novel SuperConductors and Synchrotron Radiation: state of the art and perspectives

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The critical doping effects on the electronic structure of iron-based superconductors

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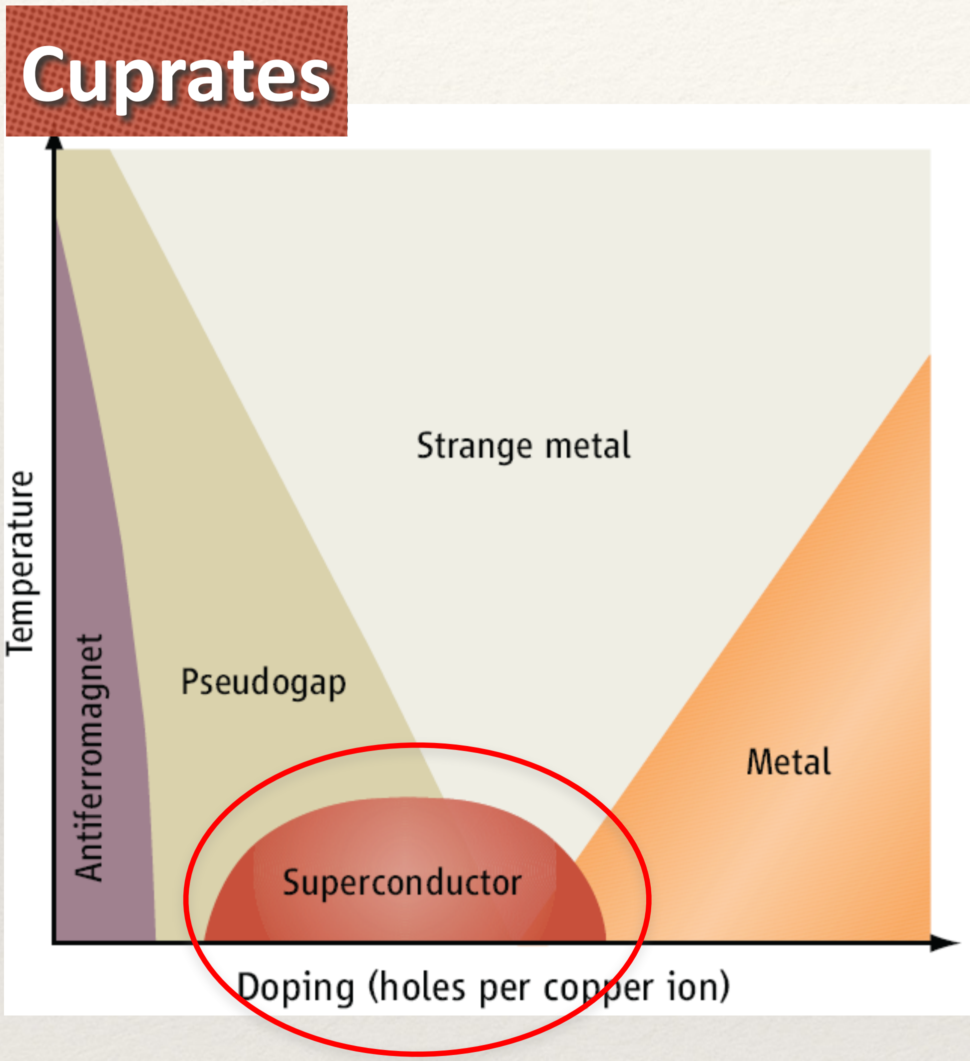
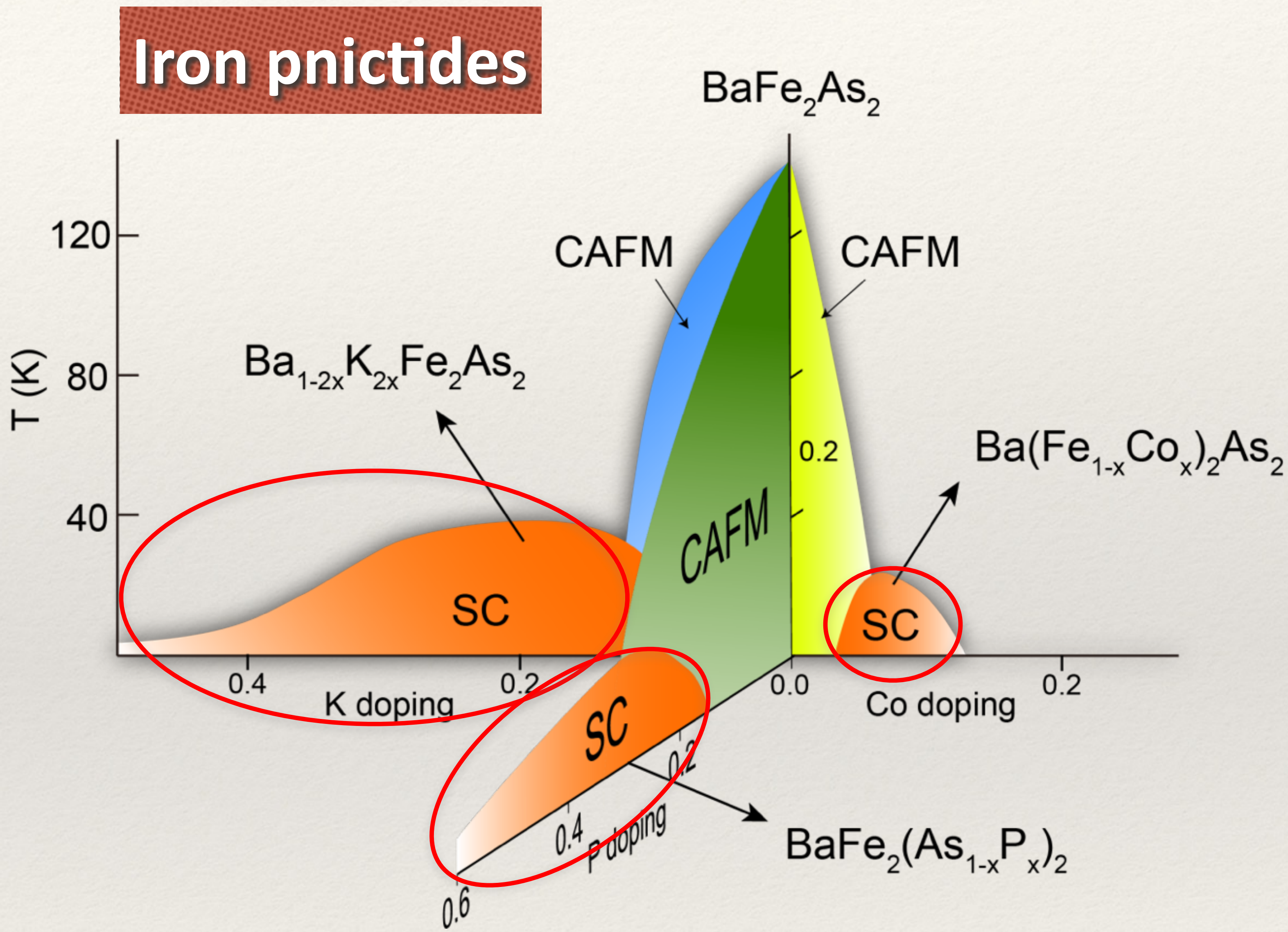
- Theory: J. P. Hu, T. Xiang, Z. Y. Lu, D. H. Lee
- NSFC, MOST

Two family of high-Tc's





The superconducting region shows a dome-like shape in the phase diagram and is sensitive to the doping level.

But we are doping a metal now ?!

- Why the iron-based superconductors (FeSC) have similar phase diagrams as that of the cuprates (doped Mott insulator) ?
- Why hetero-valent doping (electron or hole) and iso-valent doping [positive pressure (P, S), or negative pressure (Ru)] (and physical pressure) give the similar phase diagram. If it does not depend on the carrier density, what matters?
- Why the phase diagram of various FeSC's are so different in regime sizes ? Why FeSC's are less sensitive to impurities, compared with the cuprates.
- Why and how does Tc depend on the structural parameters ?

What is the universal role of dopants on the electronic structure ? and HOW does that affect the superconductivity?

Outline

- Extraordinary impurity scattering
- Alter Fermi surface
- Change bandwidth: the real universal electronic parameter
- What are more important for Tc ?

Z. R. Ye et al. PRX 4, 031041 (2014)
X. H. Niu, (in preparation)

Various iron-based systems studied

$LiFe_{1-x}Co_xAs$: x=0, 0.03, 0.09, 0.12, 0.17, 0.3

$NaFe_{1-x}Co_xAs$: x=0.045, 0.065, 0.1, 0.146, 0.32

Electron doping

$Ba_{1-x}K_xFe_2As_2$: x=0, 0.23, 0.43, 0.65, 0.86, 1

Hole doping

$BaFe_2(As_{1-x}P_x)_2$: x=0, 0.1, 0.2, 0.3, 0.5

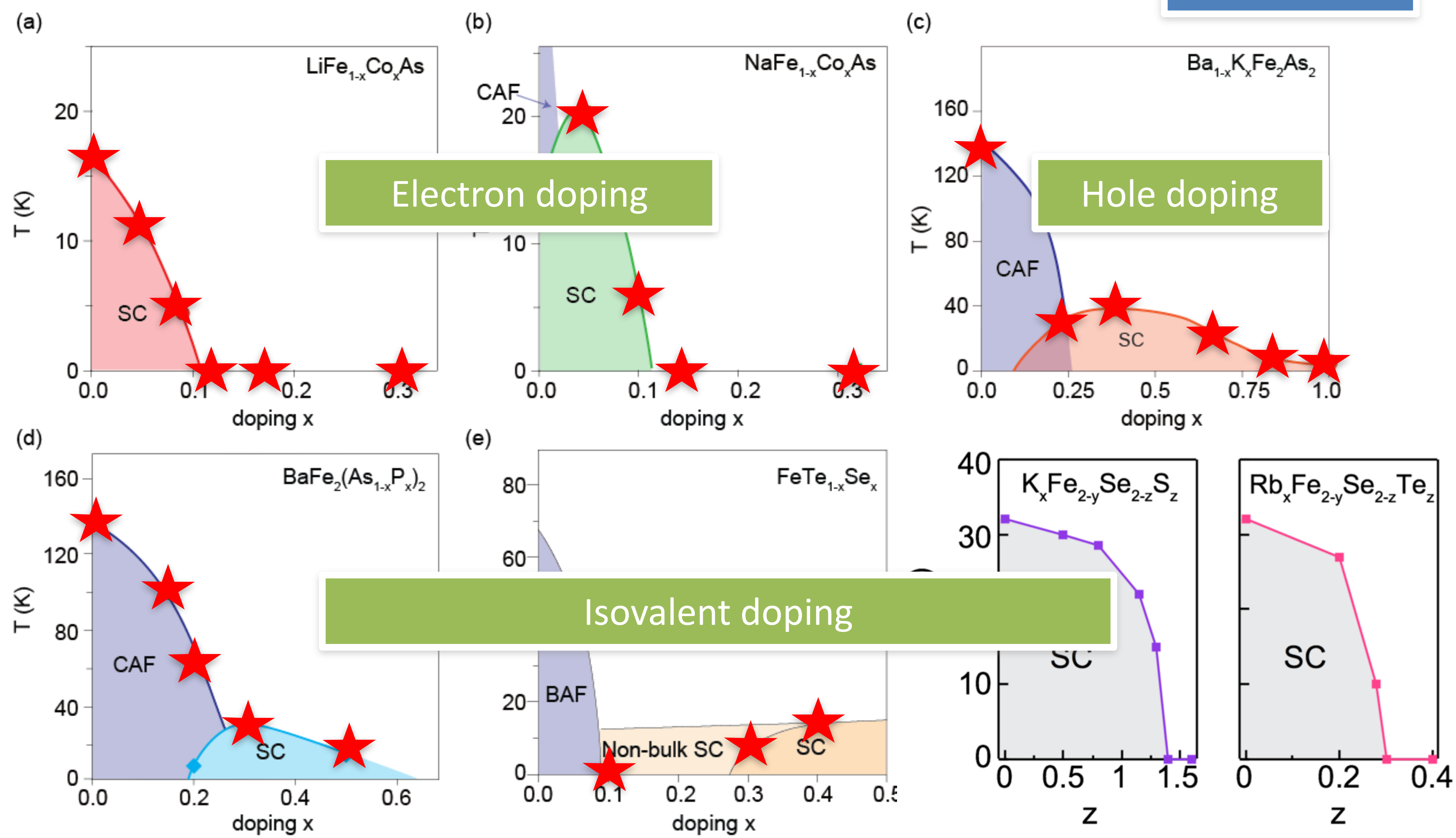
FeAs compounds

$FeTe_{1-x}Se_x$: x=0.1, 0.3, 0.4

$K_xFe_{2-y}Se_{2-z}S_z$: Z=0, …, 2 $Rb_xFe_{2-y}Se_{2-z}Te_z$: Z=0, …, 0.4

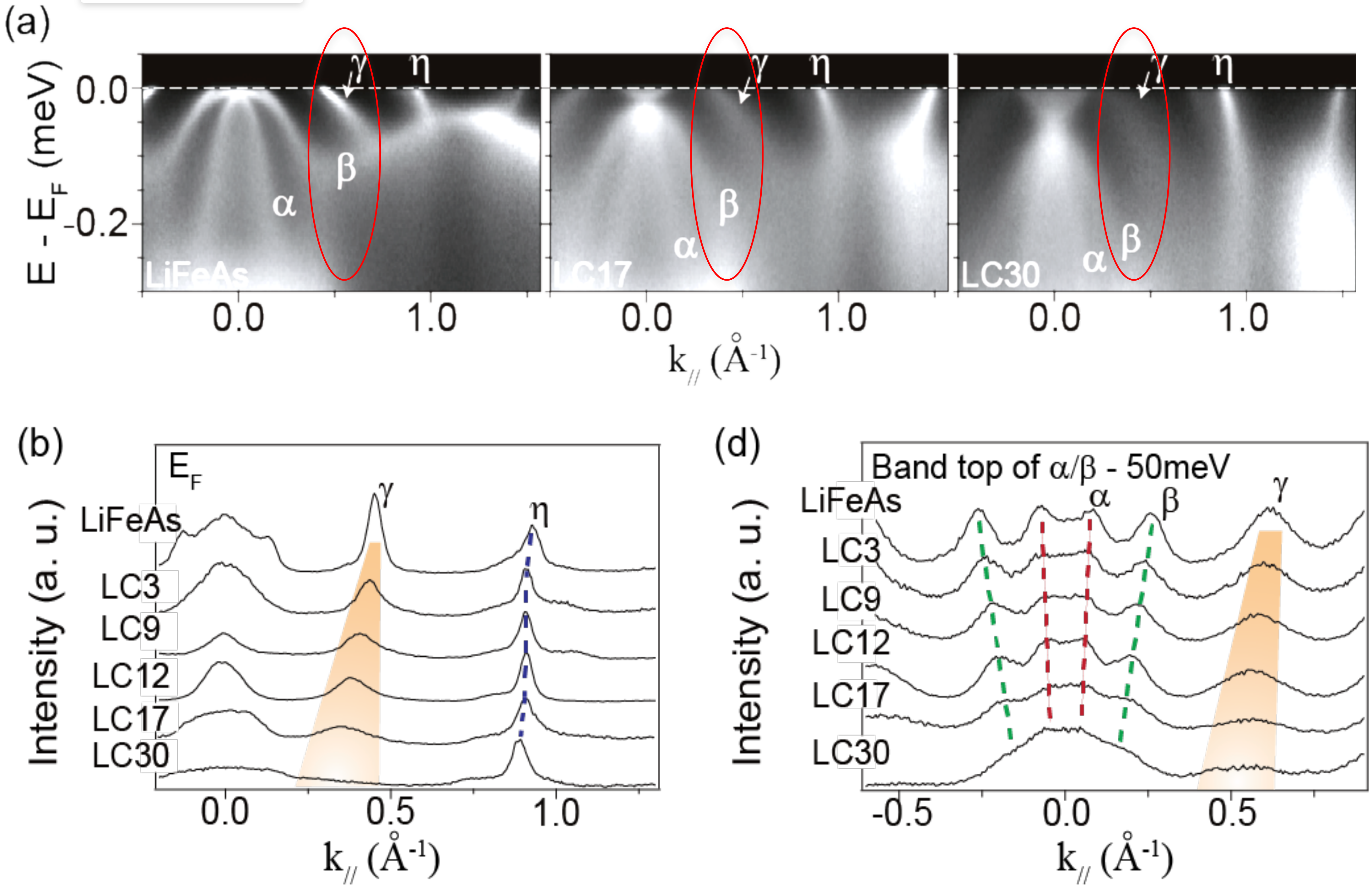
Isovalent doping

FeSe compounds



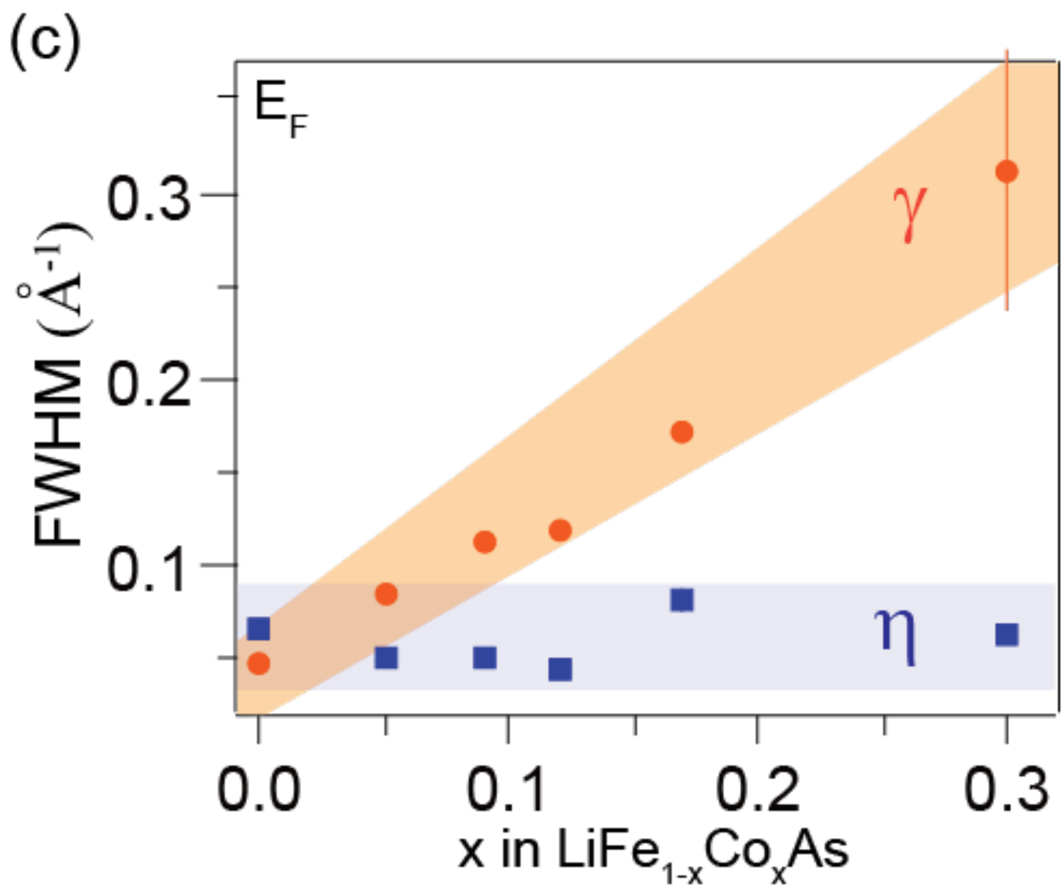
1. Impurity scattering effect

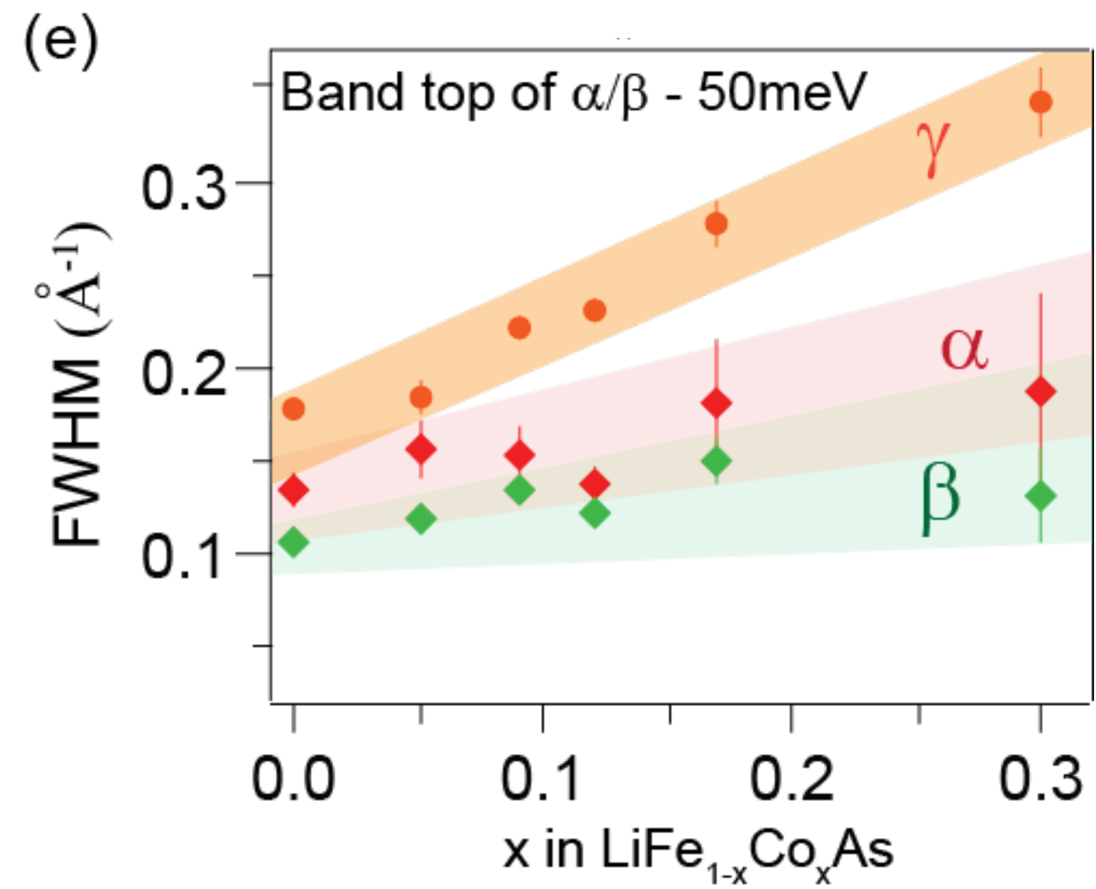
$LiFe_{1-x}Co_xAs$



with cobalt doping, the d_{xy}-based γ band becomes significantly weaker and broader.

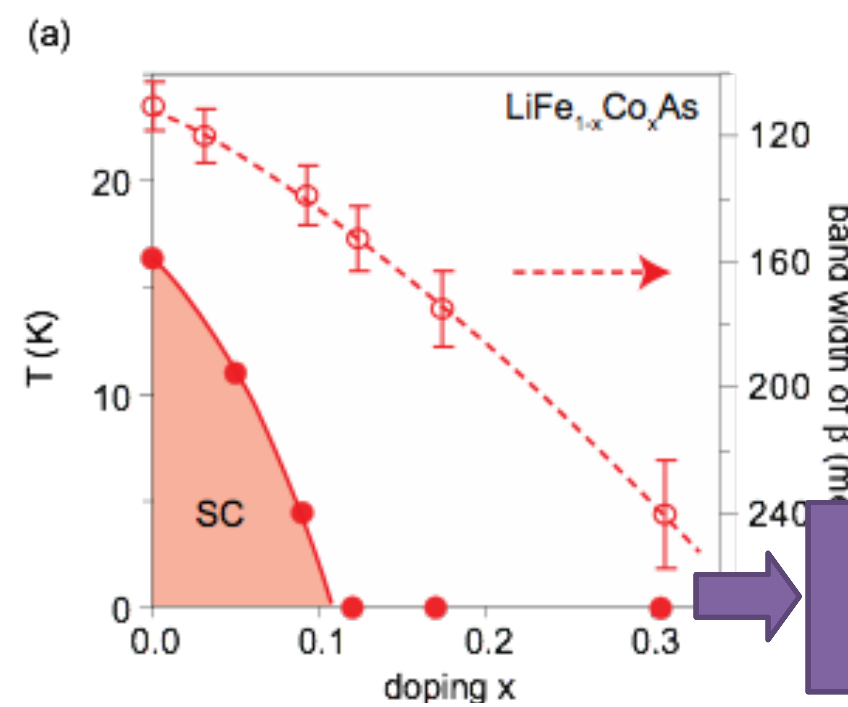
Band selective scattering





The FWHM of γ increases remarkably, compared to all the other bands.

Such a quasiparticle scattering of the γ band with d_{xy} orbital is not due to the increase of electronic correlation, as we will show later, the band renormalization decreases with doping.



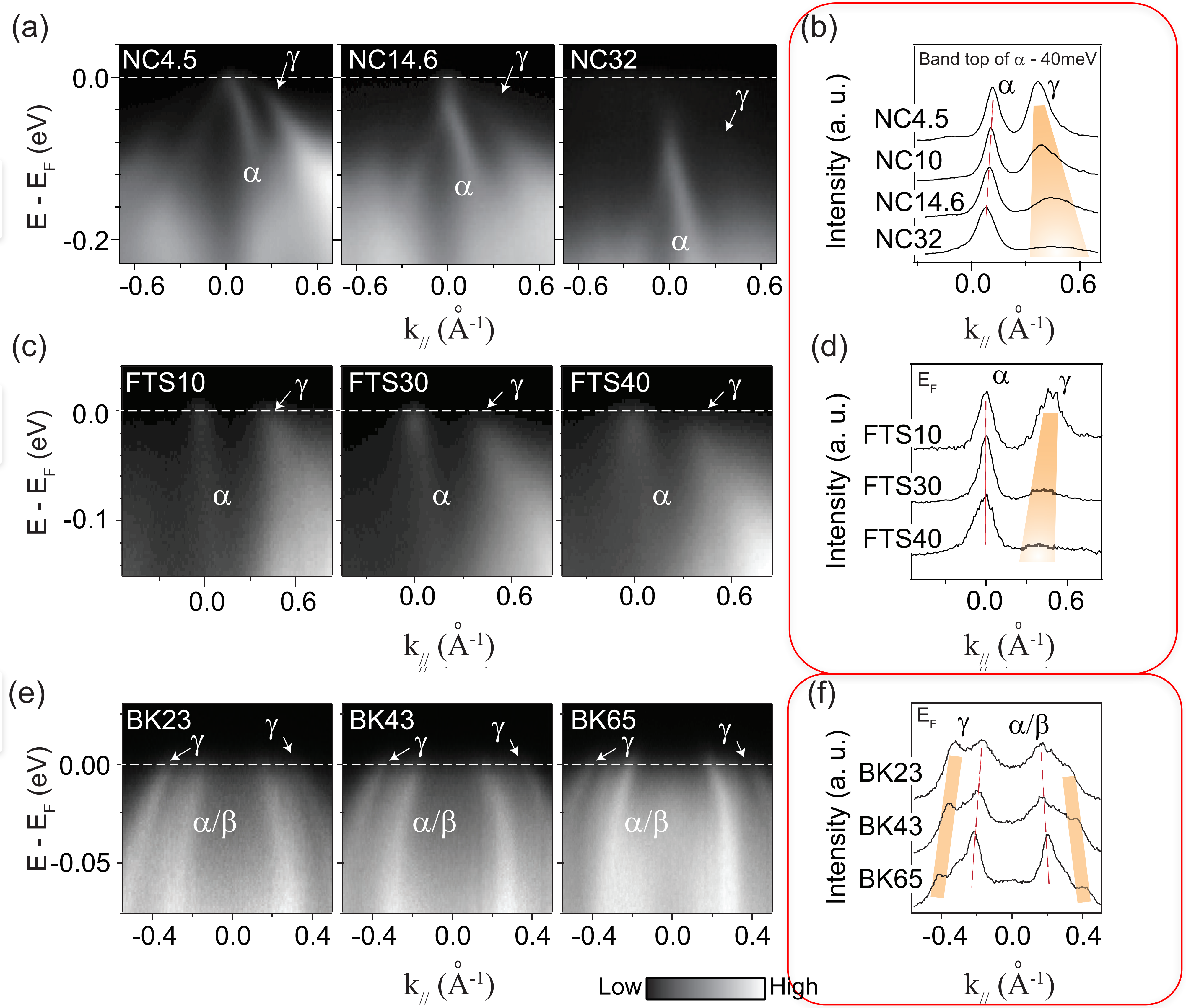
Will be shown later

site dependence

$NaFe_{1-x}Co_xAs$

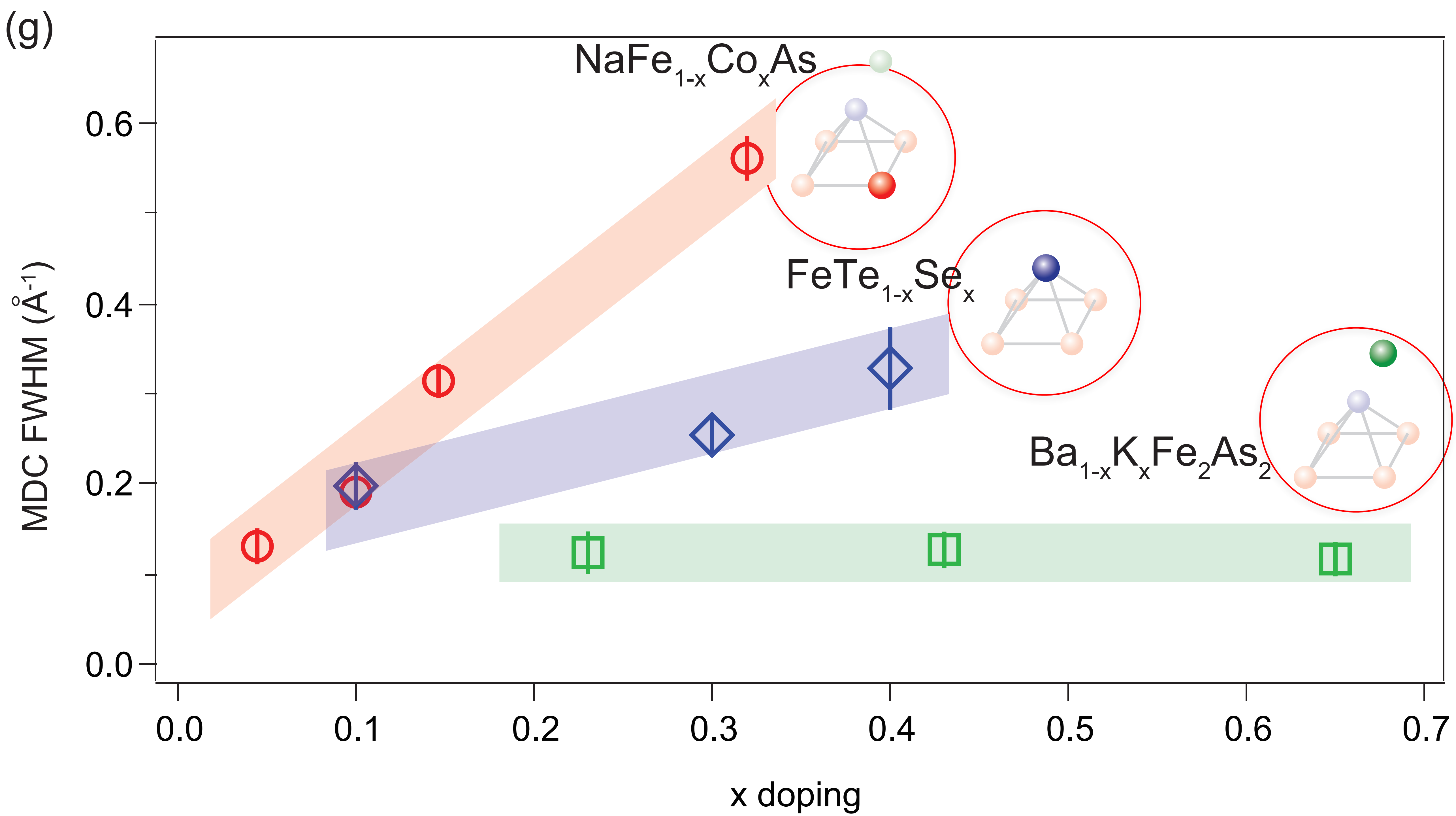
$FeTe_{1-x}Se_x$

$Ba_{1-x}K_xFe_2As_2$

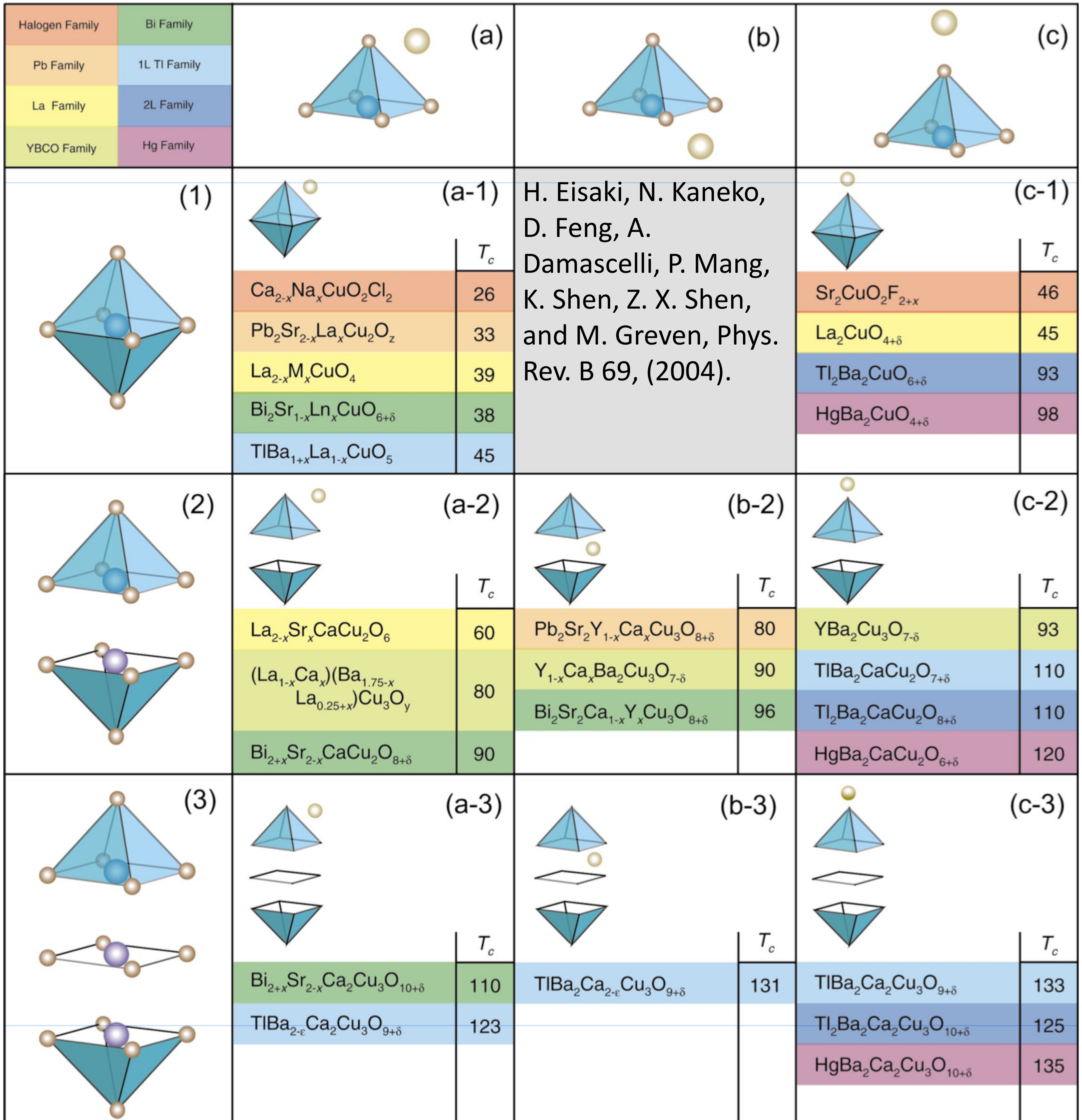


The γ band in $NaFe_{1-x}Co_xAs$ and $FeTe_{1-x}Se_x$ are broadened with doping, while for $Ba_{1-x}K_xFe_2As_2$, it is relatively unchanged.

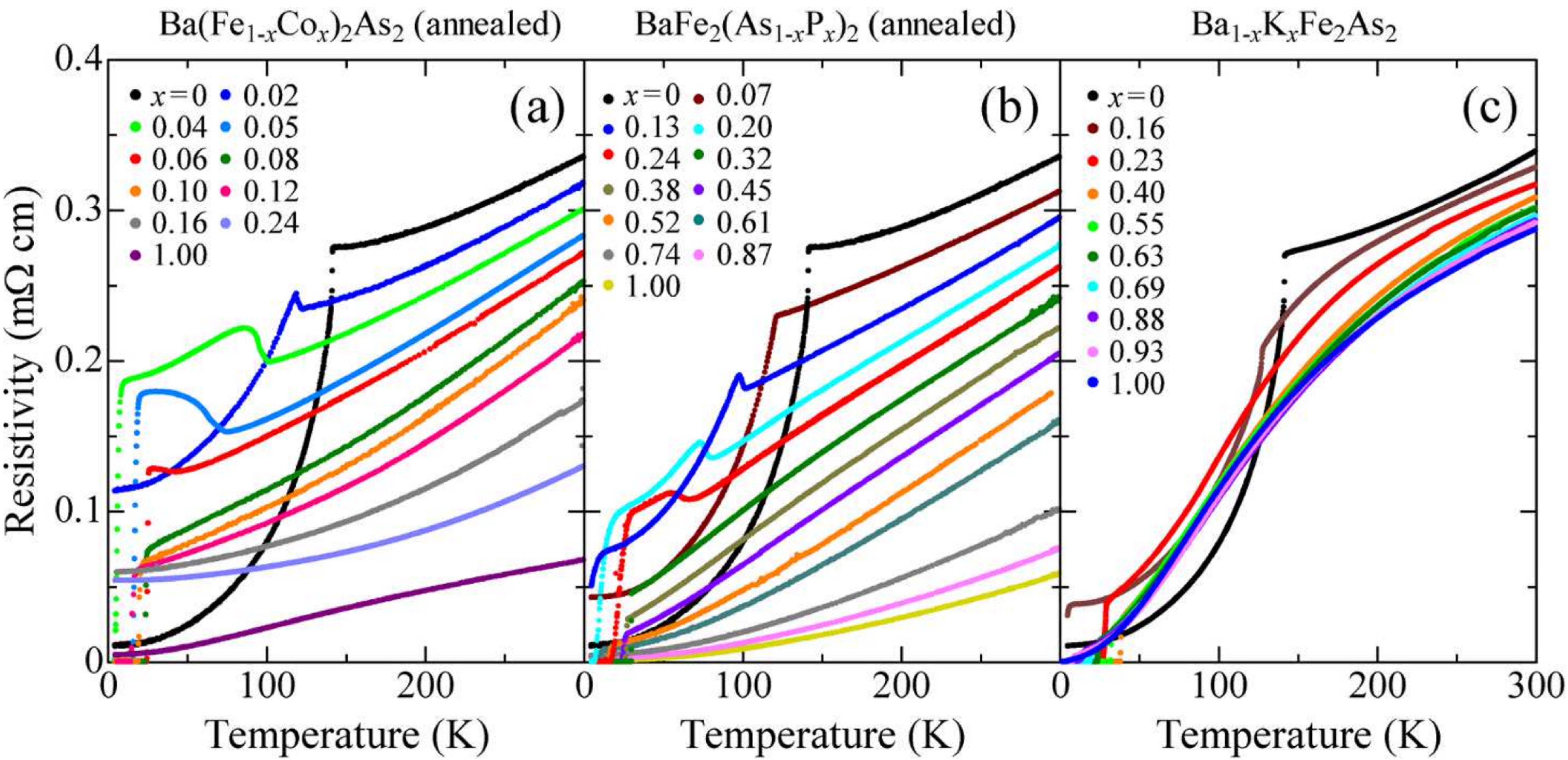
Site dependence



The scattering strength strongly depends on the dopants’ location: when the dopant moves away from the iron-anion layer, the scattering decreases.


Halogen Family
Bi Family
Pb Family
1L Tl Family
La Family
2L Family
YBCO Family
Hg Family
(a)
(b)
(c)
(1)
(a-1)
T_c
$Ca_{2-x}Na_xCuO_2Cl_2$ 26
$Pb_2Sr_{2-x}La_xCu_2O_z$ 33
$La_{2-x}M_xCuO_4$ 39
$Bi_2Sr_{1-x}Ln_xCuO_{6+\delta}$ 38
$TlBa_{1+x}La_{1-x}CuO_5$ 45
H. Eisaki, N. Kaneko, D. Feng, A. Damascelli, P. Mang, K. Shen, Z. X. Shen, and M. Greven, Phys. Rev. B 69, (2004).
(c-1)
T_c
$Sr_2CuO_2F_{2+x}$ 46
$La_2CuO_{4+\delta}$ 45
$Tl_2Ba_2CuO_{6+\delta}$ 93
$HgBa_2CuO_{4+\delta}$ 98
(2)
(a-2)
T_c
$La_{2-x}Sr_xCaCu_2O_6$ 60
$(La_{1-x}Ca_x)(Ba_{1.75-x}La_{0.25+x})Cu_3O_y$ 80
$Bi_{2+x}Sr_{2-x}CaCu_2O_{8+\delta}$ 90
(b-2)
T_c
$Pb_2Sr_2Y_{1-x}Ca_xCu_3O_{8+\delta}$ 80
$Y_{1-x}Ca_xBa_2Cu_3O_{7-\delta}$ 90
$Bi_2Sr_2Ca_{1-x}Y_xCu_3O_{8+\delta}$ 96
(c-2)
T_c
$YBa_2Cu_3O_{7-\delta}$ 93
$TlBa_2CaCu_2O_{7+\delta}$ 110
$Tl_2Ba_2CaCu_2O_{8+\delta}$ 110
$HgBa_2CaCu_2O_{6+\delta}$ 120
(3)
(a-3)
T_c
$Bi_{2+x}Sr_{2-x}Ca_2Cu_3O_{10+\delta}$ 110
$TlBa_{2-\varepsilon}Ca_2Cu_3O_{9+\delta}$ 123
(b-3)
T_c
$TlBa_2Ca_{2-\varepsilon}Cu_3O_{9+\delta}$ 131
(c-3)
T_c
$TlBa_2Ca_2Cu_3O_{9+\delta}$ 133
$Tl_2Ba_2Ca_2Cu_3O_{10+\delta}$ 125
$HgBa_2Ca_2Cu_3O_{10+\delta}$ 135

Impurity effects on resistivity



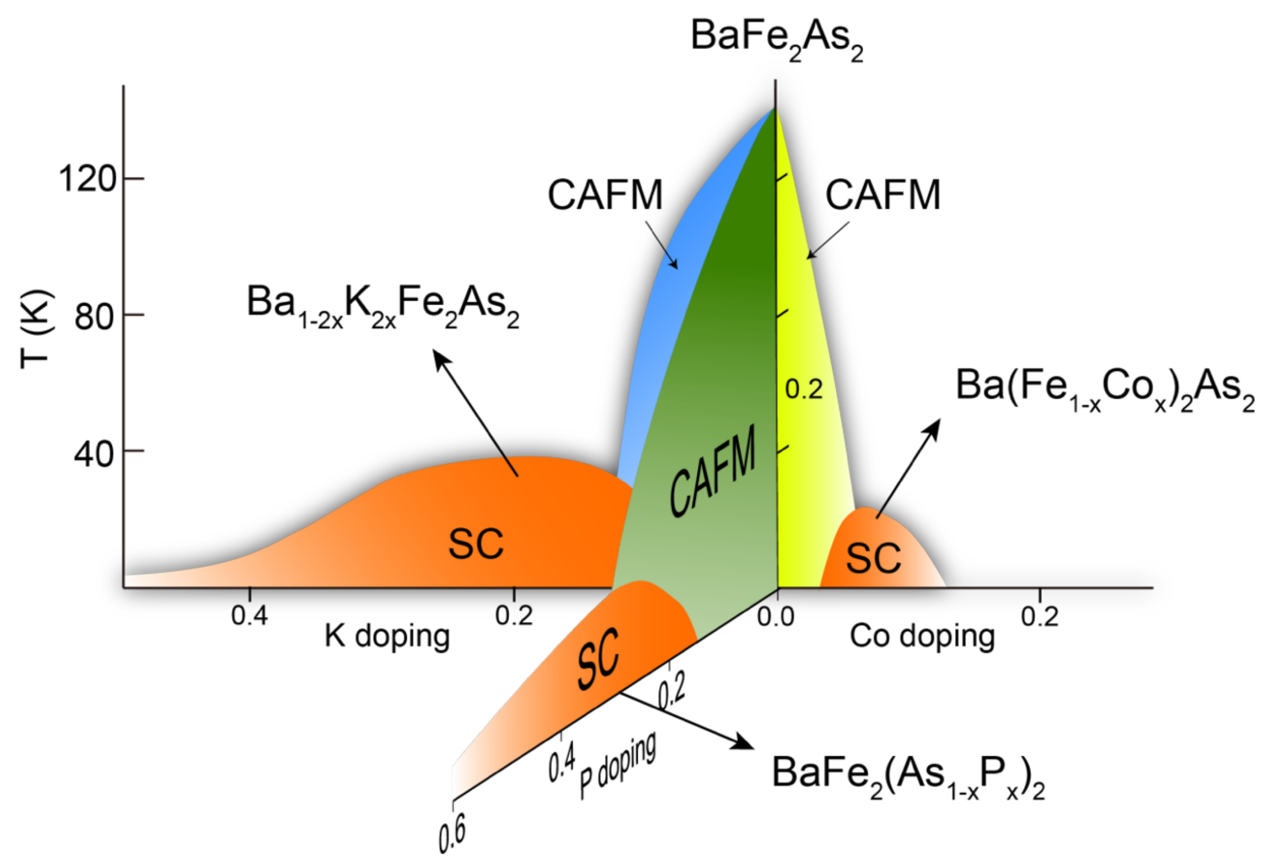
M. Nakajima et al. Arxiv/1308.1633 (S. Uchida group)

Consequences

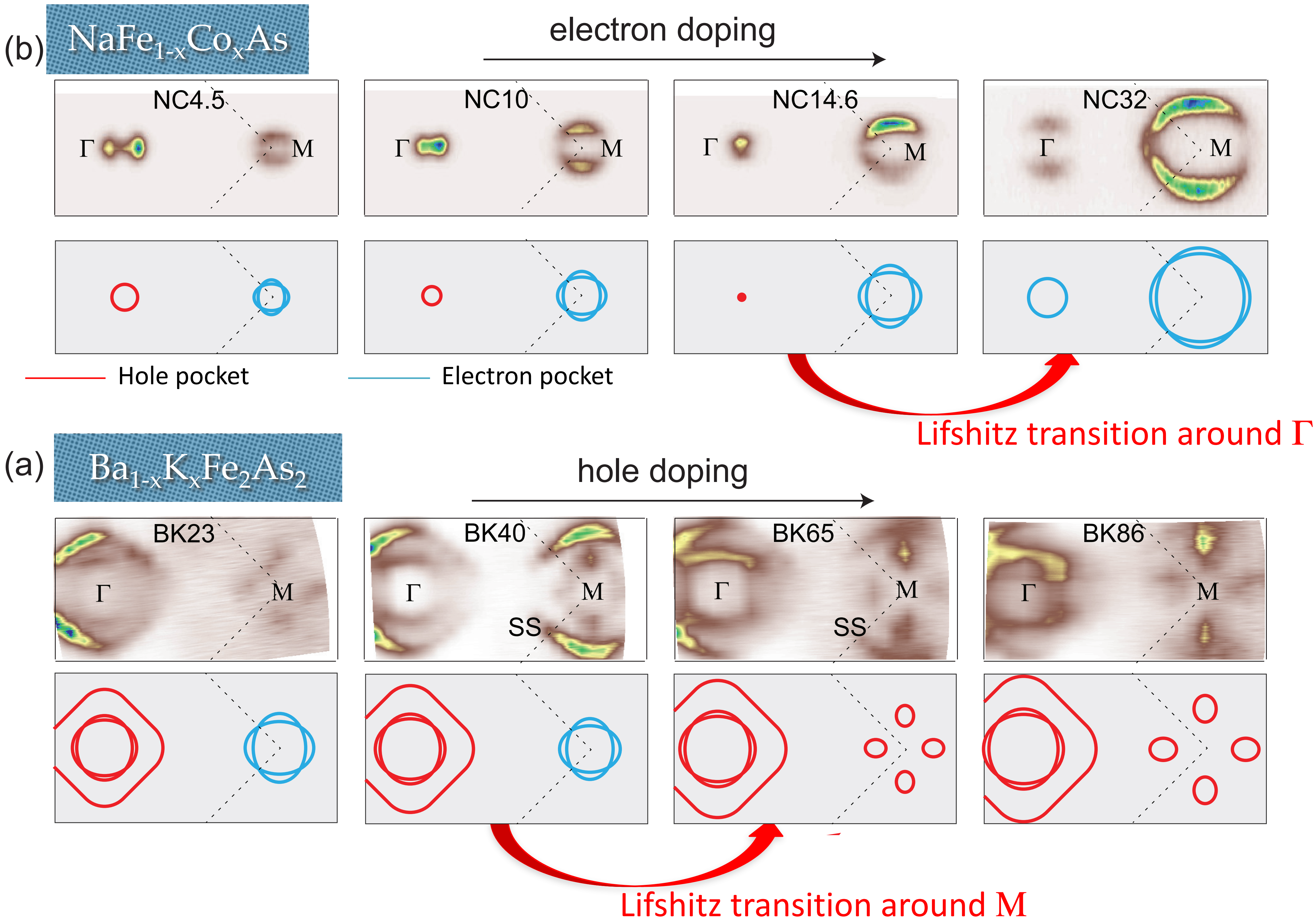
1. The band selectivity could explain the **robust superconductivity against heavy doping** in iron-based superconductors, since most bands are basically unaffected by the scattering of dopants.

2. The site dependence could understand **different optimal Tc's and SC regime sizes in different iron-based systems**.

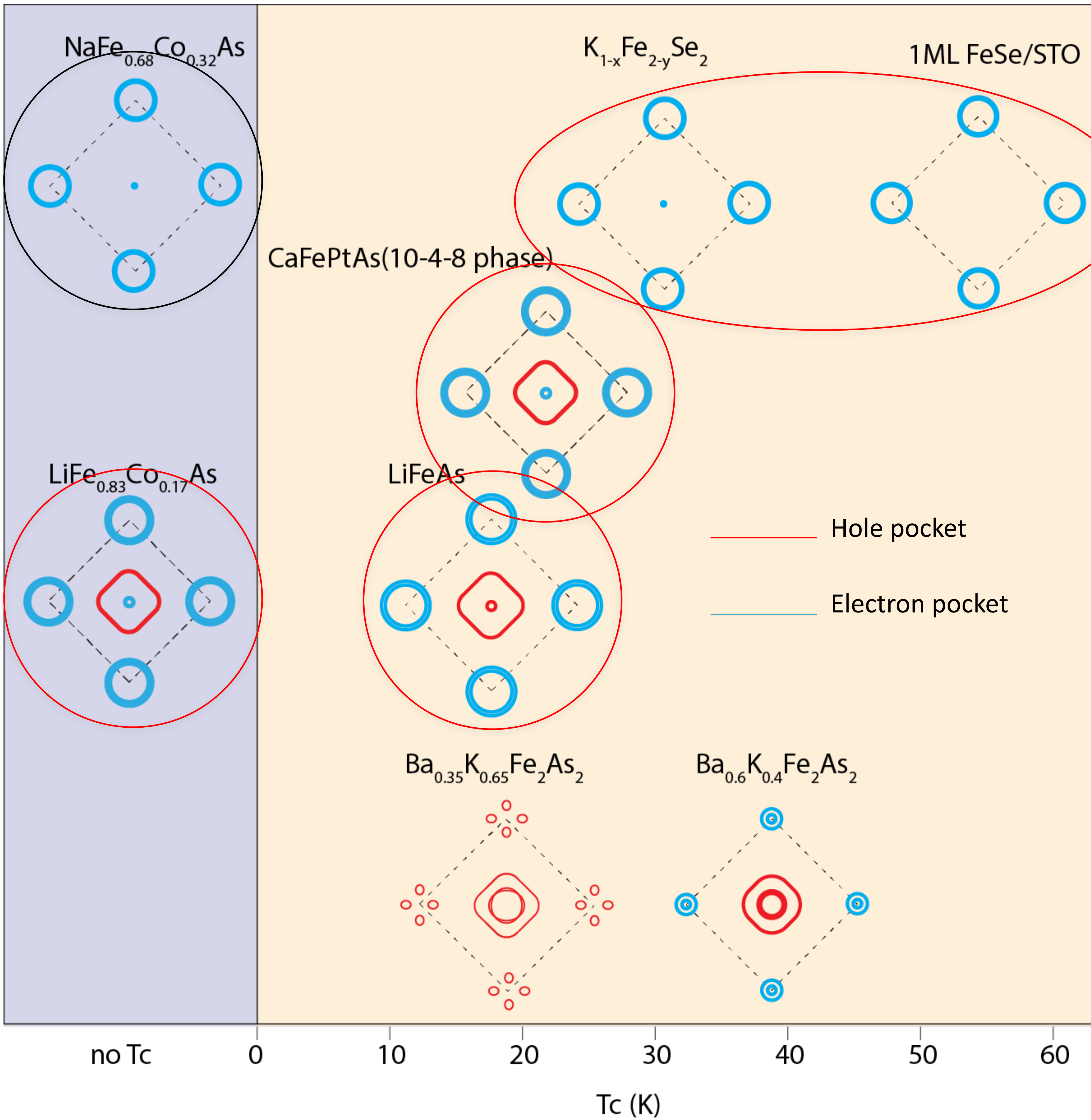
3. Lifshitz transition (**the correlation between the disappearance of Tc and the dxz/dyz hole pocket) is an accident**, as the day hole pocket is strongly scattered.



2. Fermi surface evolution and Lifshitz transition



The relation between Fermi surface and superconductivity is still under debate.



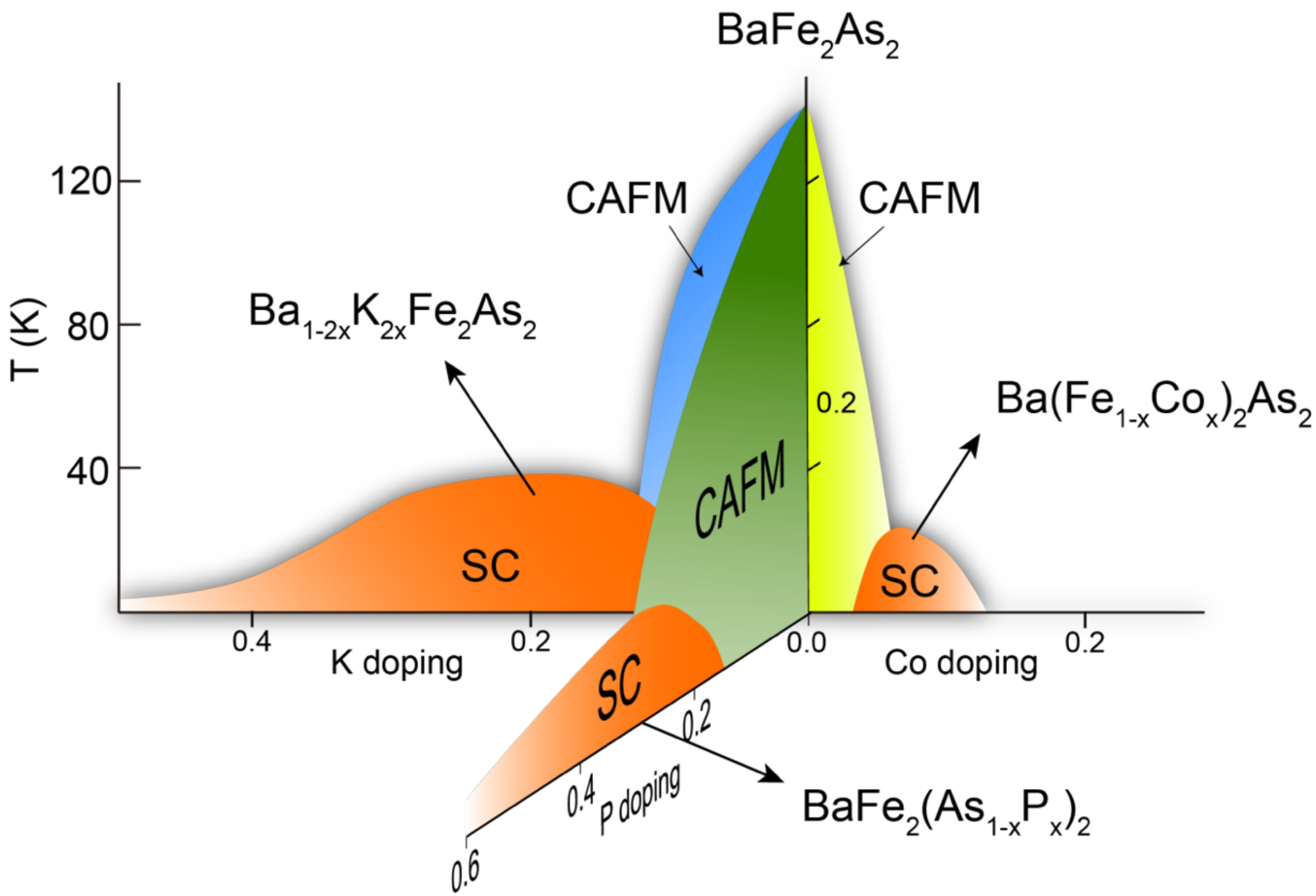
There is no systematics!

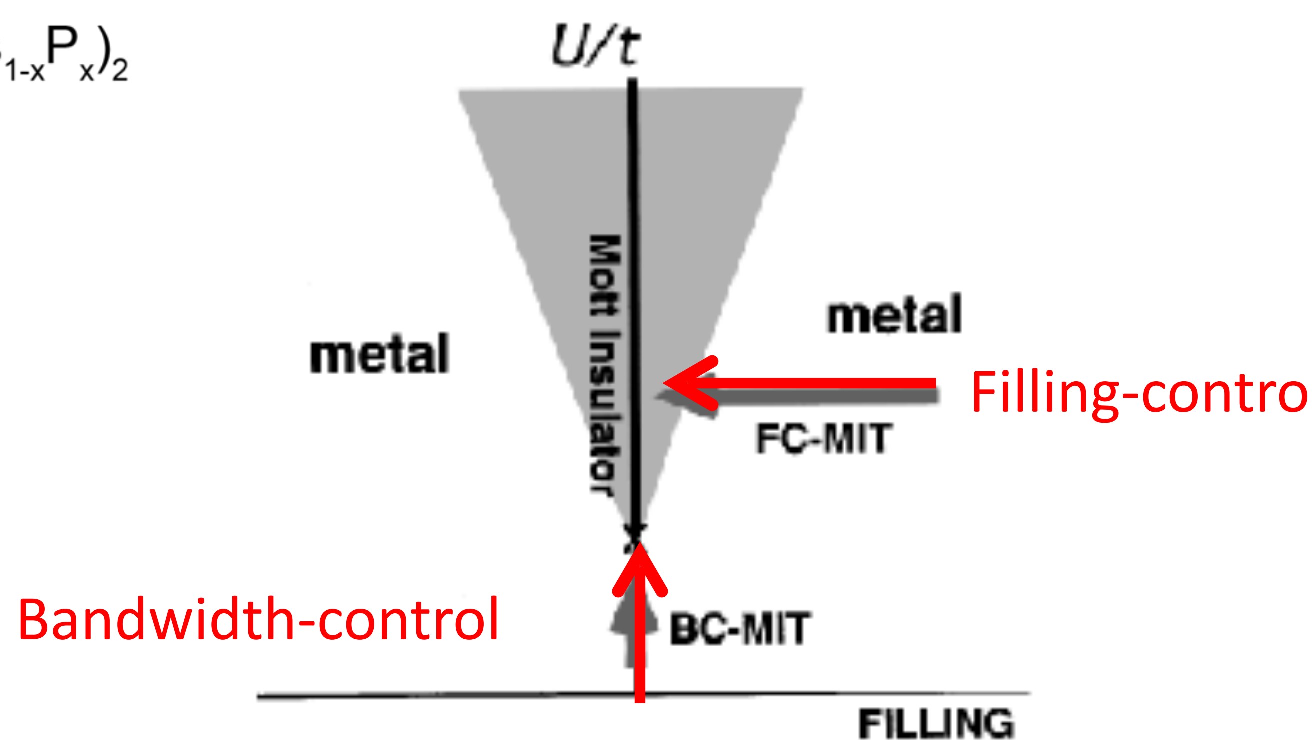
Tc is not directly related with the Fermi surface topology.

Dope a metal often does not cause much change of carrier.

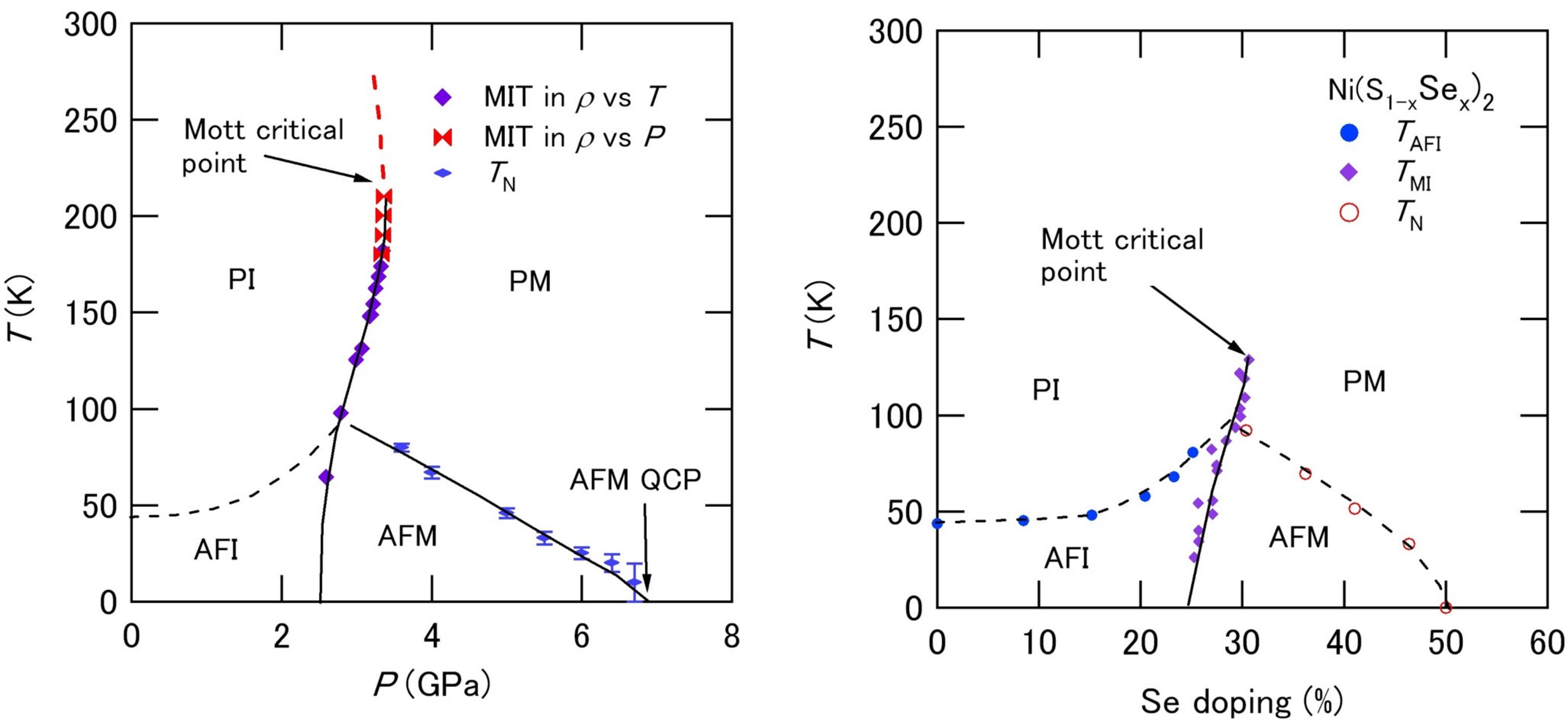
Fermi surface plays a secondary role.

dxy can sustain SC when it is not scattered strongly, eg. in the 10-4-8 phase.


BaFe2As2
T (K)
120
80
40
CAFM
CAFM
CAFM
Ba1-2xK2xFe2As2
Ba(Fe1-xCo x)2As2
SC
SC
SC
0.4
0.2
K doping
0.0
0.2
Co doping
0.2
0.2
0.4
P doping
0.6
BaFe2(As1-xPx)2

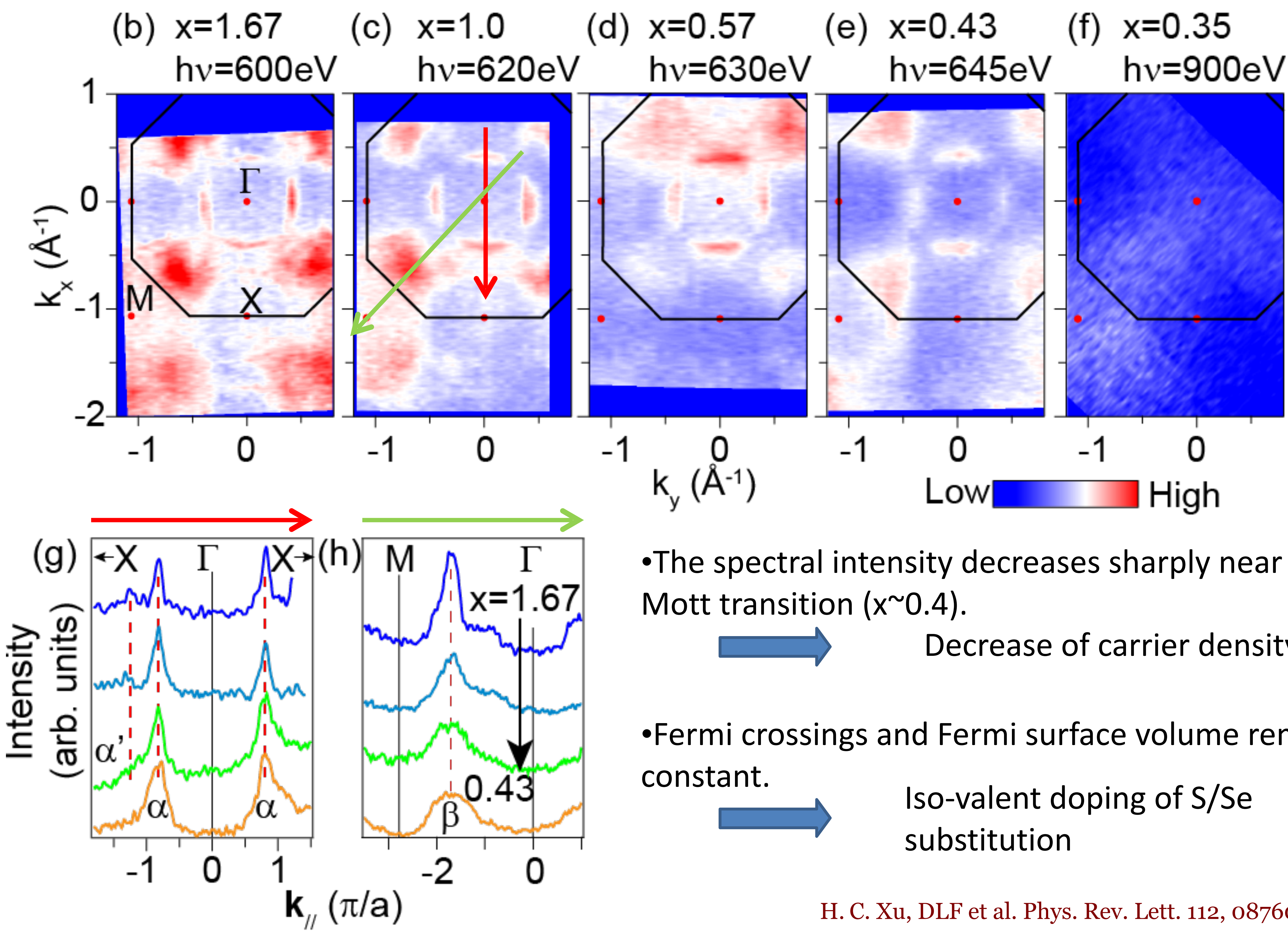

U/t
Mott Insulator
metal
metal
Filling-control
FC-MIT
Bandwidth-control
BC-MIT
FILLING

Phase diagram of NiS_2 (pressure) and $Ni(S_{1-x}Se_x)_2$ (Se substitution)



Takagi et al.

Doping-independent Fermi Surface



•The spectral intensity decreases sharply near the Mott transition (x~0.4).

Decrease of carrier density

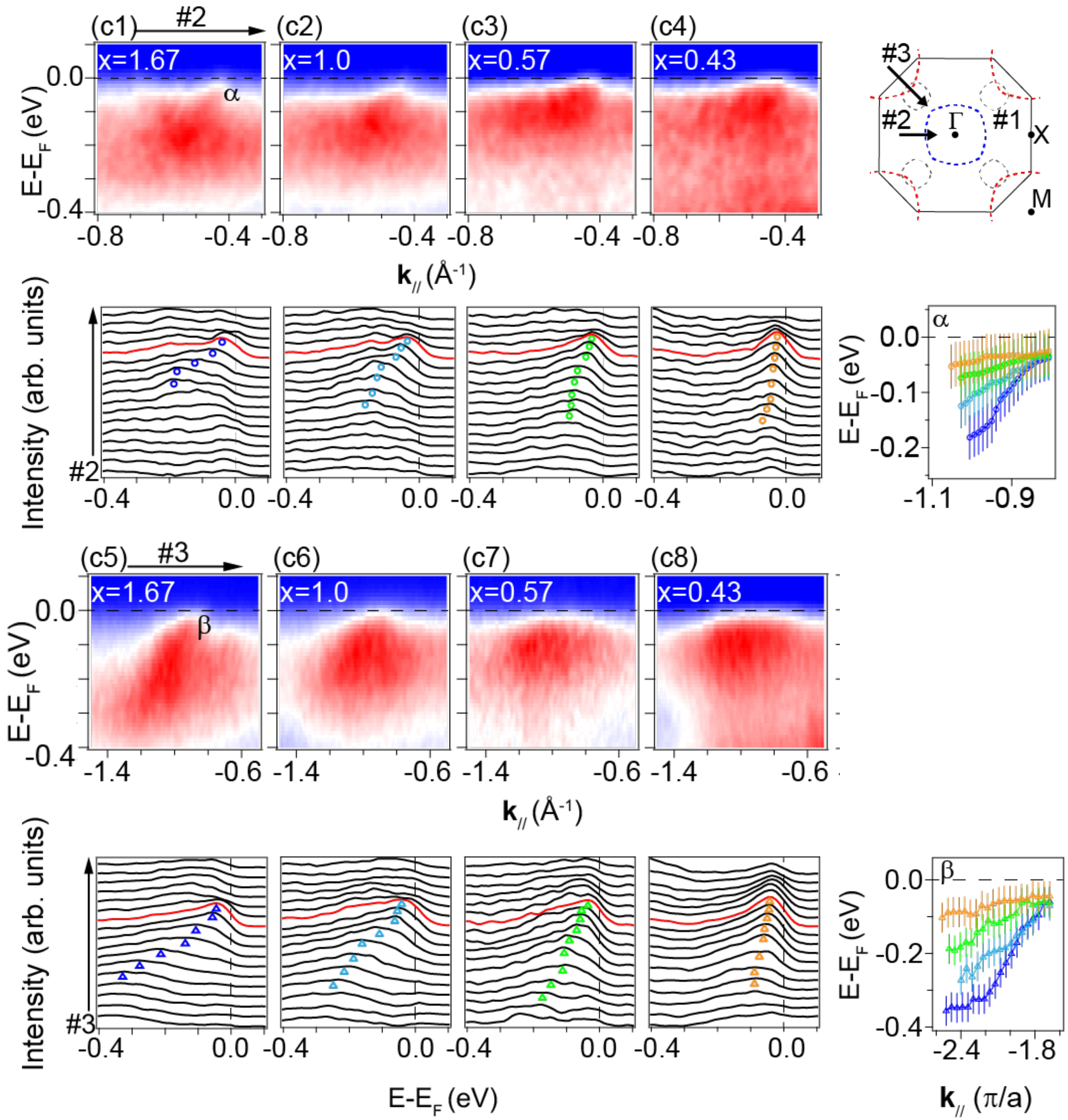
•Fermi crossings and Fermi surface volume remains constant.

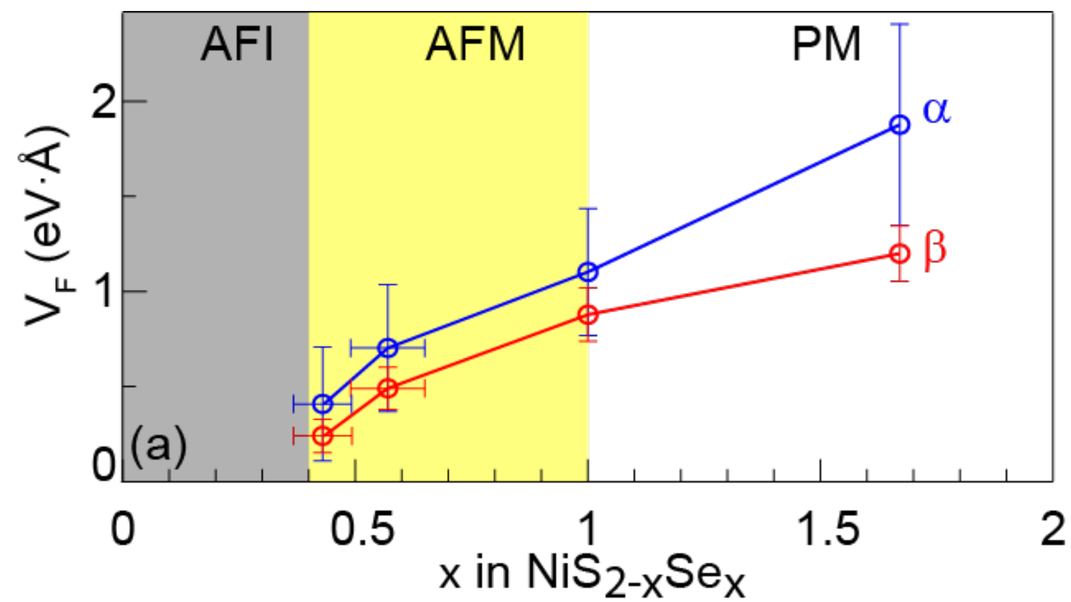
Iso-valent doping of S/Se substitution

H. C. Xu, DLF et al. Phys. Rev. Lett. 112, 087603 (2014).

Band width controlled Mott transition

•EDCs after subtracting the background





•The Fermi velocities drop rapidly as approaching the Mott transition, and diminish at the transition.

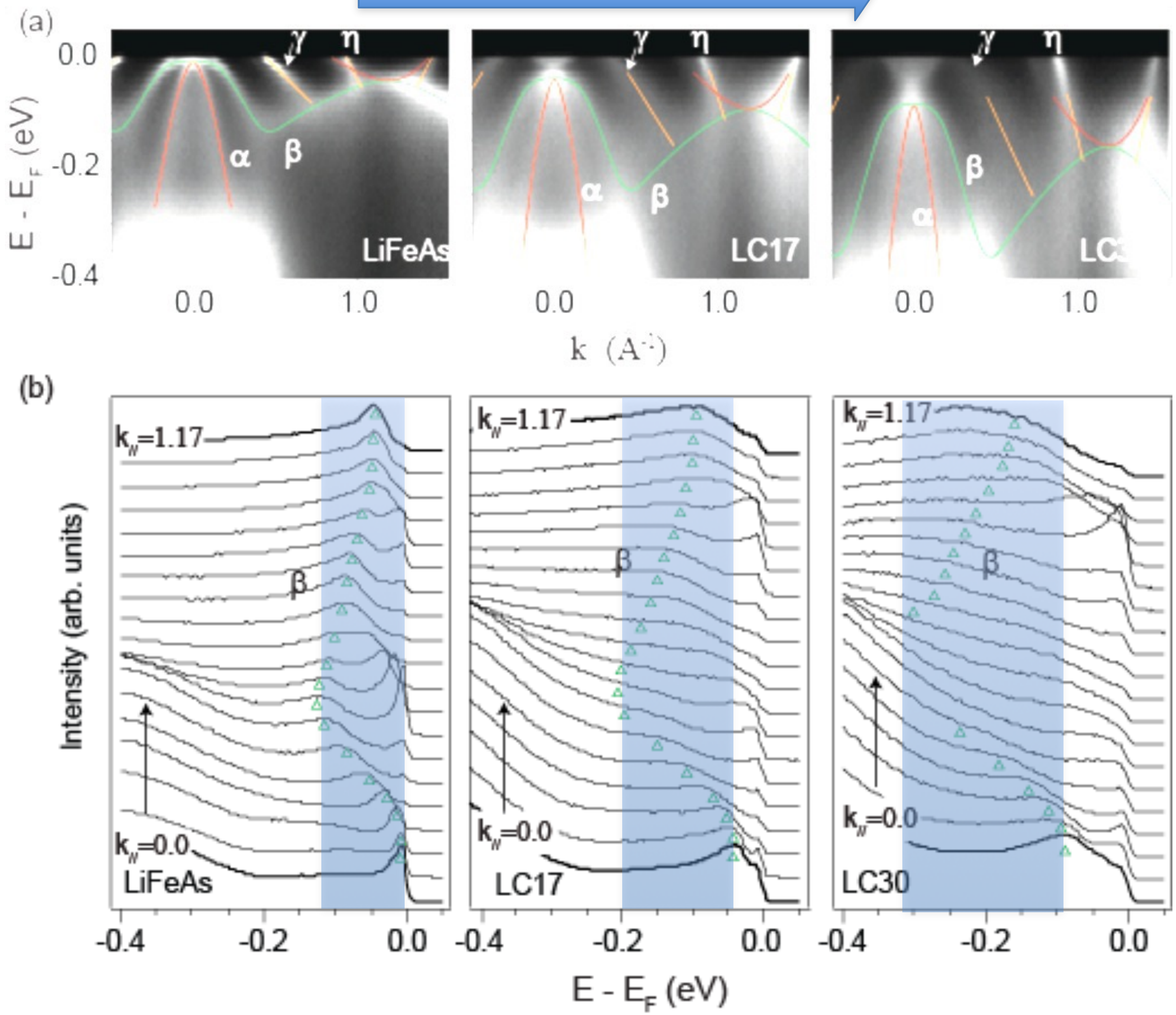
•Direct observation of quasiparticle mass divergence at bandwidth-control Mott transition

H. C. Xu, DLF et al. Phys. Rev. Lett. 112, 087603 (2014).

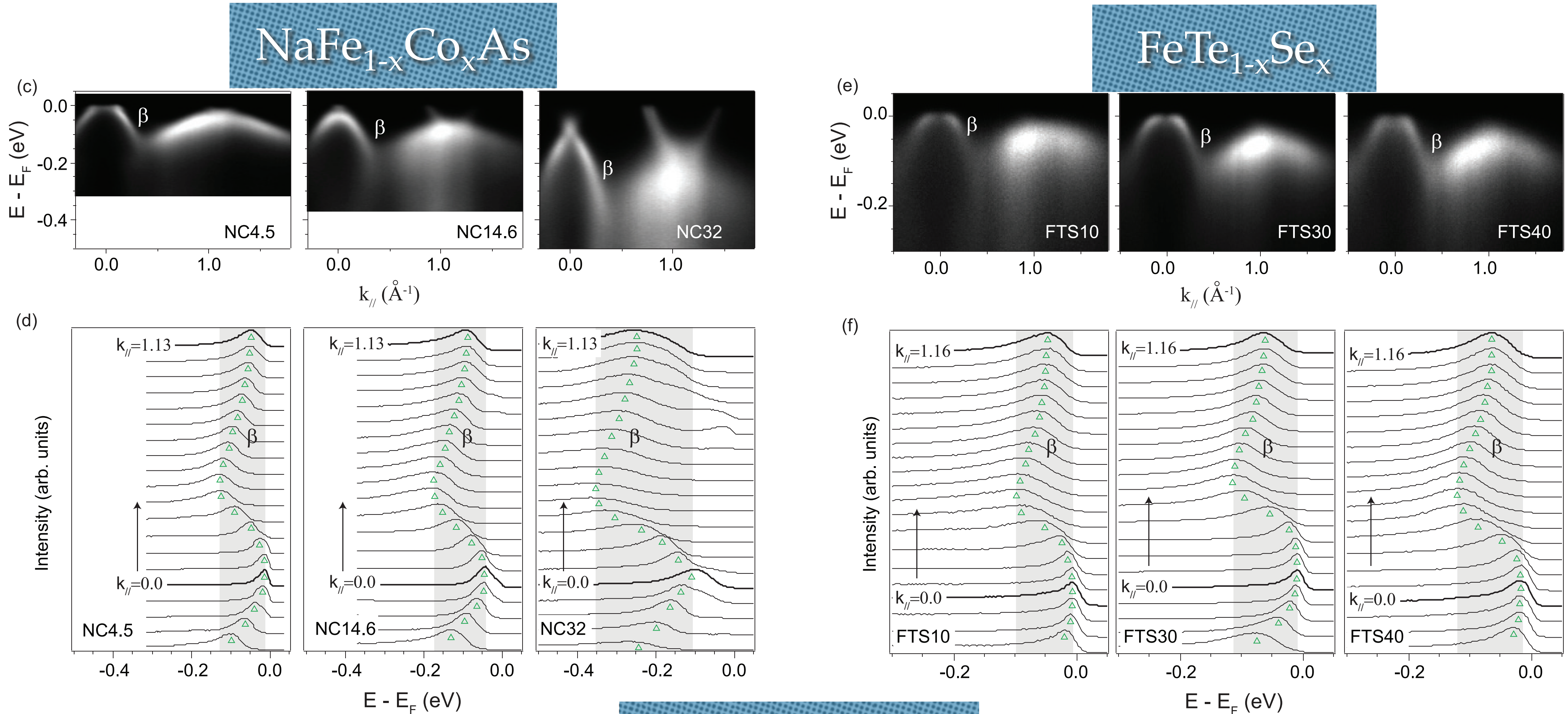
3. Bandwidth, electronic correlations

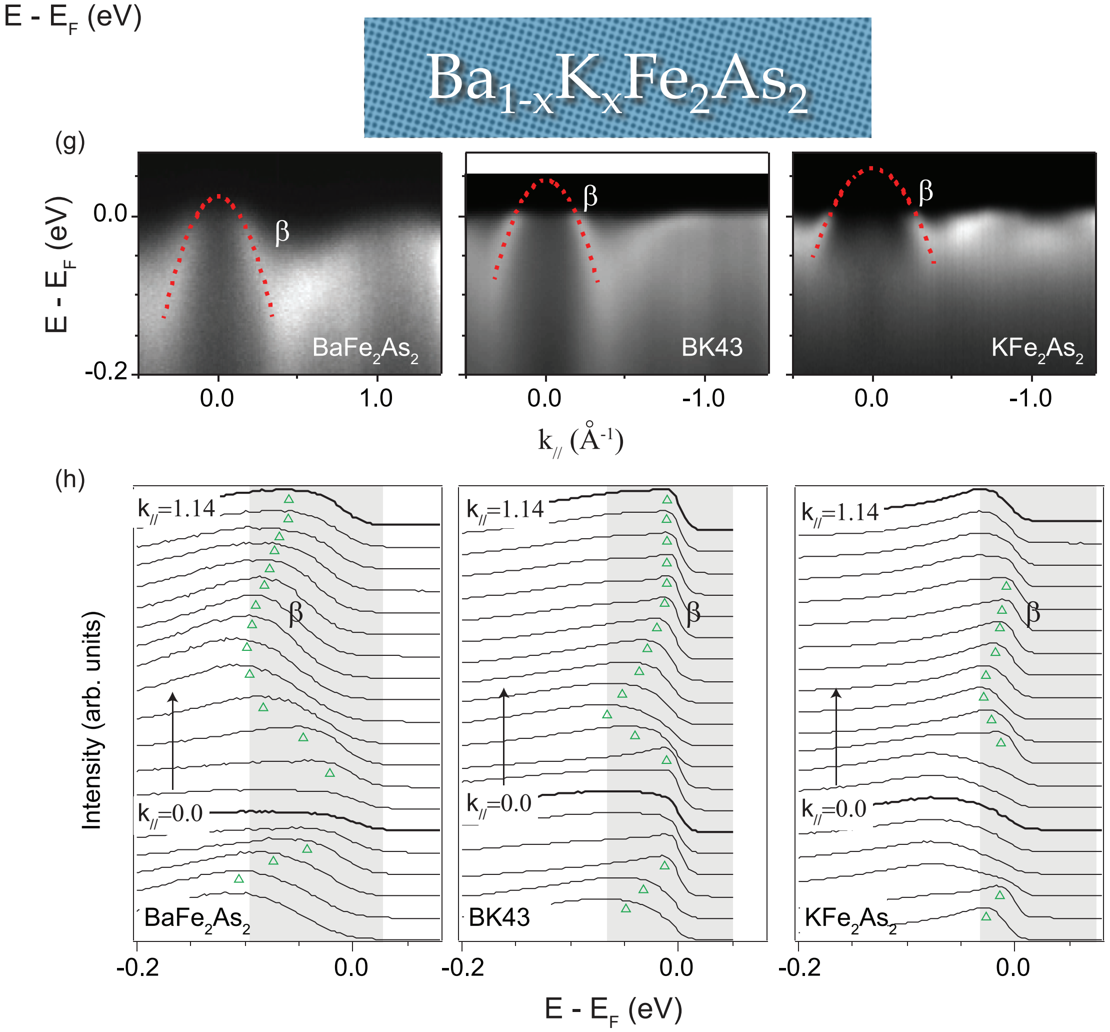
$LiFe_{1-x}Co_xAs$

Co doping

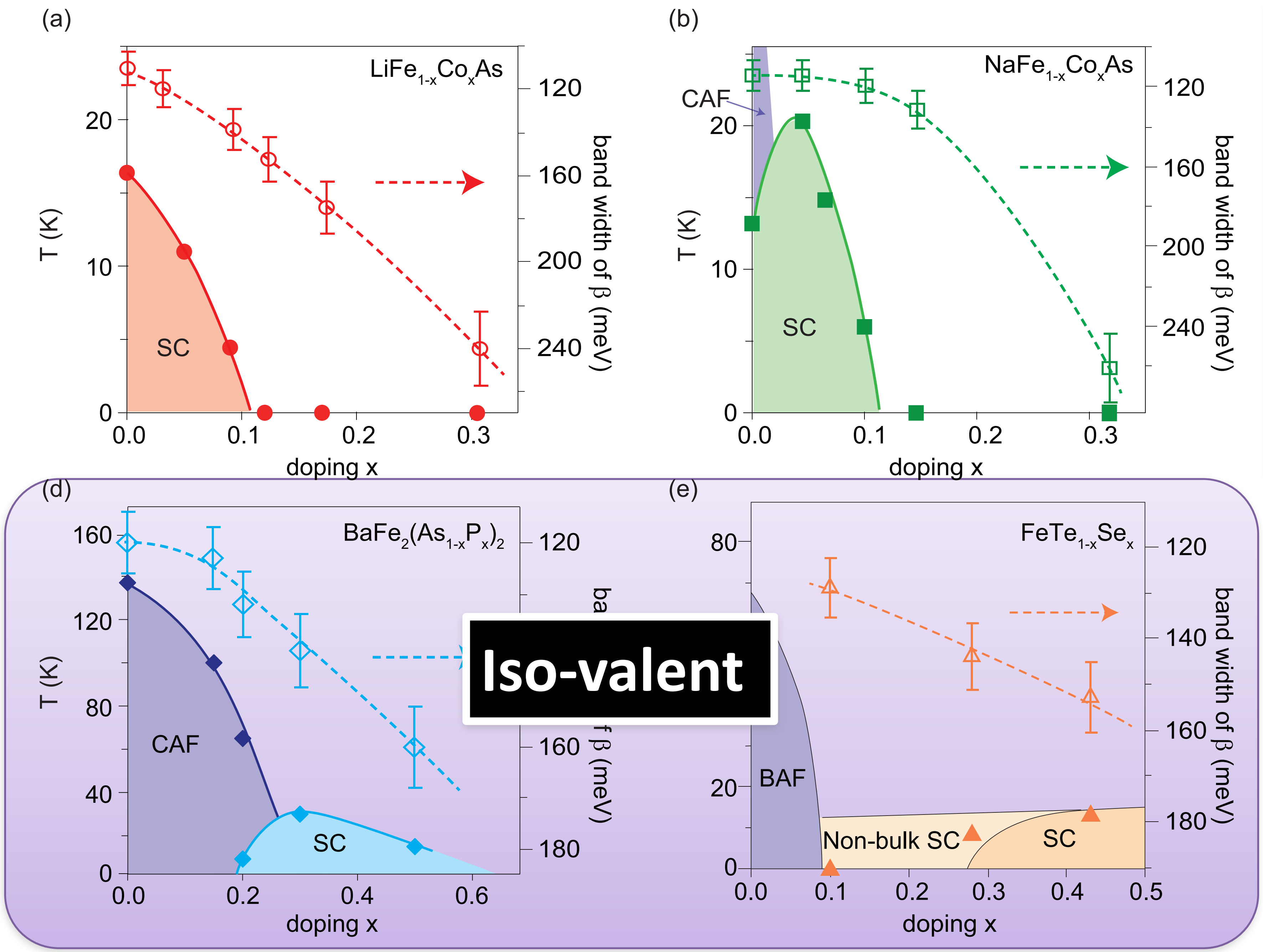


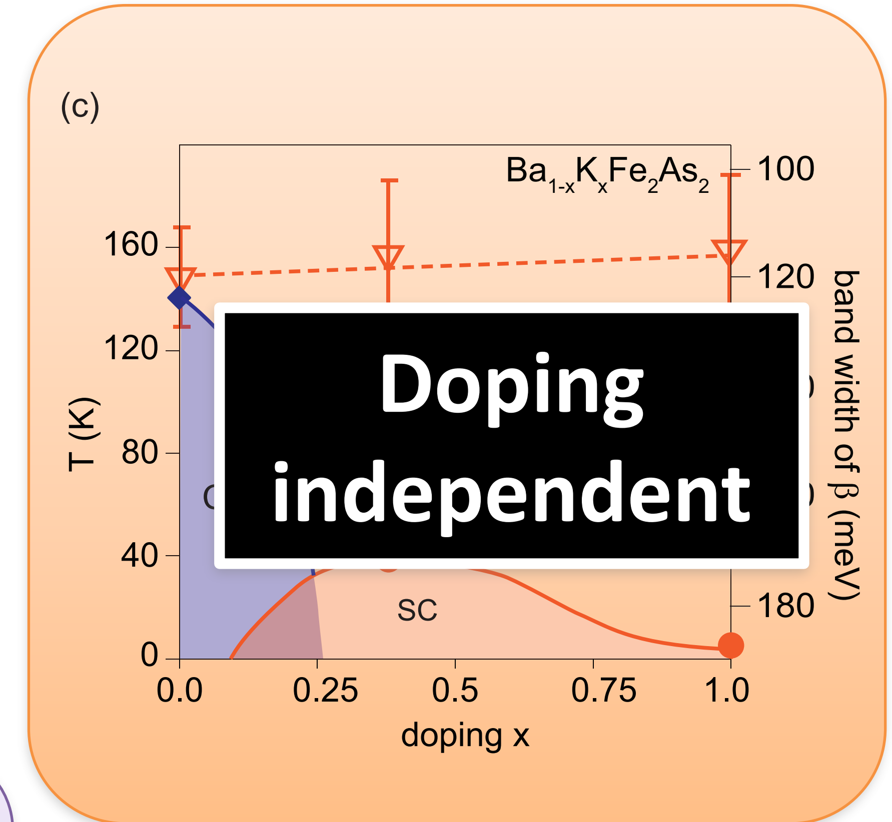
With doping, the bandwidth is increased equally for all the bands.





The same analysis on the doping evolution of the bandwidth of β was extended to $NaFe_{1-x}Co_xAs$, $FeTe_{1-x}Se_x$, and $Ba_{1-x}K_xFe_2As_2$.





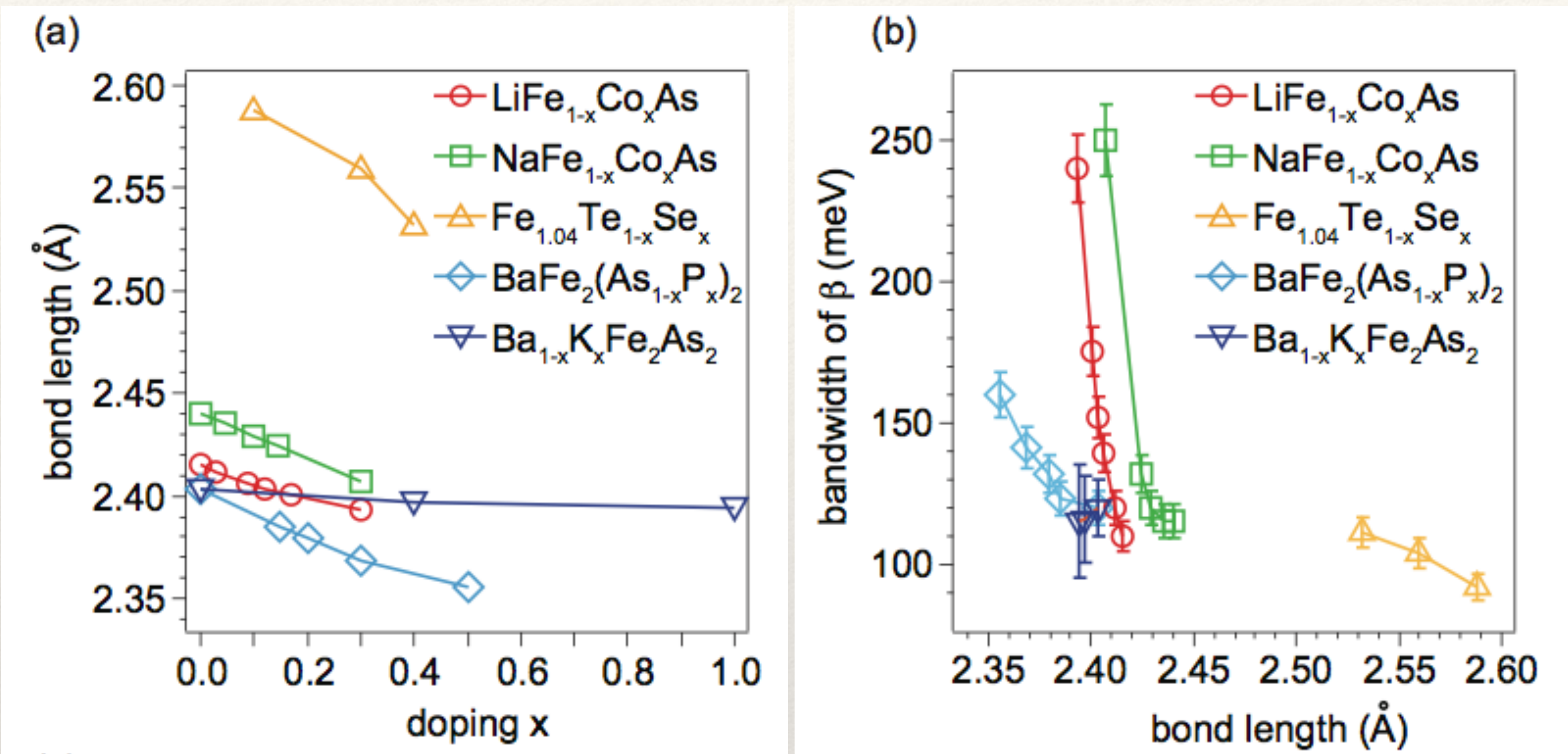
The suppression of the electronic correlation is universal for all systems except for $Ba_{1-x}K_xFe_2As_2$.

What are the causes for the change of correlation ?

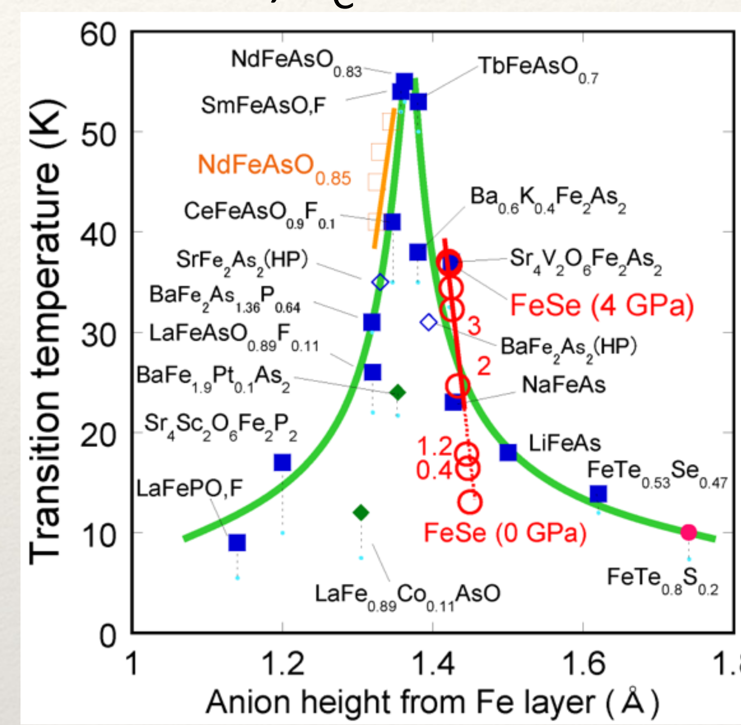
Carrier doping ?

Lattice ?

Bond length and bandwidth



H=1.38A, T_C the maximum



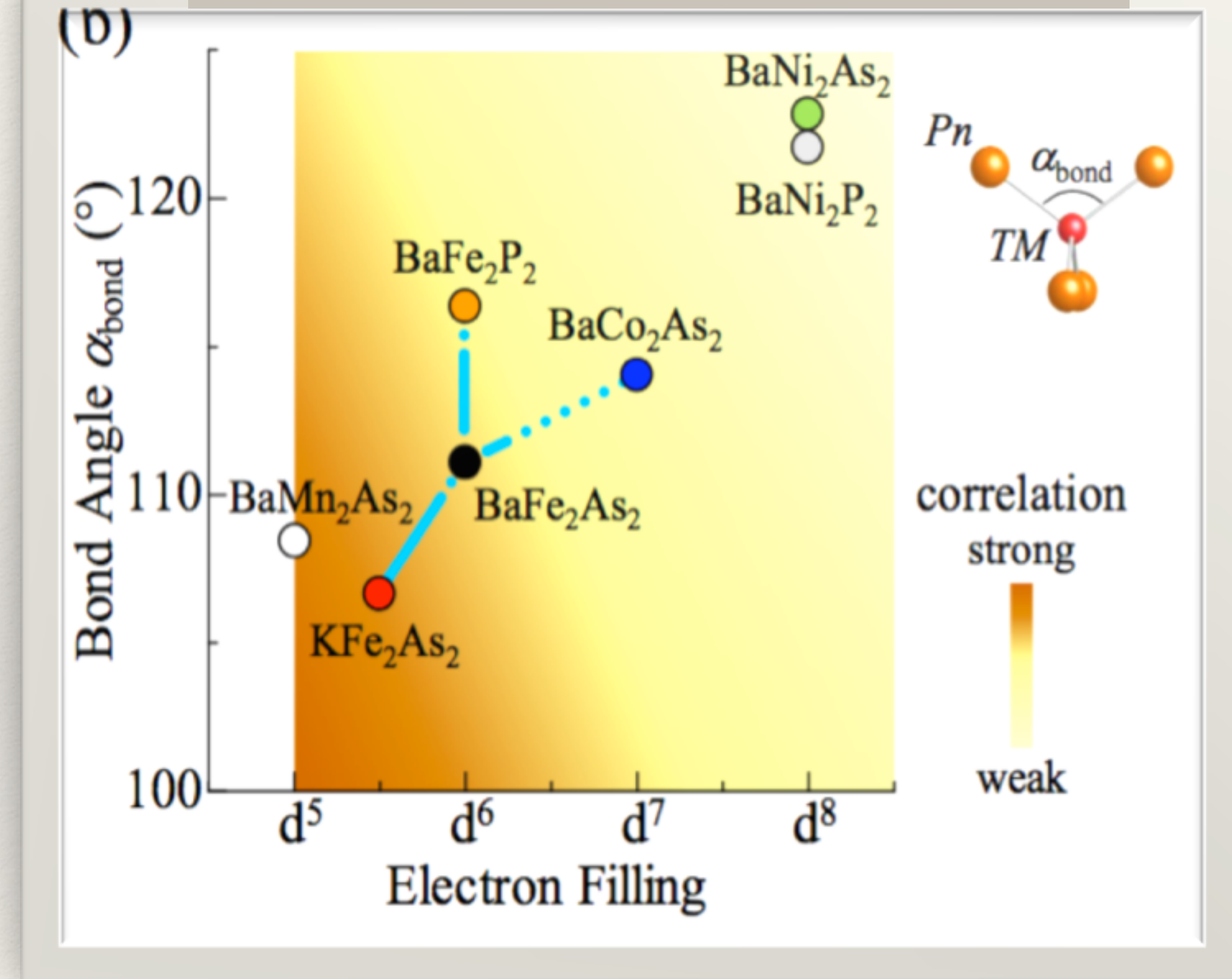
Y. Mizuguhci et al., arXiv:1001.1801v2

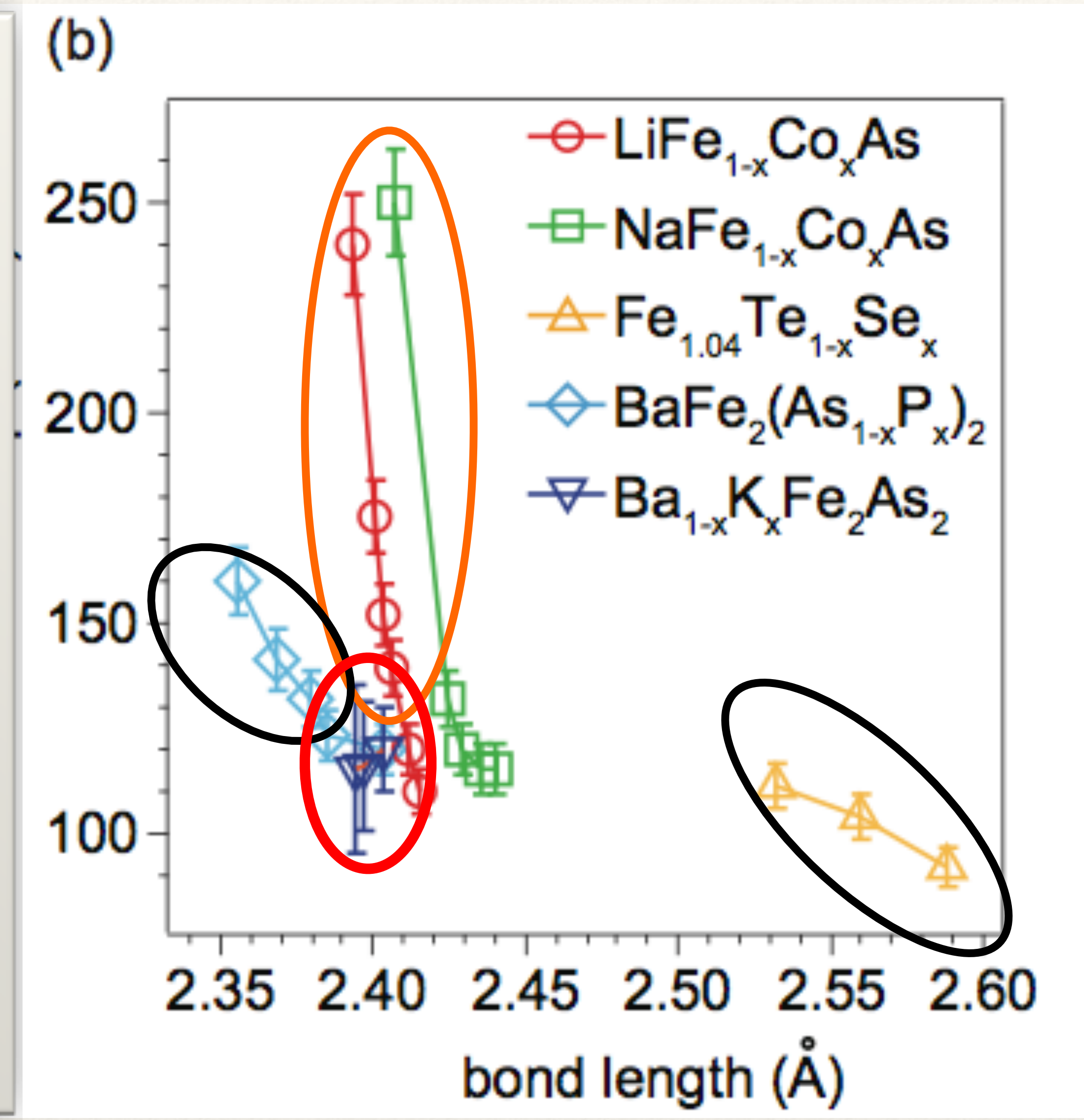
- **Lattice structure (chemical pressure) plays an important role in the bandwidth evolution.**
- **Partially explains the bandwidth change.**
- **Relates the electronic structure, structure, correlation, and Tc, which needs systematic numerical investigations, including bond angle etc.**
- **Physical pressure effects are likely due to the bandwidth change as well.**

Z. R. Ye, et al., arXiv, 1404.6716 (2014).

Particle-hole asymmetry

M. Nakajima, et al., arXiv, 1308.6113 (2013).

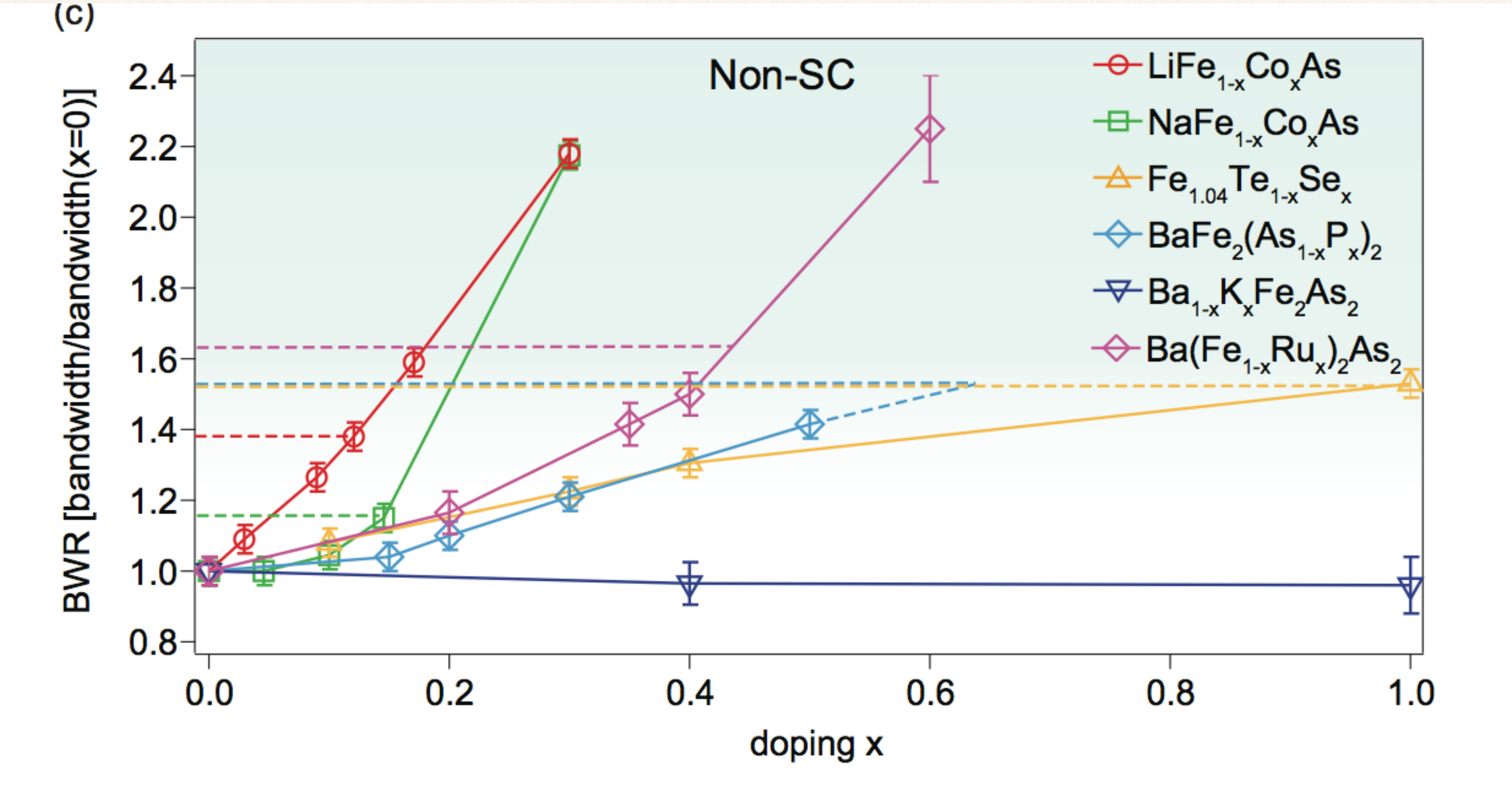




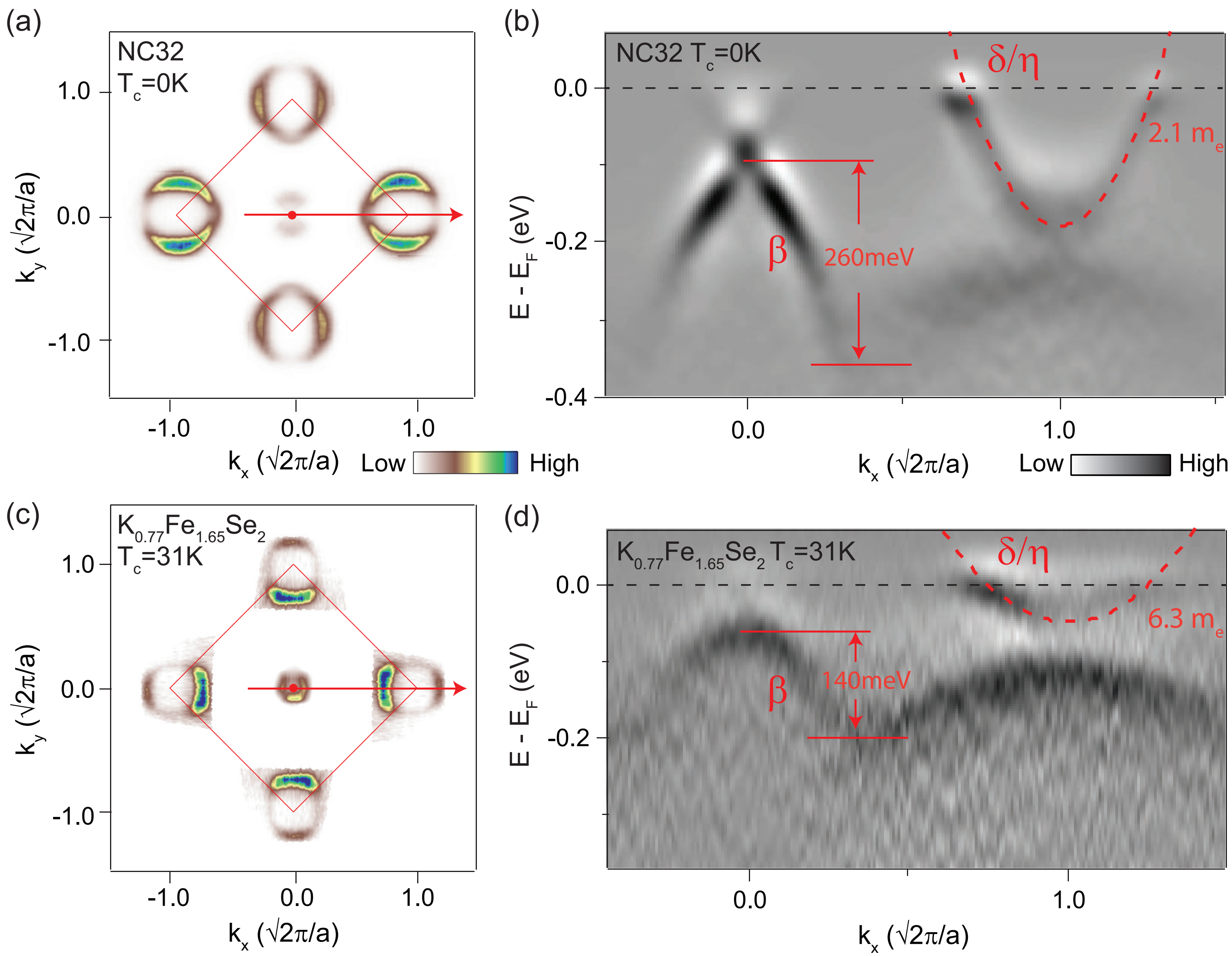
Co dopants: reduced bond length + reduced Hund's rule coupling

K dopants: hole doping drives system to $3d^5$ state, counter-balance the screening effect.

Critical role of bandwidth on SC



- **Ru doping increases bond length, however 4d electrons are more itinerant.**
- **bandwidth ratio (BWR) >~1.5, the SC disappears**



$NaFe_{1-x}Co_xAs$ (x=0.32), Tc=0K

$K_xFe_{2-y}Se_2$, Tc=31K

- The J1-J2-… local interactions seem to be arguably dominating pairing. (Hu, Lee, Ding among many others)
- Electronic correlation/bandwidth plays an important role on supporting the superconductivity in KFe_2Se_2.

What is more important for Tc ?

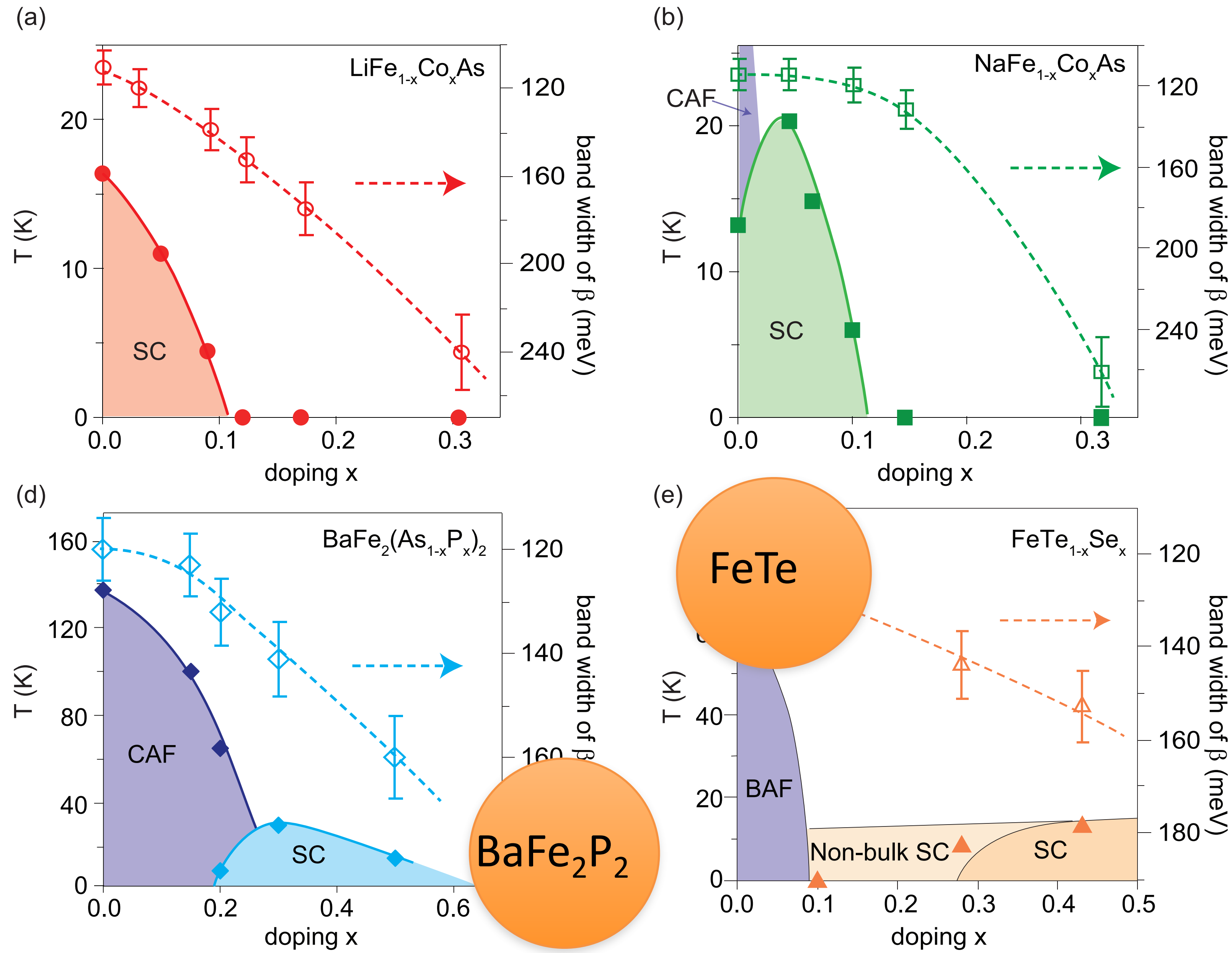
1. **Fermi surface**

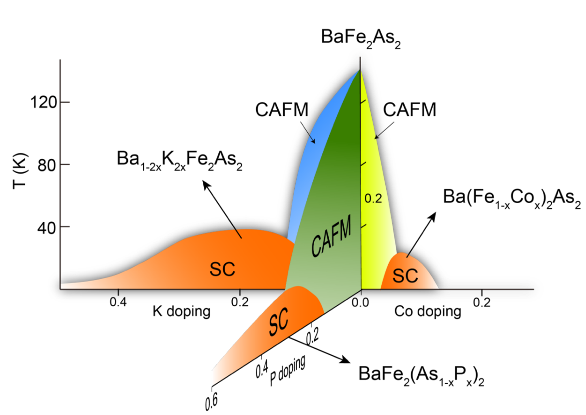
Play a secondary role

2. **Electronic correlation**

Moderate strength

3. **Impurity scattering**



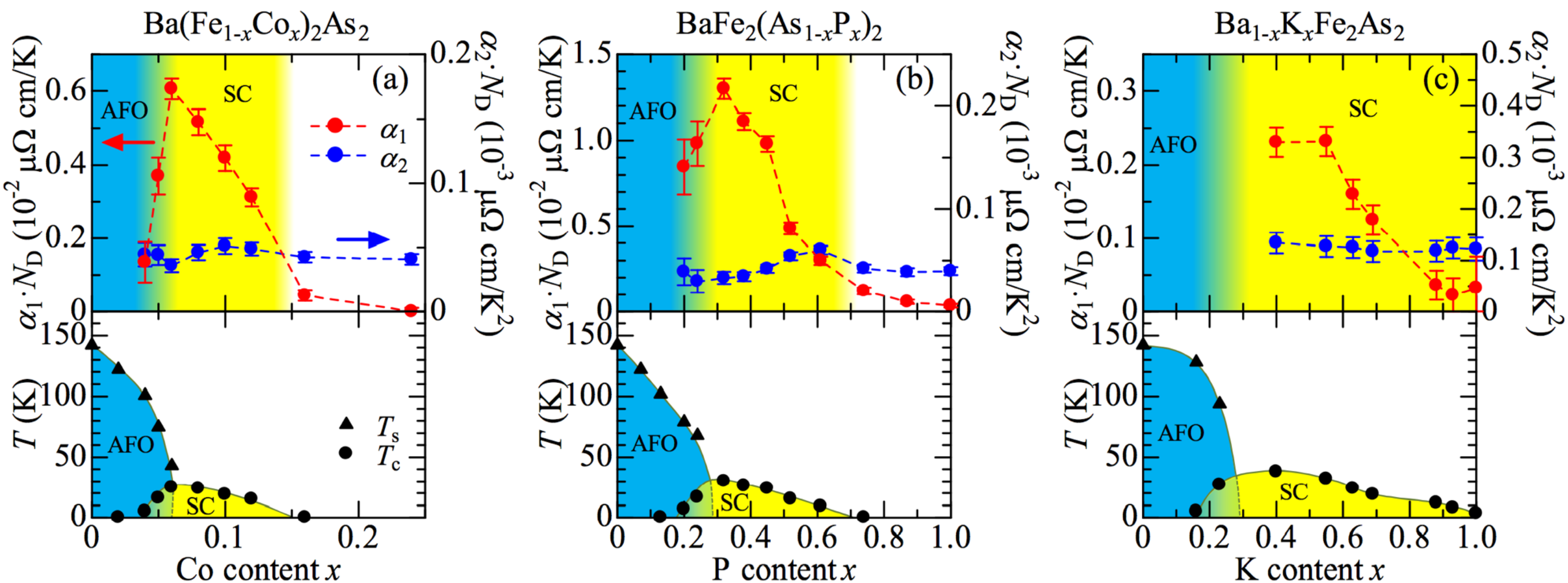


Too strong correlation: bad metal, form magnetic or orbital orderings. (FeTe)

Too small correlation: normal metal. ($BaFe_2P_2$)

Correlations matter

$$1/\rho(T) = 1/(\rho_0 + \alpha_1 T + \alpha_2 T^2) + \sigma_{\text{in}}$$



M. Nakajima et al. Arxiv/1308.1633 (S. Uchida group)

What is more important for Tc ?

1. Fermi surface

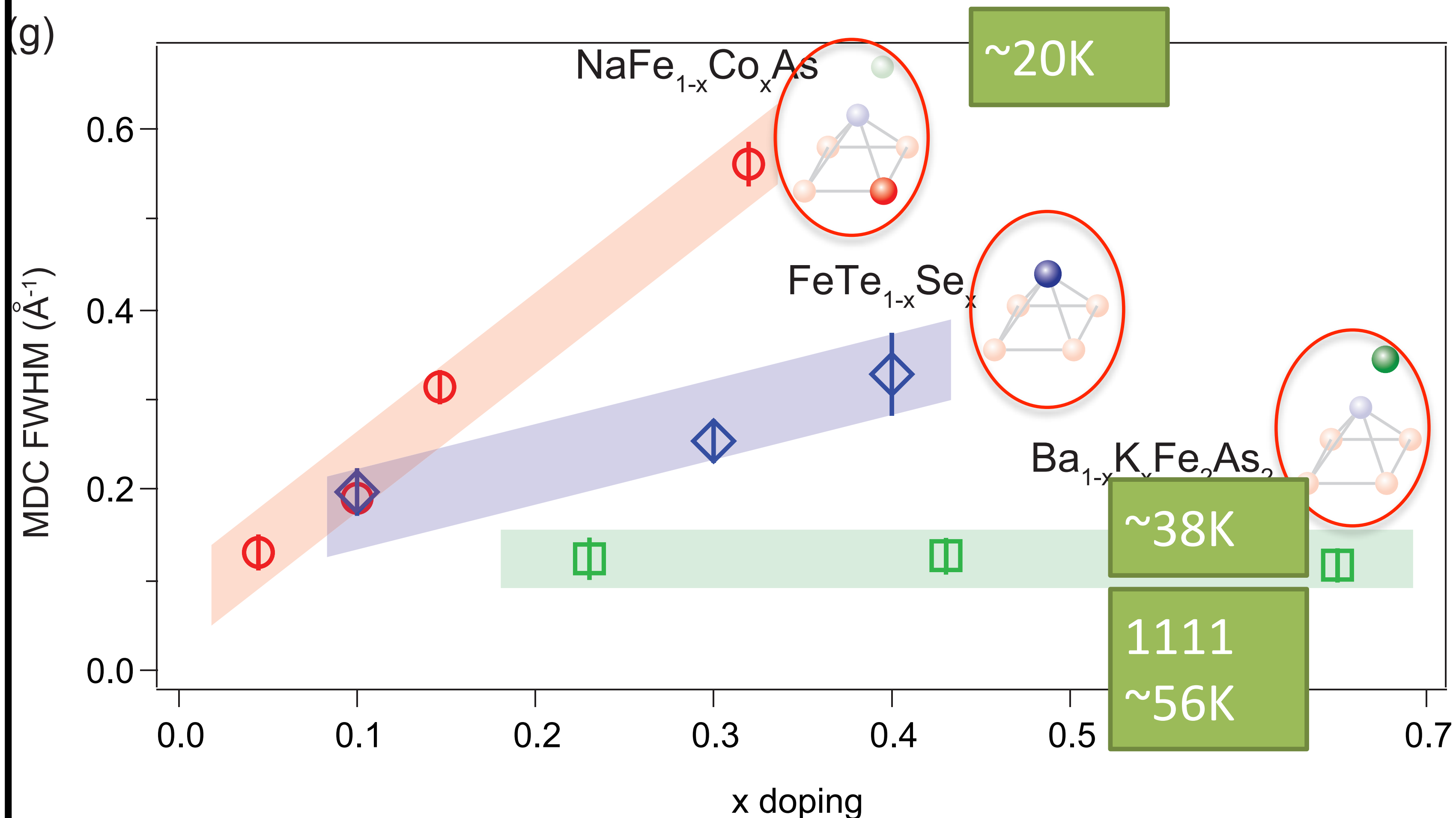
Play a secondary role

2. Electronic correlation

Moderate strength

3. Impurity scattering

Minimum impurity in iron-anion layer



The site dependence could understand different optimal Tc's in different iron-based systems.

What is more important for Tc ?

1. **Fermi surface**

   Play a secondary role

2. **Electronic correlation**

   Moderate strength

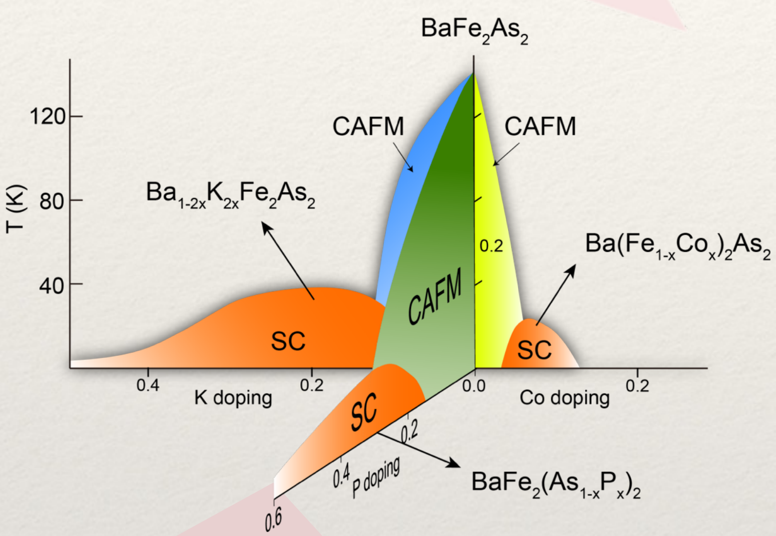
3. **Impurity scattering**

   Minimum impurity in iron-anion layer

a direction to increase Tc

Conclusion

Likely dominating



Cause the diversity and complexity

Band width

- The real universal electronic parameter
- Origin: lattice change and carrier type.
- Moderate bandwidth for maximum Tc.
- BWR>1.5, Tc disappear.
- Reflects interaction strength, DOS@EF etc.

Doping

Scattering

- Band-selective.
- Site-dependent.

Fermi surface

- Large diversities.
- Do not directly correlate with Tc.
- Plays a secondary role