

A simple effective theory for AF correlated superconductors; Interface high T_c superconductivity

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Collaborators:

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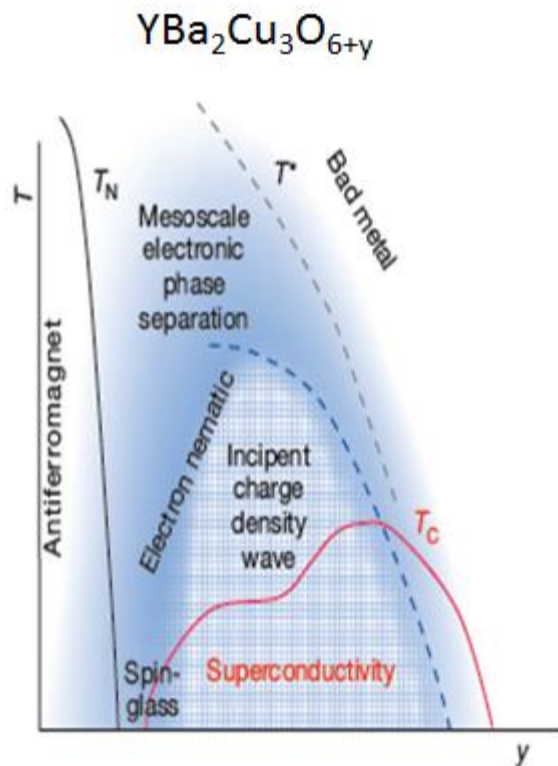
Fan Yang (Beijing Tech)

Hui Zhai (Tsinghua U)

- H. Zhai, F. Wang and D.-H. Lee, PRB 80, 064517 (2009).
- F. Wang and D.-H. Lee, Science, 332, 200 (2011)
- J.C. Davis and D.-H. Lee, PNAS 110, 17623 (2013).
- J.J Lee et al, Nature accepted.

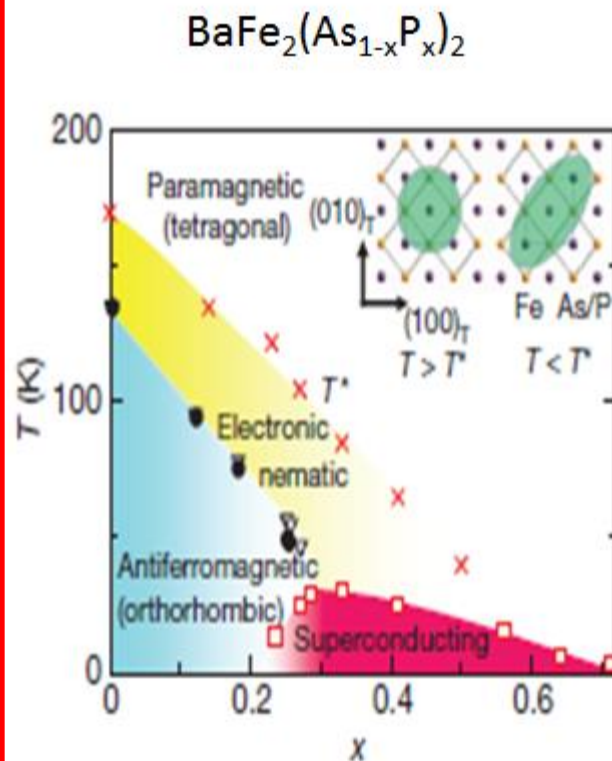
Antiferromagnetically Correlated Superconductors

Cu-based Superconductors (Cuprates)



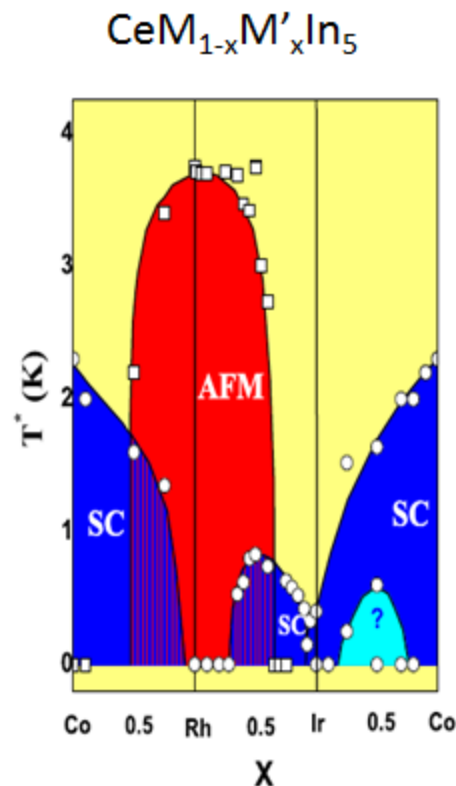
Fradkin, Kivelson, Nature Physics 864 (2012)

Fe-based Superconductors



Matsuda et al, Nature 486, 382 (2012)

Heavy fermion Superconductors



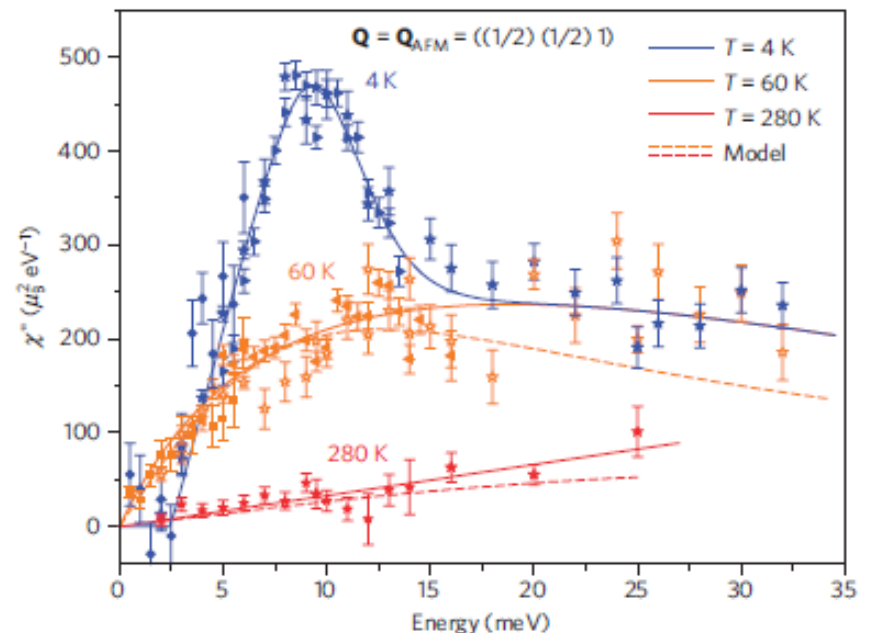
Pagliuso et al, Phys. Rev. B 64, 100503 (2001)

Note the “intertwined” orders.

Normal-state spin dynamics and temperature-dependent spin-resonance energy in optimally doped $\text{BaFe}_{1.85}\text{Co}_{0.15}\text{As}_2$

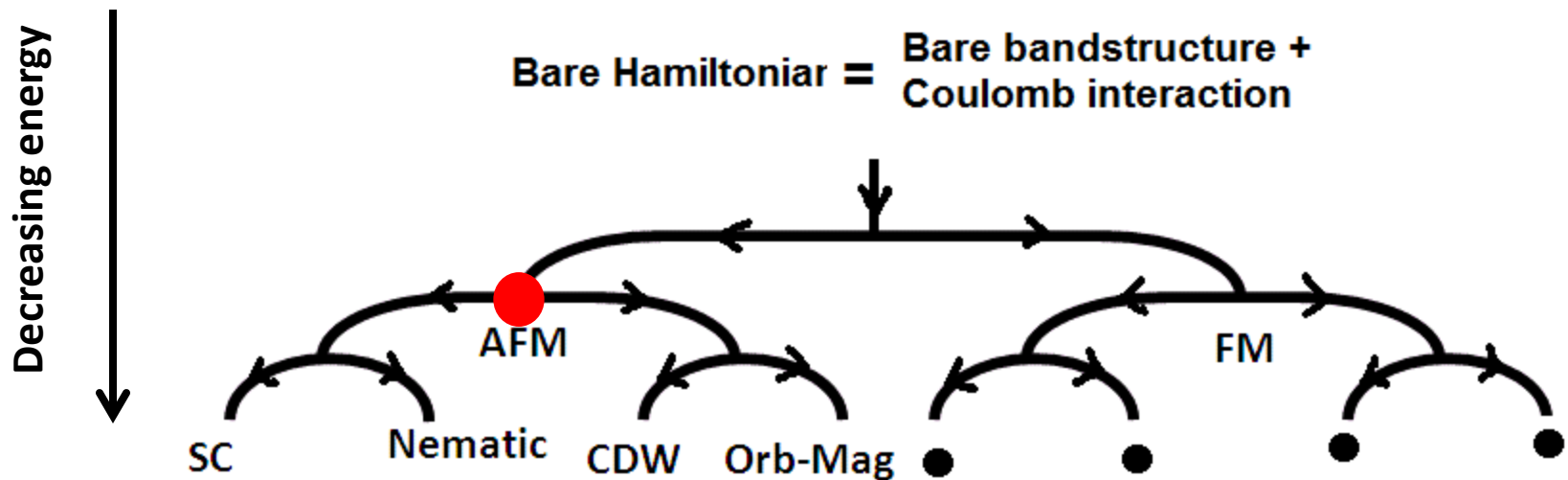
D. S. Inosov¹, J. T. Park¹, P. Bourges², D. L. Sun¹, Y. Sidis², A. Schneidewind^{3,4}, K. Hradil^{4,5}, D. Haug¹, C. T. Lin¹, B. Keimer¹ and V. Hinkov^{1*}

The total spectral weight at 60 K, integrated over Q and ω up to 35 meV, is $\chi''_{60\text{K}} = 0.17 \mu_B^2/\text{f.u.}$, and is thus comparable to underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$.



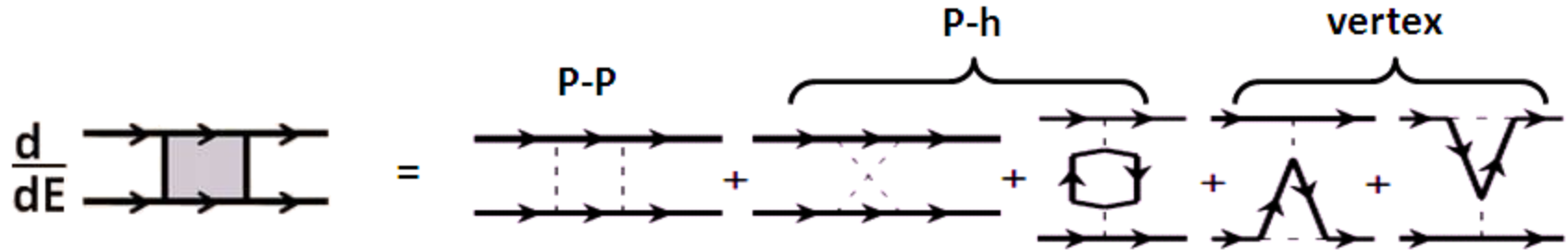
The interaction responsible for Cooper pairing is an **effective** interaction.

- For strongly correlated systems the evolution of the effective Hamiltonian as a function of energy can go through many unexpected modifications.



Capture the effective Hamiltonian at the energy scale at which bifurcation occurs helps understanding the mechanism for intertwined phases.

In recent years attempts at deriving the effective pairing interaction through perturbative renormalization group calculation have been made.



Copper-based SC

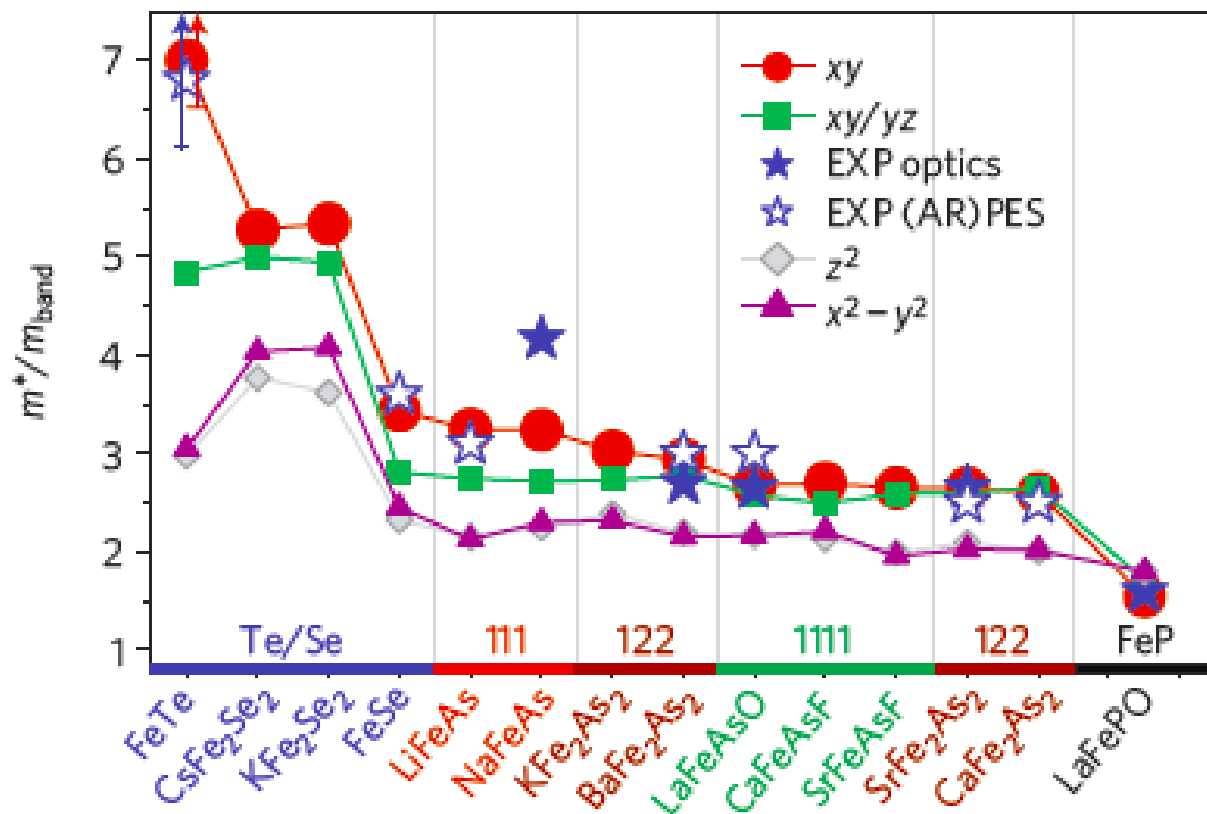
- Honerkamp, Rice *et al*, PRB 63, 035109 (2001).

Iron-based SC

- F. Wang *et al*, PRL 102,047005 (2009); H. Zhai *et al*, PRB 80, 064517 (2009); F. Wang and Lee, Science 332, 200 (2011).
R. Thomale *et al*, Phys. Rev. B 80, 180505 (2009).

*A derivation of the effective interaction valid for strong coupling is lacking.

DFT+DMFT results for the correlation strength in Fe-based superconductors



Yin, Haule, Kotliar, Nature Materials 10, 932 (2011)

Strong correlation : Q. M. Si, E. Abrahams, Phys. Rev. Lett. 101, 076401 (2008).

Functional RG results

F. Wang et al, arXiv 0805.3343 (May 2008)

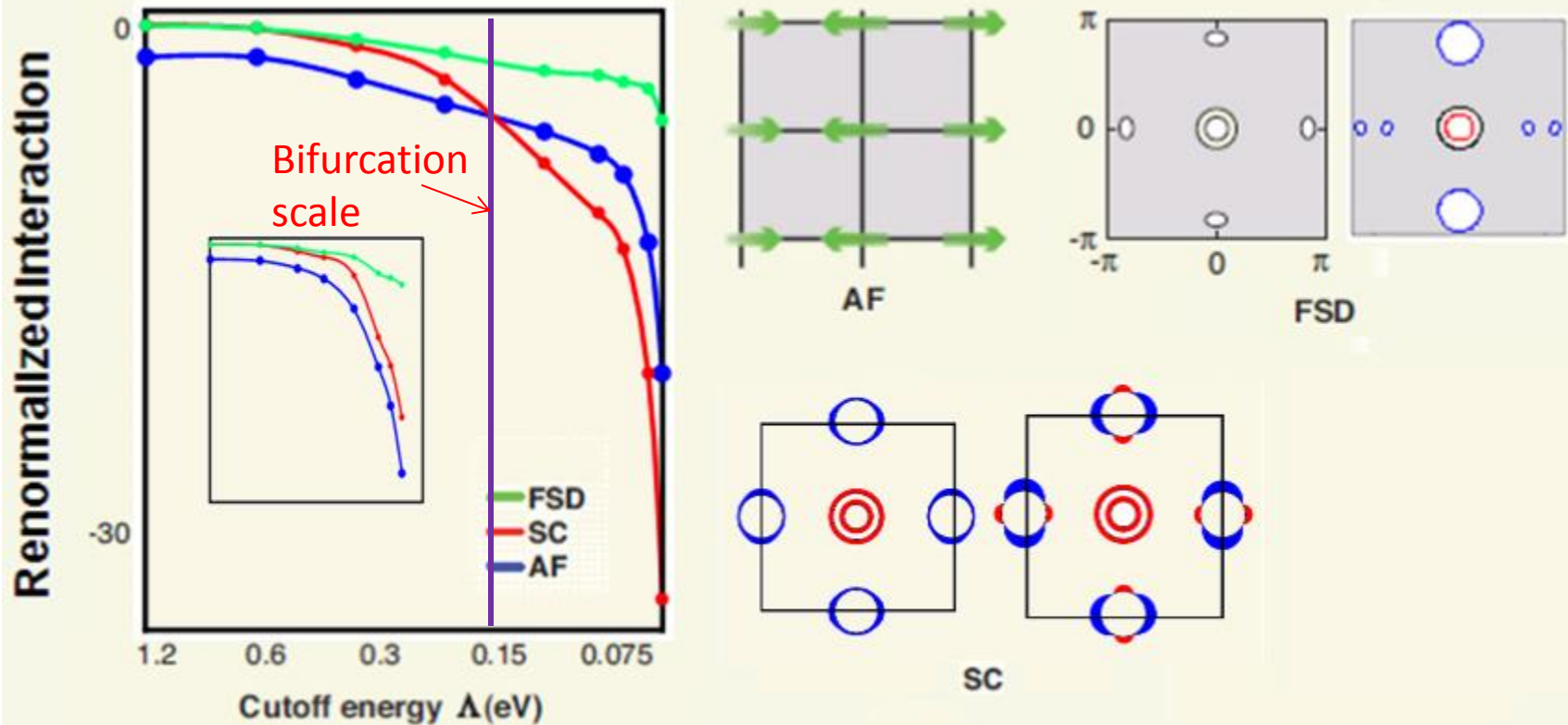
F. Wang et al, PRL 102,047005 (2009)

H. Zhai et al, Phys. Rev. B 80, 064517 (2009).

F. Wang and DHL, Science, 332, 200 (2011).

H= bandstructure + Hubbard Hunds model $U=4\text{eV}$, $V=2\text{ eV}$, $J=0.7\text{ eV}$.

Three leading instabilities



Strong correlation

A variational Monte-Carlo study using partially projected WF

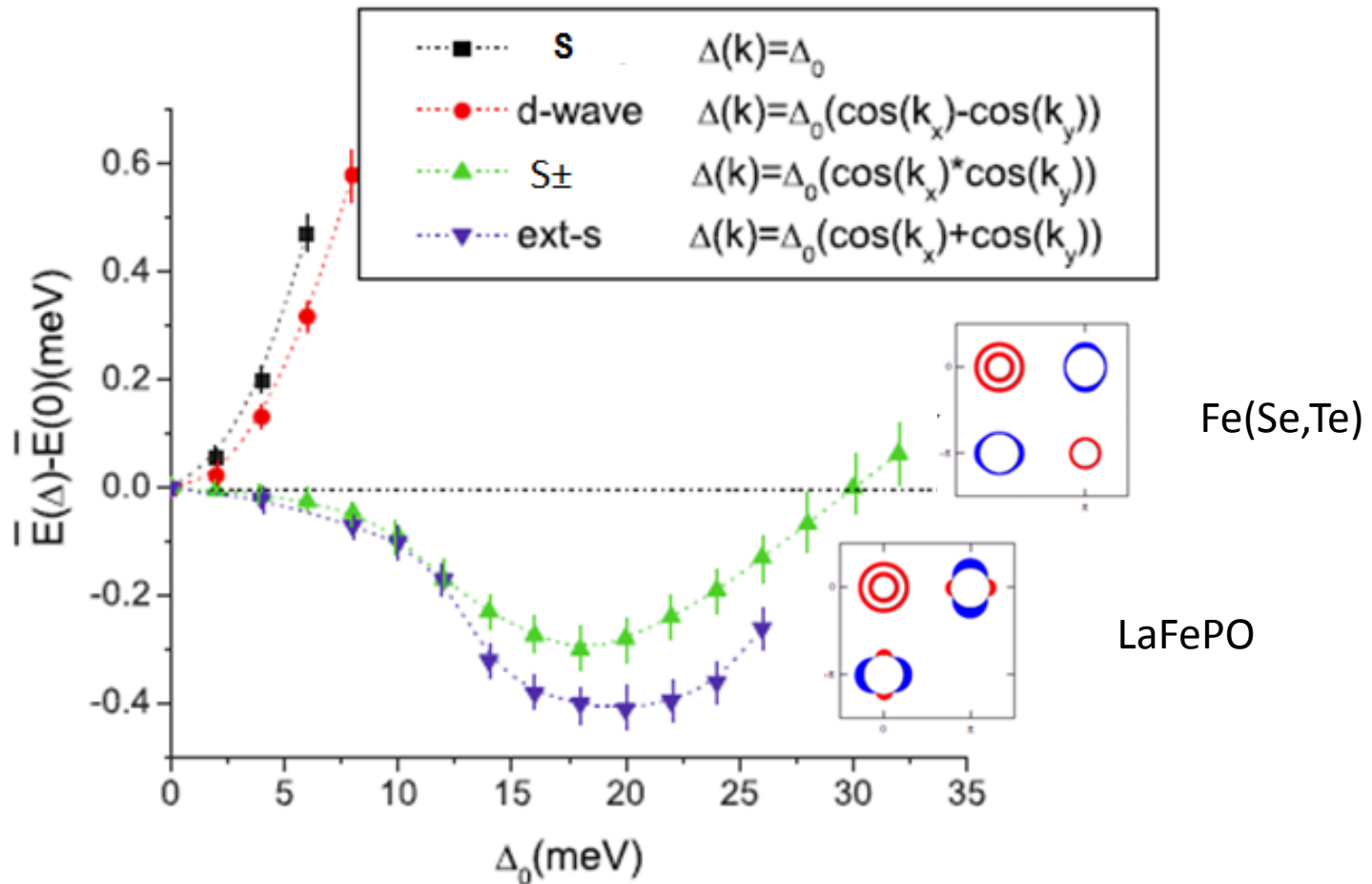
$$|\psi\rangle = g_1^{\hat{N}_1} g_2^{\hat{N}_2} \hat{P}_{N_e} |\psi_{MF}\rangle,$$

where

$$\hat{N}_1 = \sum_{i,\mu} \hat{n}_{i\mu\uparrow} \hat{n}_{i\mu\downarrow}, \quad \hat{N}_2 = \sum_{i,\mu < \nu} \hat{n}_{i\mu} \hat{n}_{i\nu}.$$

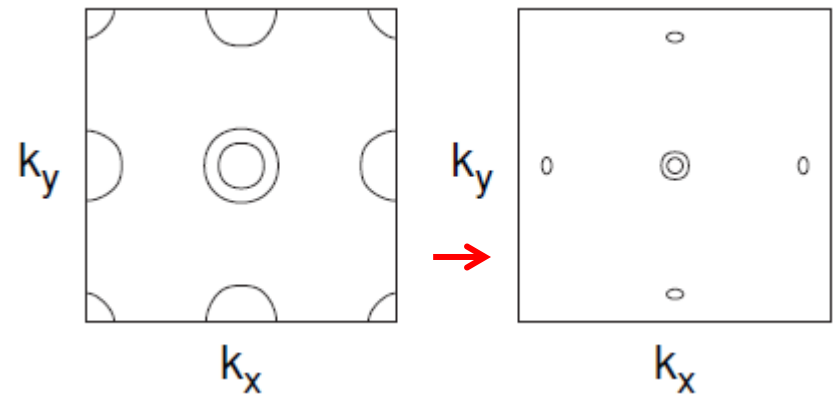
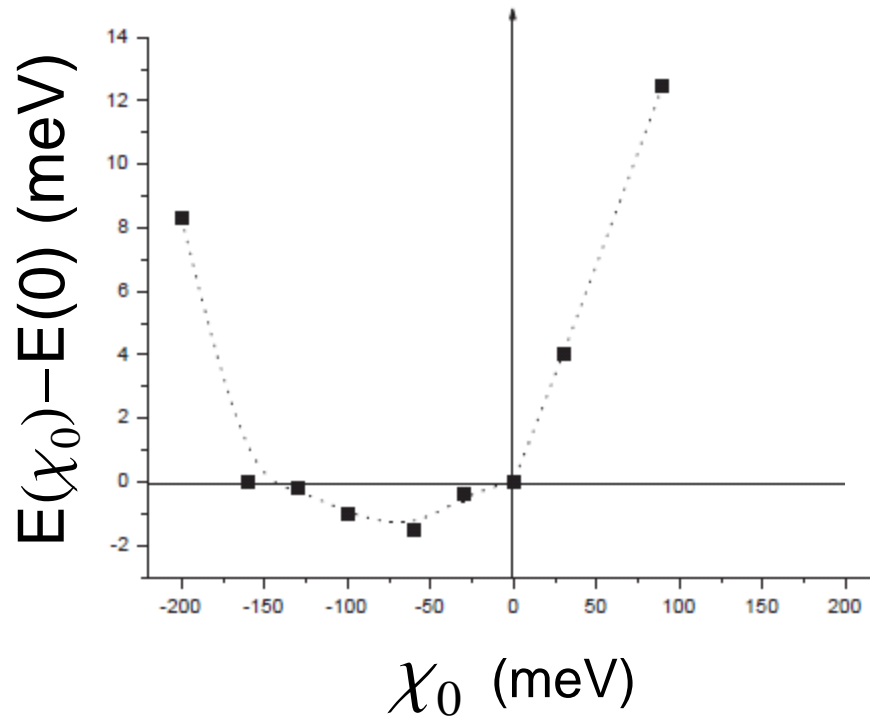
Cooper pairing

Band structure + Hubbard Hunds model $U=4\text{eV}$, $V=2\text{ eV}$, $J=0.7\text{ eV}$.



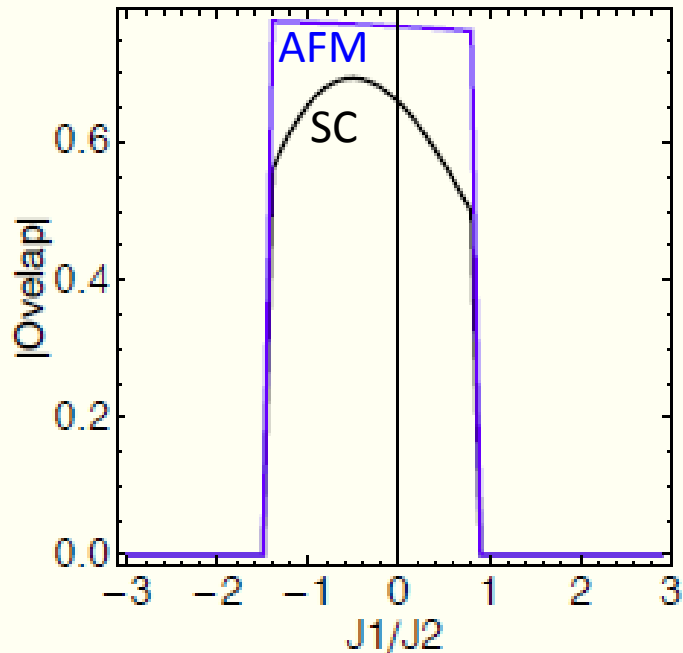
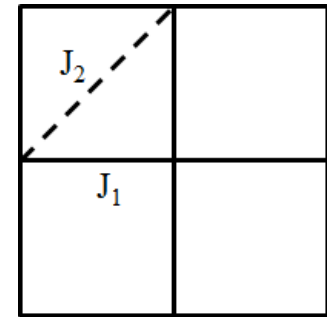
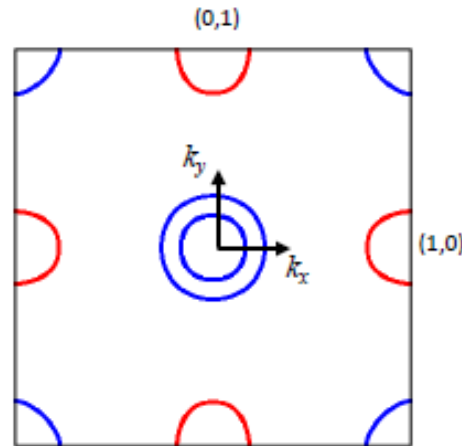
Fermi surface distortion

$$H_{MF} = \sum_{\mathbf{k}\alpha\sigma} (\varepsilon_{\mathbf{k}}^{\alpha} + \chi(\mathbf{k})) n_{\mathbf{k}\alpha\sigma} \quad \chi(\mathbf{k}) = \chi_0 \cos k_x \cos k_y$$



A hint at the effective interaction

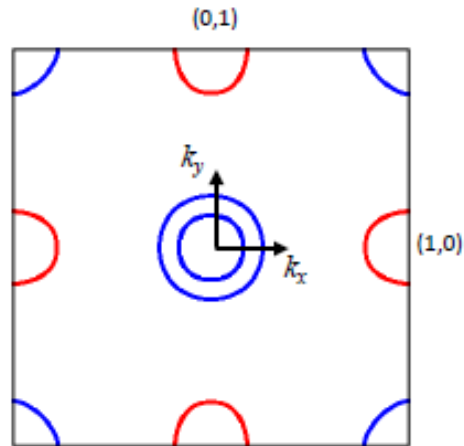
$$H_{eff} = \sum_{\mathbf{k}}' \sum_s \epsilon(\mathbf{k}) n_s(\mathbf{k}) + \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$



Overlap= the overlap between the FRG order parameters for AFM and SC with those of the effective Hamiltonian

Consequences of the effective Hamiltonian

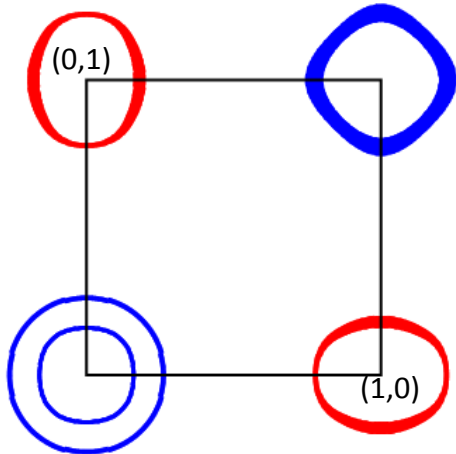
$$H_{eff} = \sum_{\mathbf{k}}' \sum_s \epsilon(\mathbf{k}) n_s(\mathbf{k}) + \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$



Iron-based SC

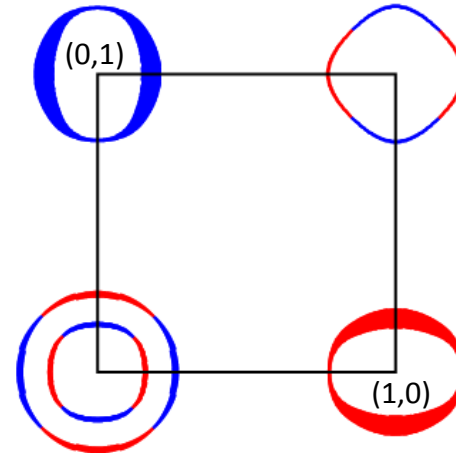
1. Cooper pairing

Leading order parameter



Symmetry : S_{\pm}

Sub-leading order parameter



Symmetry : d-wave

S. Graser et al, New J. Phys. 11, 025016 (2009)
J. Hu and H. Ding, Scientific Reports, 2, 381 (2012)
JC Davis and DHL, PNAS 110, 17623 (2013).

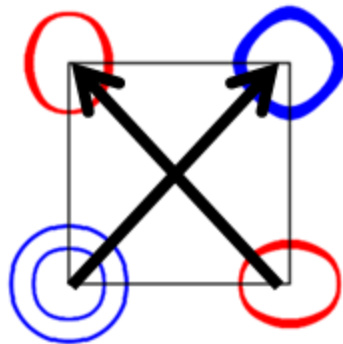
F. Wang, H. Zhai, and D.-H. Lee, EuroPhys. Lett. **85**, 37005 (2009).

Y.Y. Zhang et al, Phys. Rev. B **80**, 094528 (2009).

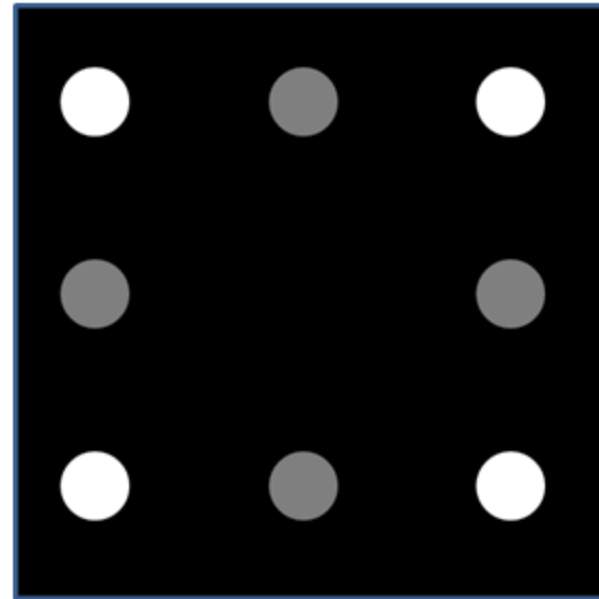
If impurity scattering is *particle-number conserving*;

$H=0$ time reversal invariant,

$H>0$ additional non-time reversal breaking terms contributes.



magnetic scattering



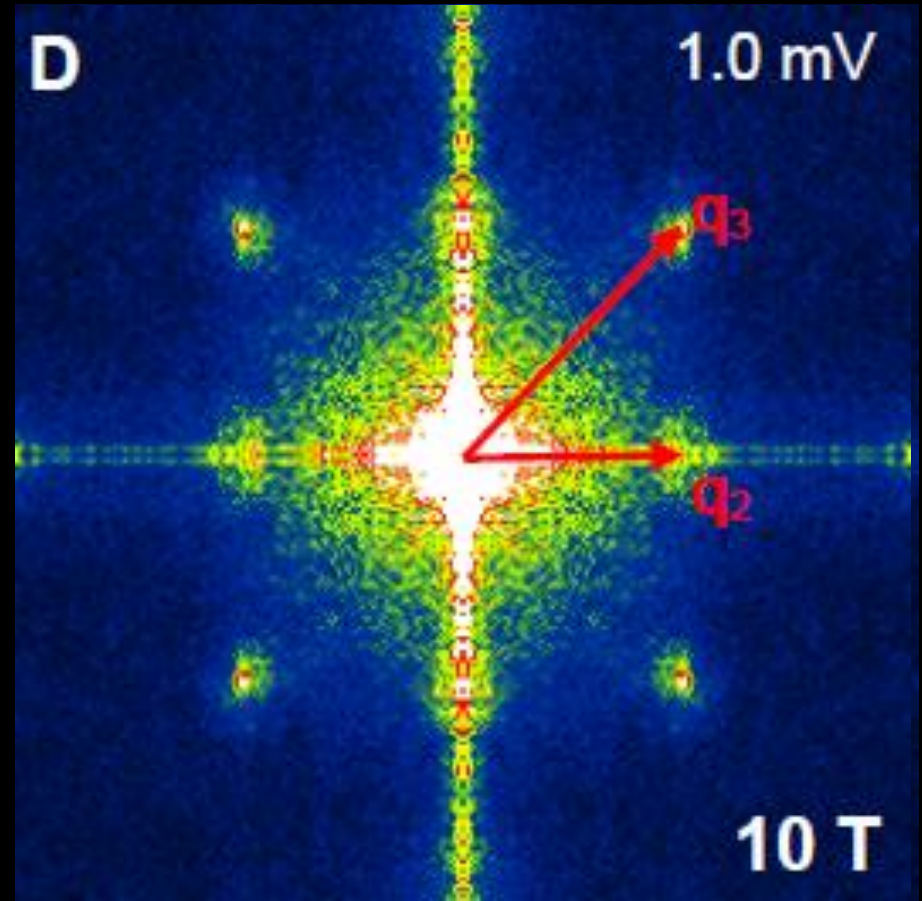
SI-STM on $\text{Fe}_{1+x}(\text{Se},\text{Te})$

$T_c \sim 13 \text{ K}$

$T \sim 1.6 \text{ K}$

$dI/dV_{+E}/dI/dV_{-E}$

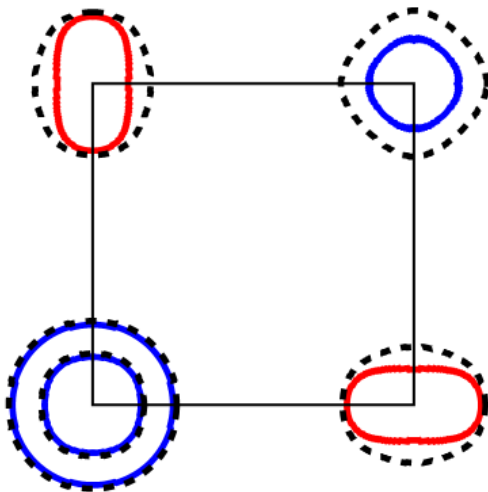
$34 \text{ nm} \times 34 \text{ nm}$, $-20 \text{ mV}/0.1 \text{ nA}$



Hanaguri et al, *Science* **328**,474 (2010)

2. $Q=0$ Fermi surface instability

Leading order parameter



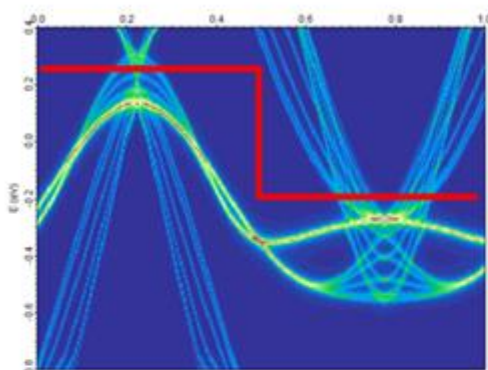
Symmetry : S-wave

No symmetry breaking

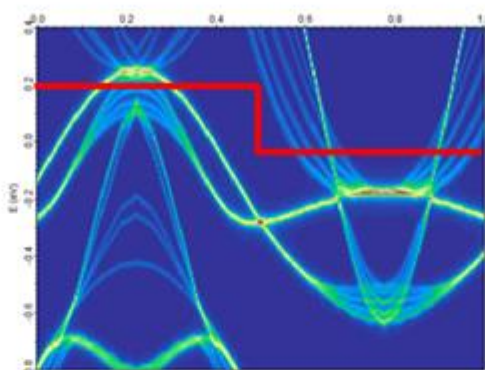
Net effect transfer of electrons from electron pockets to hole pockets \rightarrow Relative shift in the electron and hole bands.

A relative shift is necessary to make the theory band structure similar to the ARPES data

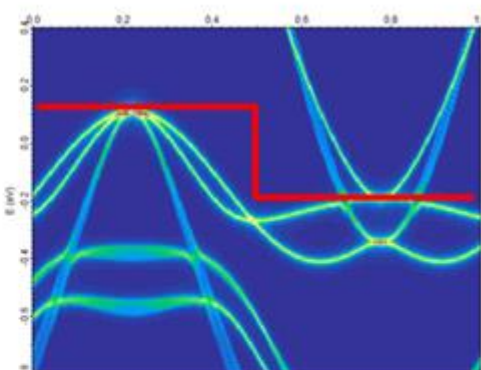
11



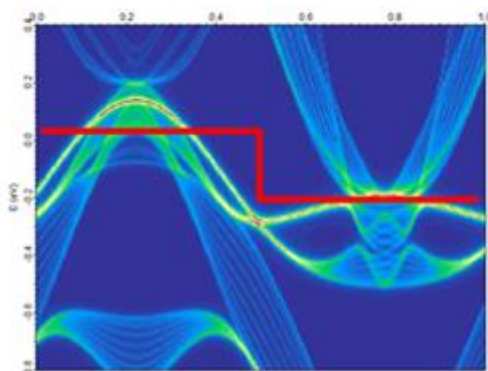
111



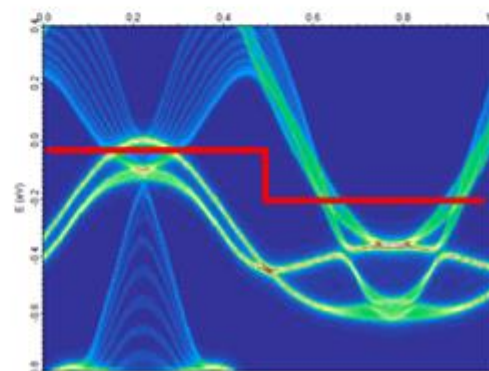
1111



122

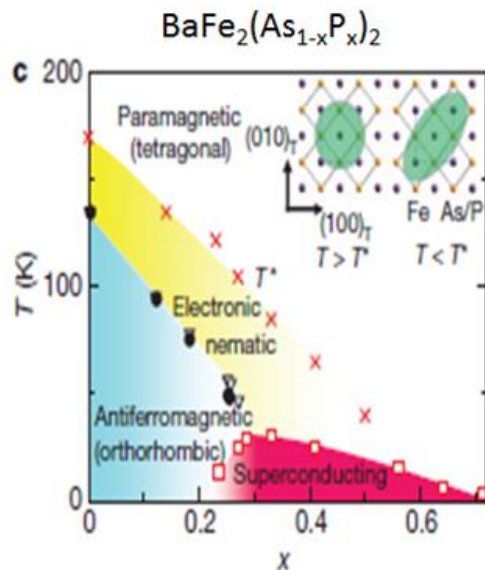


245(122)

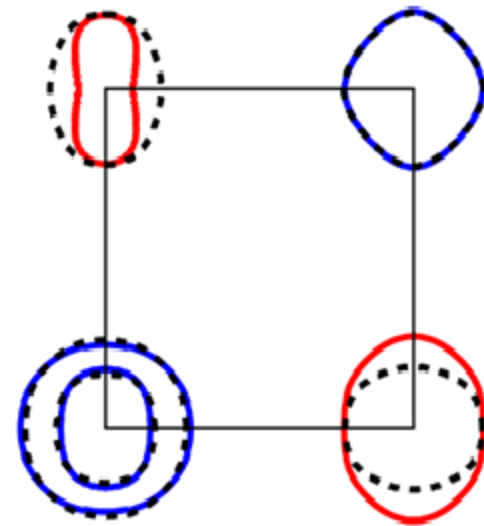


2. $Q=0$ Pomeranchuk instability

- Chuang, T. M. *et al.*, Science 327, 181–184 (2010).
- Chu, J-H. *et al.* Science 329, 824–826 (2010).
- Yi, M. *et al.* Proc. Natl Acad. Sci. USA 108, 6878–6883 (2011).
- Matsuda et al, Nature 486, 382 (2012).



Sub-leading order parameter



Symmetry : Break $C_4 \rightarrow$ nematic order

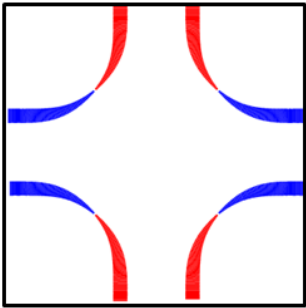
Couple to spin nematicity.

JC Davis and DHL, PNAS 110, 17623 (2013).

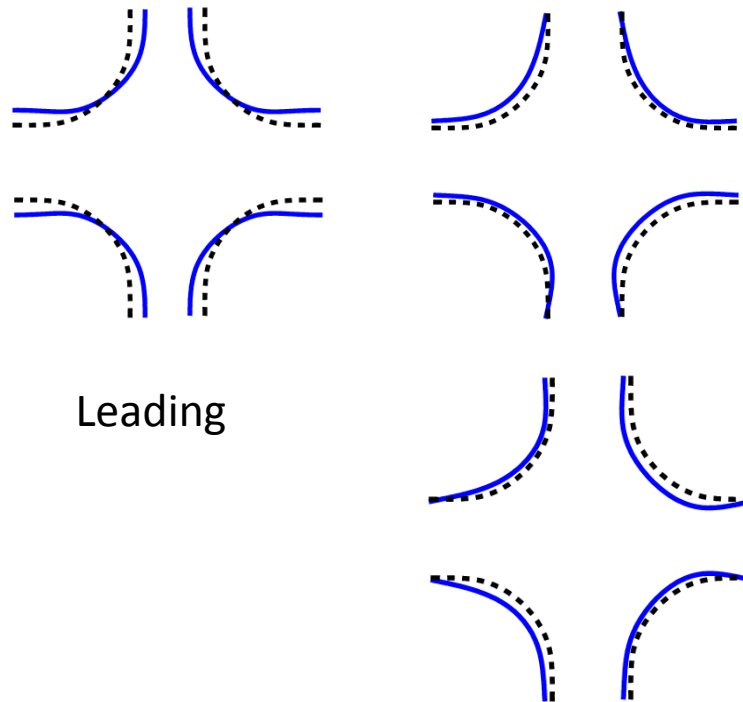
A nearest neighbor AF exchange interaction also accounts for the instabilities lurking around in the cuprates.

JC Davis and DHL, PNAS 110, 17623 (2013).

Cooper Pairing



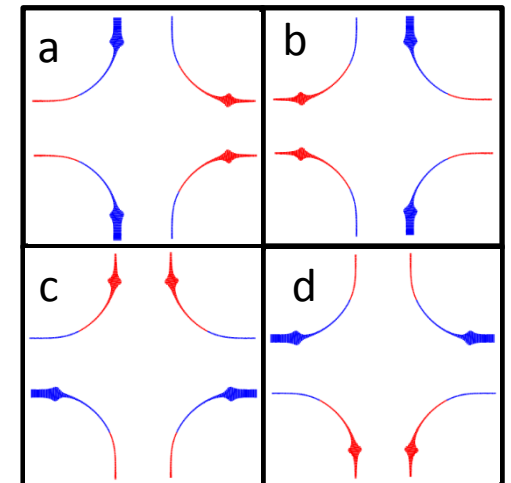
Fermi surface instabilities



Leading

Sub-leading
Break T

Charge density wave



$$\mathbf{Q} = (\pm\delta, 0), (0, \pm\delta)$$

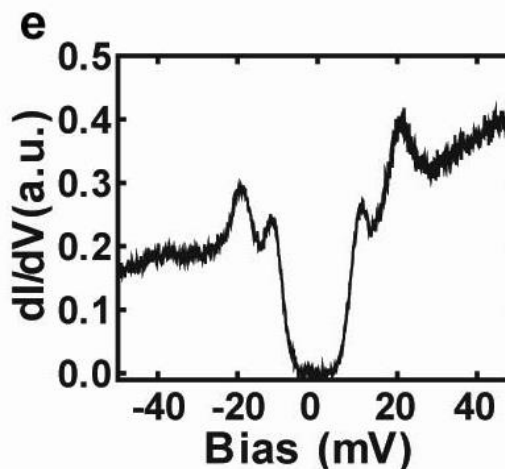
$$\Delta_{-\mathbf{q}}(\mathbf{k}) = \Delta_{\mathbf{q}}(\mathbf{k} - \mathbf{Q})^*$$

Interface high T_c superconductivity

Interface-Induced High-Temperature Superconductivity in Single Unit-Cell FeSe Films on SrTiO₃ *

WANG Qing-Yan(王庆艳)^{1,2†}, LI Zhi(李志)^{2†}, ZHANG Wen-Hao(张文号)^{1†}, ZHANG Zuo-Cheng(张祚成)^{1†}, ZHANG Jin-Song(张金松)¹, LI Wei(李渭)¹, DING Hao(丁浩)¹, OU Yun-Bo(欧云波)², DENG Peng(邓鹏)¹, CHANG Kai(常凯)¹, WEN Jing(文竞)¹, SONG Can-Li(宋灿立)¹, HE Ke(何珂)², JIA Jin-Feng(贾金锋)¹, JI Shuai-Hua(季帅华)¹, WANG Ya-Yu(王亚愚)¹, WANG Li-Li(王立莉)², CHEN Xi(陈曦)¹, MA Xu-Cun(马旭村)^{2**}, XUE Qi-Kun(薛其坤)^{1**}

c

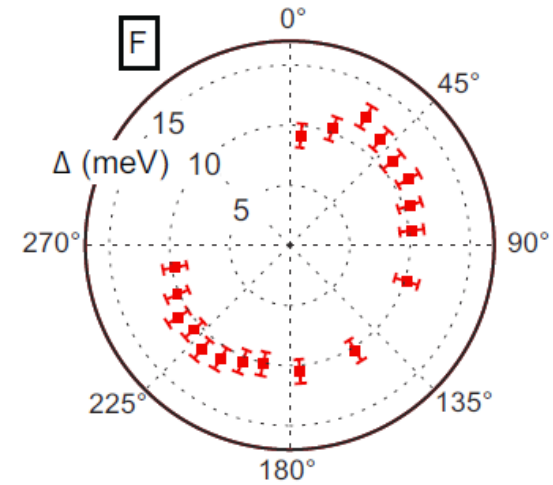
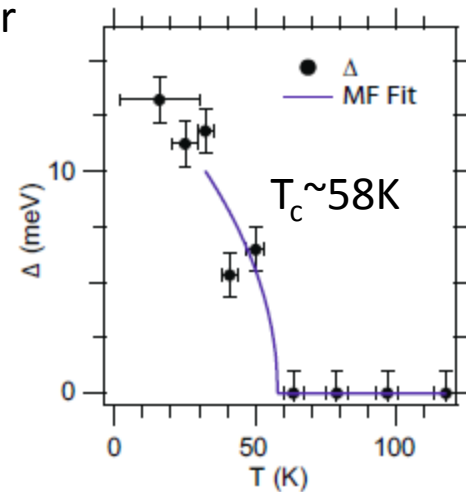
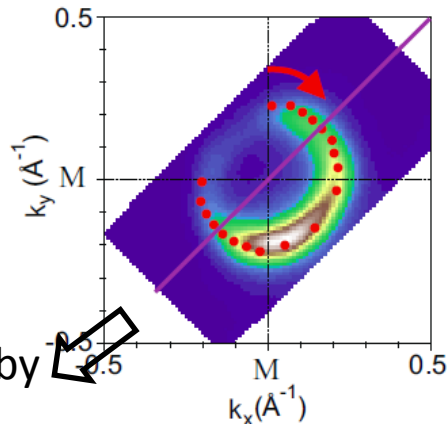


- Liu, D. *et al. Nat. Commun.* **3**, 931 (2012).
- Tan, S. *et al. Nat. Mater.* **12**, 634–640 (2013).
- He, S. *et al. Nat. Mater.* **12**, 605–610 (2013).

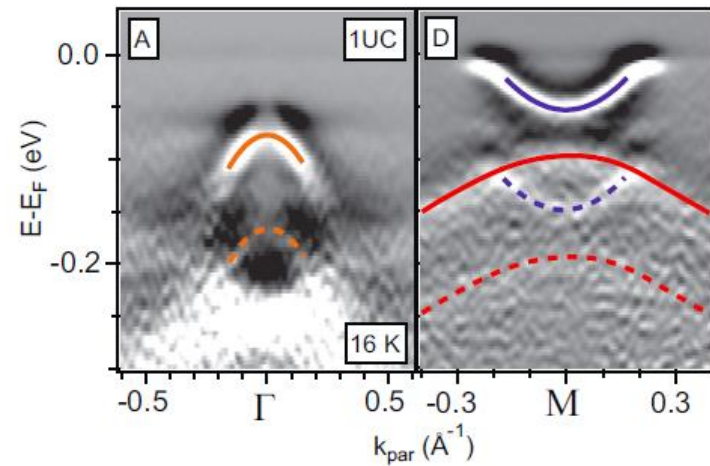
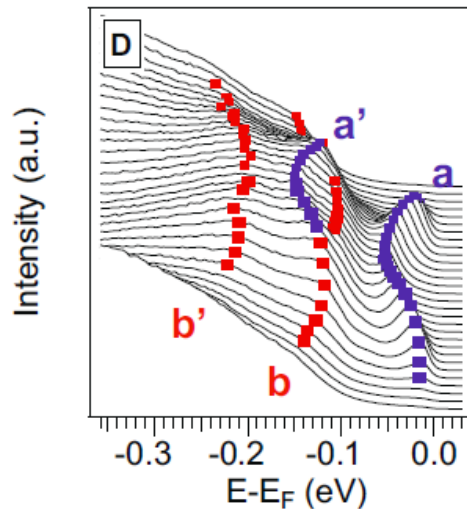
To date, highest ARPES gap opening temperature $\sim 75\text{K}$

J.J Lee et al, Nature accepted.

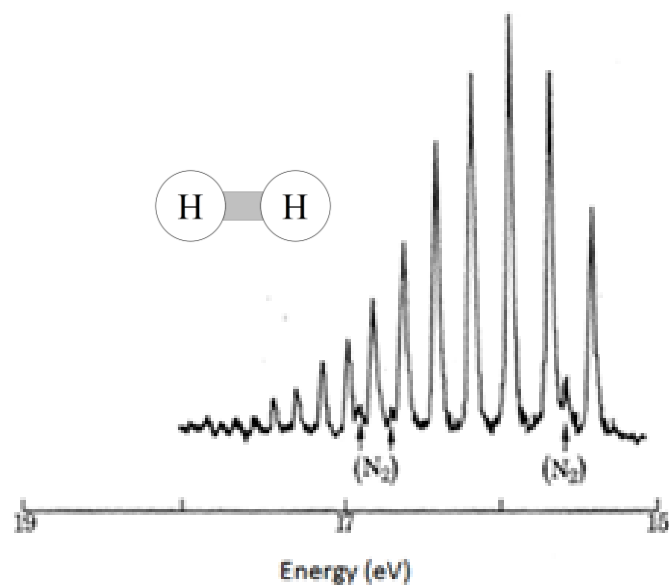
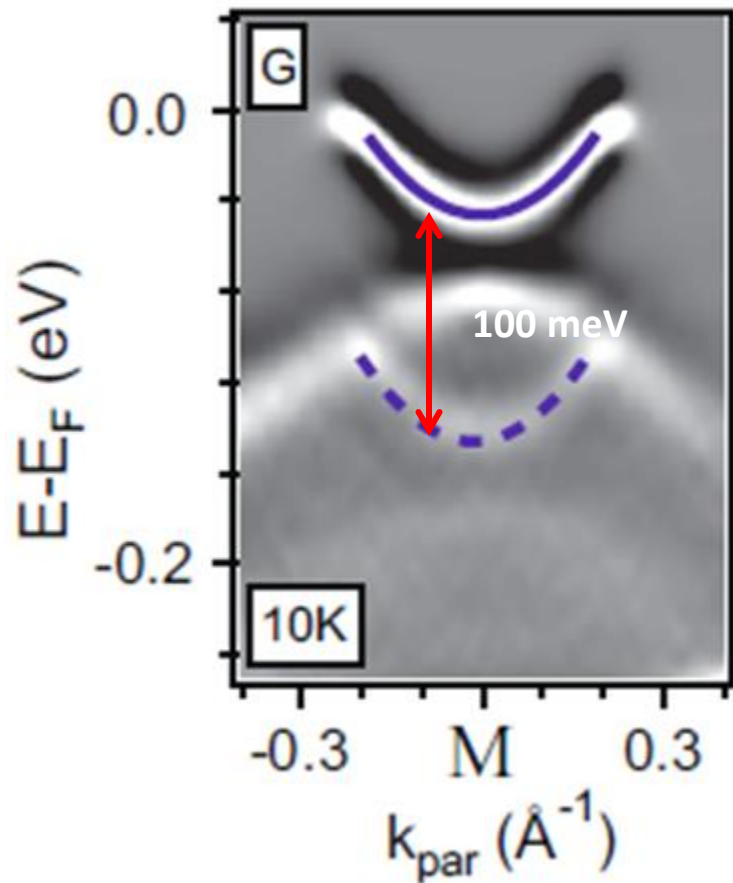
Only electron pockets
around zone corner



Electron doped by
the substrate



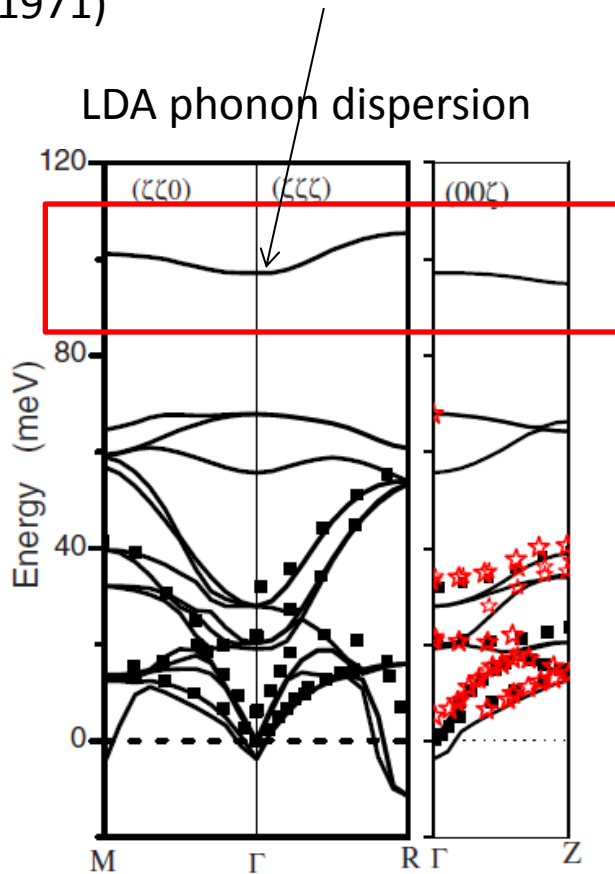
- Only 1 UC film show replica band.
- Only one unit cell film shows energy gap.
- Films with ≥ 2 UC thickness has nearly bulk FeSe bandstructure. (no charge transfer).



Turner, *Phil. Trans. Roy. Soc. Lond. A.* 268, 7 (1970)

Interpretation: replica bands are due to phonon shake off.

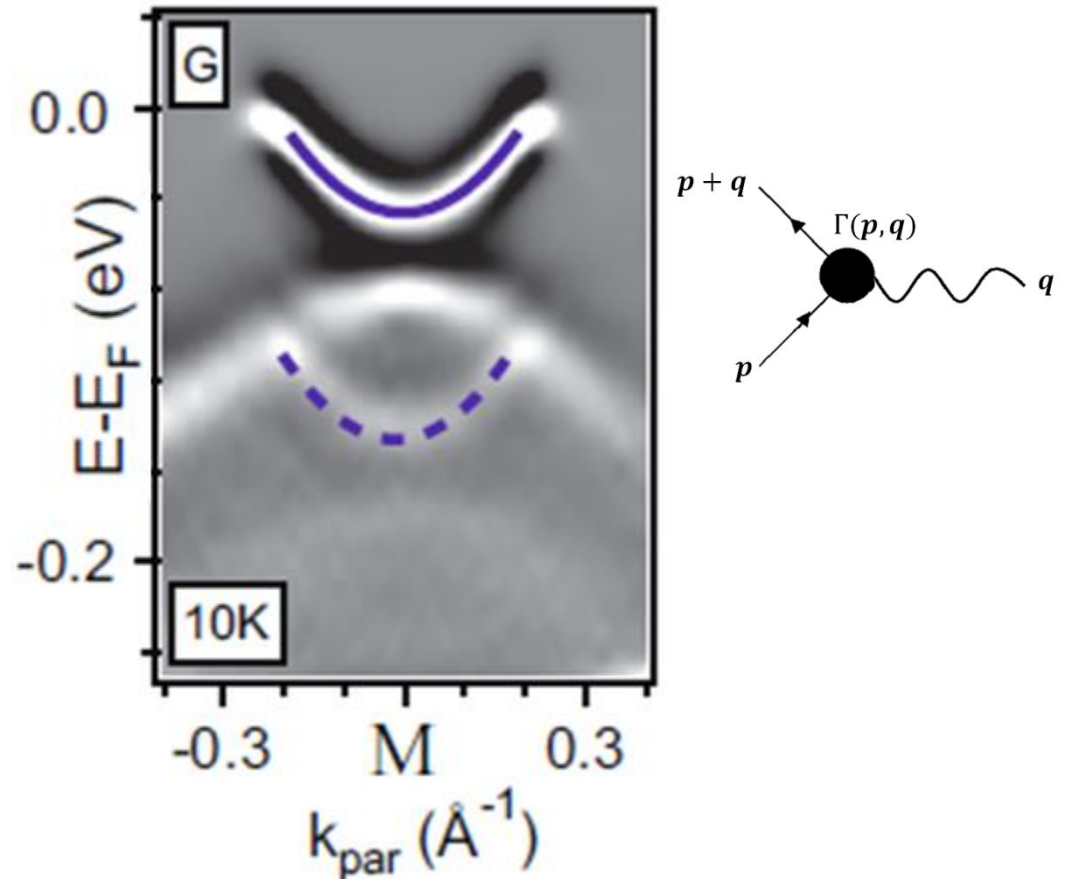
Also seen in neutron scattering by Stirling, J. Phys. C, Solid St. 5,2711 (1971)



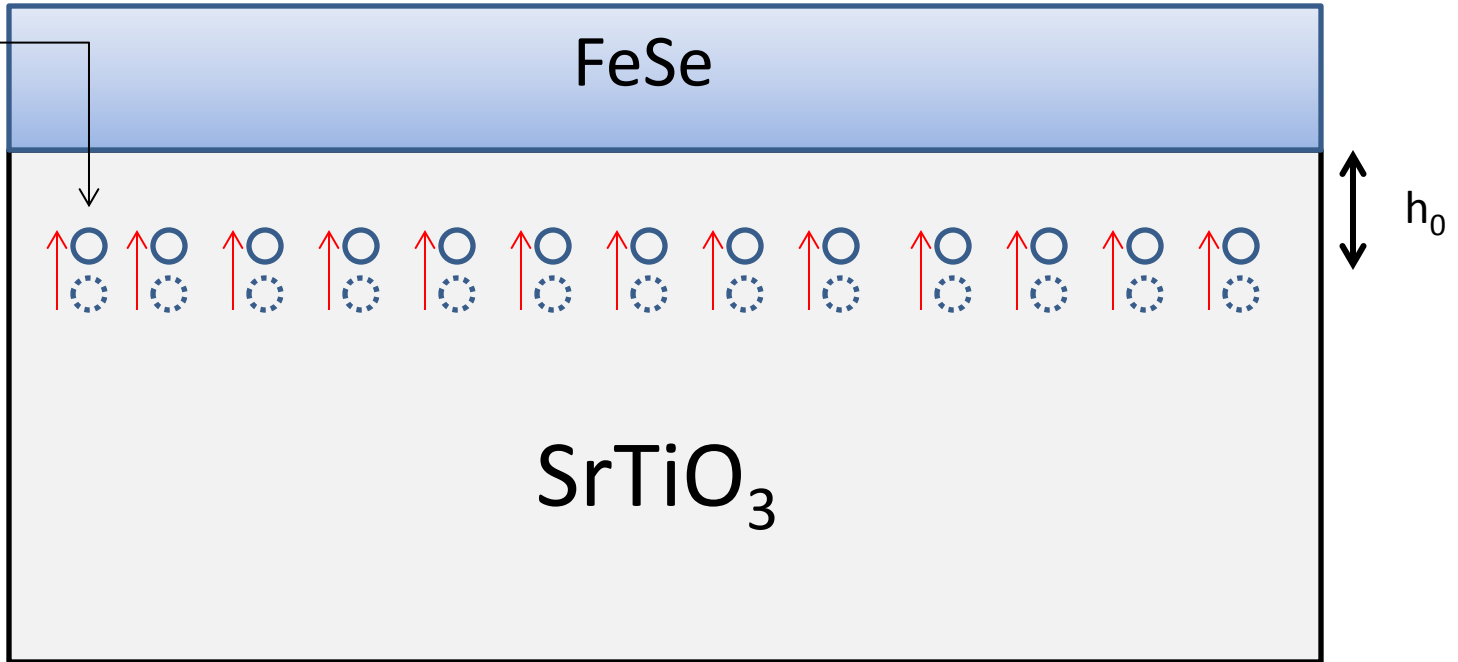
Choudhury et al, PRB **77**, 134111 (2008)

Dominant oxygen motion

In order for the replica band to follow the dispersion of the main band closely, $\Gamma(\mathbf{p}, \mathbf{q})$ needs to be sharply peaked at $\mathbf{q} = \mathbf{0}$.

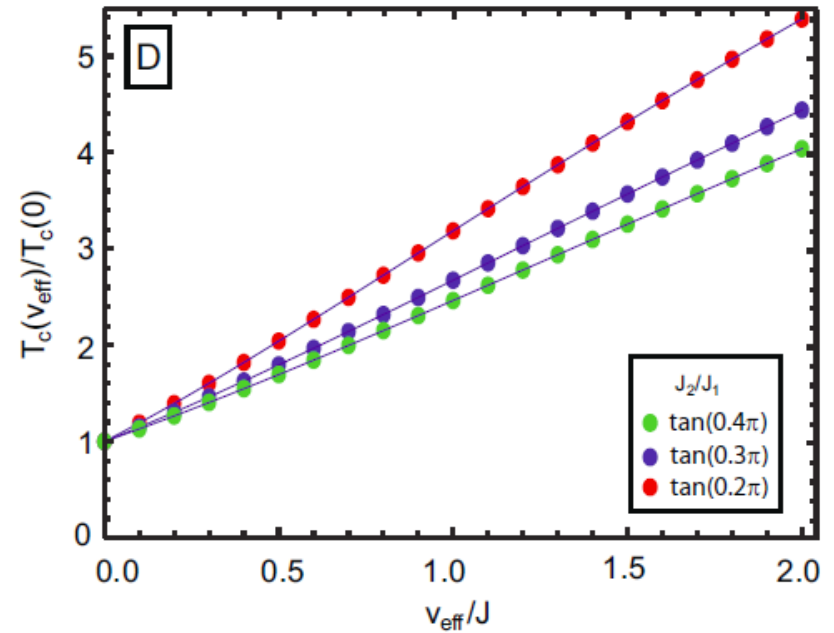
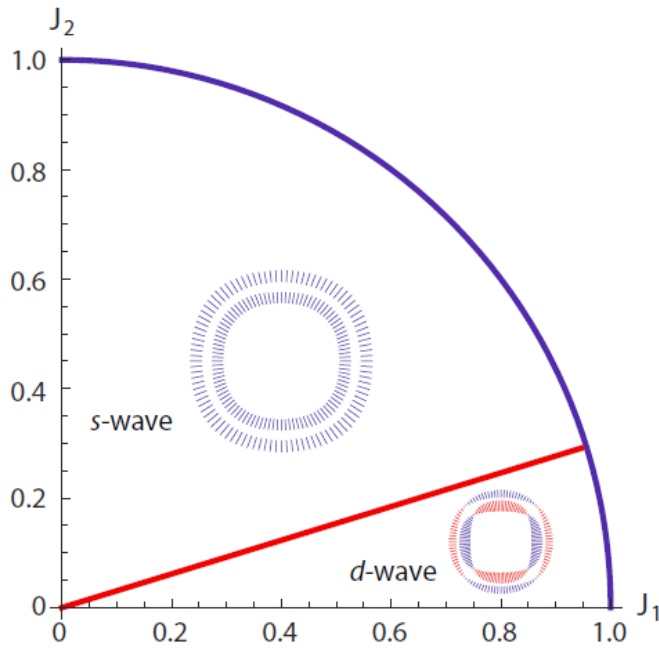


Aligned electric dipole moments near the interface caused by charge transfer



$$\delta\Phi(\mathbf{q}_{\parallel}) = \sqrt{\frac{\epsilon_{\parallel}}{\epsilon_{\perp}}} \left(\frac{2\pi q_{\text{eff}}}{\sqrt{\epsilon_{\perp}}} \right) e^{-\left(|\mathbf{q}_{\parallel}| h_0 \sqrt{\epsilon_{\parallel}/\epsilon_{\perp}}\right)} \delta h(\mathbf{q}_{\parallel})$$

$$H_{\text{eff}} = \sum_{\mathbf{k}}' \sum_{\sigma} \epsilon(\mathbf{k}) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + 2 \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j - \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} \sum_{\sigma,\sigma'} \left(\frac{v_{\text{eff}}}{2\pi q_0^2} e^{-|\mathbf{q}|/q_0} \right) c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k}\sigma} c_{\mathbf{p}-\mathbf{q}\sigma'}^{\dagger} c_{\mathbf{p}\sigma'}$$



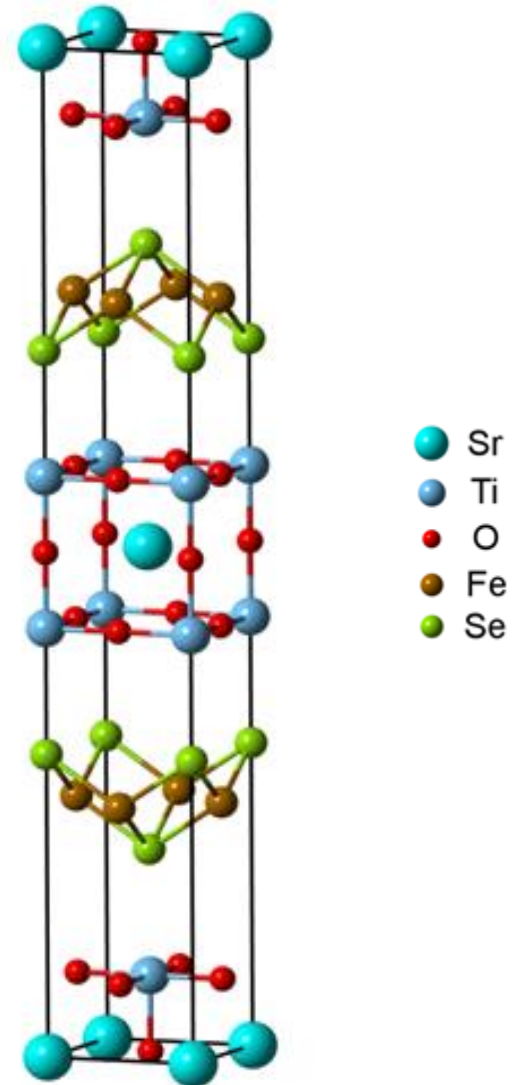
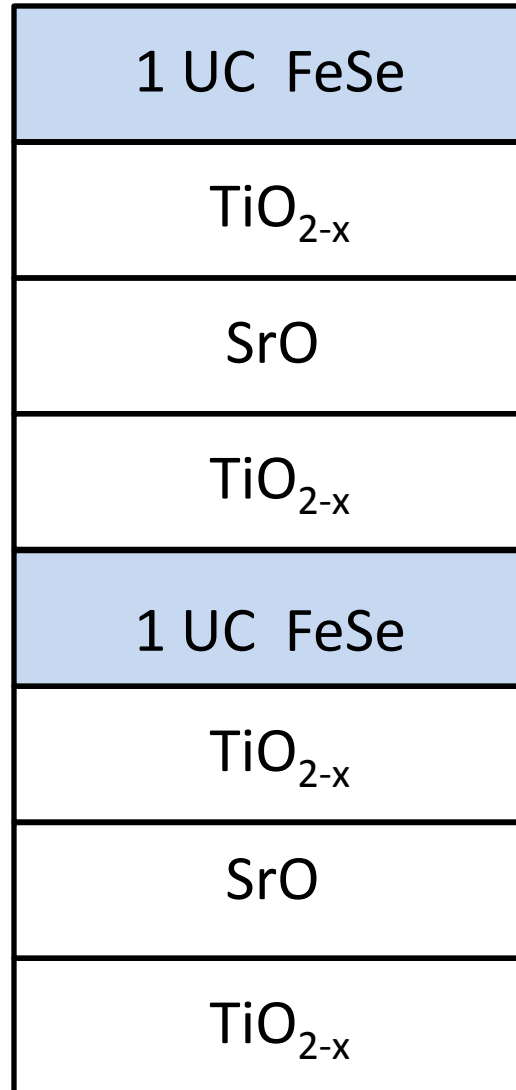
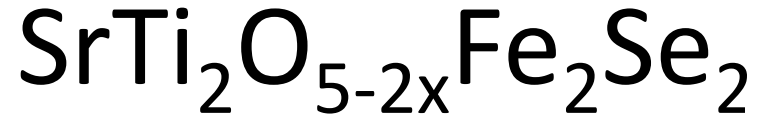
Donglai Feng, Monday talk.

Intensity of the replica band / Intensity of the main band \Rightarrow electron-phonon interaction strength \Rightarrow effective electron-electron attraction

$$\Rightarrow v_{\text{eff}} / \sqrt{J_1^2 + J_2^2} \geq \frac{1}{3} \quad \Rightarrow T_c \text{ enhancement} \geq 1.5 !$$

Y.-Y. Xiang, F. Wang, D. Wang, Q.-H. Wang, and D.-H. Lee, Phys. Rev. B 86 134508 (2012).

Proposal of a bulk High T_c superconductor



How to derive the low energy effective theory for strongly correlated materials ?

Thank you !