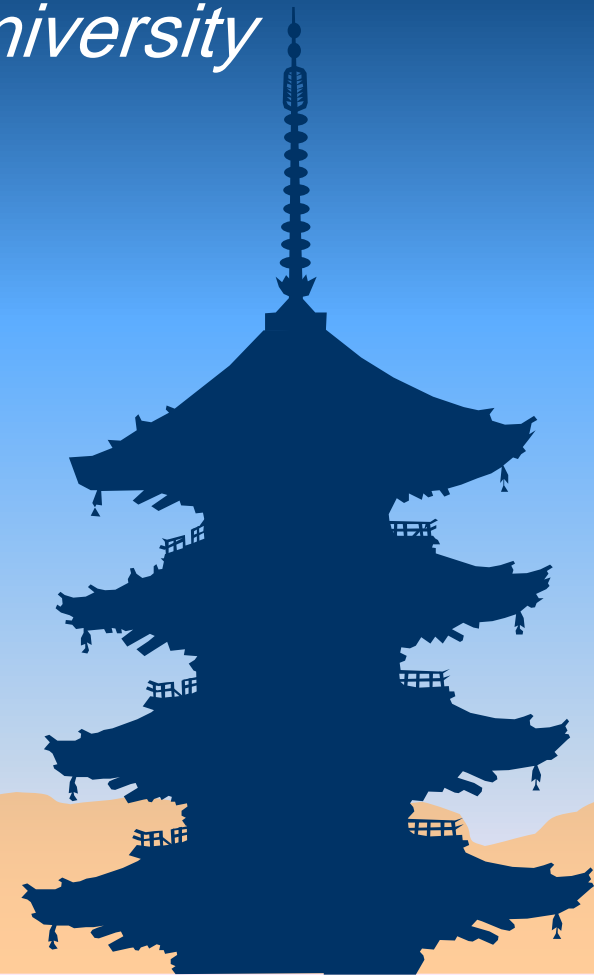


Determining gap nodal structure in isovalent doped $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

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Collaborators

Penetration depth, dHvA

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K. Hashimoto
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Univ. of Bristol, UK

Specific heat

H. Ikeda **Band calc.**
T. Iye

G.R. Stewart
J.S. Kim



P.J. Hirschfeld
Univ. of Florida

Y. Nakai
K. Ishida
Kyoto Univ.

NMR

Penetration depth

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Ames



THE Ames Laboratory
Creating Materials & Energy Solutions

Laser ARPES

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ARPES

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A. Fujimori



Univ. of Tokyo

Thermal conductivity, theory

I. Vekhter
Louisiana



A.B. Vorontsov
Montana



Outline

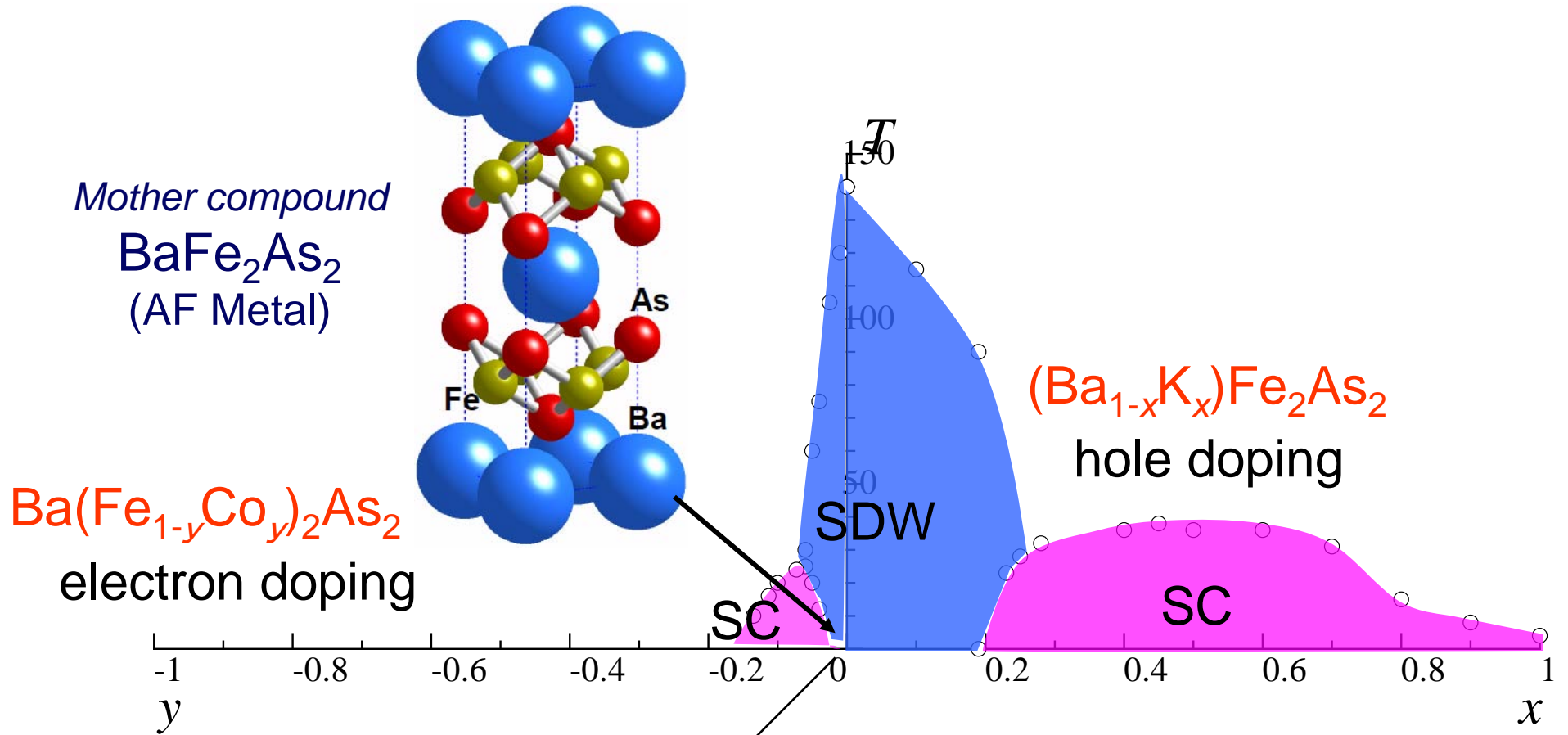
1. Introduction

2. “Iso-valent doping” system $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

3. Superconducting gap structure of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$
Evidence of line node
Pinpointing the position of line node

4. Summary

Superconductivity in BaFe₂As₂ systems



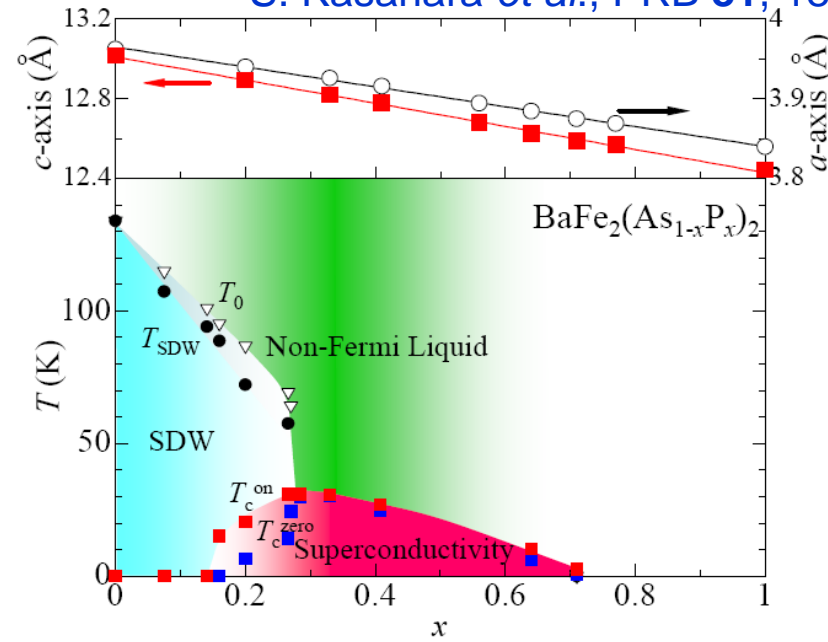
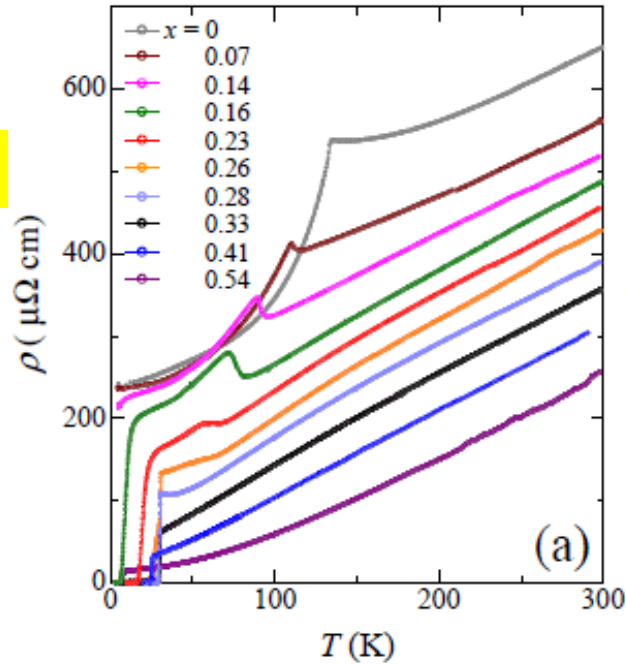
BaFe₂(As_{1-x}P_x)₂ S. Jiang *et al.* JPCM (09)

Iso-valent doping (Chemical Pressure)

Superconductivity by isovalent substitution of P for As

S. Kasahara *et al.*, PRB **81**, 184519 (2010).

P-dope



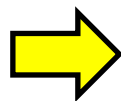
Why is the isovalent doping important?

Compensation condition ($n_e = n_h$) holds for any x .

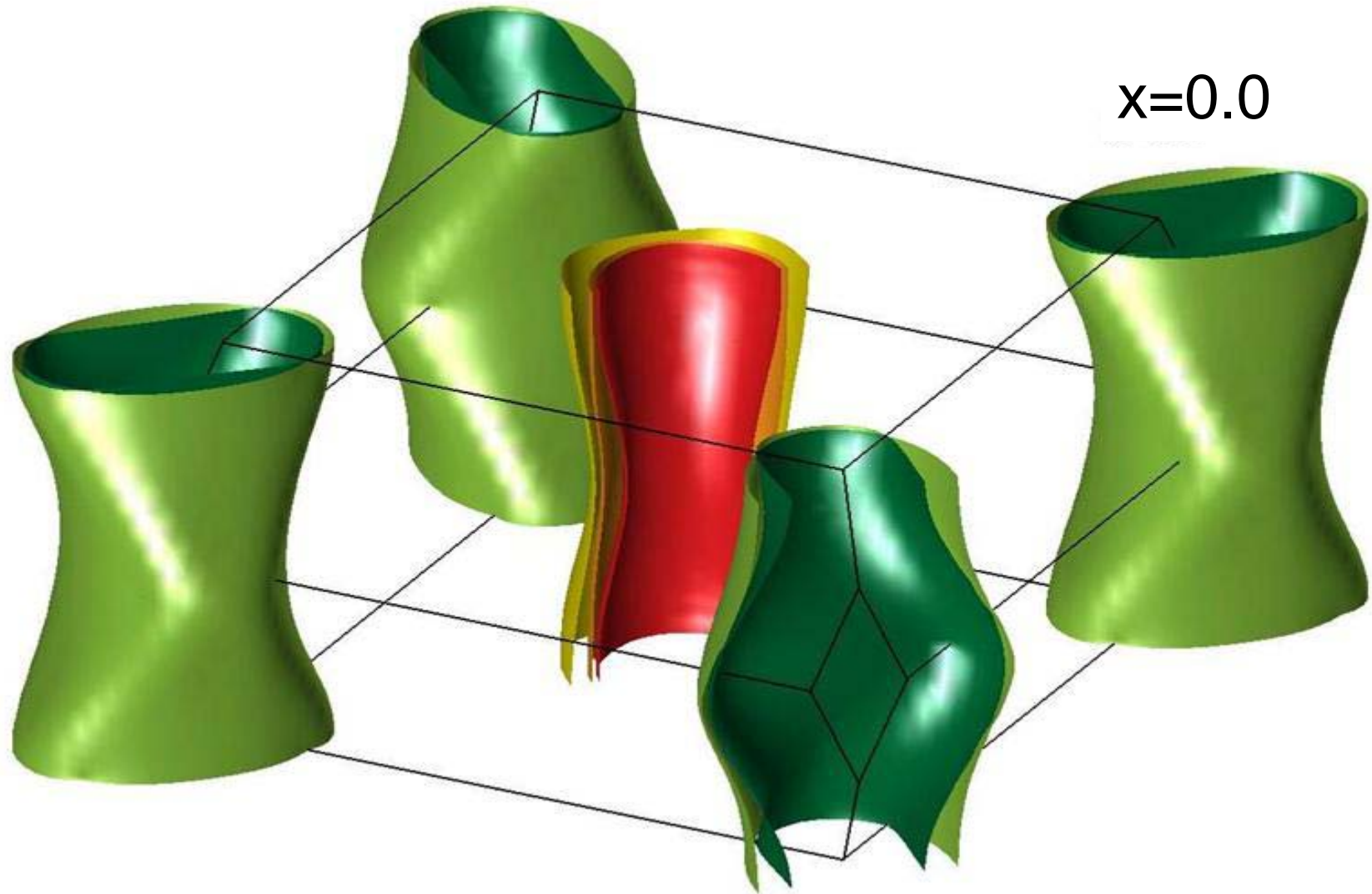
Volume of hole FSs = Volume of electron FSs

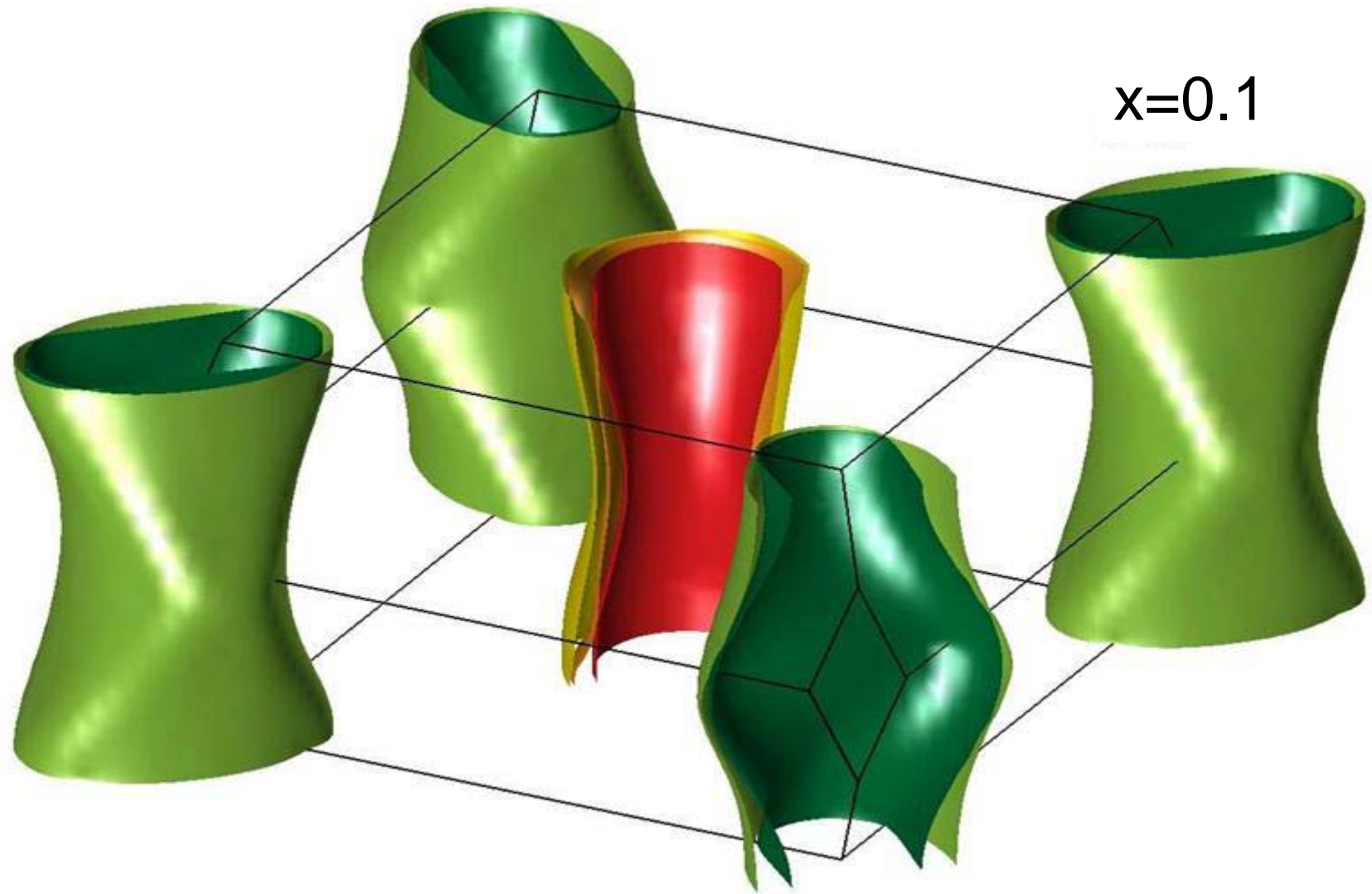
The magnetic characters can be tuned by x without doping carrier.

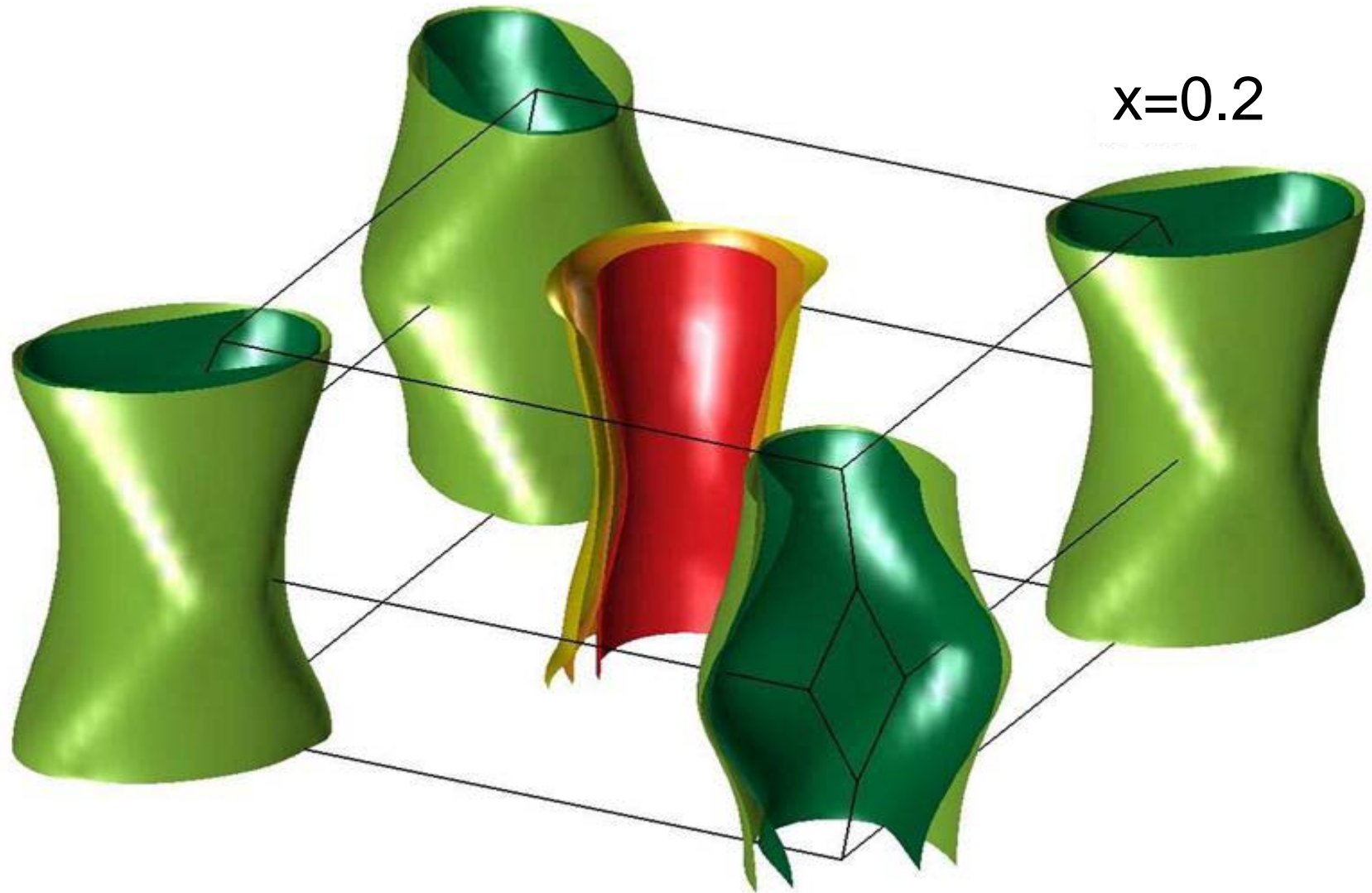
Very clean single crystals are available (quantum oscillations)

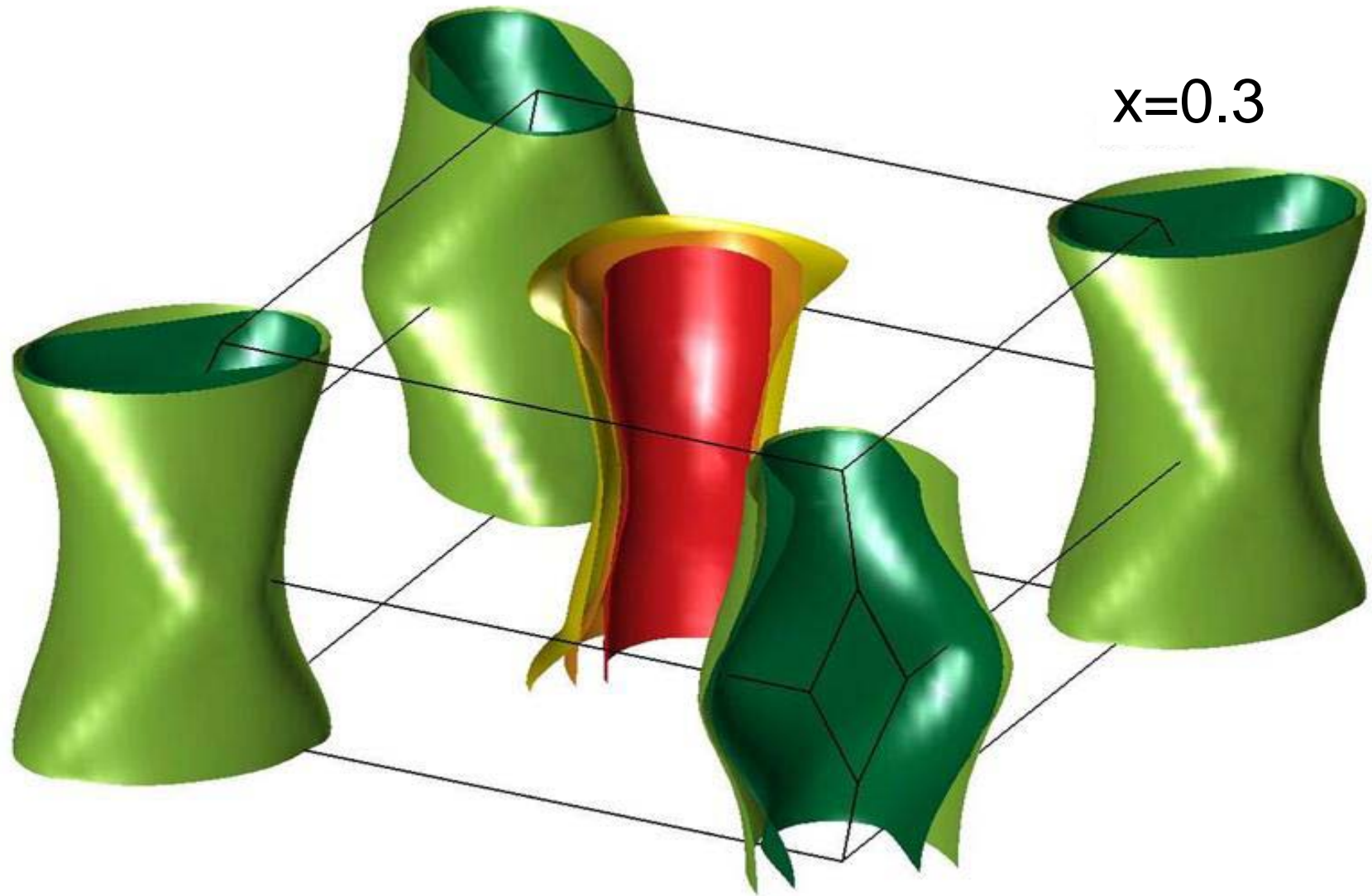


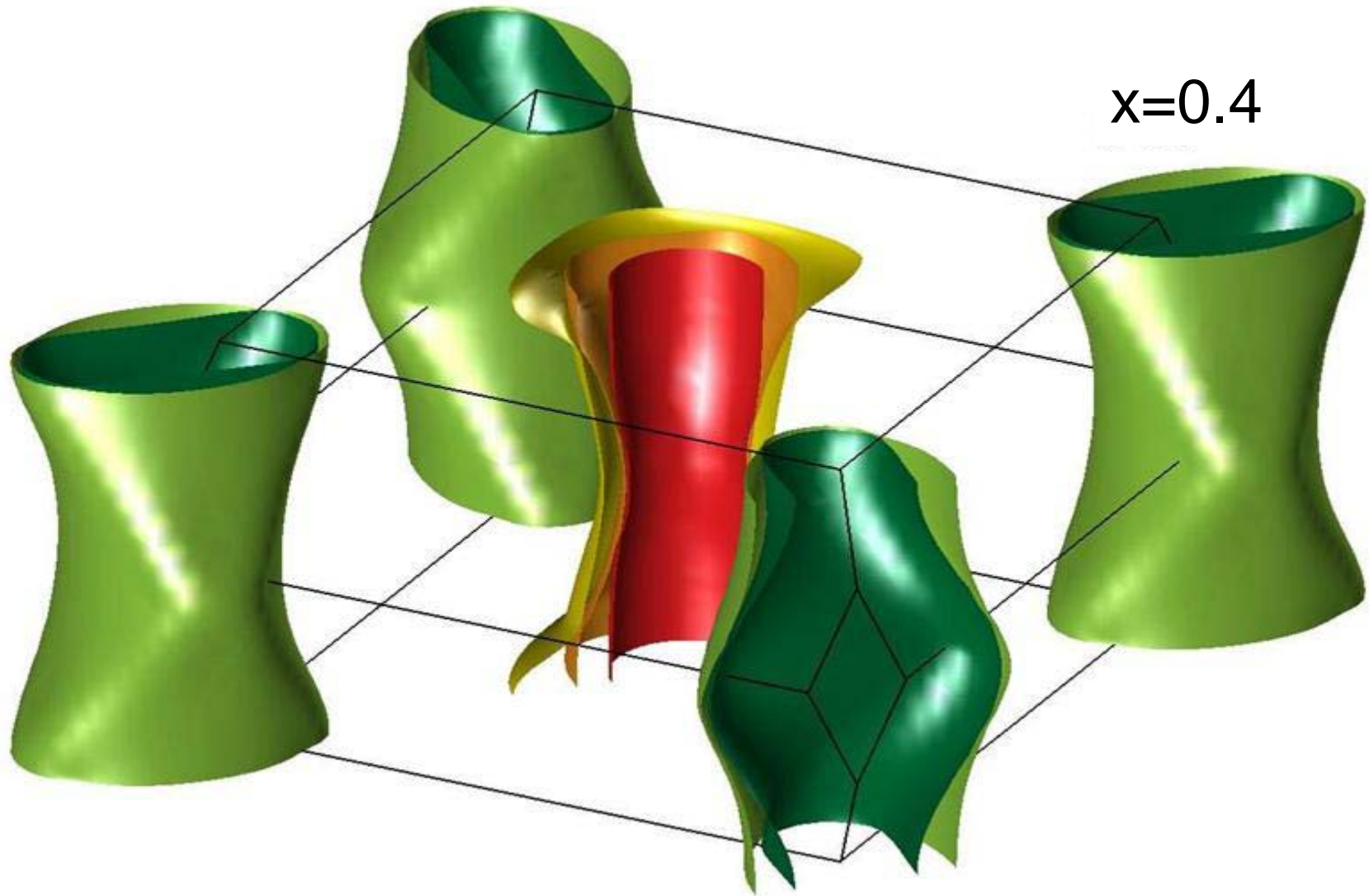
suitable for studying intrinsic physics among Fe-based SCs.

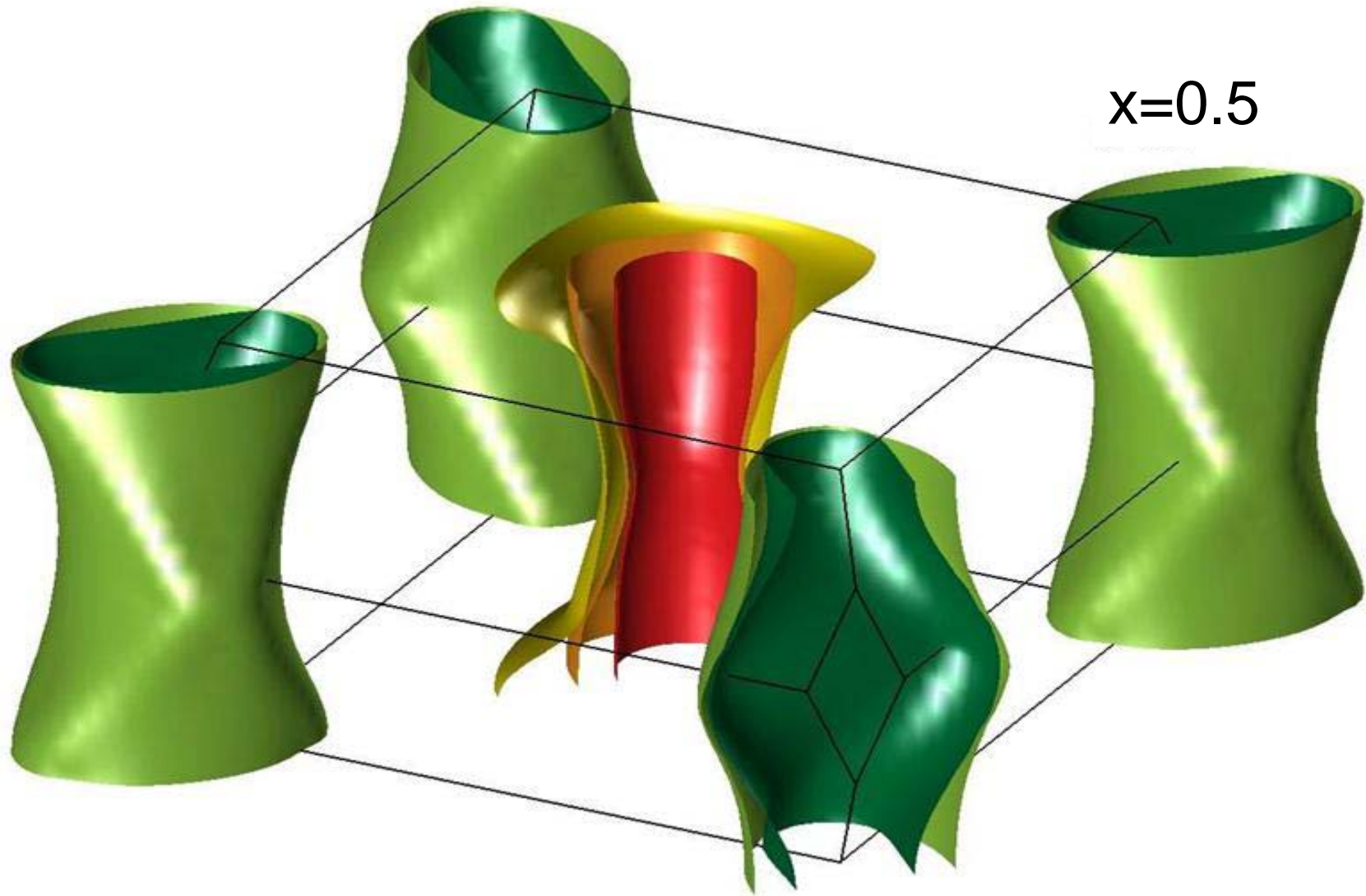


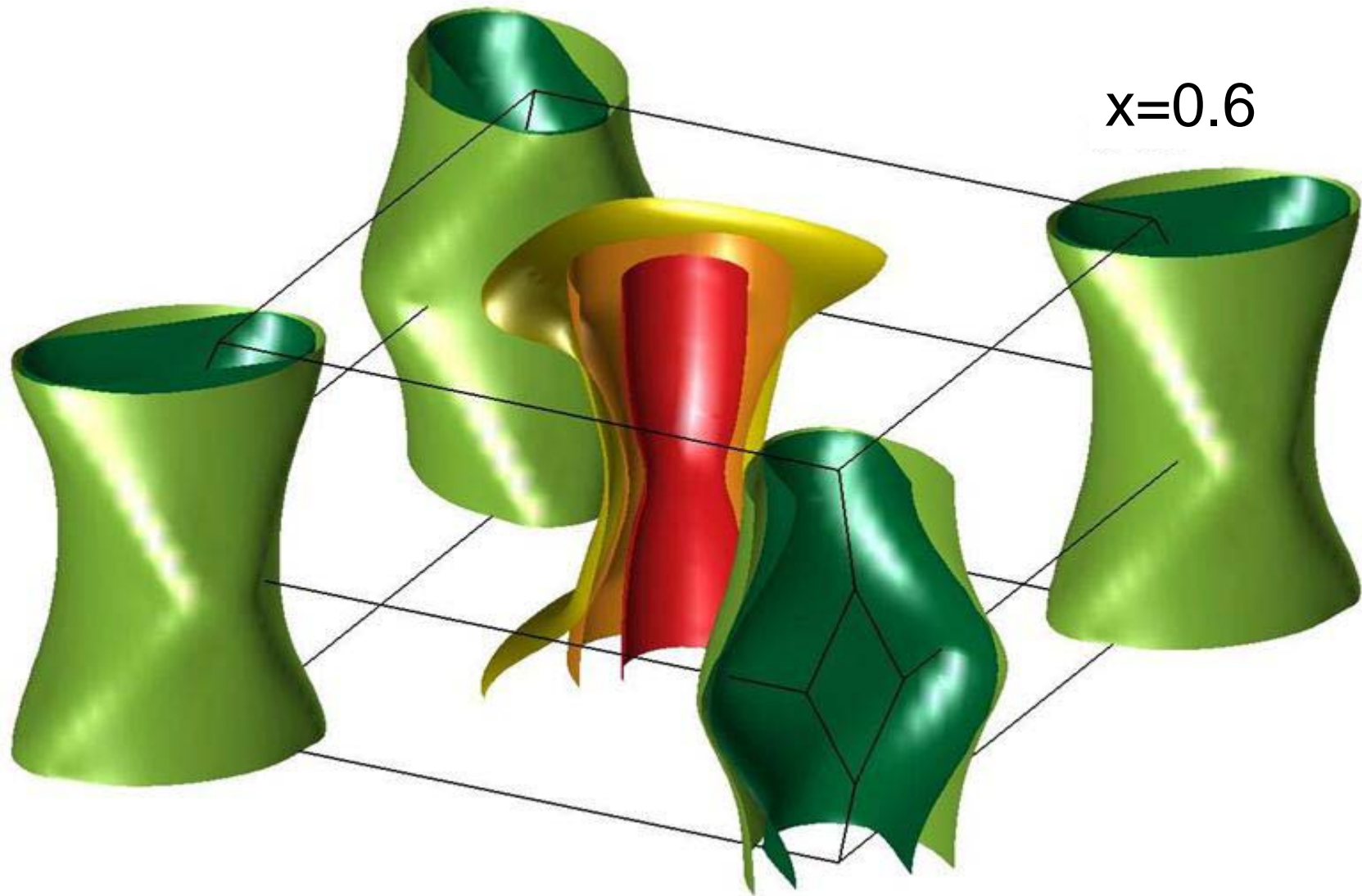


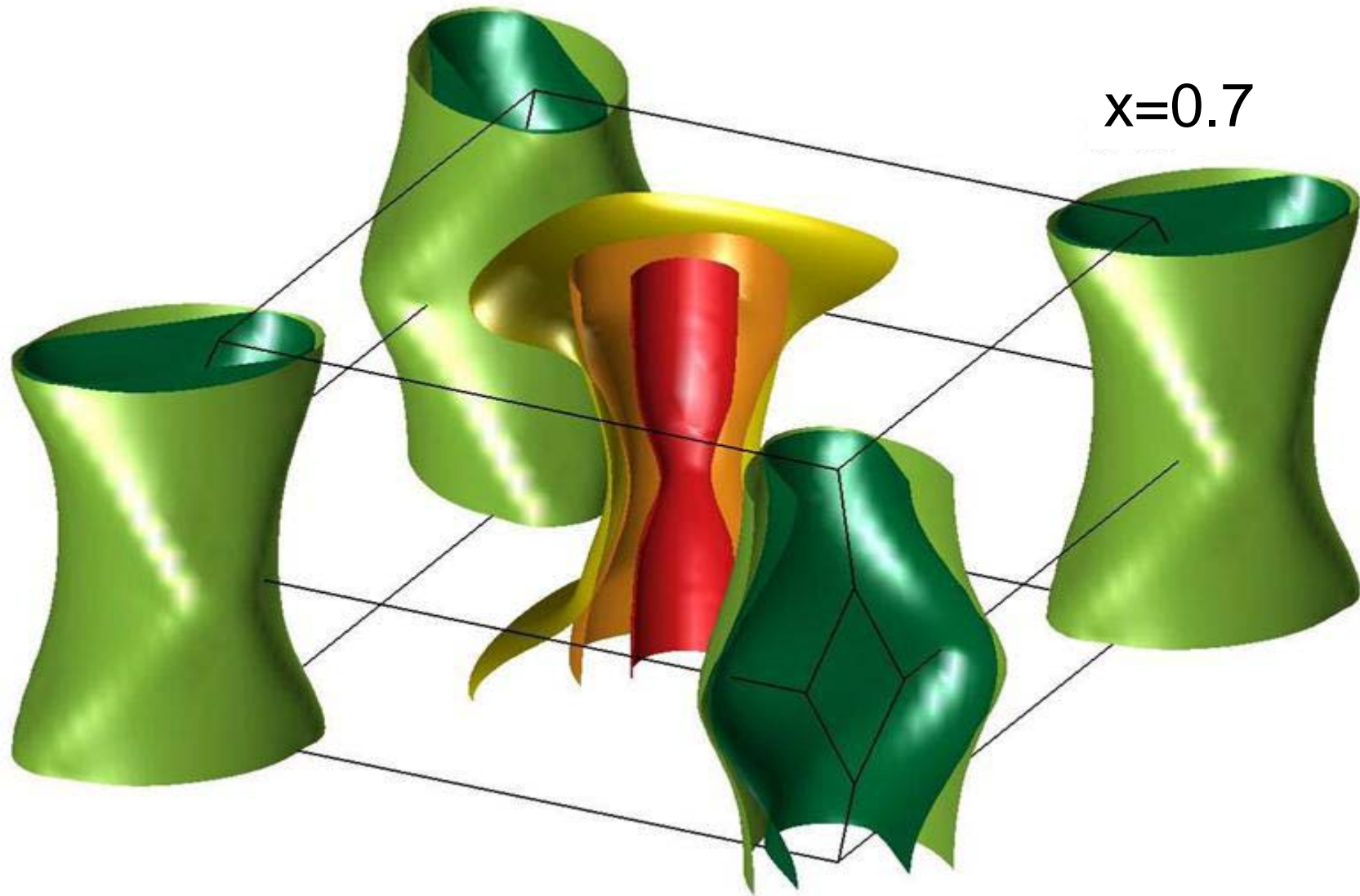


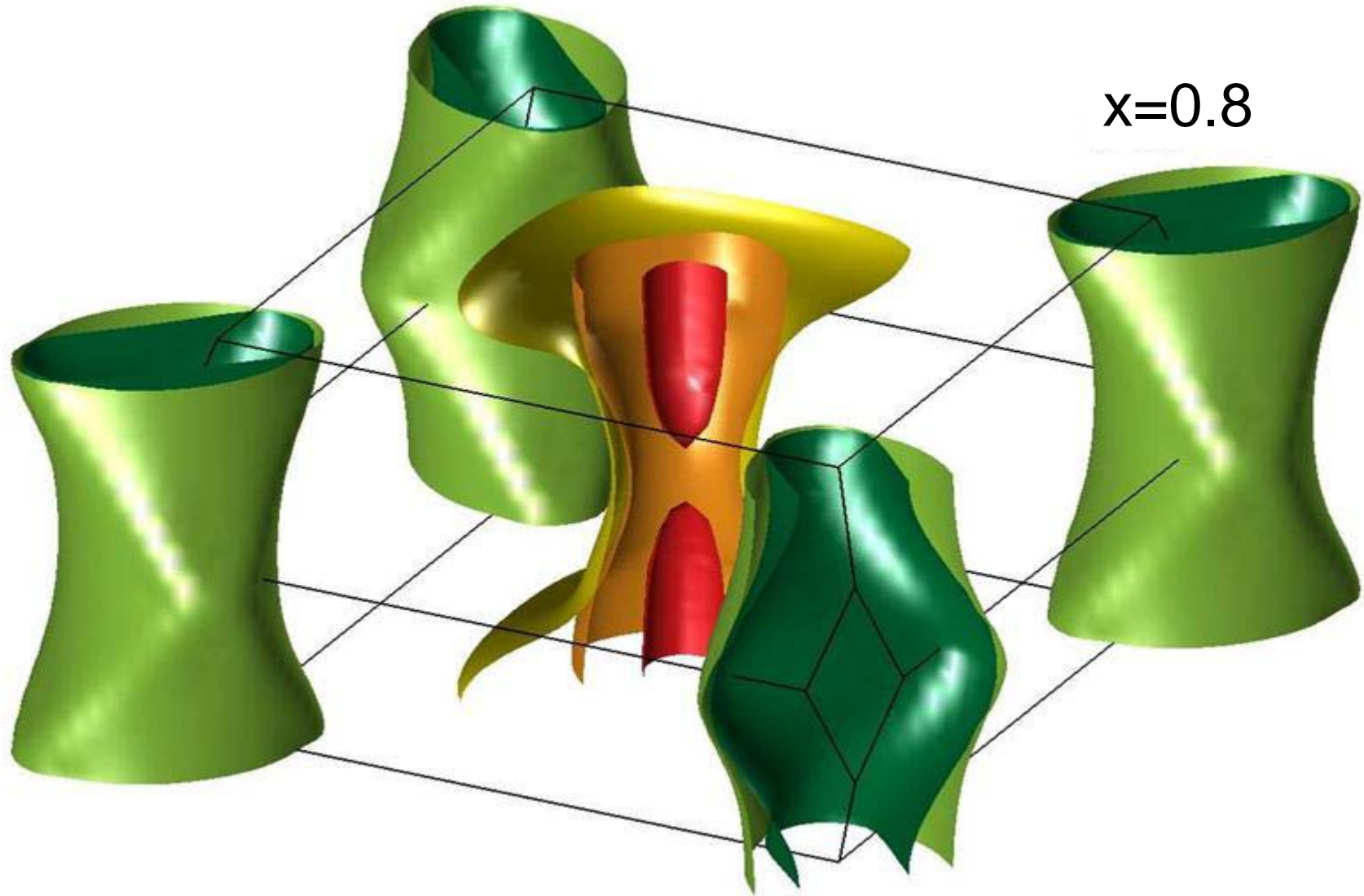


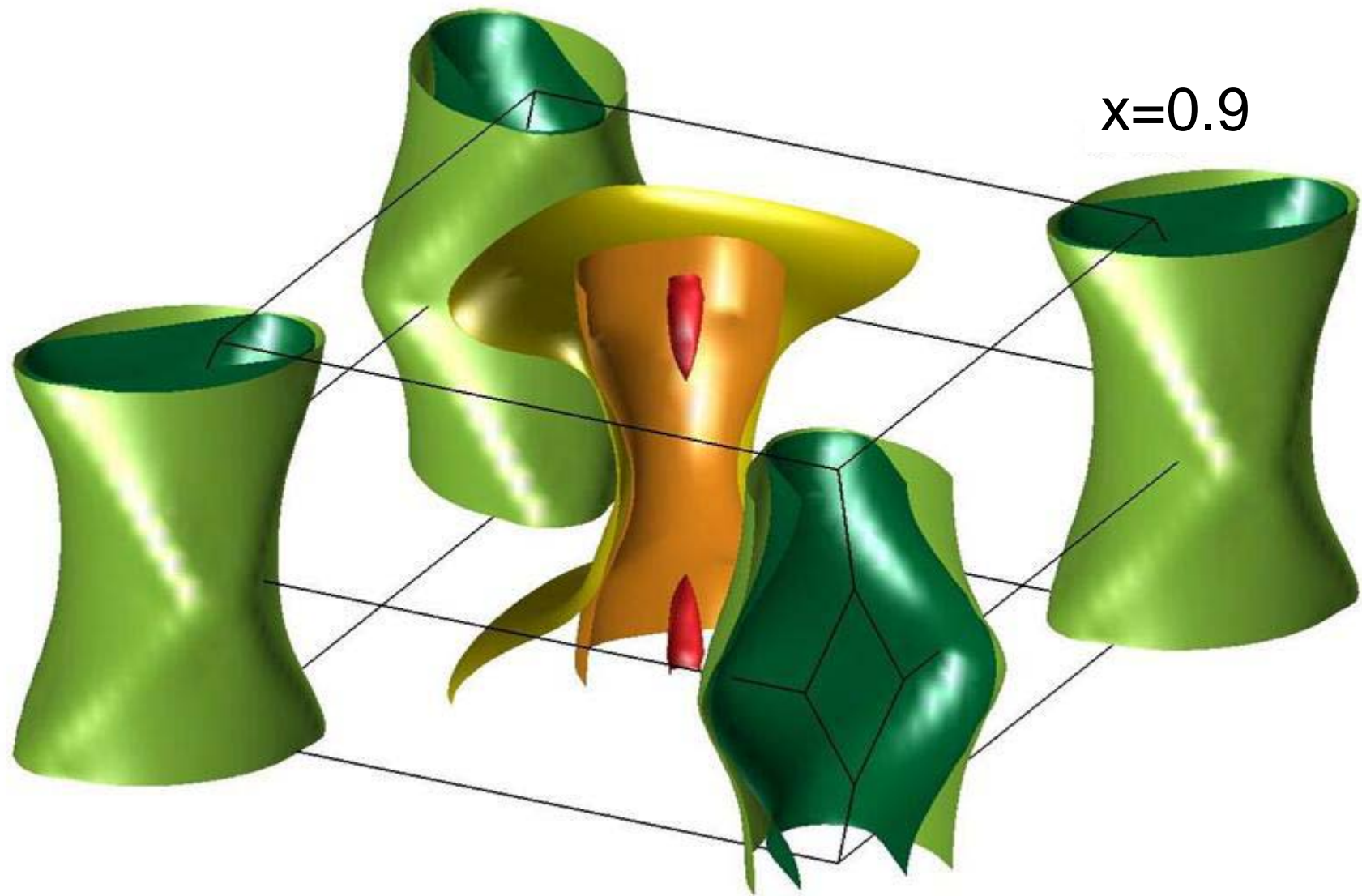


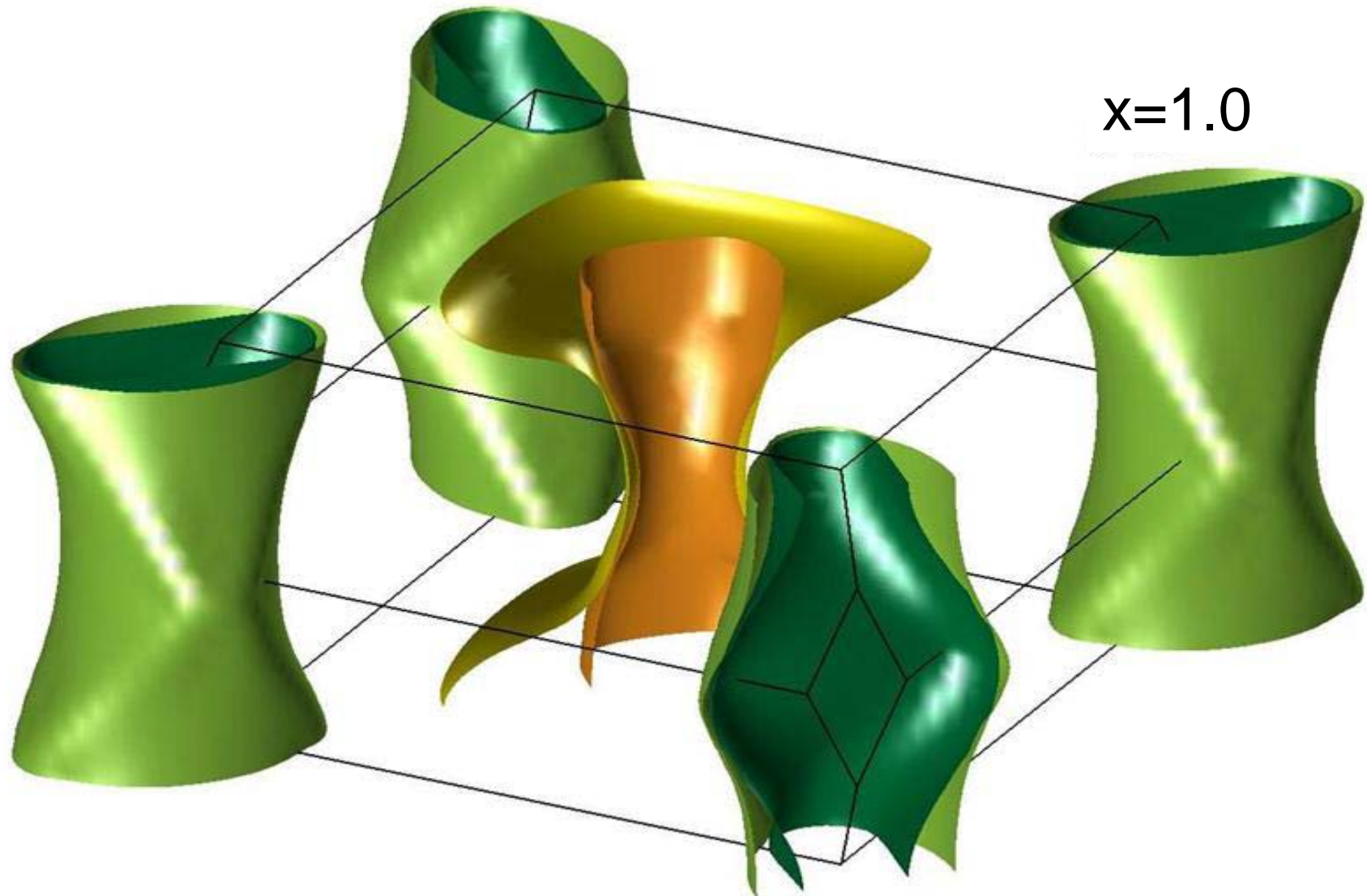








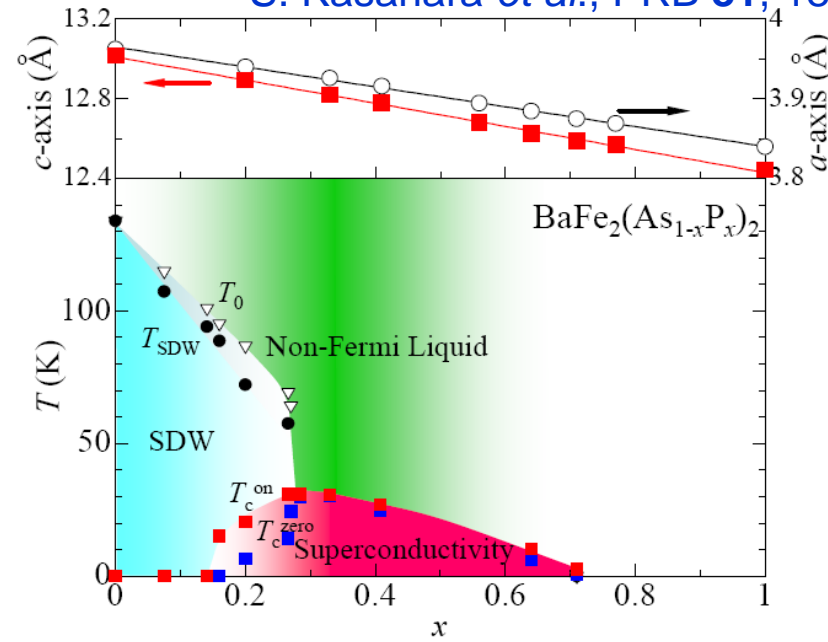
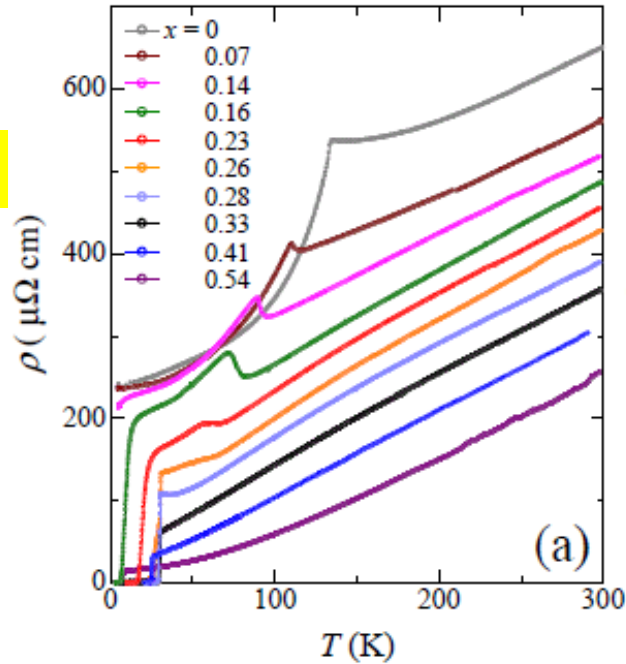




Superconductivity by isovalent substitution of P for As

S. Kasahara *et al.*, PRB **81**, 184519 (2010).

P-dope



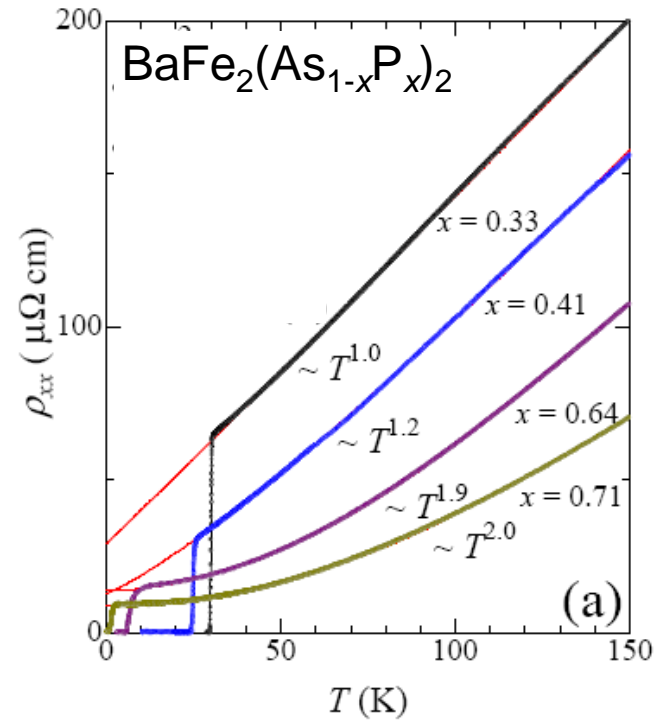
Compensation condition ($n_e = n_h$) holds for any x .

Volume of hole FSs = Volume of electron FSs

Hole band becomes more 3D-like but electron band is almost unchanged.

Nesting condition degrades with x .

Evolution of transport properties with doping

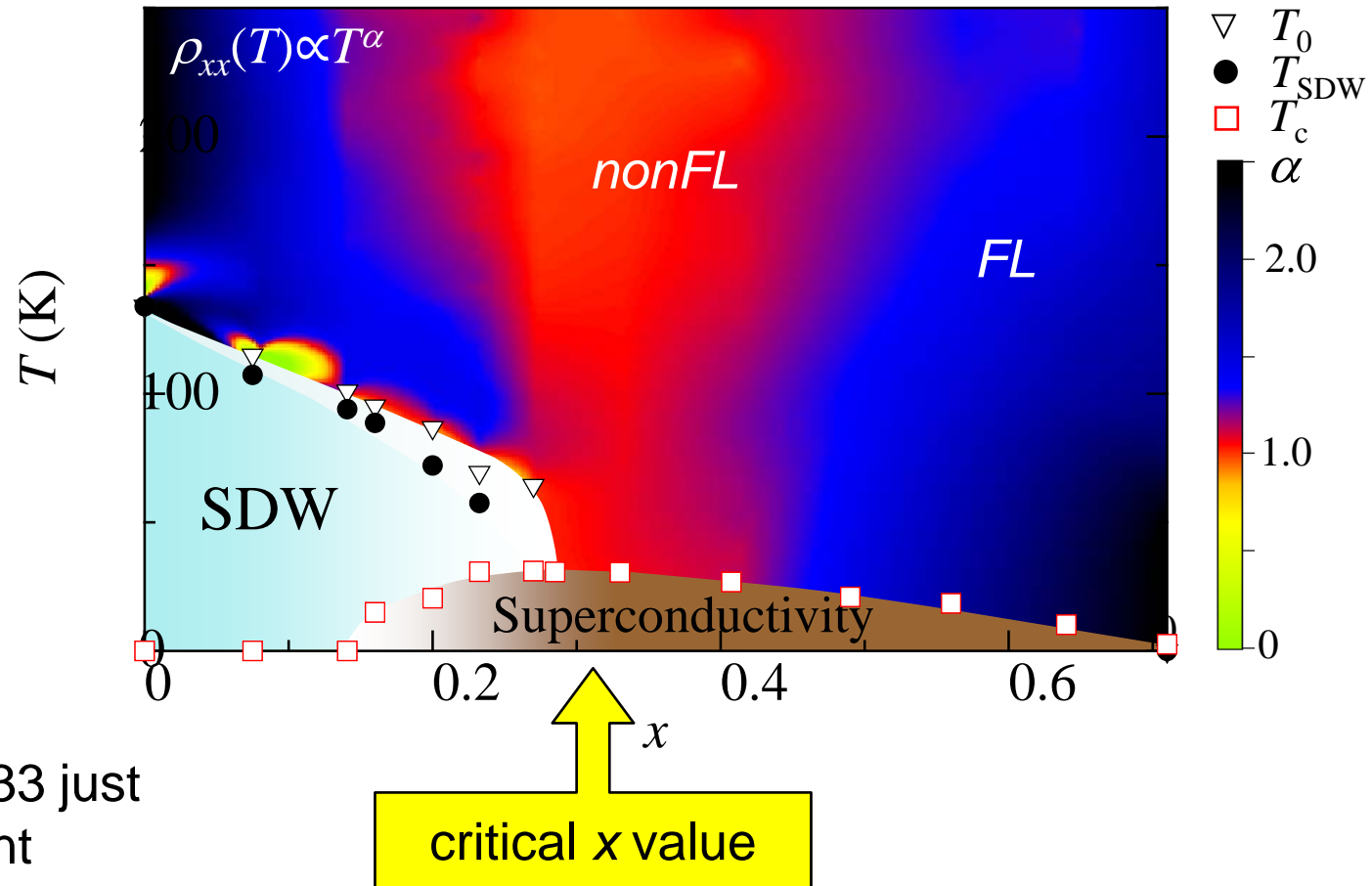


T -linear resistivity at $x=0.33$ just beyond the SDW end point

Hallmark of non-Fermi liquid

T^2 -dependence at $x=0.71$

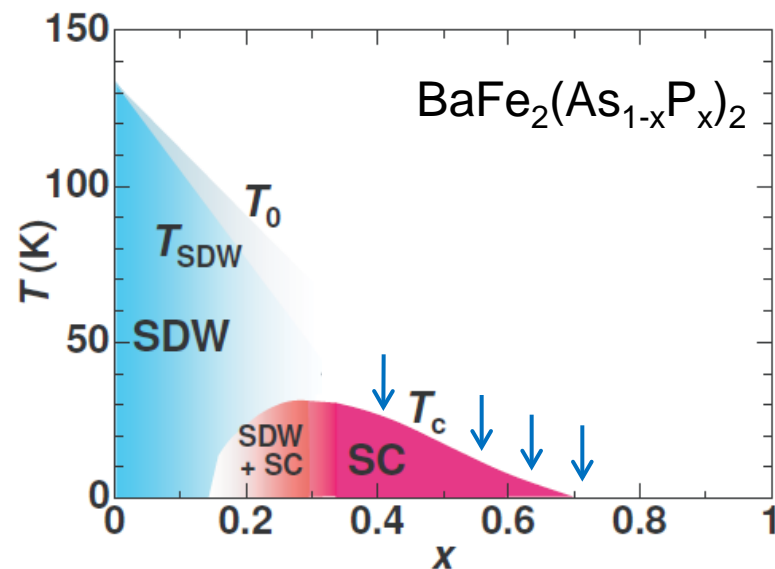
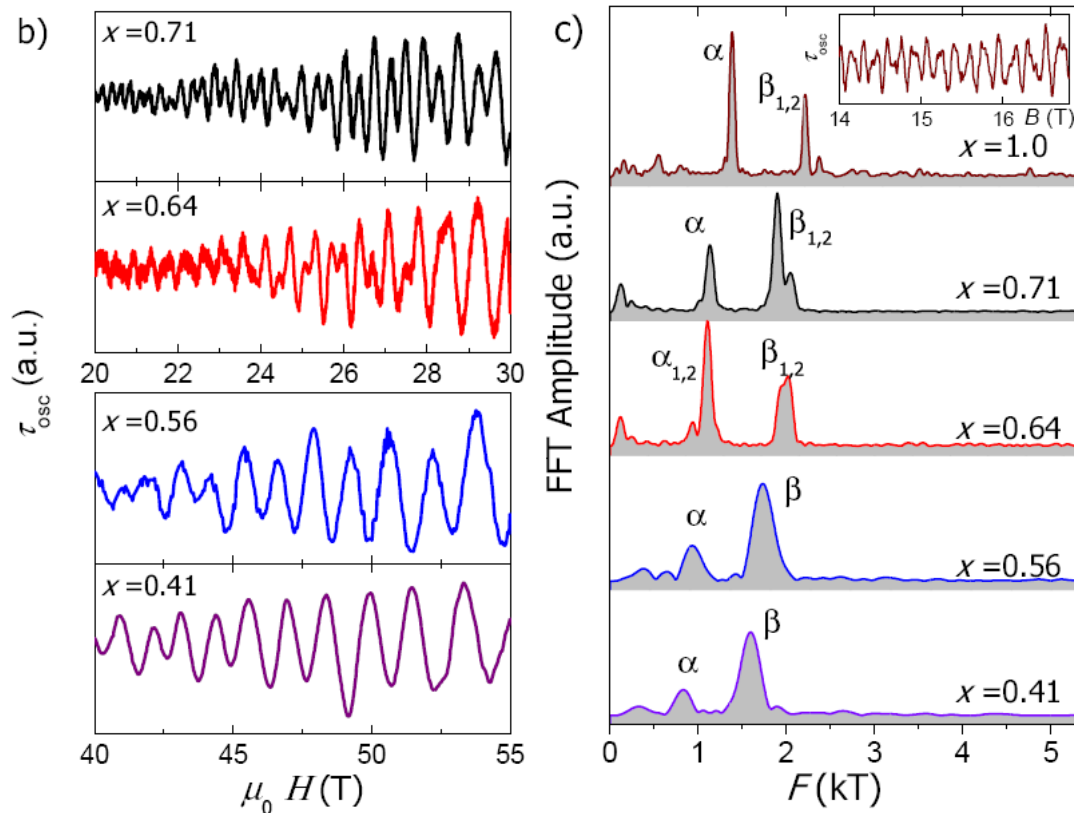
Fermi-liquid behavior



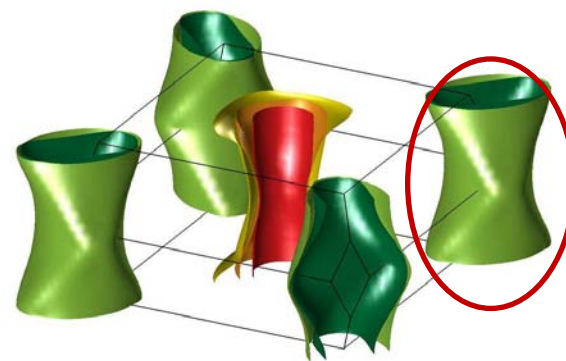
S. Kasahara *et al.*, PRB **81**, 184519 (2010)

Evolution of the Fermi surface on entering the SC dome

dHvA H. Shishido *et al.*, PRL **104**, 057008 (2010)

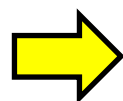


Electron bands



Hole band ($x=0.63$), J.G. Analytis *et al.* PRL (10)

Very clean single crystals are available (quantum oscillations)

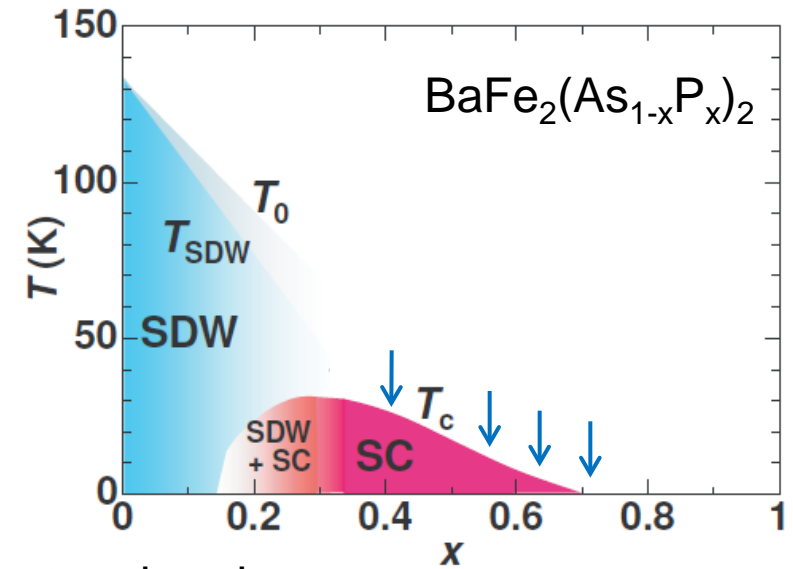
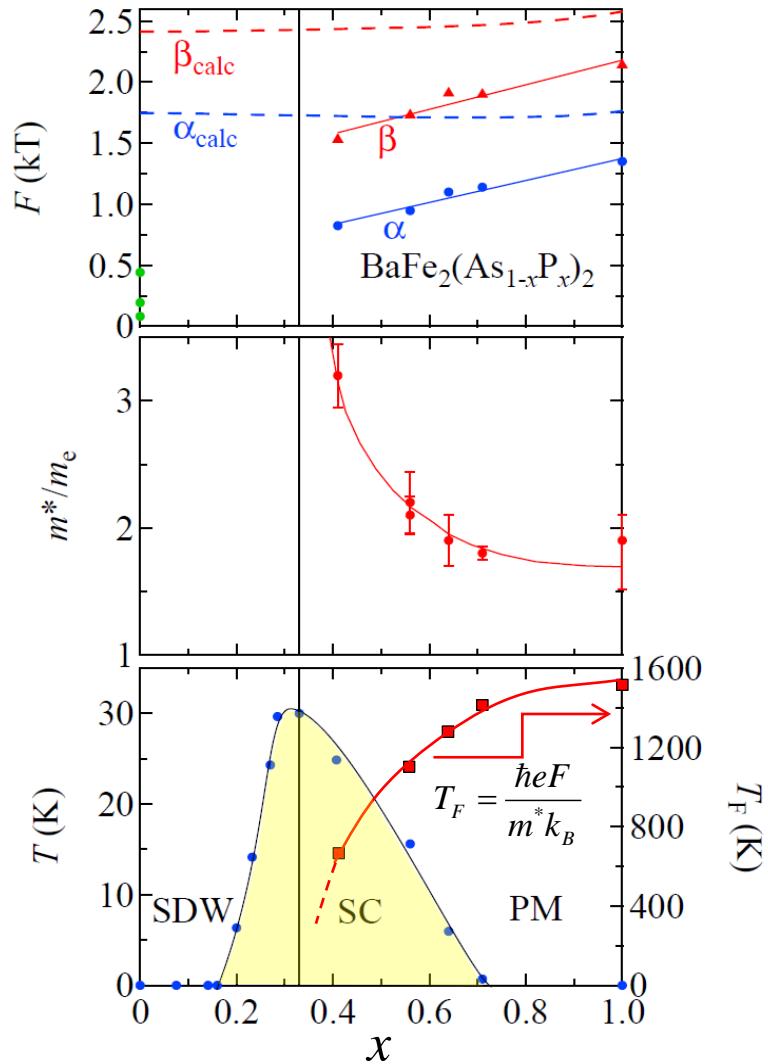


suitable for studying intrinsic physics among Fe-based SCs.

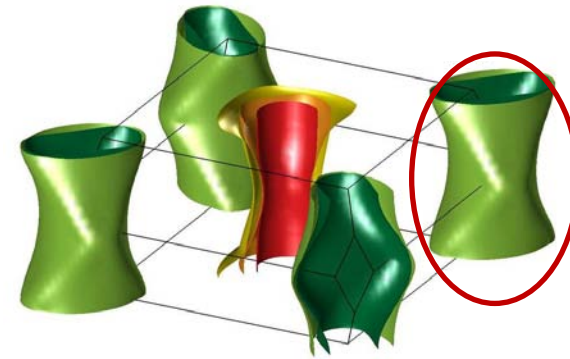
Evolution of the Fermi surface on entering the SC dome

dHvA

H. Shishido *et al.*, PRL **104**, 057008 (2010)



Electron bands



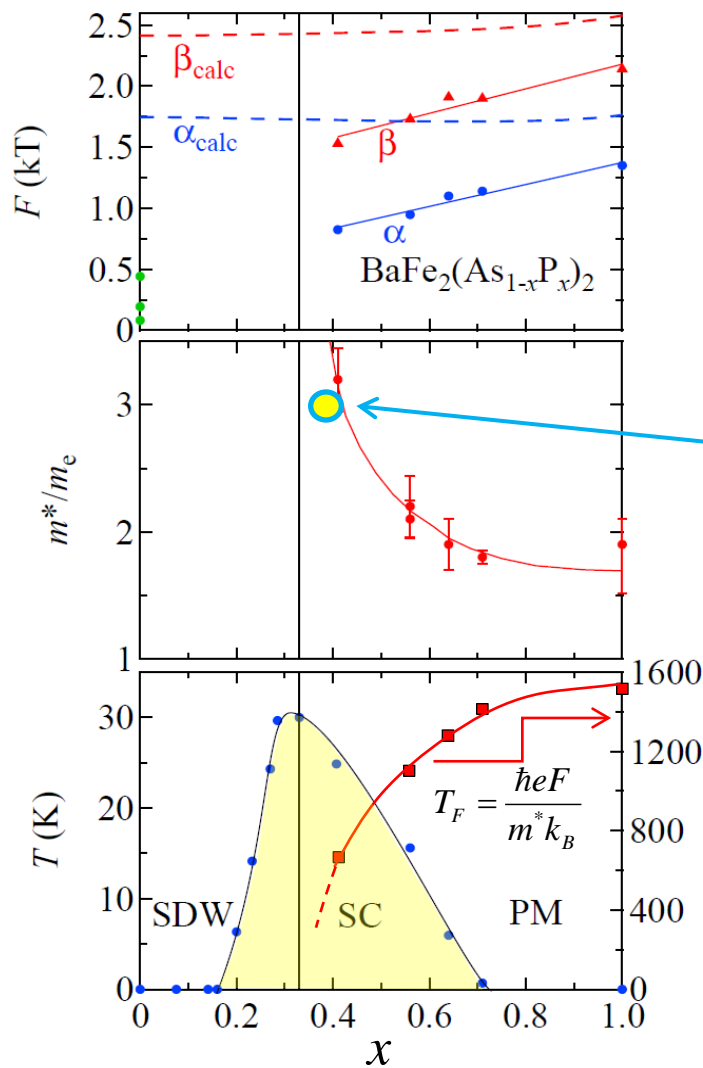
As x is tuned towards the maximum T_c ,

- Shrinkage of the FS occurs
- Effective mass m^* is strongly enhanced
- Fermi temperature $T_F = \hbar e F / m^* k_B$ decreases

Evolution of the Fermi surface on entering the SC dome

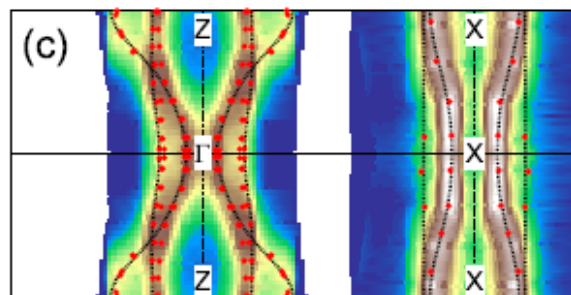
dHvA

H. Shishido *et al.*, PRL(10)

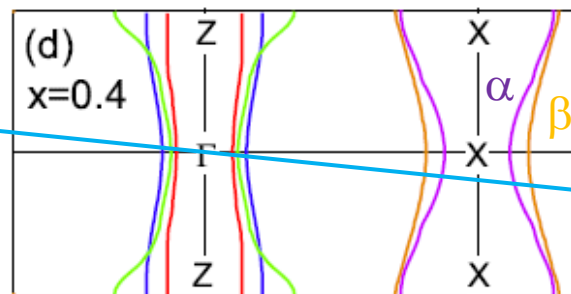


ARPES

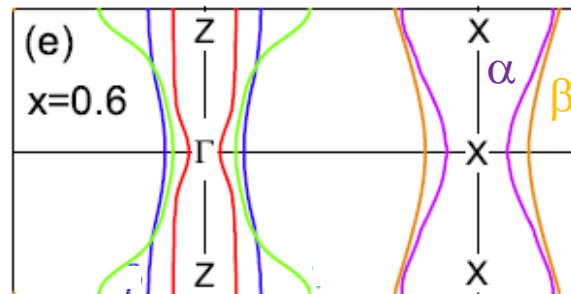
T.Yoshida *et al.* PRL in press



$\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$
 $x=0.38$



3D volume	k_z	2D area	m^*/m_e	m_b/m_e	m^*/m_b
3.9	Γ	3.9	3.8	1.3	2.9
	Z	3.8	2.5	1.2	2.1
6.0	Γ	1.0	2.6	0.9	2.9
	Z	16.3	3.9	2.3	1.7
5.3	X	5.3	2.8	0.71	3.9
3.4	X	3.0	2.0	0.93	2.1



Electron pocket

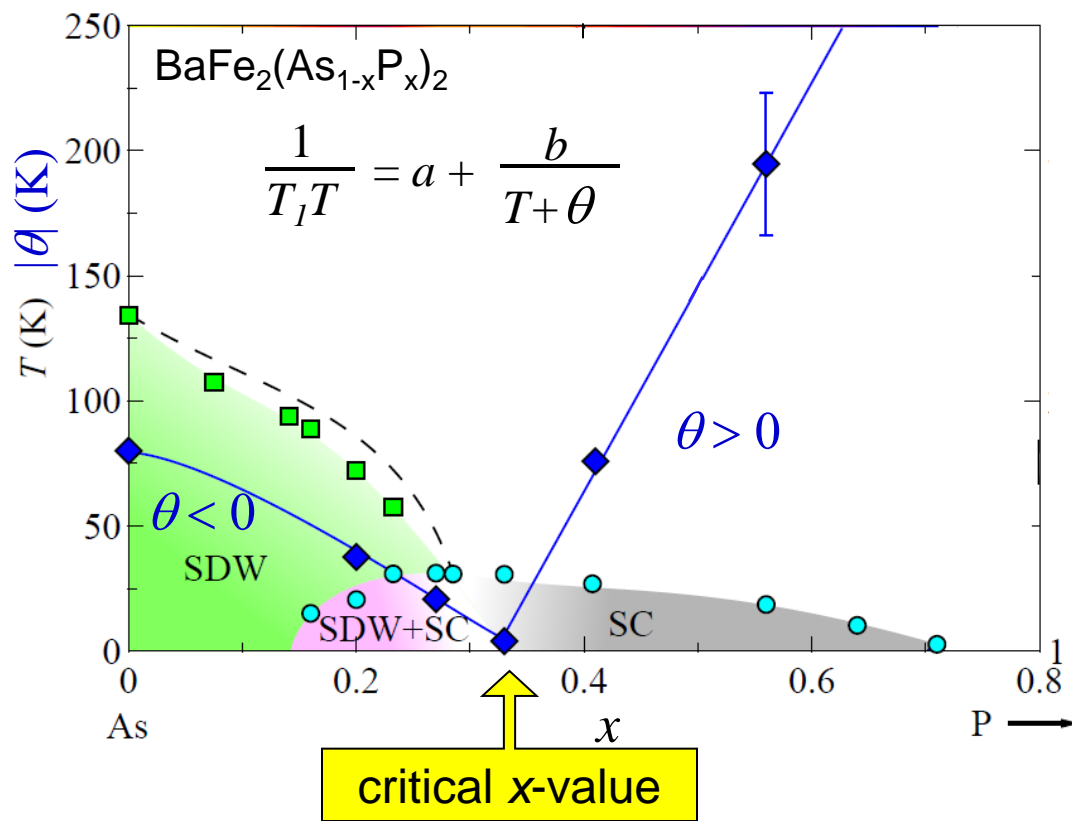
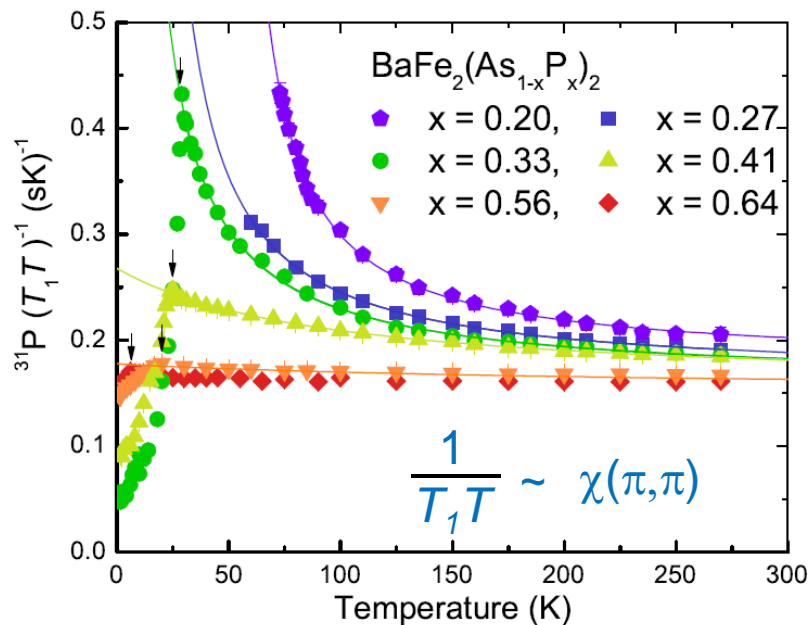
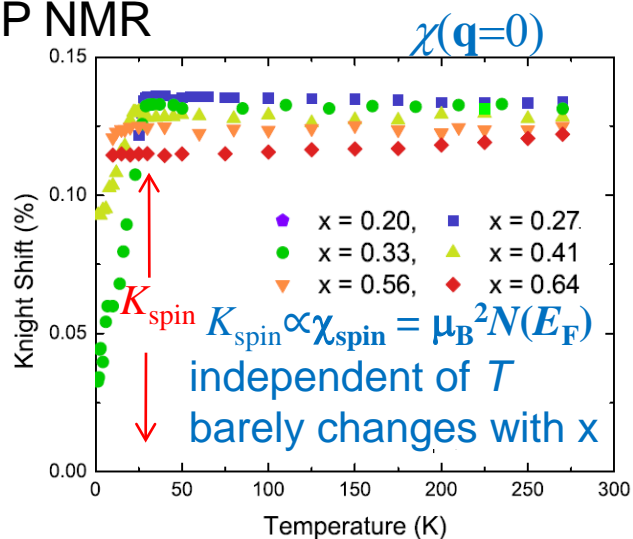
Electron correlation effect

Shrinkage of the FS occurs
 Effective mass m^* is strongly enhanced
 Fermi temperature $T_F = \hbar e F / m^* k_B$ decreases

As x is tuned towards the maximum T_C ,

Evolution of the magnetic fluctuations with doping (NMR)

^{31}P NMR

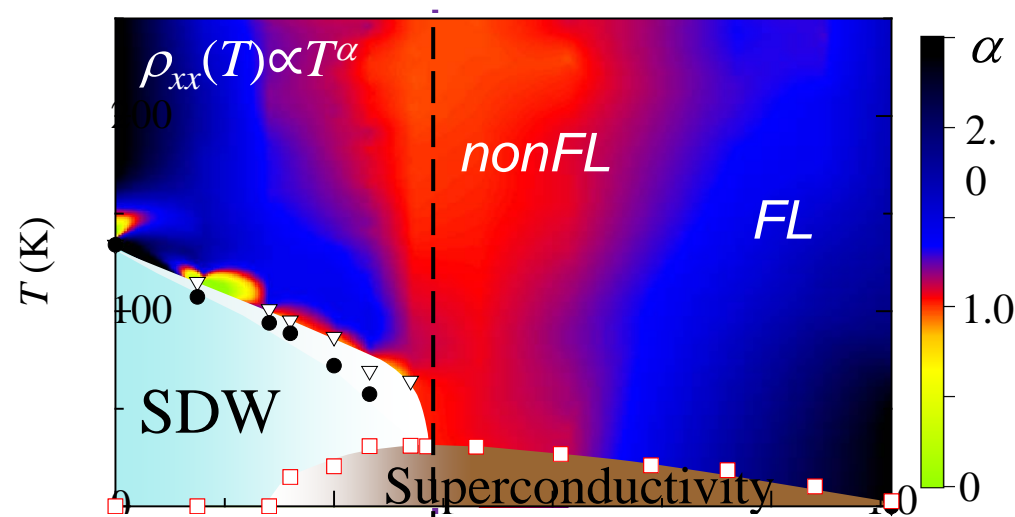


θ : Weiss temperature

θ goes to zero at $x \sim 0.33$

Y. Nakai *et al.* PRL (10)

Evolution of transport properties, magnetic properties, Fermi surface with doping in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$



In the SC dome,

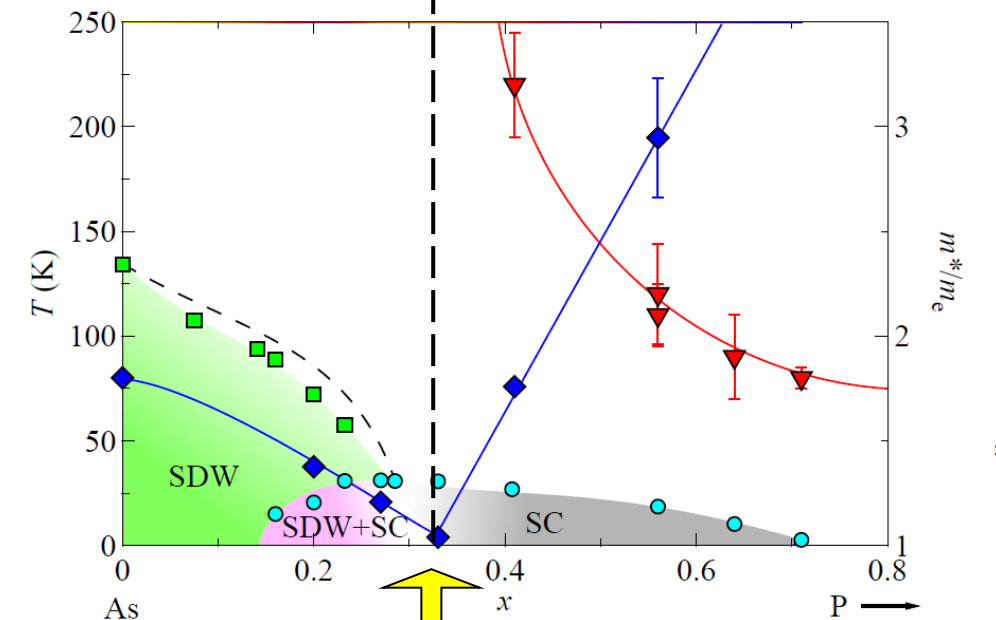
Strong enhancement of effective mass m^* (dHvA and ARPES) as x is tuned towards $x_c=0.33$

At a critical doping value $x_c=0.33$ close to the end point of SDW

T_c becomes maximum

Hallmark of non-Fermi in the transport coefficients

Weiss temperature θ (NMR) goes to zero



AFM QCP at the end point of SDW

Non-Fermi liquid properties, magnetic fluctuations, electron correlations and superconductivity are intimately linked.

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

Evidence of line node

Pinpointing the position of line node

Possible gap functions (2D)

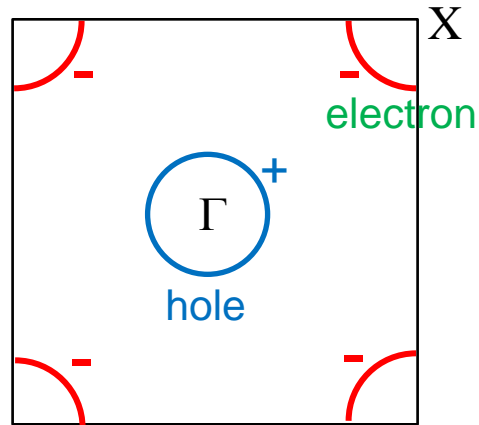
Large $\chi(\mathbf{q})$



$\Delta(\mathbf{k}+\mathbf{q})\Delta(\mathbf{k}) < 0$
Sign change

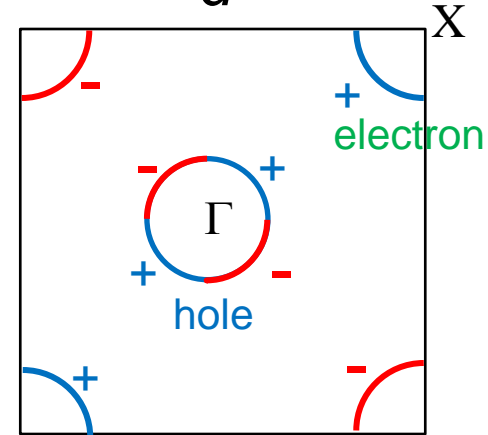
Nodeless

s_{\pm}

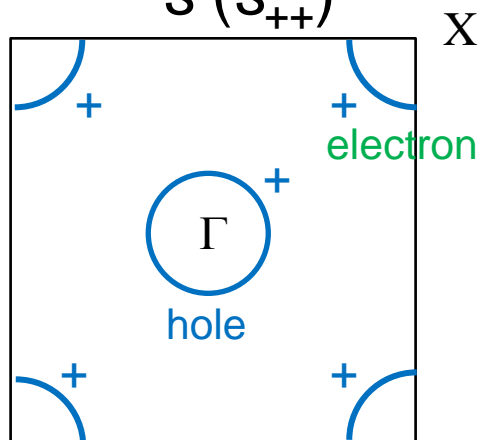


Nodal

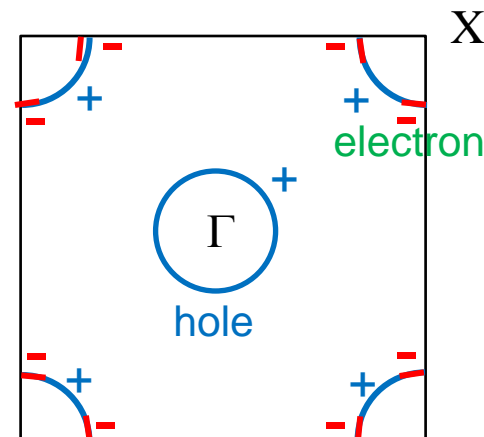
d



$s (s_{++})$

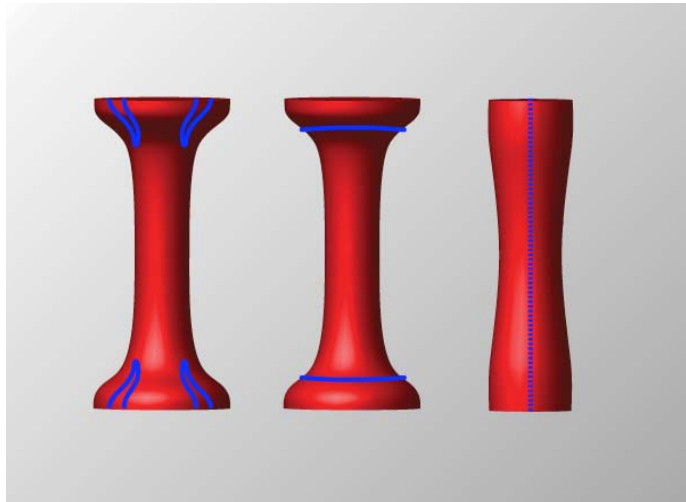


nodal S

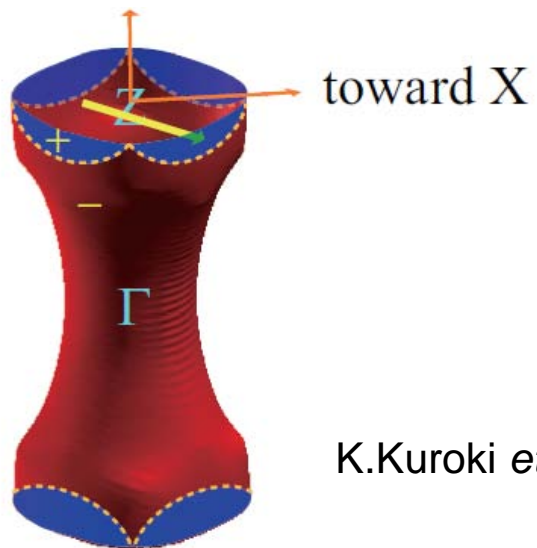


Possible gap functions (3D)

Node in the hole band



P.J. Hirschfeld and D.J. Scalapino,
Physics **3**, 64 (2010)



K.Kuroki *et al.* arXiv:1010.3542

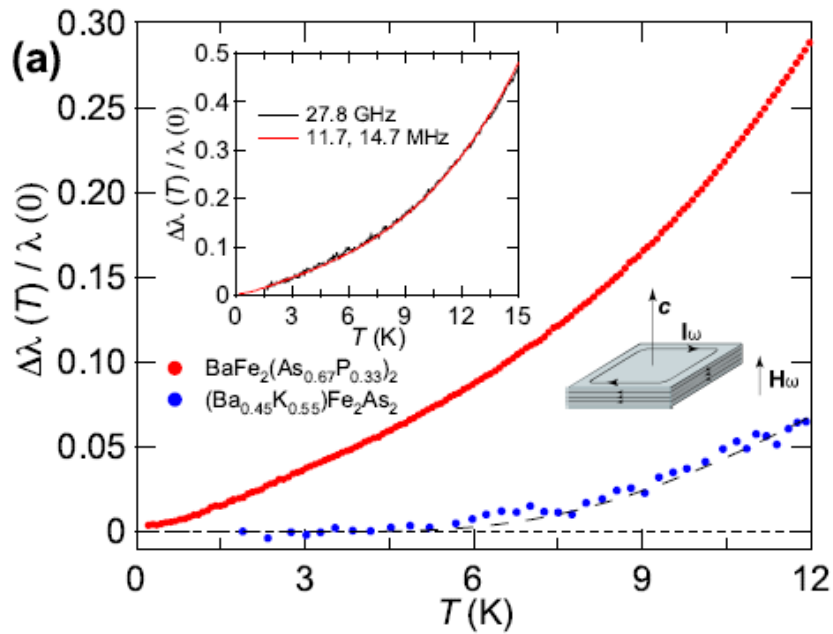
Node in the electron band



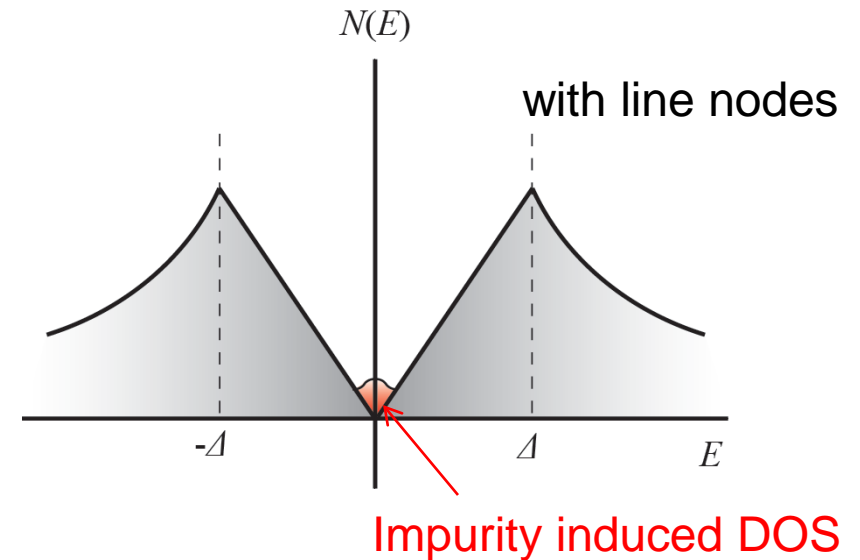
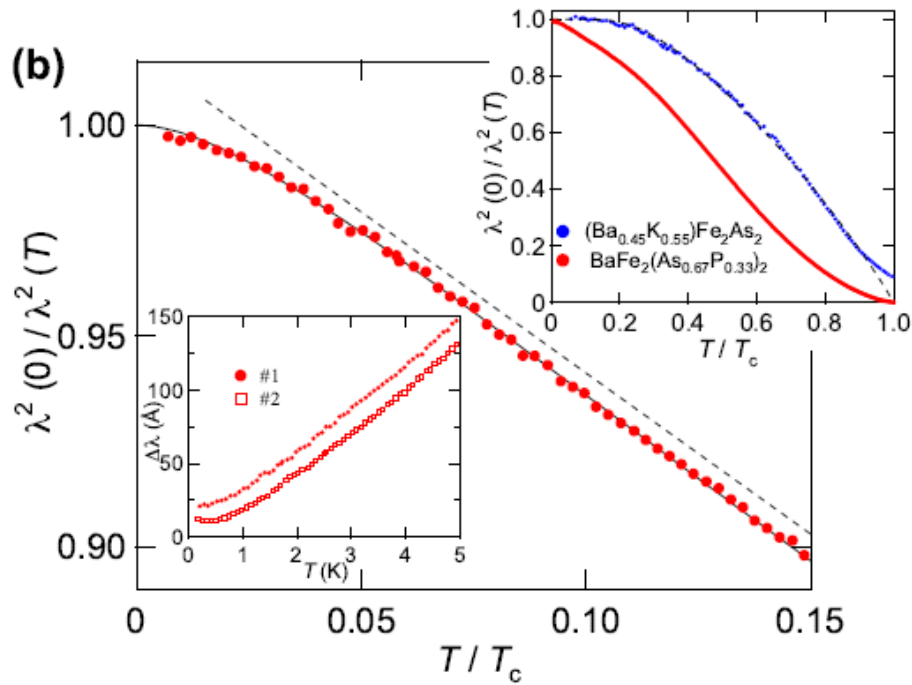
I.I. Mazin *et al.*, PRB (10)

Gap structure of $\text{BaFe}_2(\text{As}_{0.67}\text{P}_{0.33})_2$: penetration depth

K. Hashimoto *et al.*, PRB **81**, 220501(R) (2010).



- T -linear penetration depth in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ ($T_c \sim 30$ K, $x=0.33$) clearly indicates the **line nodes** in the gap.

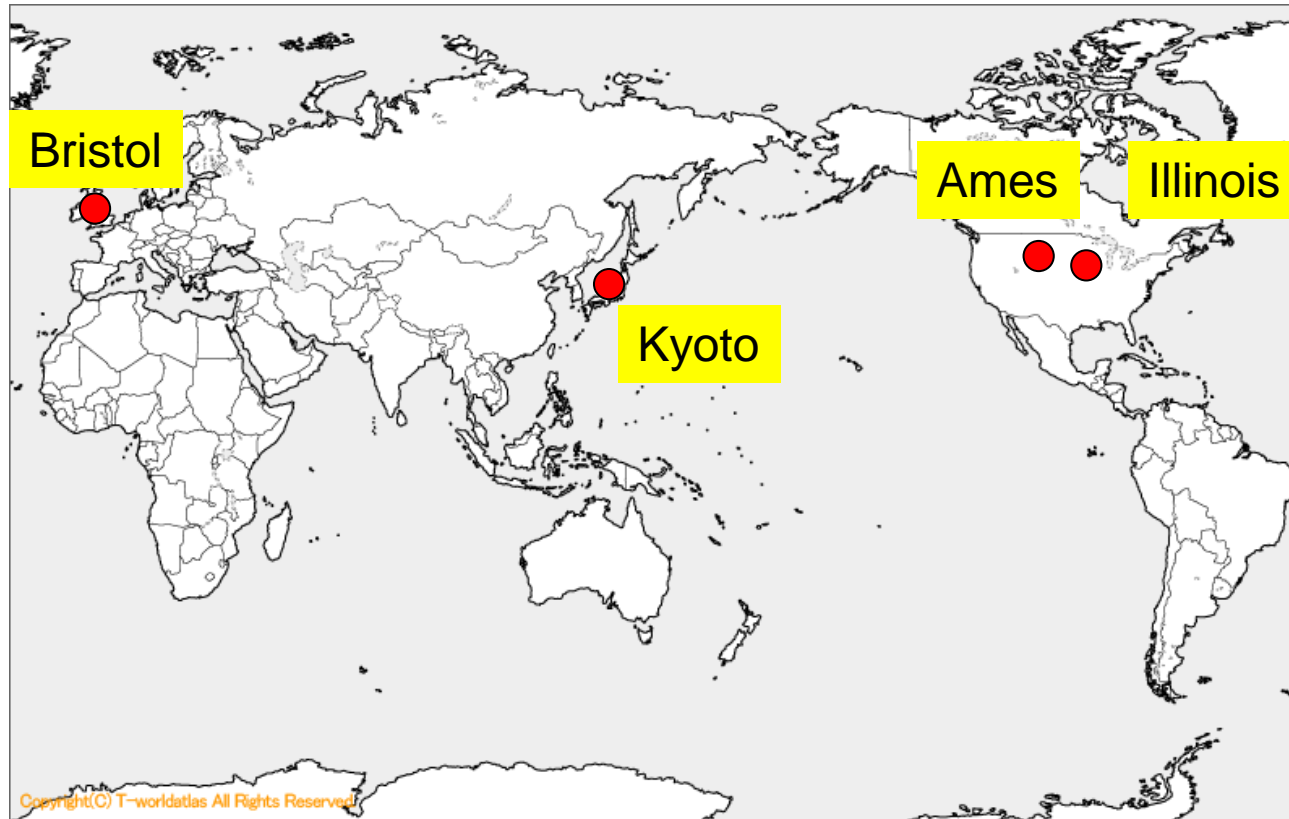


$$\Delta\lambda(T) \sim T^2/(T+T^*) \quad T^*=1.3 \text{ K}$$

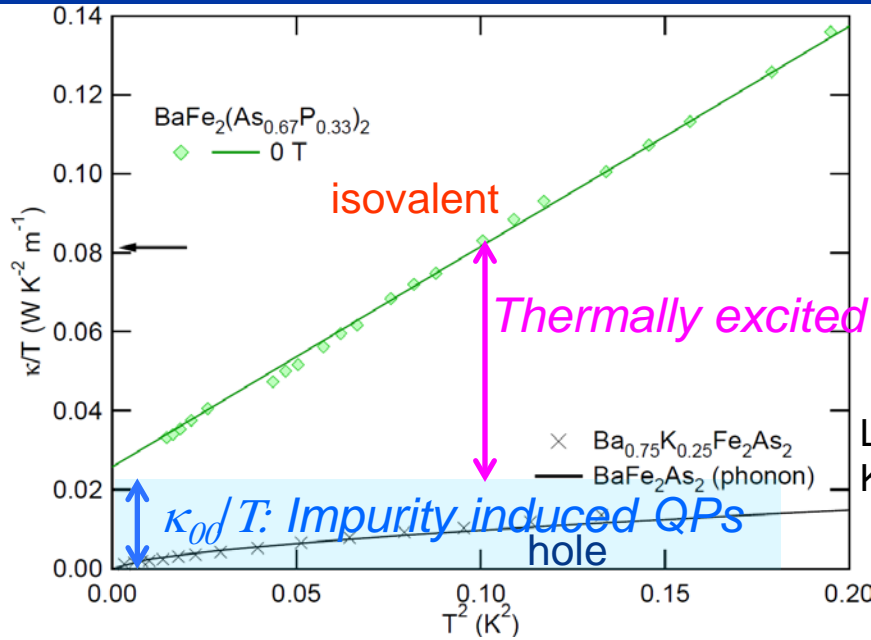
cf. clean YBCO $T^* \sim 1$ K

Gap structure of $\text{BaFe}_2(\text{As}_{0.67}\text{P}_{0.33})_2$: penetration depth

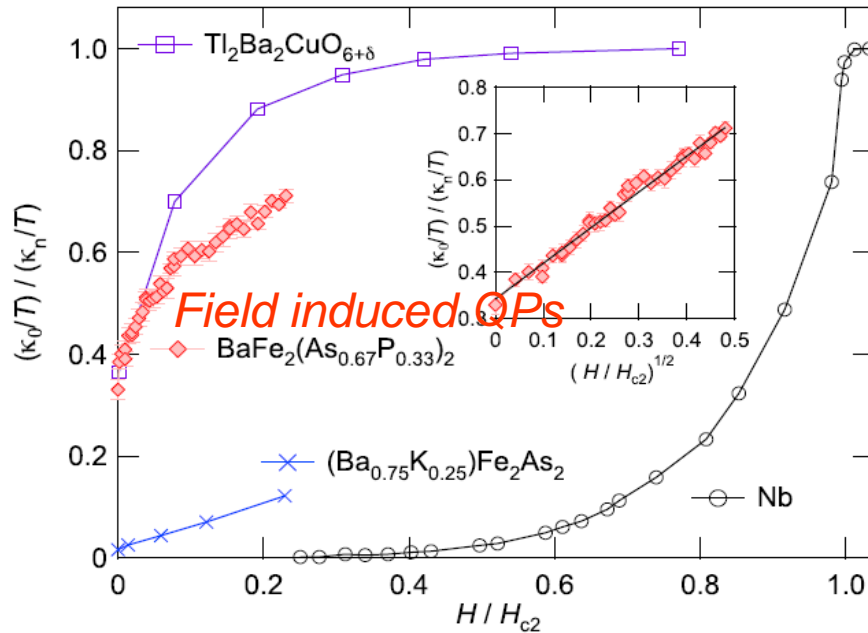
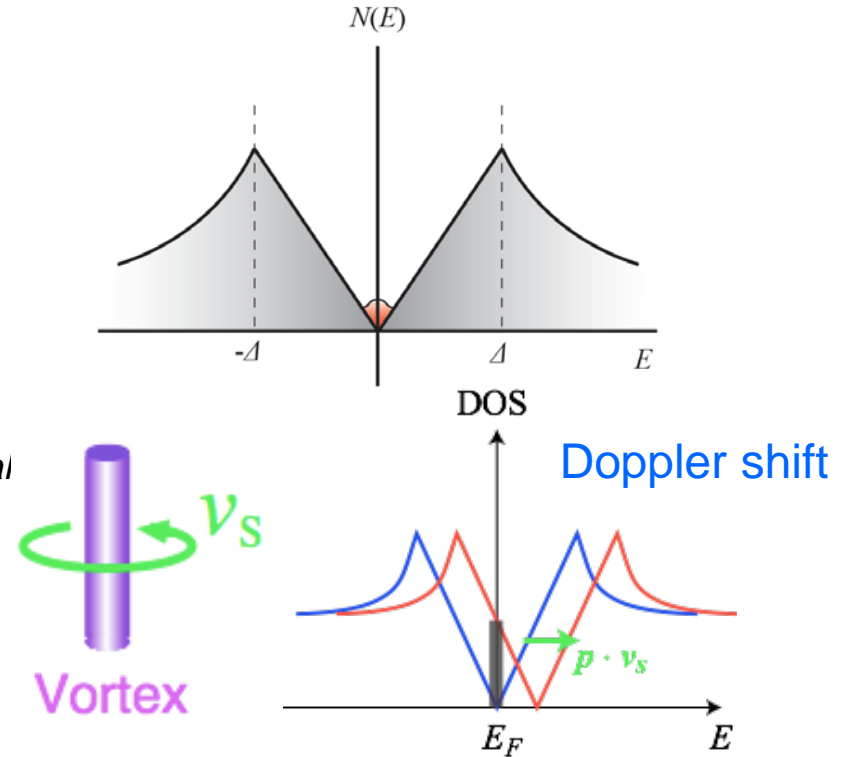
The T -linear dependent penetration depth of $\text{BaFe}_2(\text{As}_{0.67}\text{P}_{0.33})_2$ ($T_c=31\text{K}$) has been confirmed in four laboratories



Gap structure of $\text{BaFe}_2(\text{As}_{0.67}\text{P}_{0.33})_2$: thermal conductivity



Luo et al.
Kurita et al

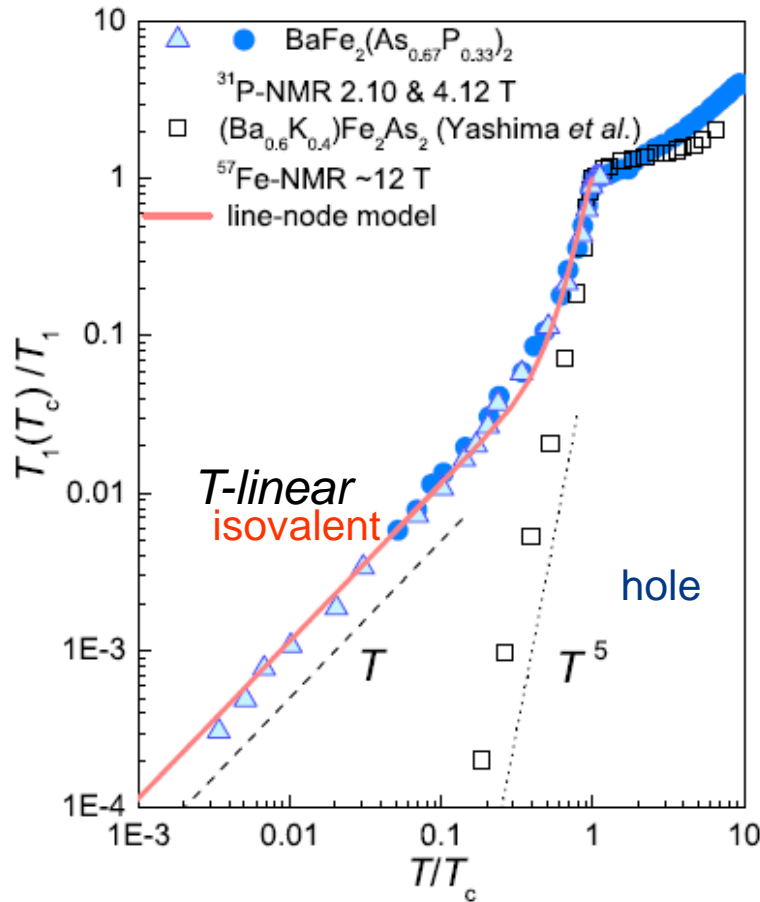


- Finite κ_0/T in the $T \rightarrow 0$ K limit
- Thermally excited QPs
- Steep increase with H

$$\kappa_0/T(T \rightarrow 0) \sim \sqrt{H}$$

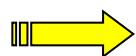
Clear evidence for *line node with sign change* in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

Gap structure of $\text{BaFe}_2(\text{As}_{0.67}\text{P}_{0.33})_2$: NMR



Y.Nakai *et al.* PRB (2010)

$T_1 T$ becomes constant at very low temperature

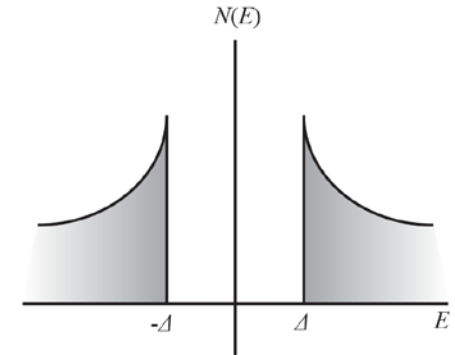


Residual DOS due to line node

Hole dope



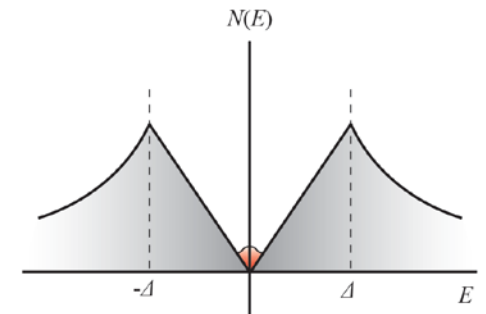
Full gap



Isovalent dope



Line node



NMR results are consistent with the penetration depth and thermal conductivity

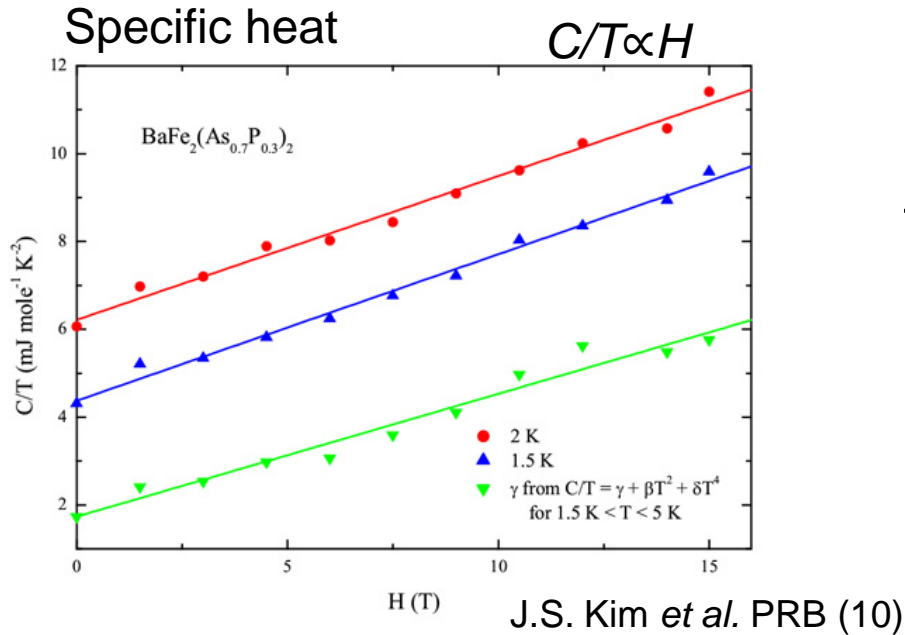
Superconducting gap structure of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

Evidence of line node

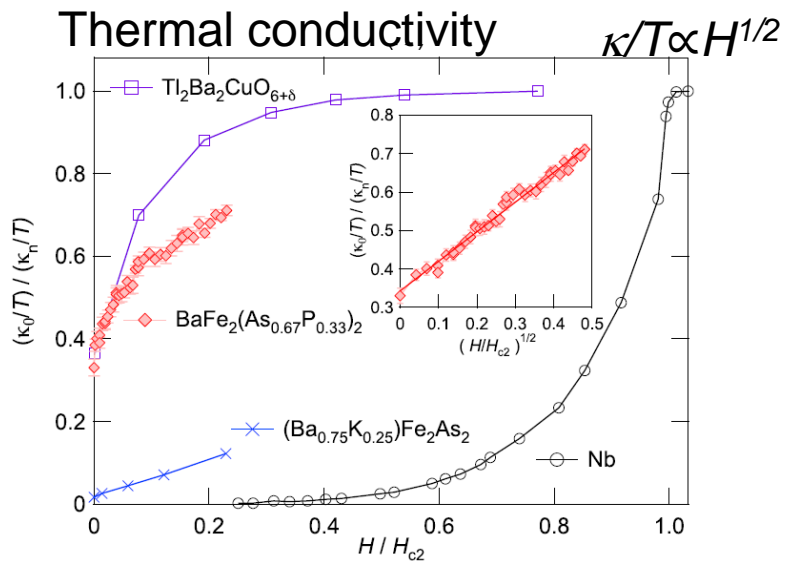
Pinpointing the position of line node

Where is the line node ?

Gap structure probed by specific heat and thermal conductivity



$H^{1/2}$ -component is less than 5% of the total specific heat



$H^{1/2}$ -component is more than 30% of the total thermal conductivity

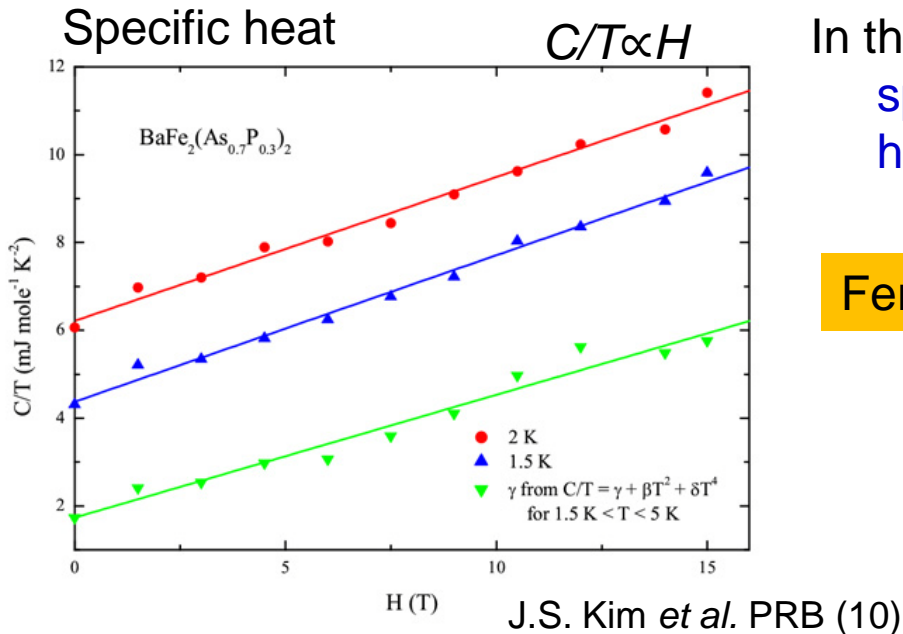
K. Hashimoto *et al.*, PRB (10).

Where is the line node ?

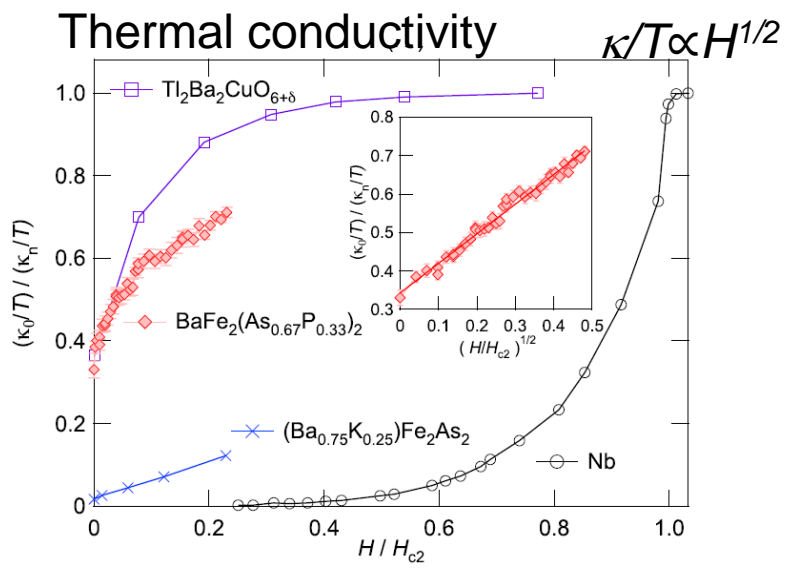
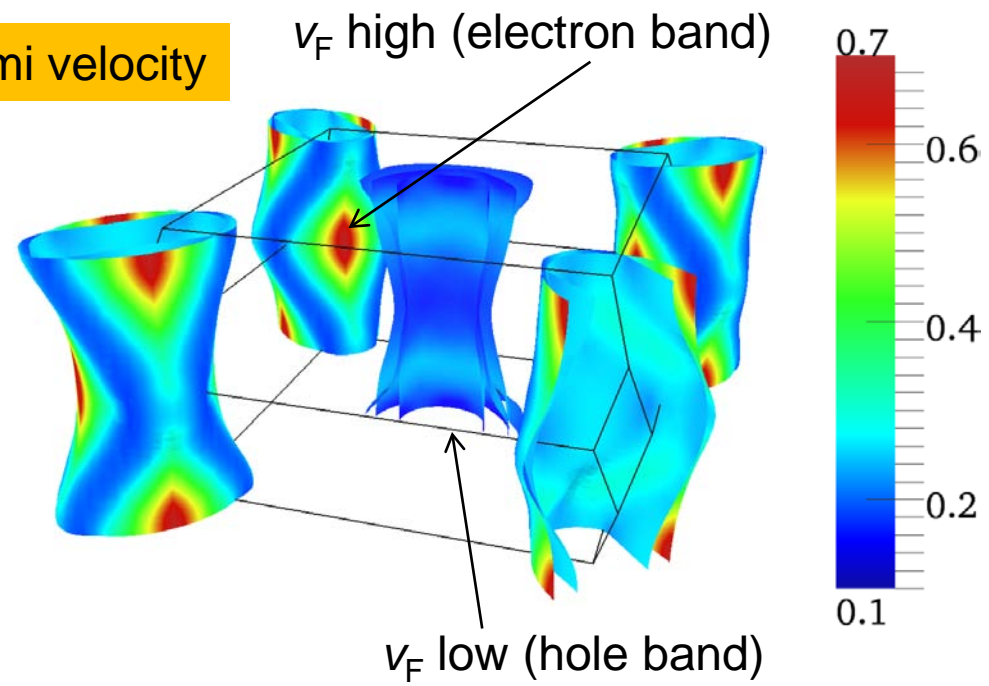
Gap structure probed by specific heat and thermal conductivity

In the multiband system,

specific heat is dominated by the heavy mass band
 heat conductivity is dominated by light mass band



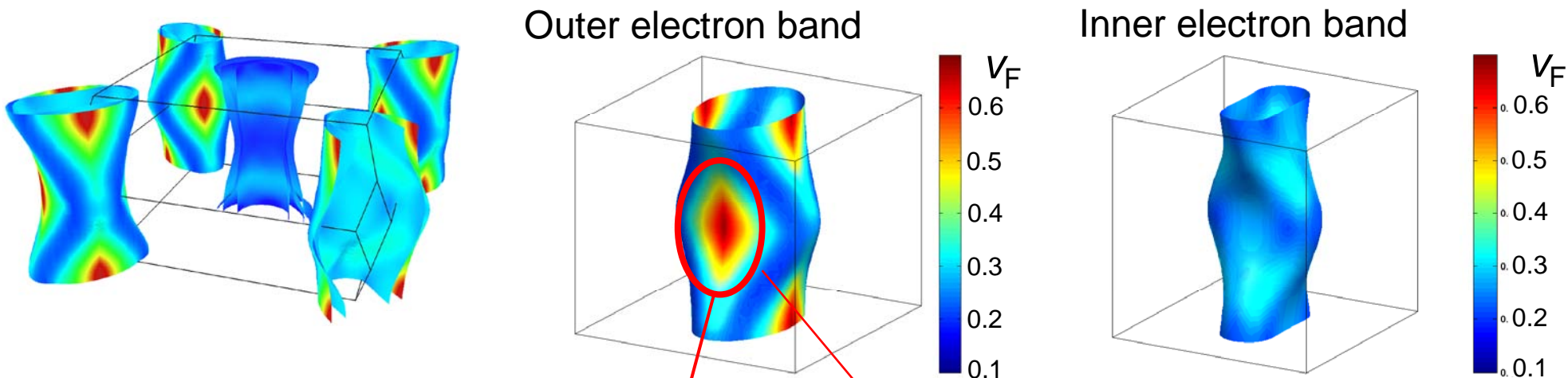
Fermi velocity



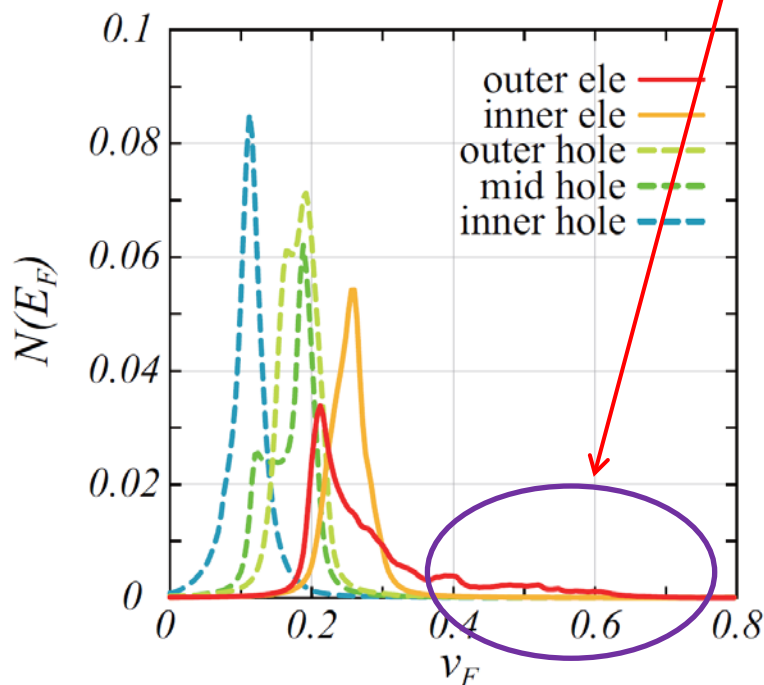
Specific heat is dominated by hole band
 Thermal conductivity is dominated by the electron band

K. Hashimoto *et al.*, PRB (10).

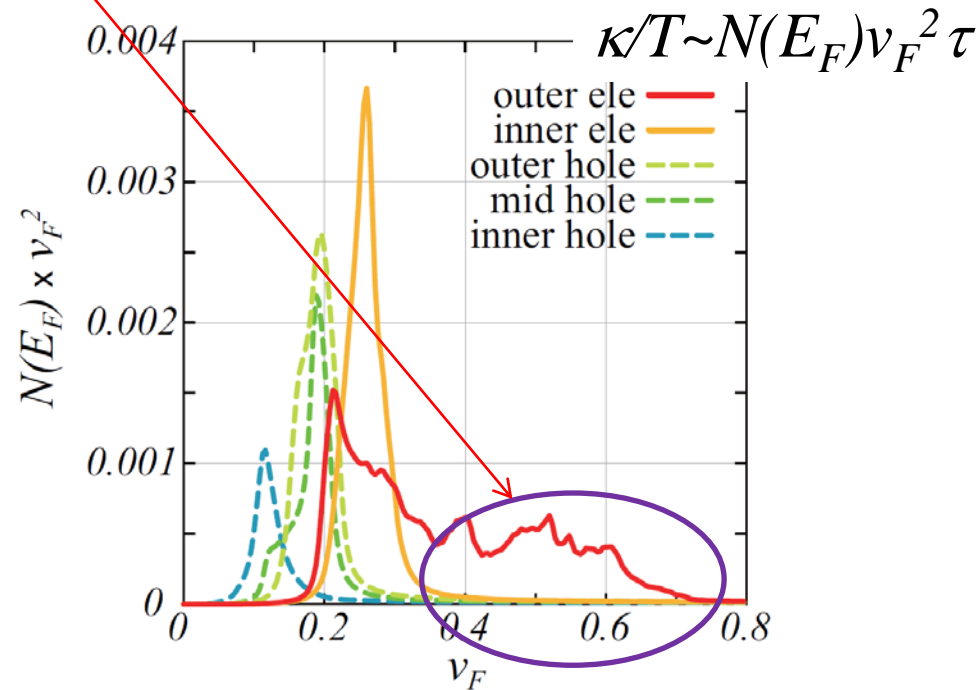
Where is the line node ?



Less than 5% of total DOS



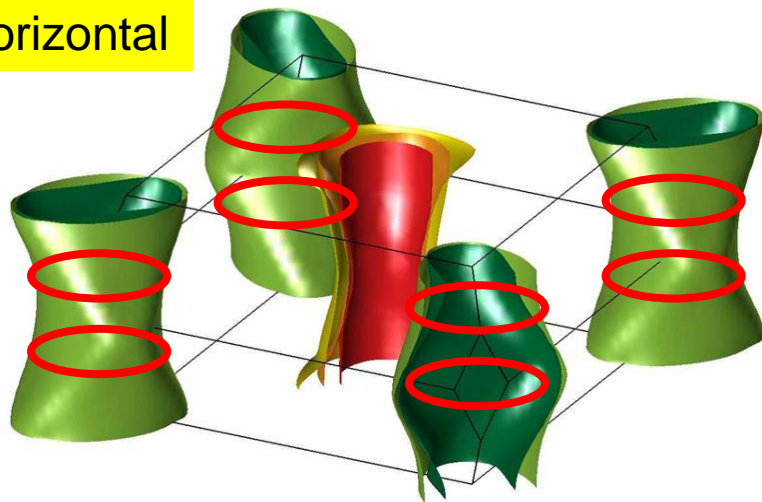
More than 20% of total thermal conductivity



Where is the line node in $\text{BaFe}_2(\text{As}_{0.67}\text{P}_{0.33})_2$ ($T_c=31$ K) ?

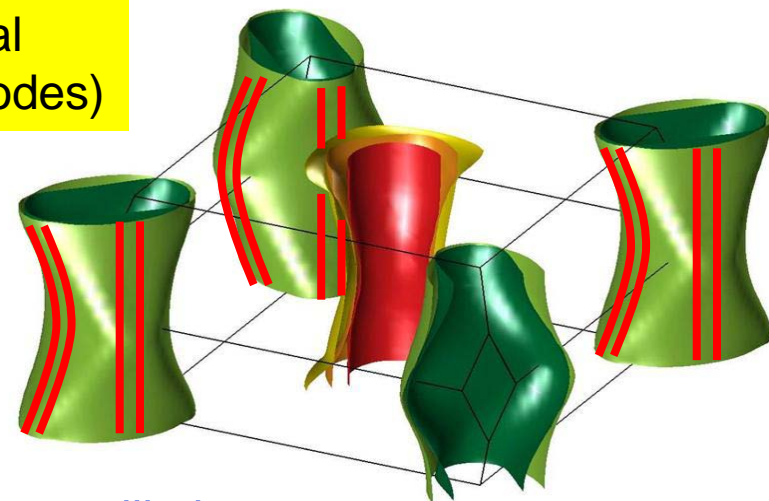
Pinpointing line node by angle-resolved thermal conductivity

i) Horizontal



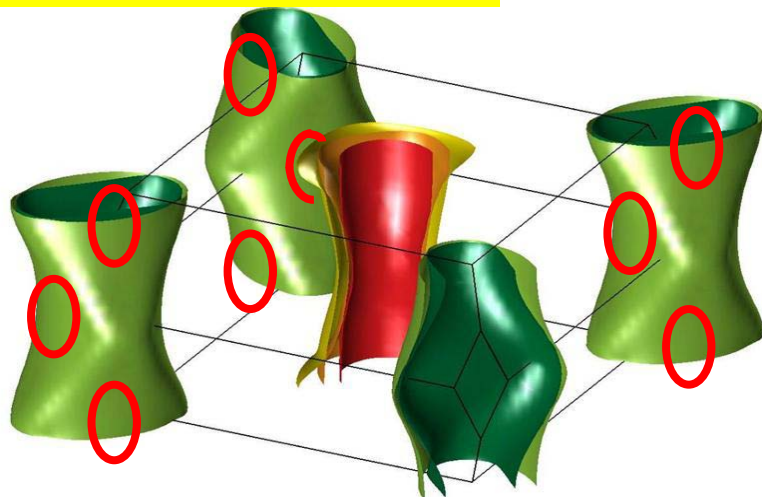
incompatible with the angle-resolved thermal conductivity

ii) Vertical
(8 line nodes)

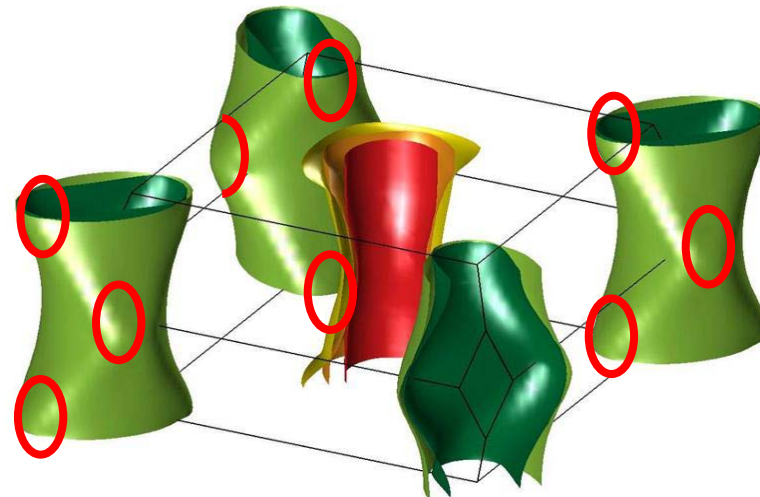


Seems unlikely
Has a symmetry higher than electron FS

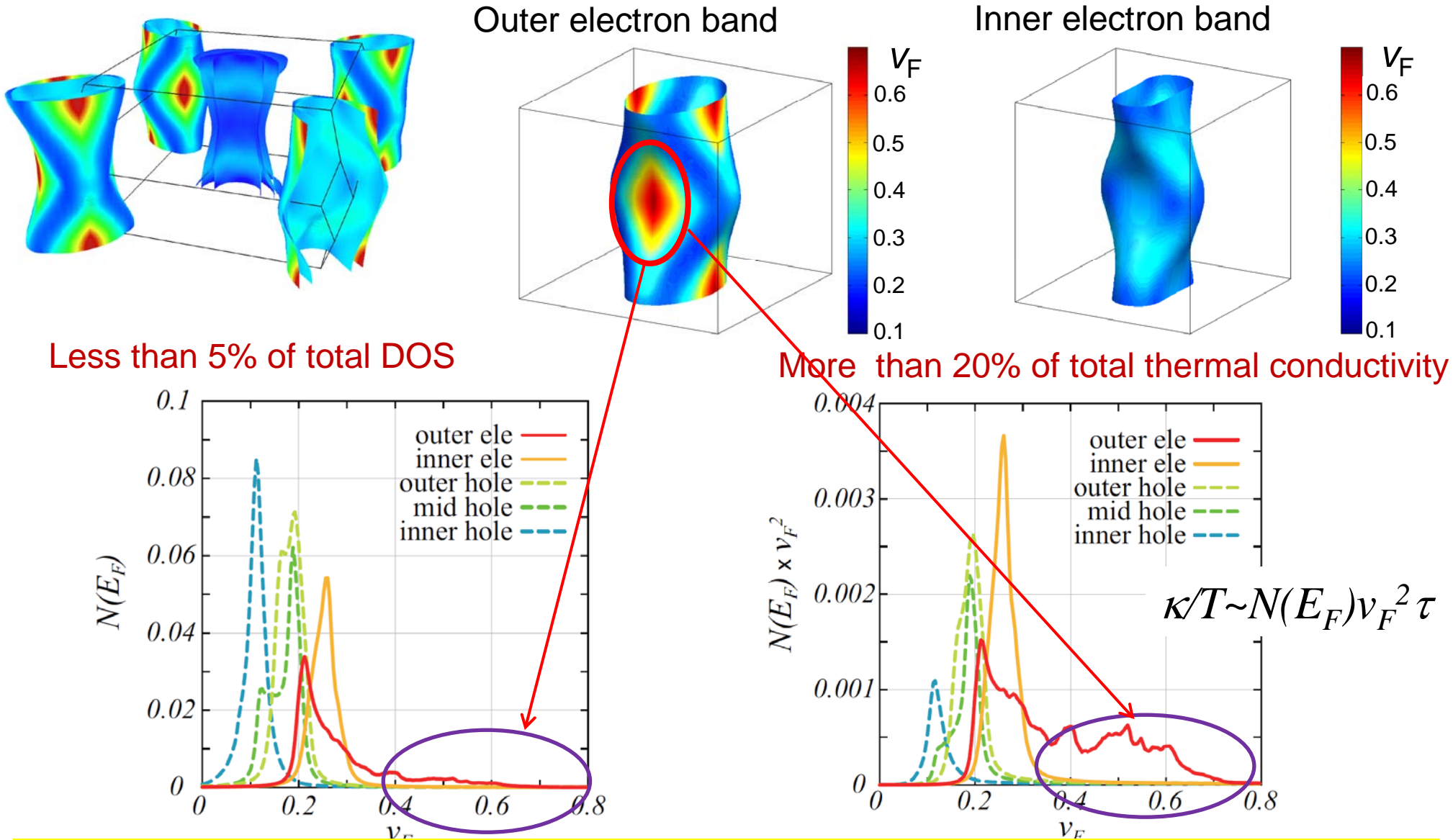
iii) Loop (Flat part of the FS)



iv) Loop (High curvature part of the FS)



Where is the line node in $\text{BaFe}_2(\text{As}_{0.67}\text{P}_{0.33})_2$ ($T_c=31$ K) ?



Line nodes are most likely to be located at the region with the largest Fermi velocity (flat part) in the electron sheet

Summary of the nodal structure of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

Penetration depth measures large v_F region

Node in the electron band

Thermal conductivity measures large v_F region

Node in the electron band

Specific heat measures large DOS region

No evidence of nodes in the hole band

ARPES measures particular hole FS

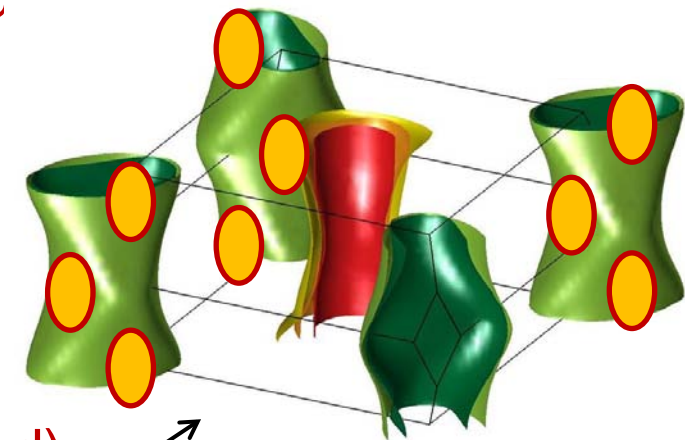
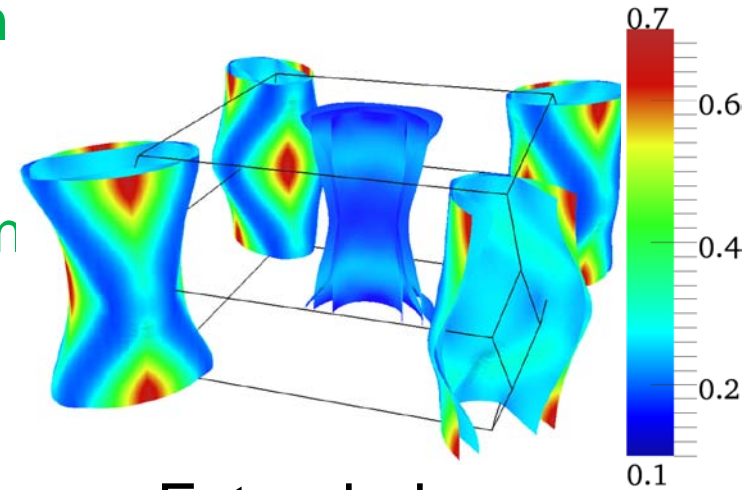
No nodes at hole FS

Angular-resolved thermal conductivity

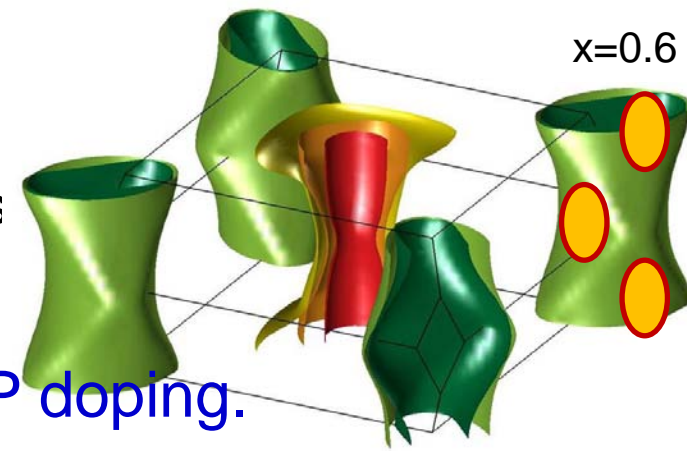
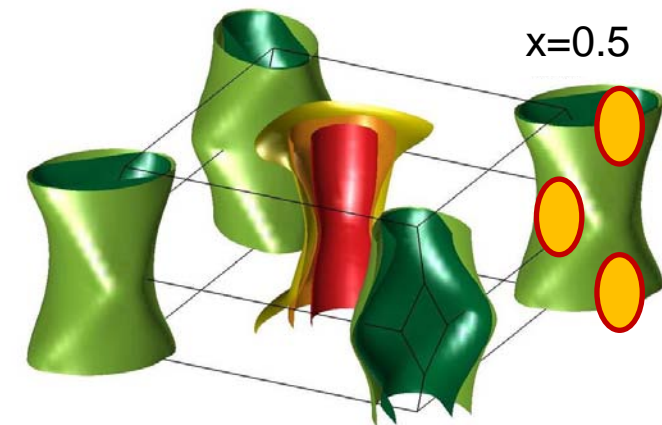
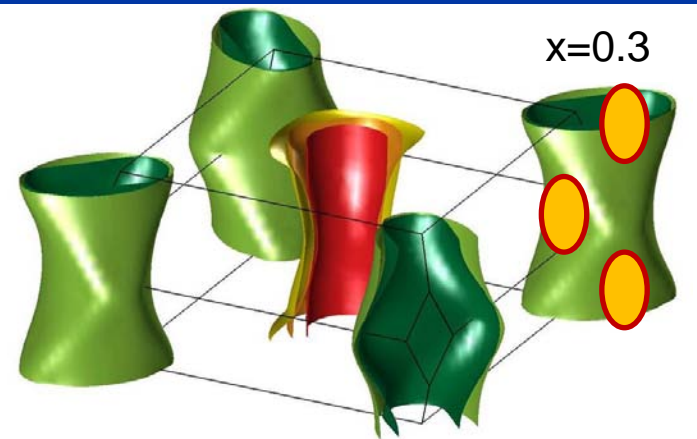
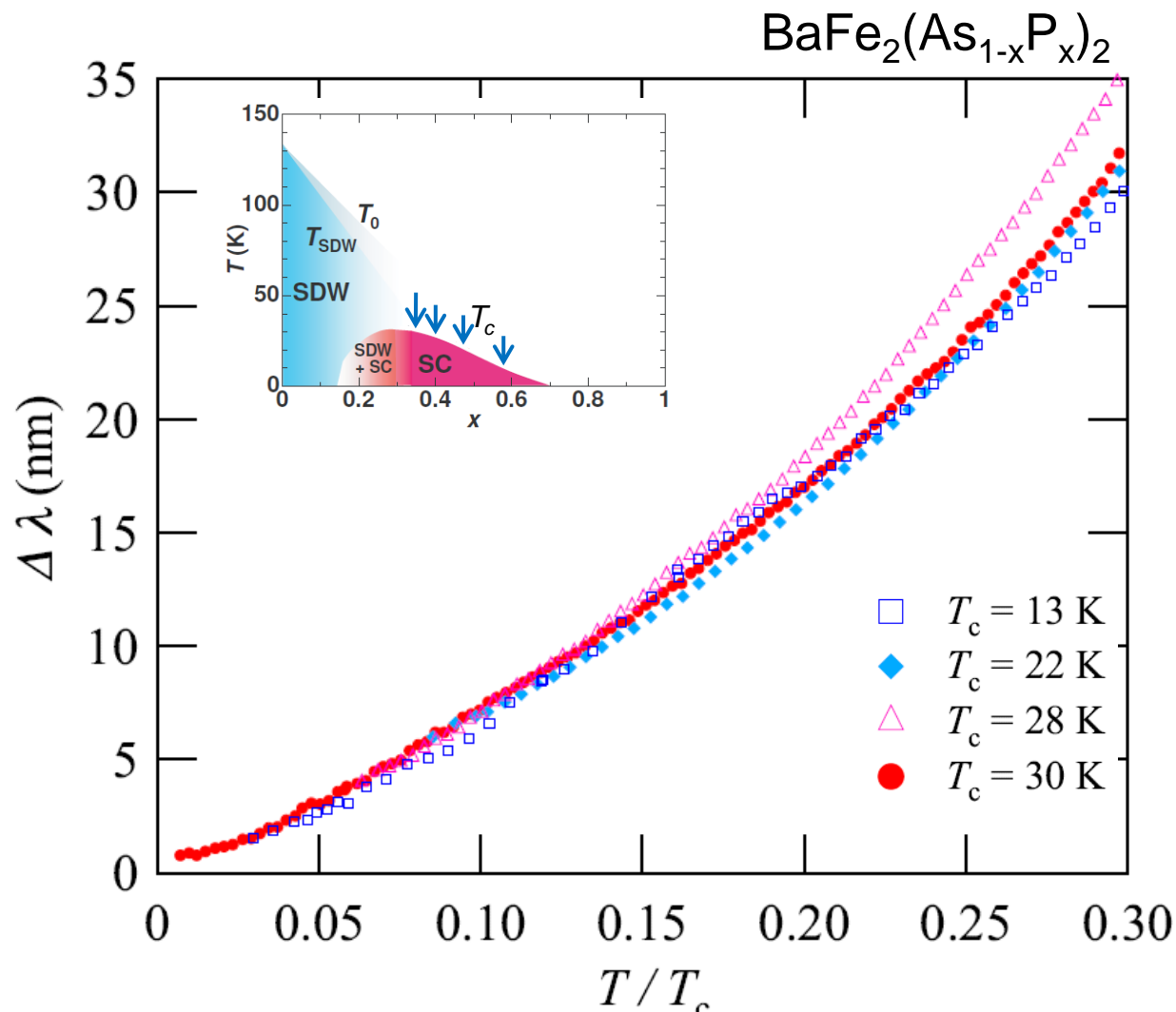
Node locates near Γ X-line (Fe-Fe bond)

All results above are consistent with this nodal structure

Line nodes are most likely to be located at the region with the largest Fermi velocity (flat part) in electron sheet



Doping dependence of the gap structure

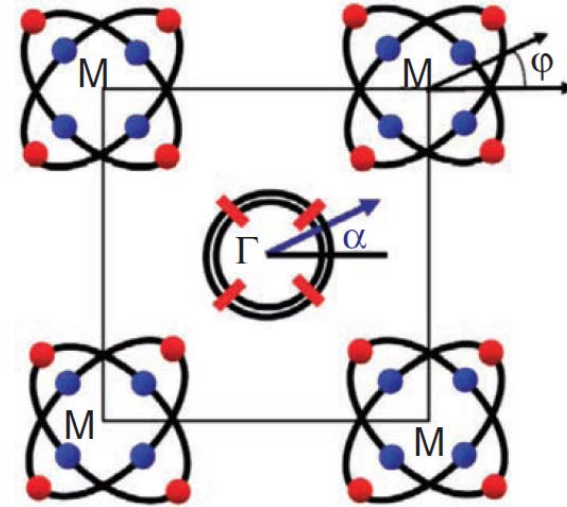
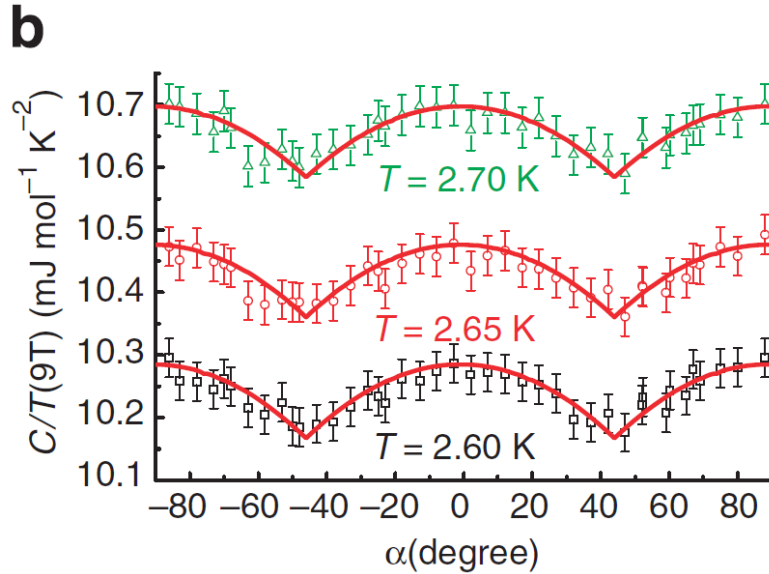


$\Delta\lambda(T)$ behavior is very similar in different doping levels

$$\Delta\lambda \sim N_0(\hat{\mathbf{k}}_n) \frac{T}{T_c}$$

The location of line node remains same with P doping.

Angle-resolved specific heat



Gap minimum (not node) along the Γ M
(Fe-Fe bond) direction

Summary

Determining gap nodal structure in isovalent doped $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

Thermal conductivity, penetration depth and NMR all consistently support the presence of line nodes in the superconducting gap.

Combined the above results with angle-resolved thermal conductivity, heat capacity, Laser ARPES, ARPES and band calculation, the line nodes are most likely to be located at the region with the largest Fermi velocity (flat part) in electron band.

The location of line node remains same with P doping.

