Respective roles of electrons and holes in the transport properties of pnictides

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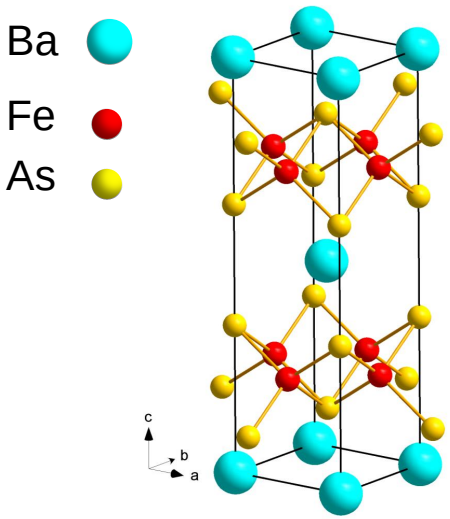
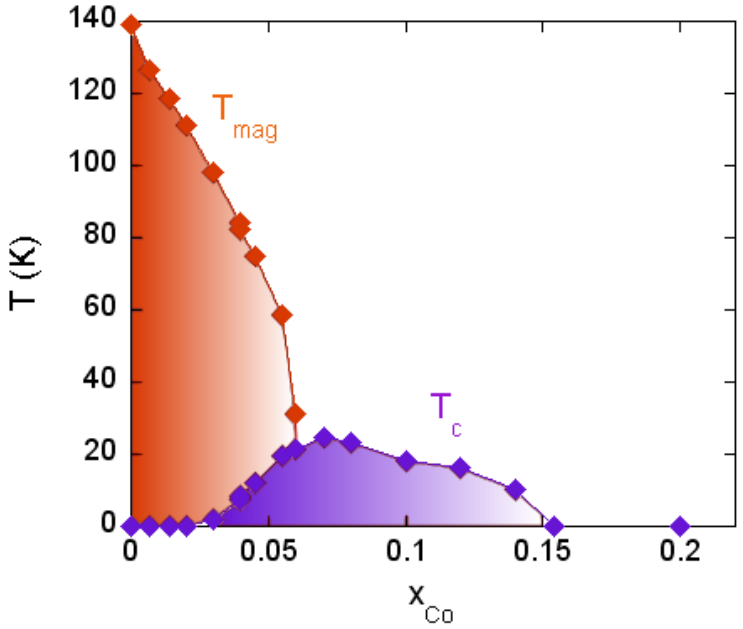




F. Rullier-Albenque et al. PRL 103 (2009)
V. Brouet et al., PRB 80 (2009)
Y. Laplace et al., PRB 80 (2009)
EPJB (2009)

B. Mansart et al. PRB 80 (2009)
L. Chauvière et al., PRB 80 (2009)
P. Bonville et al., arxiv 1002.0931

Outline

- The *"122" phase: $BaFe_2As_2$: electron doped* $Ba(Fe_{1-x}Co_x)_2As_2$

- Analysis of the transport properties of $Ba(Fe_{1-x}Co_x)_2As_2$

  Resistivity and Hall effect

  Carrier content, scattering processes and magnetic transitions

- Isovalent substitution : $Ba(Fe_{1-x}Ru_x)_2As_2$:

  Contribution of holes and electrons to the transport properties

- Summary

122 Phase : $BaFe_2As_2$

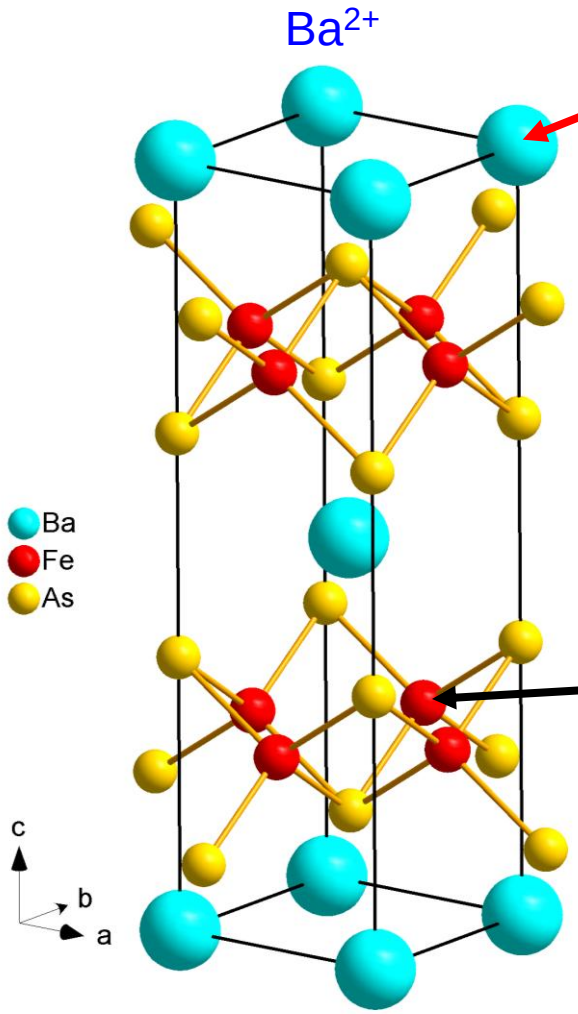
Possibility to get large single crystals

$BaFe_2As_2$

Tetragonal (I4/m m m)
a= 3,9625(1) Å
c= 13,0168(3) Å

Ba-As: 3,38 Å
Fe-As: 2,40 Å
Fe-Fe: 2,80 Å
As-Fe-As: 111,1 et 108,7°

Rotter et al., PRL 2008



Hole-doped
T_c^{max} =36K

Ru on Fe site
P on As Site

Isovalent substitution

Co : $3d^7$ **Rh : $4d^7$**
Ni : $3d^8$ **Ir : $5d^9$**

Electron-doped
T_c^{max} =25K

122 Phase $BaFe_2As_2$: crystal growth

Self flux method

a)
$$Fe + As \xrightarrow{800°C} FeAs$$
$$Fe + Co \xrightarrow{700°C} CoAs$$

b)
Ba + FeAs, with excess of CoAs
↓
$Ba(Fe_{1-x}Co_x)_2As_2$

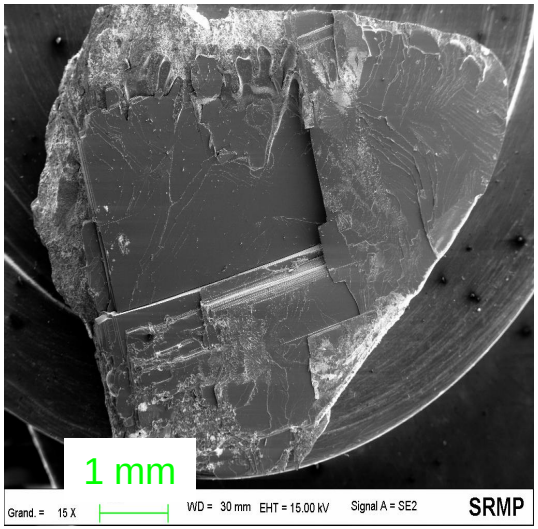
Weighing and mixing in a glove box under Ar atmosphere : ~2 g powder, Al_2O_3 crucibles

Synthesis in quartz tubes, sealed under vacuum

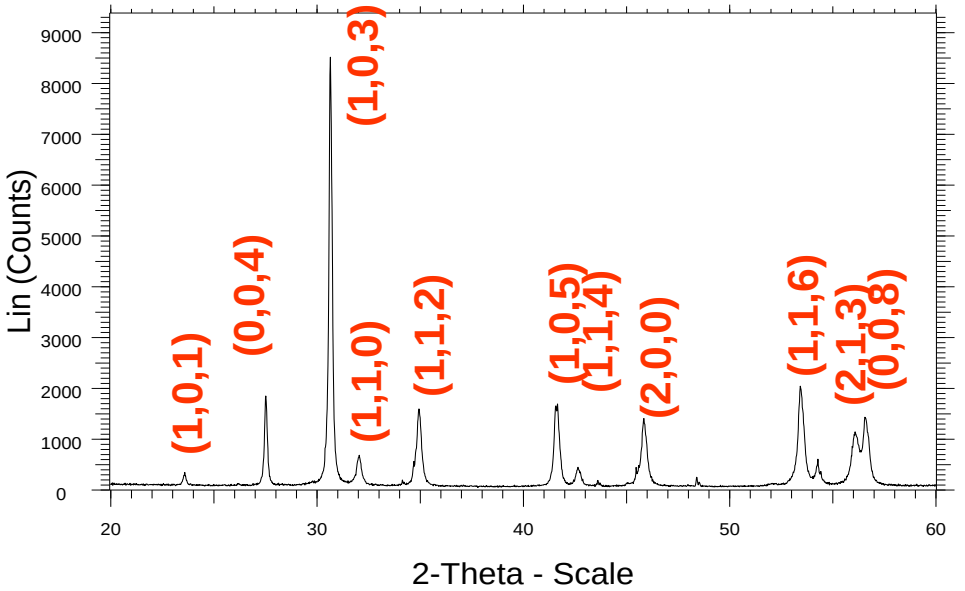
Kept at 1180°C for 4h and cooling at 5°C/h ⟶ 1000°C for 6h

Cooled down to room T

Mechanical extraction of platelets single crystals,



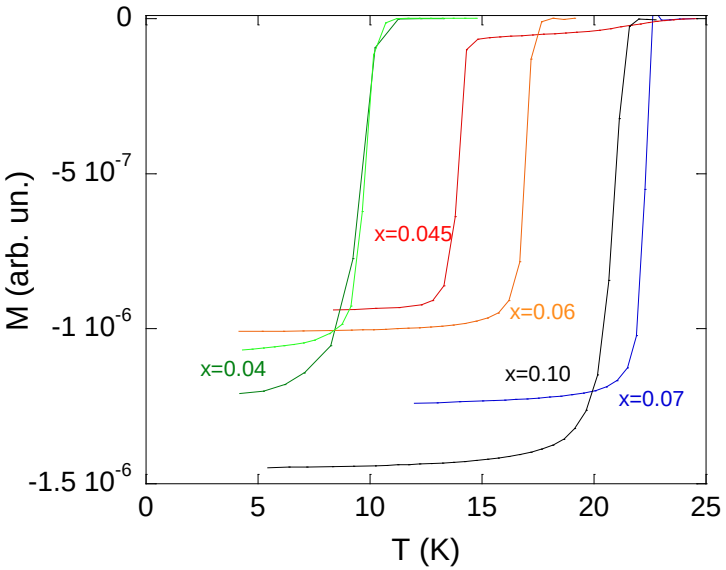
RX diagram



Co-doped: $Ba(Fe_{1-x}Co_x)_2As_2$

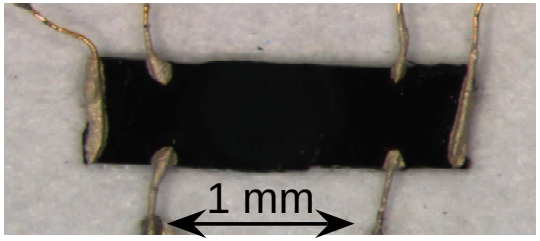
Co content determined by wave length dispersive X-ray spectroscopy

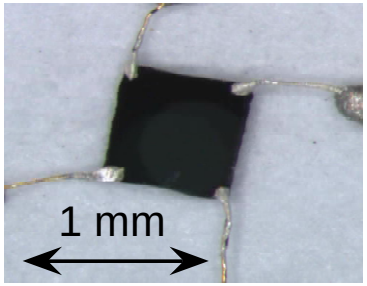
$0 \leq x \leq 0.3$ With a precision of 10%

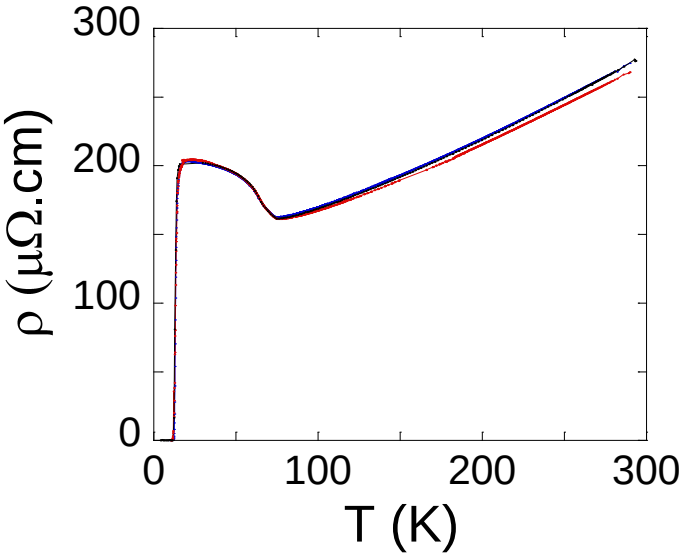


Resistivity and Hall effects measurements

Thickness between 10 to 30 μm



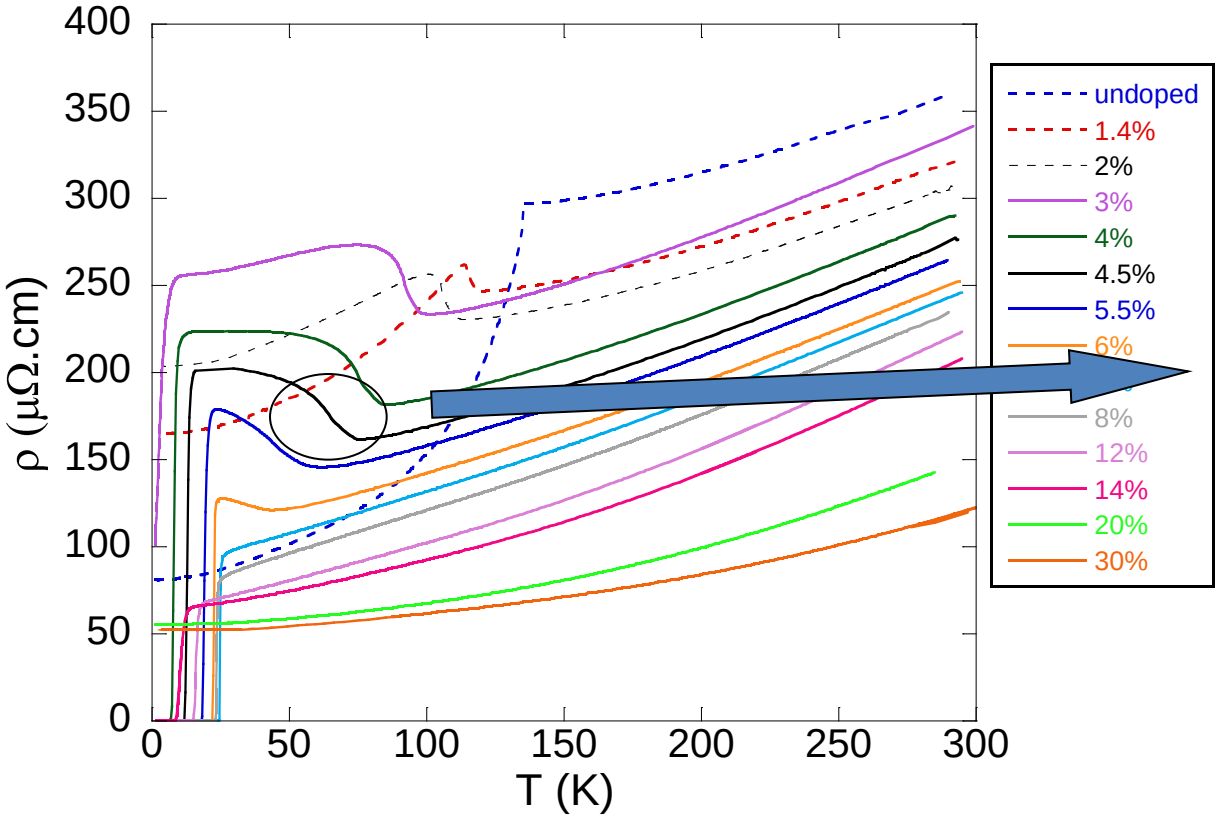




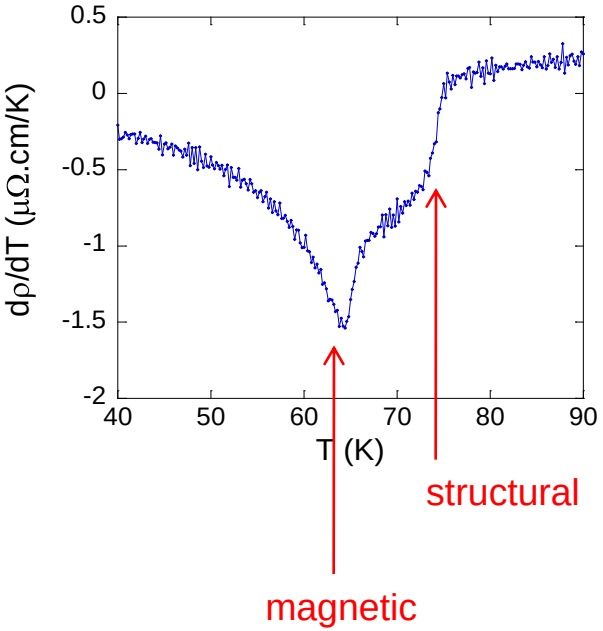
Good reproducibility of the measurements
Absolute values of the resisitivity

Resisitivity curves all over the phase diagram

Co-doped: $Ba(Fe_{1-x}Co_x)_2As_2$



Structural and magnetic transitions

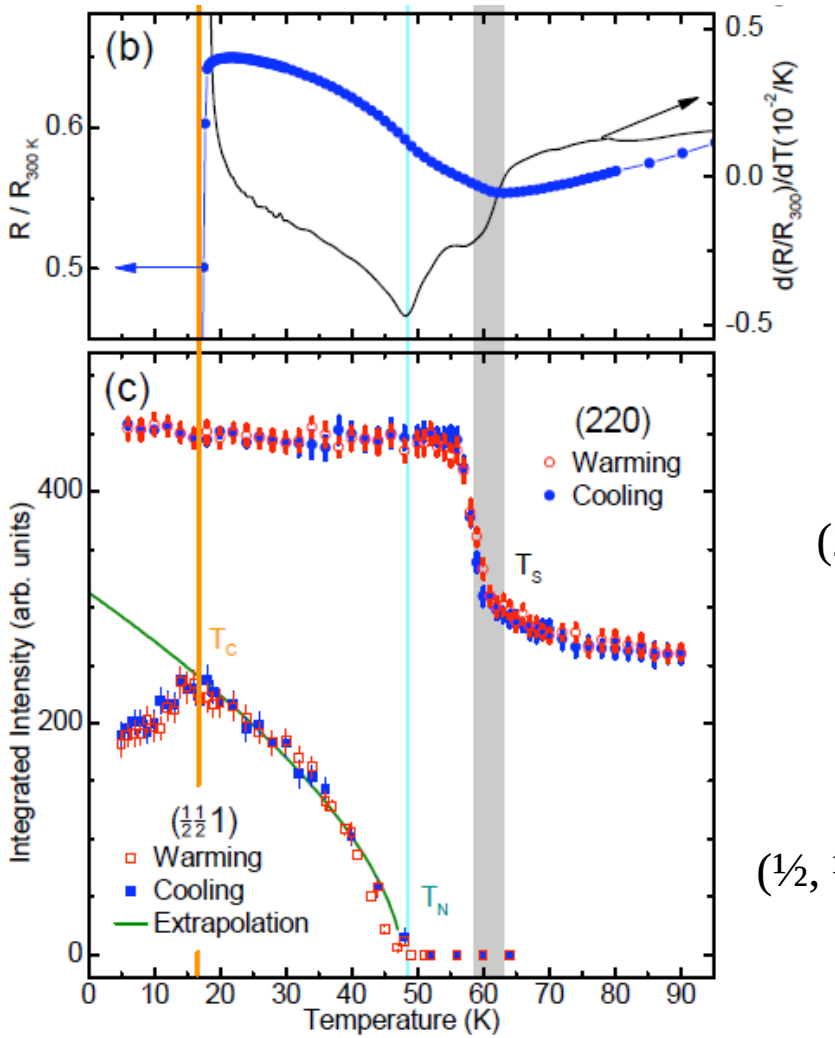


Very homogeneous samples

See also Y. Laplace et al., EJPB (2009)

Structural and magnetic transitions

$Ba(Fe_{0.953}Co_{0.047})_2As_2$

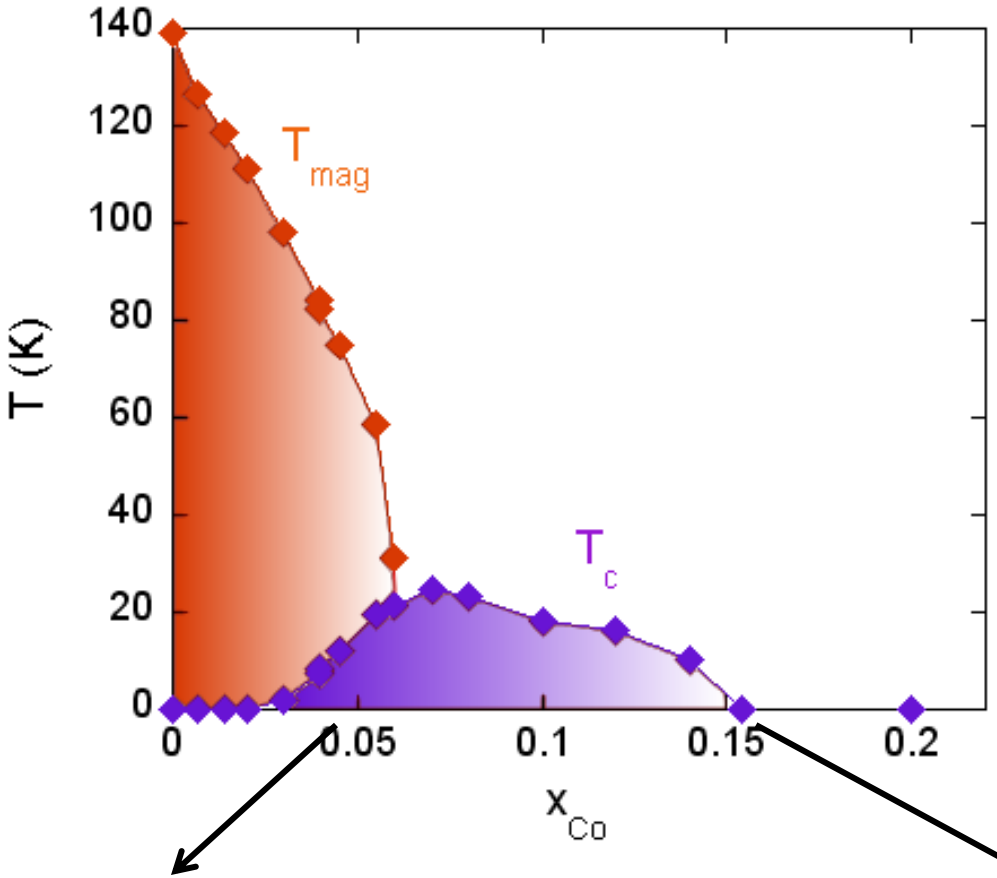


(220) nuclear reflection

(½, ½,1) magnetic reflection

D.K. Pratt et al., PRL (2009)

Phase diagram of $Ba(Fe_{1-x}Co_x)_2As_2$



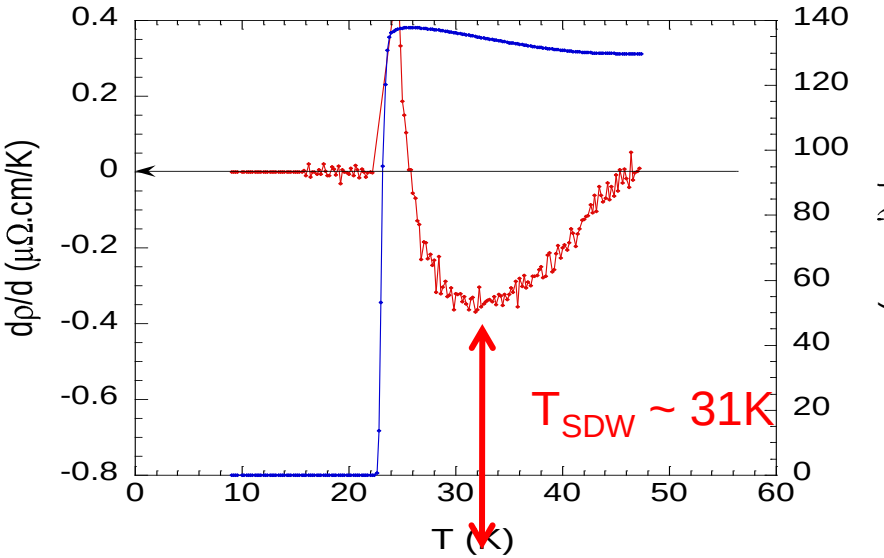
3% < x < 7% coexistence magnetism and superconductivity

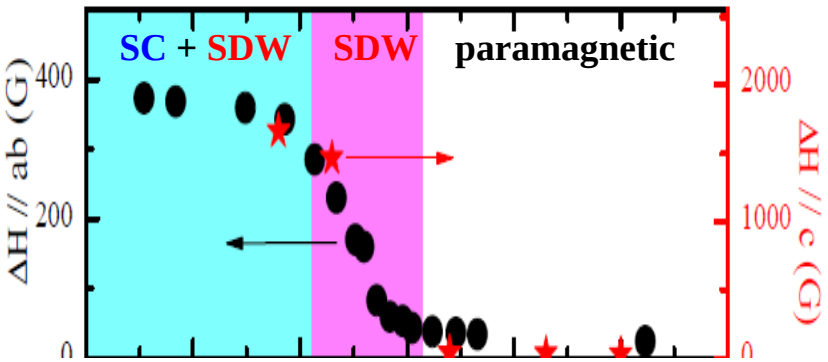
$T_c = 0$ for x > 15.5%

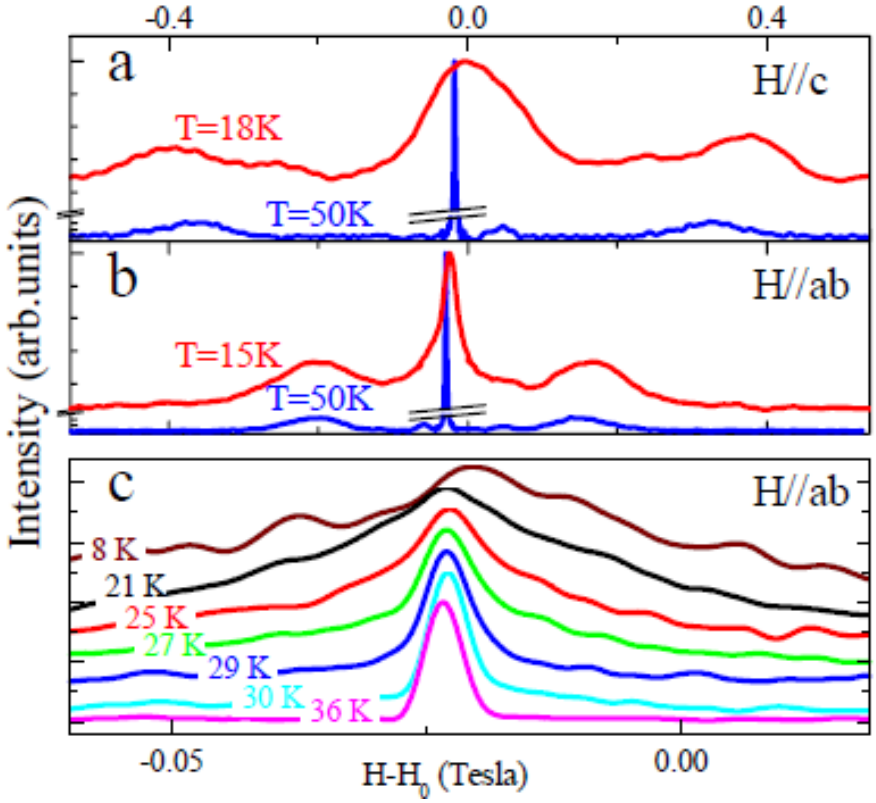
Coexistence of superconductivity and magnetism at the atomic scale

NMR on single crystal with 6%Co

Y. Laplace et al. PRB 80 (2009)





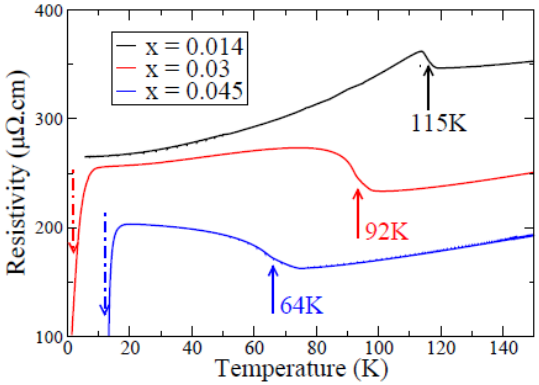


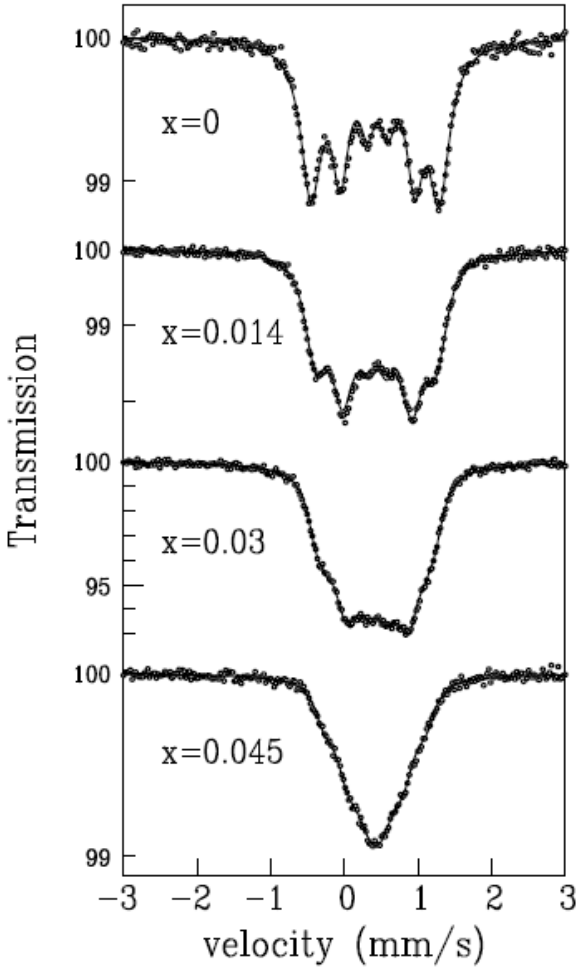
Incommensurate magnetic order

Very small deviation ε ~ 4%

Mössbauer spectroscopy - Incommensurate magnetic order

B. Bonville et al., arXiv 1002.0931





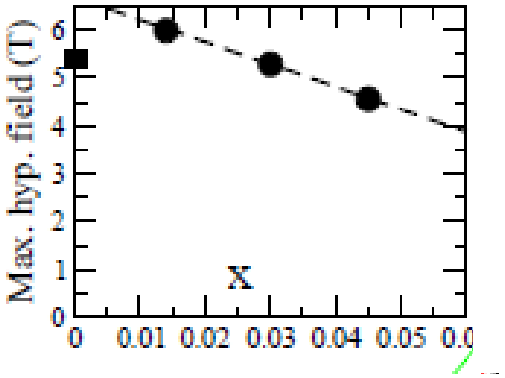
Single magnetic hyperfine pattern

6 lines

H_{hf} ~ 5.4T

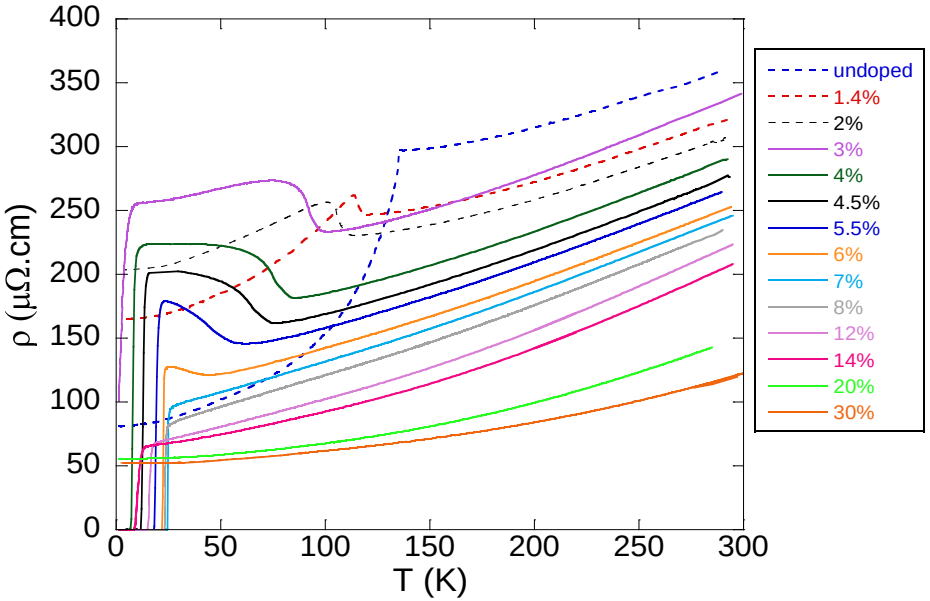
Distribution of hyperfine fields

Incommensurate modulated magnetic structure



This incommensurability has not be seen by neutron diffraction up to now.

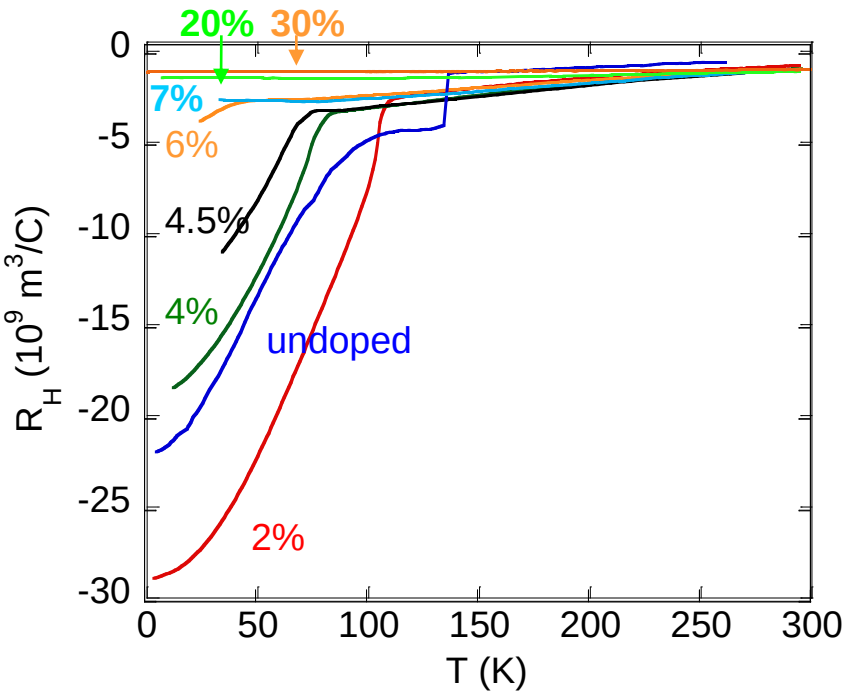
Resisitivity and Hall effect all over the phase diagram



$$\rho = \frac{m^*}{ne^2\tau}$$

Multiband system:

$$\sigma = \sigma_e + \sigma_h$$

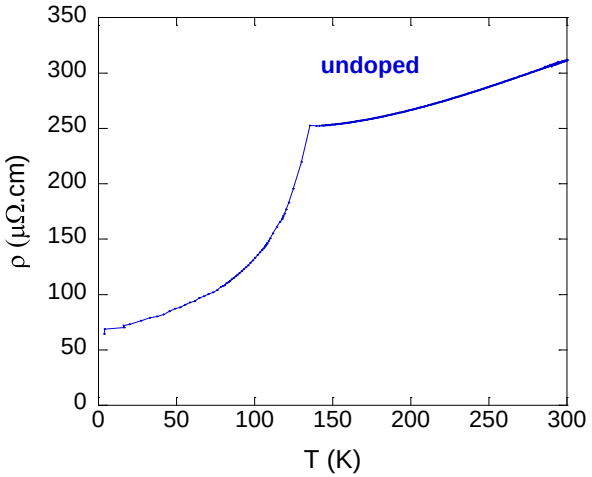


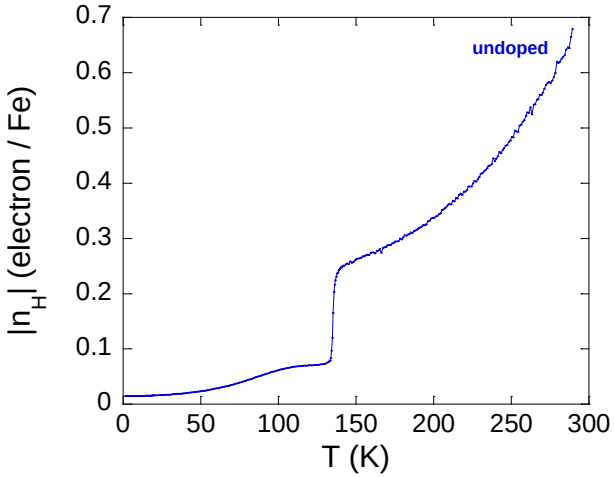
Drop in the absolute value of R_H at the magnetic transition.

R_H always negative

Transport dominated by electrons all over the phase diagram

Undoped compound $BaFe_2As_2$



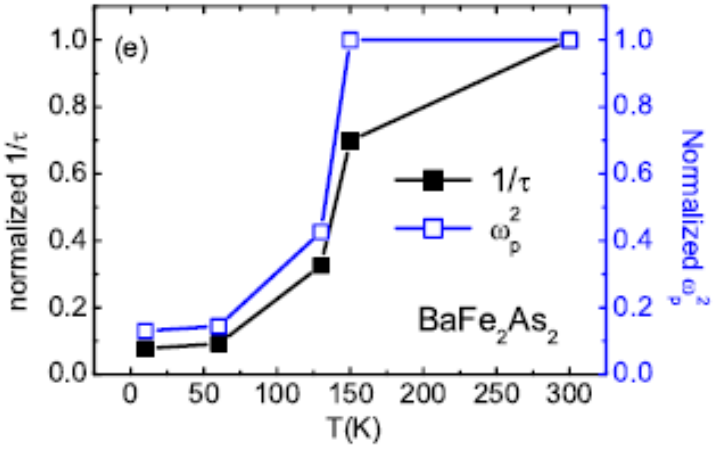


Double step
in the SDW transition

Drop of ρ attributed to a decrease of the scattering rate at T_{SDW}

Overcomes the reduction of carrier contents due to a partial gapping of the Fermi surface

Confirmed by optical measurements

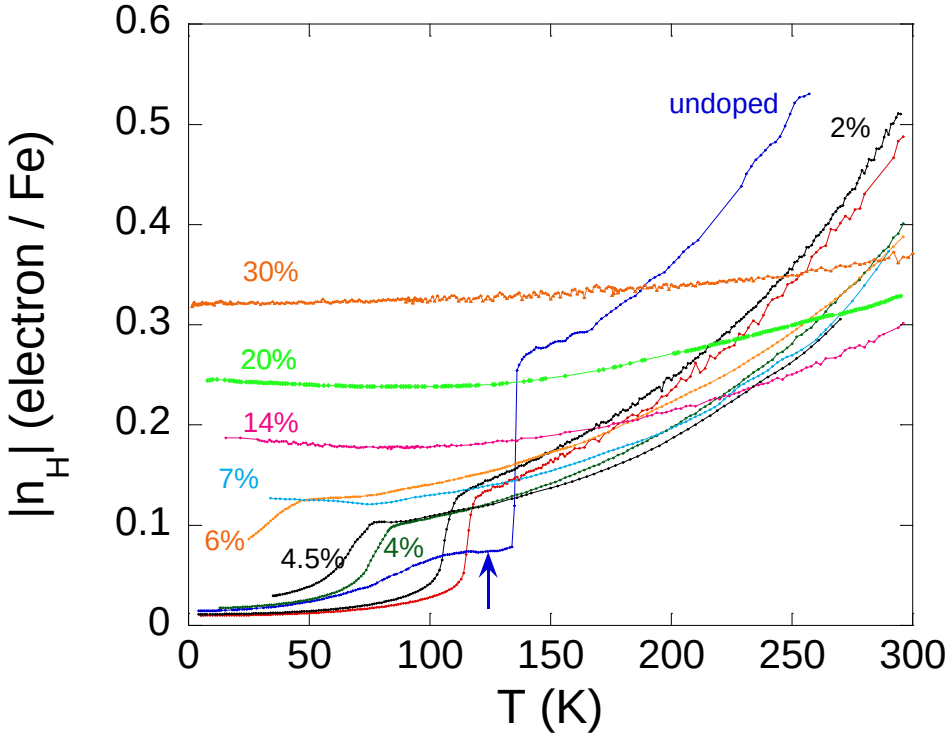


Reduction of the carrier content by a factor 8
Reduction of the scattering rate by a factor 13

This can account for a factor ~2 reduction of the resistivity

Hall effect measurements

$$|n_H| = \frac{1}{e|R_H|}$$



In a two-band model:

$$\frac{1}{n_H e} = R_H = \frac{-R_e\sigma_e^2 + R_h\sigma_h^2}{(\sigma_e + \sigma_h)^2}$$

electrons holes

$$R_e = \frac{1}{n_e e} \qquad R_h = \frac{1}{n_h e}$$

$|n_H|$ upper bound for n_e

4 unknown quantities:
n_e, n_h, σ_e, σ_h

But only 3 relations

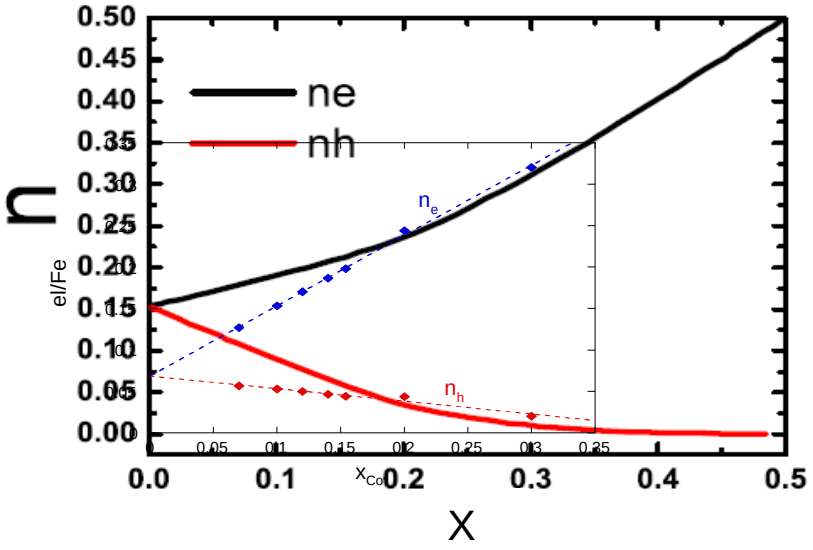
Conductivity: $\sigma = \sigma_e + \sigma_h$

Hall effect

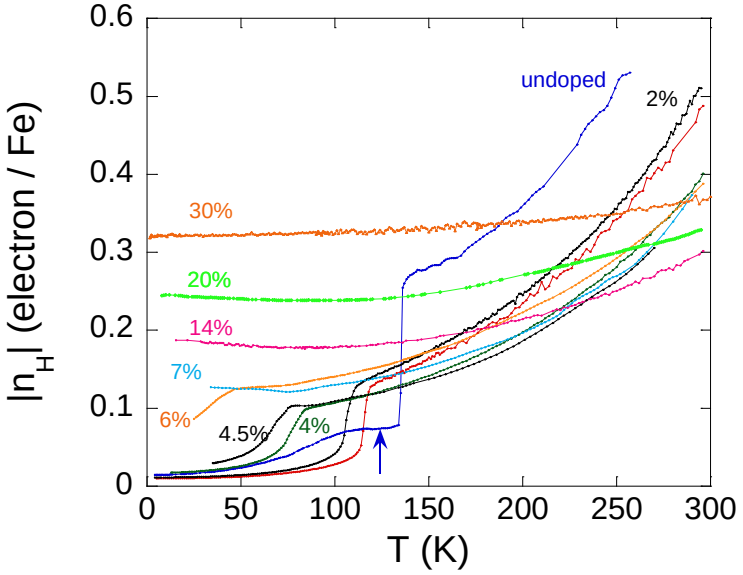
$$n_e = n_h + x_{Co}$$

Using LDA calculations to determine n_e and n_h

L. Fang et al., PRB 80 (2009)



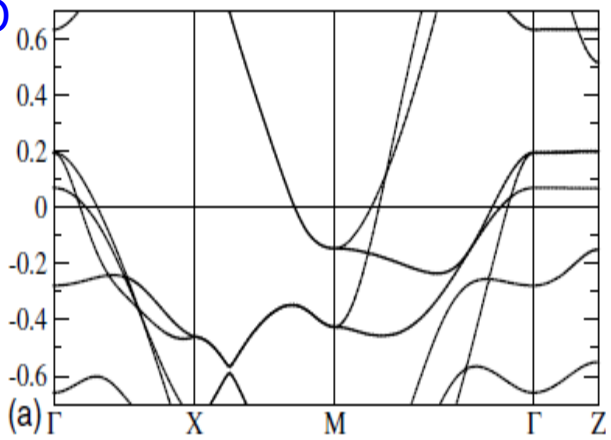
$|n_H|$ upper bound for n_e



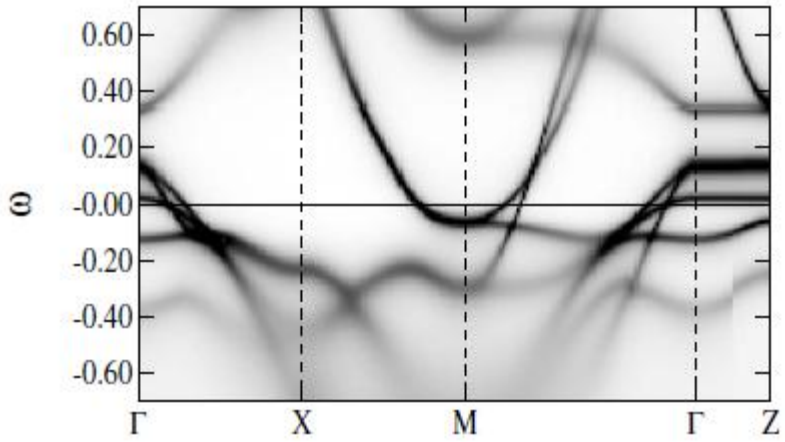
LDA calculations appear to overestimate the number of electrons and holes up to x~0.2

LaFeAsO

LDA



LDA +DMFT

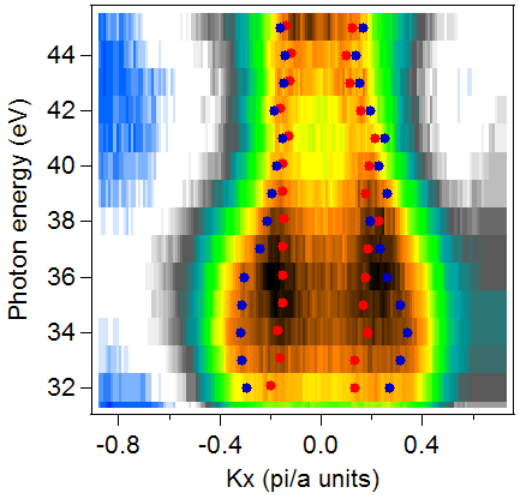


M. Aichhorn et al. PRB 80 (2009)

Using ARPES measurements to determine n_e and n_h

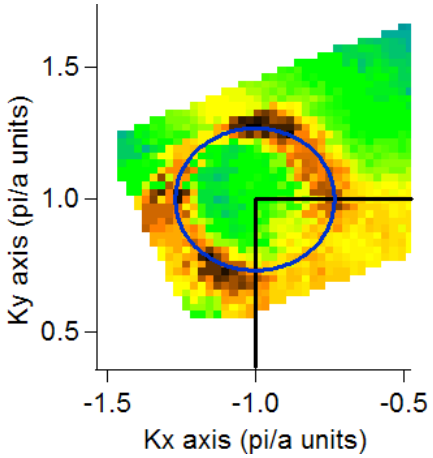
V. Brouet et al., PRB (2009)

Hole bands: two 2D, one 3D

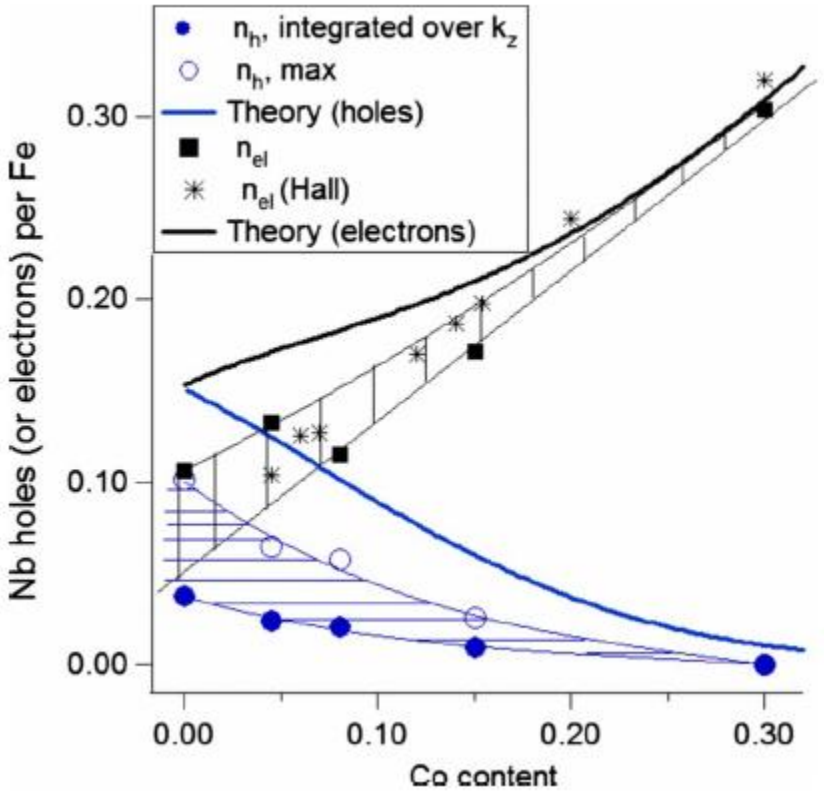


4% Co

2 degenerate electron bands: 2D



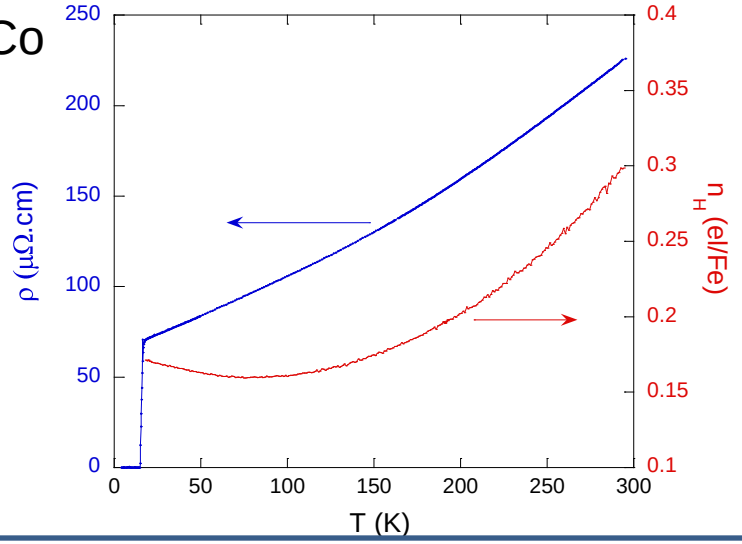
7% Co



Good agreement between ARPES and transport data

Analysis of resistivity and Hall effect in a two-band model with T independent n_e and n_h

10% Co

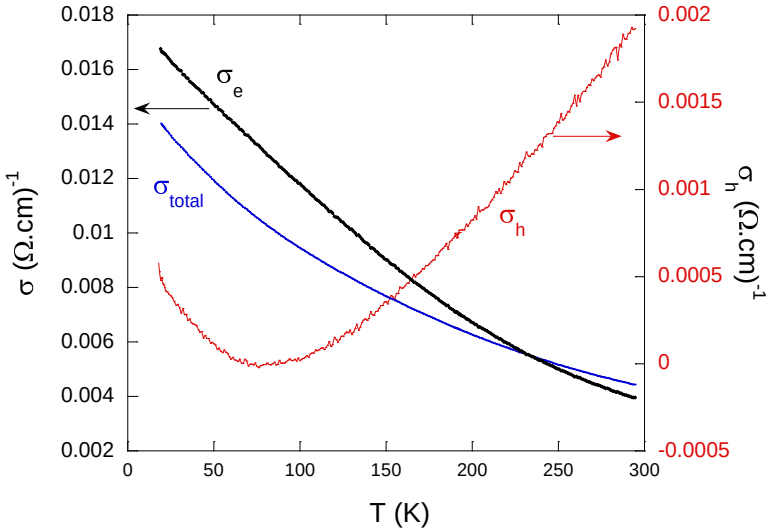


Minimal value of $n_H \approx n_e$

For large Co doping : $n_h << n_e$

$$n_H \approx n_e(1+2\frac{\sigma_h}{\sigma})$$

$$\sigma = \sigma_e + \sigma_h$$



Minimal value for σ_h

Mobility of the holes increases with T!

Opposite to what expected for a metallic system

Assumption of constant n_e and n_h with T is not valid

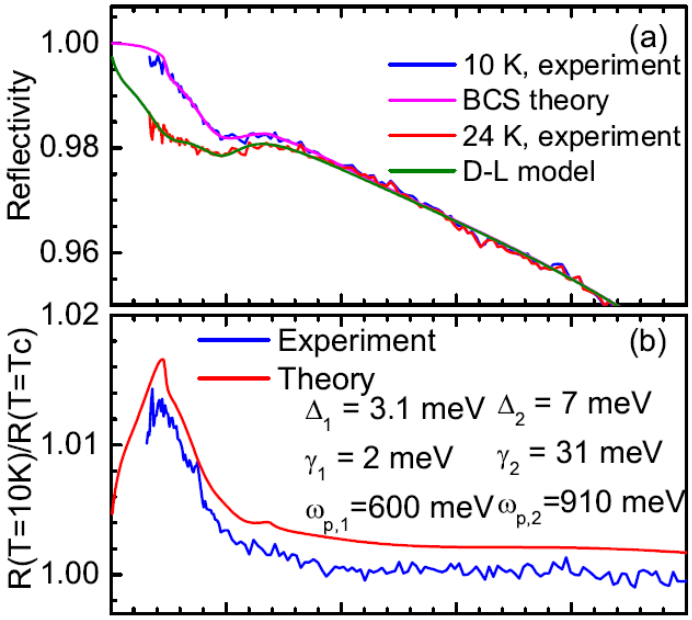
Holes not directly visible in the transport properties

Optical measurements in $Ba(Fe_{1-x}Co_x)As_2$

➡ One type of carriers more strongly scattered than the other one

Superconducting state for x=7%

E. Van Heumen et al., arXiv 0912.0636

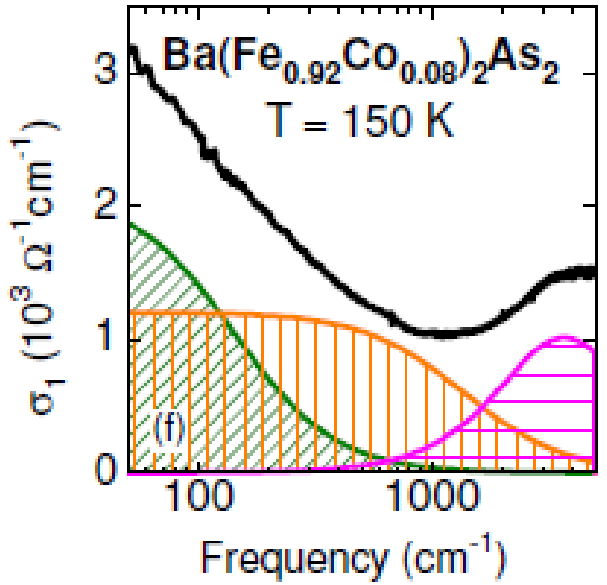


The holes are 15 times more scattered than the electrons

Interband scattering more efficient for the holes than for the electrons

Normal state for x=7%

D. Wu et al., arXiv 0912.3334

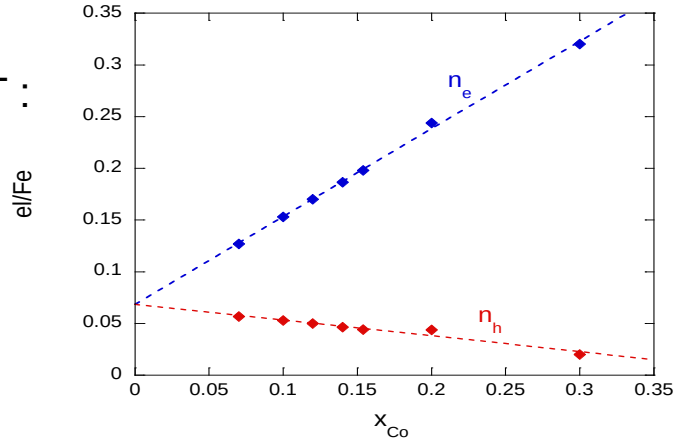


Two Drude components with very different scattering rates

Carrier content vs Co doping and temperature

Variation with Co content

At low T :



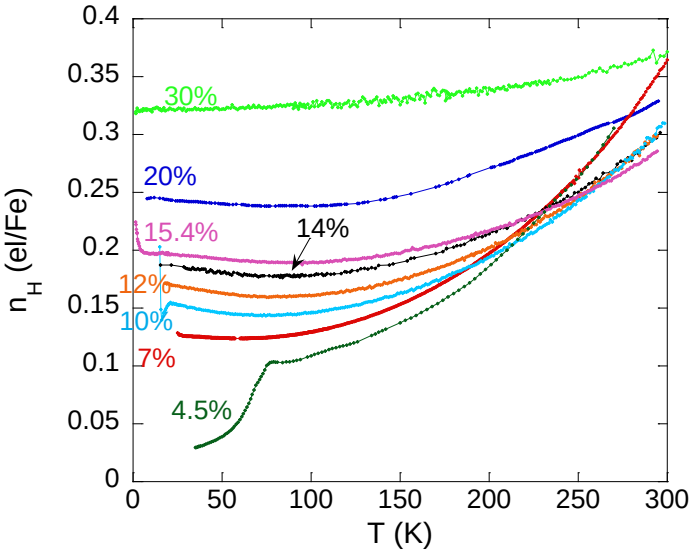
Each Co adds ~0.9el/Fe

$n_e = n_h + x_{Co}$ ⇒ n_h

This result can be explained if the shapes of electron and hole pockets are different

Shift of the Fermi level ⇒ Different changes of n_e and n_h.

Variation with T



For $T \leq 150$ K and $x \geq 4.5\%$:
rather weak T dependence

$BaFe_2As_2$: semimetal with the bottom of the electron bands and the top of the hole bands very near E_F (20-40meV)

Increasing T ⇒ Shift of the chemical potential

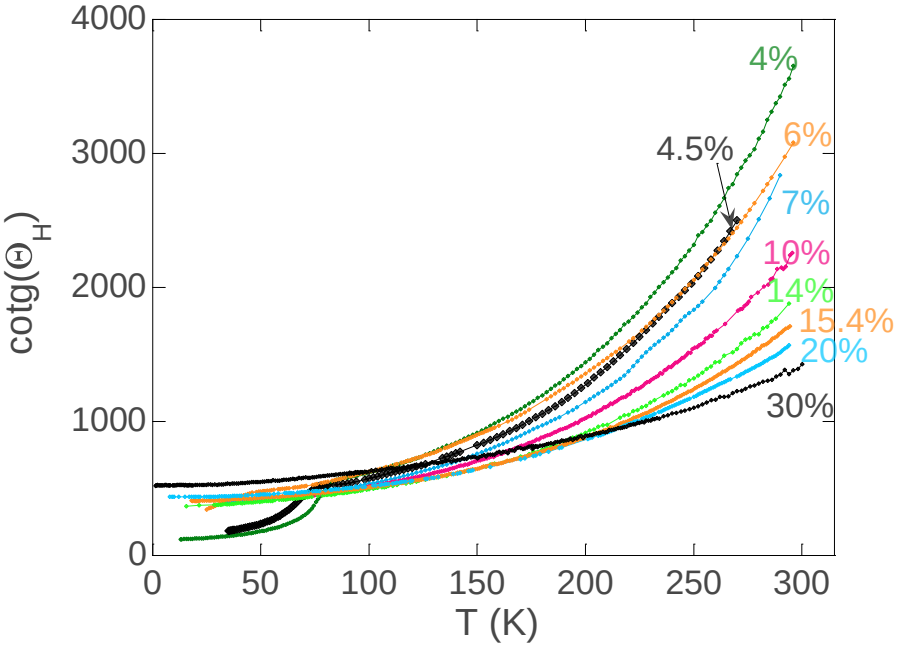
⇒ Equal modification of n_e and n_h

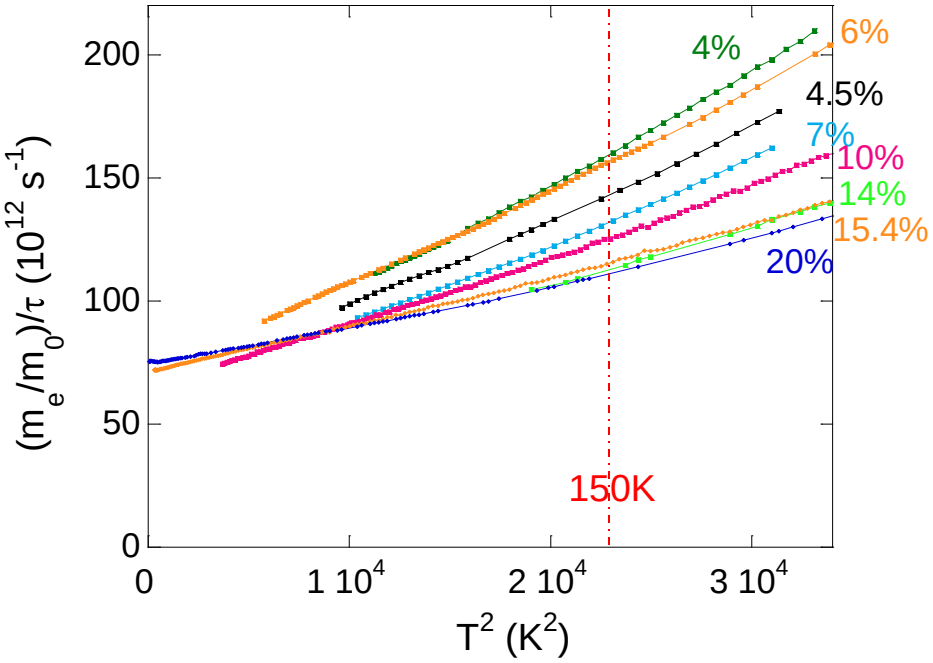
Electronic scattering rates

$$n_e(T) = n_H(T)$$

$$\rho(T) = \frac{m_e}{n_e(T) e^2 \tau(T)}$$

$$\cot(\Theta_H) = \rho / |R_H| = m_e / e\tau$$



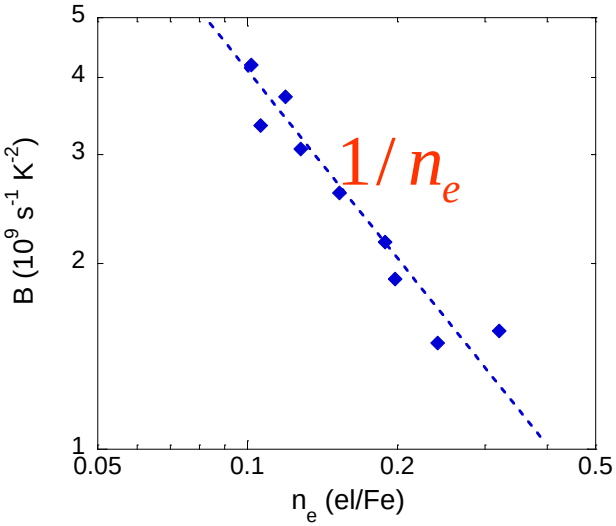


Up to 150K: $1/\tau = 1/\tau_0 + BT^2$ ➡ Electron-electron interaction

$1/\tau_0$ independent on Co doping for $x \leq 20\%$

No contribution of phonons nor spin fluctuations to the electronic scattering rates

Fermi liquid behavior



Electron-electron scattering process:

$$\frac{\hbar}{\tau_e(T)} \propto \frac{(k_B T)^2}{E_F}$$

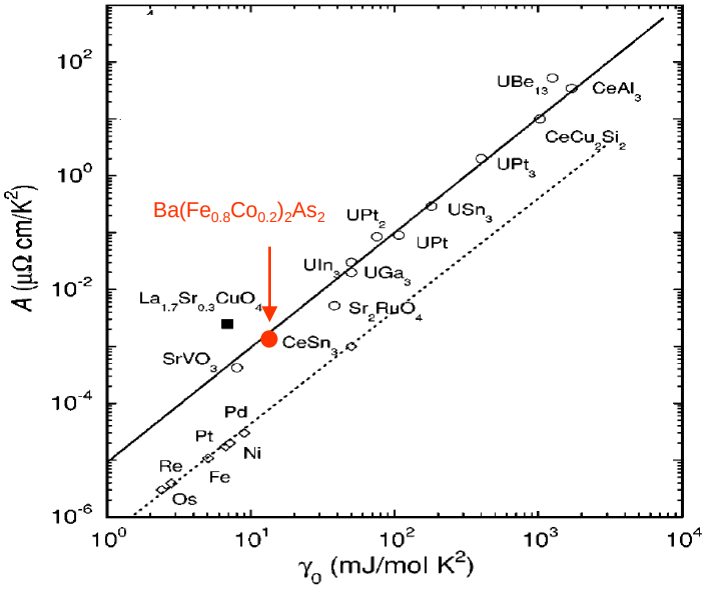
In agreement with $E_F \propto n_e$ in 2D

Comparison with Kadowaki woods ratio :
relation between
the T^2 coefficient of the resistivity A
and
the electronic specific heat γ_0

x =20%

A = 1.4 nΩ.cm/K^2

γ_0 ~ 10-15mJ/mol K^2



This corroborates our analysis in terms of transport dominated by electrons with a T variation of carriers

Fermi liquid vs non Fermi liquid behavior

Observation of a T linear resistivity near optimal doping

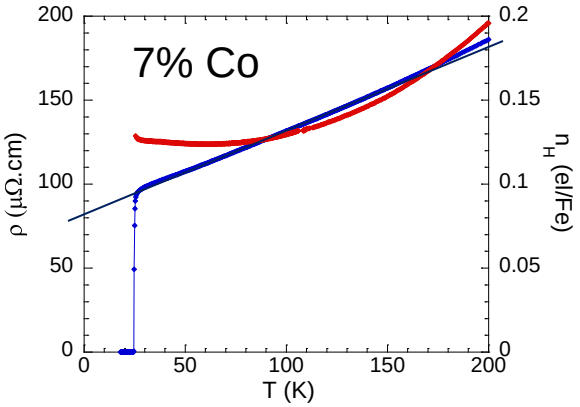
Non Fermi liquid behavior

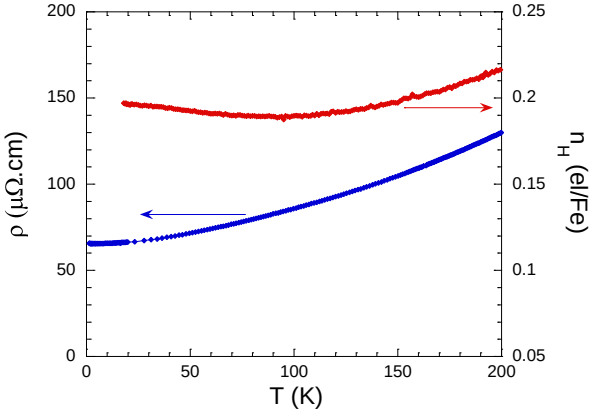
More precisely in the overdoped regime

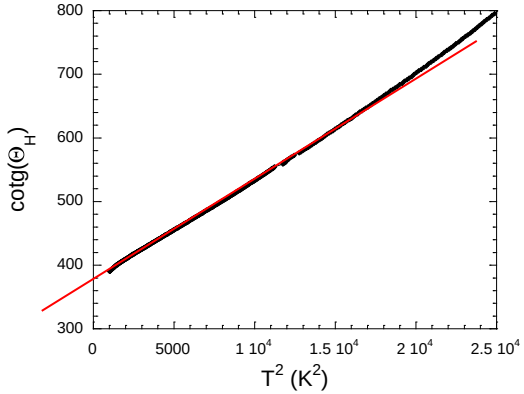
$\rho(T)=\rho_0+ AT+BT^2$ with A = 0 when $T_c=0$

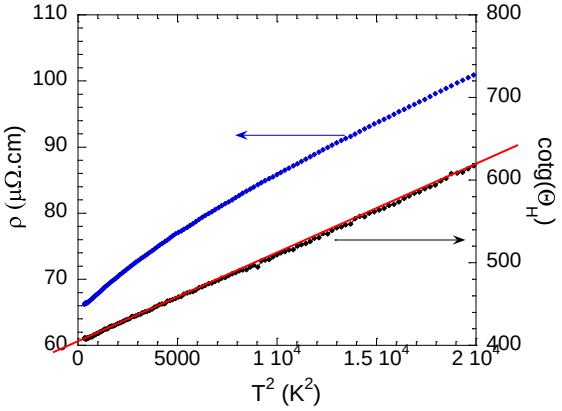
N. Doiron-Leyraud et al., PRB (2009)

15.5% Co – T_c=0K







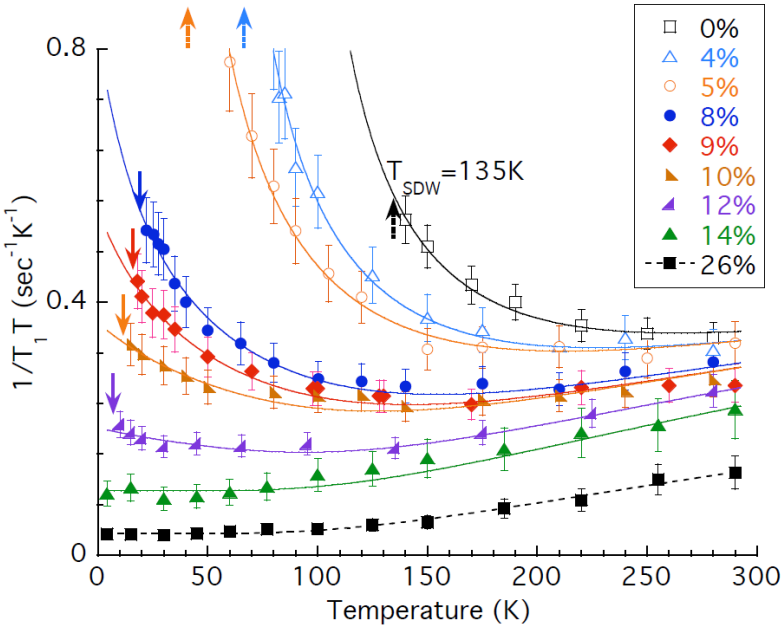


A very small variation of the number of carriers with temperature can be responsible for an apparent T linear resistivity

Why the spin fluctuations are not directly apparent in the transport?

As NMR in underdoped and overdoped $Ba(Fe_{1-x}Co_x)As_2$

Ning et al. Arxiv 0907.3875



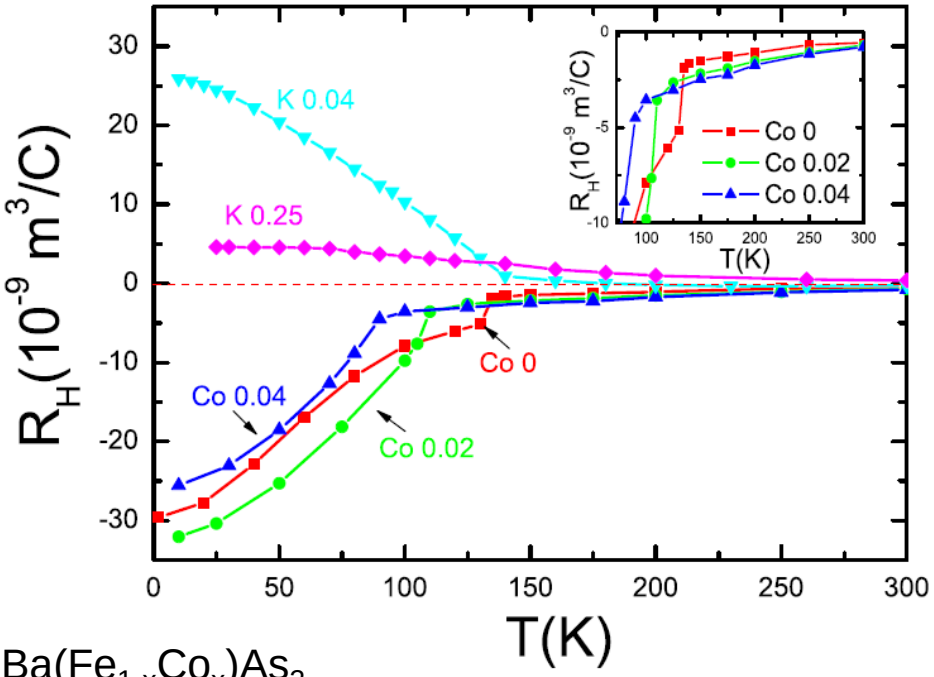
Huge increase of $1/T_1T$ below 10%

Are the holes localized by the spin fluctuations?

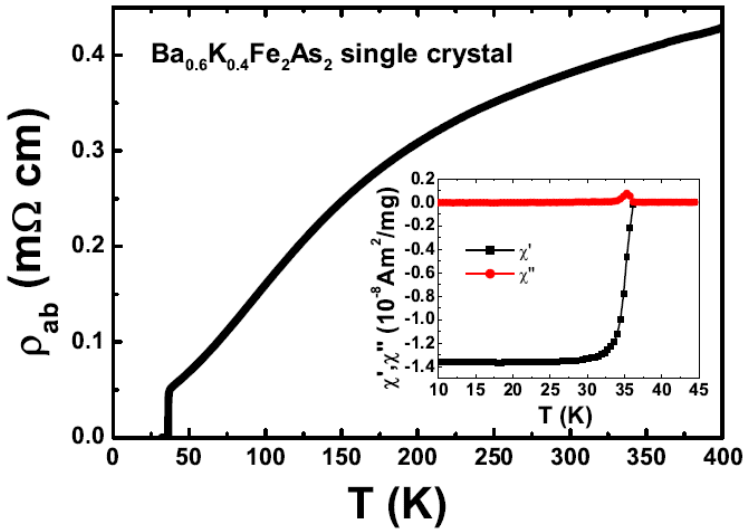
Why the electron transport is not affected?

Electron-Hole asymmetry in the 122 family

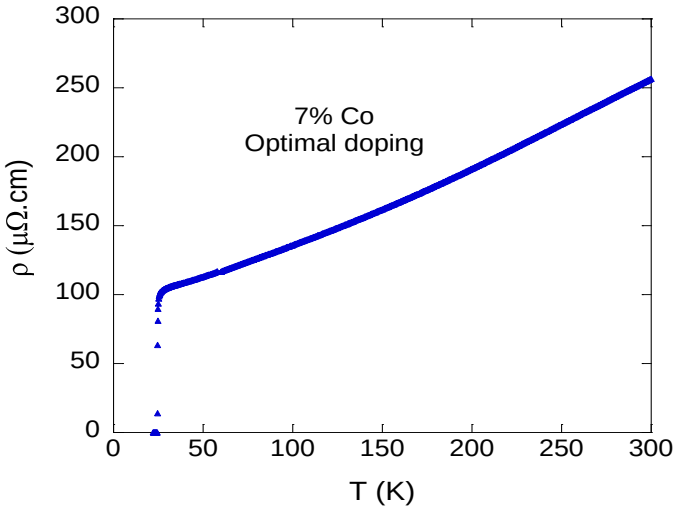
L. Fang et al., PRB (2009)



$Ba_{1-x}K_xFe_2As_2$



$Ba(Fe_{1-x}Co_x)As_2$



Very different ρ(T) curves

Ru-doped: $Ba(Fe_{1-x}Ru_x)_2As_2$

Isovalent substitution $n_e = n_h = n$

LDA calculations :

L. Zhang and D.J. Singh, PRB (2009)

Electronic structure near the Fermi level quite similar in $BaFe_2As_2$ and Ru-$BaFe_2As_2$

Results on polycrystalline samples

S. Paulraj et al., arXiv 0902.2728

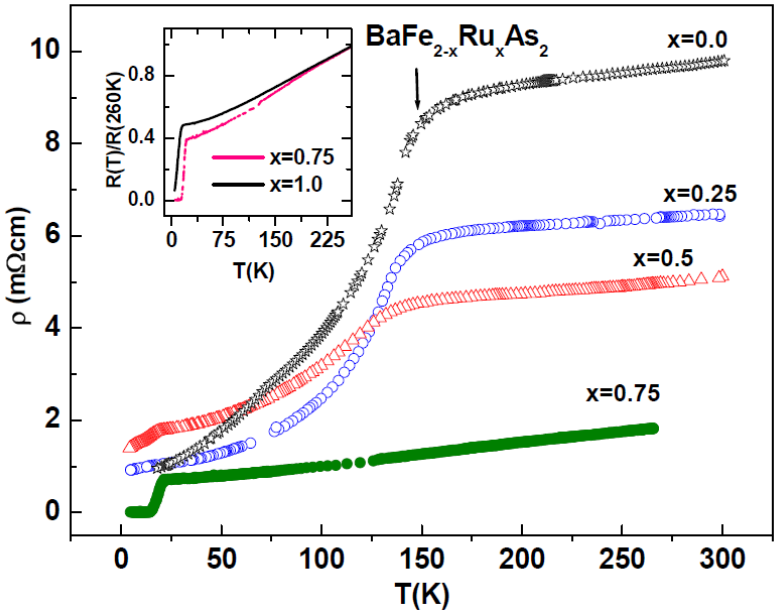
Weak suppression of magnetism

Superconductivity for x ~0.35

:

But negative Hall coefficient

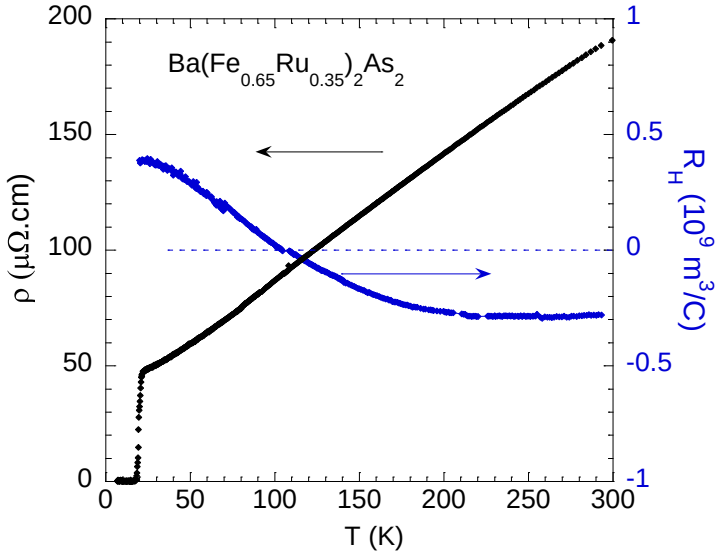
Electron doped?



Negative Hall coefficient also in single crystals of $BaFe_2(As_{1-x}P_x)_2$

S. Kasahara et al., arXiv0905.4427

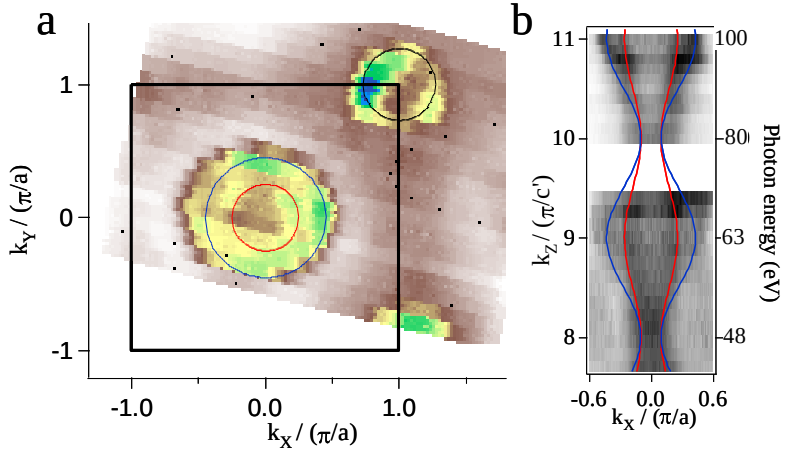
Transport and ARPES in $Ba(Fe_{1.65}Ru_{0.35})_2As_2$



The Hall coefficient changes sign
at low temperature

Mobility of holes larger than the one of electrons

ARPES measurements : See Poster by V. Brouet

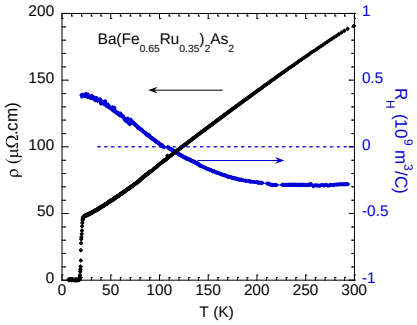


For the hole pockets:
FS significantly warped along k_Z

$$n_e = n_h = n = 0.11/Fe$$

Number of carriers nearly twice the one found by ARPES in $BaFe_2As_2$

Analysis of the transport data for $Ba(FeRu_{0.35})_2As_2$



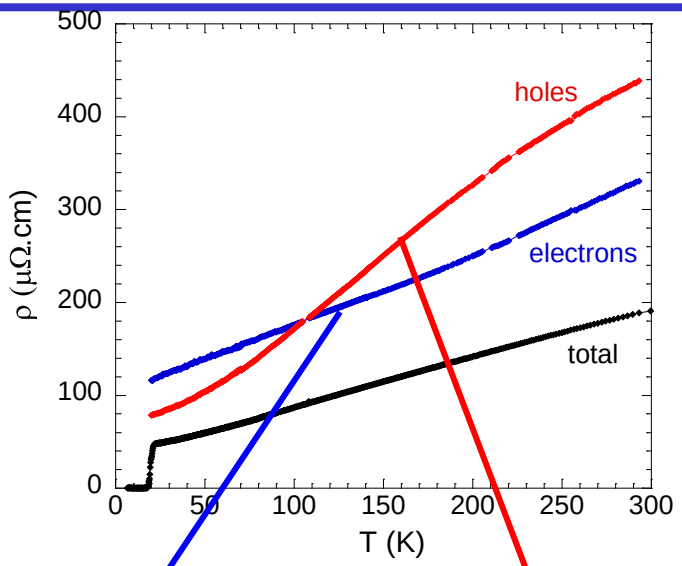
Compensated semi-metal

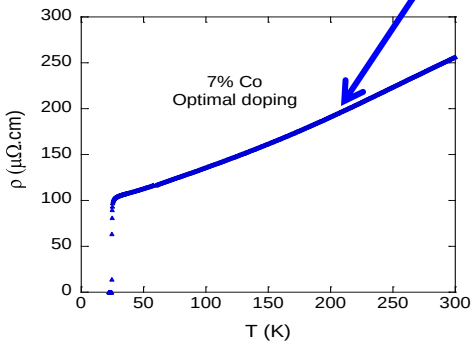
In a two-band model:

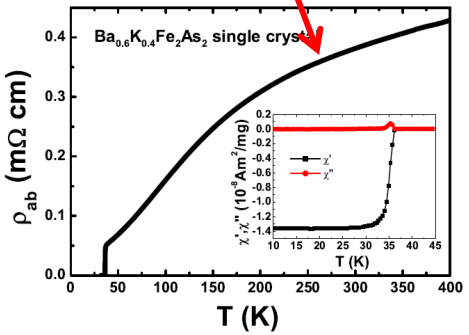
$$R_H = \frac{1}{ne}\frac{(\sigma_h - \sigma_e)}{(\sigma_h + \sigma_e)}$$

$$\sigma = \sigma_e + \sigma_h$$

$$n = 0.11el/Fe$$







Why are the holes less scattered in Ru doped compounds than in the undoped parent?

Spin fluctuations?

Modification of the electronic structure : weaker correlations – See poster by V. Brouet

Summary

- Coherent picture of the charge transport in $Ba(Fe_{1-x}Co_x)_2As_2$ at low T
  - Transport dominated by the electrons
  - The T variation of the Hall number explained by a T variation of the number of carriers

- Scattering processes : Fermi liquid behavior
  - *Spin fluctuations not directly visible in the transport properties*
  - Residual scattering rates independent on Co doping

- Ru-substituted $BaFe_2As_2$
  - Phase diagram very similar to the one found for Co or K doped compounds
  - Electrons and holes contribute to the transport.
  - Modification of the electronic structure