# Electronic Correlations and Multiorbital Effects in Iron Pnictides and Chalcogenides

**Rong Yu**

Renmin University of China

Sep. 24 , 2014

KITP Conference on Strong Correlations and Unconventional Superconductivity

# Collaborators

*Theory*

Emilian Nica (Rice)

Wenxin Ding (Rice)

Qimiao Si (Rice)

Jian-Xin Zhu (LANL)

*ARPES*

Ming Yi (Berkeley)

Donghui Lu (SLAC)

Zhi-Xun Shen (Stanford)

*Neutron Scattering*

Chenglin Zhang (Rice)

Pengcheng Dai (Rice)

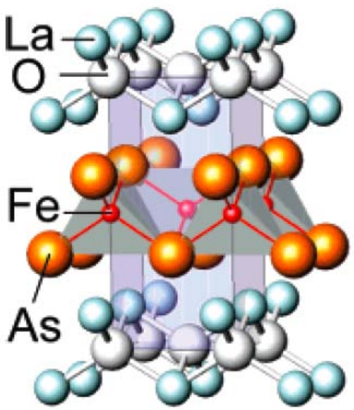
# Outline

- Introduction--electron correlations in iron-based superconductors
- Metal-insulator transition in multiorbital models for iron-based superconductors
  - Slave-spin formulation for multi-orbital models
  - Mott transitions in iron pnictides: phase diagram
  - Alkaline iron selenides: Mott  localization and orbital-selective Mott phase
- Pairing amplitudes: orbital selective pairing
- Summary

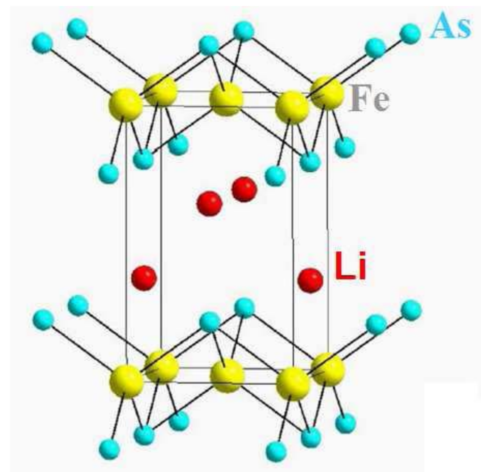
# Family of Iron Based Superconductors

<u>pnictides</u>:

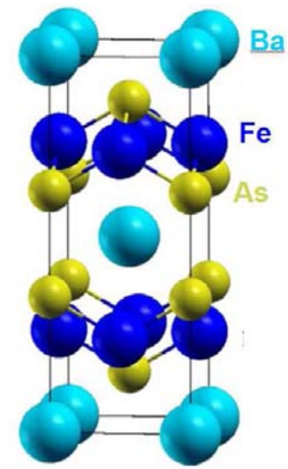
1111: LaOFeAs




111: LiFeAs

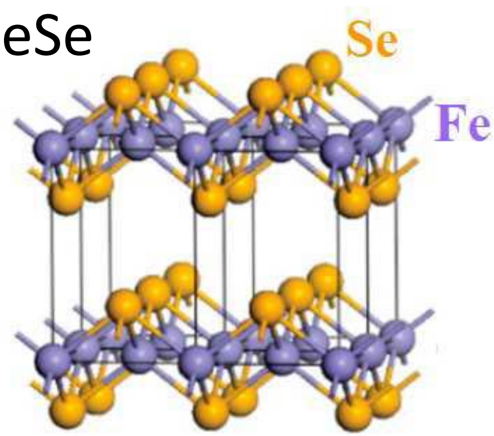



122: BaFe2As2

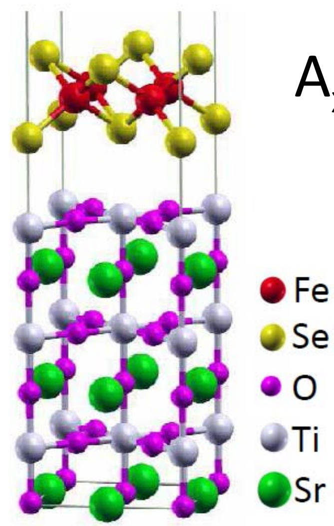



<u>chalcogenides</u>:

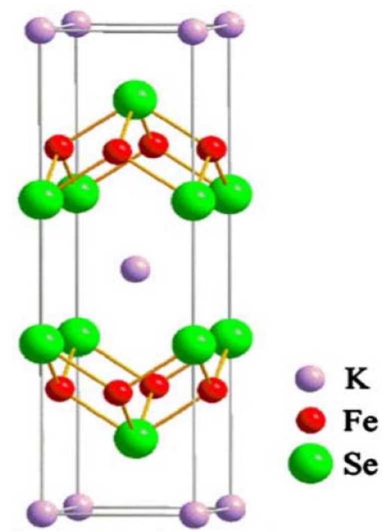
11: FeSe



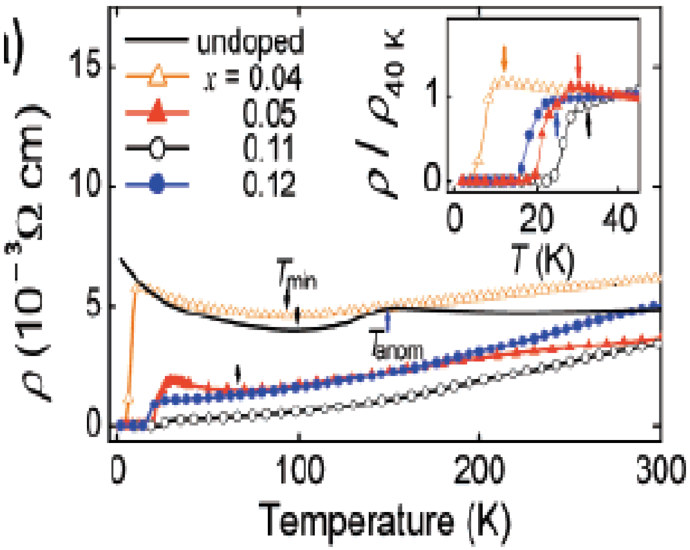

1-layer FeSe



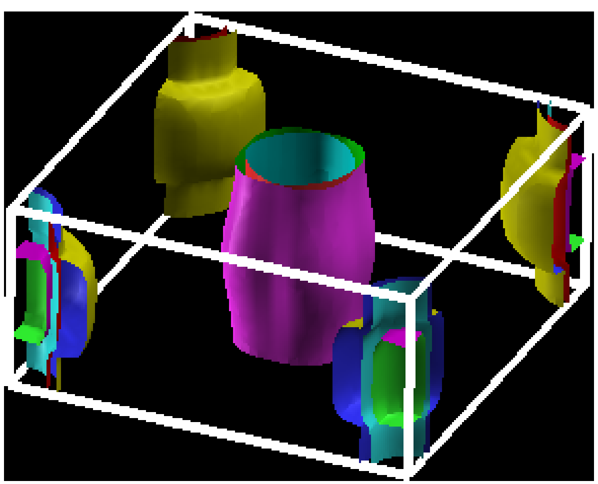

$A_xFe_{2-y}Se_2$



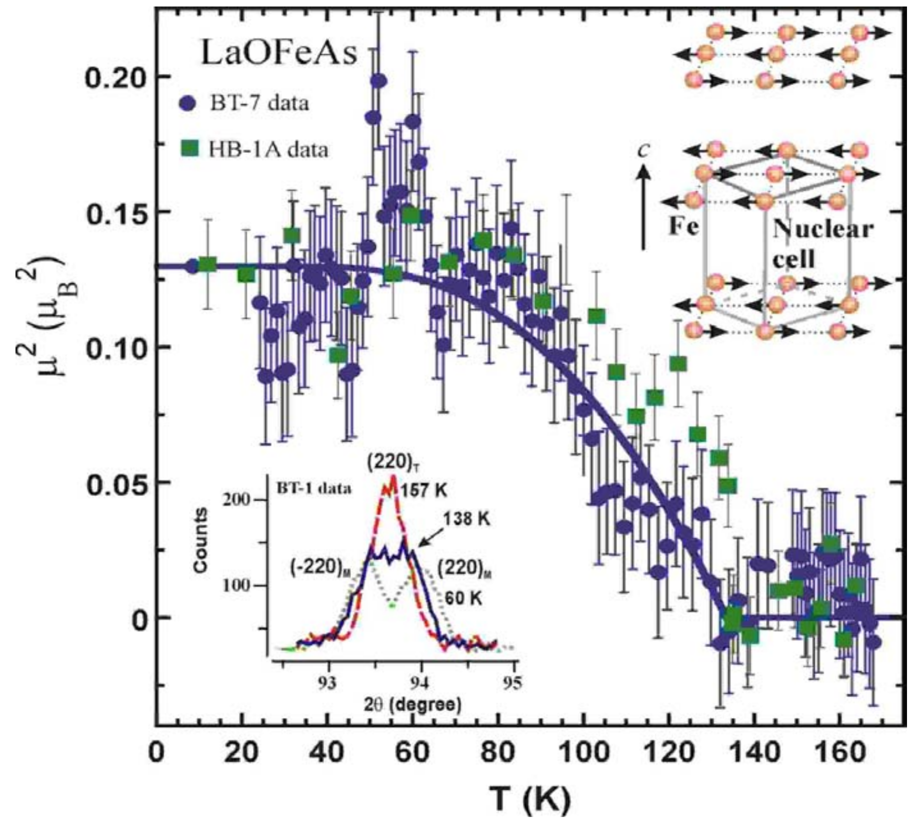
# Parent Pnictides: Electronic Properties




Kamihara et al, JACS **130**, 3296 (2008)



Singh & Du, PRL **100**, 237003 (2008)

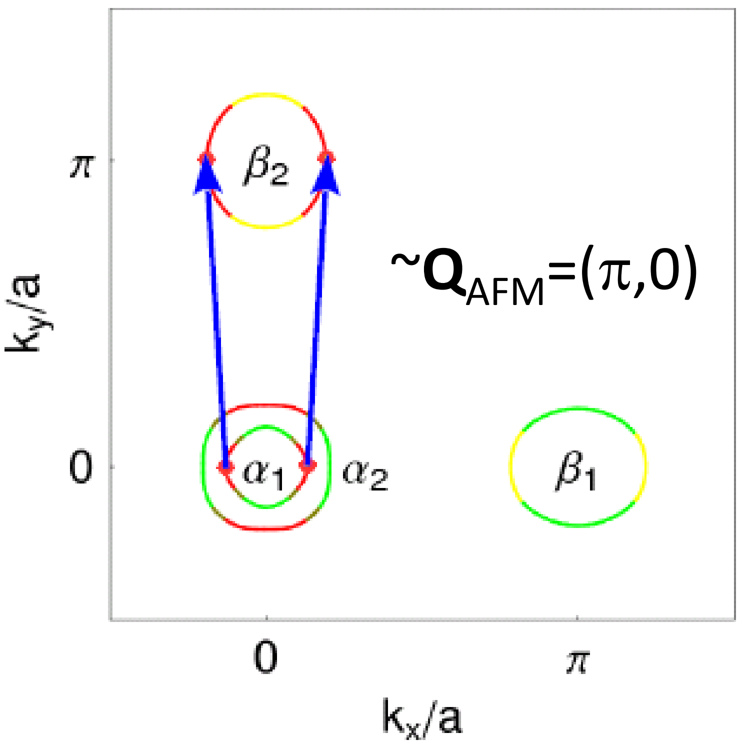



de la Cruz et al., Nature **453**, 899 (2008)

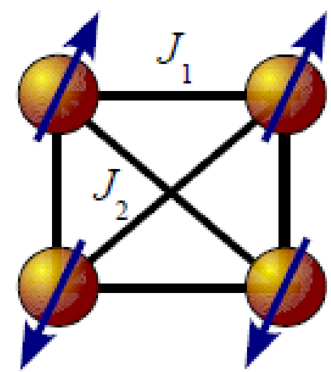
columinar $(\pi,0)$ antiferromagnetic metal with small electron & hole pockets

# Understanding the Magnetic Order in Iron Pnictides

weak coupling:
Fermi surface nesting




strong coupling:
Interacting local moments




$J_2>J_1/2$

# Evidence for Electron Correlations

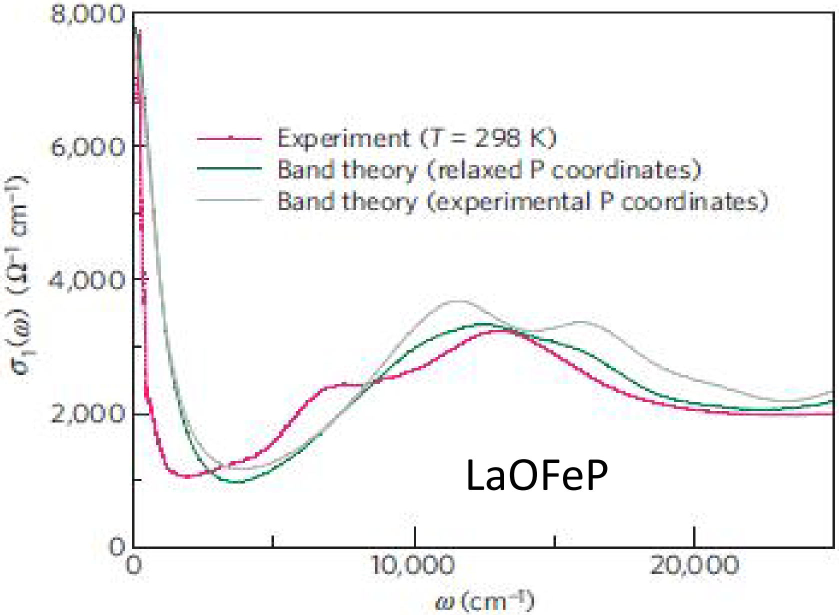
Bad metal behavior of the parent compound

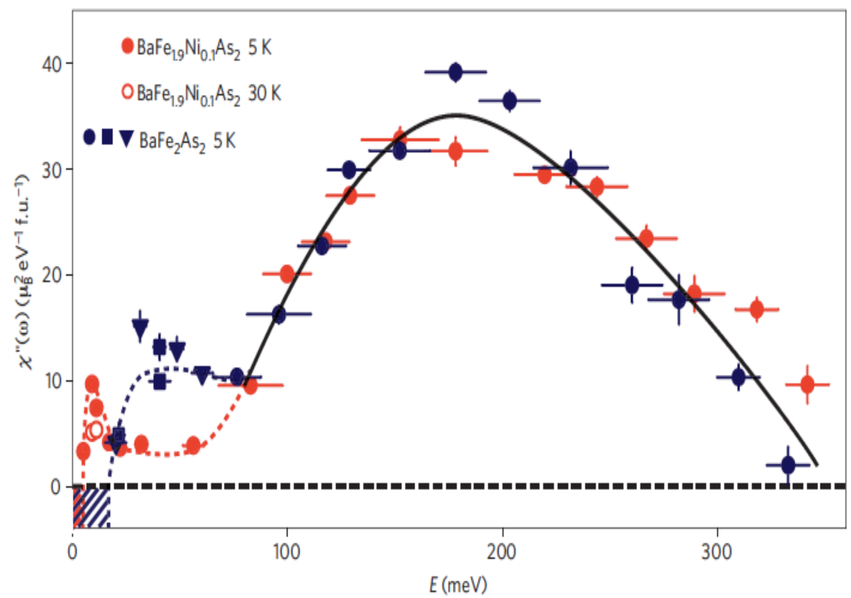
✓Transport: large room-T resistivity, reaches the Ioffe-Regel limit

✓Spectroscopy:

reduction of Drude weight

large overall spin spectral weight

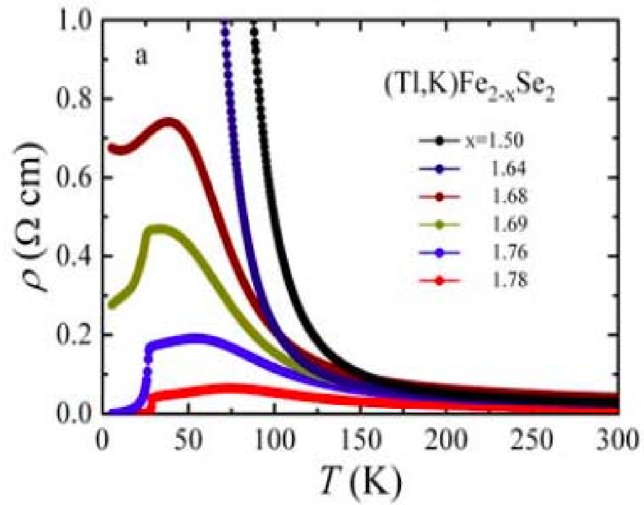


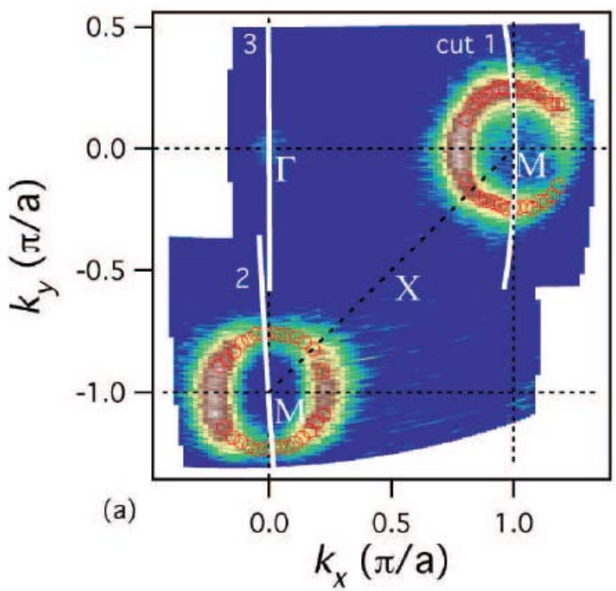

Qazilbash et al, Nat. Phys. **5**, 647 (2009)

Liu et al, Nat. Phys. **8**, 376 (2012)

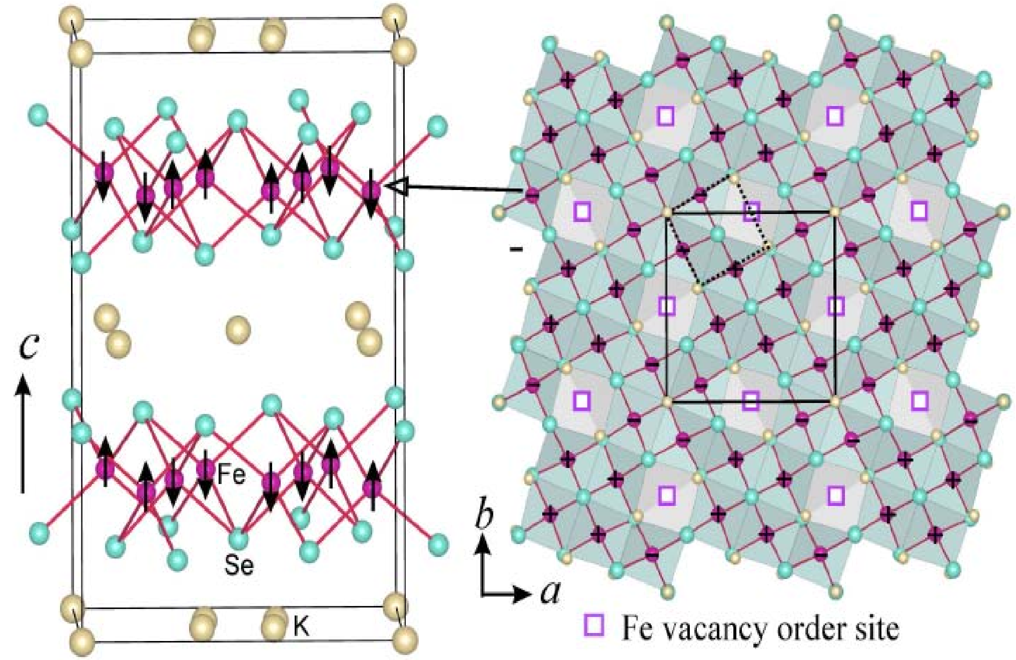
# Properties of Alkaline Iron Selenides




Fang et al, EPL **94**, 27009 (2011)



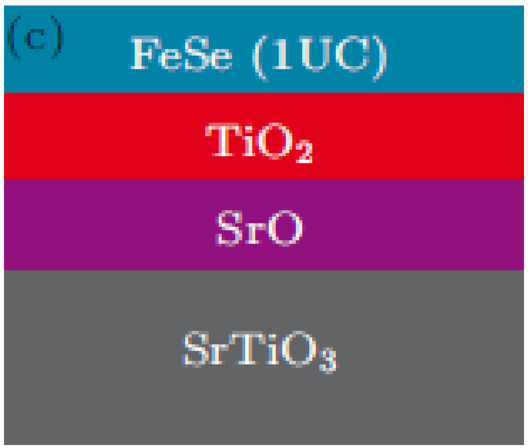

Qian et al., PRL **106**, 187001 (2011)

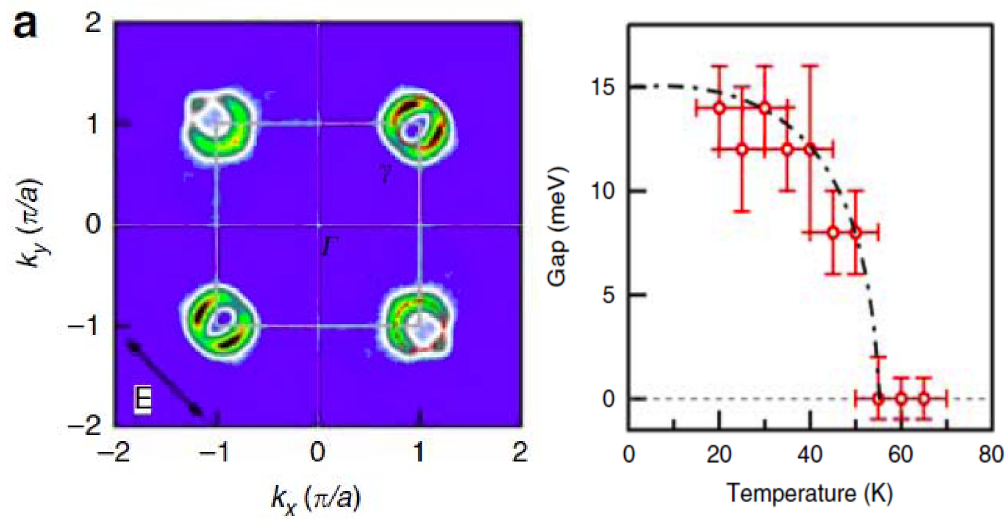



Bao et al., CPL **28**, 086104 (2011)

- Metallic/Insulating, depending on Fe content
- Fermi surface: electron pockets only
- Magnetic order influenced by ordered Fe vacancies

# Properties of Single-Layer FeSe/$SrTiO_3$



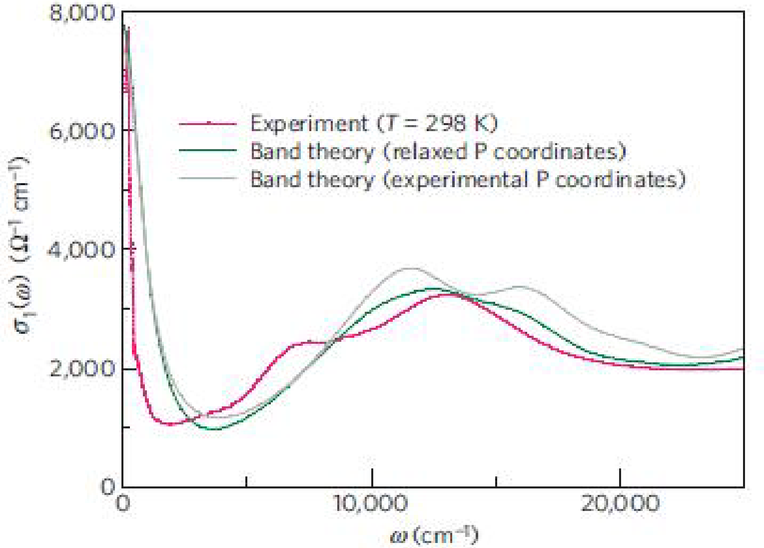




Liu et al., Nat. Comm. **3**, 931 (2012).

- ✓ Electron pockets only
- ✓ $T_c$>=60 K from ARPES, STM and transport measurements

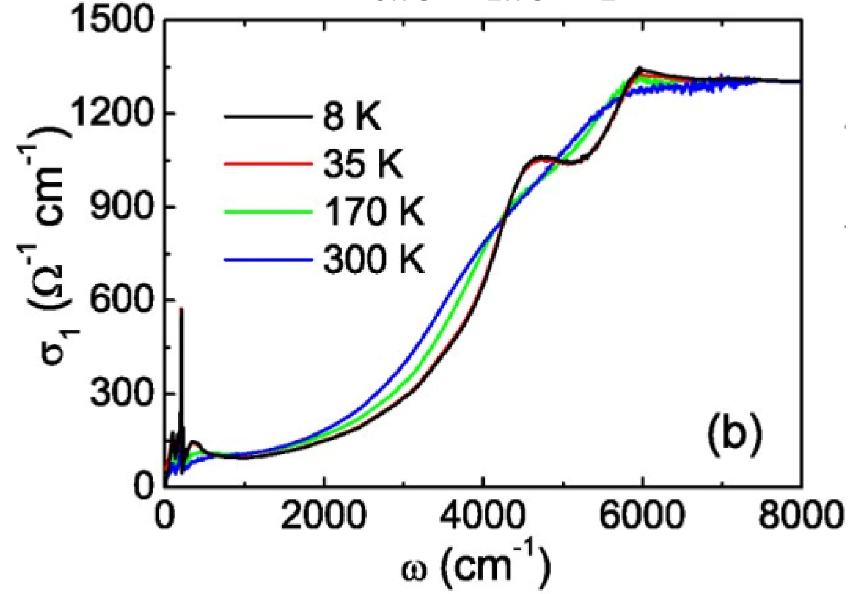
# Electron Correlations and Mott Localization

LaOFeP

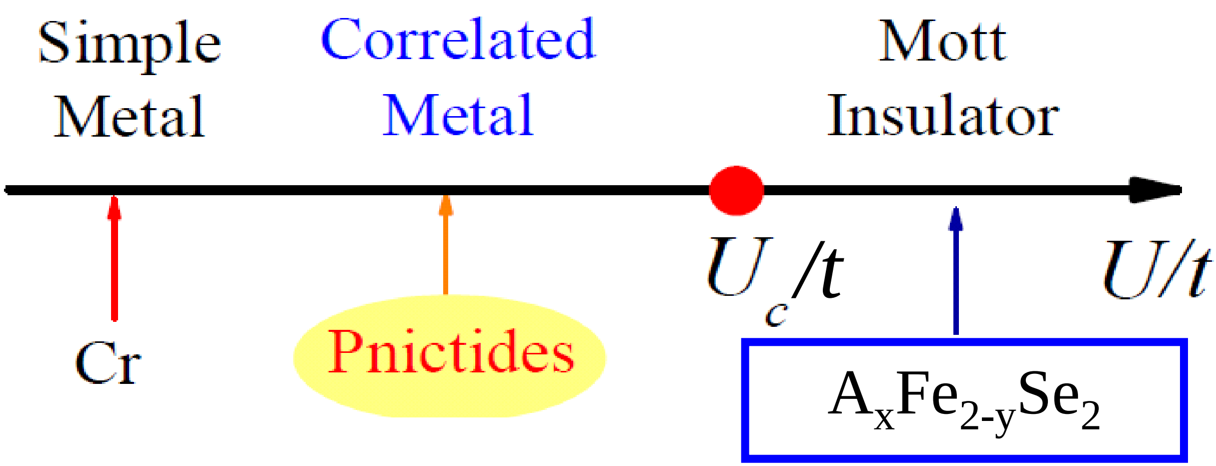



Qazilbash et al, Nat. Phys. **5**, 647 (2009)

$K_{0.75}Fe_{1.75}Se_2$




Yuan et al., Sci. Rep. **2**, 221 (2012).



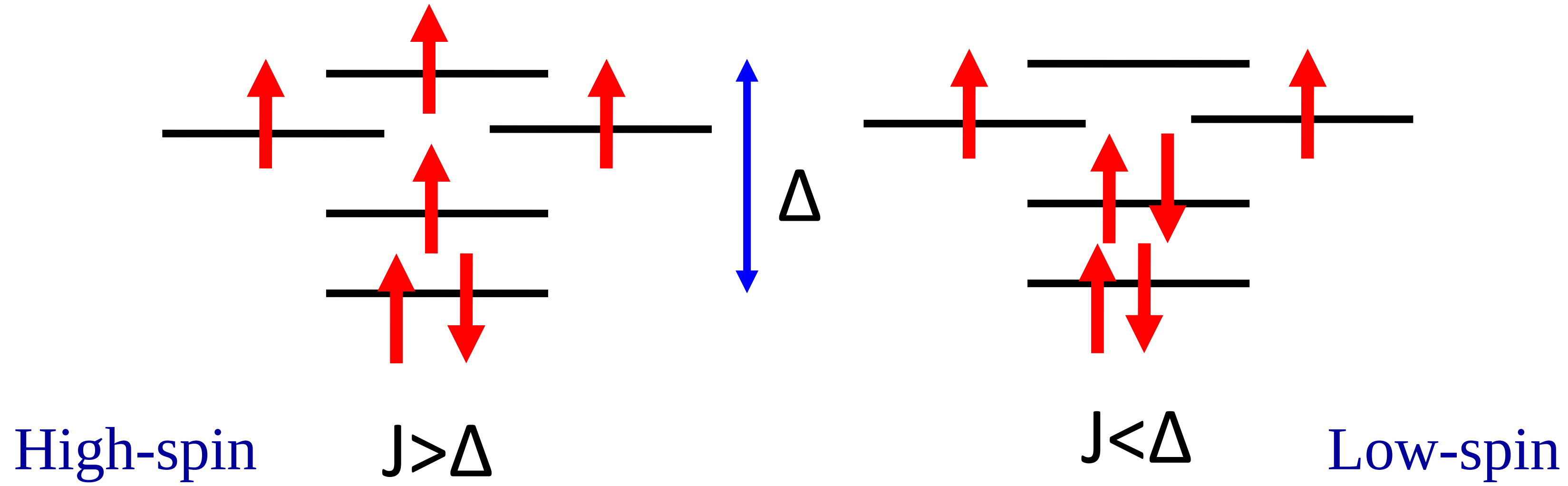
How will the Mott transition take place in the multi-orbital iron-based systems with even number of electrons per unit cell?

# Multi-Orbital Hubbard Model

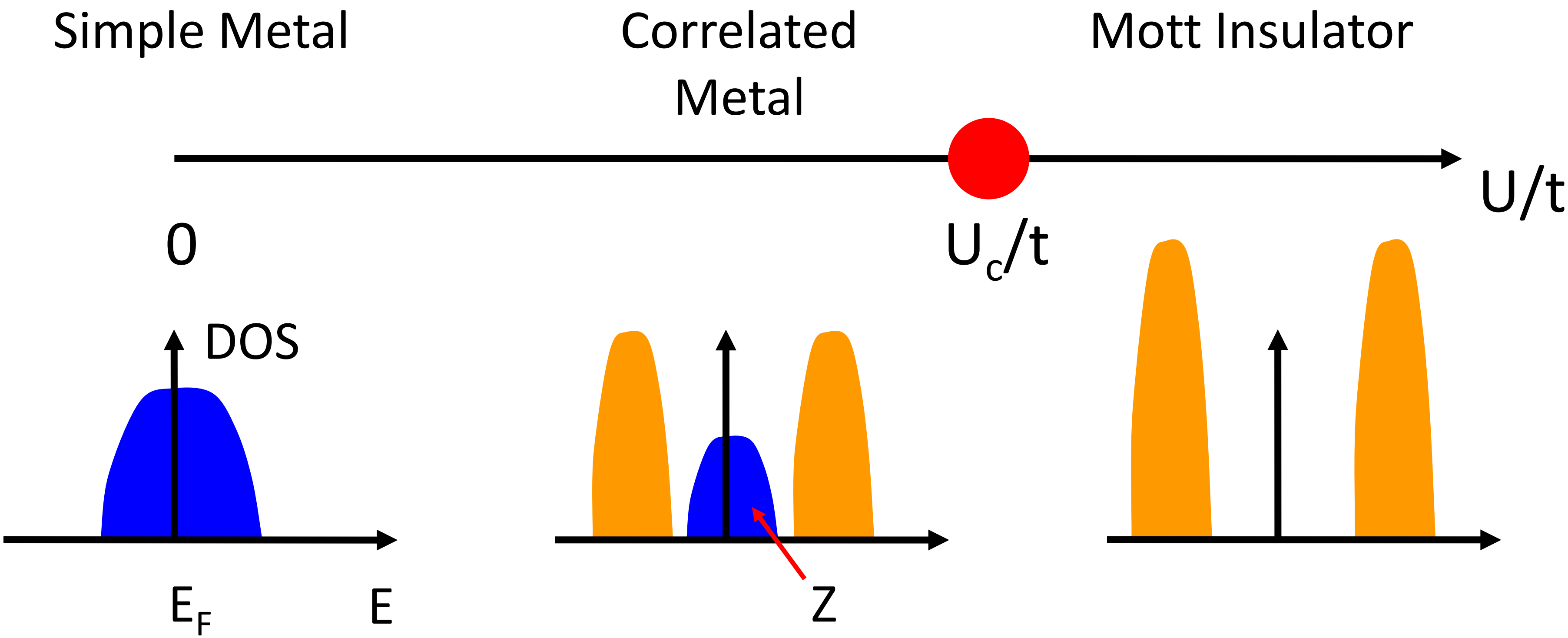
$$H = H_{\rm TB} + H_{\rm int}$$

$$H_{\rm int} = U \sum_{\mathbf{i},\alpha} n_{\mathbf{i},\alpha,\uparrow} n_{\mathbf{i},\alpha,\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\alpha<\beta} n_{\mathbf{i},\alpha} n_{\mathbf{i},\beta}$$
$$- 2J \sum_{\mathbf{i},\alpha<\beta} \mathbf{S}_{\mathbf{i},\alpha} \cdot \mathbf{S}_{\mathbf{i},\beta} - J \sum_{\mathbf{i},\alpha<\beta} (d^{\dagger}_{\mathbf{i},\alpha,\uparrow} d^{\dagger}_{\mathbf{i},\alpha,\downarrow} d_{\mathbf{i},\beta,\uparrow} d_{\mathbf{i},\beta,\downarrow} + \text{H.c.})$$

Systems filled with even electrons



# Mott Transition




Requiring theoretical tool that is able to access the phases on both sides of the transition

# U(1) Slave-Spin Theory

$$d^\dagger_{i\alpha\sigma} = S^+_{i\alpha\sigma} f^\dagger_{i\alpha\sigma}$$

constraint:

$$S^z_{i\alpha\sigma} = f^\dagger_{i\alpha\sigma} f_{i\alpha\sigma} - \frac{1}{2}$$

Schwinger boson representation: $S^+_{i\alpha\sigma} = a^\dagger_{i\alpha\sigma} b_{i\alpha\sigma}$

$$d^\dagger_{i\alpha\sigma} = z^\dagger_{i\alpha\sigma} f^\dagger_{i\alpha\sigma} \qquad z^\dagger_{i\alpha\sigma} = P^-_{i\alpha\sigma} a^\dagger_{i\alpha\sigma} b_{i\alpha\sigma} P^+_{i\alpha\sigma}$$

$$Z_{i\alpha\sigma} = |\langle z_{i\alpha\sigma}\rangle|^2 \qquad P^\pm_{i\alpha\sigma} = 1/\sqrt{1/2 + \delta \pm (a^\dagger_{i\alpha\sigma} a_{i\alpha\sigma} - b^\dagger_{i\alpha\sigma} b_{i\alpha\sigma})/2}$$

Determining renormalization amplitudes:

$$H_f^{\mathrm{mf}} = \frac{1}{2} \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \langle z^\dagger_{i\alpha\sigma} z_{j\beta\sigma}\rangle f^\dagger_{i\alpha\sigma} f_{j\beta\sigma} + \sum_{i\alpha\sigma} (\Delta_\alpha - \lambda_{i\alpha\sigma} - \mu) f^\dagger_{i\alpha\sigma} f_{i\alpha\sigma},$$

$$H_S^{\mathrm{mf}} = \frac{1}{2} \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \langle f^\dagger_{i\alpha\sigma} f_{j\beta\sigma}\rangle z^\dagger_{i\alpha\sigma} z_{j\beta\sigma} + \sum_{i\alpha\sigma} \frac{\lambda_{i\alpha\sigma}}{2} (\hat{n}^a_{i\alpha\sigma} - \hat{n}^b_{i\alpha\sigma}) + H_{\mathrm{int}}$$

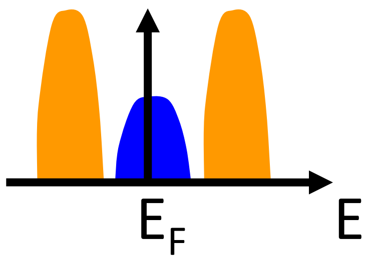
RY and Q. Si, PRB **86**, 085104 (2012),
Cf. ($Z_2$ slave-spin theory): L. de'Medici et al., PRB **72**, 205124 (2005).

# Possible Ground States

- Metal:

  ordered slave spins (Z>0);

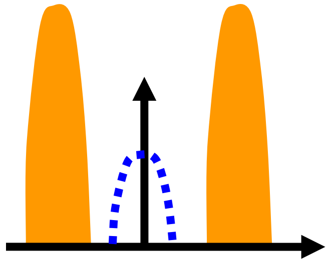
  gapless electrons (finite electron Fermi surface)




- Mott Insulator

  disordered slave spins (Z=0);

  gapless spinons (finite spinion Fermi surface)

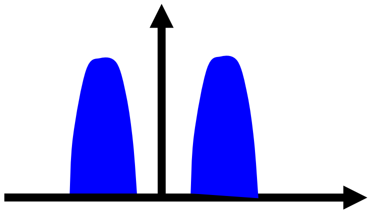


- Band Insulator

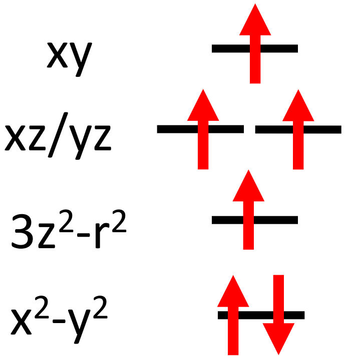
  ordered slave spins (Z>0);

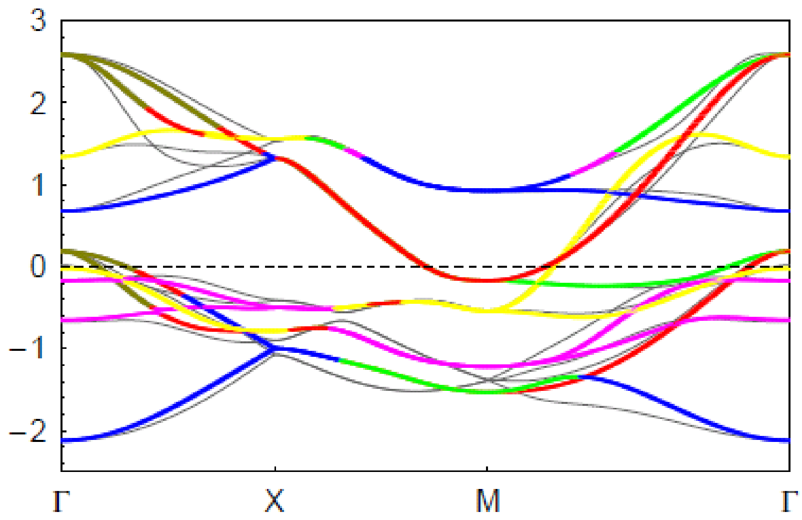
  gapped spinons

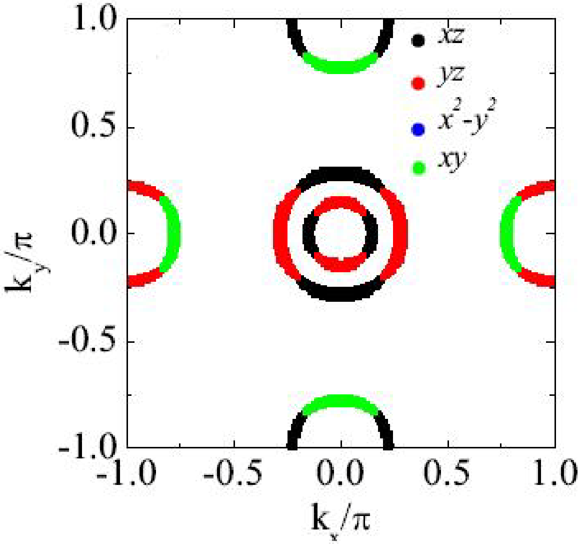
  gapped electrons



# Kinetic Part of the Multiorbital Model for Iron Pnictides



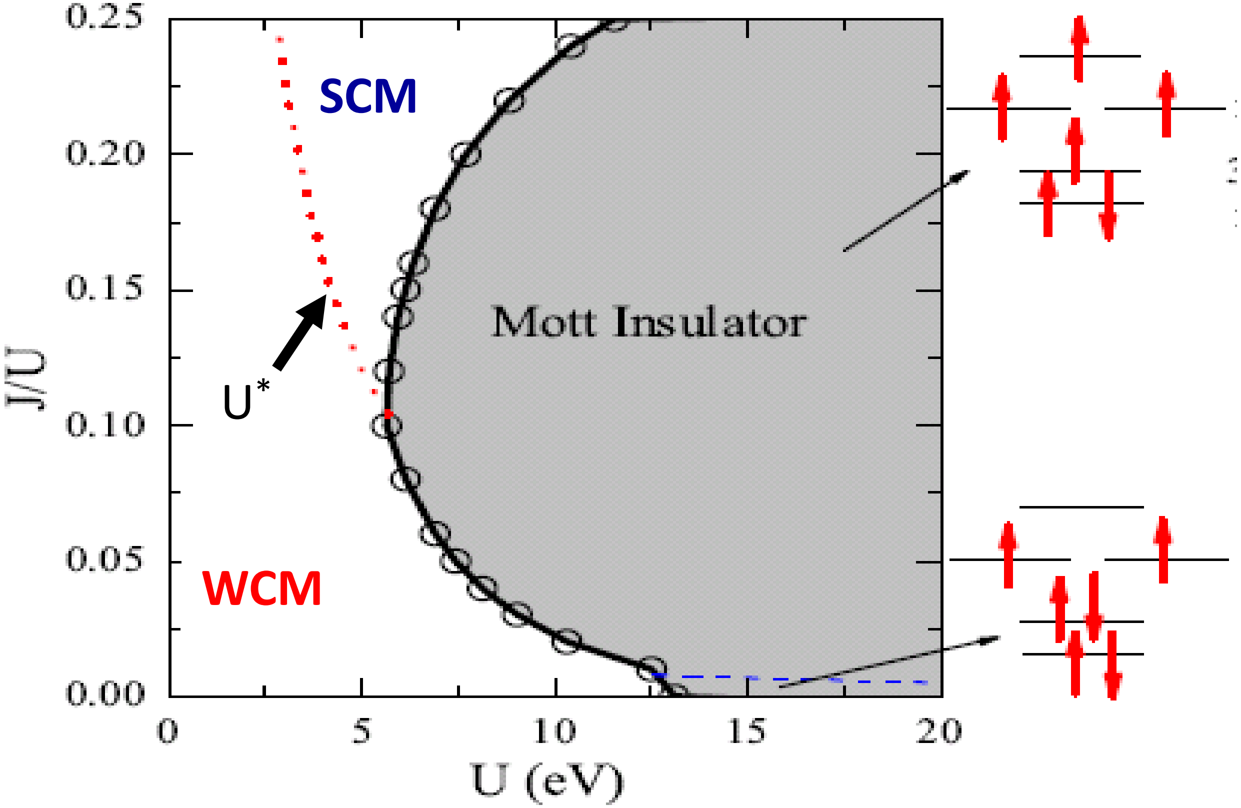

S. Graser et al., New J. Phys. **11**, 025016 (2009).

✓ tight-binding model involving five Fe 3d orbitals

✓ nonzero crystal field splitting

✓ double degenerate xz and yz orbitals

# Mott Transition in the Five-Orbital Model




crossover between:

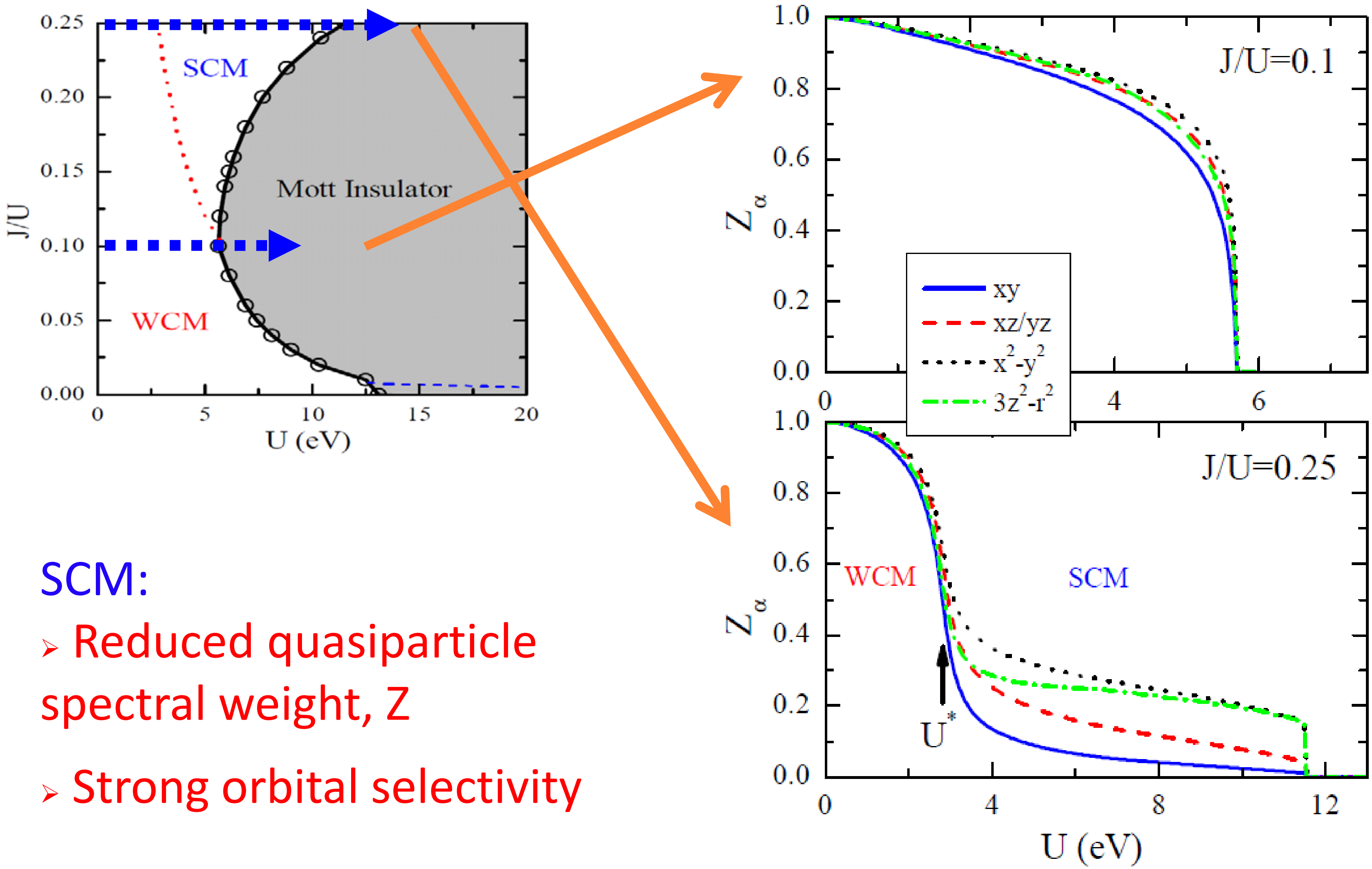
Strongly Correlated Metal

&

Weakly Correlated Metal

RY and Q. Si, PRB **86**, 085104 (2012)

# Correlation Effects in Metallic State



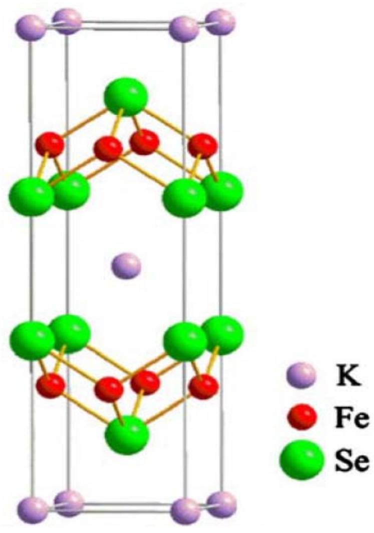

SCM:

- Reduced quasiparticle spectral weight, Z
- Strong orbital selectivity

RY and Q. Si, PRB **86**, 085104 (2012)

# Mott Localization in Alkaline Iron Selenides

**$A_xFe_{2-y}Se_2$**




Vacancy Order

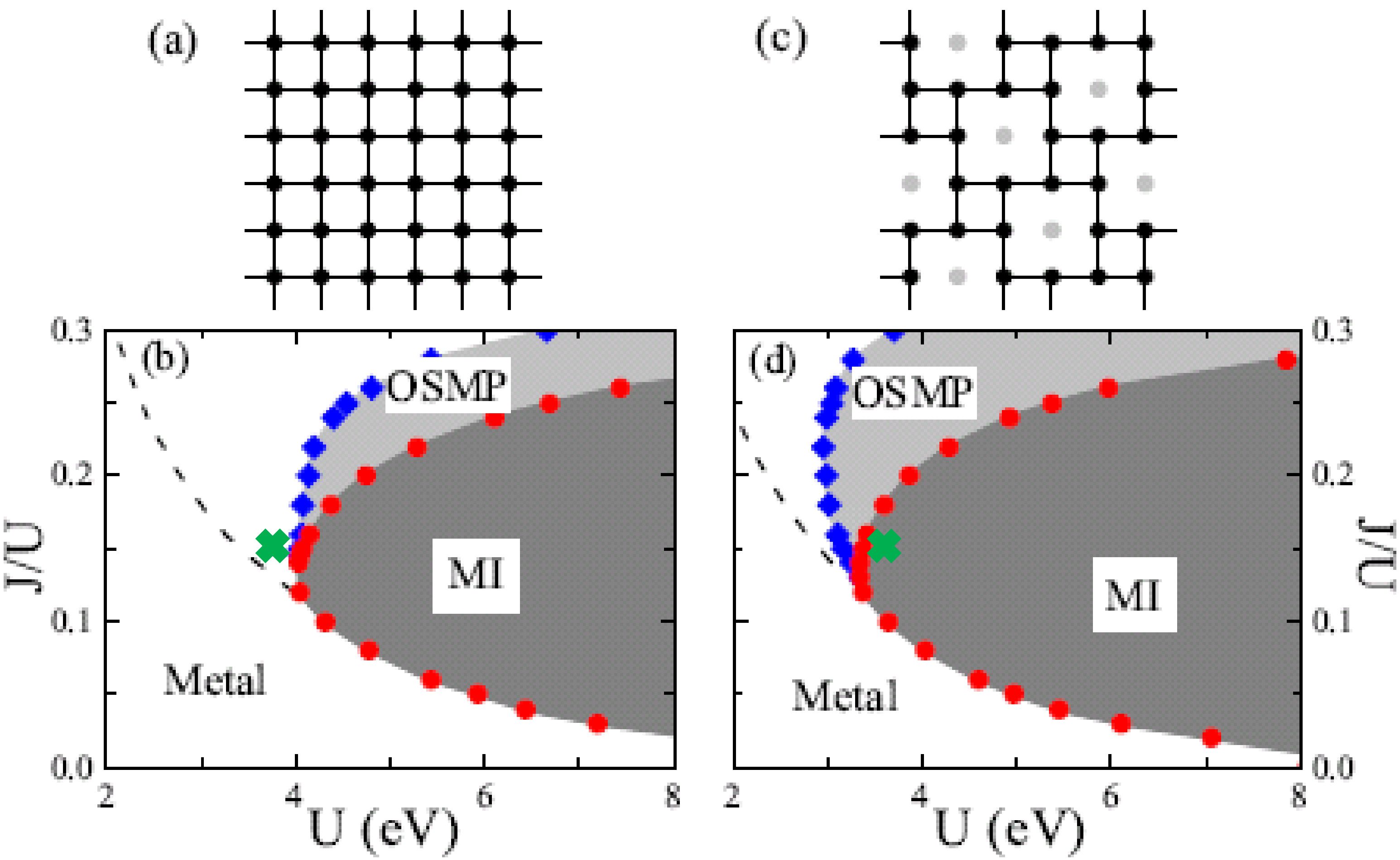
vs

Mott Localization

# Metal-to-Insulator Transition in Parent $K_xFe_{2-y}Se_2$

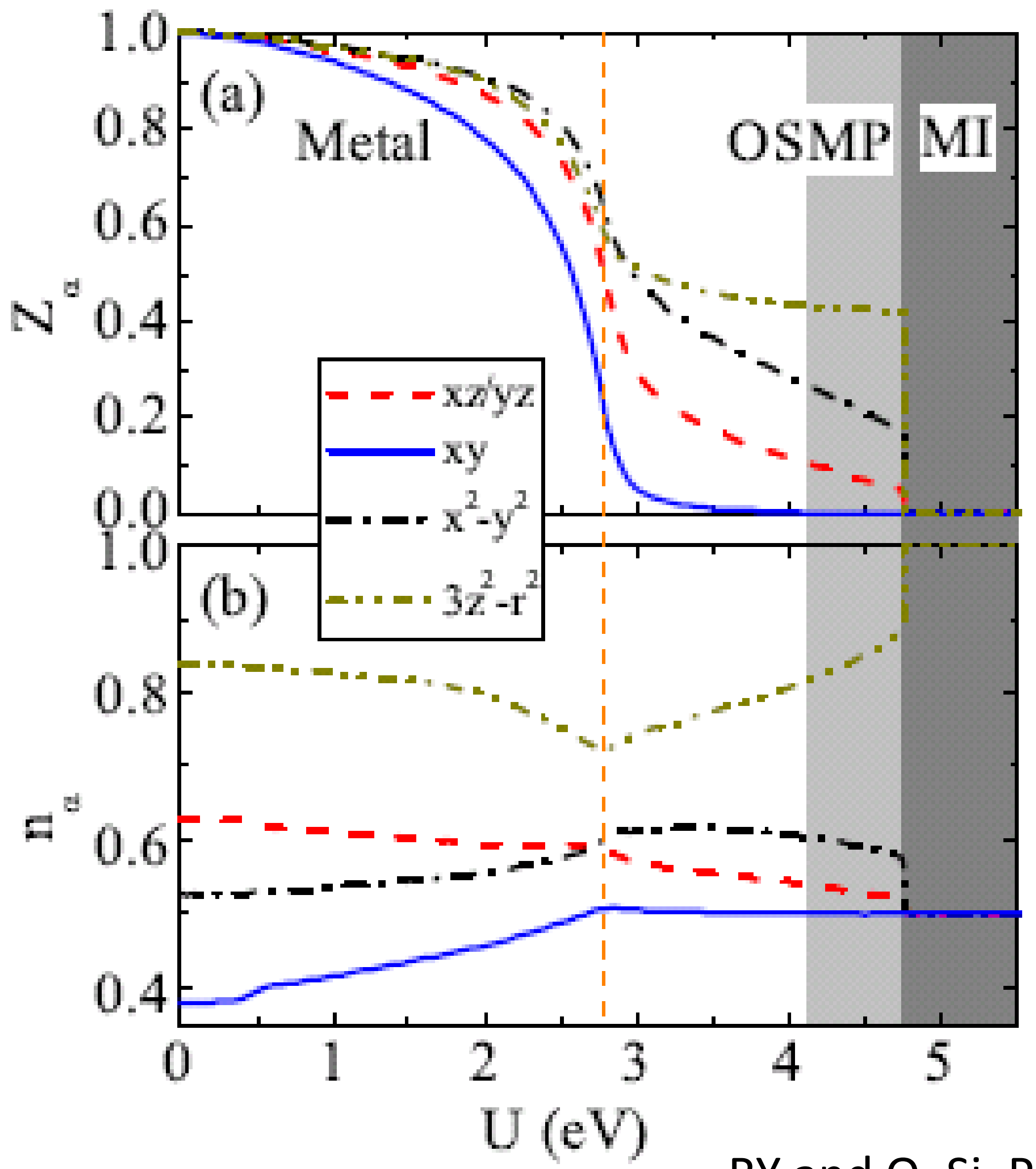
filling n=6 kinetic energy reduction by ordered vacancies

No Vacancy √5×√5 Vacancy Ordered




RY and Q. Si, PRL **110**, 146402 (2013)

# Evolution of QP Weight Z with U

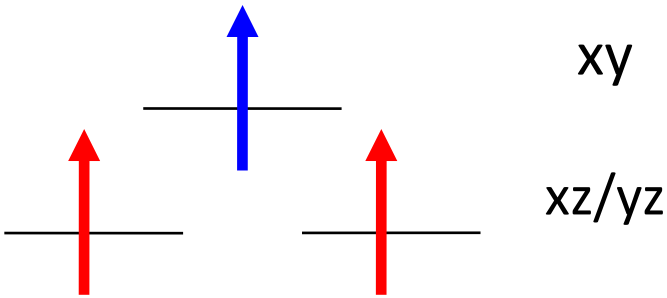


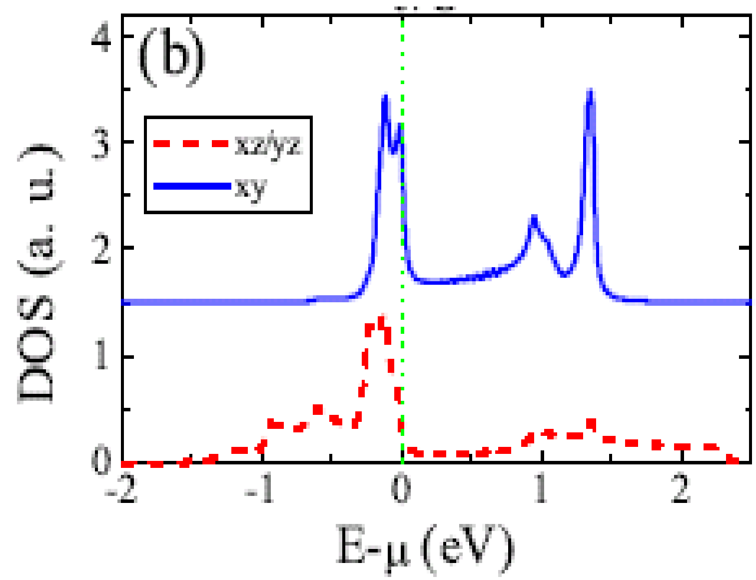

n=6, J/U=0.2

OSMP:
xy orbital localized;
others itinerant.

RY and Q. Si, PRL **110**, 146402 (2013)

# Nature of the Orbital-Selective Mott Phase




✓ crystal level splitting: lowest filling in dxy

✓ dxy bands is narrower than dxz/yz bands

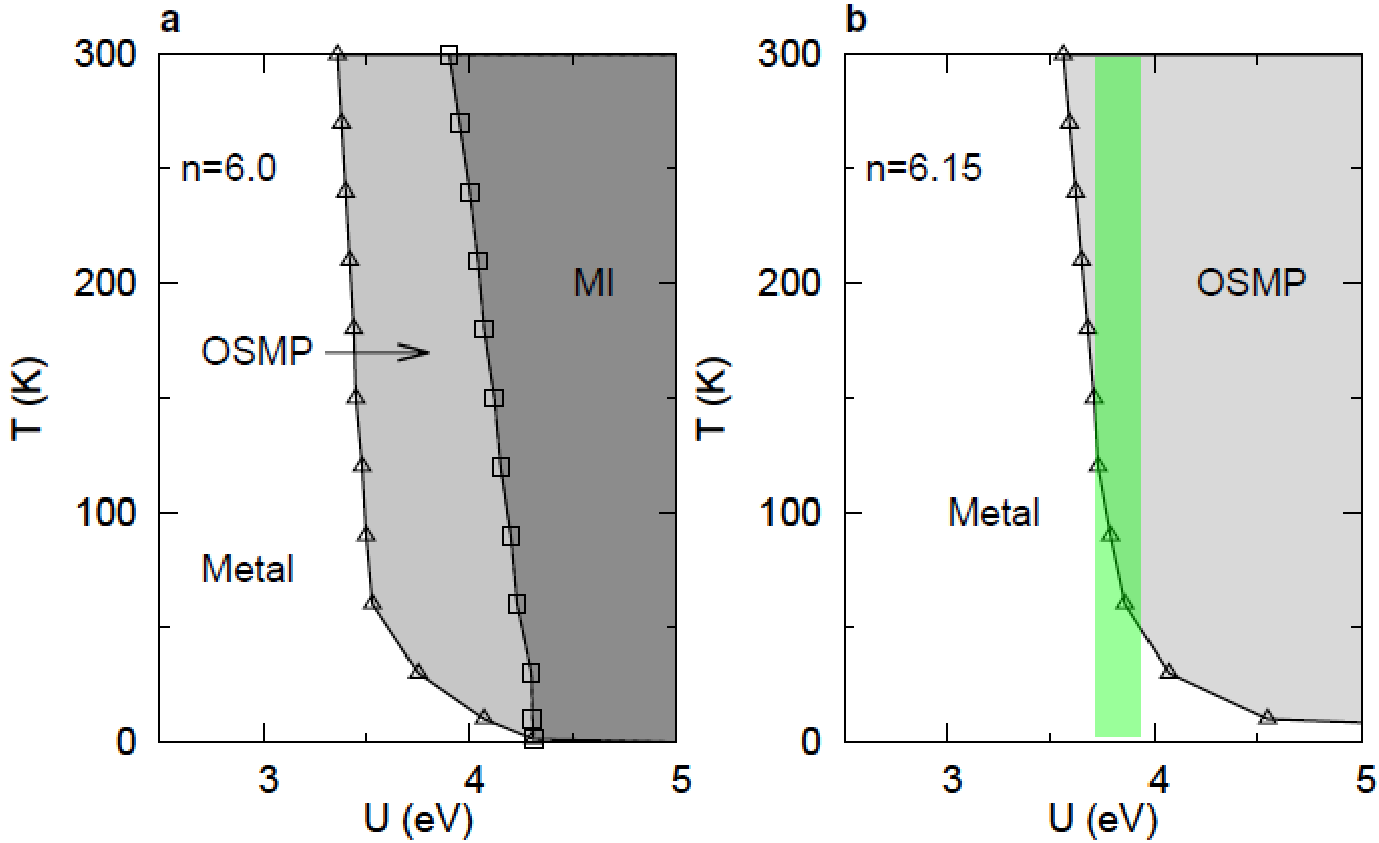
✓ Hund's coupling reduces orbital fluctuations

Cf. (other contexts/regimes):

Anisimov et al, Eur. Phys. J. B **25**, 191 (2002);

de' Medici et al, PRL **102**, 126401 (2009).

# Temperature Induced Mott Localization

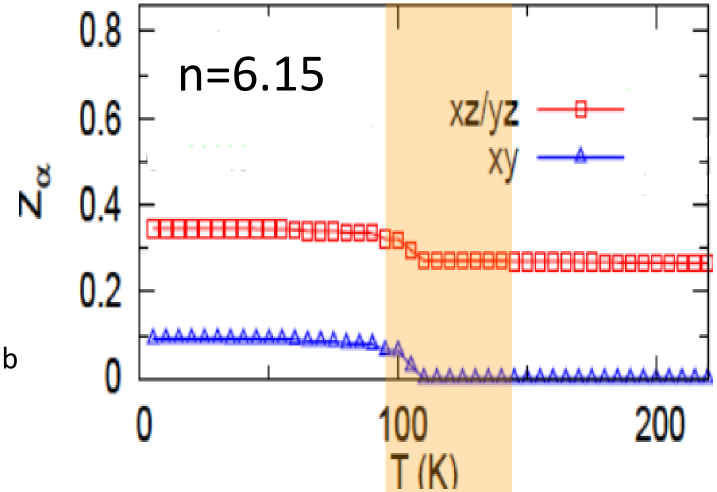


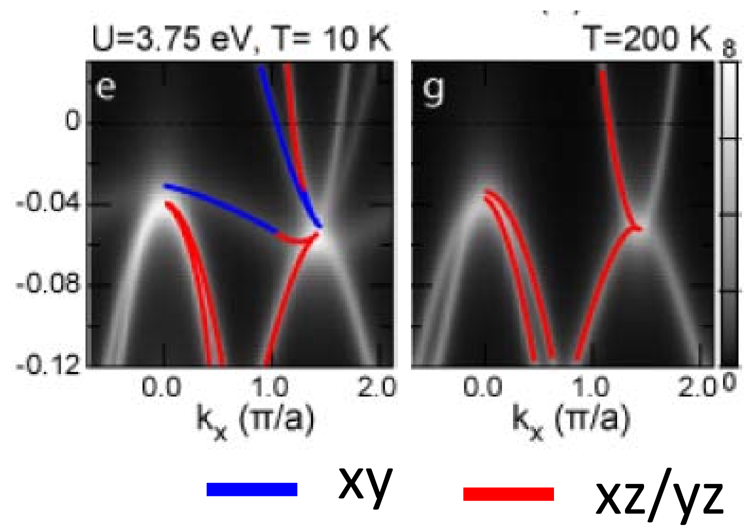

M. Yi, RY, et al., PRL **110**, 067003 (2013)

# Temperature Induced OSMT in $K_xFe_{2-y}Se_2$

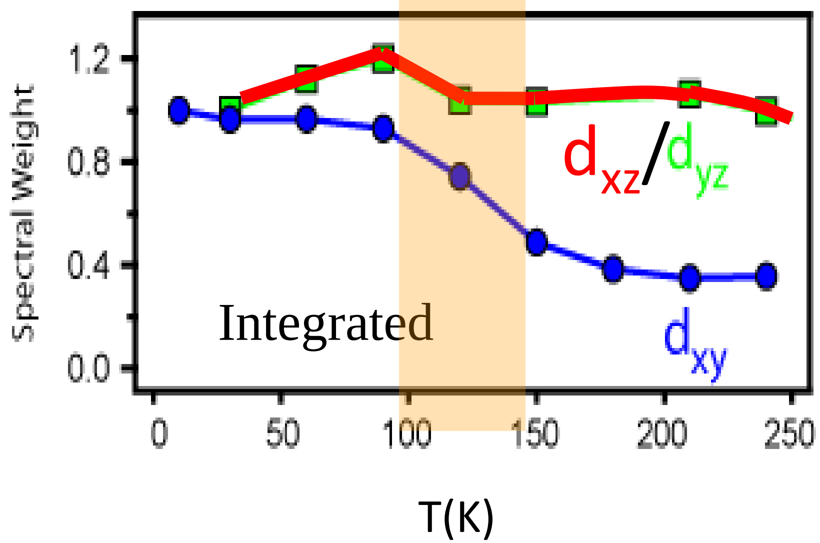
Theory

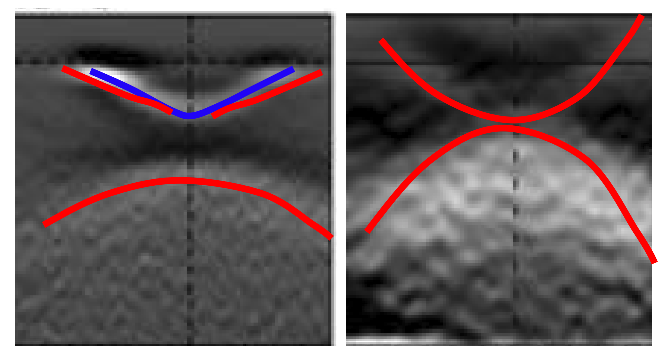
$1/Z \sim m^*/m_b$




ARPES

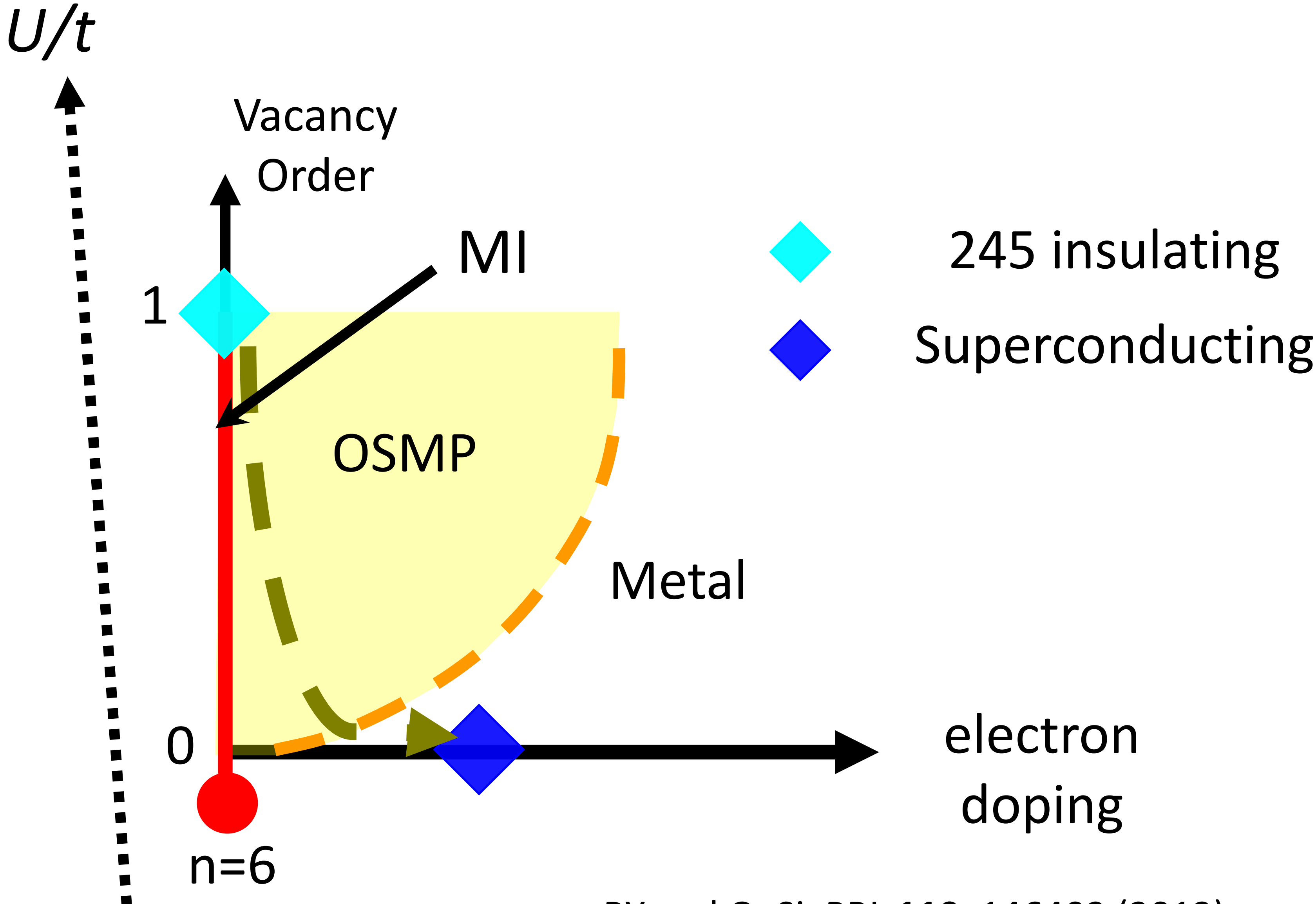


M. Yi, RY, et al., PRL **110**, 067003 (2013)

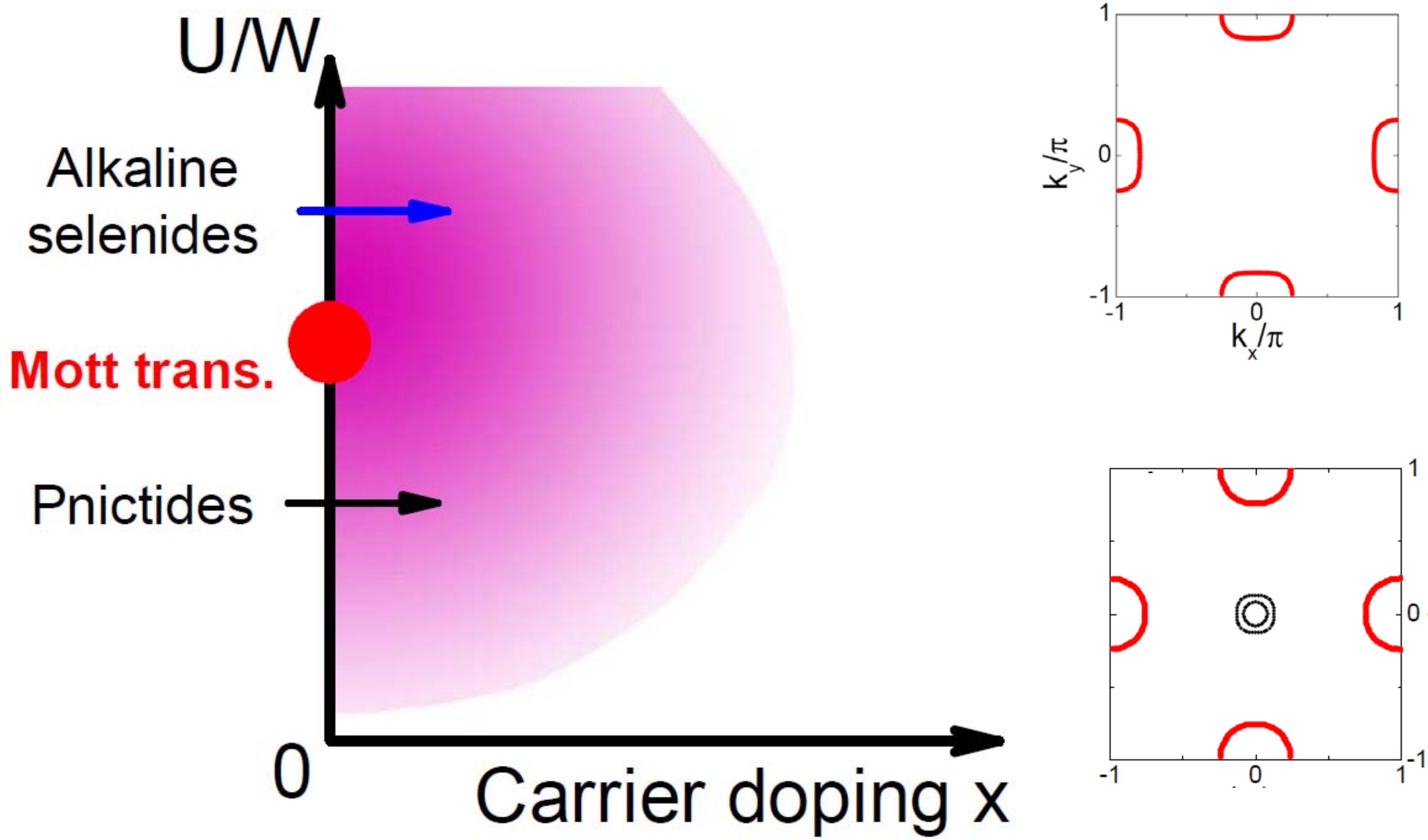
- Similar strong orbital selective behavior also observed in sinlge-layer FeSe/STO (M. Yi's talk on Monday)

# Phase Diagram for $A_xFe_{2-y}Se_2$




RY and Q. Si, PRL **110**, 146402 (2013)

# A Unified Phase Diagram




comparable Tc for iron pnictides & alkaline iron selenides

# Effective Exchange Interactions near a Mott Transition

- One band Hubbard model

$$H = \sum_{(ij),\sigma} t_{ij} d_{i\sigma}^{+} d_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

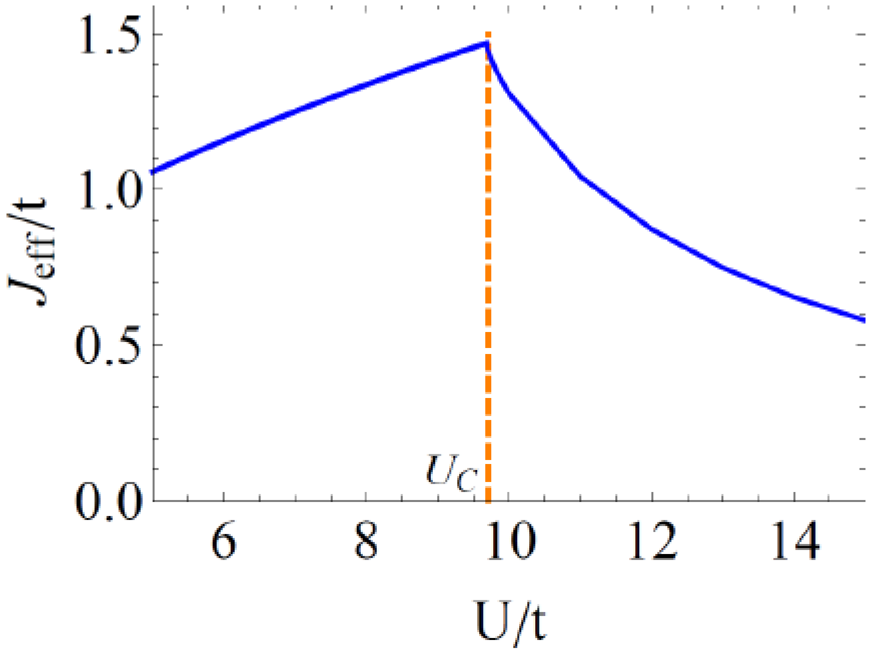
- Slave rotor representation

$$d_{i\sigma} = e^{-i\theta_i} f_{i\sigma}$$

S. Florence and A. Georges,
Phys. Rev. B **70**, 035114 (2004).

- Effective exchange couplings among spinons

$$H_{\text{ex}} = J_{\text{eff}} f_{i\sigma}^{+} f_{i\sigma'} f_{j\sigma'}^{+} f_{j\sigma}$$




W. Ding et al., unpublished.

# Superconducting pairing in multiorbital t-$J_1$-$J_2$ model

$$H = -\sum_{i<j,\alpha,\beta,s} t_{ij}^{\alpha\beta} c_{i\alpha s}^{\dagger} c_{j\beta s} + h.c. - \mu \sum_{i,\alpha} n_{i\alpha}$$
$$+ \sum_{\langle ij\rangle,\alpha,\beta} J_1^{\alpha\beta} \left( \vec{S}_{i\alpha} \cdot \vec{S}_{j\beta} - \frac{1}{4} n_{i\alpha} n_{j\beta} \right) + \sum_{\langle\langle ij\rangle\rangle,\alpha,\beta} J_2^{\alpha\beta} \left( \vec{S}_{i\alpha} \cdot \vec{S}_{j\beta} - \frac{1}{4} n_{i\alpha} n_{j\beta} \right)$$

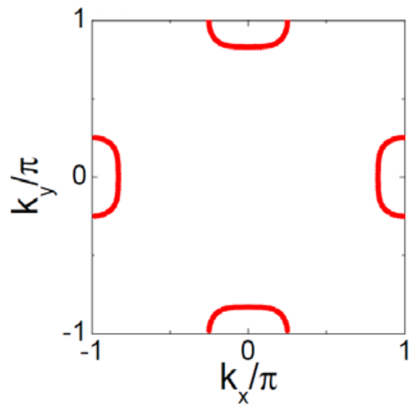
- ✓ decomposing the $J_1$, $J_2$ interactions in pairing channels
- ✓ intra-orbital singlet pairings
- ✓ do not address coexistence of SC and AFM

P Goswami et al., *EPL* **91**, 37006 (2010)

**RY** et al., *Nat Commun* **4**, 2783 (2013)

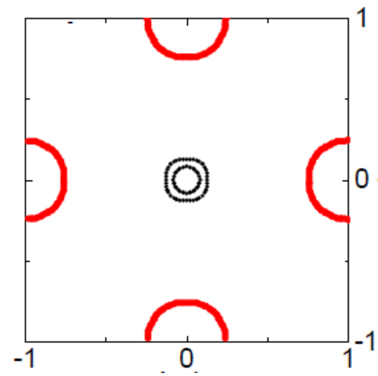
# Comparable Pairing Amplitudes

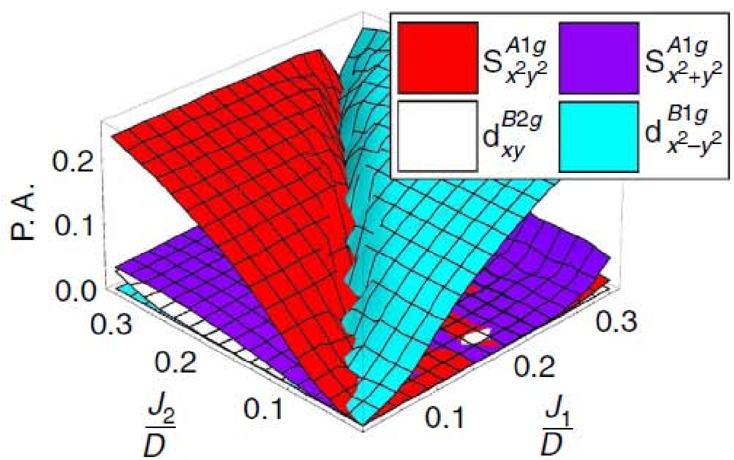
Alkaline iron selenide

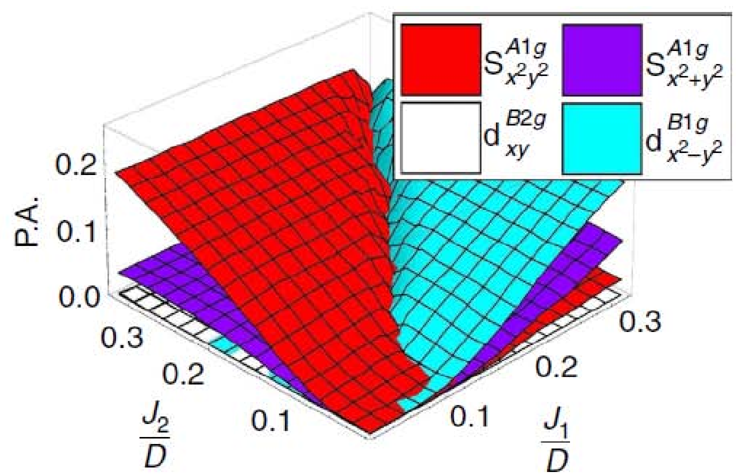



$\delta = 0.15$

Iron pnictide



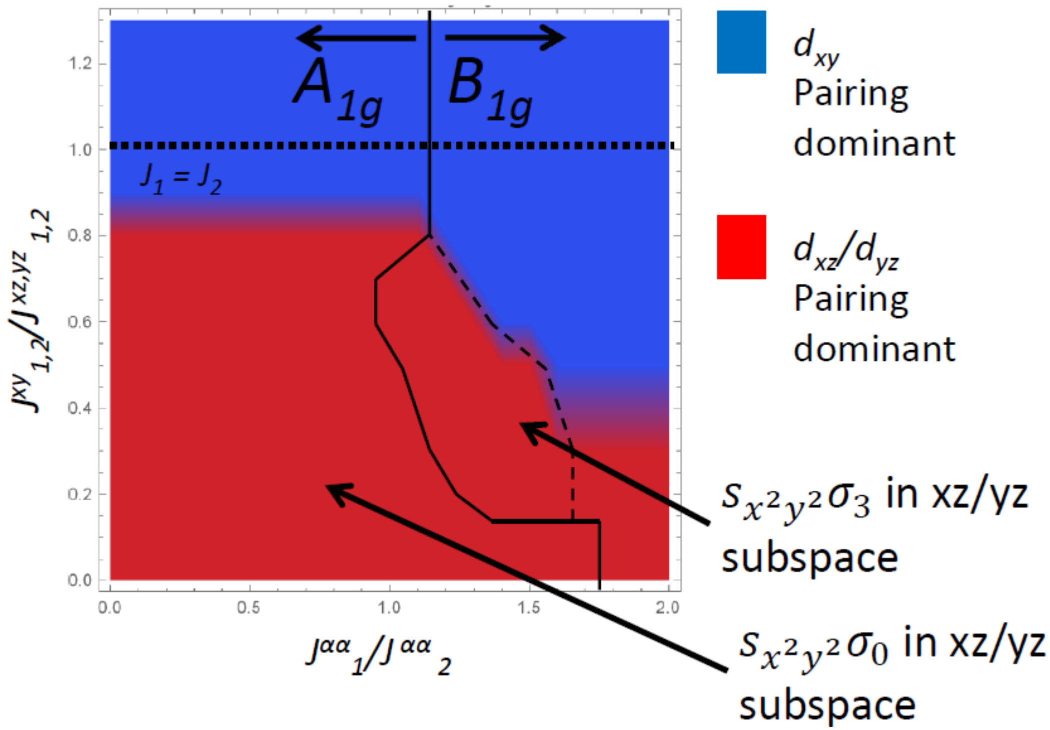




- Similar results also for 1-layer FeSe/STO

**RY** et al., *Nat Commun* **4**, 2783 (2013)

# Orbital-Selective Pairing in Multiorbital $t$-$J_1$-$J_2$ model



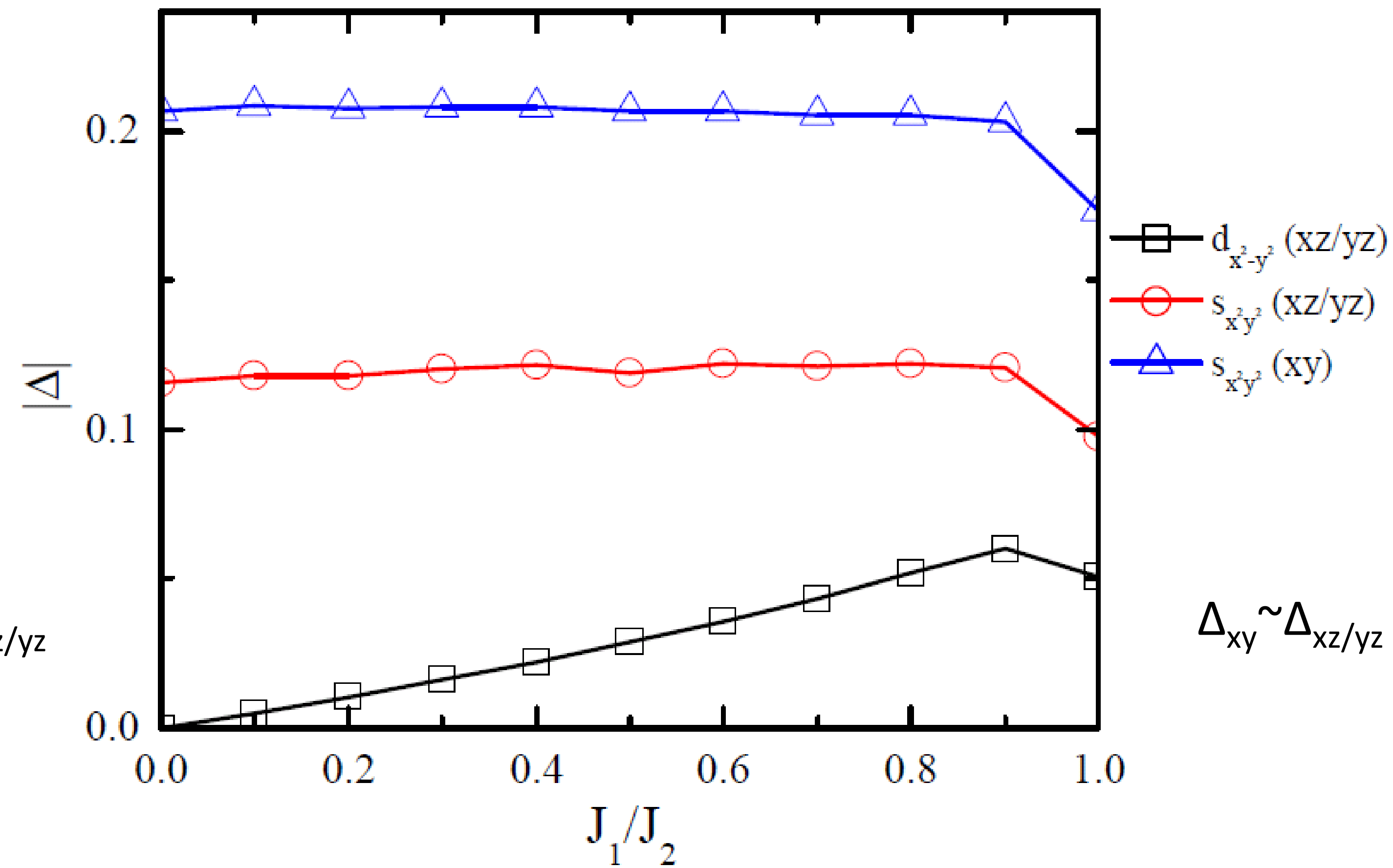

- ✓ diagonal but orbital dependent J matrix, $r_O = J^{xy}_{1(2)} / J^{xz/yz}_{1(2)}$
- ✓ competition between s-$A_{1g}$ and d-$B_{1g}$ pairing channels
- ✓ s-$B_{1g}$ pairing stabilized at intermediate $r_O$.

E Nica, et al, unpublished.

# Orbital-Selective Pairing Amplitudes

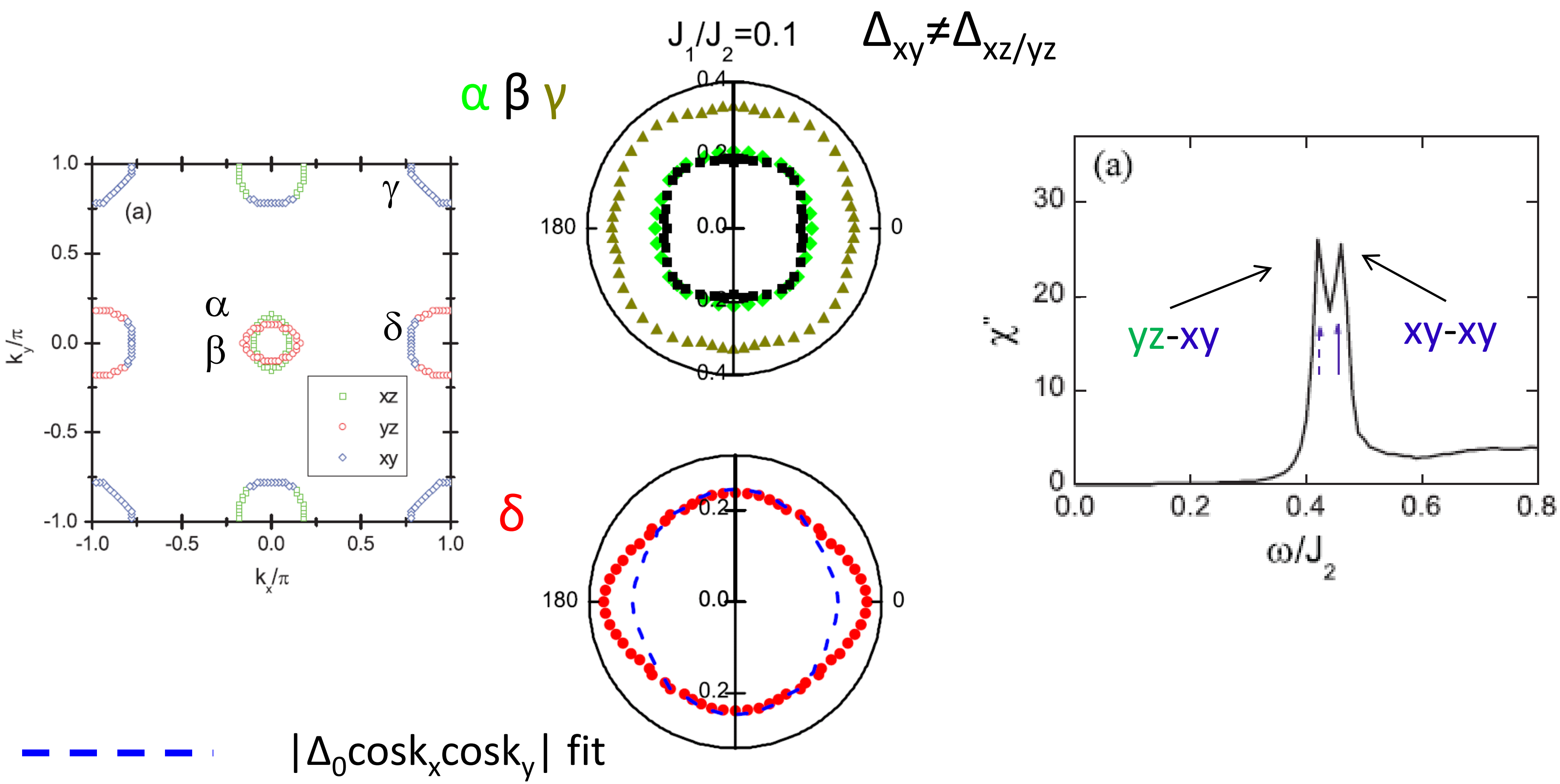
Dominant pairing channels with $A_{1g}$ symmetry at $r_O=1$

$\Delta_{xy} \neq \Delta_{xz/yz}$




$\Delta_{xy} \sim \Delta_{xz/yz}$

# Anisotropic Superconducting Gap and Splitting of Spin Resonance Peaks

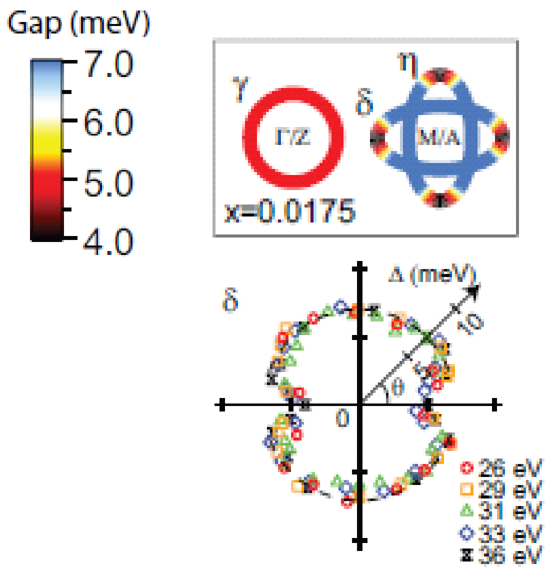



Yu, Zhu, and Si, PRB **89**, 024509 (2014)

# Anisotropic SC Gap and Double Spin Resonances in underdoped Na 111

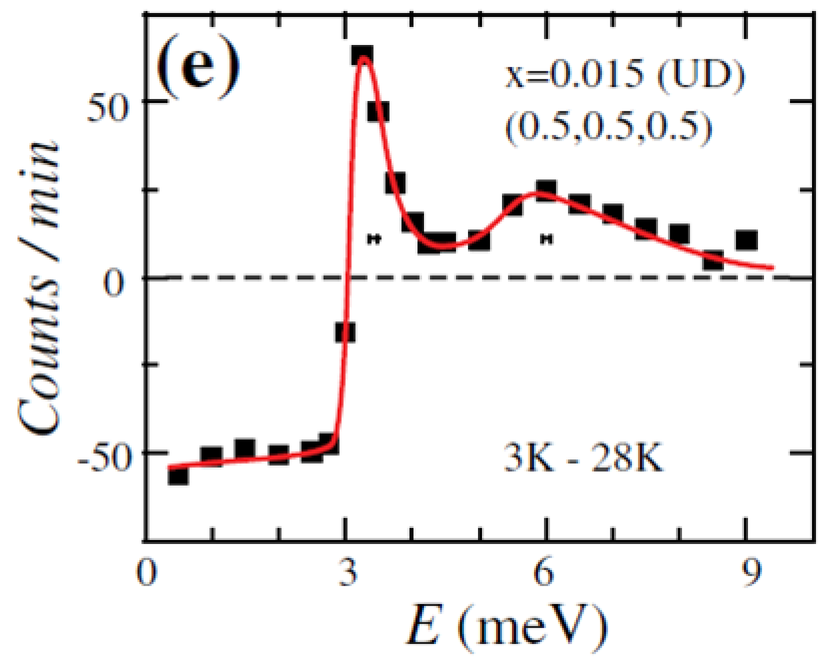
$NaFe_{1-x}Co_xAs$

ARPES




NOT compatible with $\cos k_x \cos k_y$

Neutron Scattering




Q Q Ge et al., *PRX* **3**, 011020 (2013)

C Zhang, **RY** et al., *PRL* **111**, 207002 (2013)

# Summary

- Metal-to-Mott-insulator transition studied by slave-spin method in multi-orbital Hubbard models for iron-based superconductors
- Mott localization influenced by various factors: Hund's coupling, Fe vacancy order, crystal level splitting ...
- Strong orbital-selective Mott physics in iron chalcogenides
- Comparable pairing amplitudes for iron pnictides and alkaline iron selenides
- Strong orbital dependent superconducting pairing: gap anisotropy and splitting of neutron resonance in the superconducting state