis!



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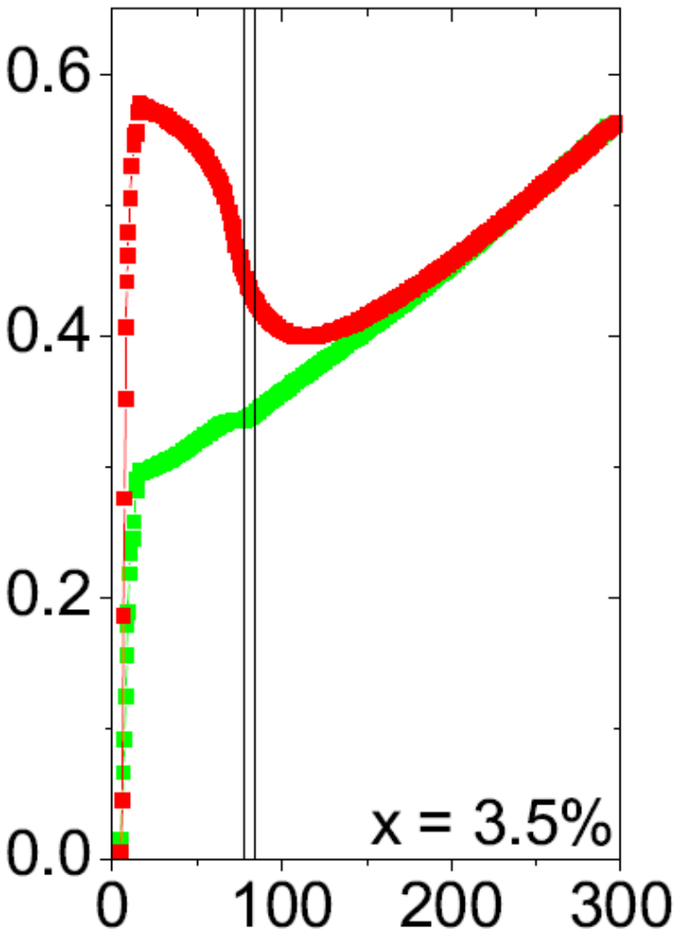

Are the pnictides important?

pnictides d^6
bad metals
multi-orbital
low-moment
moderate
T_c

Cuprates d^9
(one-unpaired electron),
single-orbital
Mott-system,
low-moment,
high T_c

pnictides d^6
bad metals
multi-orbital
low-moment
moderate
T_c

Cuprates d^9
(one-unpaired electron),
single-orbital
Mott-system,
low-moment,
high T_c

pnictides d^6
bad metals
multi-orbital
low-moment
moderate
T_c

Cuprates d^9
(one-unpaired electron),
single-orbital
Mott-system,
low-moment,
high T_c

manganites
multi-orbital
high-moment
no T_c

pnictides d^6
bad metals
multi-orbital
low-moment
moderate
T_c

Cuprates d^9
(one-unpaired electron),
single-orbital
Mott-system,
low-moment,
high T_c

pnictides d^6
bad metals
multi-orbital
low-moment
moderate
T_c

Cuprates d^9
(one-unpaired electron),
single-orbital Mott-system,
low-moment,
high T_c

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

pnictides d^6
bad metals
multi-orbital
low-moment
moderate T_c

Does multi-orbital physics (>1 e/unit cell) increase T_c?

Cuprates d^9
(one-unpaired electron),
single-orbital Mott-system,
low-moment,
high T_c

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

pnictides d^6
bad metals
multi-orbital
low-moment
moderate T_c

Possible systems (multi-orbital Mott systems) ?

Simple

$NiO_{1-x}F_x$

hole-doping a d^8 system.
Does it superconduct?

complex (oxychalchogenides

$A_2O_3Fe_2M_2$

A= La, Y
M=Se, S, Te

Co and Cu- based

$La_2Co_2Se_2O_3$

$Na_2OCu_4OSe_2$

J|A|C|S ARTICLES

Published on Web 04/28/2010

$La_2Co_2Se_2O_3$: A Quasi-Two-Dimensional Mott Insulator with Unusual Cobalt Spin State and Possible Orbital Ordering

Cao Wang,† Ming-qiu Tan,† Chun-mu Feng,‡ Zhi-feng Ma,† Shuai Jiang,† Zhu-an Xu,†,§ Guang-han Cao,*,†,§ Kazuyuki Matsubayashi,|| and Yoshiya Uwatoko||

Department of Physics, Test and Analysis Center, and State Key Lab of Silicon Materials, Zhejiang University, Hangzhou 310027, People's Republic of China, and Institute for Solid State Physics, The University of Tokyo, Kashiwanoha, Kashiwa, Chiba 277-8581, Japan

Received January 7, 2010; E-mail: ghcao@zju.edu.cn

Abstract: The new oxyselenide $La_2Co_2Se_2O_3$, containing Co_2O square-planar layers, has been successfully synthesized using solid-state reactions under vacuum. The compound crystallizes in space group *I*4/*mmm* with lattice parameters $a = 4.0697(8)$ Å and $c = 18.419(4)$ Å. Magnetic susceptibility measurements indicate an antiferromagnetic transition at ~220 K. The magnetic entropy associated with the transition is close to $R\ln 2$, suggesting an unusual low-spin state for the Co^{2+} ions. The as-prepared sample shows insulating behavior with room-temperature resistivity of $\sim 10^7$ Ω cm, which decreases by 4 orders of magnitude under a pressure of 7 GPa. Band structure calculations using the LSDA+*U* approach reproduce the insulating ground state with low spin for Co and suggest strong orbital polarization for the valence electrons near the Fermi level. It is also revealed that the spin and orbital degrees of freedom in the antiferromagnetic checkerboard spin−lattice are mutually coupled.

PHYSICAL REVIEW B **82**, 020410(R) (2010)

Electronic structure, spin state, and magnetism of the square-lattice Mott insulator $La_2Co_2Se_2O_3$ from first principles

Hua Wu

II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

(Received 2 June 2010; revised manuscript received 7 July 2010; published 30 July 2010)

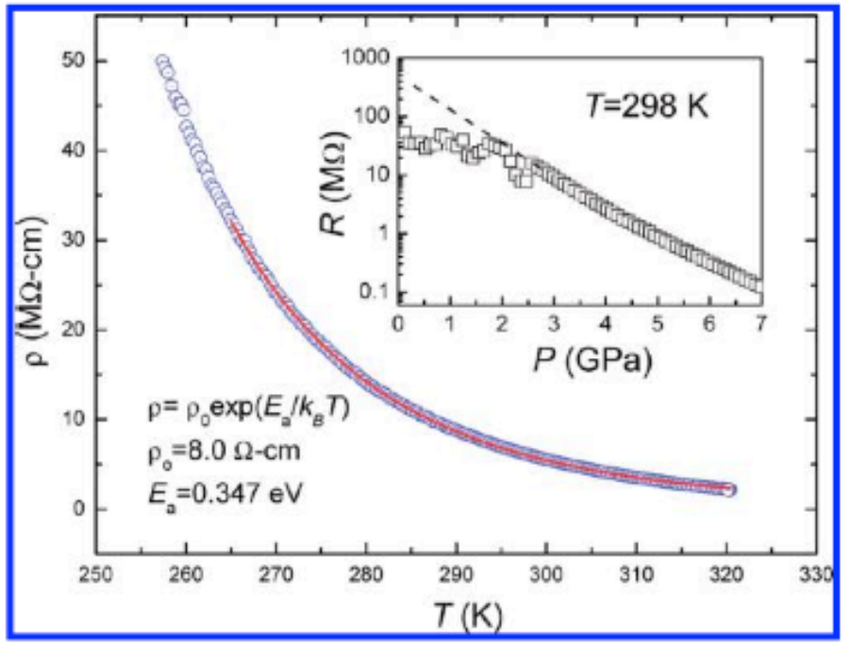

Figure 2. Temperature dependence of resistivity for the $La_2Co_2Se_2O_3$ polycrystalline sample. The inset shows the pressure dependence of resistance at room temperature. Note that the resistance at ambient pressure is too high to be measured accurately.

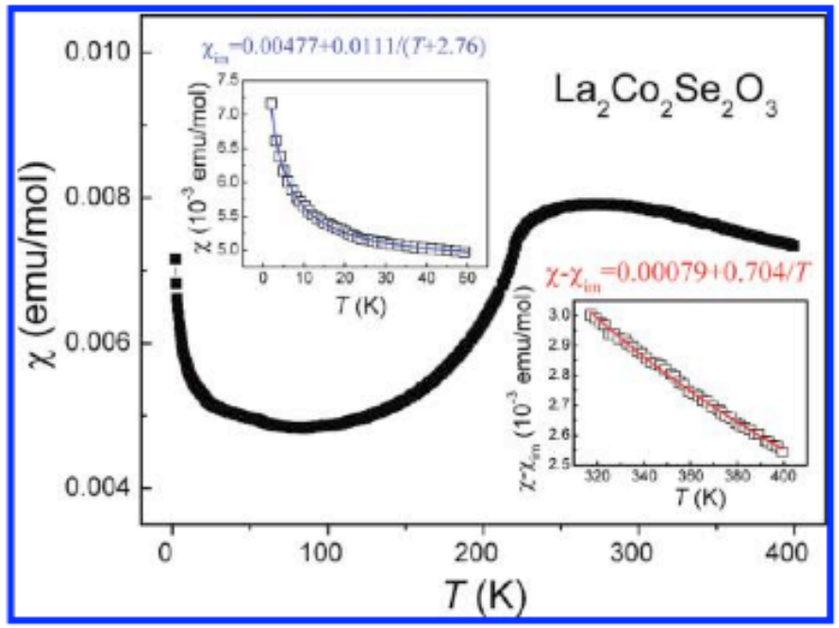

Figure 3. Temperature dependence of the magnetic susceptibility for $La_2Co_2Se_2O_3$. The applied field is 1000 Oe. The data fittings in the insets are based on Curie−Weiss law.

PHYSICAL REVIEW B **81**, 214433 (2010)

Low-temperature nuclear and magnetic structures of $La_2O_2Fe_2OSe_2$ from x-ray and neutron diffraction measurements

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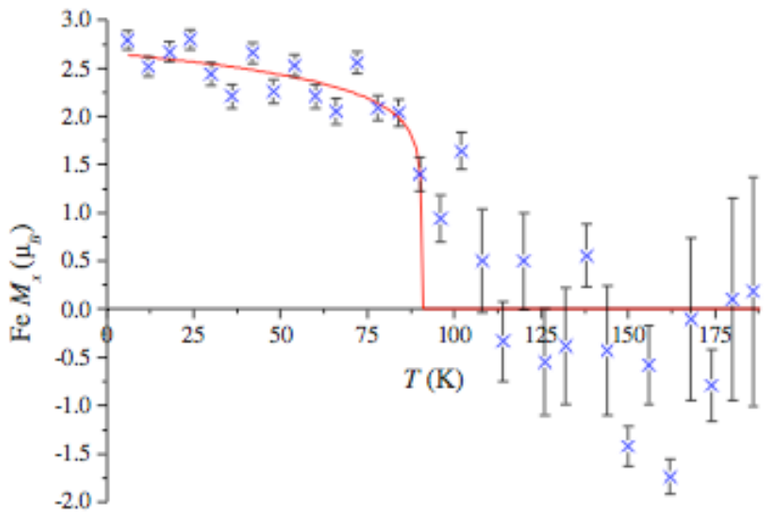
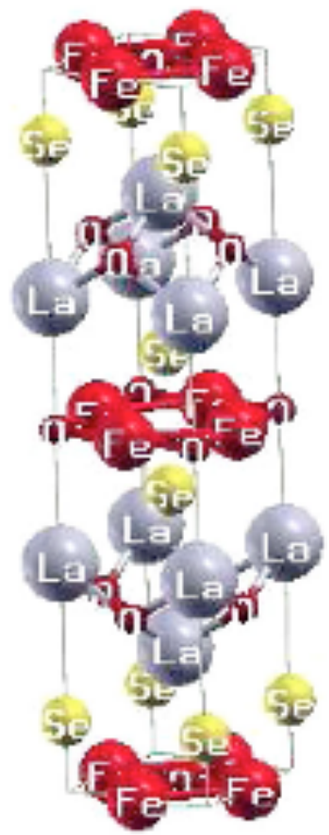
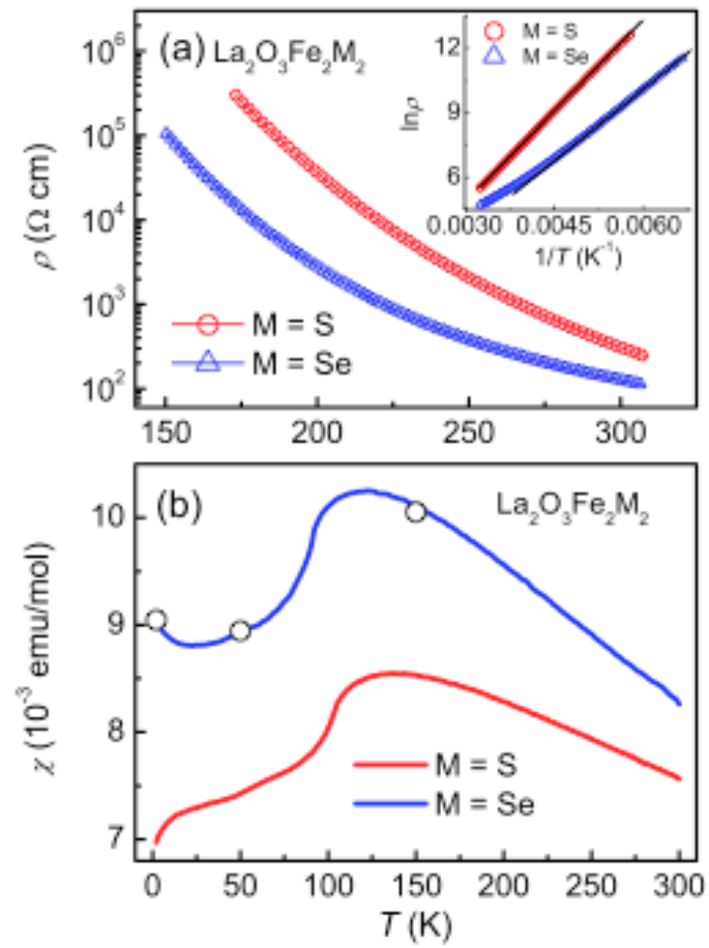
Band Narrowing and Mott Localization in Iron Oxychalcogenides $La_2O_2Fe_2O(Se, S)_2$

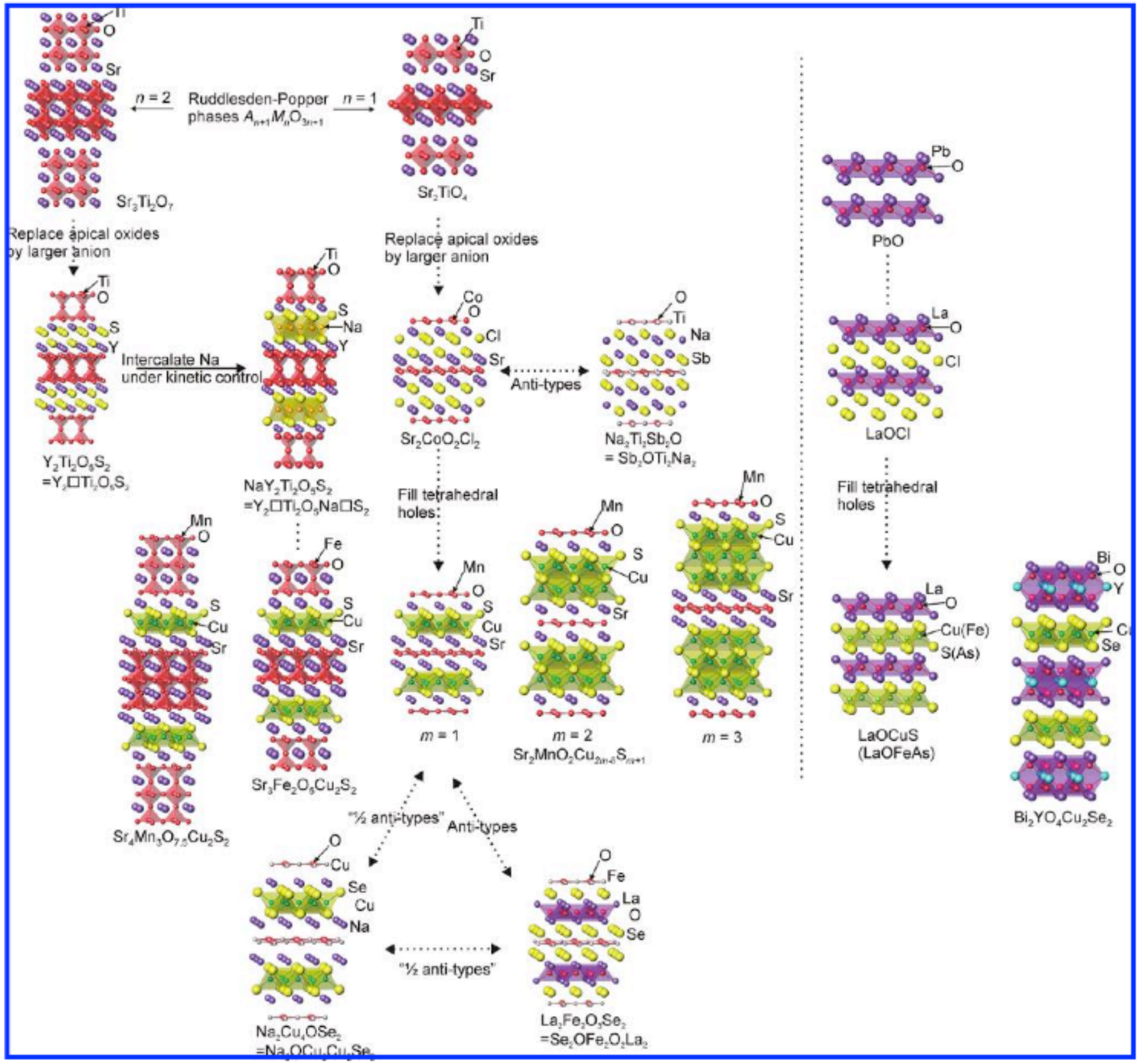
Jian-Xin Zhu,[1] Rong Yu,[2] Hangdong Wang,[3] Liang L. Zhao,[2] M. D. Jones,[4] Jianhui Dai,[3] Elihu Abrahams,[5,*] E. Morosan,[2] Minghu Fang,[3] and Qimiao Si[2]

b)








Ti
O
Sr
n = 2
Ruddlesden-Popper phases $A_{n+1}M_nO_{3n+1}$
n = 1
$Sr_3Ti_2O_7$
Sr_2TiO_4
Replace apical oxides by larger anion
Replace apical oxides by larger anion
S
Y
Na
Intercalate Na under kinetic control
$Y_2Ti_2O_5S_2$
$=Y_2\square Ti_2O_5S_2$
$NaY_2Ti_2O_5S_2$
$=Y_2\square Ti_2O_5Na\square S_2$
Co
Cl
$Sr_2CoO_2Cl_2$
Anti-types
Na
Sb
$Na_2Ti_2Sb_2O$
$= Sb_2OTi_2Na_2$
Pb
PbO
La
LaOCl
Fill tetrahedral holes
Fill tetrahedral holes
Mn
Cu
$Sr_4Mn_3O_{7.5}Cu_2S_2$
Fe
$Sr_3Fe_2O_5Cu_2S_2$
m = 1
m = 2
$Sr_2MnO_2Cu_{2n-\delta}S_{n+1}$
m = 3
Cu(Fe)
S(As)
LaOCuS
(LaOFeAs)
Bi
Y
Se
$Bi_2YO_4Cu_2Se_2$
"½ anti-types"
Anti-types
"½ anti-types"
$Na_2Cu_4OSe_2$
$=Na_2OCu_2Cu_2Se_2$
$La_2Fe_2O_3Se_2$
$=Se_2OFe_2O_2La_2$

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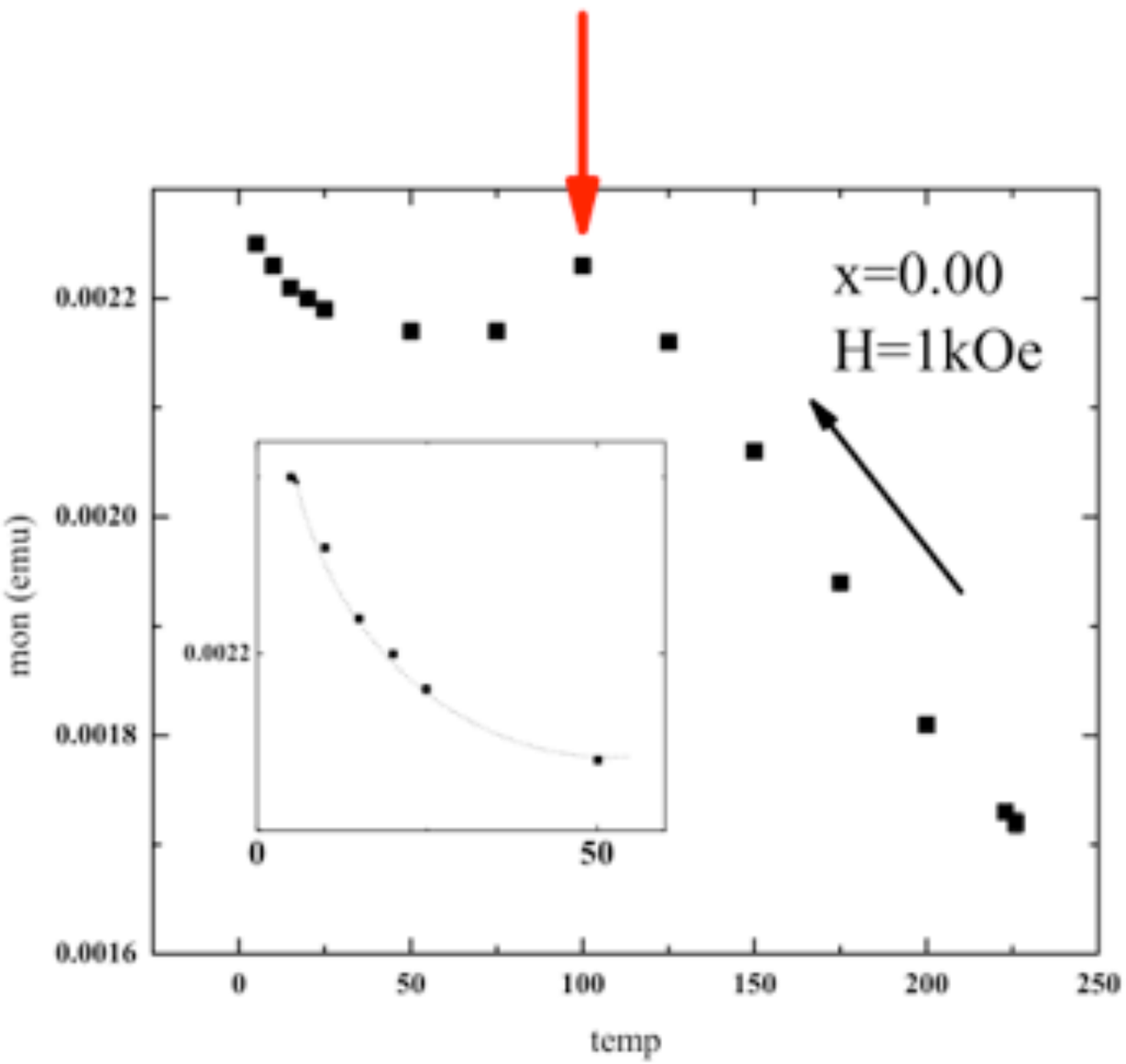
HMI, Berlin

T_N ~ 100K as reference



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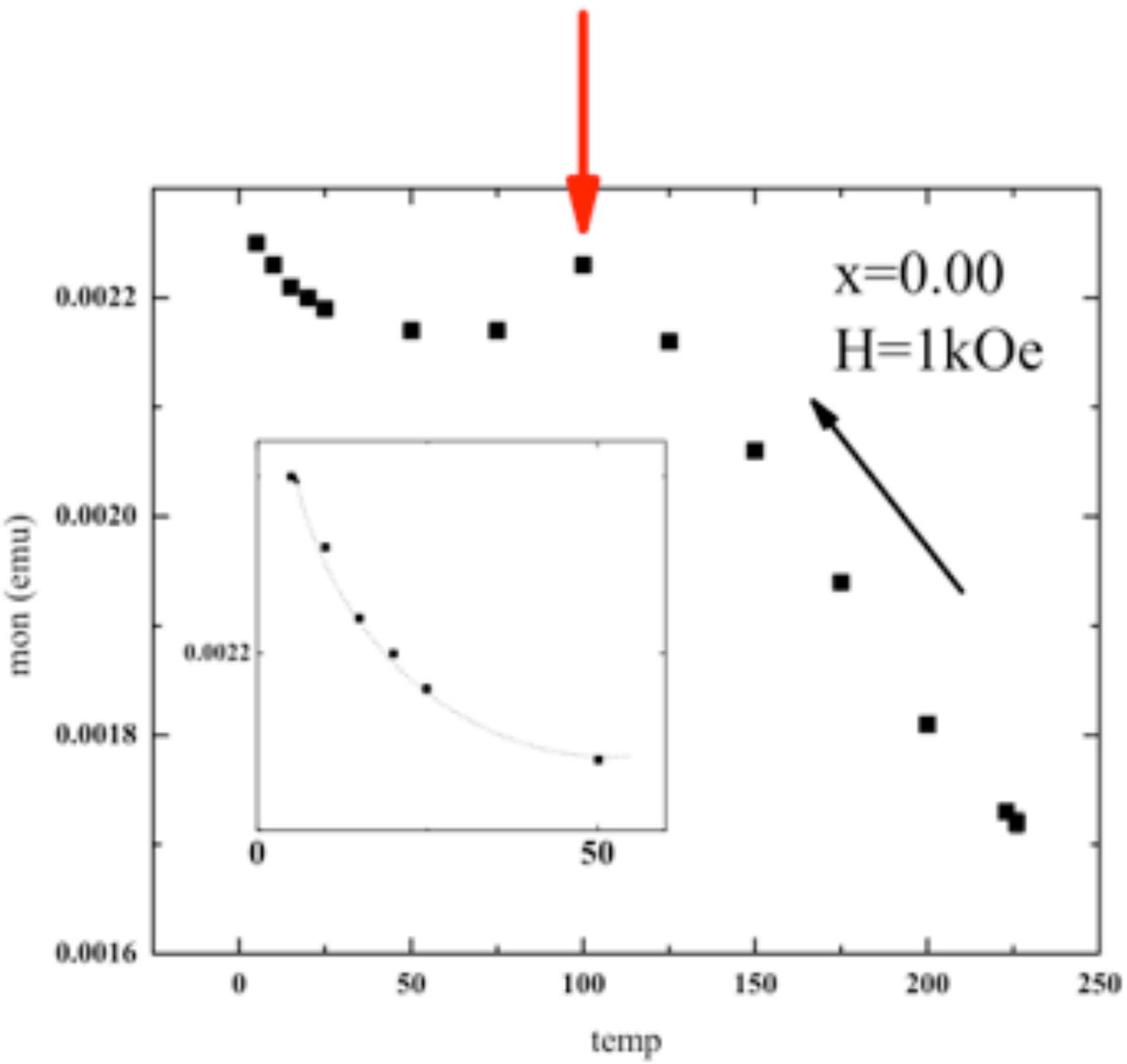
T_N ~ 100K as reference



what about the doped system?
superconductivity?

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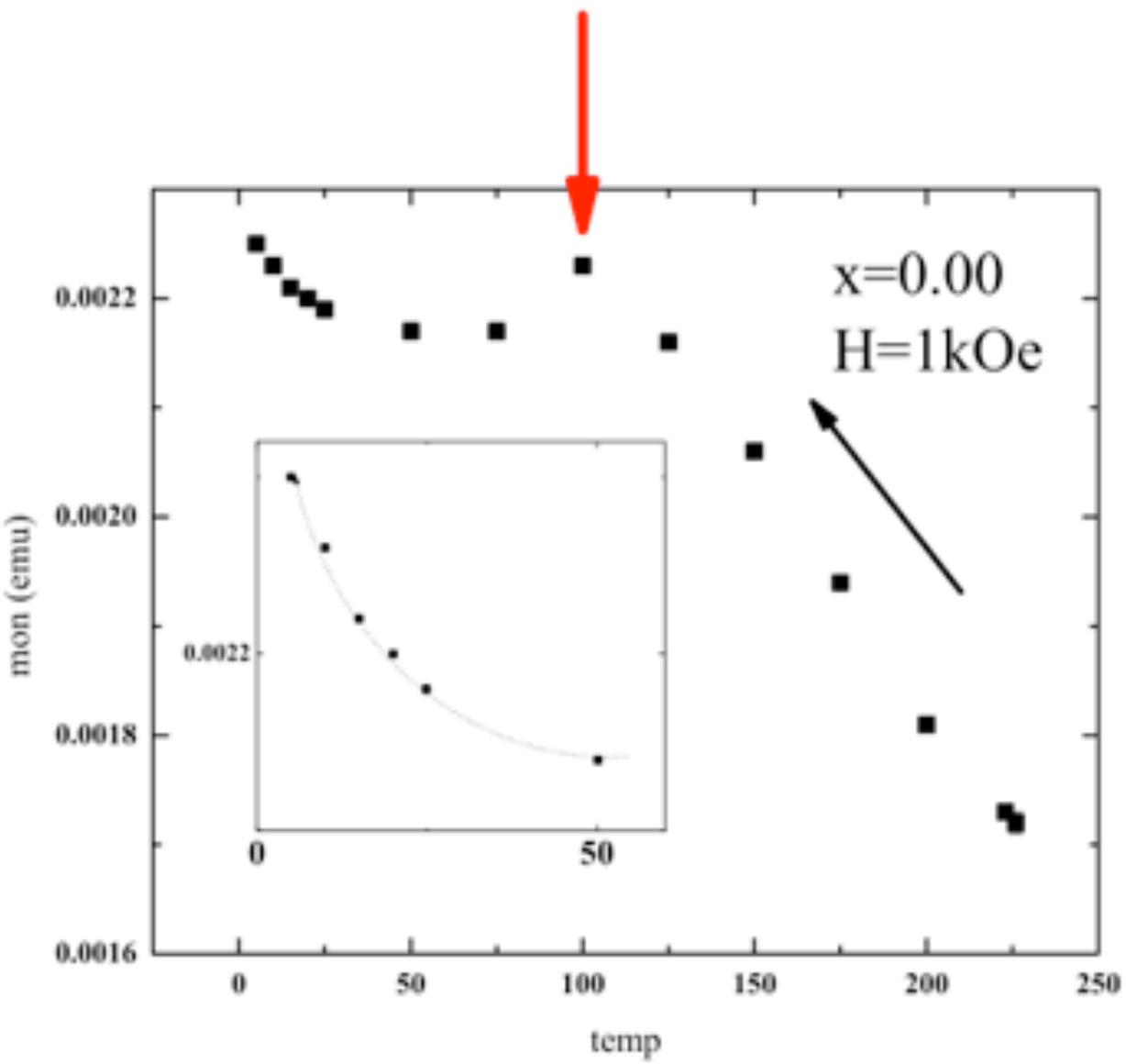
T_N ~ 100K as reference



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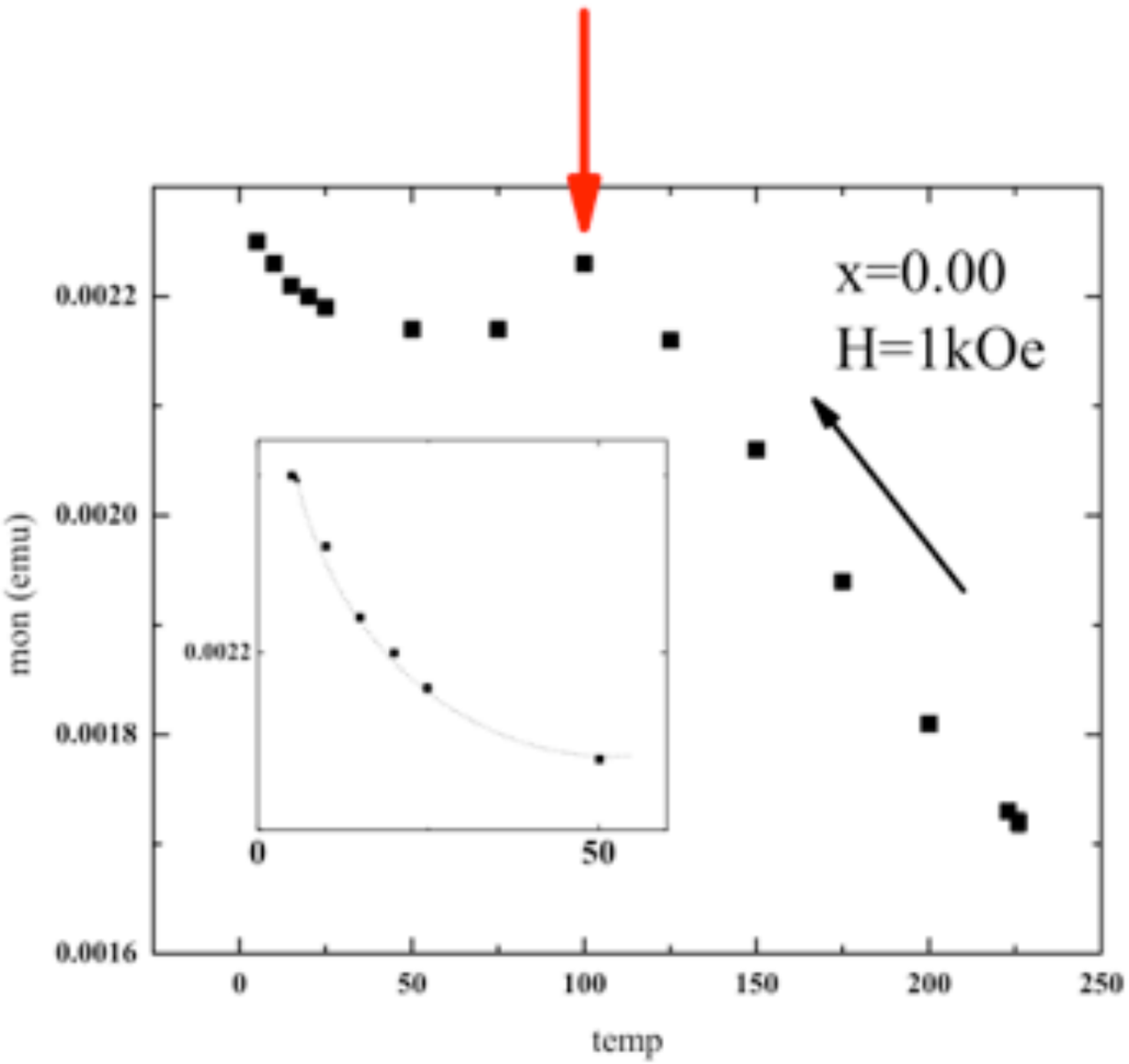

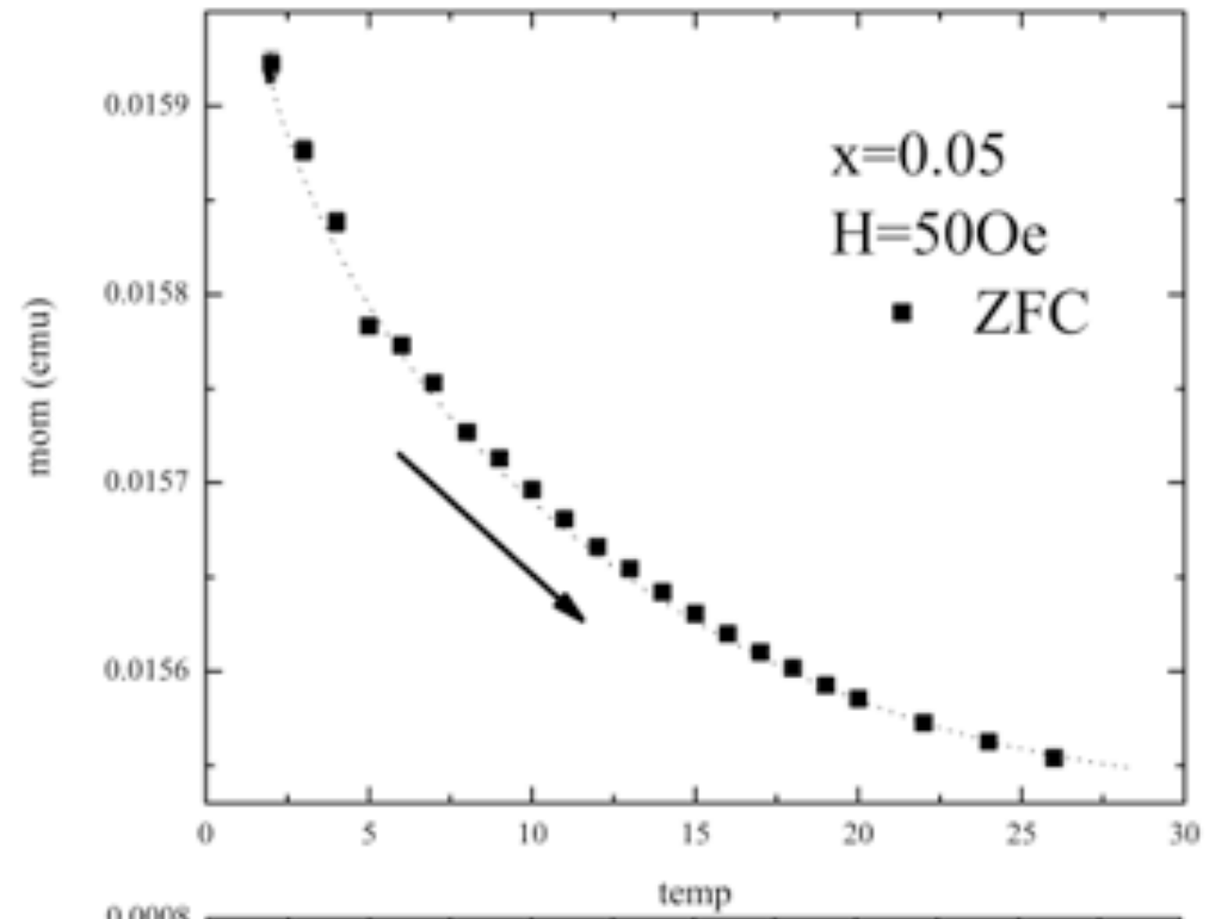

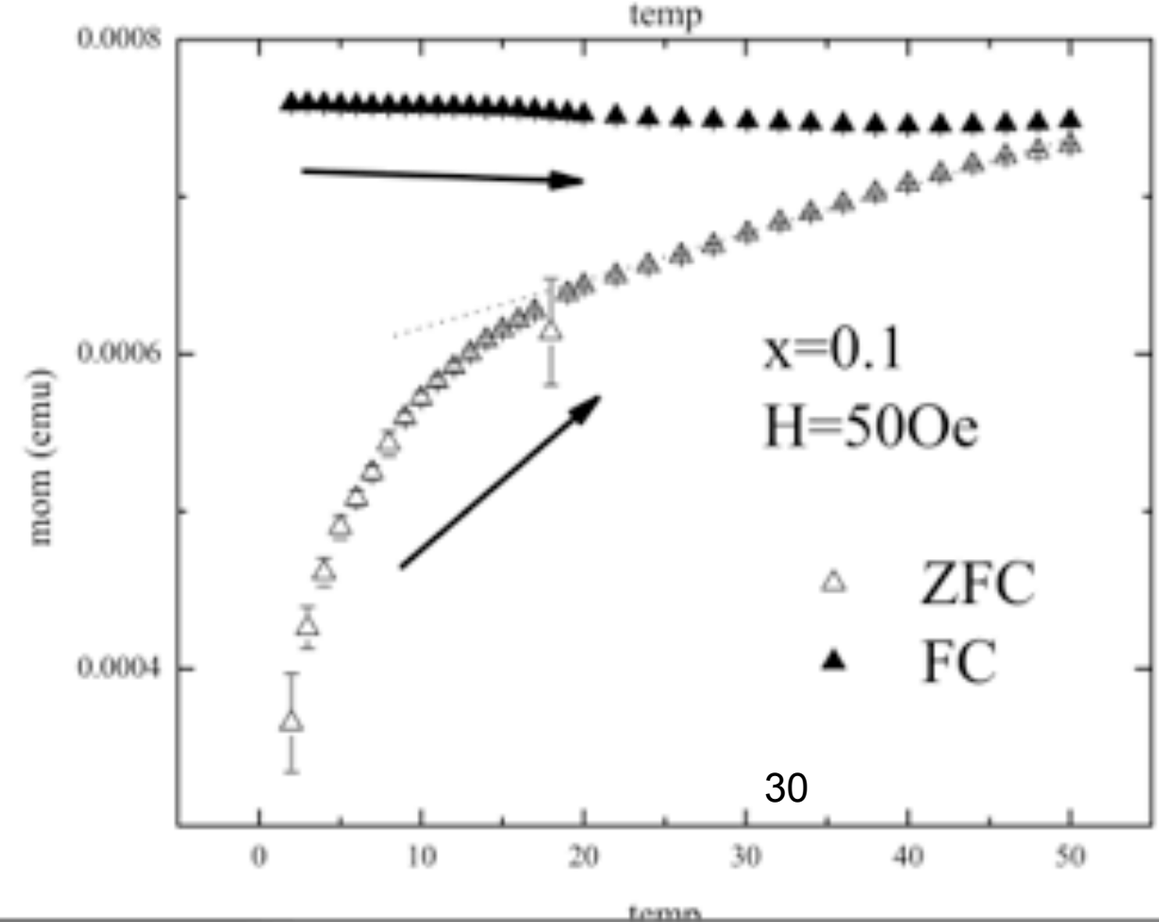

Do the doped oxychalcogenide superconduct? multi-orbital Mott systems?

Thanks to D. Argyriou, W-C Lee, F. Kruger, W-C. Lv, J. Wu

Superconductors come of age

A South Korean company has placed by far the biggest commercial order for superconducting wires.

Superconducting wires could soon help to light up Seoul.

iStockphoto.com / Min-Gyu Seong

American Superconductor have not disclosed the value of the deal. But Jason Fredette, managing director of corporate communications at the company, says that LS Cable will use the wire to make about 20 circuit kilometres of cable as part of a programme to modernize the South Korean electricity network starting in the capital, Seoul.