

高温超伝導体の角度分解光電子分光 - PF BL-28Aの成果から -

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ISSP-Workshop

「東京大学アウトステーション (SPring-8 BL07LSU) での物性研究の新展開」

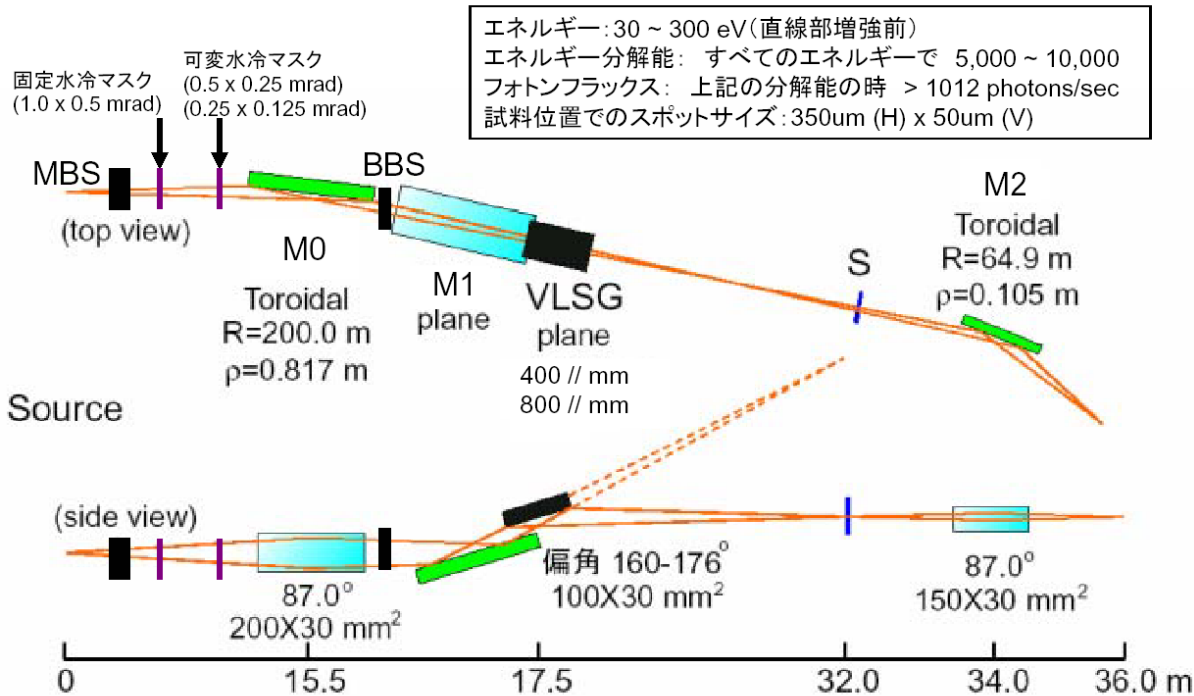
- BL-28A の紹介
 ビームライン、エンドステーション
 進行中の研究課題
- 鉄系高温超伝導体の角度分解光電子分光

 等原子価置換された $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

 不純物置換による電子ドーピング系
 $\text{Ba}(\text{Fe}_{1-x}\text{TM}_x)_2\text{As}_2$ (TM=Ni, Cu)

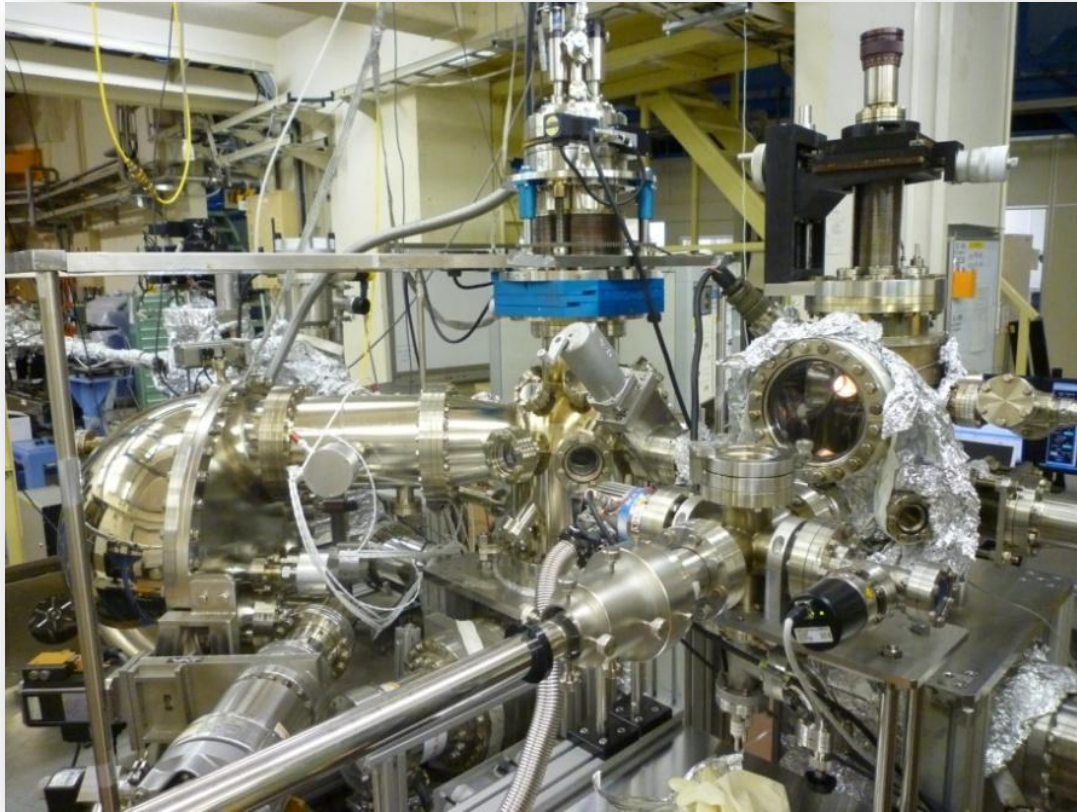
PF BL-28A ビームライン

BL-28 可変偏角不等間隔平面回折格子分光器のレイアウト



入射スリットレスでエネルギー分解能と光子フラックスを両立
可変偏角のMonk-Gillieson型不等間隔平面回折格子分光器
(前置集光鏡+平面回折格子)

K. Amemiya and T. Ohta, J. Synchrotron Rad. 11, 171 (2004).



基本性能データ

SES-2002

エネルギー分解能:
0.9 meV

(Pass energy 2 eV)

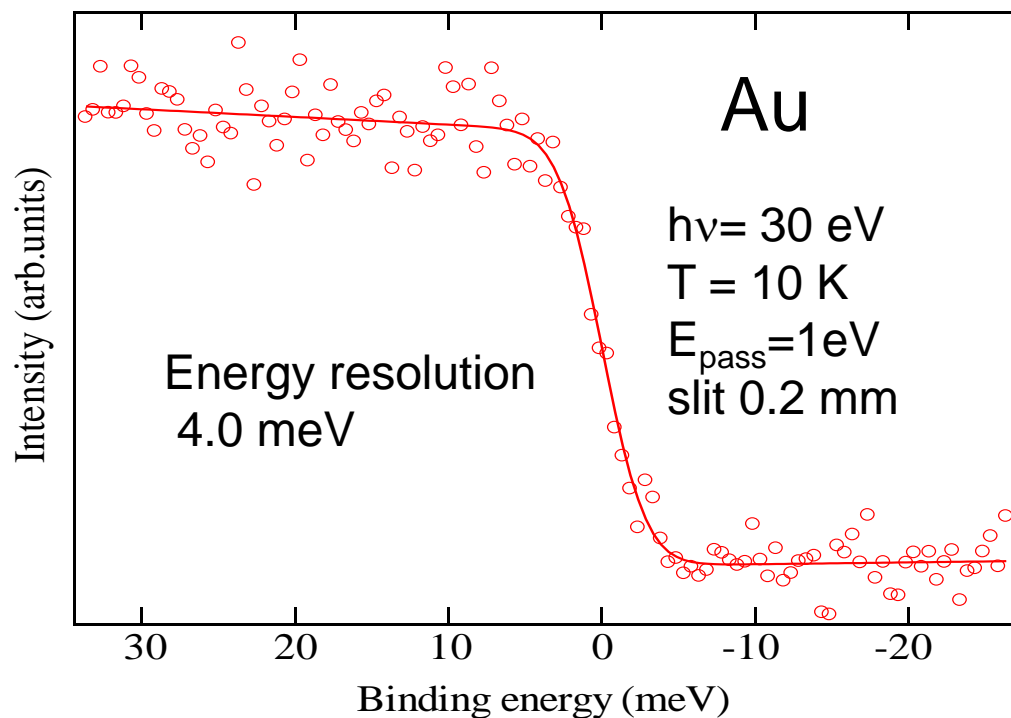
角度分解能: $\pm 0.1^\circ$

角度分解モード取り込み角:
 $\pm 6^\circ$

測定温度領域: 7 ~ 300 K

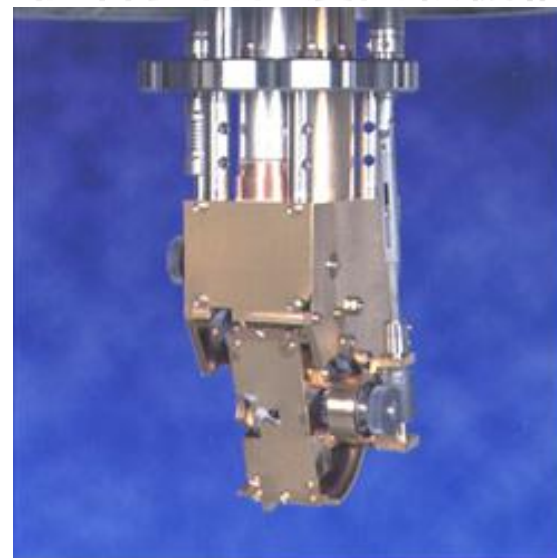
測定槽到達真空度:
 1.0×10^{-8} Pa

エネルギー分解能評価



- 光源とアナライザーを合わせたエネルギー分解能は4meVを達成している
- 超高真空中で低温10K以下を保ちつつ試料を多自由度で回転できるため運動量空間の走査を効率よく行うことができる。

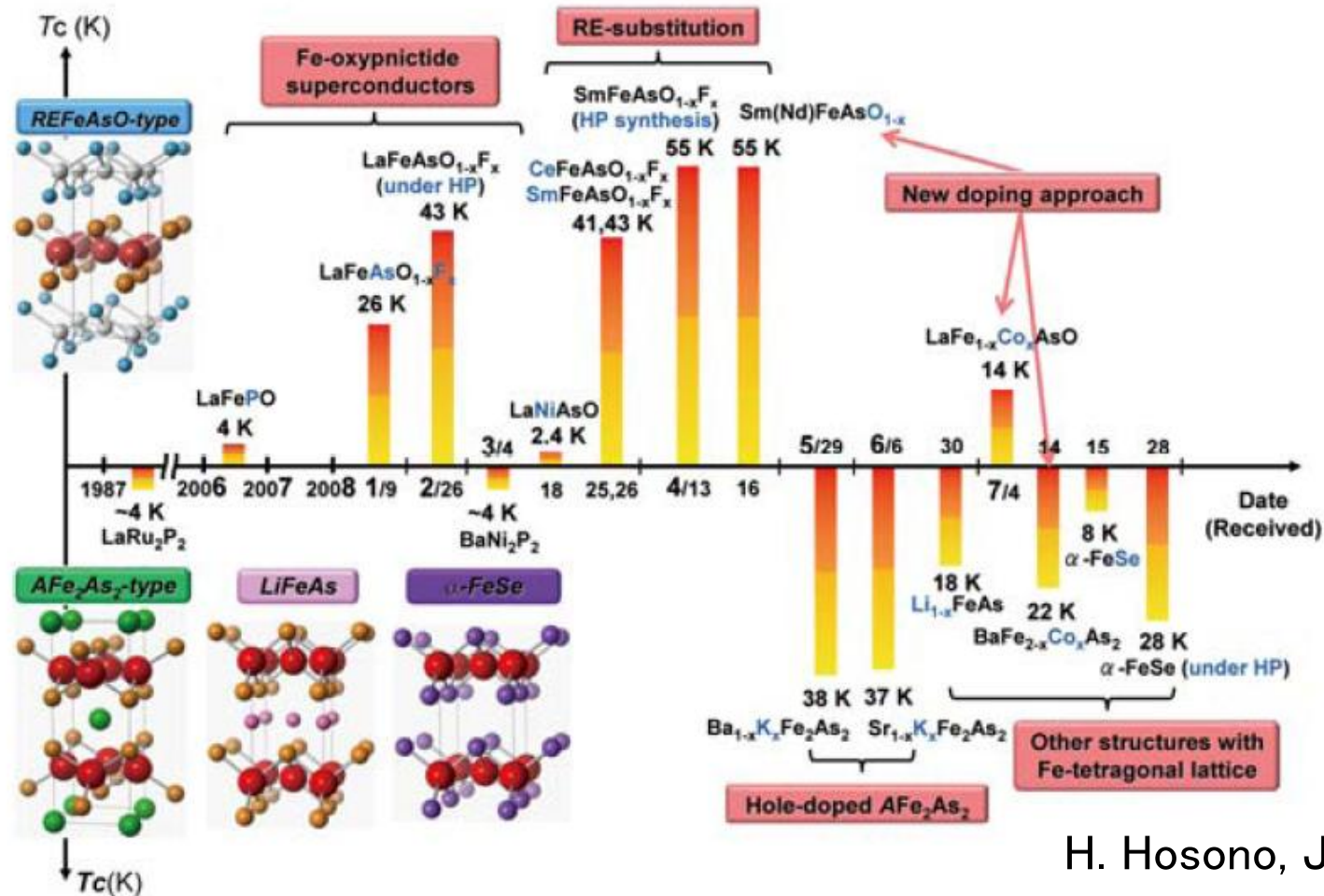
試料多自由度回転機構



アールデック社製
2軸回転マニピュレータ
i-GONIOにより試料角度を
2軸回転可能

i-GONIO
(アールデック社、
産総研共同開発)
Y. Aiura *et al.*, *Rev. Sci.
Instrum.*, **74**, 3177 (2003).

鉄系超伝導体の発見と物質探索の経過



H. Hosono, JPSJ '08

2008年2月の鉄系高温超伝導体の発見以来、様々な類似した超伝導物質が見つかった。超伝導メカニズムを明らかにするために、電子構造の研究が必要とされている。

「新規高温超伝導体および関連化合物の高分解能角度分解光電子分光」 (課題番号 2009S2-005)

実験組織

研究代表者： 藤森淳（東大理）

吉田鉄平（東大理）、中山耕輔、相馬清吾、佐藤宇史、高橋隆（東北大理）、
齋藤智彦（東理大理）、久保田正人、小野寛太（PF物構研）

研究目的

高分解能角度分解光電子分光(ARPES)を用いて新型鉄系高温超伝導体の電子状態を精密に決定し、超伝導発現機構の解明を目指した研究を行う。フェルミ面、バンド分散、エネルギーギャップ、準粒子スペクトルの微細構造の精密測定を行い、電子状態の基礎的理解を構築する。また、銅酸化物やグラファイト超伝導体など新規超伝導物質との比較研究を行い、電子構造の類似点/相違点を明らかにする。

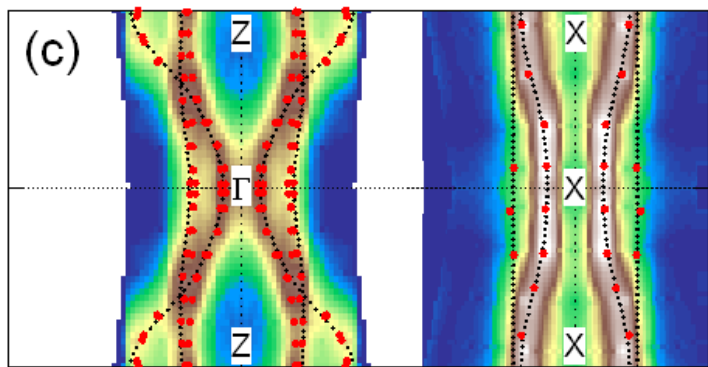
JST-TRIP

「鉄系超伝導体の低エネルギー電子状態の解明」(代表:吉田鉄平)

「高分解能ARPESによる鉄系高温超伝導体の微細電子構造の研究」(代表:佐藤宇史)

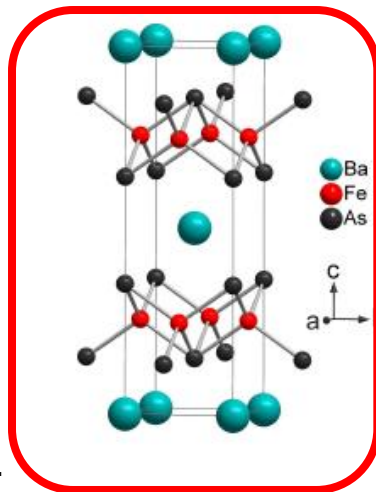
PF BL-28A における研究展開

BaFe₂(As,P)₂

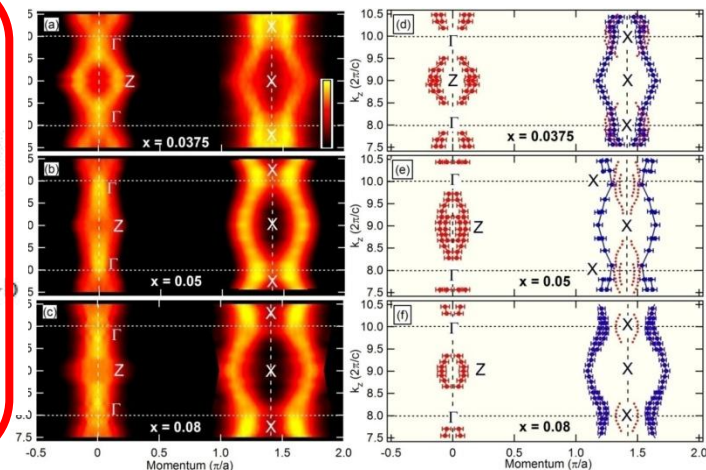


T. Yoshida *et al.*, Phys. Rev. Lett. *in press.*

BaFe₂As₂の結晶構造

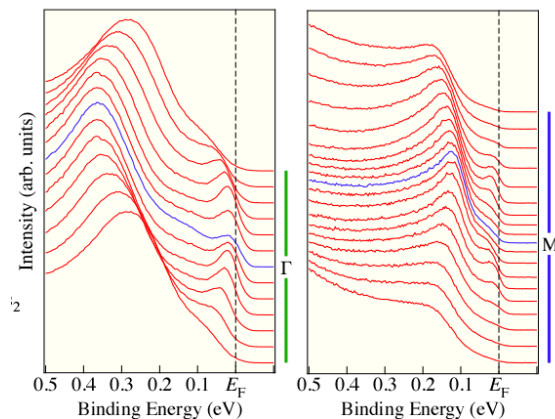
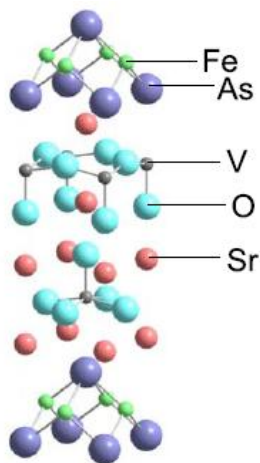


Ba(Fe,Ni)₂As₂



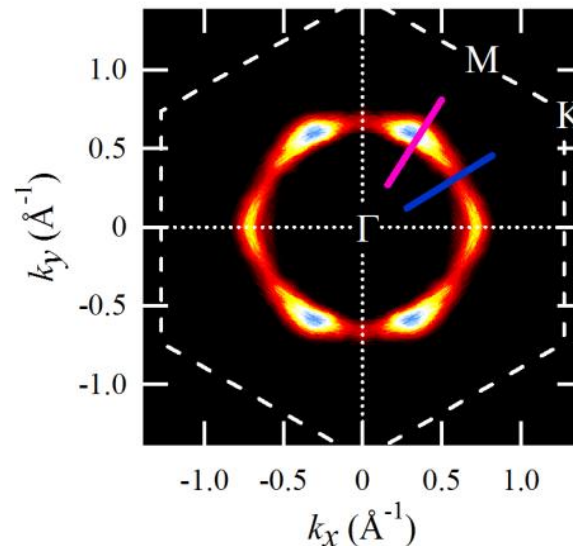
S. Ideta *et al.*,

Sr₄V₂O₆Fe₂As₂



T. Qian *et al.*,
arXiv:1008.4905.

水を含んだK_{0.5}CoO₂

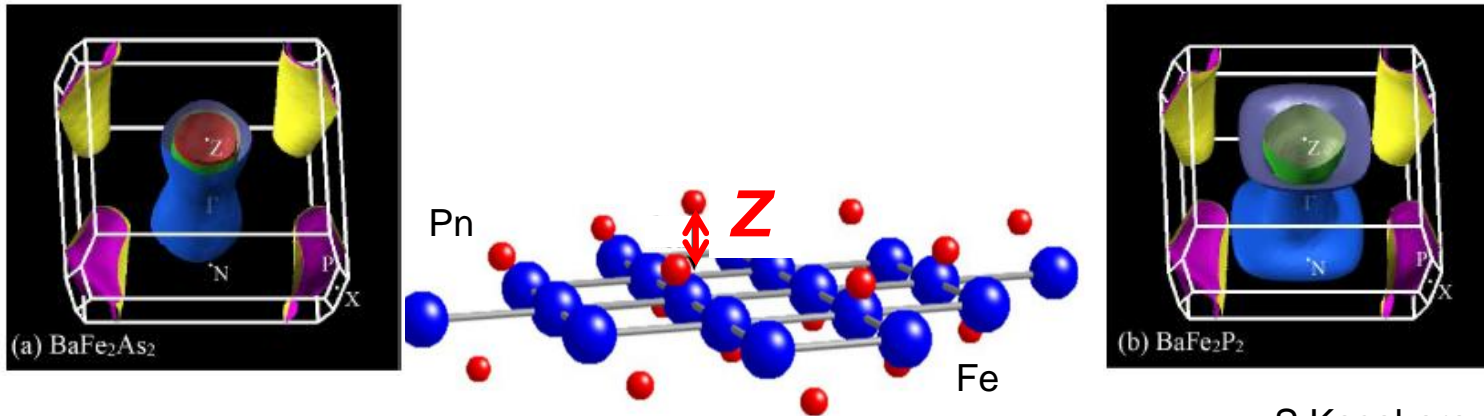


H. Usui *et al.*,
Physica C (2010).

Three-dimensional Fermi surface of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

**T. Yoshida et al.,
arXiv:1008.2080
Phys. Rev. Lett. in press.**

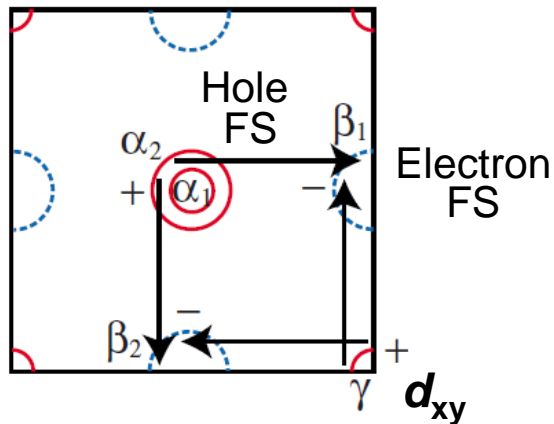
Pnictogen-height dependence of electronic structure and pairing symmetry



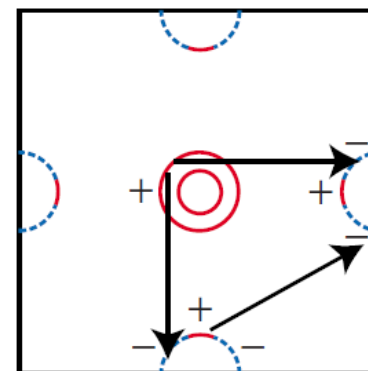
S.Kasahara et al., PRB '10.

high ← Pnictogen height Z → low

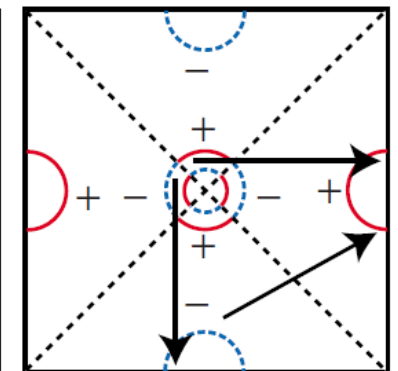
fully gapped $s \pm$ wave



nodal $s \pm$ wave



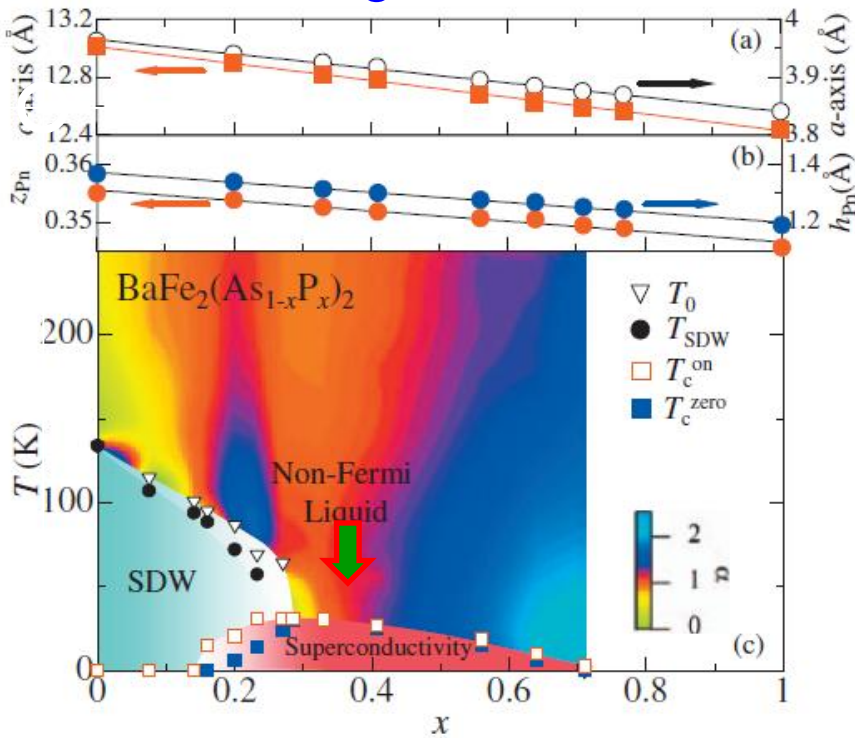
d-wave



K. Kuroki et al., PRB '09

Isovalent doping system $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

Phase diagram

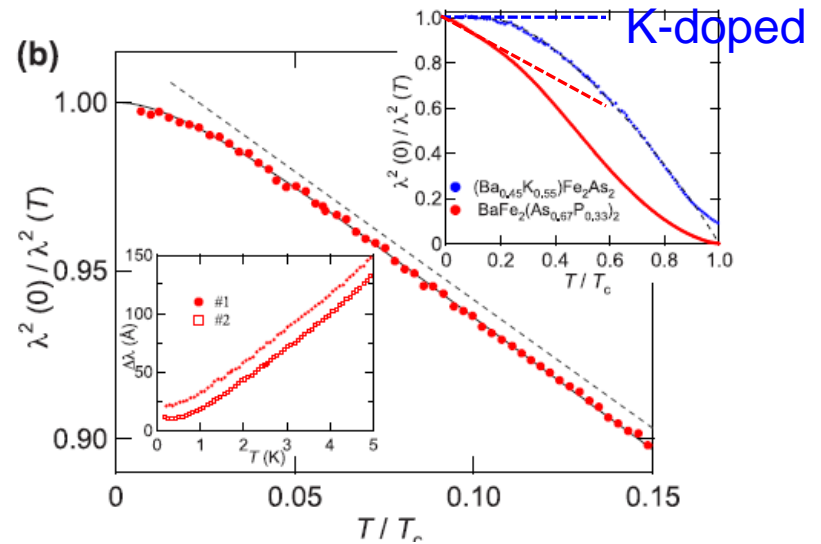


S.Kasahara *et al.*, PRB '10.

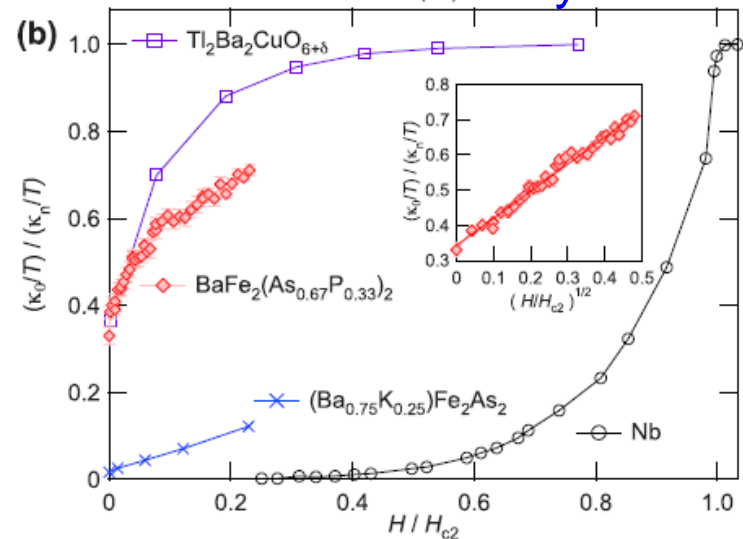
- Number of Fe 3d electron is constant.
- Pnictogen height h_{Pn} decreases.

line node in SC gap

Penetration depth

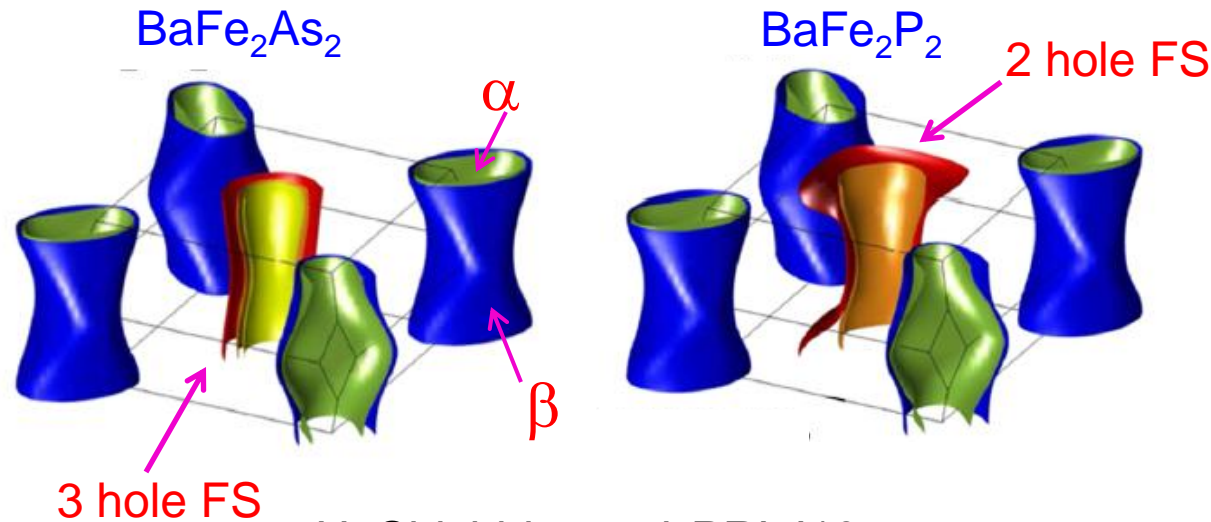
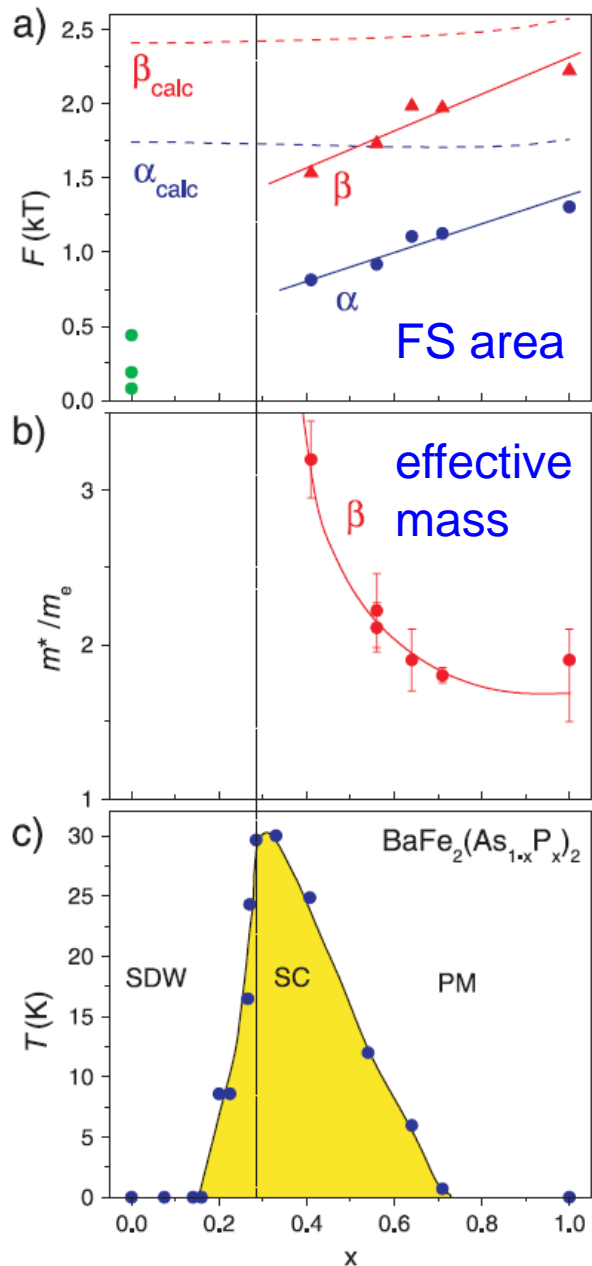


Thermal conductivity



K. Hashimoto *et al.*, PRB '10.

dHvA result of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

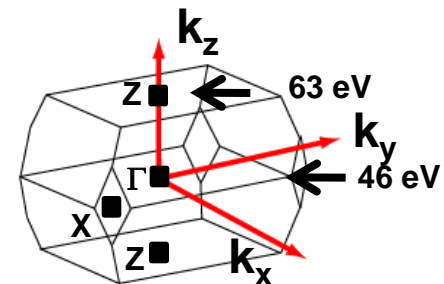
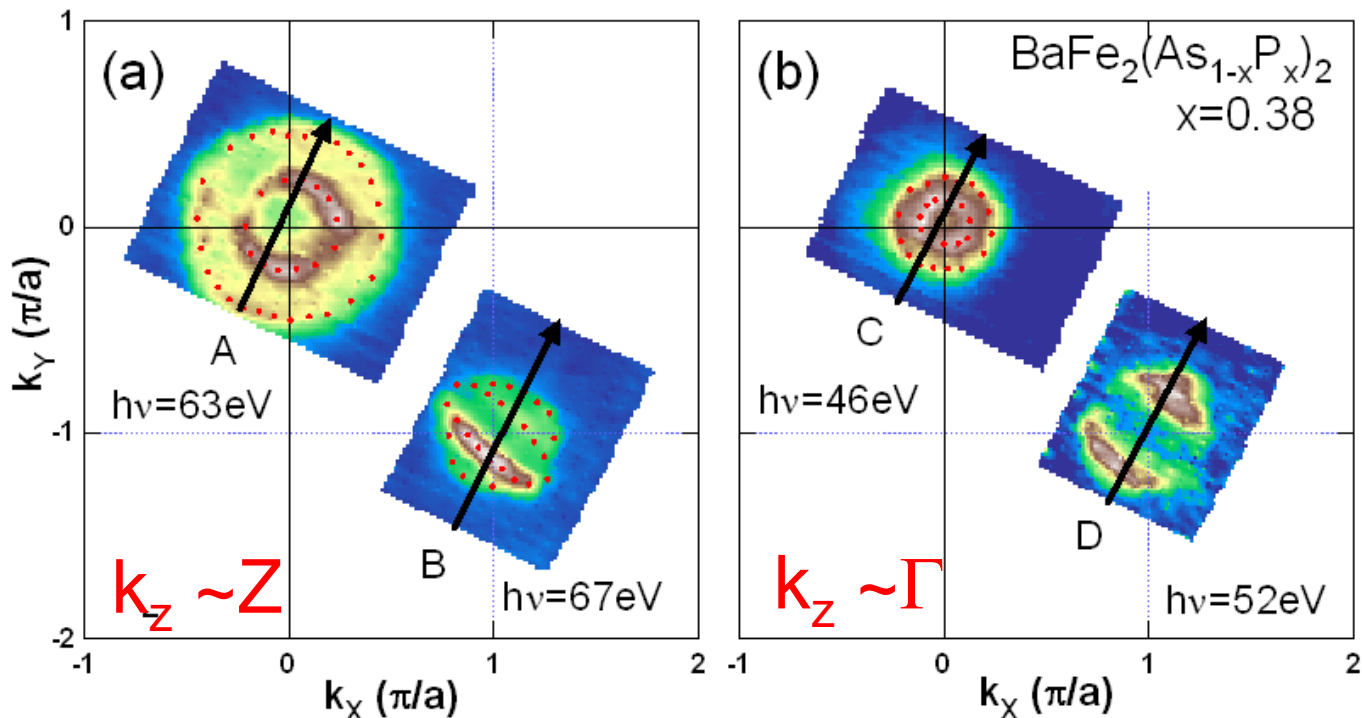


H. Shishido *et al*, PRL '10.

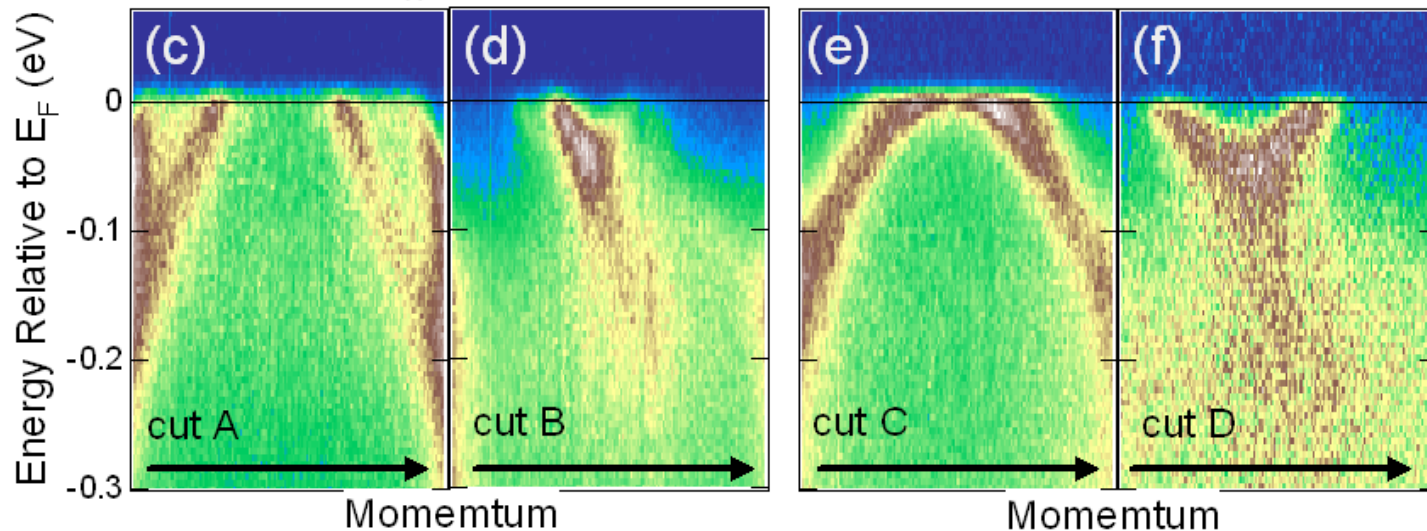
- Electron FSs are smaller than the prediction by the band-structure calculation.
inter-band scattering?
- Electron mass enhancement
Quantum critical behavior?

Direct observation of the FSs by ARPES

Fermi surface mapping of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$



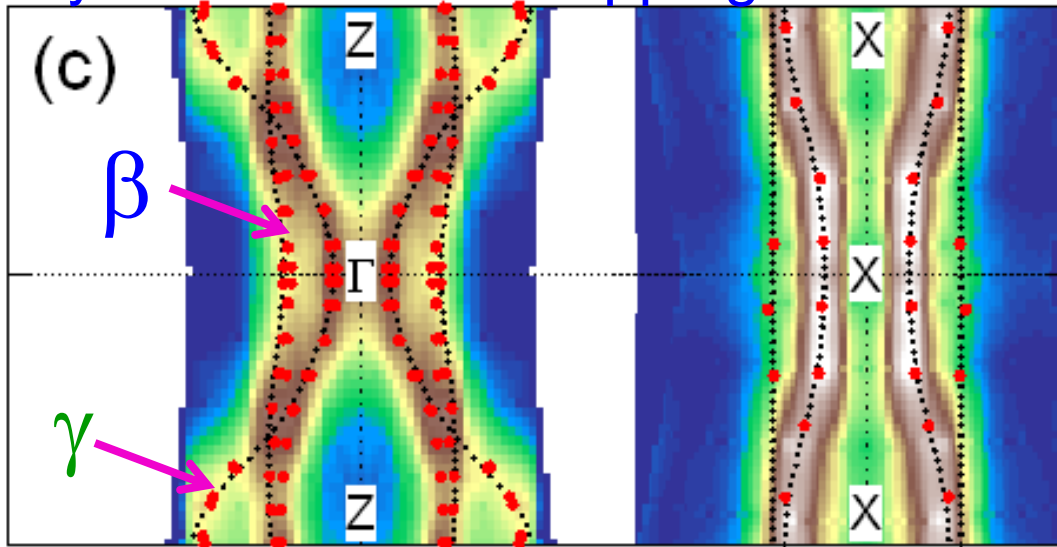
Strong three-dimensional



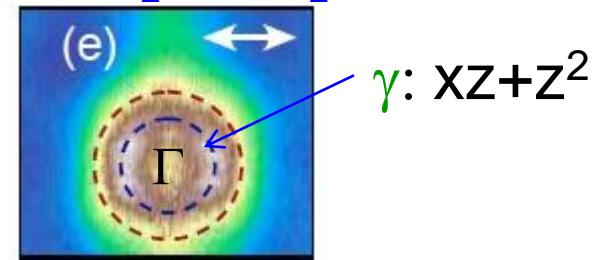
inner potential $V_0=13.5\text{ eV}$

Three-dimensional FSs

Symmetrized FS mapping

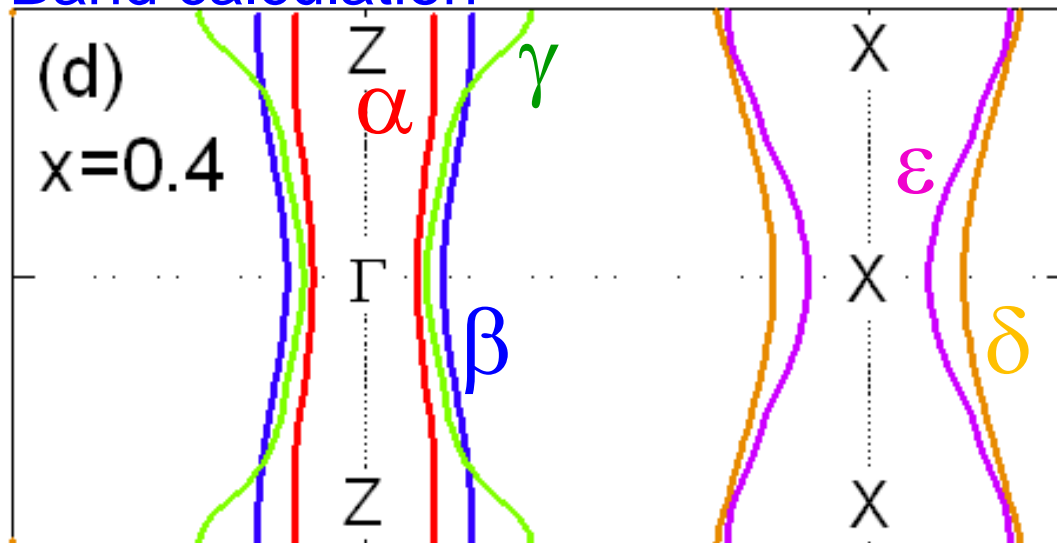


EuFe₂(As,P)₂



S. Thirupathiah *et al.*, arXiv '10

Band calculation



$\alpha: xy$

$\beta: yz$

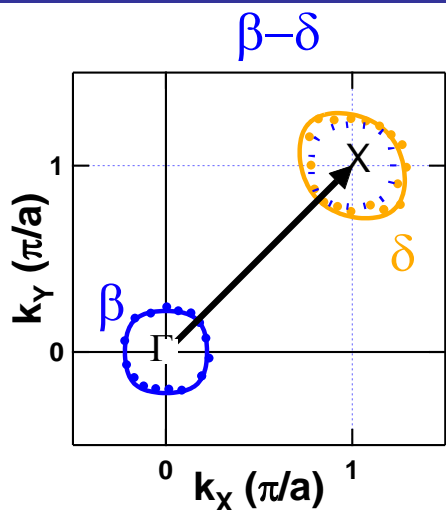
$\gamma: xz+z^2$

$\epsilon: yz$

$\delta: xy$

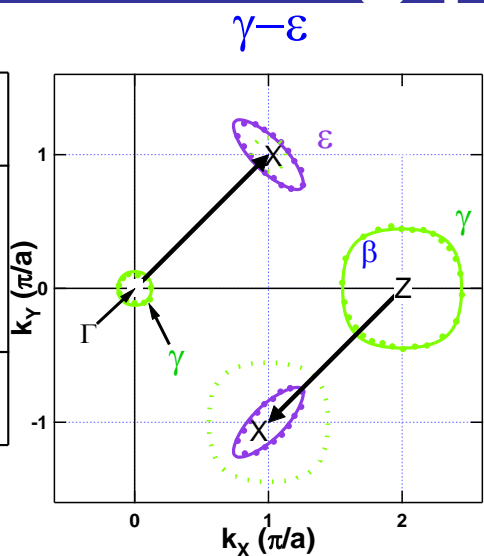
Matrix element of the d_{xy} orbital is small around the Γ point .

Nesting properties



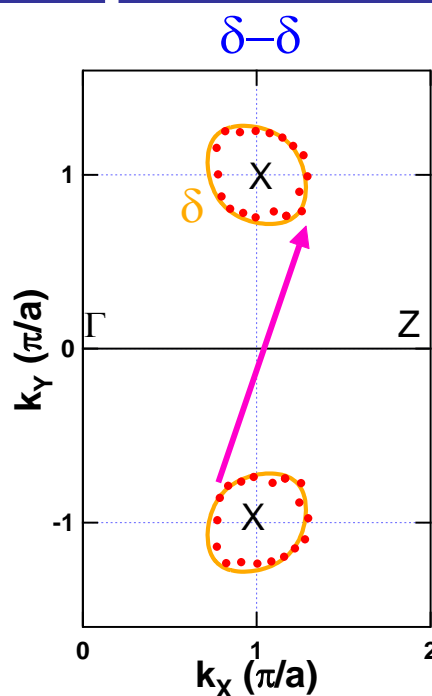
Different orbital character

“Poor nesting”



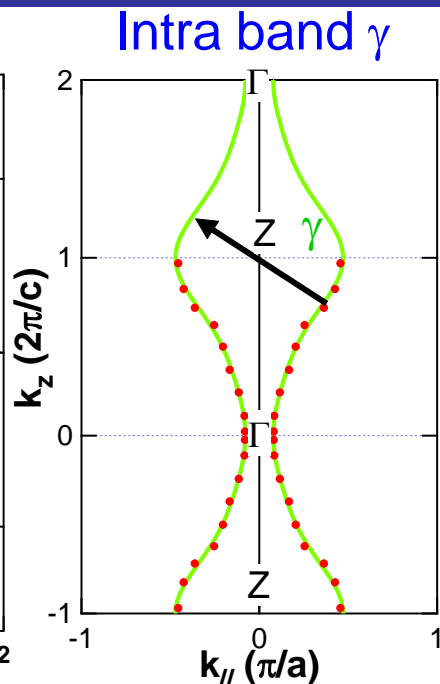
Three-dimensional γ FS

Poor nesting



Same orbital character

Partial nesting



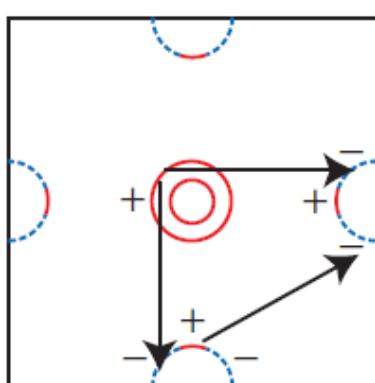
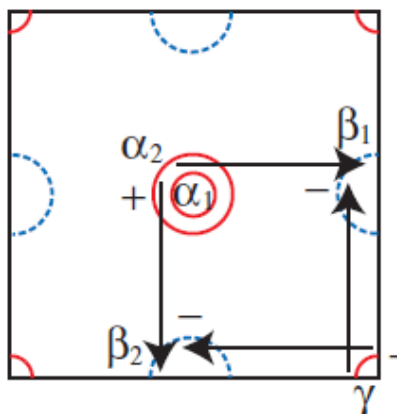
Horizontal node

Kuroki *et al.*,
Graser *et al.*, PRB '10

Theoretical prediction of line-node in SC gap

fully gapped $s \pm$ wave

nodal $s \pm$ wave



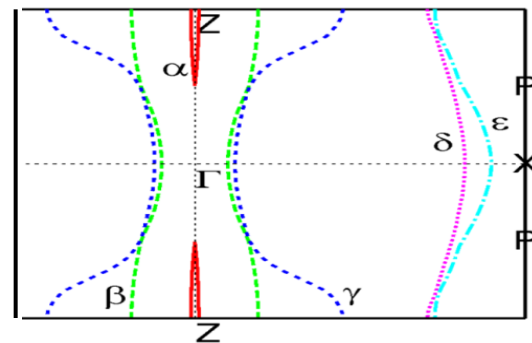
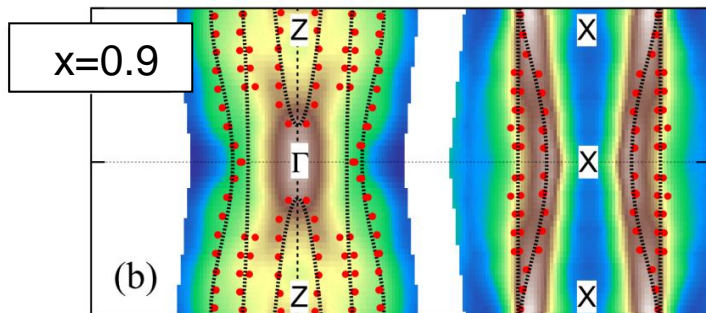
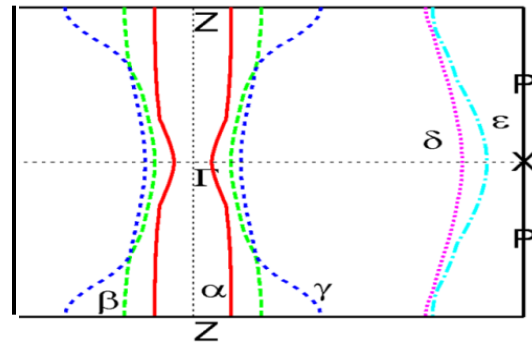
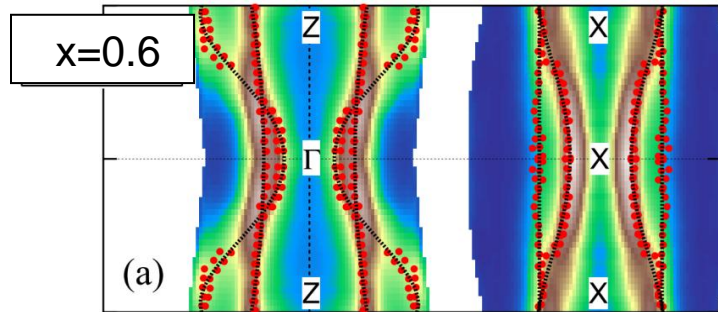
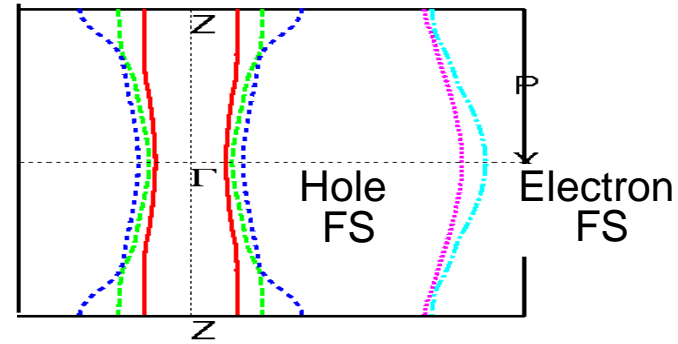
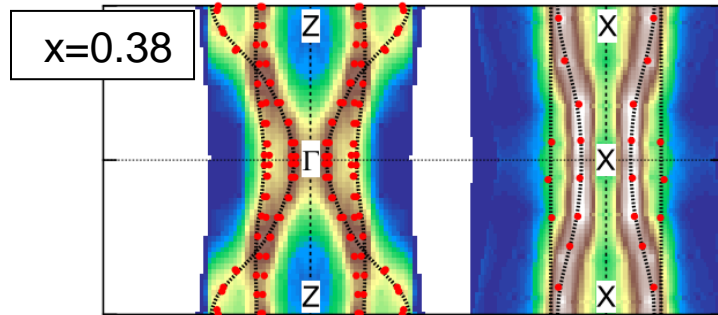
Kuroki *et al.*,
PRB '09.

Node in the
superconducting gap is
likely to be realized.

Modulation of Fermi surfaces along the k_z direction in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

ARPES intensity plot & k_F

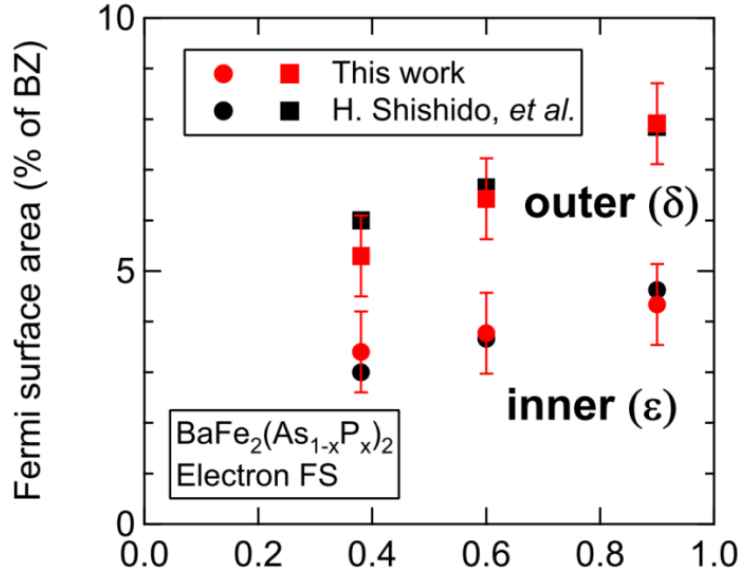
LDA calc



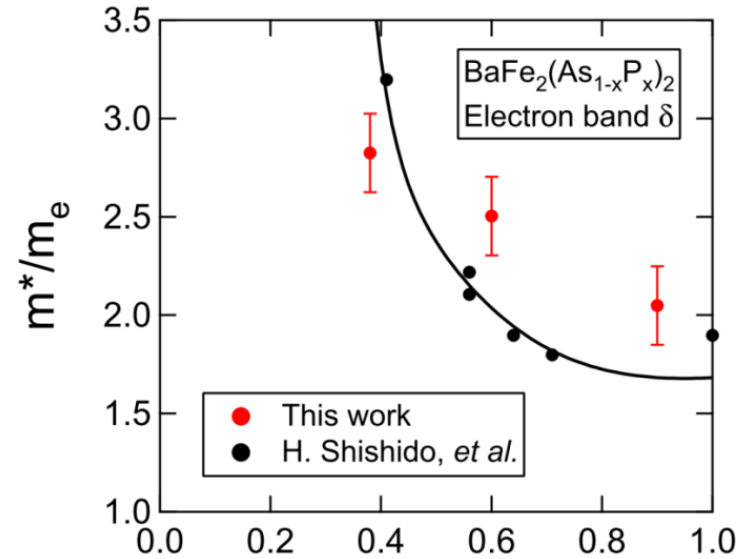
T. Yoshida et al.,
to appear in PRL
I. Nishi et al.,

Fermi surface volumes and effective masses in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

Area of electron FS's

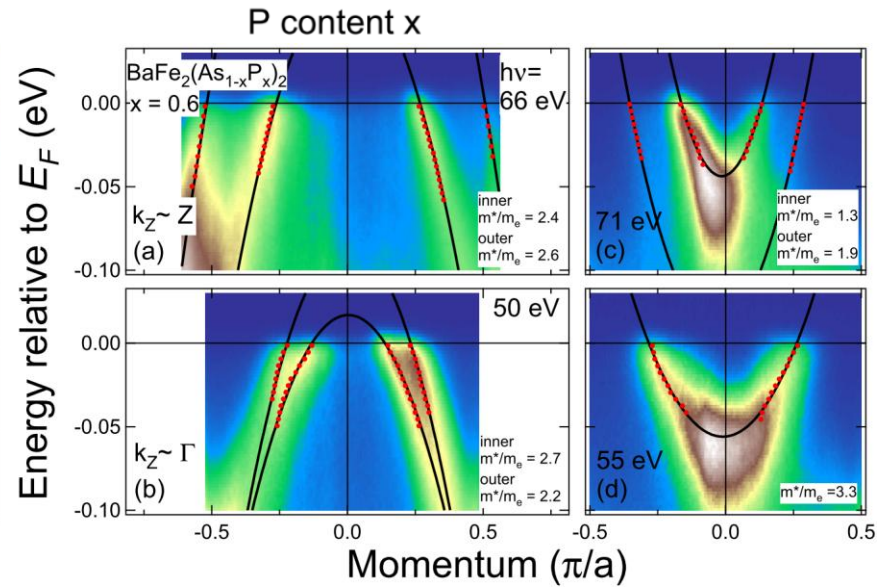
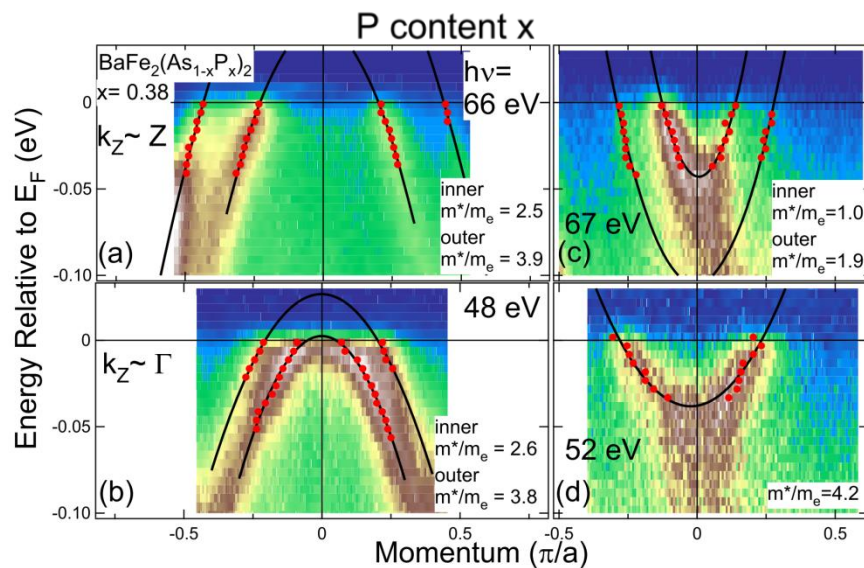


Effective masses of electron band

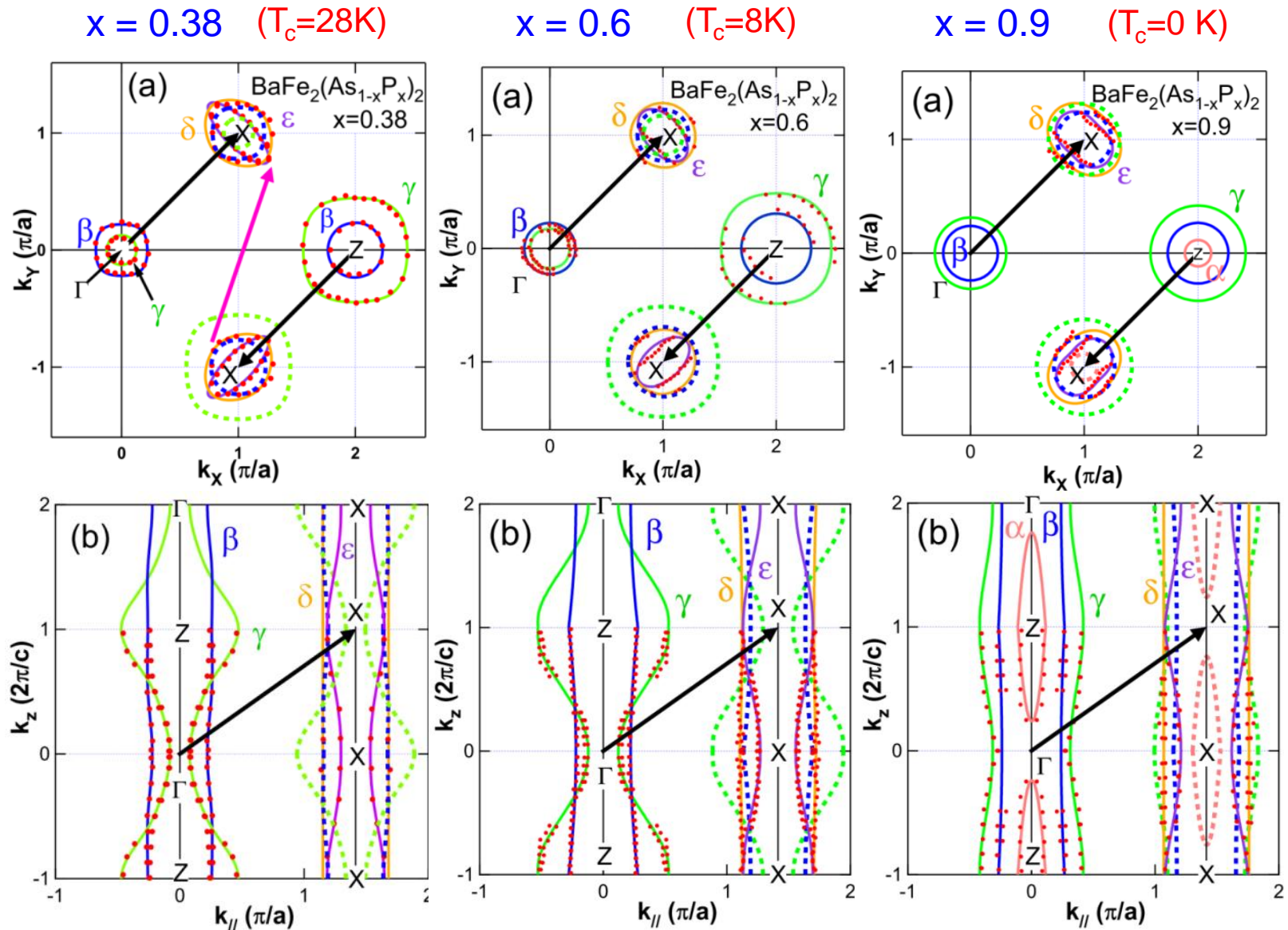


I. Nishi *et al.*

dHvA: H. Shishido
et al., PRL '10



Composition dependence of the Nesting properties

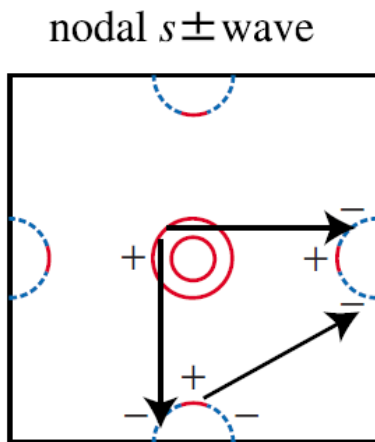
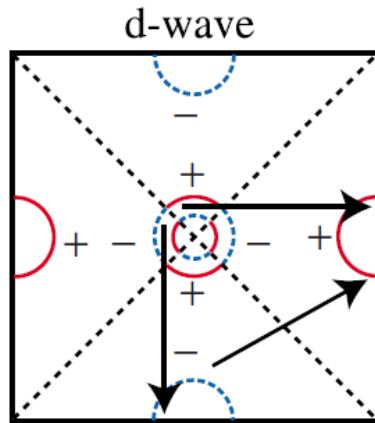


The nesting properties for $x = 0.6$ seem to be almost the same as those for $x = 0.38$.

suppression of
superconductivity

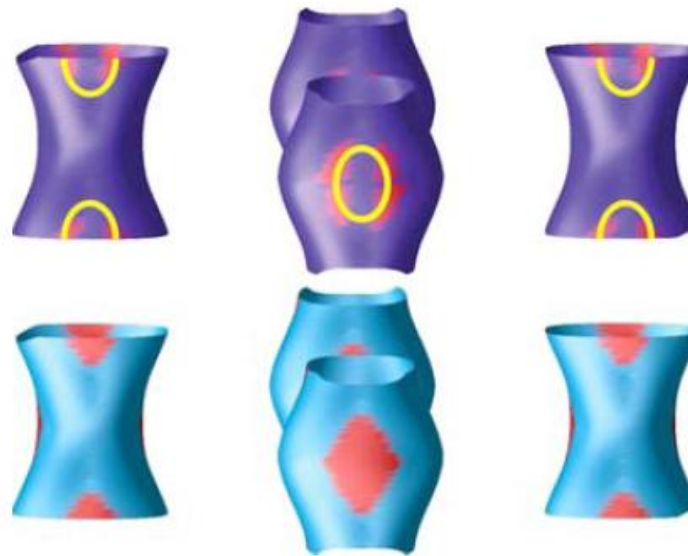
Possible line nodes in the superconducting gaps of Fe pnictides

“Vertical” line node



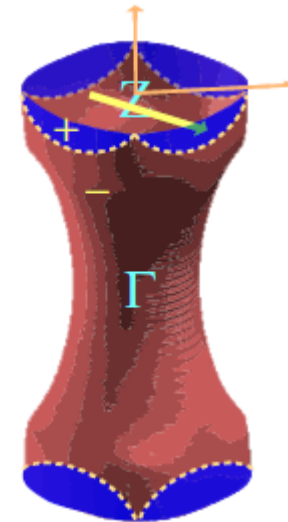
K. Kuroki et al., PRB '09

Loop-like line node on electron Fermi surface



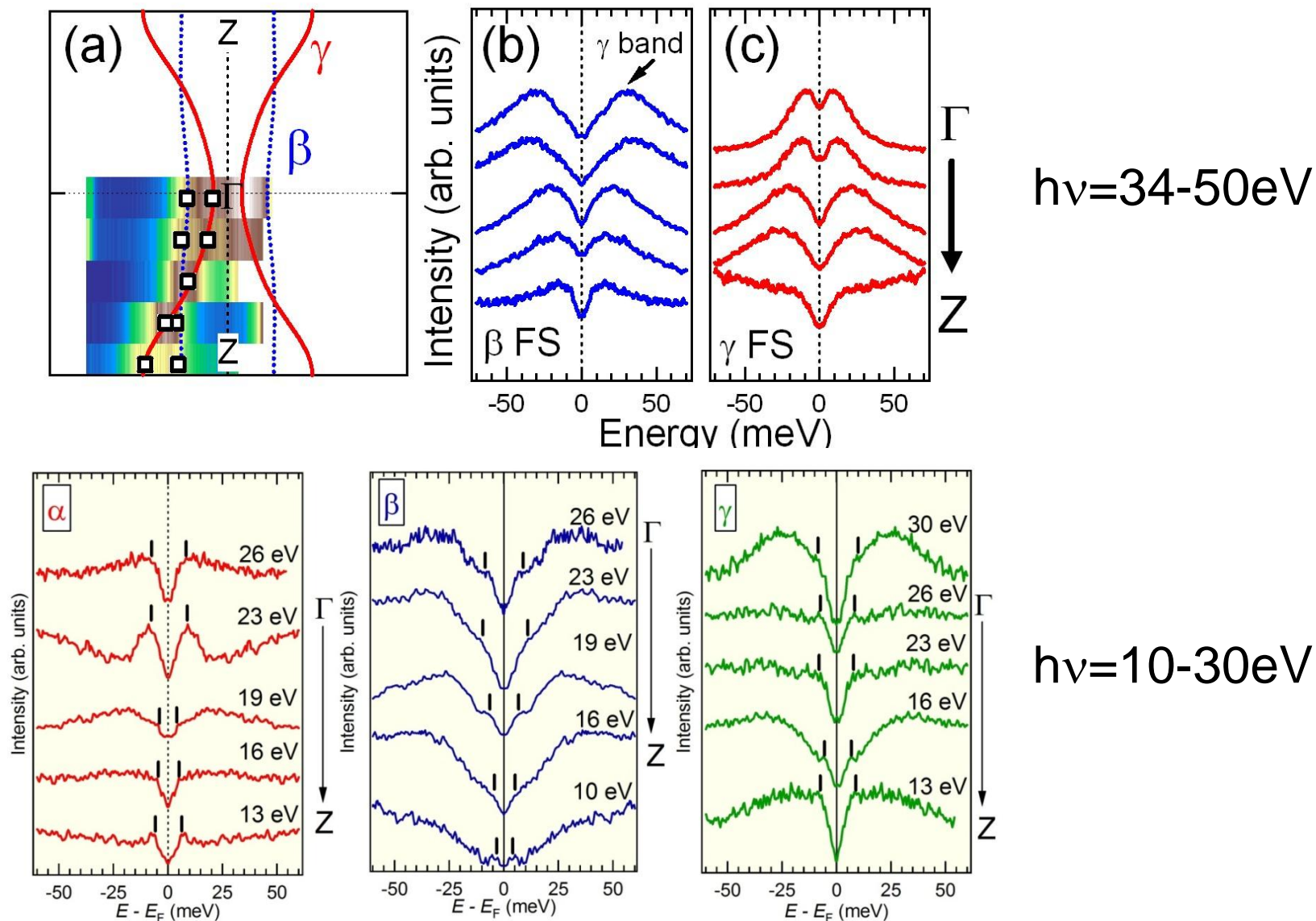
I. Mazin et al., PRB '10

Horizontal line node on hole Fermi surface



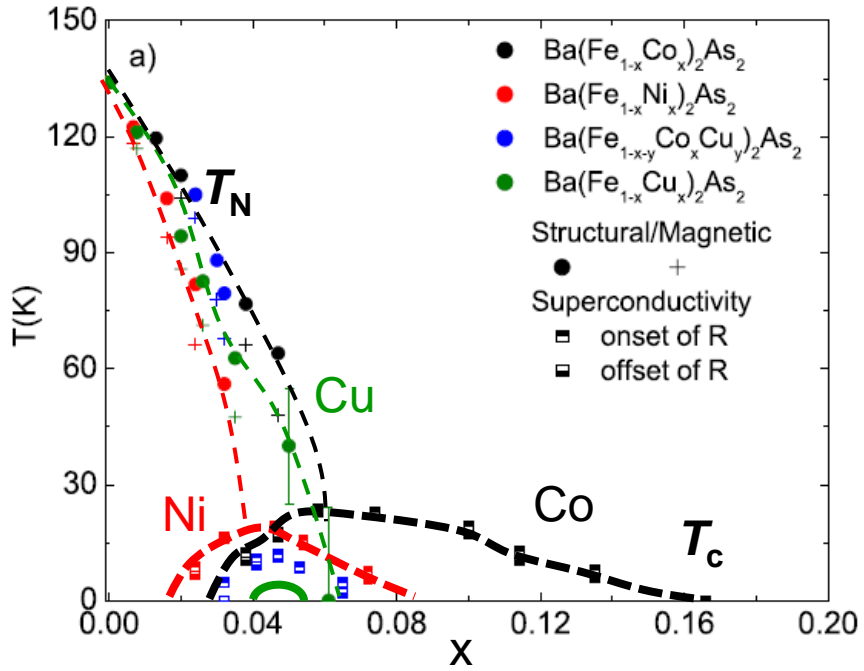
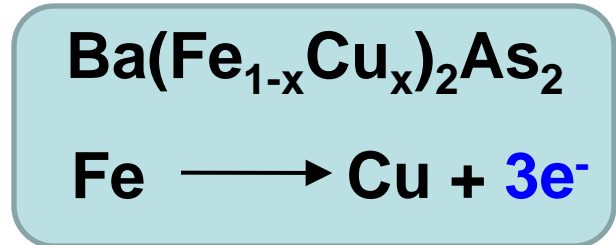
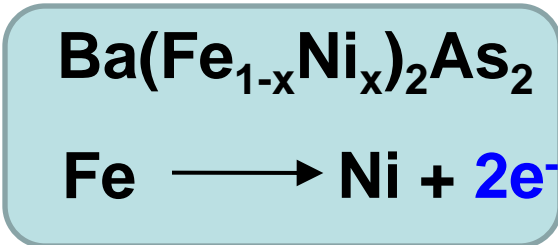
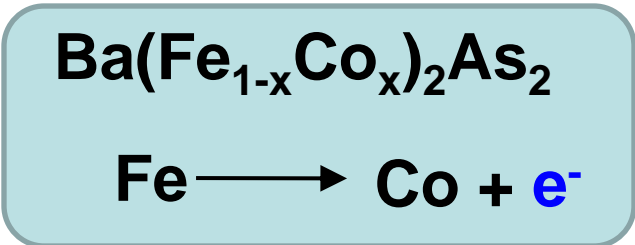
K. Suzuki et al., JPSJ '11

k_z dependence of the superconducting gap

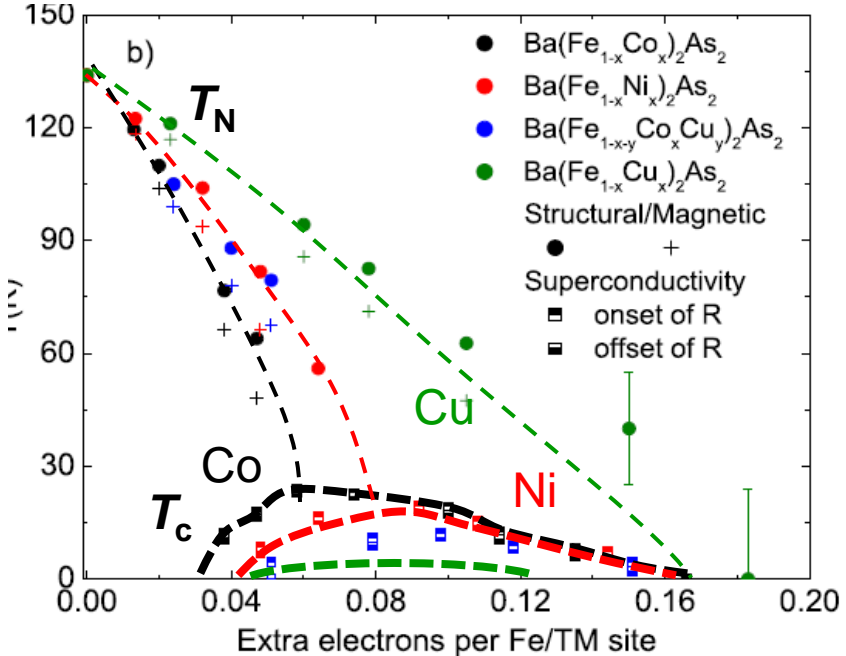


Non-rigid-band-like behavior in
Ba (Fe_{1-x}TM_x)₂As₂ (TM=Ni, Cu)

Electron-doped iron-based superconductors



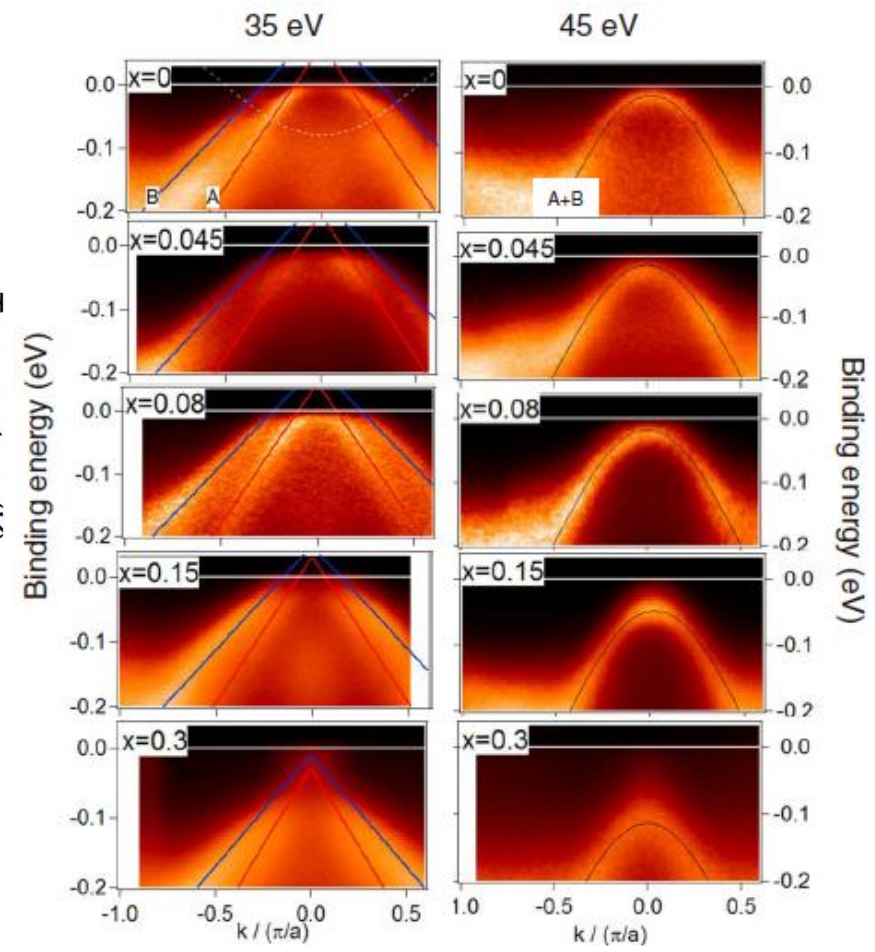
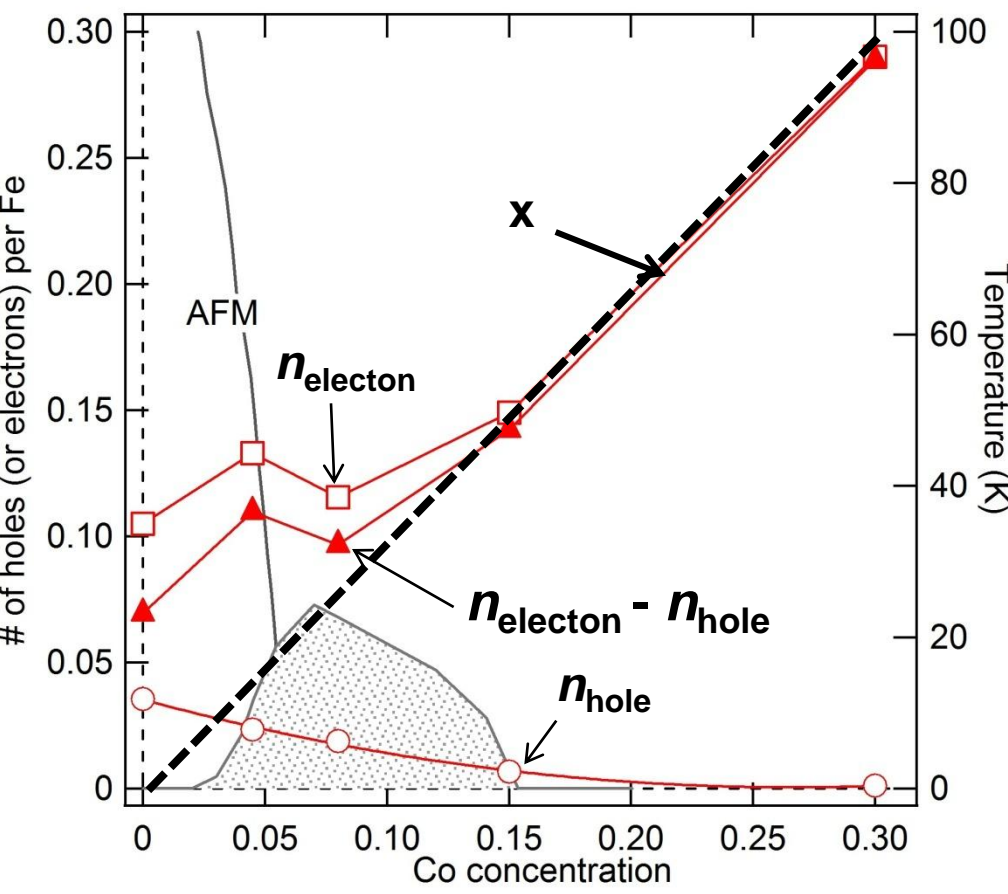
(x: Nominal TM content)



P.C. Canfield et al., PRB '09
 N. Ni et al., PRB '10

Estimation of carrier number in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

ARPES



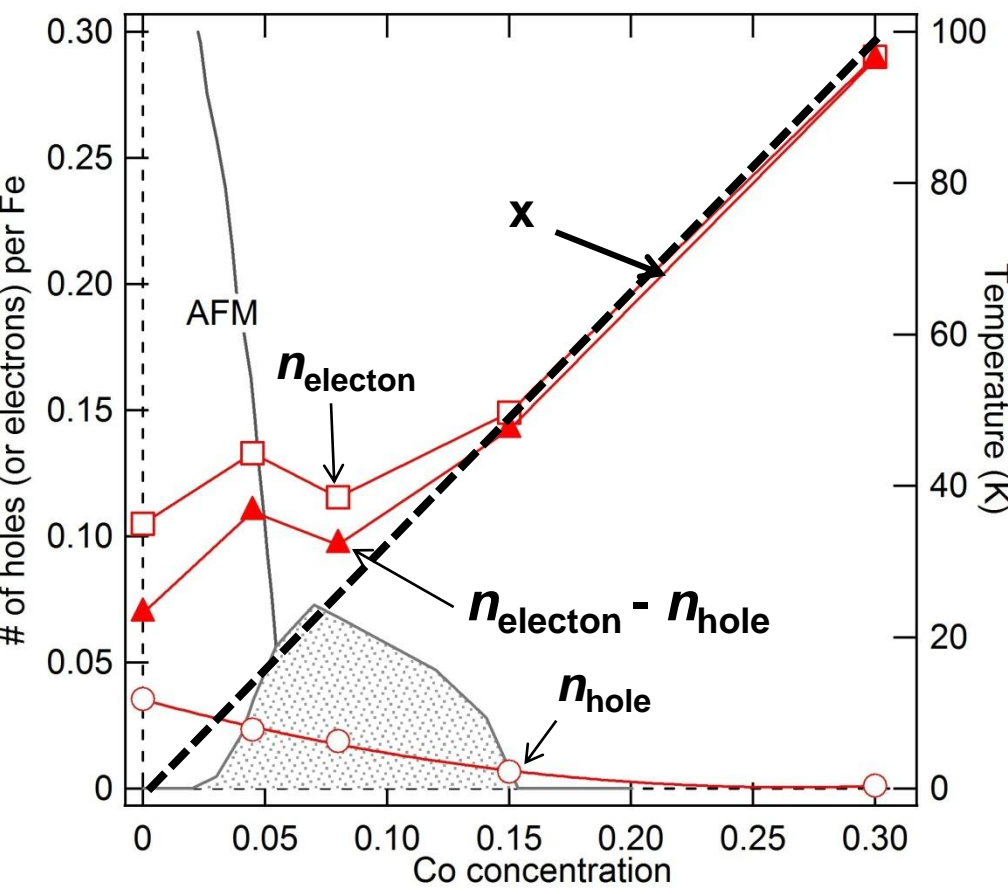
V. Brouet *et al.*, PRB **80**, 165115 (2009).

- $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$
- n_{el} (ARPES)
- n_{h} (ARPES)
- ▲— $n_{\text{el}} - n_{\text{h}}$ (ARPES)
- ▨ T_c
- T_{AFM}

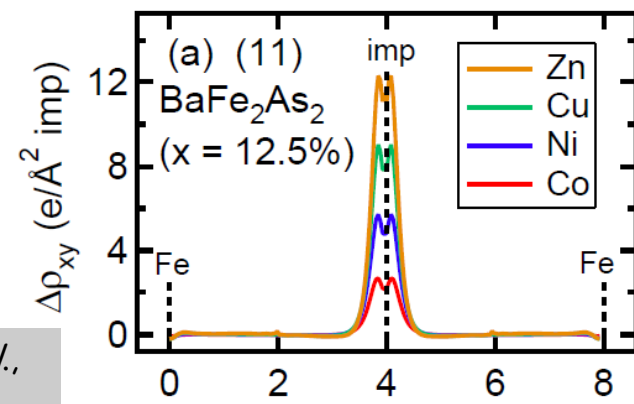
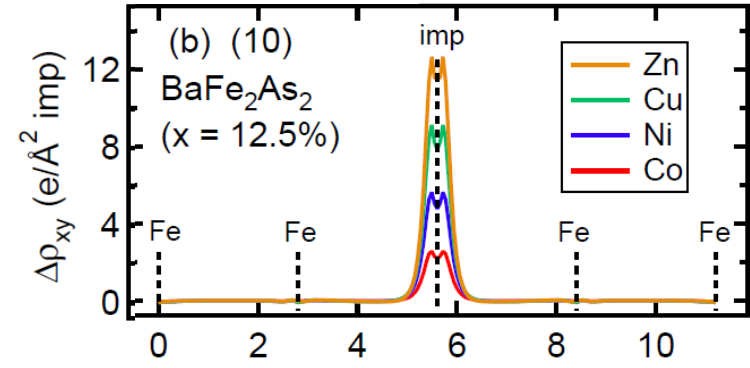
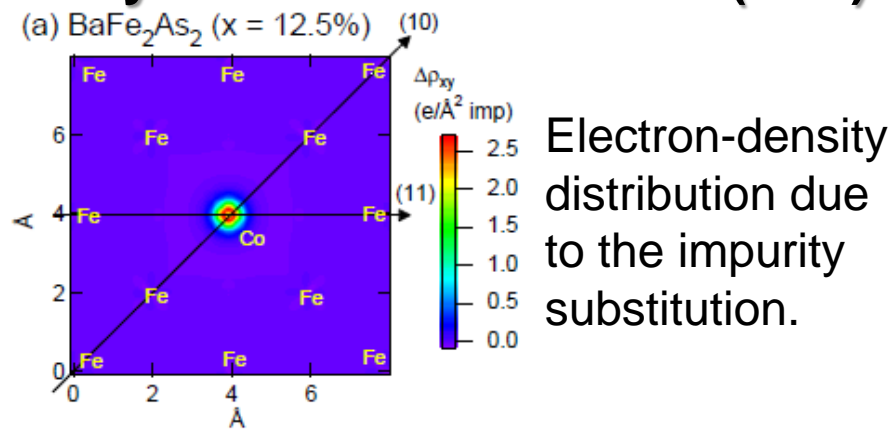
- Rigid-band-like shift
- $n_{\text{electron}} \sim x$

Estimation of carrier number in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

ARPES



Density functional calculation (DFT)



$\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

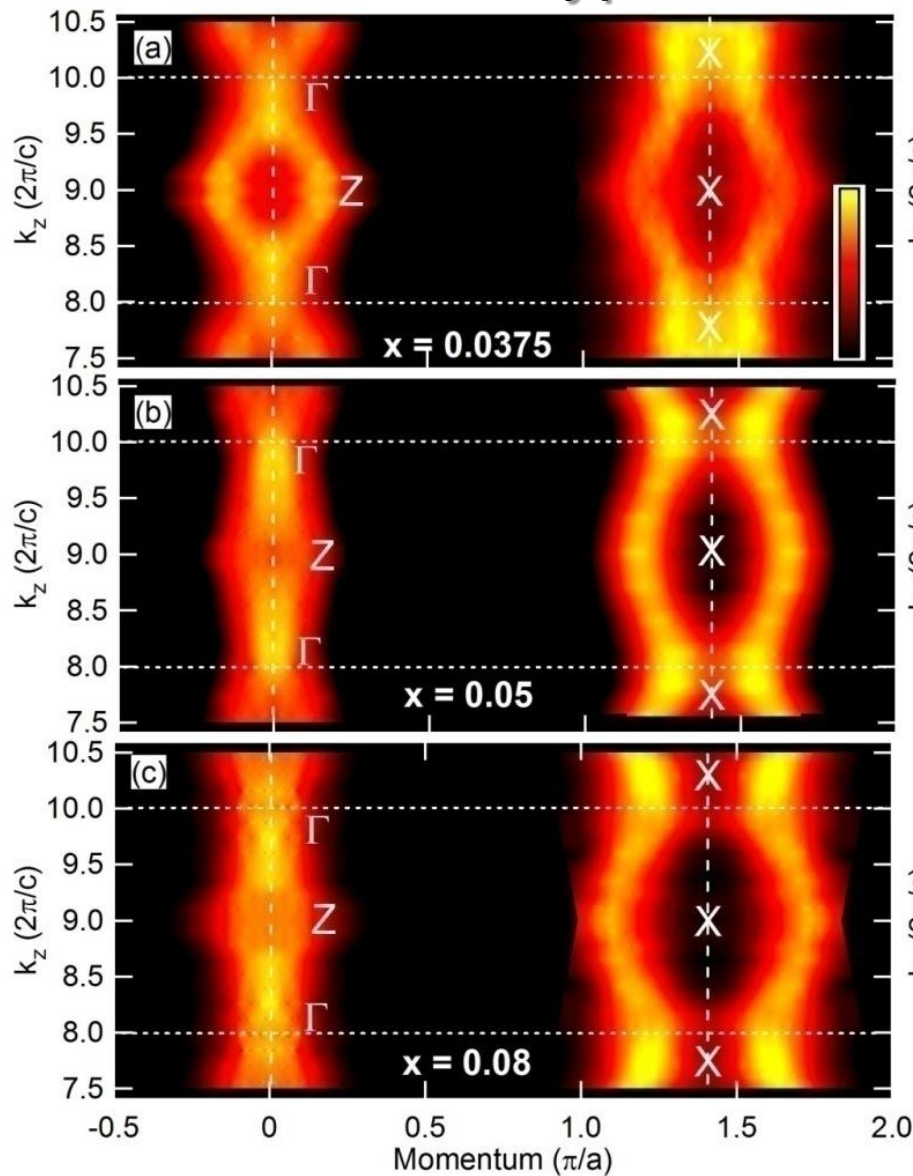
- n_{el} (ARPES)
- n_h (ARPES)
- ▲— $n_{el} - n_h$ (ARPES)
- ▨ T_c
- T_{AFM}

V. Brouet *et al.*, PRB **80**, 165115 (2009).

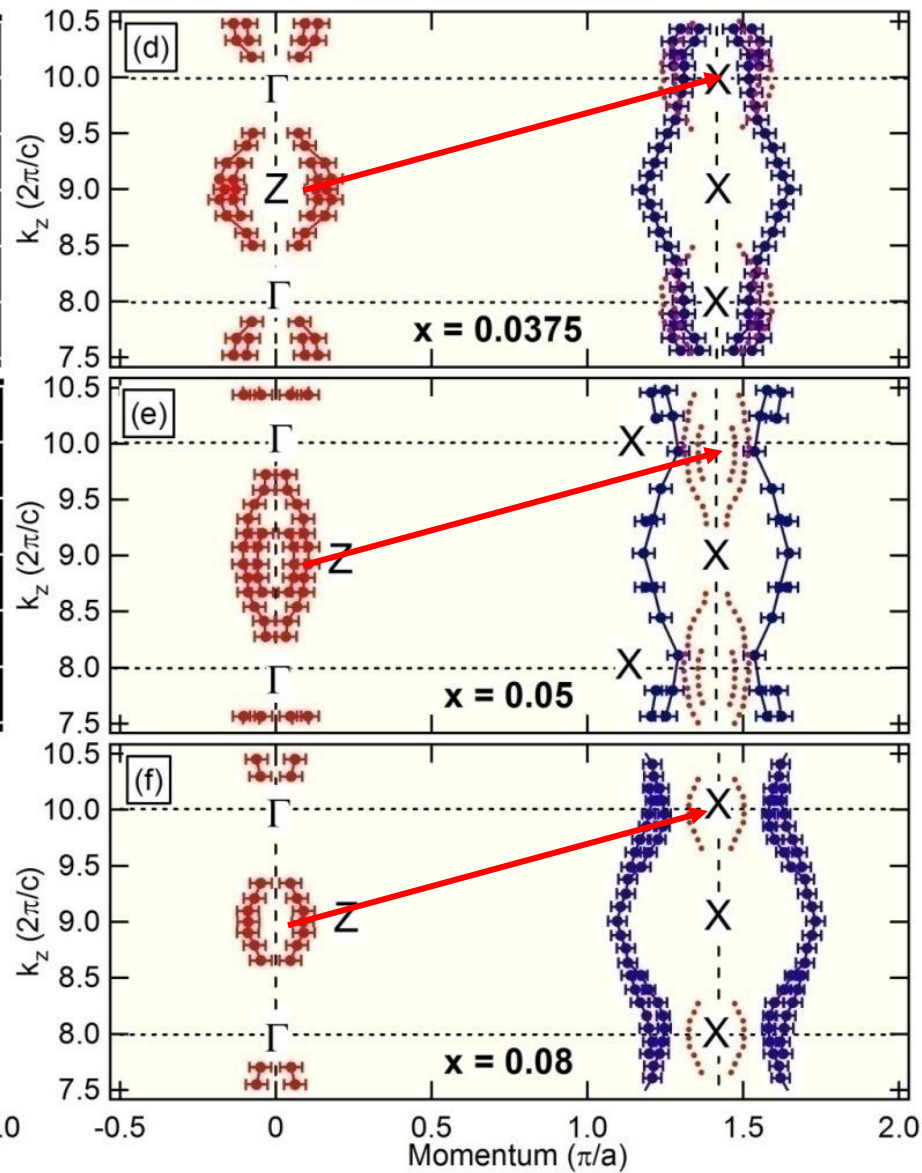
H. Wadati *et al.*, PRL (2010).

Modulation of Fermi surfaces along the k_z direction in $\text{Ba}(\text{Fe}_{1-x}\text{Ni}_x)_2\text{As}_2$

ARPES intensity plots



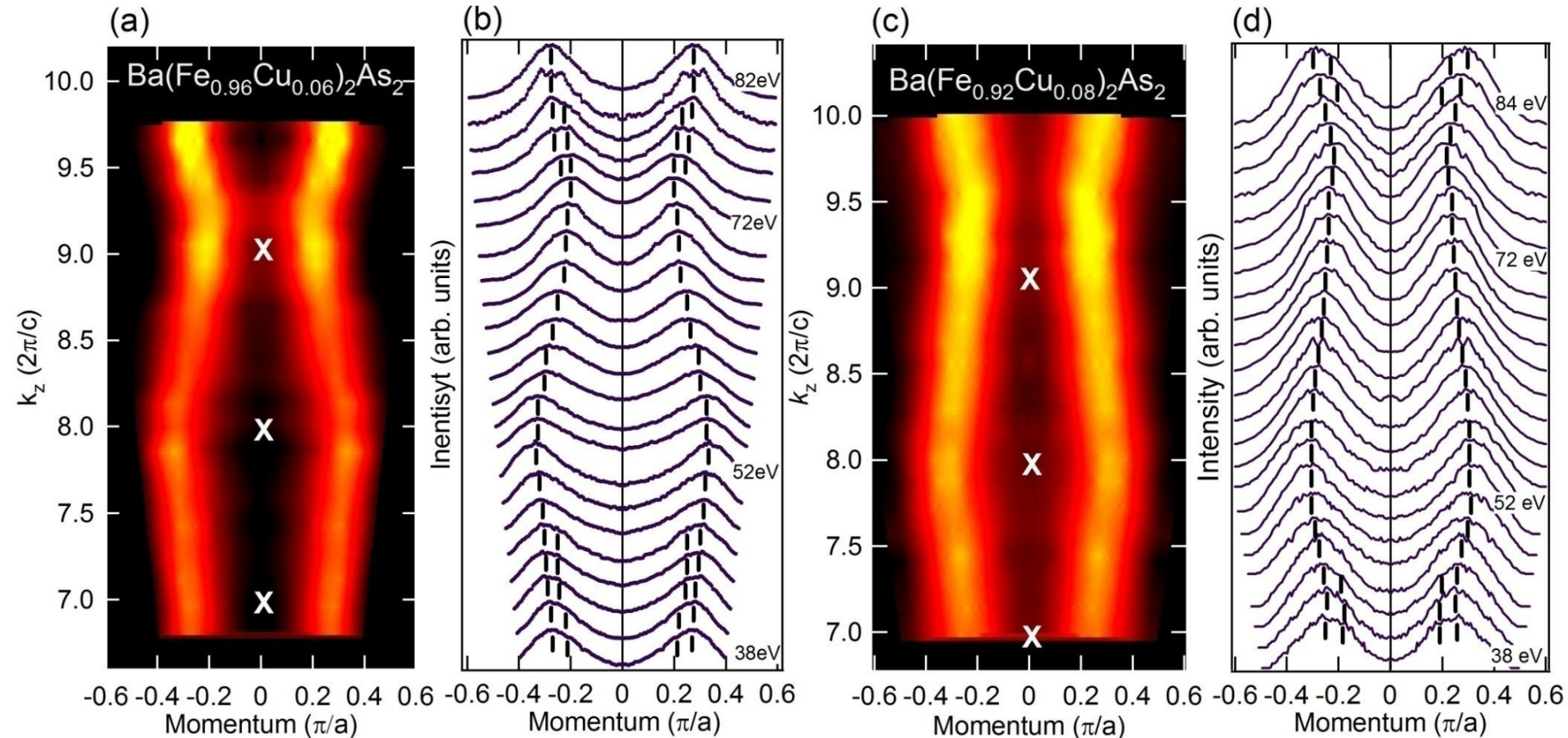
k_F plots estimated from MDCs



Modulation of Fermi surfaces along the k_z direction for $\text{Ba}(\text{Fe}_{1-x}\text{Cu}_x)_2\text{As}_2$

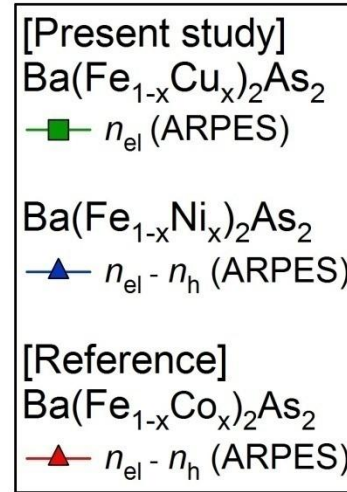
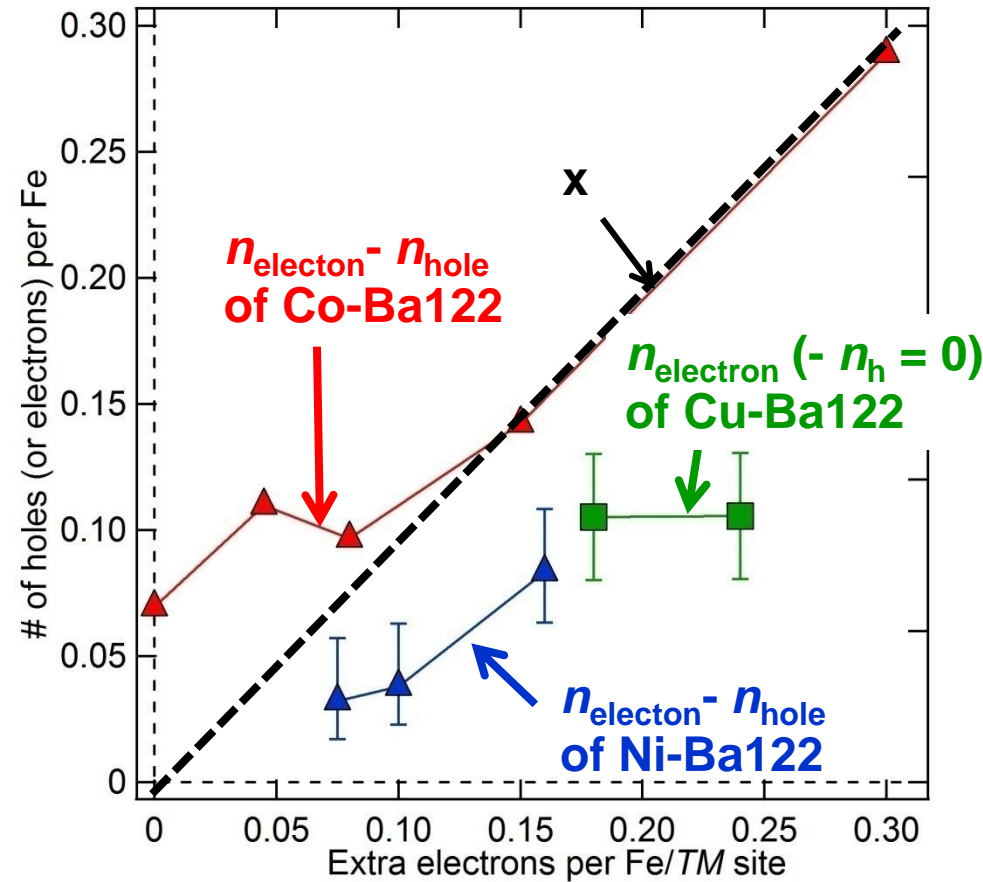
$x = 0.06$

$x = 0.08$

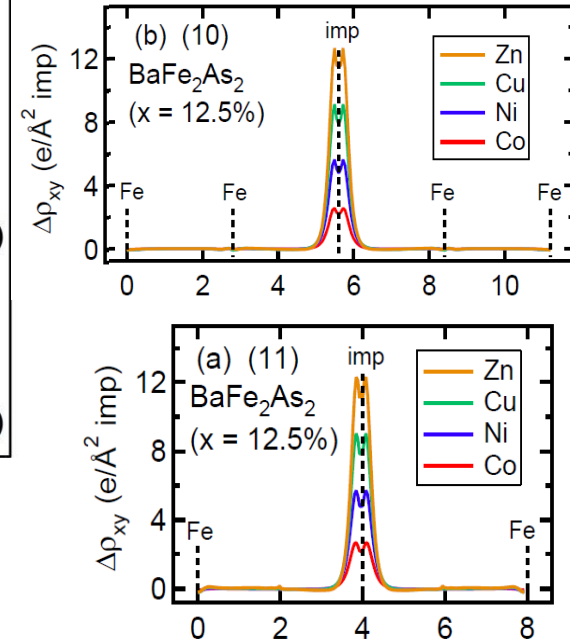


The volume of electron FS of the Cu-Ba122 dose not show a large difference between the $x = 0.06$ and 0.08 sampels.

$n_{el} - n_h$ for $Ba(Fe_{1-x}TM_x)_2As_2$ ($TM = Co, Ni, Cu$)



Density functional calculation (DFT)



H. Wadati *et al.*,
PRL (2010).

- The number of electron in Ni-Ba122 and Cu-Ba122 deviates from that of Co-doped Ba122.
- Co-Ba122 behaves like a rigid-band shift.
- Effect of localized d electron has been observed with changing Co, Ni, and Cu ? (Wadati *et al.*)

Summary

We have performed ARPES studies of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{TM}_x)_2\text{As}_2$ (TM=Ni, Cu) to clarify the three-dimensional electronic structure.

$\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

- The disconnection of the FS in $x=0.9$ seems to deteriorate nesting properties and may lead to the suppression of superconductivity.
- The energy gaps in the hole FSs have been observed for a wide range of k_z .

$\text{Ba}(\text{Fe}_{1-x}\text{TM}_x)_2\text{As}_2$ (TM=Ni, Cu)

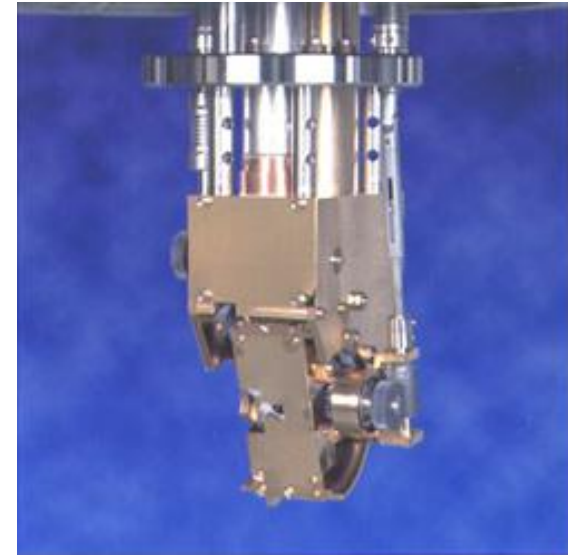
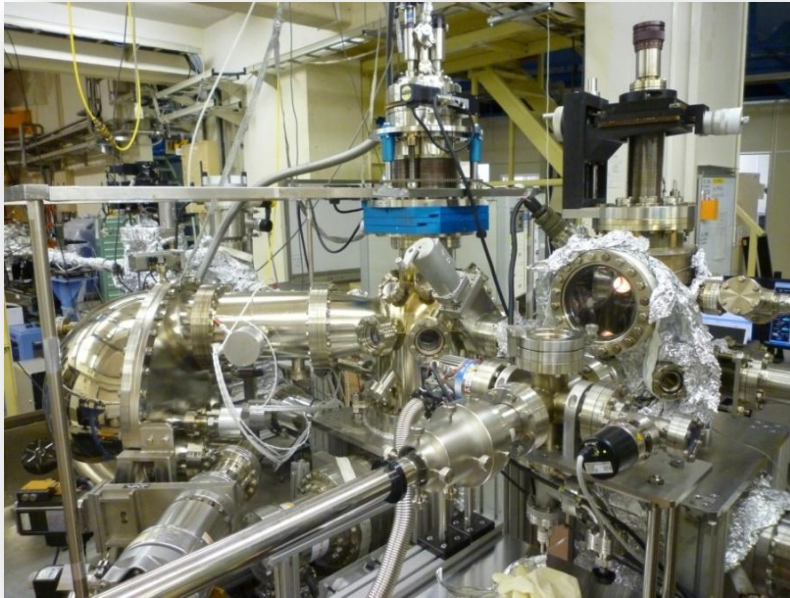
- Nesting condition becomes worse than that of the hole-doped Ba122 even in the optimally doped $\text{Ba}(\text{Fe},\text{Ni})_2\text{As}_2$.
- The electron carrier numbers estimated from FS volume of $\text{Ba}(\text{Fe},\text{Ni})_2\text{As}_2$ and $\text{Ba}(\text{Fe},\text{Cu})_2\text{As}_2$ are much smaller than those of the nominal electron number, indicating localization of the doped electrons.

Future work

- Observation of the node in the superconducting gap.
- Fine structure such as kink should be investigated.
- Relation between orbital character and superconductivity.

BL-28A Outlook

- アナライザー更新
R4000導入
- フェルミ面マッピングの自動化



Collaborators

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