

ARPES Results of '122' Iron-based Superconductors

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Solid State II

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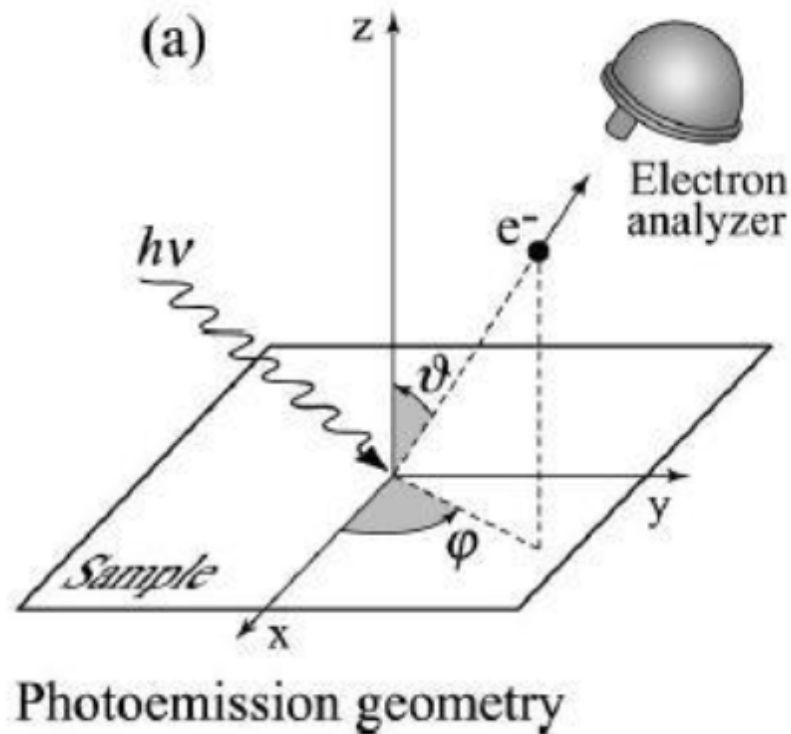
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OUTLINES

1. Angle-Resolved PhotoEmission Spectroscopy (ARPES)
2. Crystal structure of "122" system
3. Experimental results
4. Theoretical results
5. Conclusions

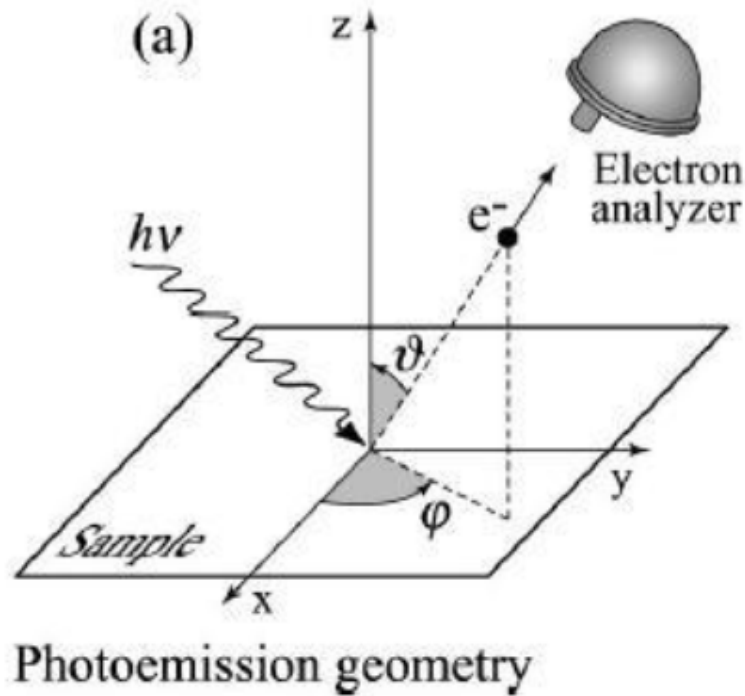
ARPES



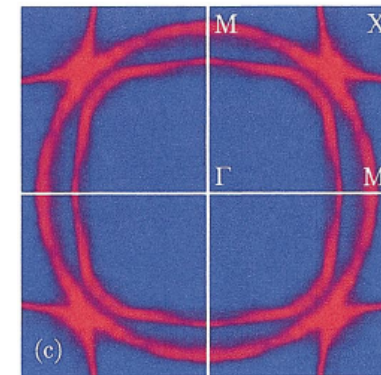
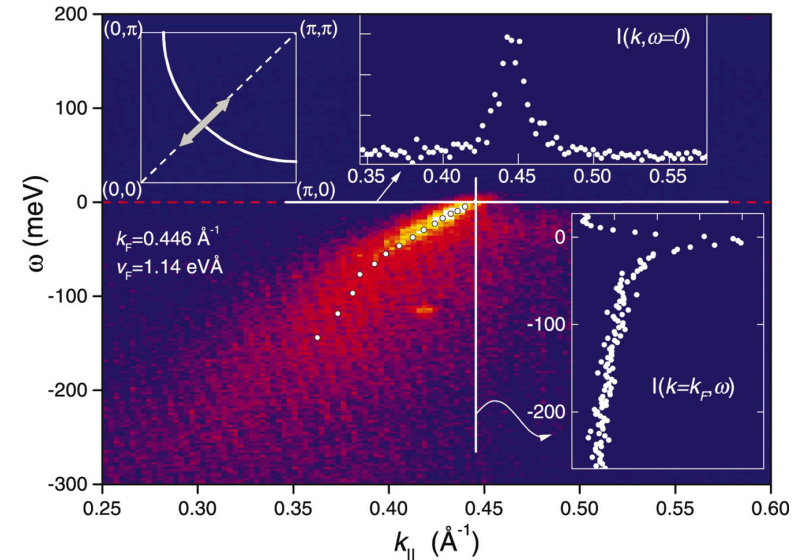
- based on Photoelectric Effect (Hertz 1887, Einstein 1905)
- powerful technique to measure the electronic structure directly (Energy vs. Momentum)

Damascelli, Hussain and Shen, Rev.Mod.Phys., **75**, 473 (2003)

ARPES



- incidence of monochromatic photons
- photoelectrons with different energy and momentum



(c)
 Sr_2RuO_4 cleaved at 180 K
 $T = 10 \text{ K}$ $h\nu = 28 \text{ eV}$

Damascelli, Hussain and Shen,
 Rev.Mod.Phys. **75**, 473 (2003)

Crystal Structure

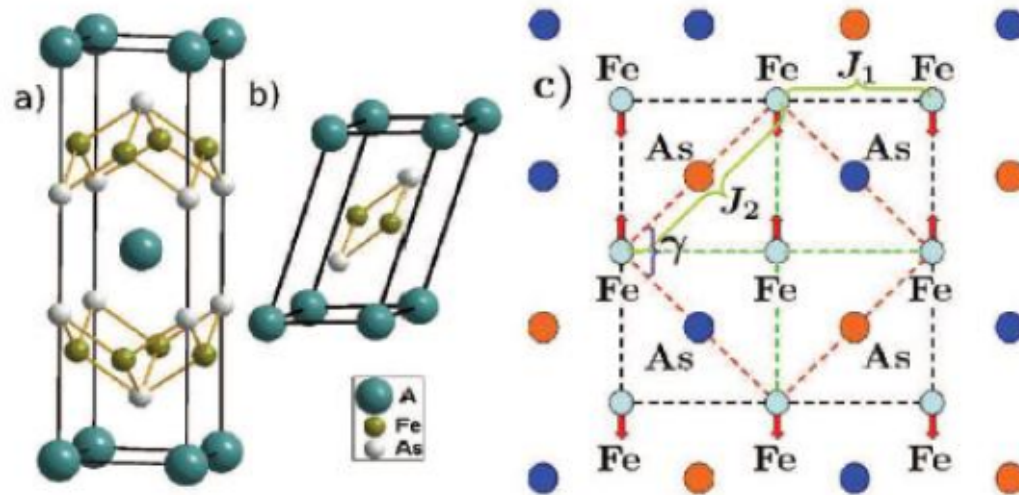
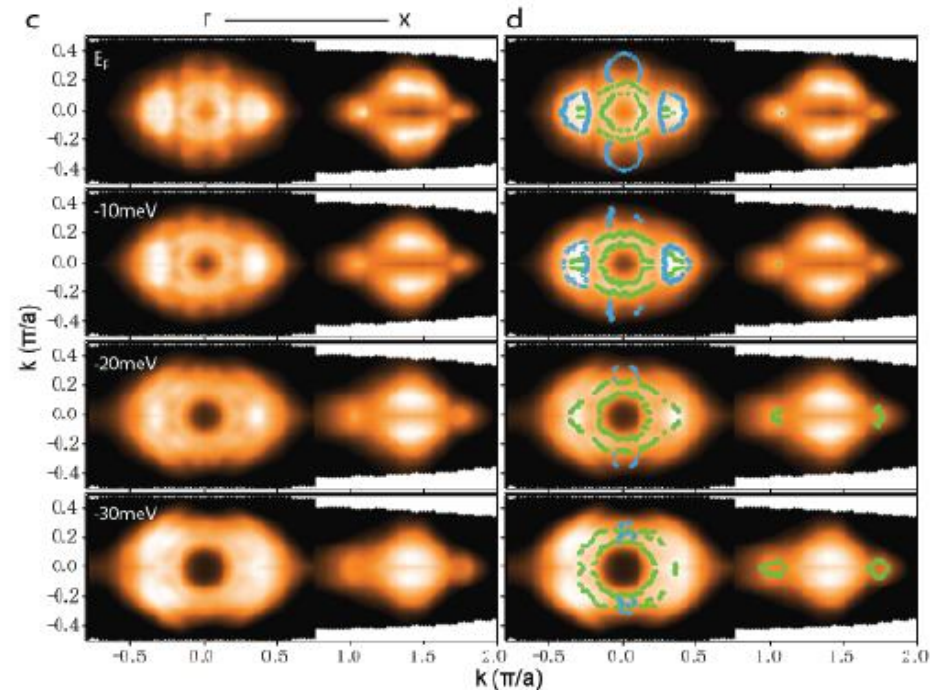
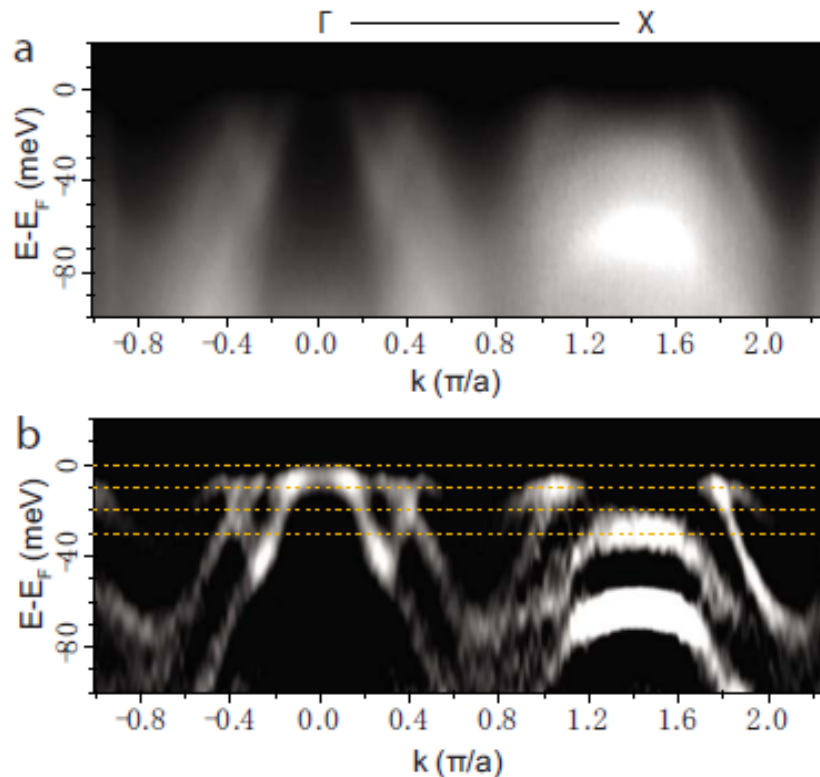


FIG. 2: Crystal structure of AF_2As_2 ($A = Ba, Sr, Ca$).

F. Ma, et al, arXiv:0806.3526v2

- The parent compounds undergo a tetragonal to orthorhombic structural transition together with a magnetic transition

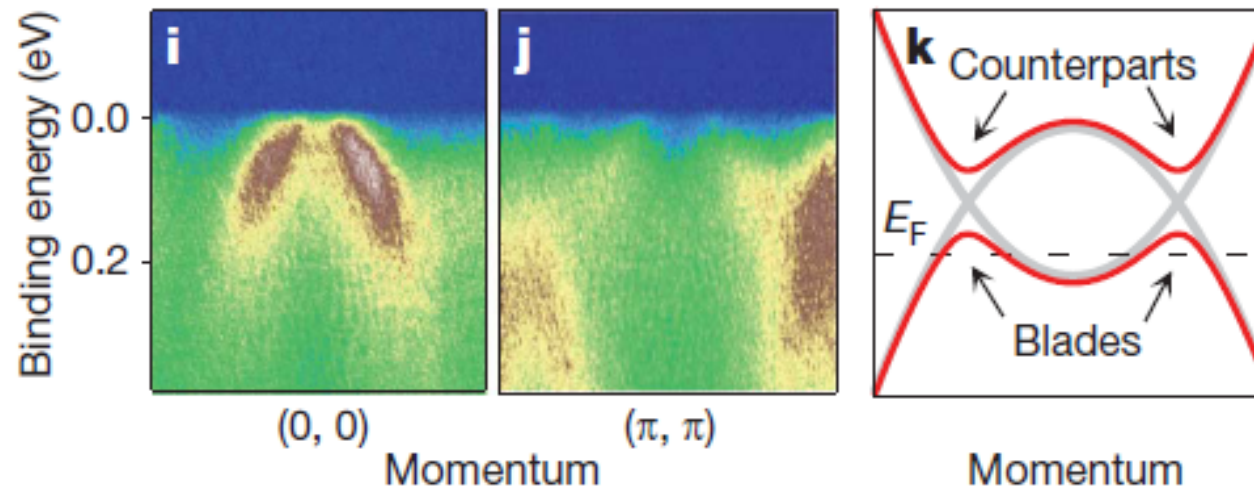
Experiments: BaFe₂As₂



M. Yi, et al, PRB, **80**, 174510 (2009)

- below T_{SDW}
- two enclosed hole-like pockets around the zone center
- four petal-like electron-like pockets below T_{SDW}
- an electron-like pocket around zone corner

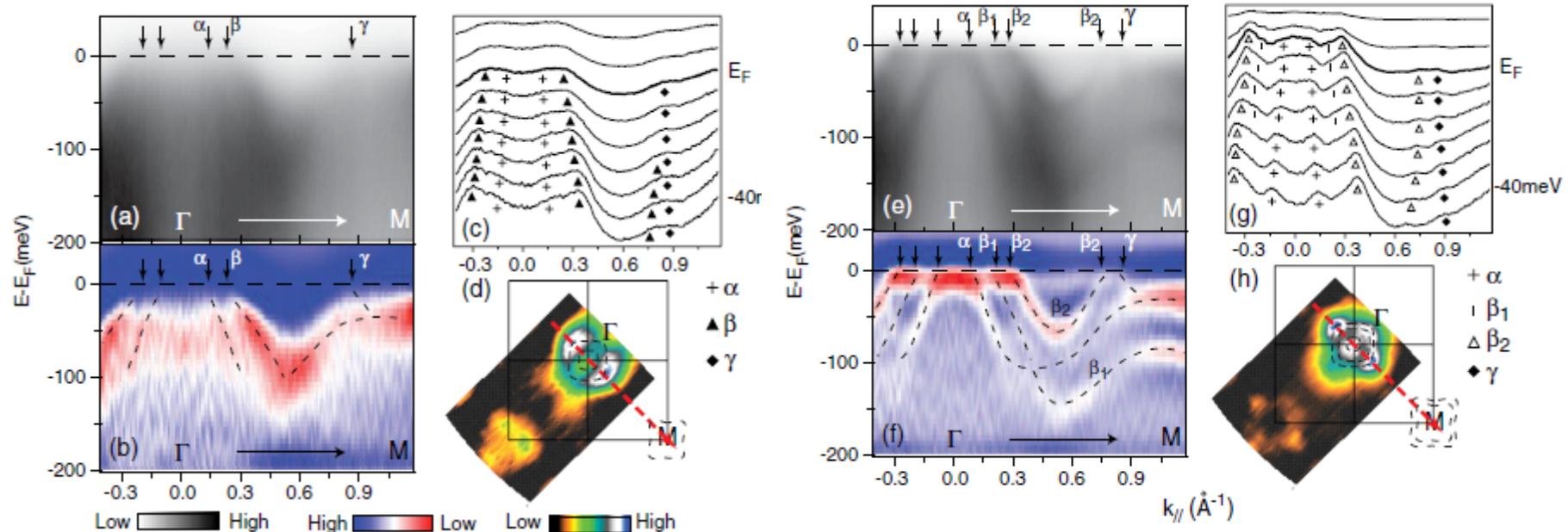
Experiments: BaFe₂As₂



V.B. Zabolotnyy, et al, Nature, **457**, 569 (2009)

- Nesting: replica of Γ -centred hole-like band (grey)
- electron-like band (grey)
- interaction of these two bands opens a gap and forms the blades (red)

Experiments: SrFe₂As₂



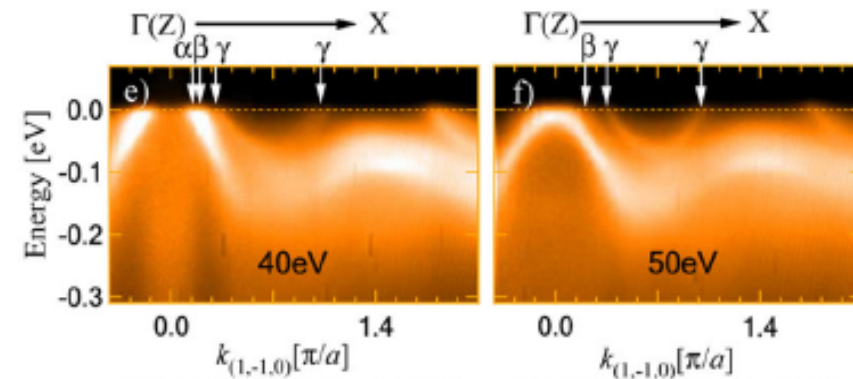
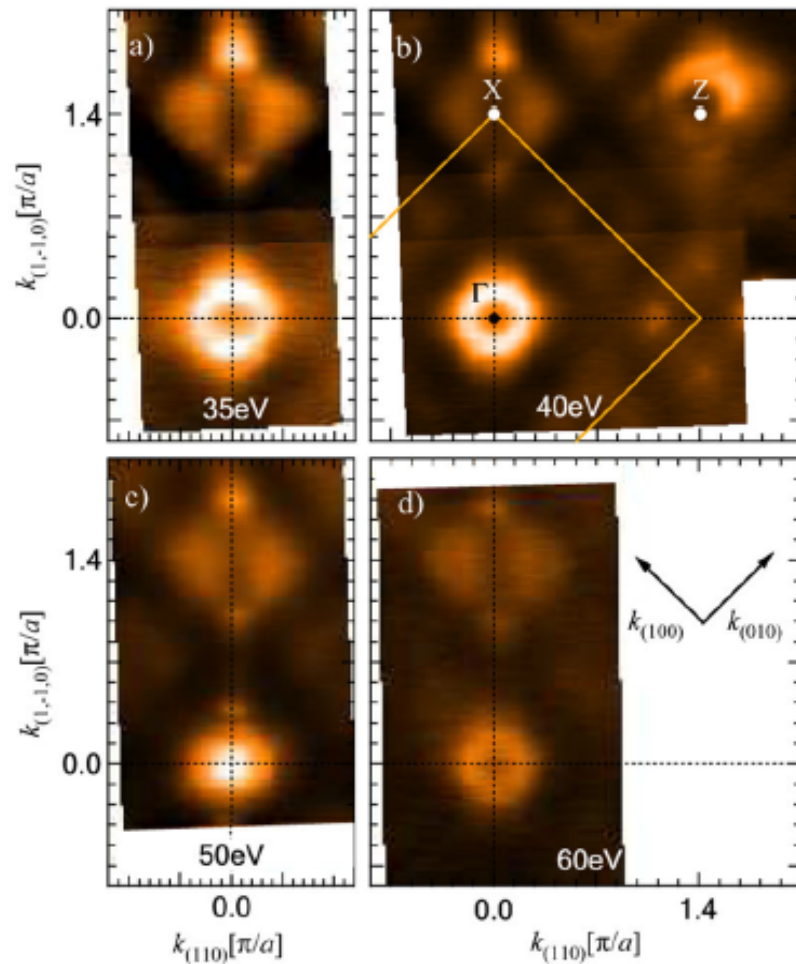
Y. Zhang, et al, PRL, **102**, 127003 (2009)

Normal state (T = 230 K)

SDW state (T = 10 K)

- High T, only two hole-like pockets at zone center and one electron-like pocket at zone corner.
- Low T, β band split into two bands β_1 β_2 . And the petal-like pockets appear, but hole-like.

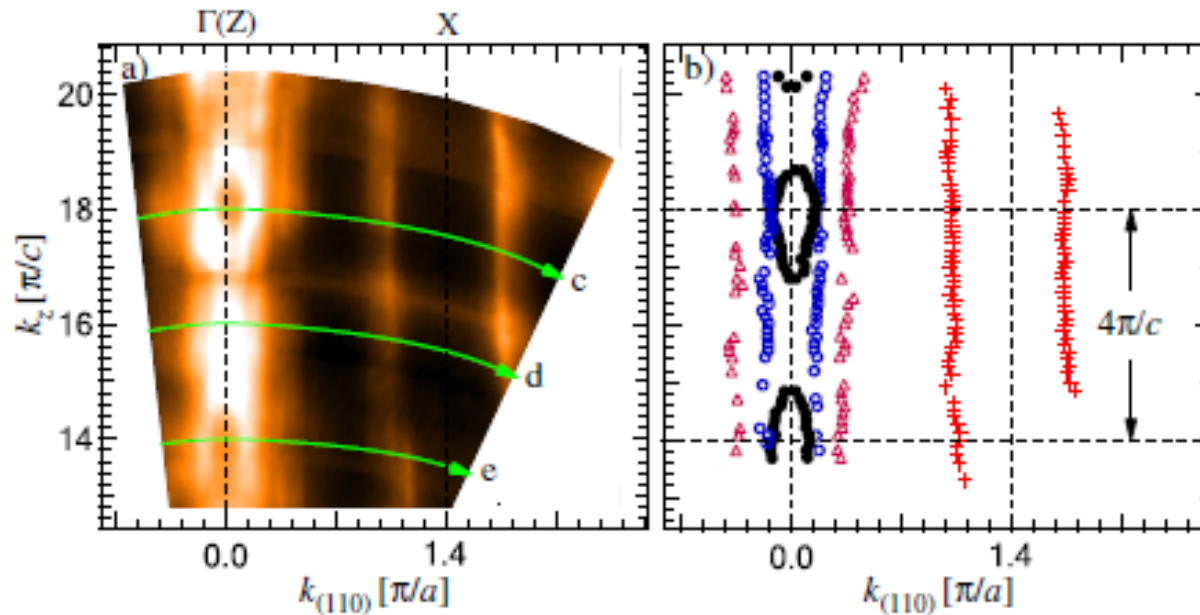
Experiments: CaFe_2As_2



- two hole-like pockets around zone center and one electron-like pocket around zone corner

C. Liu, et al, PRL, **102**, 167004 (2009)

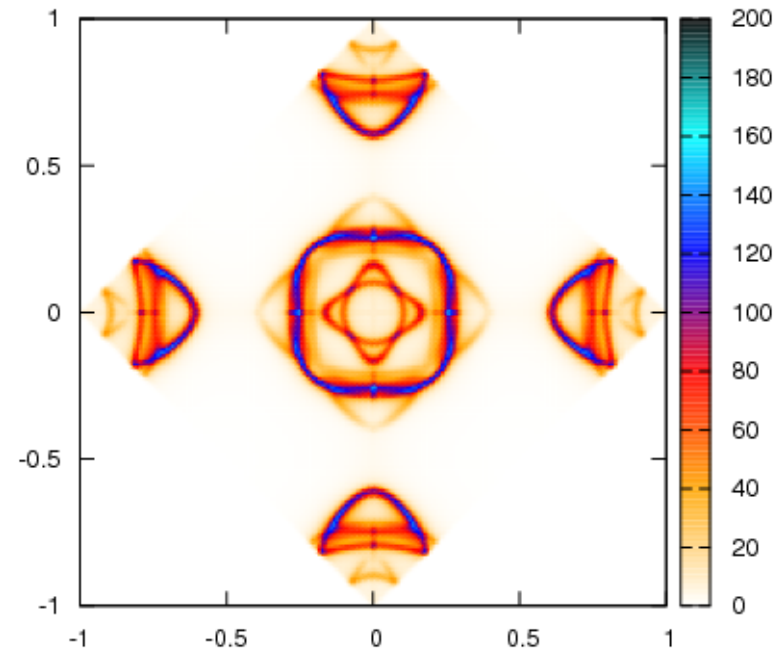
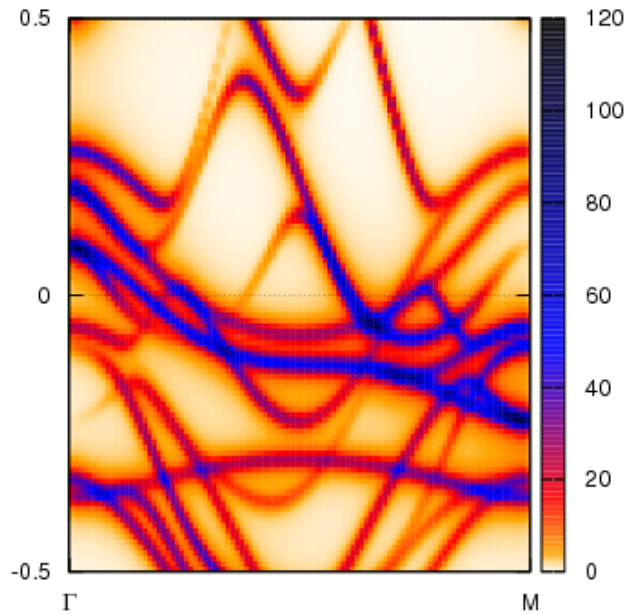
Experiments: CaFe_2As_2



C. Liu, et al, PRL, **102**, 167004 (2009)

- z component of momentum is identified by the incident energy of photon.
- the bands around Γ point is more 3D than the bands around M point.

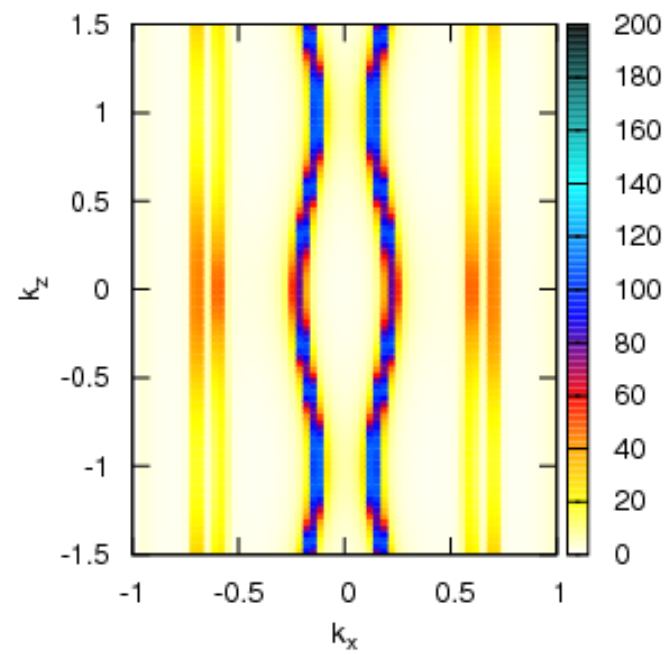
my results



- Five-orbital model + MFA

$$H_0 = \sum_{\mathbf{k}, \sigma} \sum_{\alpha, \beta} (\xi_{\alpha\beta}(\mathbf{k}) + \epsilon_{\alpha} \delta_{\alpha\beta}) d_{\alpha\sigma}^{\dagger}(\mathbf{k}) d_{\beta\sigma}(\mathbf{k}) \quad H_{\text{int}} = U \sum_{\mathbf{i}, \alpha} n_{\mathbf{i}, \alpha, \uparrow} n_{\mathbf{i}, \alpha, \downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i}, \alpha < \beta} n_{\mathbf{i}, \alpha} n_{\mathbf{i}, \beta} - 2J \sum_{\mathbf{i}, \alpha < \beta} \mathbf{S}_{\mathbf{i}, \alpha} \cdot \mathbf{S}_{\mathbf{i}, \beta}.$$

my results



Conclusions

- two hole-like enclosed pockets and four petal-like pockets around zone center
- one electron-like enclosed pocket and four petal-like pickets around zone corner
- more 3D than cuprates
- MFA of 5-orbital model gives consistent results with experiments

References

- Damascelli, Hussain and Shen, *Rev. Mod. Phys.*, **75**, 473 (2003)
- F. Ma, et al, [arXiv:0806.3526v2](https://arxiv.org/abs/0806.3526v2)
- M. Yi, et al, *PRB*, **80**, 174510 (2009)
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- Y. Zhang, et al, *PRL*, **102**, 127003 (2009)
- C. Liu, et al, *PRL*, **102**, 167004 (2009)