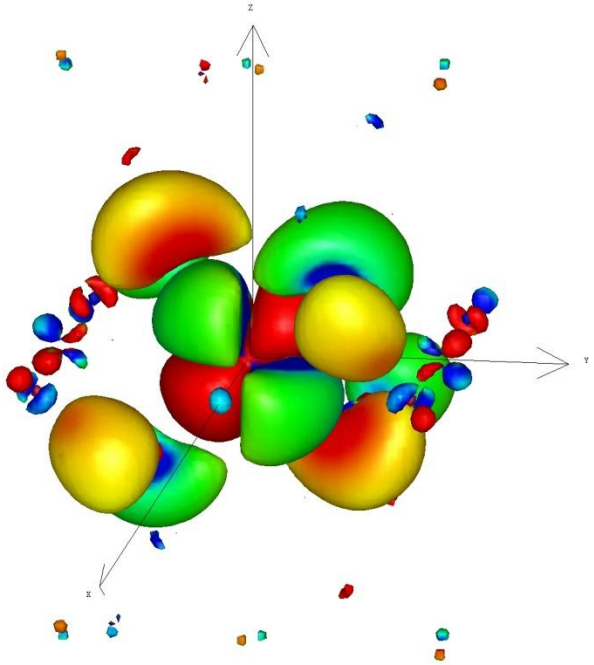
Anisotropic Magnetic Structures in Iron-Based Superconductors



Chi-Cheng Lee, Weiguo Yin & **Wei Ku**

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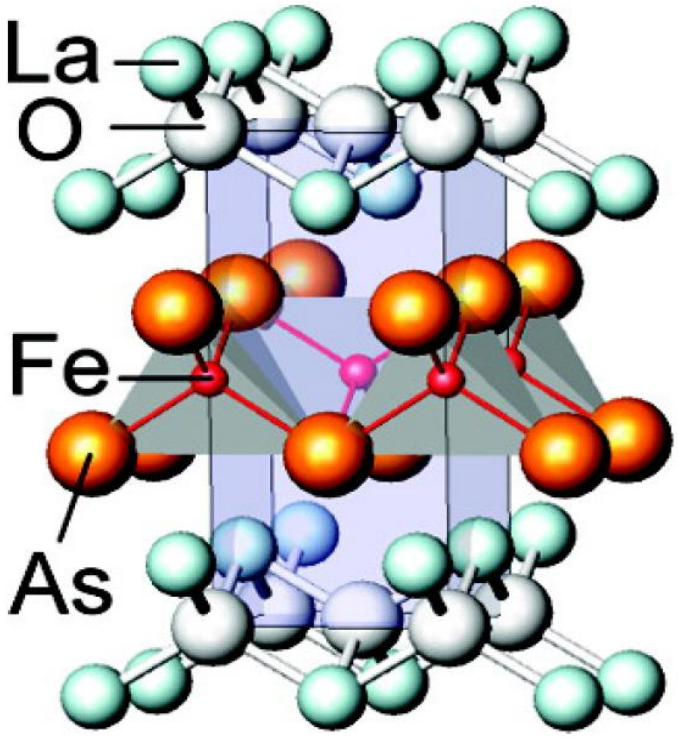
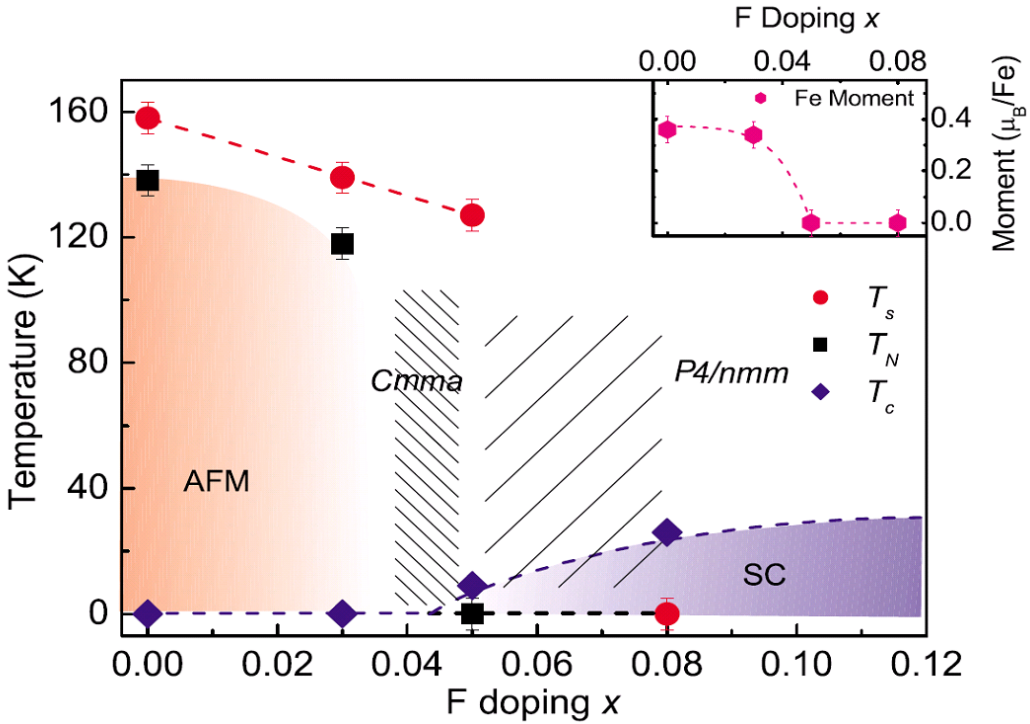
Department of Physics, SUNY Stony Brook

Another example of SC by doping away from AFM





Clarina de la Cruz et al., Nature 453, 899 (2008)
Y. Kamihara et al., J. Am. Chem. Soc. **130**, 3296-3297 (2008)

Q. Huang et al., PRB **78**, 054529 (2008)

- Long standing questions about AFM and SC
- Electronic structure of the undoped magnetic system?
- Similar to the cuprates?

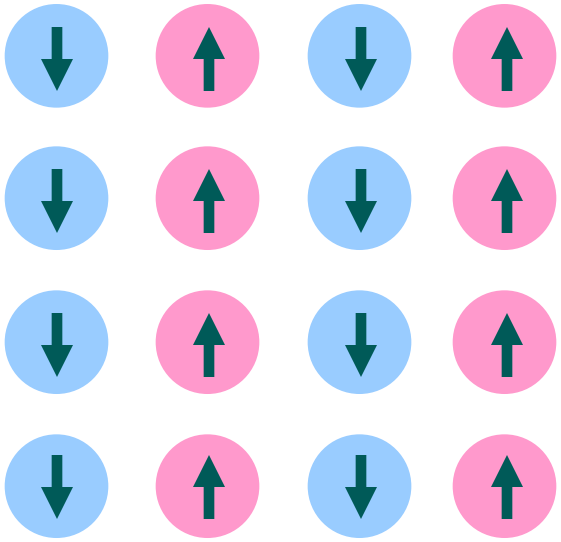
Stripy magnetic and lattice structure

- DFT gives:
  - E^{total} (AFM) best even in the doped system without LRO
    - → short-range correlation necessary for short-range bonding!
  - AFM LRO too strong: Δ^{AF} too big & moment too big
    - → ordered moment vs. fluctuating moment
      - → seriously beyond mean-field?
    - → strong short-range magnetic correlation in doped system (neutron)
    - → robust local moment (against doping/temperature, NMR/neutron) ?
    - → competition of different length scale?
  - long bond in AFM phase is stronger for phonon (~exp), why?
- Local magnetic moment or itinerant?
- Strongly correlated or not?
  - SC is a correlated state.
    - → High-T_c implies strong correlation in the pairing channel
    - → not necessary resulting from intra-atomic correlation

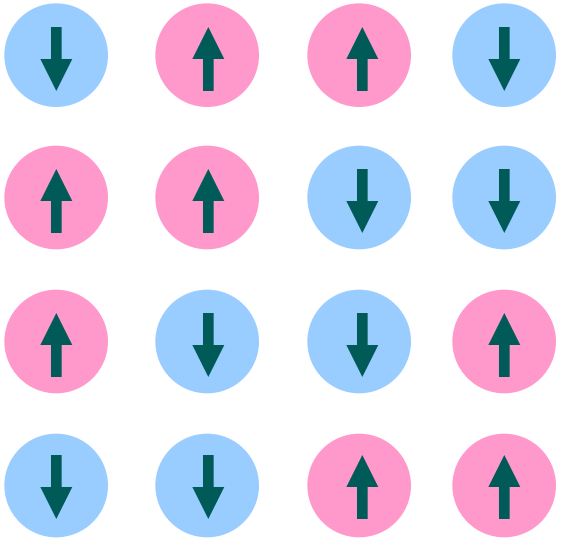
Families of Fe-based High Temperature Superconductor

Magnetic structure of parent undoped compound

C-type
stripe-like
collinear



E-type
double stripe
bicollinear



1111 (e.g. $LaO_{1-x}F_xFeAs$)
122 (e.g. $Ba_{1-x}K_xFe_2As_2$)
111 (e.g. Li_xFeAs)

11 (e.g. $FeTe_{1-x}Se_x$)

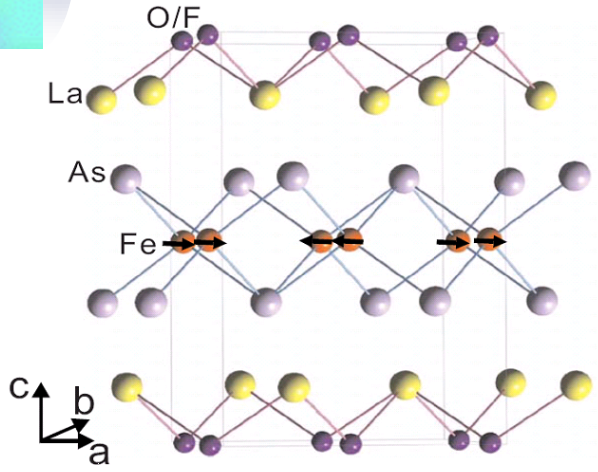
Representative parent compound **LaOFeAs**

Ferro-orbital order & anisotropic magnetic structure in 1111 (&122)

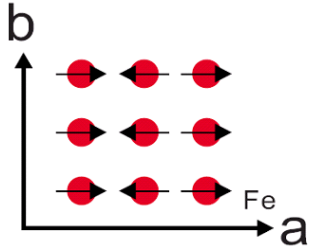
Chi-Cheng Lee, Weiguo Yin & Wei Ku

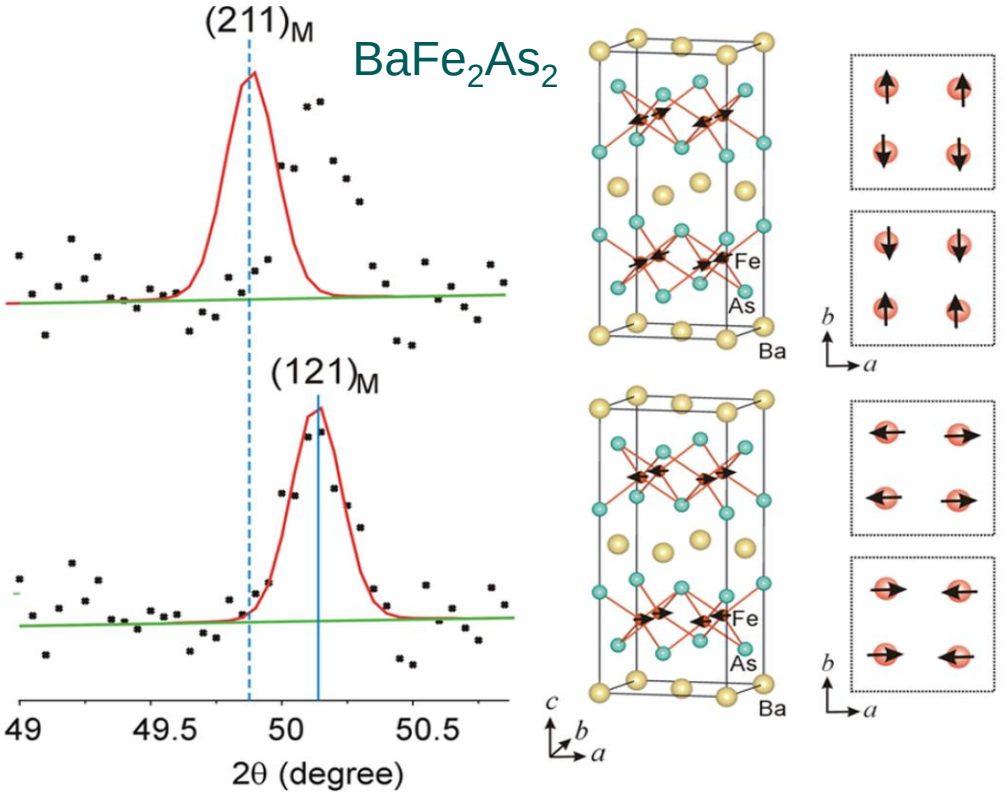
Phys. Rev. Lett. **103**, 267001 (2009)

Stripy magnetic and lattice structure



Phys. Rev. B **78**, 054529 (2008)



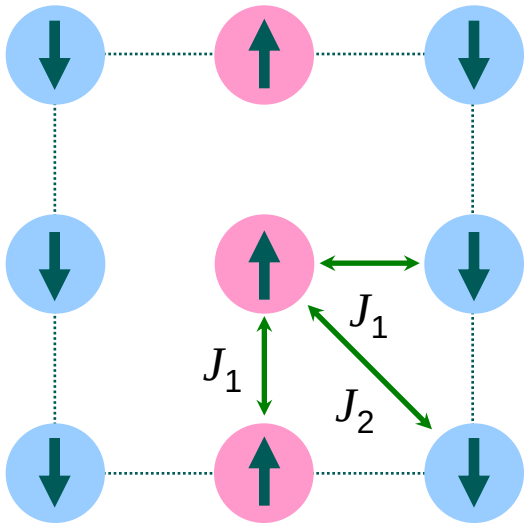


Q. Huang et al., PRL **101**, 257003 (2008)

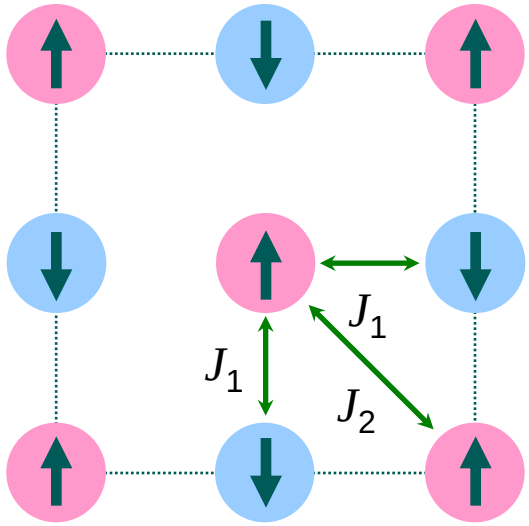
- Structure transition at 155k; Stripy AFM order at 137K (AF bond longer?)
- What drives the magnetic transition?
  Fermi surface instability? (SDW due to nesting?)
- What drives the structural transition?
  Transition temperature so close to magnetic T_N : related?
- Implications to electronic structure and superconductivity?

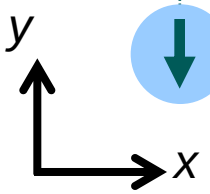
Microscopic mechanisms for stripy magnetic structure

C-type AF: $E = -2J_2S^2$

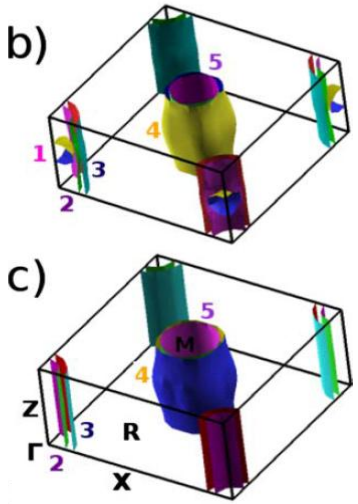


G-type AF: $E = -(2J_1 - 2J_2)S^2$





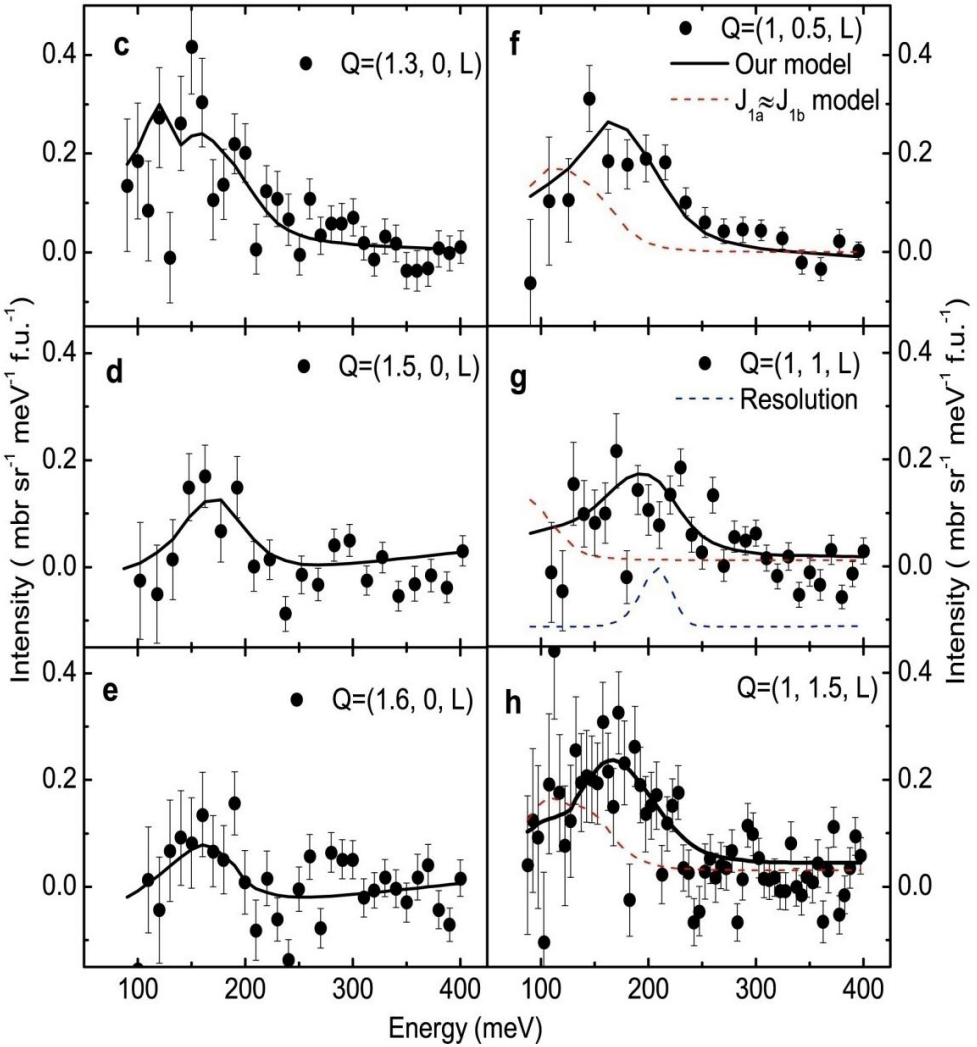
T. Yildirim, PRL **101**, 057010 (2008)



F. Ma et al., PRB **78**, 033111 (2008)

- Competing C-AF & G-AF ($2J_2 > J_1$) ?
- How can T_N be so high (~ 137K)?
- Or, SDW via Fermi surface nesting?

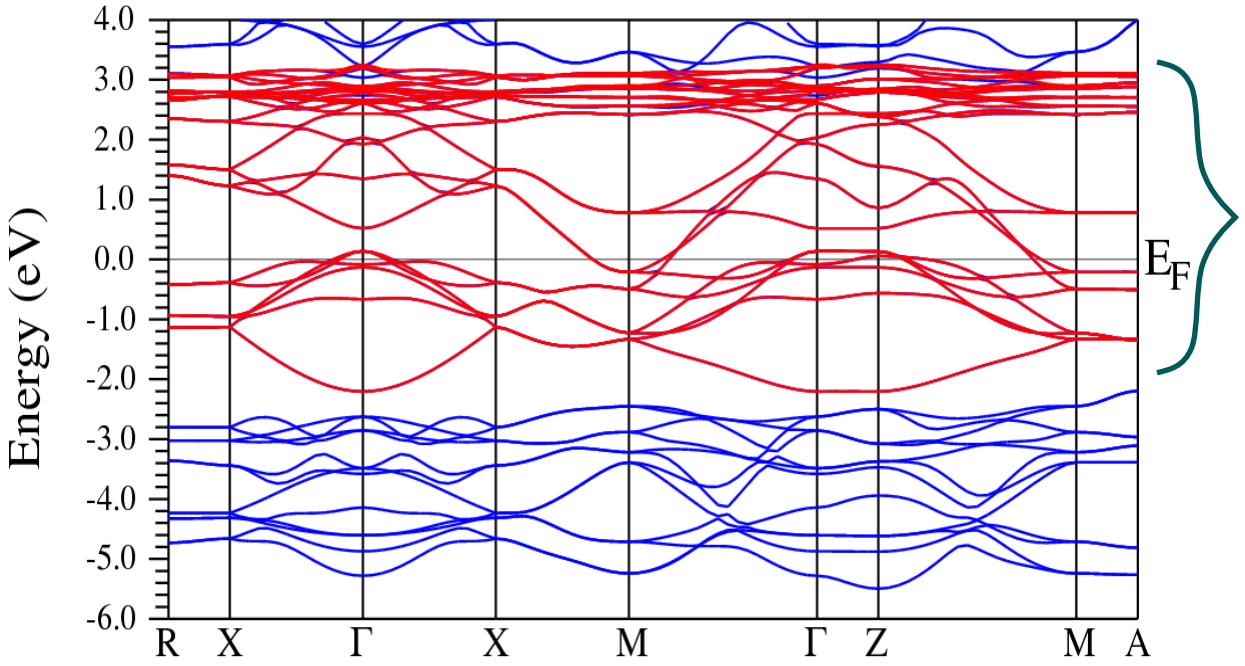
Huge anisotropy found via inelastic neutron scattering



J. Zhao et al., arXiv:0903.2686 (2009)

- Magnon dispersion from INS → huge anisotropy : $J_{1x} >> J_{1y}$
  - → broken rotational symmetry?
  - → too large to be explained by SDW picture

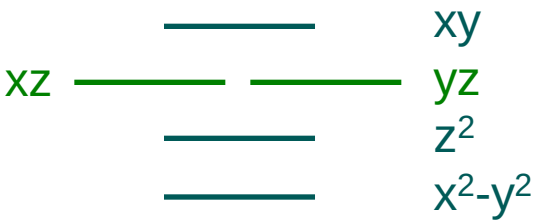
Energy resolved, symmetry respecting Wannier function



$$|\vec{R}n\rangle = \sum_{\vec{k}m}^{(\text{energy window})} |\vec{k}m\rangle\langle\vec{k}m|\vec{R}n\rangle$$

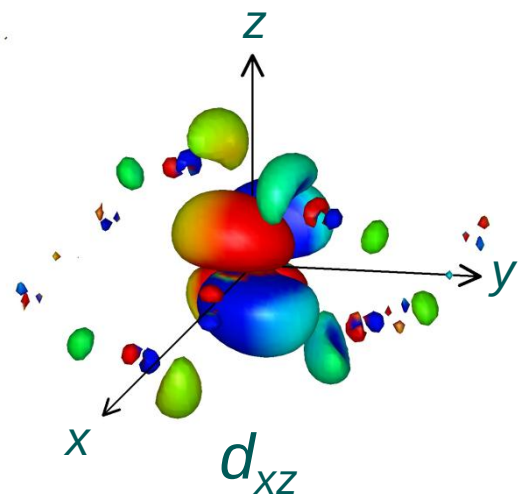
$$= \frac{1}{\sqrt{N_{cell}}} \sum_{\vec{k}m} |\vec{k}m\rangle e^{-i\vec{k}\cdot\vec{R}} U_{mn}^{(\vec{k})}$$

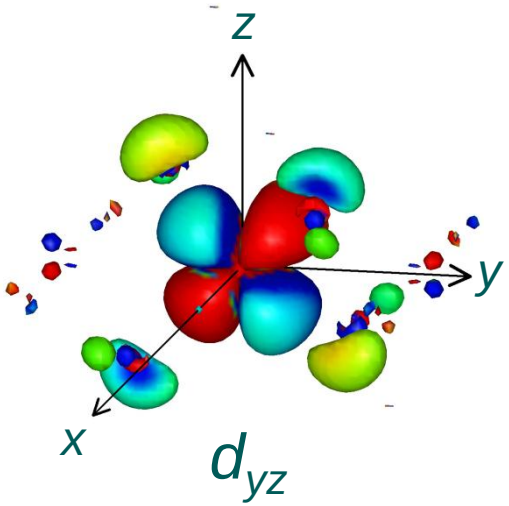
$$= \frac{1}{\sqrt{N_{cell}}} \sum_{\vec{k}} \left(\sum_{m} U_{mn}^{(\vec{k})} |\vec{k}m\rangle \right) e^{-i\vec{k}\cdot\vec{R}}$$



NM onsite energy (eV)

z^2	-0.03
x^2-y^2	-0.20
yz	0.10
xz	0.10
xy	0.34

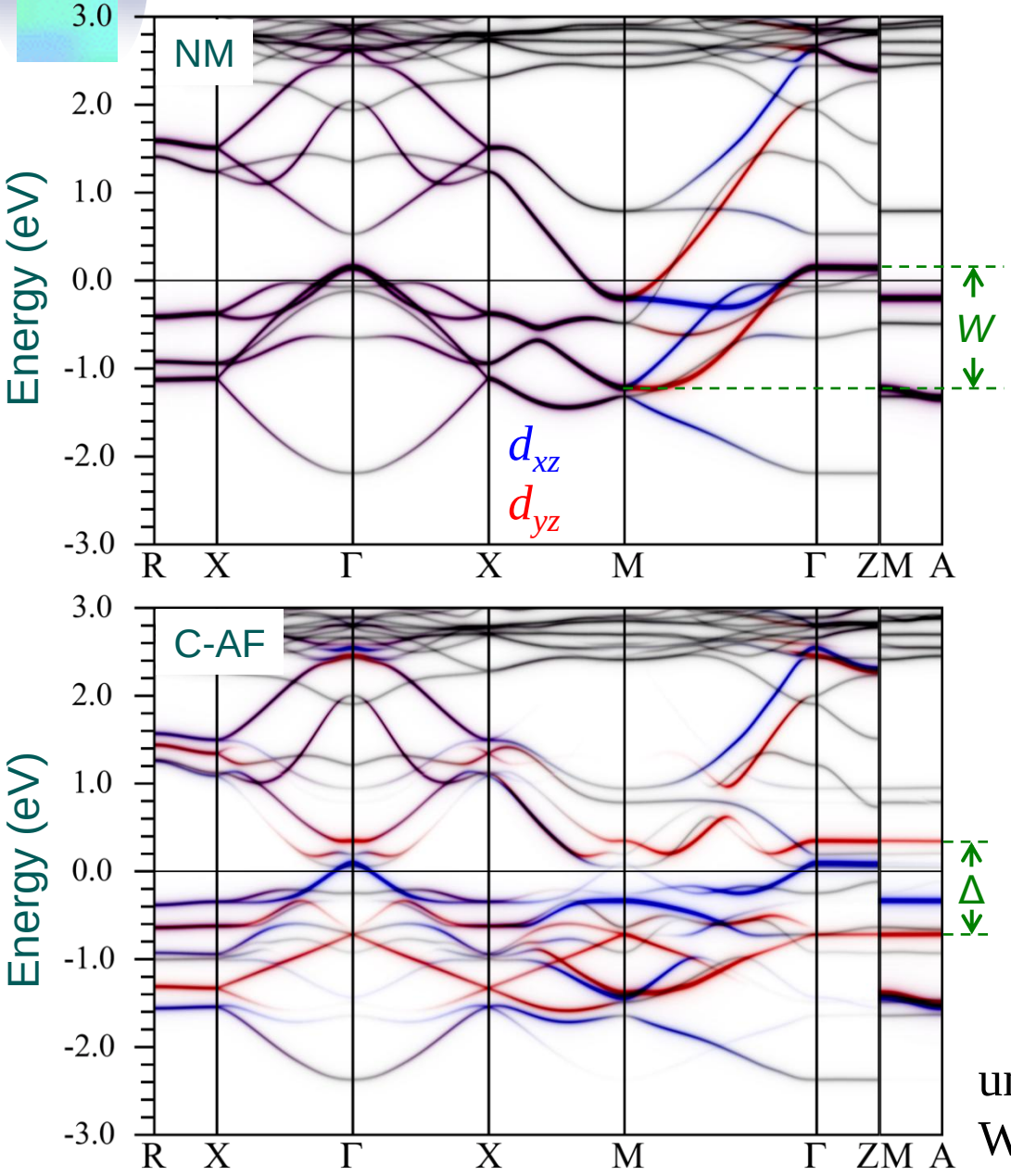




- small crystal field splitting!

methods see: W. Ku et al., PRL 89, 167204 (2002); W. Yin et al., PRL 96, 116405 (2006)

Comparing LDA band structures



- in NM 1st-BZ
- d_{xz} & d_{yz} most relevant to the low-E
- Only d_{yz} splits strongly near E_F
- d_{yz} more spin polarized ~0.34μ_B than d_{xz} (~0.15μ_B)
- more different with U=2eV
  0.58 vs. 0.23μ_B

→ orbital symmetry broken

- $\Delta \sim W$

→ large (ω,**k**)-space involved

→ local picture more suitable

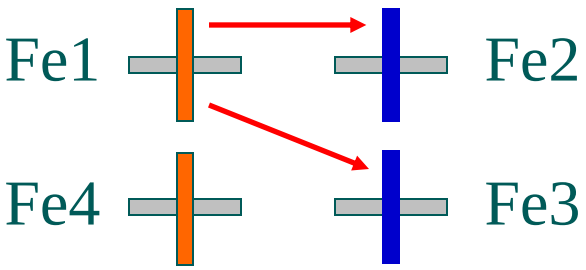
→ Fermi surface nesting not essential

→ SDW less convenient

unfolding methods see:
Wei Ku *et al.*, PRL **104**, 216401 (2010)

Anti-intuitive hopping parameters

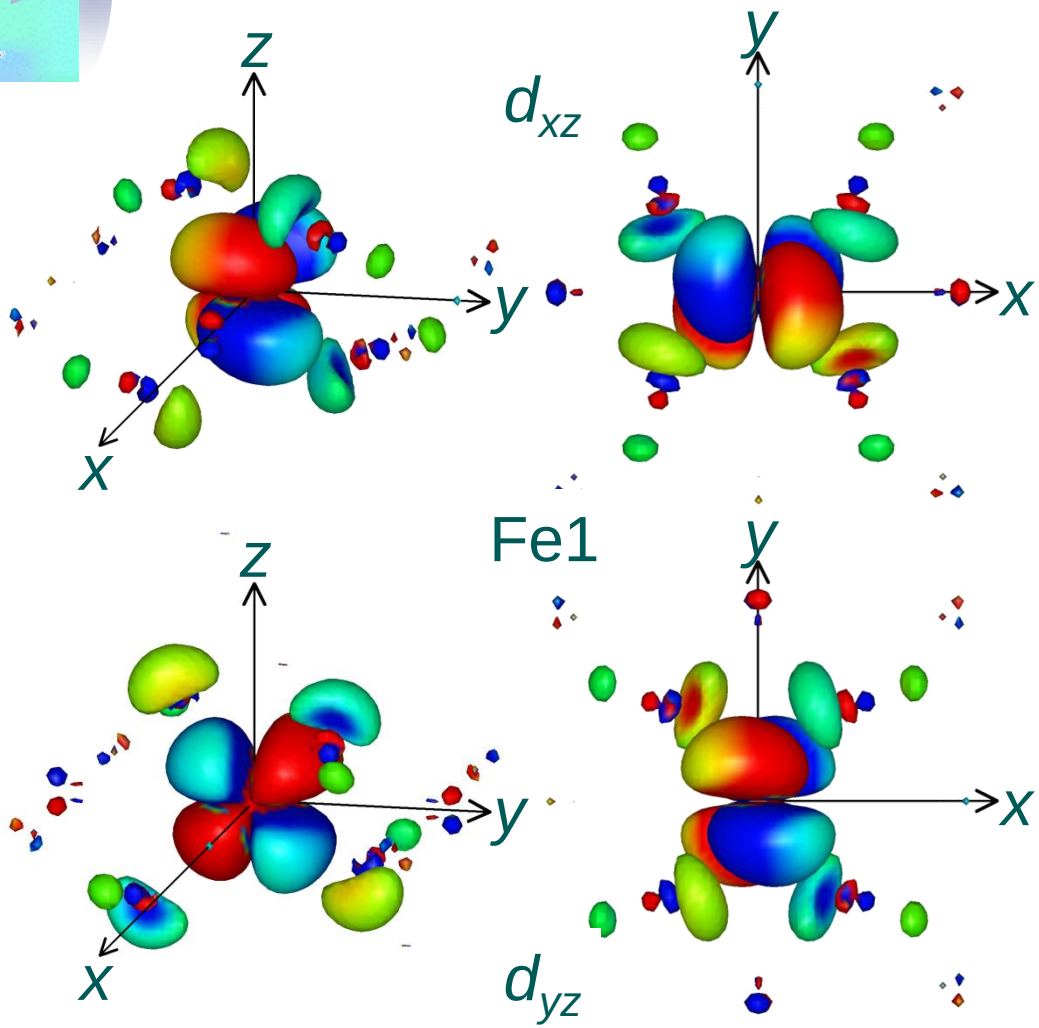
<WFs|H|WFs>	Fe1 z^2	x^2-y^2	yz	xz	xy
Fe2 (Fe4) z^2	0.13	0.31 (-0.31)	-0.10 (0.00)	0.00 (0.10)	0.00
x^2-y^2	0.31 (-0.31)	-0.32	0.42 (0.00)	0.00 (0.42)	0.00
yz	-0.10 (0.00)	0.42 (0.00)	-0.40 (-0.13)	0.00	0.00 (0.23)
xz	0.00 (0.10)	0.00 (0.42)	0.00	-0.13 (-0.40)	-0.23 (0.00)
xy	0.00	0.00	0.00 (0.23)	-0.23 (0.00)	-0.30
Fe3 z^2	0.06	0.00	-0.08	0.08	0.26
x^2-y^2	0.00	-0.10	0.12	0.12	0.00
yz	0.08	-0.12	0.25	-0.07	-0.05
xz	-0.08	-0.12	-0.07	0.25	0.05
xy	0.26	0.00	0.05	-0.05	0.16

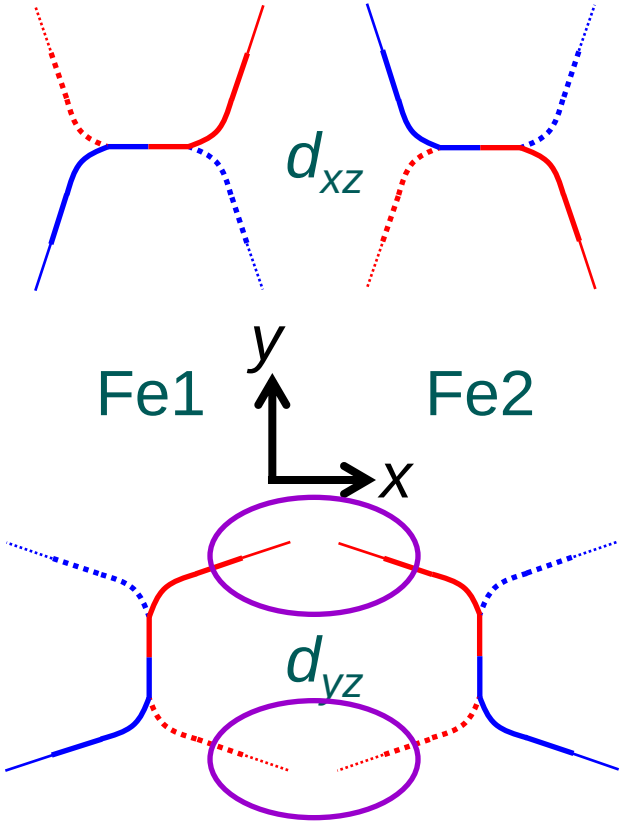


- Unusual coupling direction
- Cubic symmetry broken seriously by As
  → Fe-As phonon modes important
- Perpendicular hopping direction!

Chi-Cheng Lee *et al.*, PRL **103**, 267001 (2009)

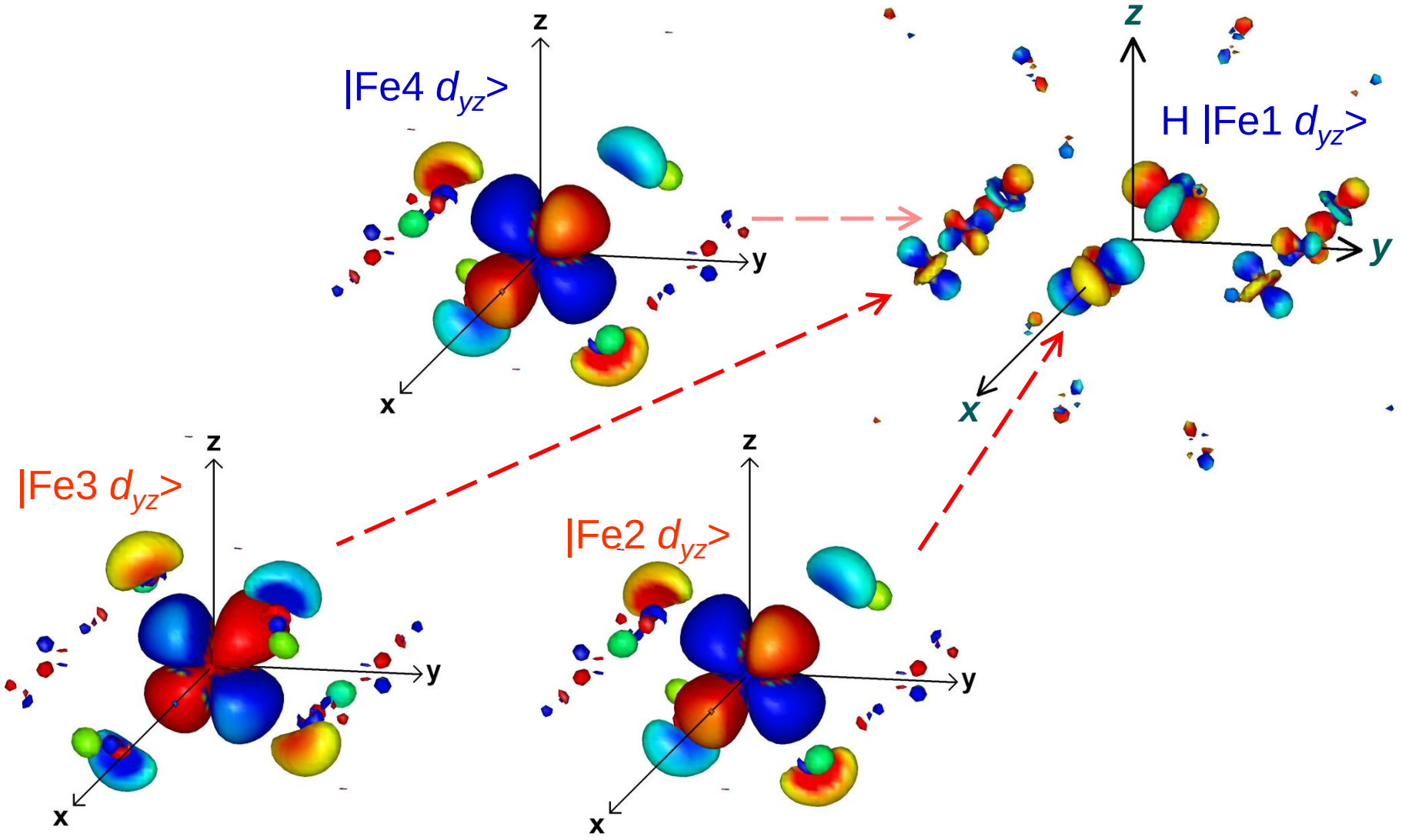
Examples of low-E Wannier functions



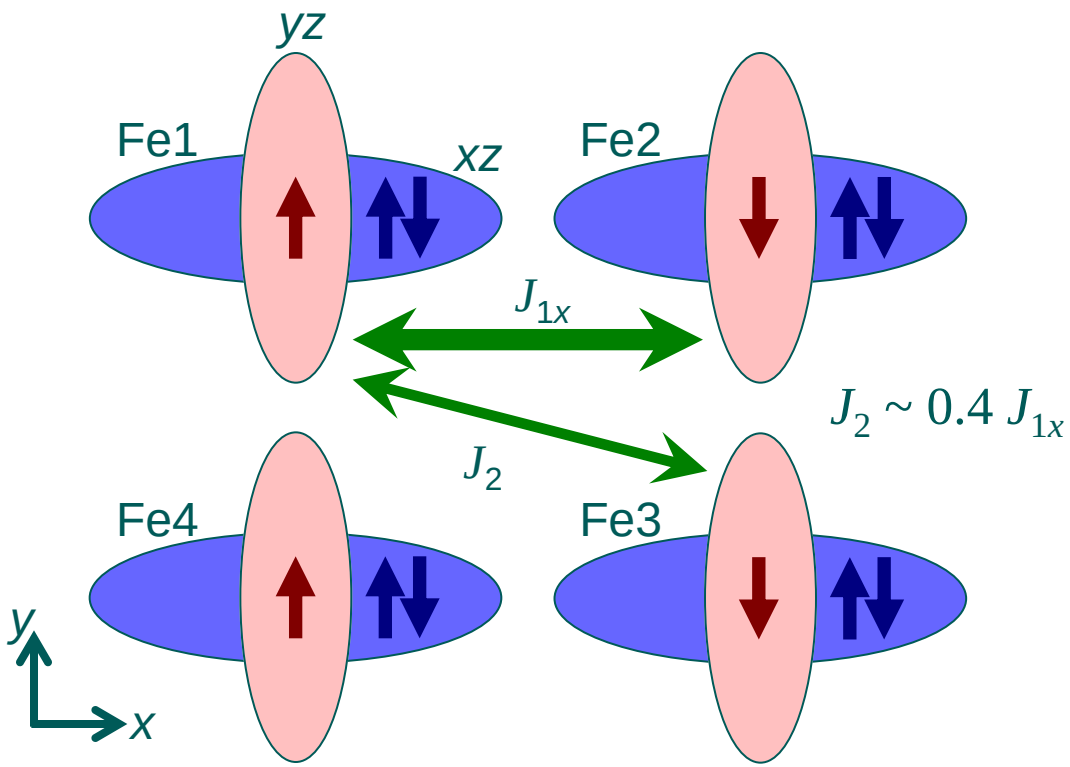


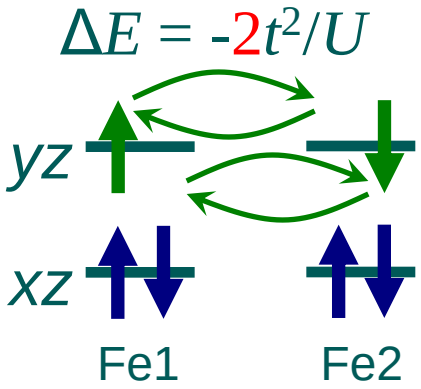
- Most relevant to the low-E
- The only ones that knows x != y
- Perpendicular extension of the hybridization tail due to As atoms !

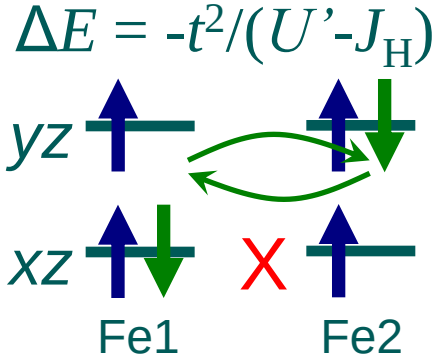
Unusual coupling made possible by As tetrahedron



C-AF magnetic structure and ferro-orbital order



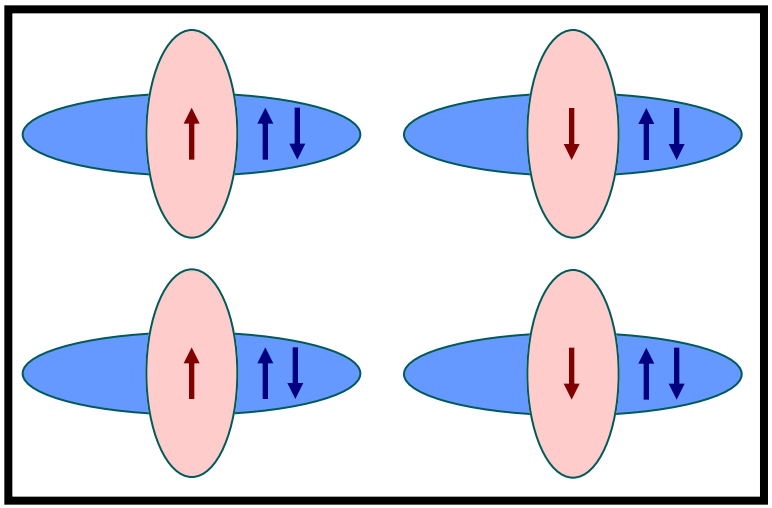


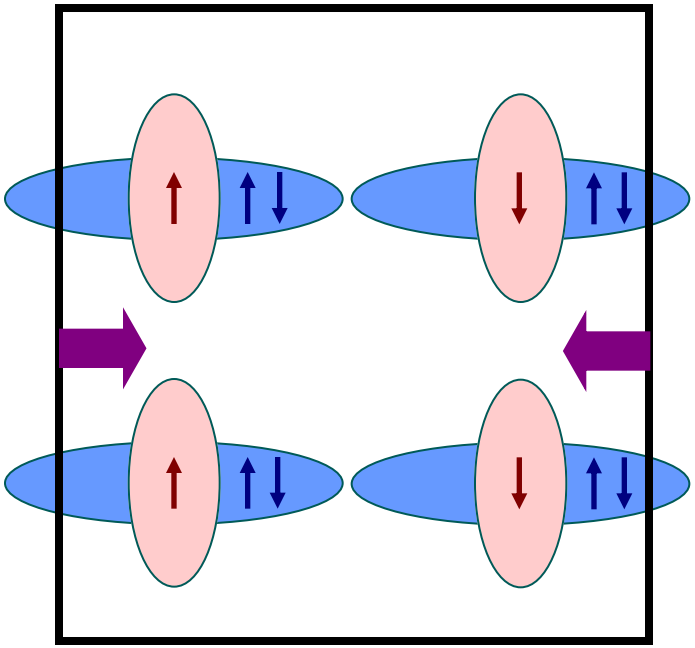


- Strongly anisotropic super-exchange: $J_{1x} > J_2 >> J_{1y}$
  - → no competition with G-AF at all ! $J_1 \sim 2J_2$ irrelevant !
  - → single orbital Heisenberg model inadequate
- Orbital polarization and ferro-orbital correlation important
  - → rotational symmetry breaking
- Unusual coupling direction !
  - → common staggered OO loses
  - → *a* > *b*: AF across long bond (rare)

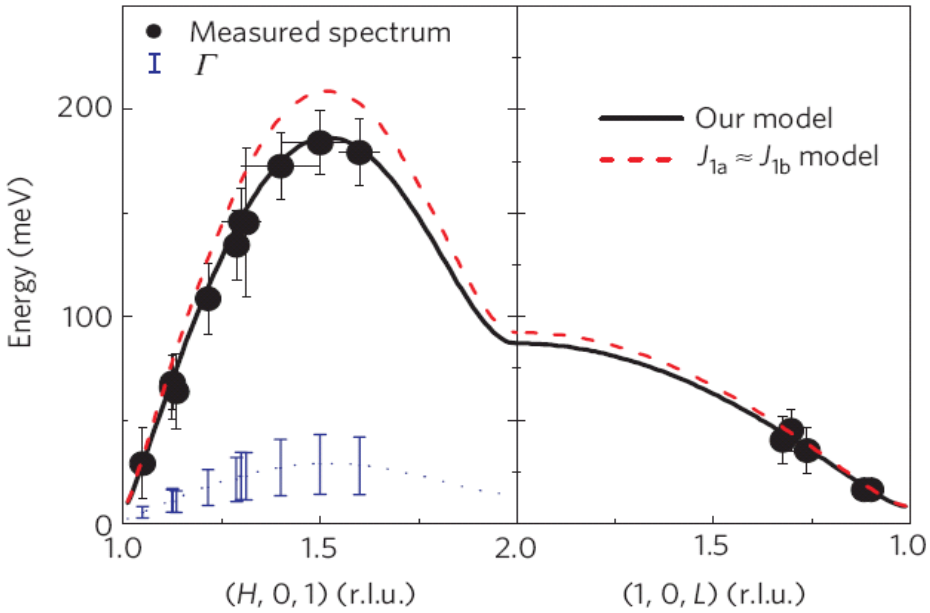
Strong coupling between magnon & light orbiton

Weak electron-lattice coupling
(ΔE <10meV/Fe compared to >100meV/Mn)





Inelastic Neutron Scattering



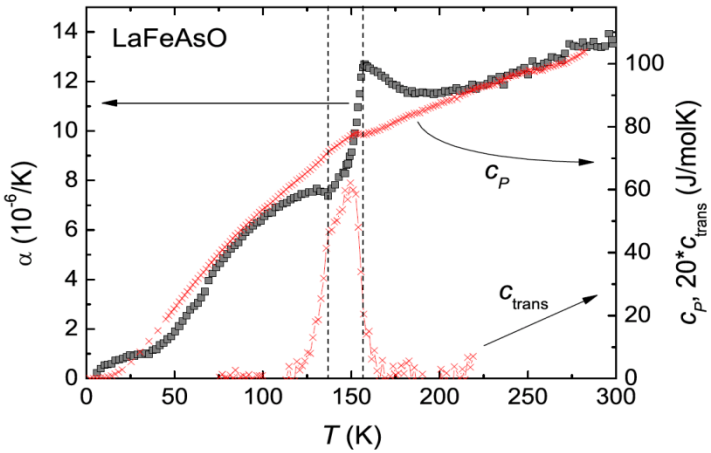
J. Zhao *et al.*, Nature Phys. **5**, 555 (2009)

magnon decay at larger q ?

Lattice, spin, & orbital

- ΔE < 10 meV with frustrated lattice distortion ($a < b$)
  - → negligibly weak "Jahn Teller" effects
  - → lattice just follows OO at $T_s = T_{OO} \sim 155$
  - → lattice does not help OO → $T_{OO} \sim T_N$
  - → OO has entirely electronic origin
  - → short-range orbital correlation above TOO
  - → anomalous thermal expansion up to T_s+40K
  - → light orbiton mass
- Same kinetic energy that drives C-AF and OO
  - → cooperative C-AF & OO → $T_N \sim T_{OO}$
  - → strong coupling between magnon & orbiton
  - → magnon decay at larger q? (J. Zhao et al., arXiv:0903.2686 (2009))
  - → large isotope effects in magnon & orbiton dispersion

(R. H. Liu, arXiv:0810.2694 (2009))



(Wang et. al., cond-mat 0903.1235)

Strongly correlated metal & implications to SC

- Success of local MB considerations
  - → Fermi surface nesting not necessary
  - → more general, no need for good coherence
  - → UD Fe-pnictides are likely strongly correlated metals
  - → reduction of average moment?
- New class of correlated materials
  - high-T_c as in cuprates, but
  - orbital freedom → fundamentally distinct from cuprates
  - orbital physics as in manganites, but
  - weak coupling to JT modes and light orbiton mass
    → qualitatively different physics from manganites
- Implications to SC
  - pairing via exchanging orbiton?
  - inclusion of orbiton coupling to magnon necessary
  - correlated nature → stronger coupling to all glues than MF estimation
  - SC at UD Fe-pnictides likely in strong coupling regime
    → low superfluid density with high T_c

(H. Luetkens, PRL **101**, 097009 (2008))

Summary

- Stripy C-AF spin correlation ⇔ ferro-orbital correlation
- Anisotropic coupling
  - → No competition with G-type AF
  - → Orbital degree of freedom essential
  - → Single orbital Heisenberg model inadequate
  - → Fundamentally distinct from cuprates
  - → Unusual hopping direction due to As tetrahedron → AF bond longer ☺
- Robust short-range correlation
  - Fermi surface nesting unnecessary (more general than standard SDW)
  - Allows incoherent but coupled orbital and spin fluctuation

How about superconductivity?

- Implies strong electron coupling to magnon + orbiton

  explicit inclusion of orbital freedom needed
- Also implies stronger coupling to phonon than previously estimated

  mean-field approaches not good enough
- UD systems likely in strong coupling regime

Unified picture of magnetism of C-type (1111, 122,…) & E-type (11)

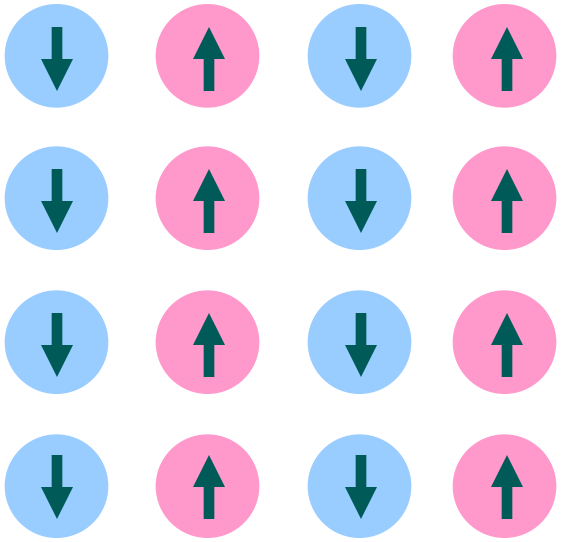
Weiguo Yin, Chi-Cheng Lee & Wei Ku

Phys. Rev. Lett. **105**, 107004 (2010)

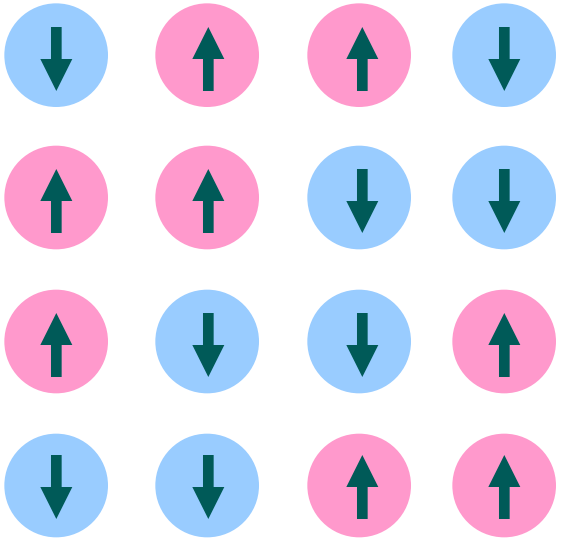
Families of Fe-based High Temperature Superconductor

Magnetic structure of parent undoped compound

C-type
stripe-like
collinear



E-type
double stripe
bicollinear



1111 (e.g. $LaO_{1-x}F_xFeAs$)
122 (e.g. $Ba_{1-x}K_xFe_2As_2$)
111 (e.g. Li_xFeAs)

11 (e.g. $FeTe_{1-x}Se_x$)

Orbital-degenerate double-exchange model

$$H = -\sum_{ij\gamma\gamma'\sigma} (t_{ij}^{\gamma\gamma'} d_{i\gamma\sigma}^{\dagger} d_{j\gamma'\sigma} + h.c.) - K \sum_{i} \vec{s}_i \cdot \vec{S}_i + \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

- "Itinerant" electrons: xz and yz.
- "Localized" spins: the rest of Fe 3d orbitals.

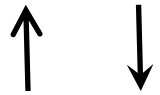
Background

- *Solvation of U but not J.* Sawatzky et al., *EPL* 86, 17006 (2009).
  - *U*=2 eV, *J*=0.8 eV, Yang et al., PRB 80, 014508 (2009).
- *Reversed strong anisotropy in the n.n. hoppings of xz and yz*
  - Lee et al., PRL 103, 267001 (2009).
- *Strongly spin-dependent electron transport in $BaFe_2As_2$.*
  - Chuang et al., *Science* 327, 181 (2010).

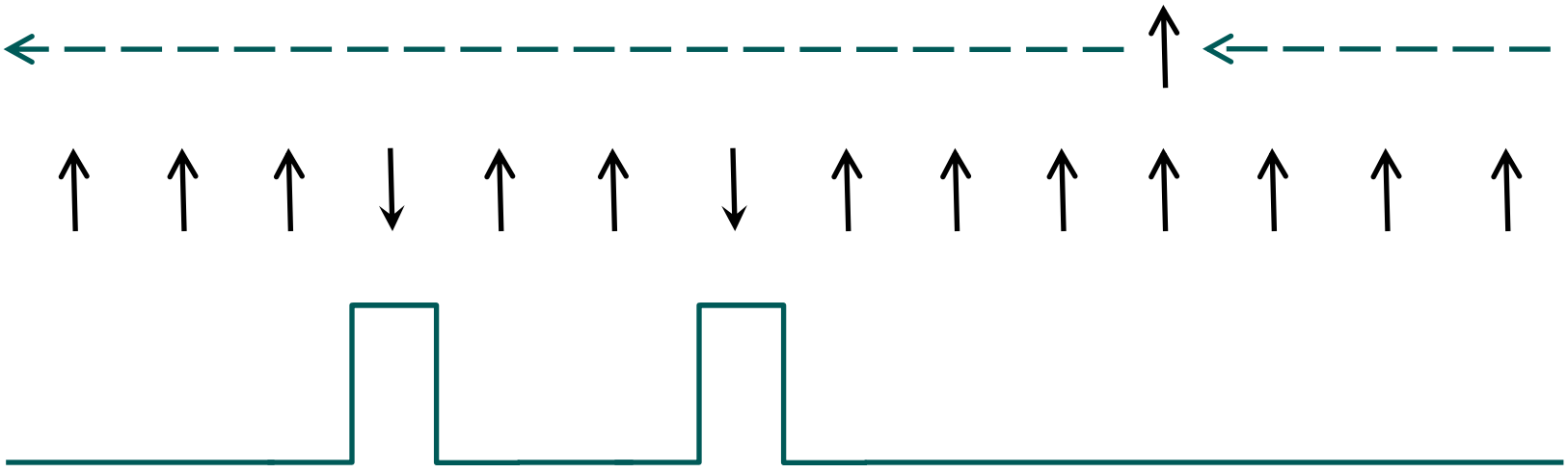
W.-G. Yin et al, PRL **105**, 107004 (2010)

Super Exchange vs. Double Exchange

- Super exchange between local moments → local AF coupling

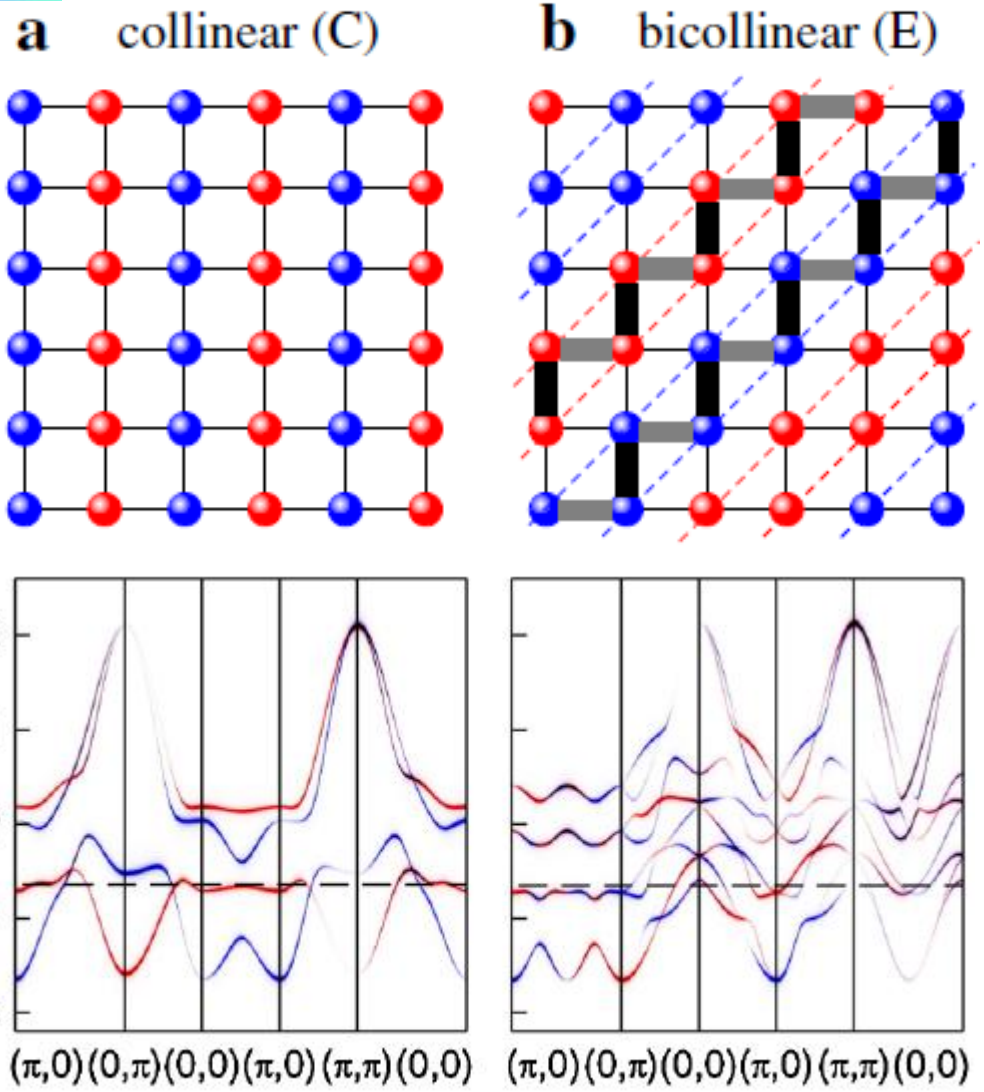


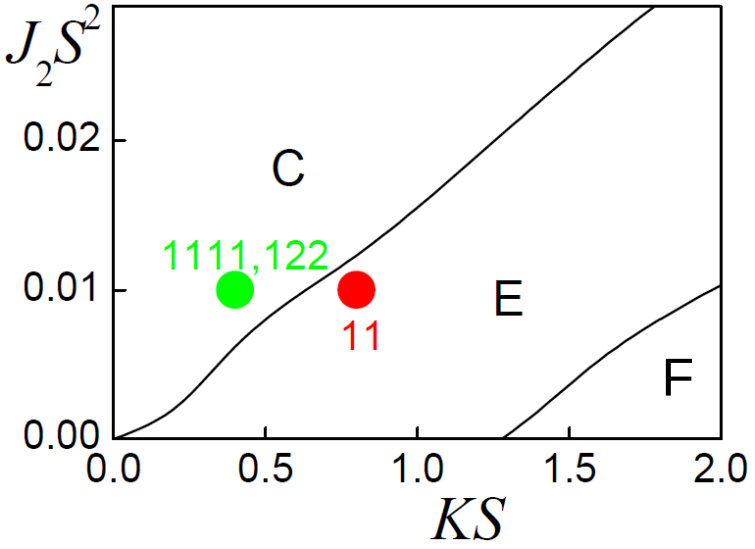
- Double exchange effects → range-dependent FM coupling



→ intrinsic instability with AF-coupled 1D FM chains

Simple mean-field estimation

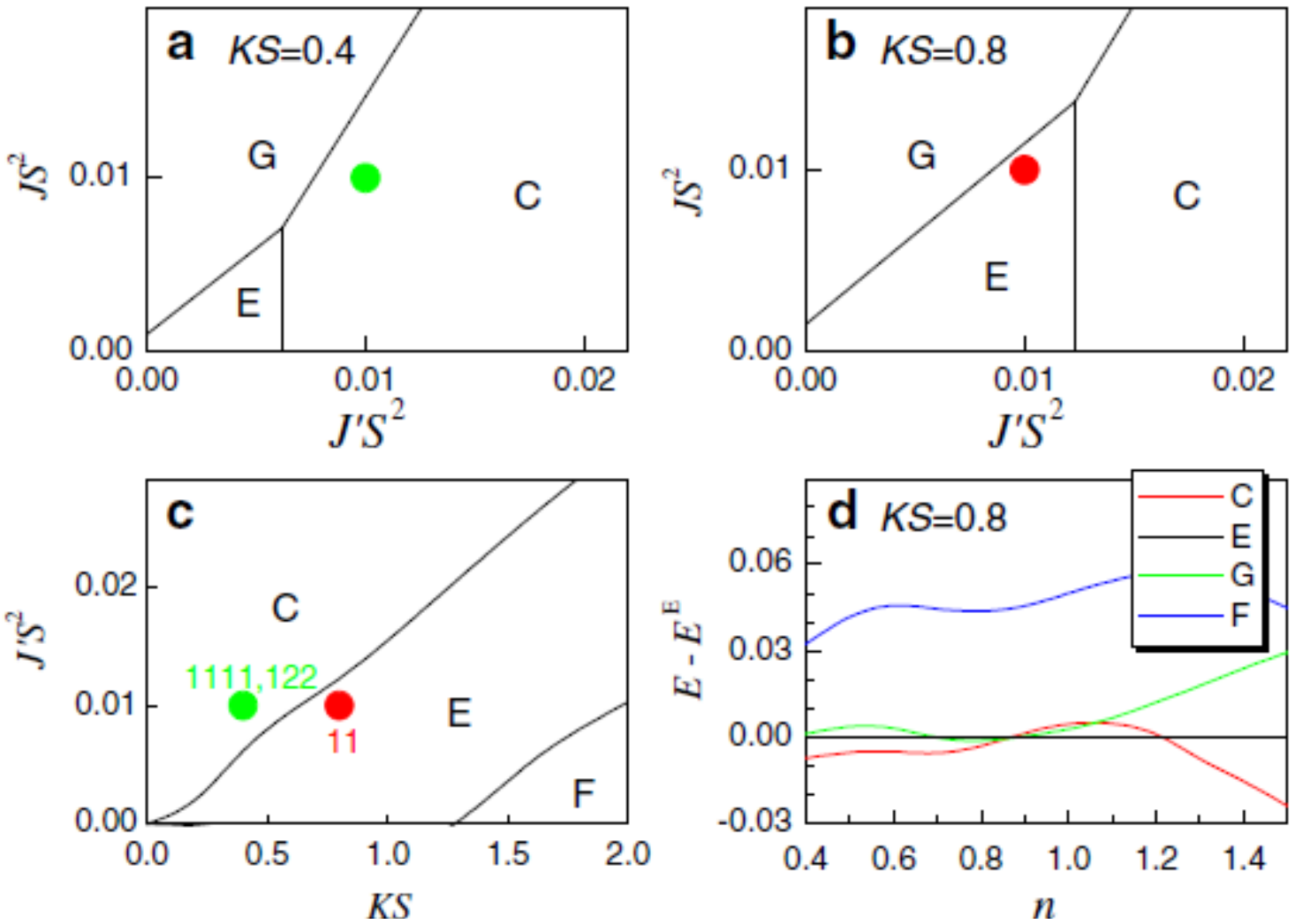




- C-type ← J_2S^2
- E-type ← KS & KE

W.-G. Yin et al, PRL **105**, 107004 (2010)

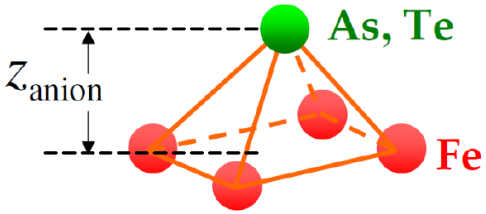
Simple mean-field estimation



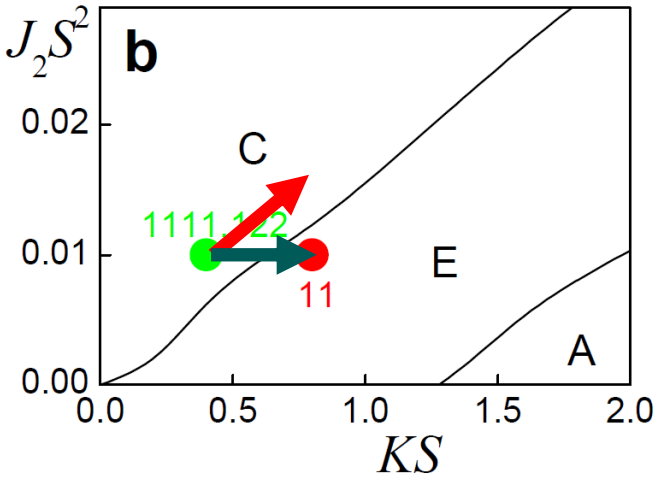
- Suppression of F-type → one less competitor for SC
- Vulnerability of E-type against doping → ~ exp.

W.-G. Yin et al, PRL **105**, 107004 (2010)

Verification using first-principles calculations



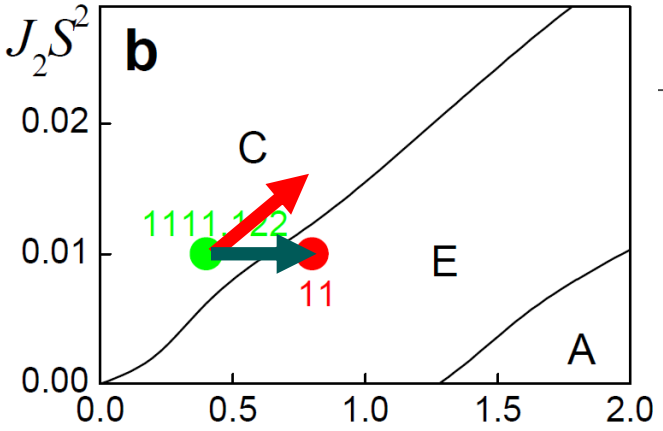
	LaOFeAs (Ref. 7)	$BaFe_2As_2$ (Ref. 8)	$Fe_{1.068}Te$ (Ref. 9)
z_{anion} (Å)	1.31	1.35	1.73
Magnetic moment (μ_B)	0.36	0.87	1.70



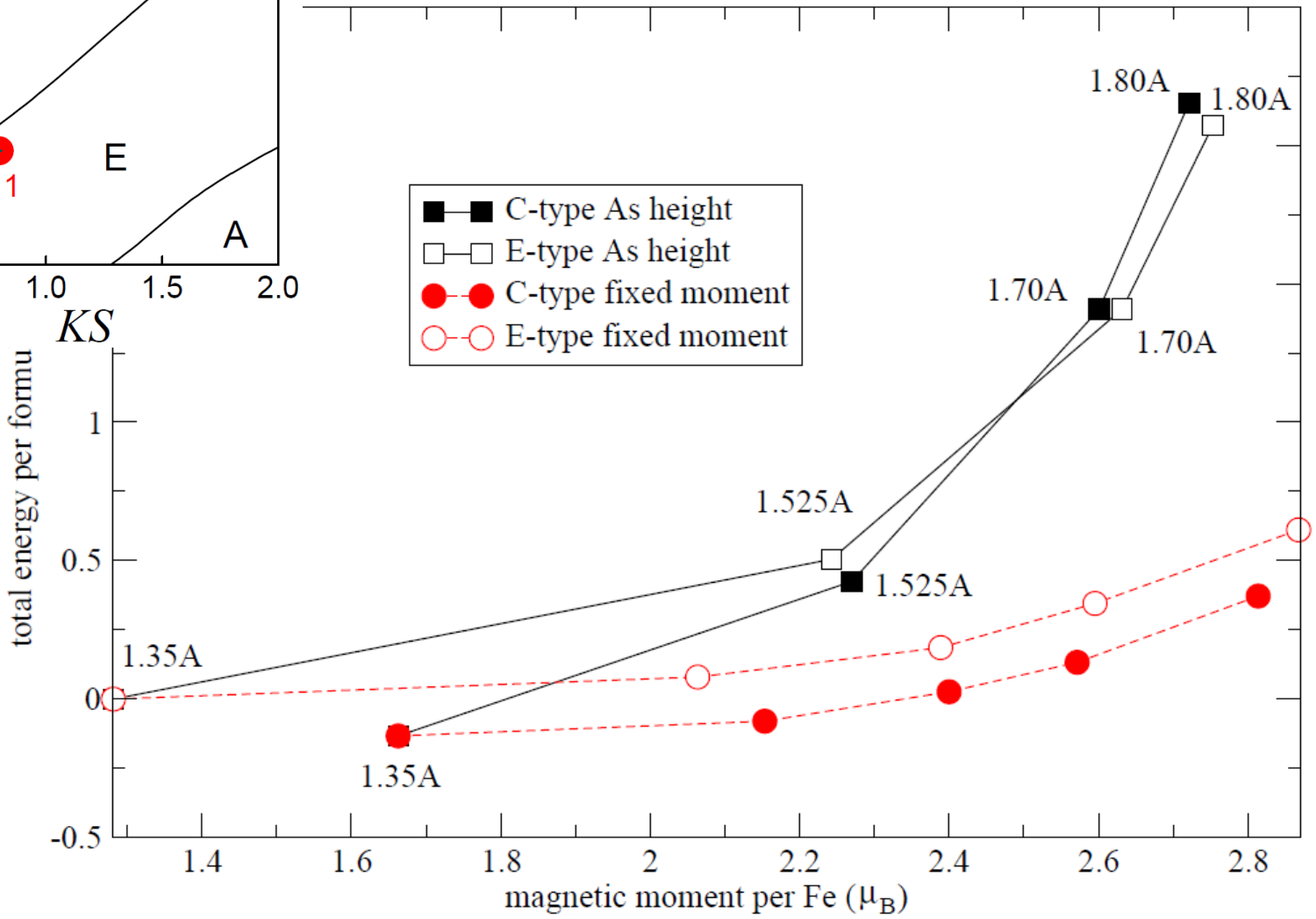
- Path 1: KS → increasing z_{anion}
- Path 2: S → increasing spin

C.-C. Lee et al, in preparation

Verification using first-principles calculations



$BaFe_2As_2$



C.-C. Lee et al, in preparation

Summary

$$H = -\sum_{ij\gamma\gamma'\sigma} (t_{ij}^{\gamma\gamma'} d_{i\gamma\sigma}^{\dagger} d_{j\gamma'\sigma} + h.c.) - K\sum_{i} \vec{s}_i \cdot \vec{S}_i + \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

- Unifying magnetic correlations

  → essentially all observed magnetic correlations included in the zero-order
- Unveiling strong correlated nature

  → quantum spin

  → incoherent normal-state electron transport, similar to manganites

  → Not proximity to the Mott state

Conclusion

- Stripy C-AF spin correlation ⇔ ferro-orbital correlation
- Anisotropic coupling
  - → No competition with G-type AF
  - → Orbital degree of freedom essential
  - → Single orbital Heisenberg model inadequate
  - → Fundamentally distinct from cuprates
  - → Unusual hopping direction due to As tetrahedron → AF bond longer ☺
- Robust short-range correlation
  - Fermi surface nesting unnecessary (more general than standard SDW)
  - Allows incoherent but coupled orbital and spin fluctuation
- Unification via degenerate double exchange model
  - → Competition between KE of itinerant electron and SE of local spins

How about superconductivity?

- Implies strong electron coupling to magnon + orbiton

  explicit inclusion of orbital freedom needed
- UD systems likely in strong coupling regime