Multiband effect and electron-hole asymmetry in the transport properties of iron pnictides

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energie atomique • energies alternatives

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Agence Nationale de la Recherche ANR

TRIANGLE DE LA PHYSIQUE

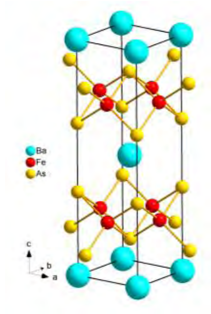
The different families of pnictides

1111 $SmFeAsO_{1-x}F_x$

Highest T_c =57K

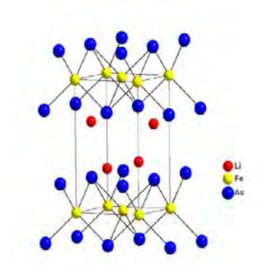
Synthesis of single crystals difficult
Few results
Chemical composition

122 $BaFe_2As_2$
$SrFe_2As_2$
$CaFe_2As_2$



A very rich family
Good single crystals

111 LiFeAs



Good single crystals
Stoechiometric ⟶ low defect content
Very sensitive to air

Chalcogenides

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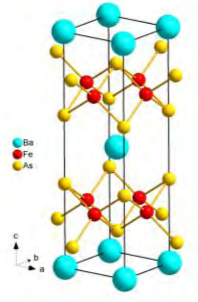

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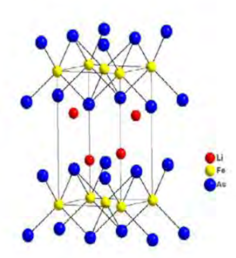

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Chalcogenides

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Transport measurements in the 122 family : Overview of the resistivity and Hall effect data

Necessity of a multiband description

Analysis of the resistivity and Hall effect measurements in a minimal two-band model: electron doped $BaFe_2As_2$ with Co and Ni substitution

Strong electron-hole asymmetry in the scattering rates

Comparison with ARPES results

Isovalent substitution: Ru/Fe

Resistivity, Hall effect and magnetoresistance

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LiFeAs Resistivity, Hall effect and magnetoresistance

Analysis in relation with ARPES and quantum oscillations data

Beyond the two-band model

The 122 Phase AFe_2As_2 (A=Ba, Sr, Ca, Eu)

Possibility to get large single crystals

Ba^{2+}, Sr^{2+}, Ca^{2+}, ..

Pr^{3+}, La^{3+}

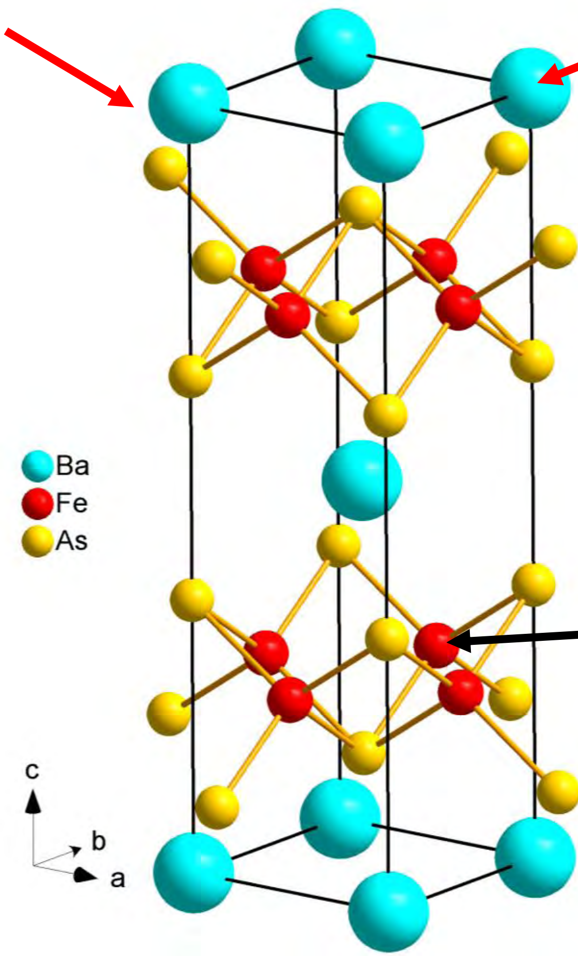
Electron-doped

T_c^{max} ~ 45K in $CaFe_2As_2$

K^+

Hole-doped

T_c^{max} =37K



Ru on Fe site
P on As Site

Isovalent substitution

26 Fe	27 Co	28 Ni
44 Ru		

Co : $3d^7$
Ni : $3d^8$

Rh : $4d^7$
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

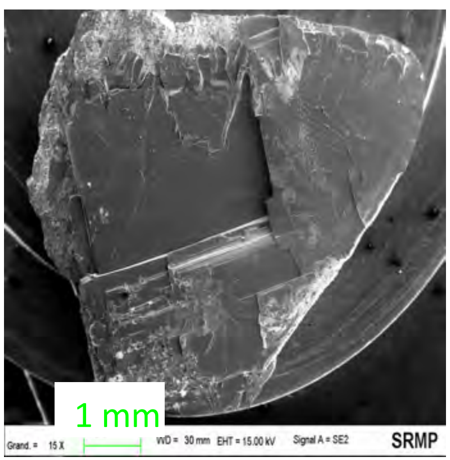
↓

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

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

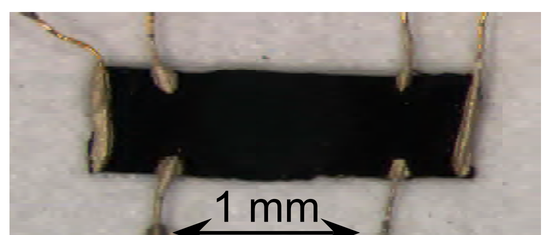
Mechanical extraction of platelets single crystals,

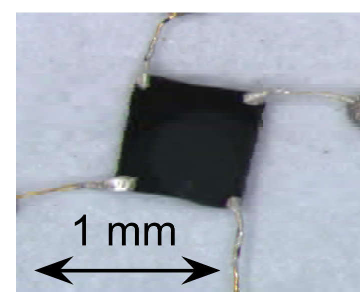


Co content determined by wave length dispersive X-ray spectroscopy

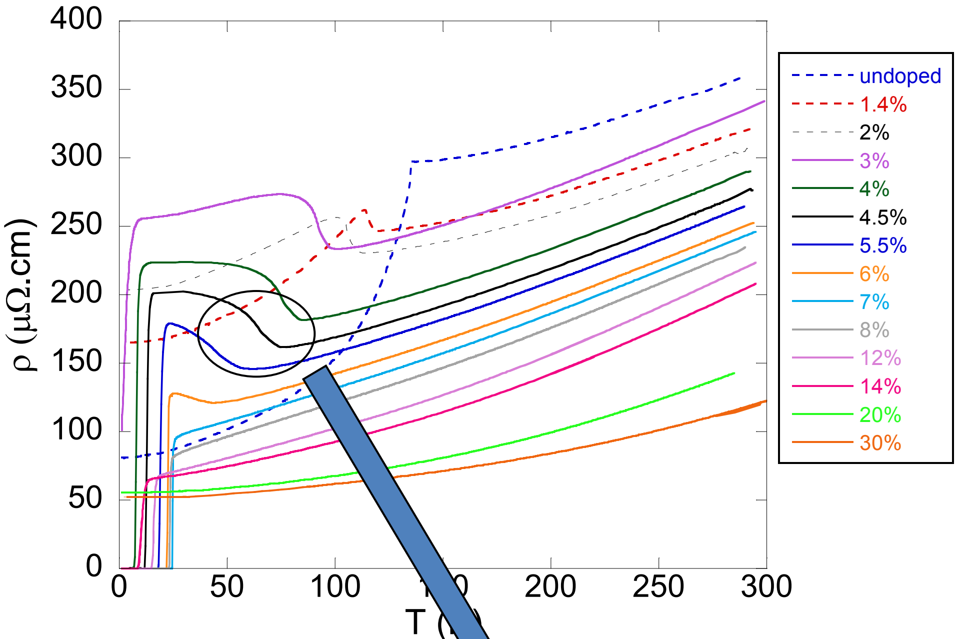
Measurements of Transport properties

Thickness between 10 to 30 mm

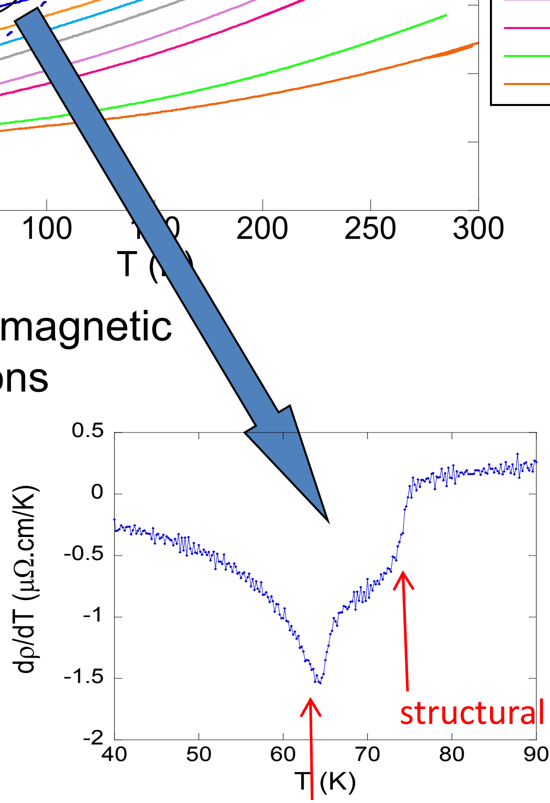


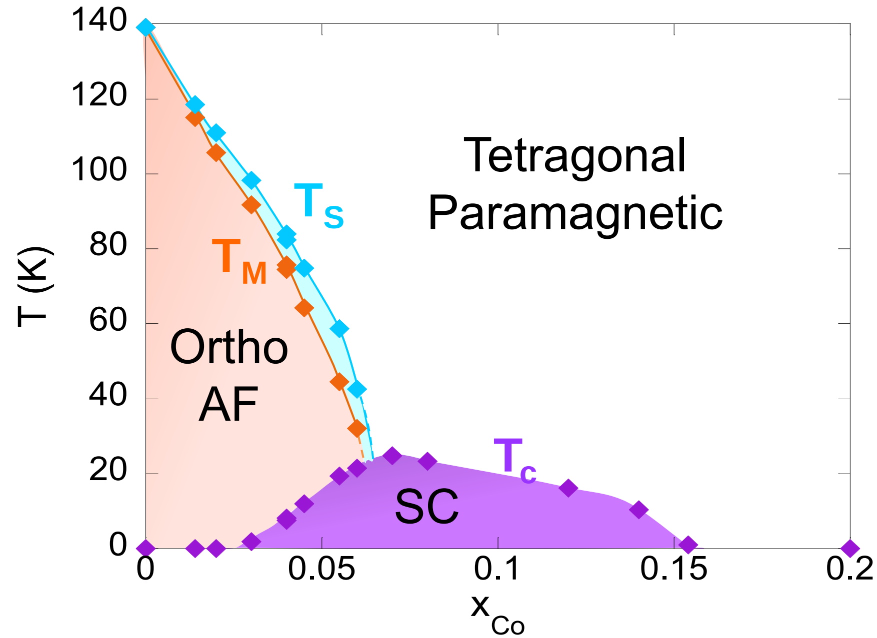


Transport properties of $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals



Structural and magnetic transitions





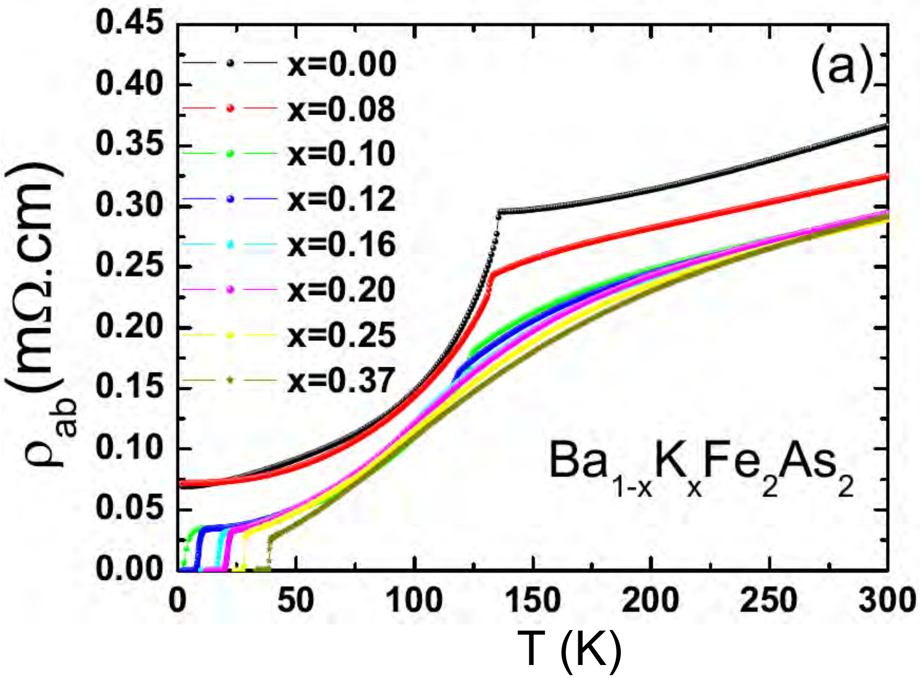
Coexistence of AF and SC states at local scale

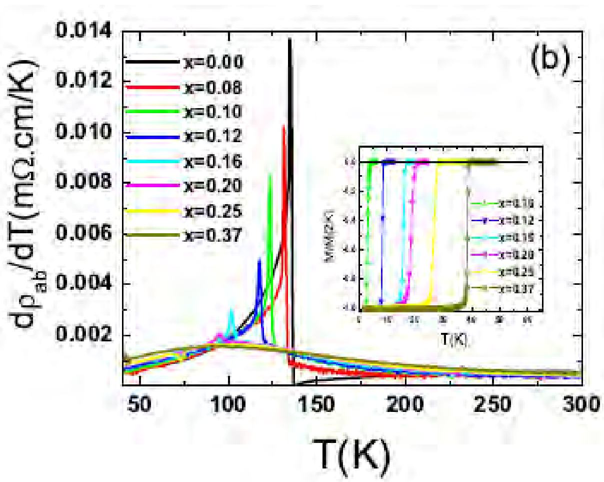
NMR : Y. Laplace et al. PRB (2009)

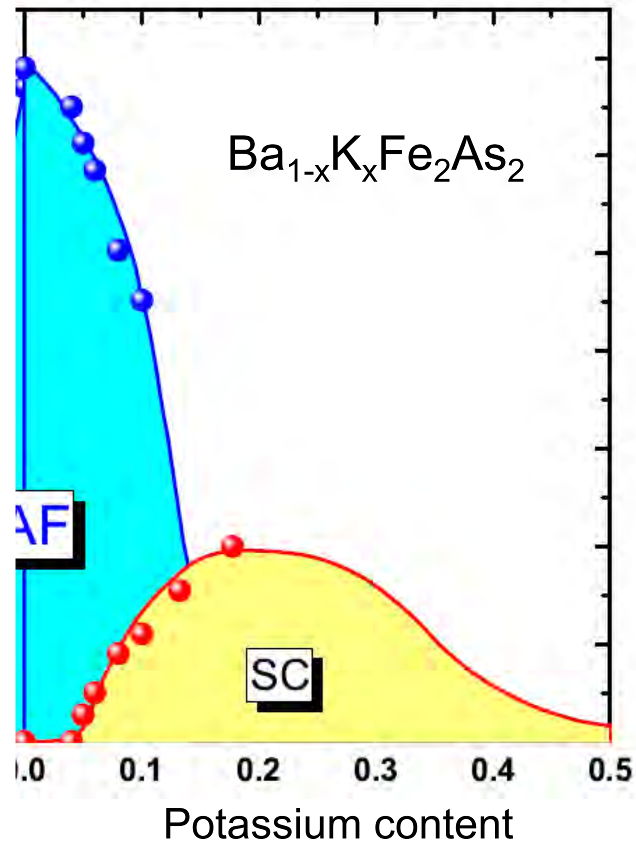
FRA et al. PRL 2009

Ni et al. PRB (2008), J.H. Chu et al., PRB (2009), L. Fang et al., PRB 2009

Transport properties of $Ba_{1-x}K_xFe_2As_2$ single crystals





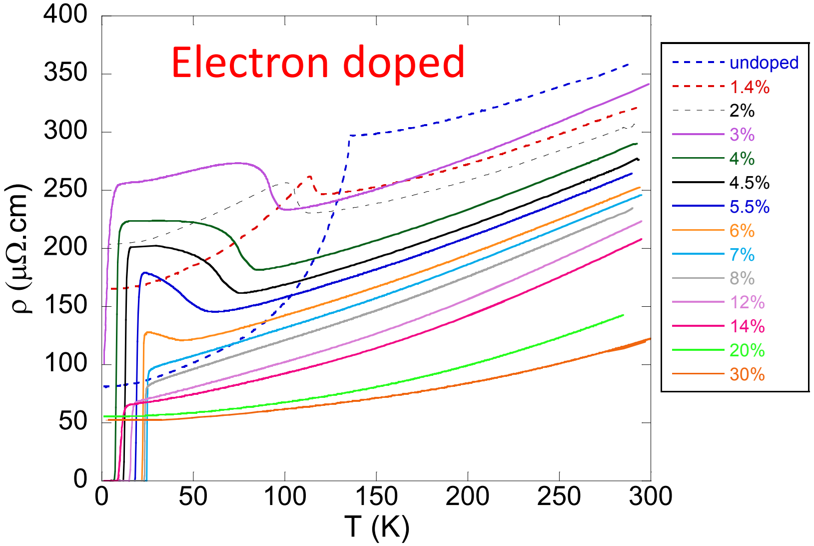


No splitting between structural and AF transitions

B. Shen et al., PRB (2011)

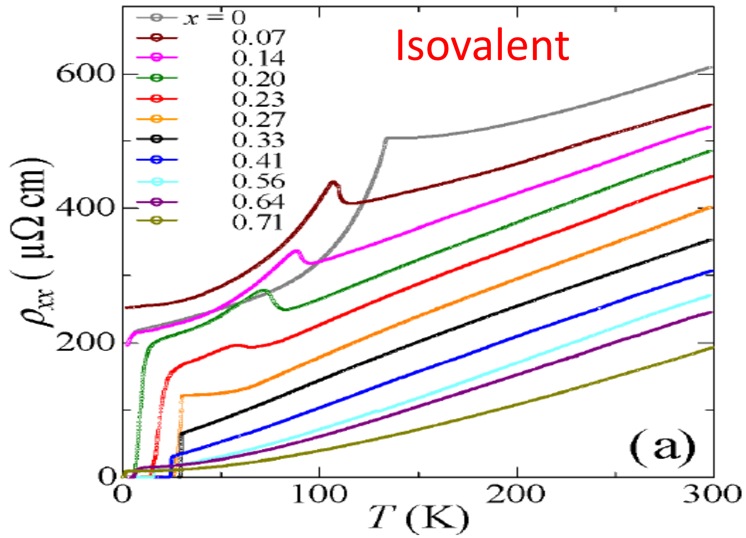
Resistivity evolution by substitution in the $BaFe_2As_2$ family

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

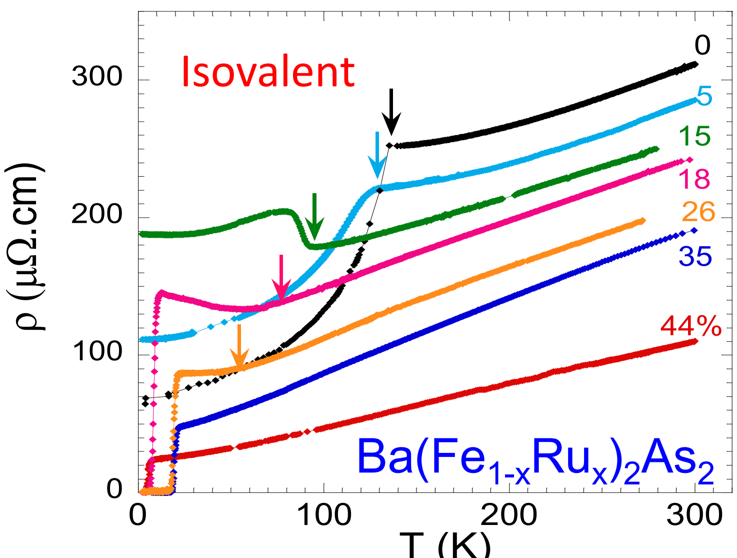


F. R.A. et al., PRL 2009

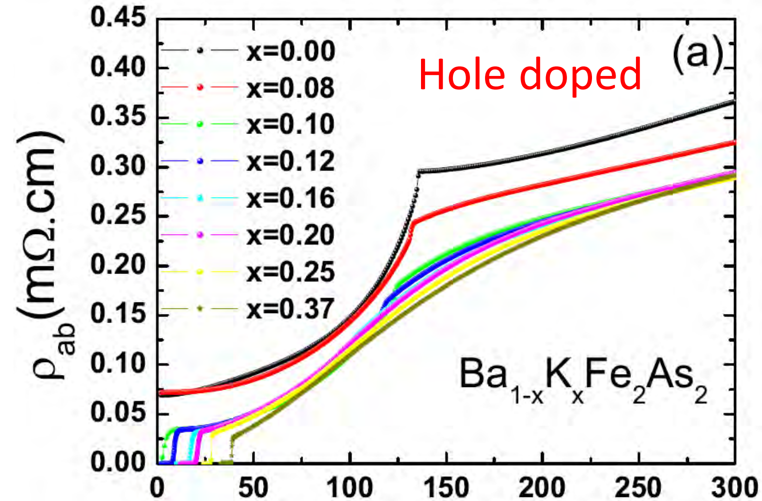
$BaFe_2(As_{1-x}P_x)_2$



S. Kasahara et al., PRB 2010



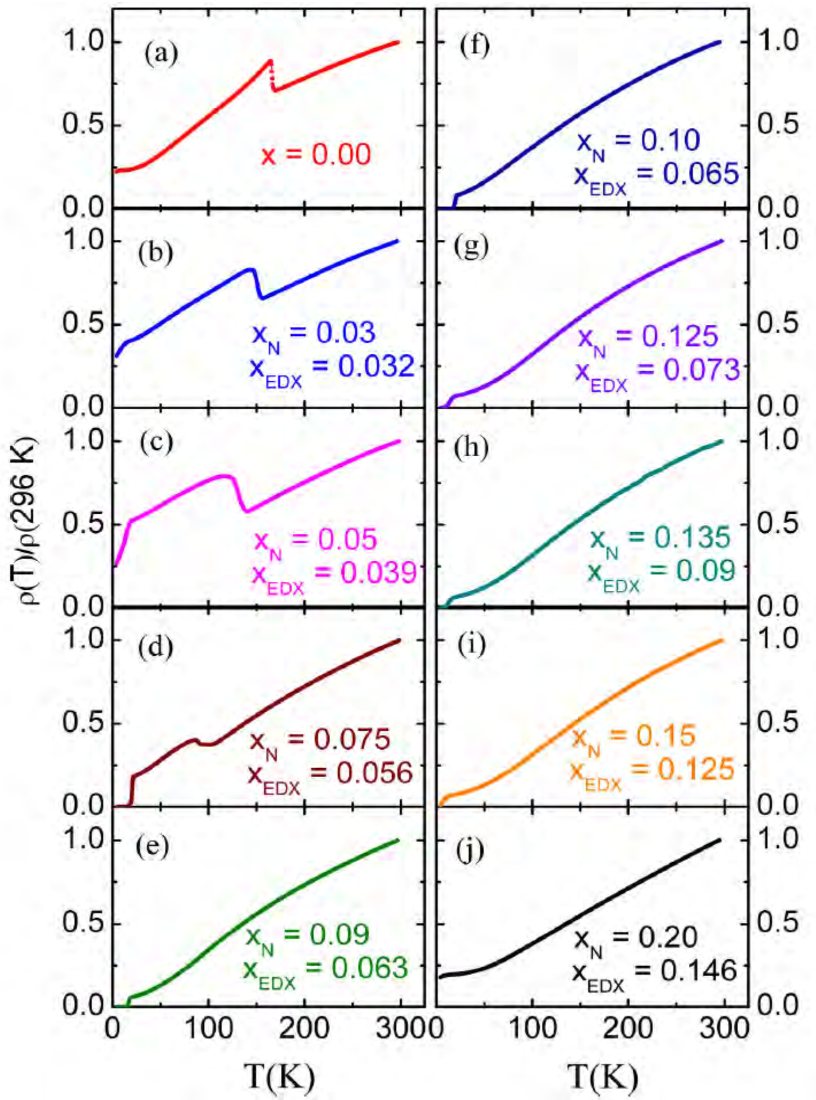
F. R.A. et al., PRB 2010



B. Shen et al., PRB (2011)

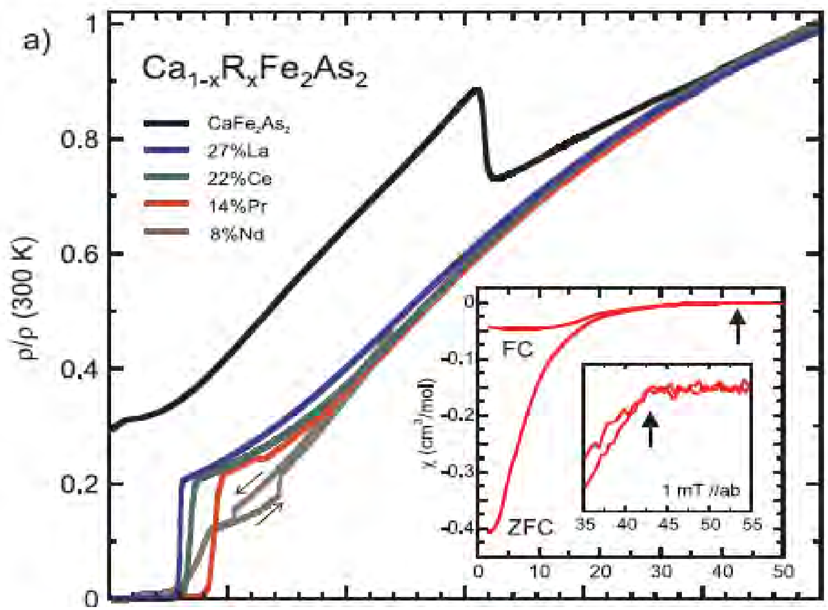
The $CaFe_2As_2$ family

$Ca(Fe_{1-x}Co_x)_2As_2$



L. Harnagea et al., arXiv 1011.2085

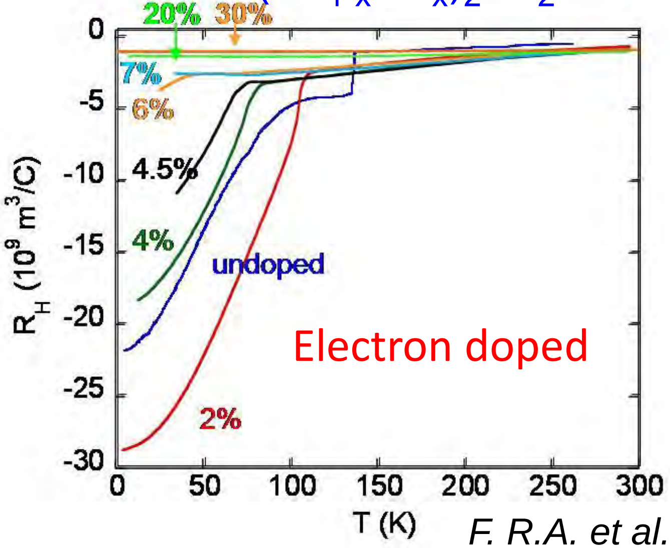
$Ca_{1-x}R_xFe_2As_2$



S.R. Saha et al., arXiv 1105.4798

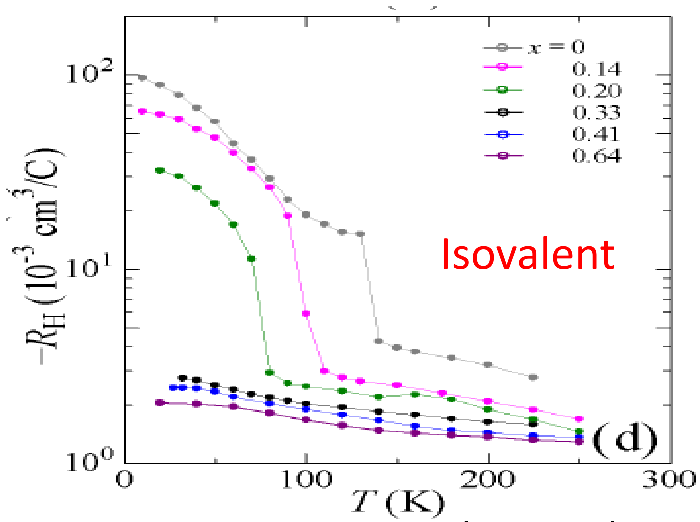
Hall effect : Large variation with temperature

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



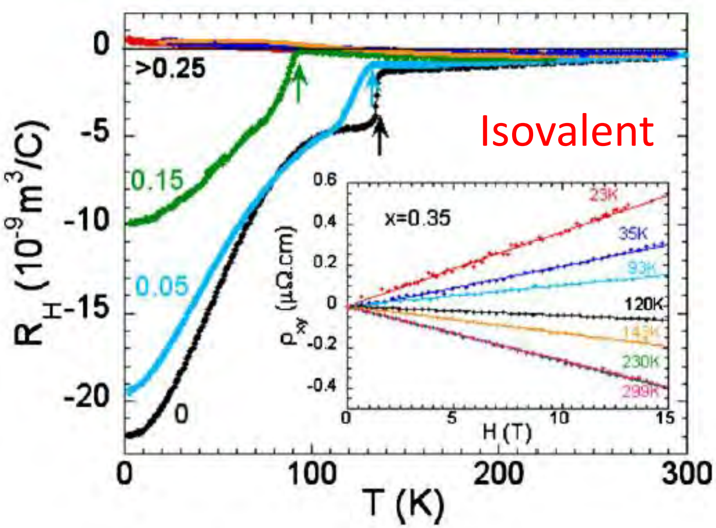
F. R.A. et al., PRL 2009

$BaFe_2(As_{1-x}P_x)_2$



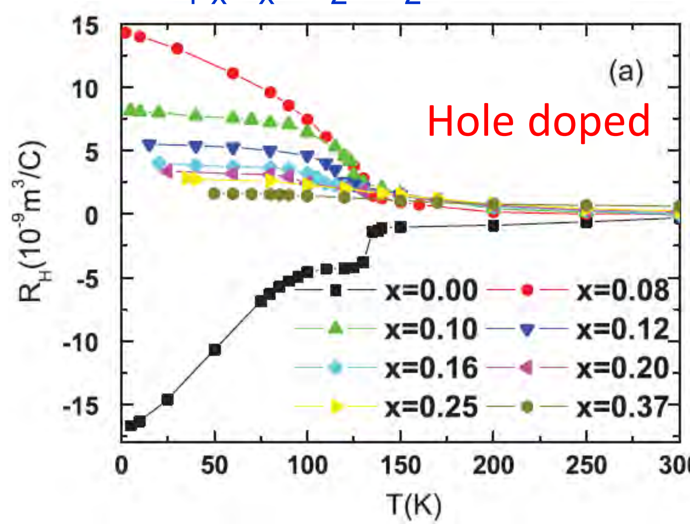
S. Kasahara et al., PRB 2010

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



F. R.A. et al., PRB 2010

$Ba_{1-x}K_xFe_2As_2$

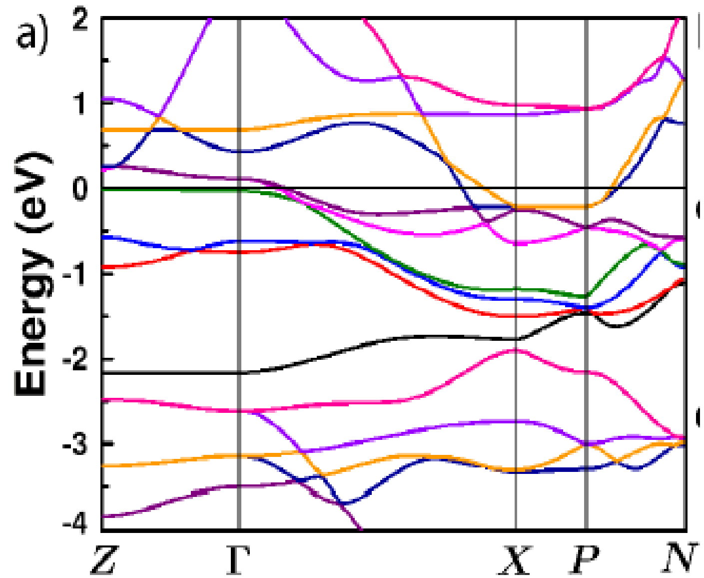


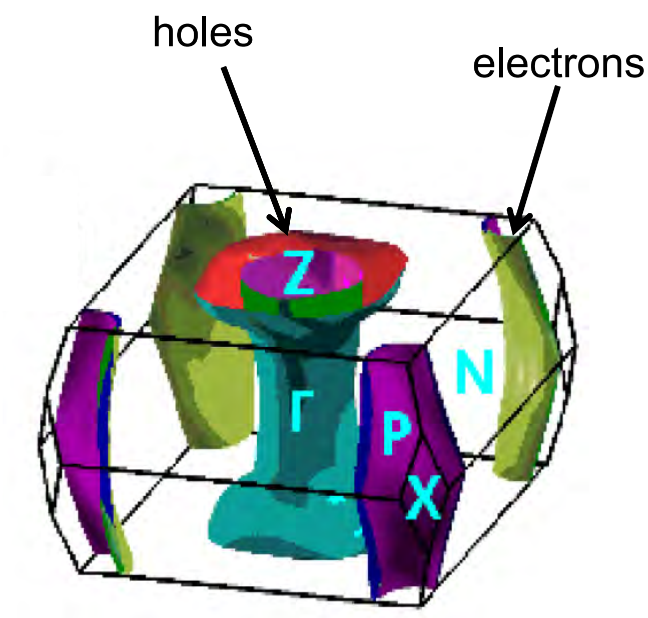
B. Shen et al., PRB (2011)

The Iron based superconductors: multiband structure

Electronic structure: band structure calculation

$BaFe_2As_2$





Compensated semimetal: $n_e = n_h$

Multiband effects

Modification by doping

→ Strong influence on transport properties

Resistivity, Hall effect, magnetoresistance, …

One-band versus multiband

Single band metal

Drude formula

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

Hall effect

$$R_H = \frac{1}{ne}$$

Iron-based superconductors

Minimal two-band model

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

$$1/\rho = 1/\rho_e + 1/\rho_h \qquad \rho_{e,h} = \frac{m^*_{e,h}}{n_{e,h}e^2\tau_{e,h}}$$

$$R_H = \frac{1}{e}\frac{(-n_e\mu_e^2 + n_h\mu_h^2)}{(n_e\mu_e + n_h\mu_h)^2}$$

$$\frac{\delta\rho}{\rho(0)} = \frac{\sigma_e\sigma_h(\mu_e + \mu_h)^2}{(\sigma_e + \sigma_h)^2}H^2$$

$$\mu_{e,h} = \frac{e\tau_{e,h}}{m^*_{e,h}}$$

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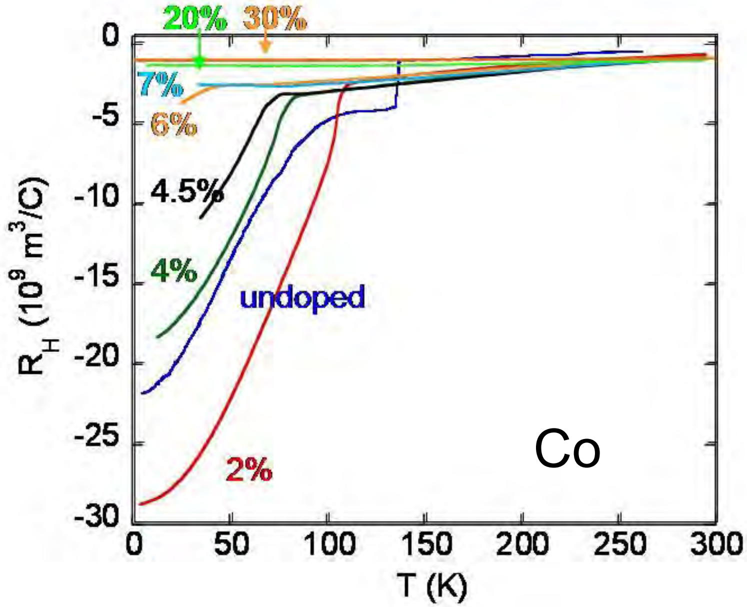
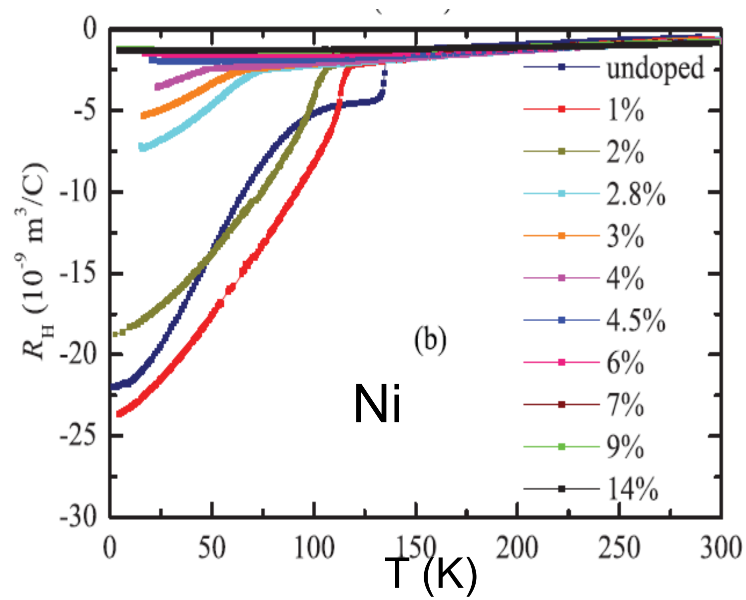
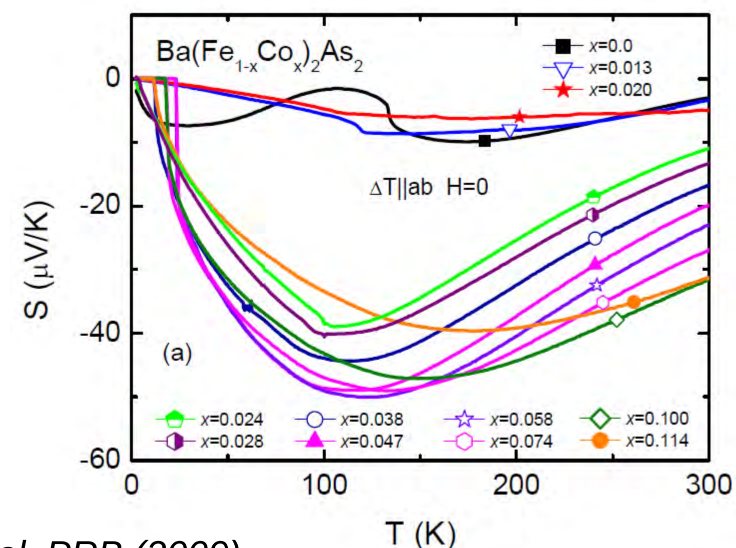
Hall effect: $Ba(Fe_{1-x}Co_x)_2As_2$ and $Ba(Fe_{1-x}Ni_x)_2As_2$





Transport dominated by the electrons all over the phase diagram

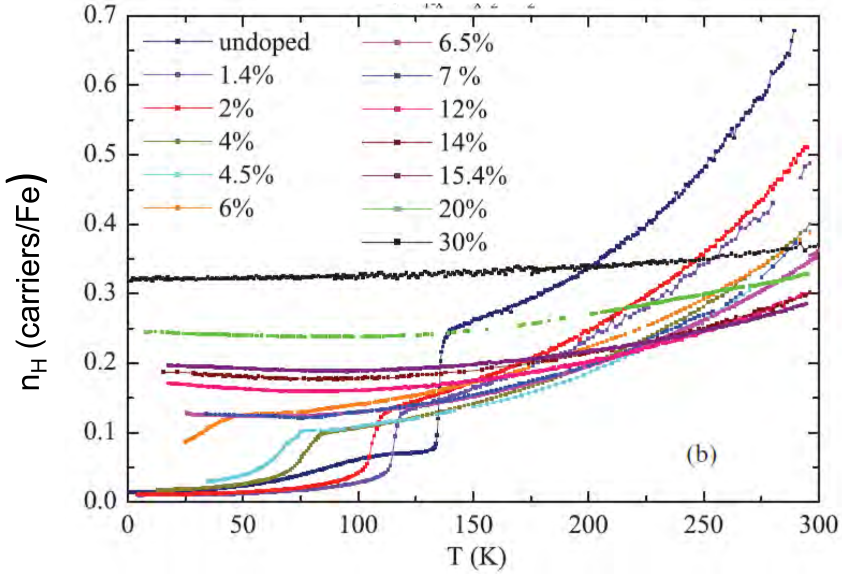
Drastic change of the Hall coefficient
in the AFM state near x~0.02
Seen also by thermopower measurements



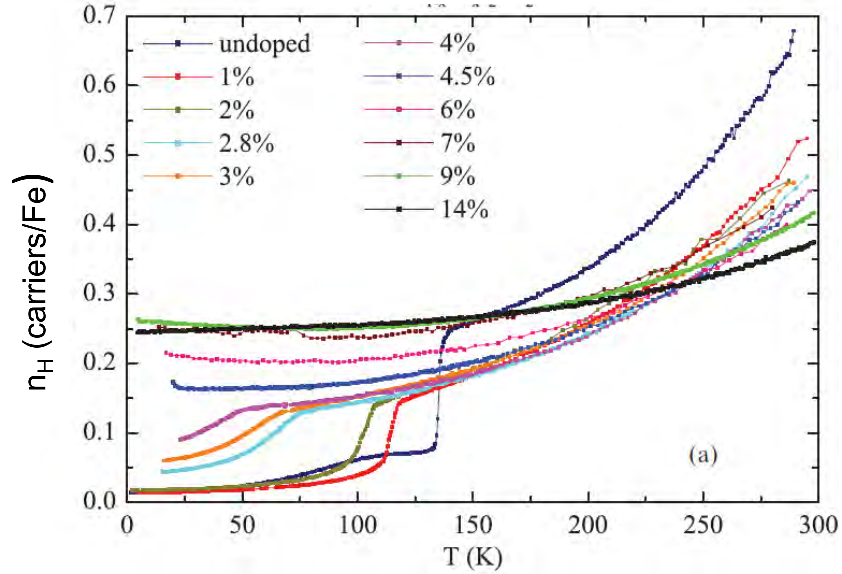
E.D. Mun et al. PRB (2009)

Hall number: $Ba(Fe_{1-x}Co_x)_2As_2$ and $Ba(Fe_{1-x}Ni_x)_2As_2$

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



$Ba(Fe_{1-x}Ni_x)_2As_2$



In a two-band model:

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

electrons

$$R_e = \frac{1}{n_e e}$$

holes

$$R_h = \frac{1}{n_h e}$$

$\Rightarrow$ n_H upper bound for n_e

Analysis in a two-band model

One electron band and one hole band : 4 unknown quantities : n_e, n_h, τ_e, τ_h

Experimentally : 3 equations

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

Hall effect: $$\frac{1}{n_H e} = \left| R_H \right| = \frac{\left| -R_e \sigma_e^2 + R_h \sigma_h^2 \right|}{(\sigma_e + \sigma_h)^2}$$

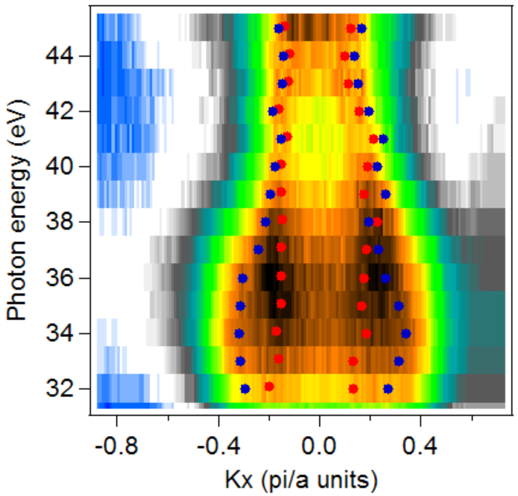
Charge conservation: $n_e = n_h + x_{Co}$

➡ Estimate of the electron density : ARPES measurements

Using ARPES measurements to determine n_e and n_h

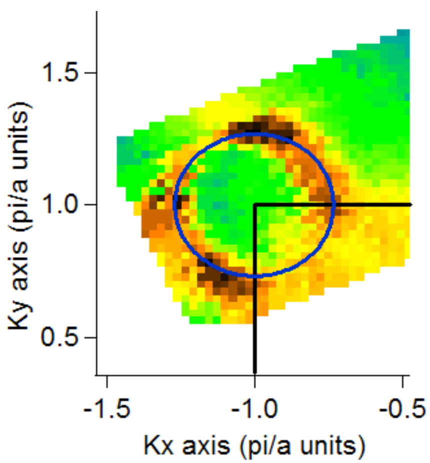
V. Brouet et al., PRB (2009)

Hole bands: two 2D, one 3D

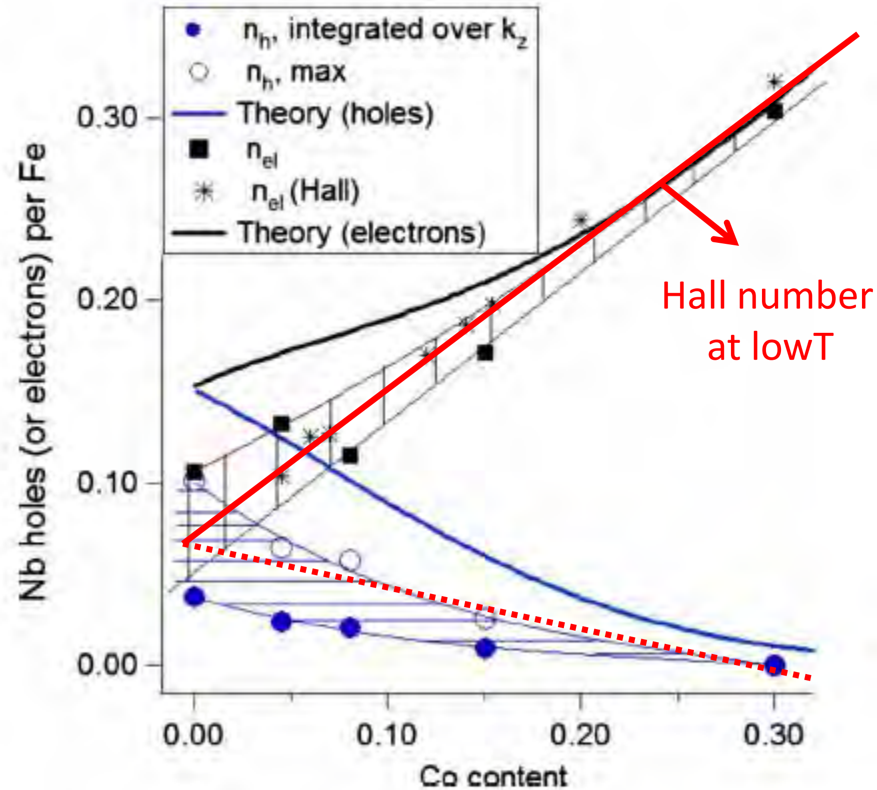


4% Co

2 degenerate electron bands: 2D



7% Co



$n_e - n_h = x_{Co}$

Good agreement between ARPES and transport data

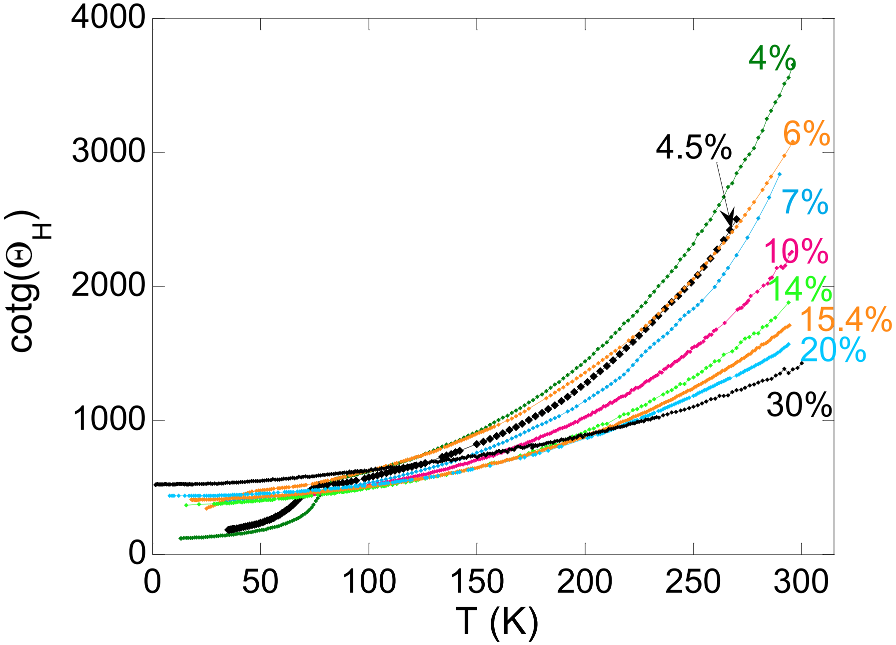
Holes not directly visible in the transport properties

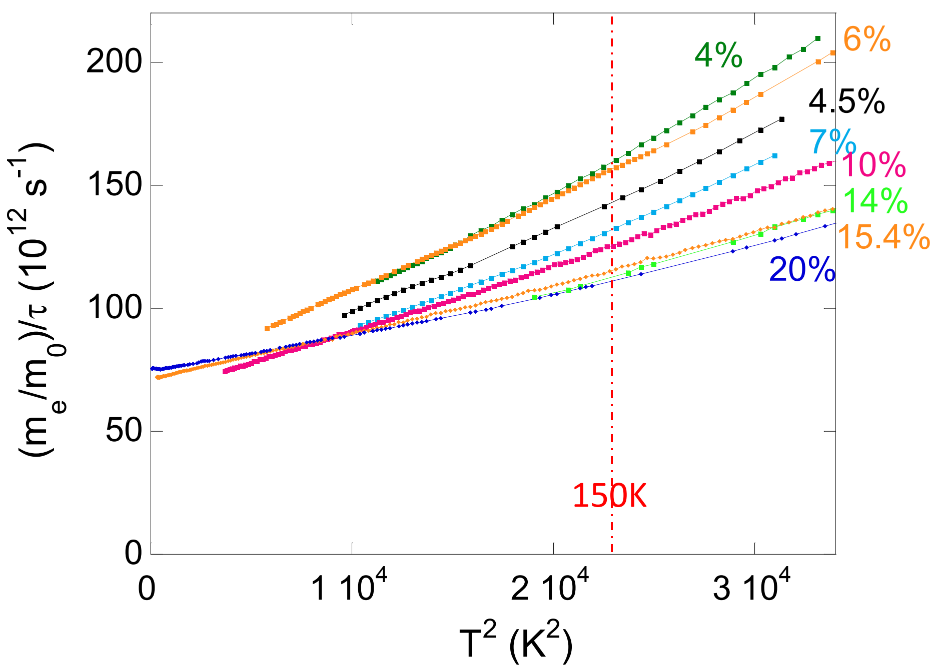
Electronic scattering rates

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

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

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





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

Fermi liquid behavior

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

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

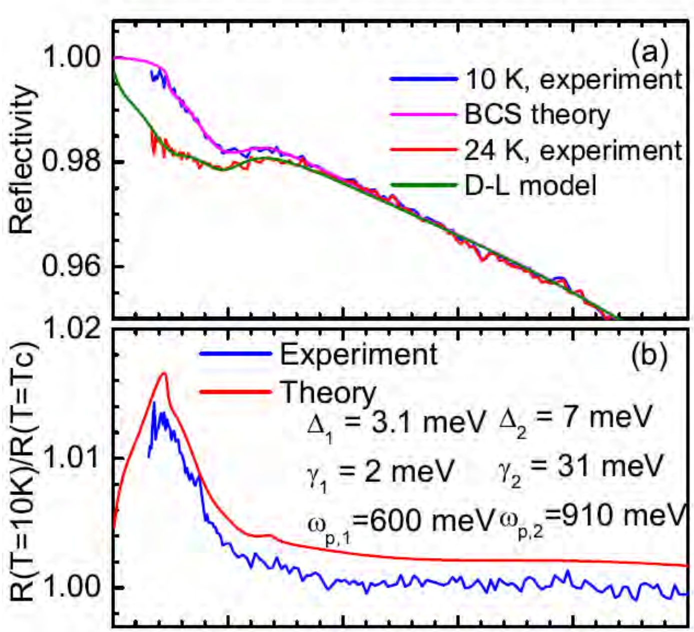
Electron and hole mobilities in $Ba(Fe_{1-x}Co_x)_2As_2$

→ Holes more strongly scattered than electrons

Optical measurements

E. Van Heumen et al., arXiv 0912.0636

Superconducting state for x=7%

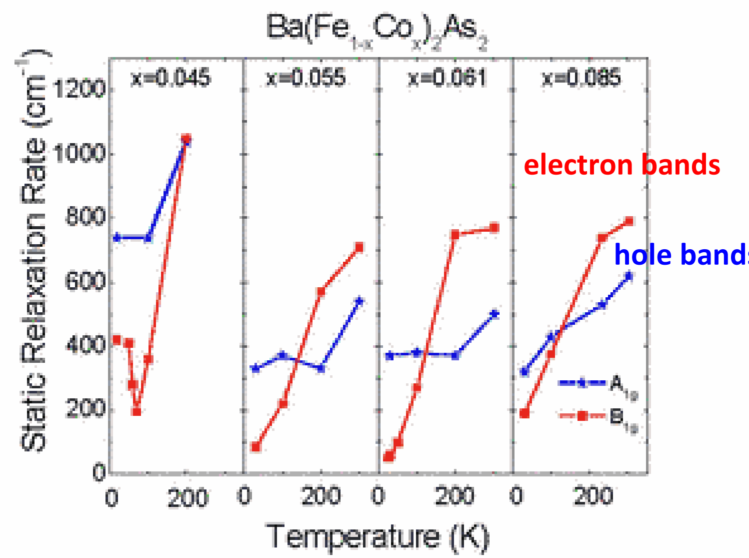


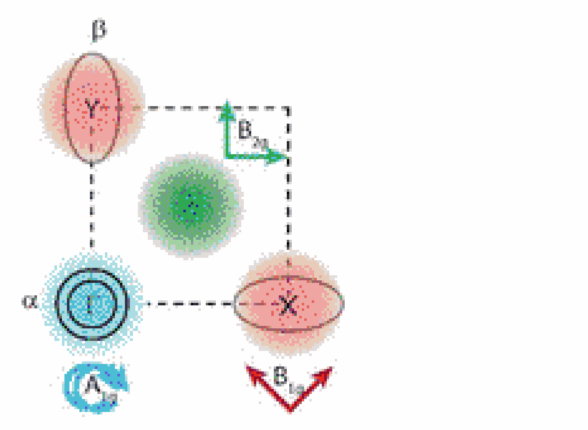
The holes are 15 times more scattered than the electrons

Interband scattering more efficient for the holes than for the electrons

Electronic Raman scattering

R. Hackl et al.

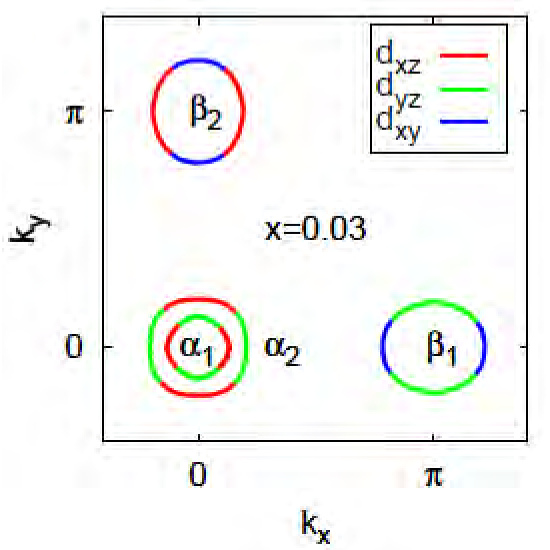




Anisotropy of the scattering rates along the FS sheets

Multiorbital composition of each Fermi pocket

A.F. Kemper et al. PRB 2011



d_{xz}, d_{yz}, d_{xy}

➡ Anisotropy of the effective mass and Fermi velocity

Scattering by spin fluctuations

One particle scattering rates affected by
- the orbital character of the initial and final states
- momentum dependence of the spin susceptibility

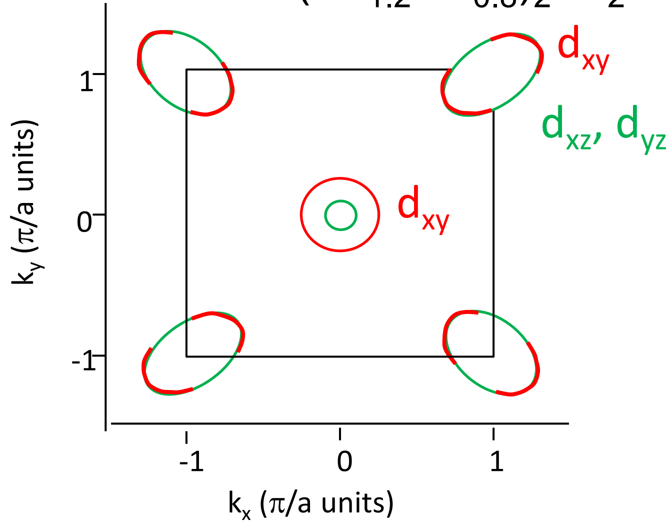
⬇

Strong anisotropy of the scattering rates

Transport dominated by small parts of the electron FS sheets with d_{xy} character with long lifetimes and large v_F

Anisotropy of the scattering rates along the FS sheets

ARPES: in $Ba(Fe_{1.2}Co_{0.8})_2As_2$: *V. Brouet et al.,arXiv 1105.5604*



lifetimes about twice longer
on the d_{xy} parts of the SF sheets
both for the hole and electrons pockets

$1/l = 1/v_F\tau$

	k_F (π/a)	v_F (eV.Å)	m*/m$_b$	$\delta k(E_F)$ (π/a)
hole d_{xz}/d_{yz}	0.06	0.5	2.7	0.11
hole d_{xy}	0.22	0.4	2.3	0.07
electron d_{xz}/d_{yz}	0.25	0.6	2.4	0.09
electron d_{xy}	0.30	0.7/1.2	5/2.9	0.04

n (carr/Fe)	$\hbar/\tau$ (meV)
0.006	44
0.038	22
0.12	43
	22/38

Seems difficult to reconcile with the Hall effect dominated by the electrons

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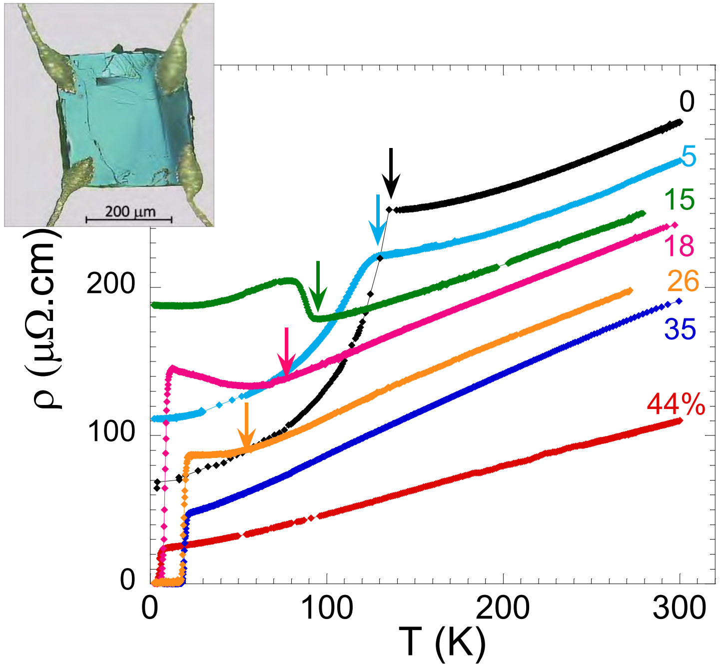
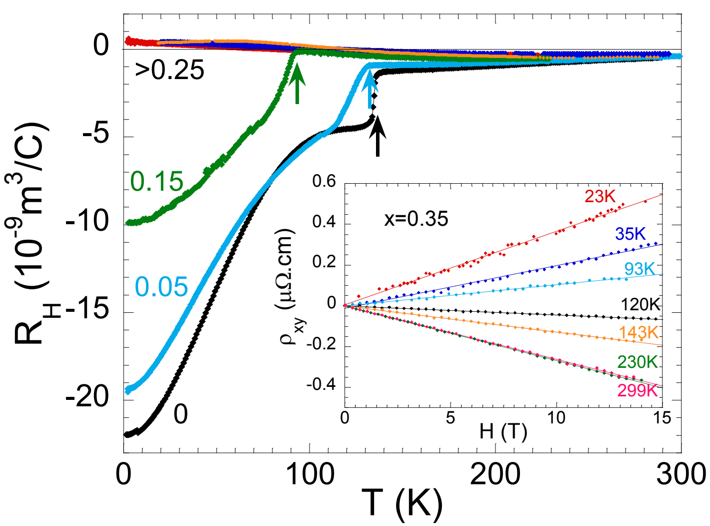
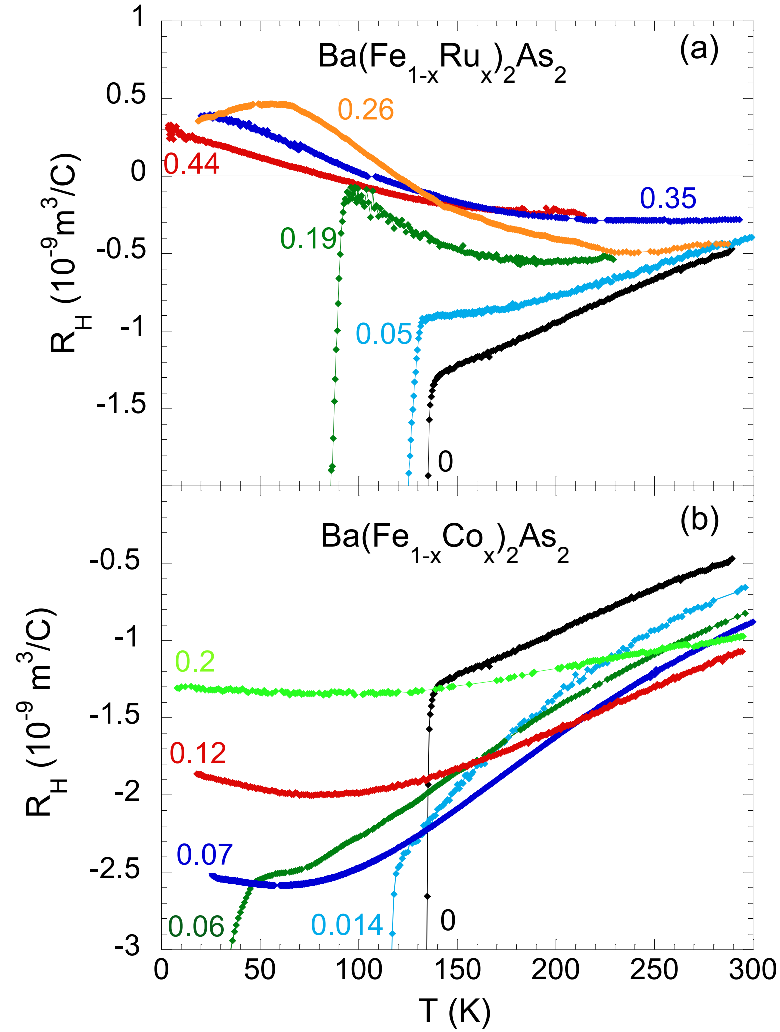
Transport properties of Ru-substituted $BaFe_2As_2$

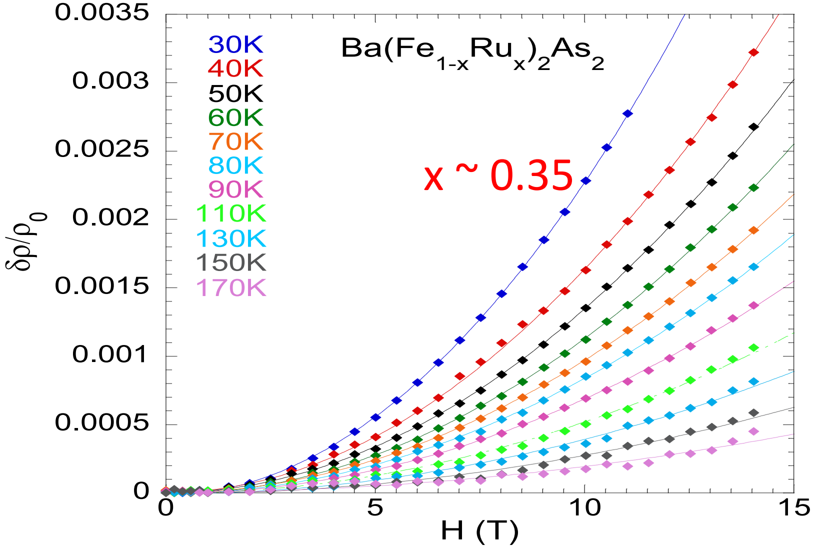






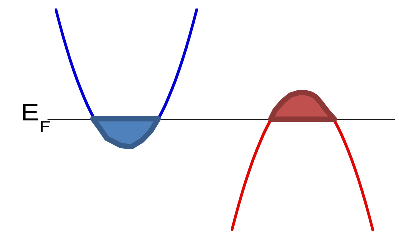
In a two band model :
mobility of holes overcomes that of electrons
at low T for x > 0.25

$Ba(Fe_{1-x}Ru_x)_2As_2$: ρ, R_H, Magnetoresistance



$$\delta\rho / \rho(0) = a(T)H^2$$

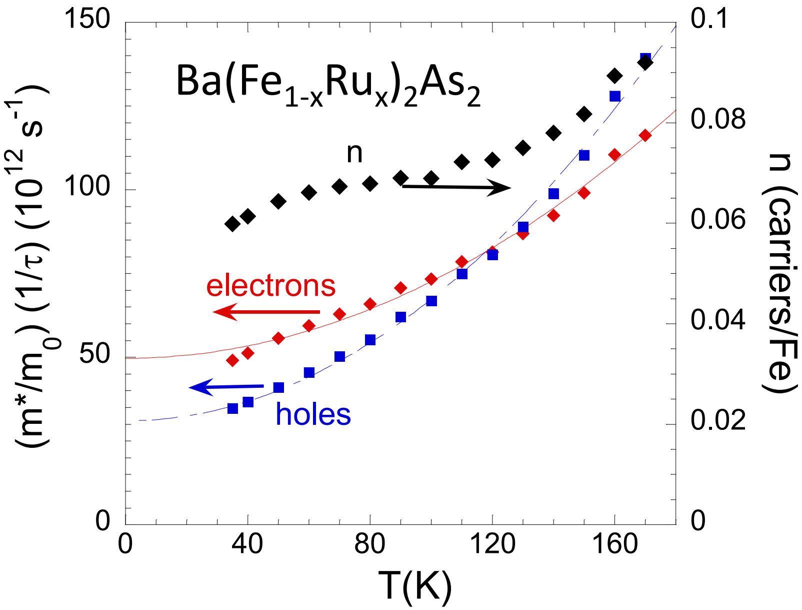
For a compensated semi-metal: $n_e = n_h = n$



$$R_H / \rho = \mu_h - \mu_e$$

$$\frac{\delta\rho}{\rho(0)} = \mu_e \mu_h H^2 \quad \Rightarrow \quad n, \mu_e, \mu_h$$

$$1/\rho = (\mu_h + \mu_e) ne$$



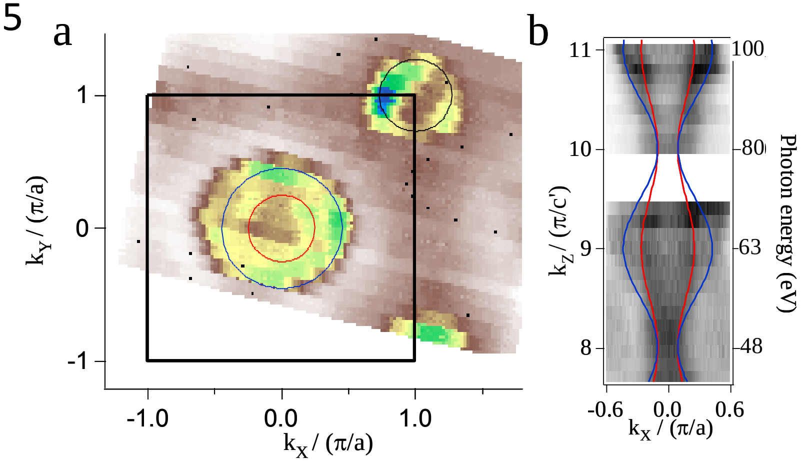
T^2 behavior for both holes and electrons

Fermi liquid

Comparaison with ARPES measurements

V. Brouet et al, PRL (2010)

x ~0.35



Modification of the band structure

For the hole pockets:

FS significantly warped along k_Z

Ru : isovalent substitution

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

But other ARPES studies show

no change of the carrier concentration

R. Dhaka et al. PRL(2011), N. Xu et al. PRL (2012)

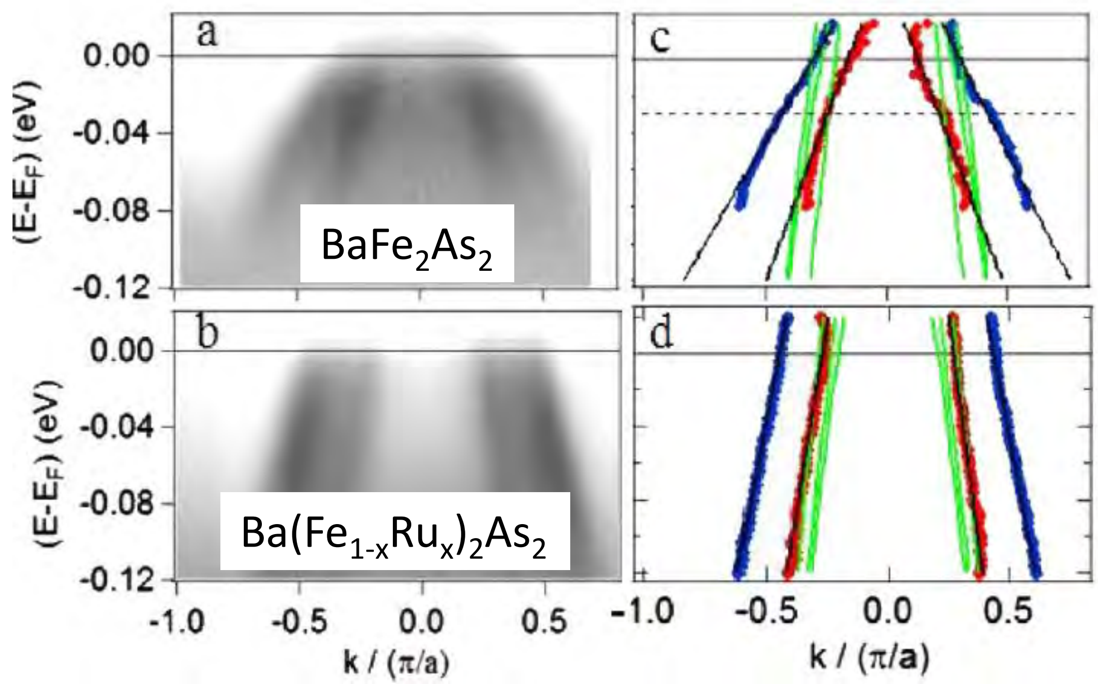
Electronic correlations

strongly reduced

v_F nearly three times larger

Might explain the increase of

the hole mobility



Outline

Transport measurements in the 122 family : Overview of the resistivity and Hall effect data

Necessity of a multiband description

Analysis of the resistivity and Hall effect measurements in a minimal two-band model: electron doped $BaFe_2As_2$ with Co and Ni substitution

Strong electron-hole asymmetry in the scattering rates

Comparison with ARPES results

Isovalent substitution: Ru/Fe

Resistivity, Hall effect and magnetoresistance

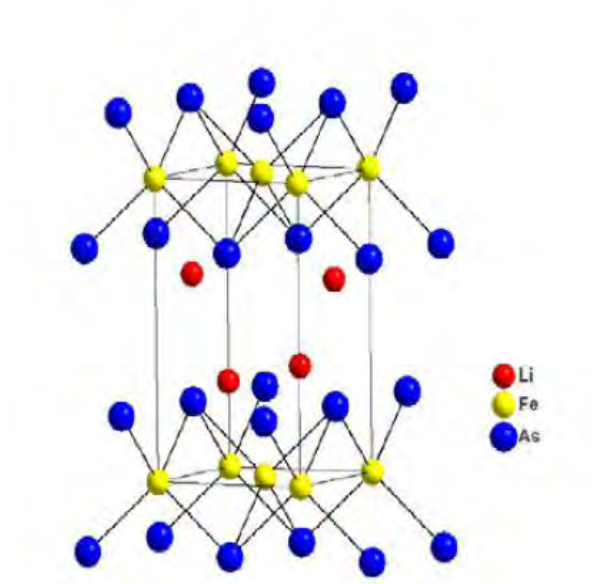
Description in a two band model

LiFeAs Resistivity, Hall effect and magnetoresistance

Analysis in relation with ARPES and quantum oscillations data

Beyond the two-band model

LiFeAs



$a=b=3.7715(2)$Å, $c=6.3574(3)$Å

T_c ~ 17-18K
Stoechiometric
Nearly compensated semi-metal

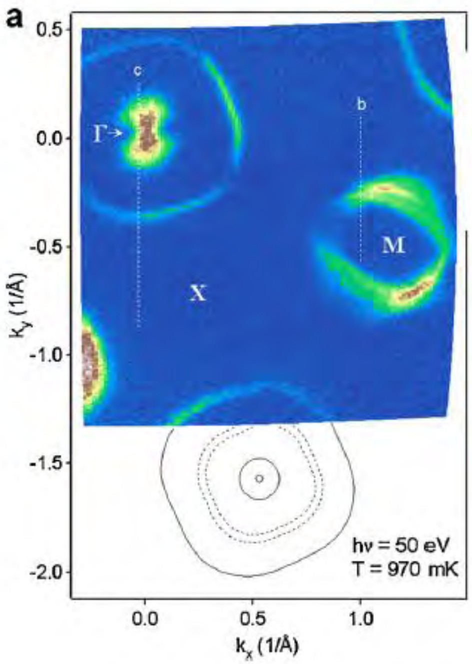
Defect free
Small upper-critical fields
Quantum oscillation measurements

Non polar surface : ARPES

Drawback: Very sensitive to air

Mechanism of superconductivity?
- Absence of nesting: Spin fluctuations?
- Orbital fluctuations : s_{++}

ARPES results on LiFeAs



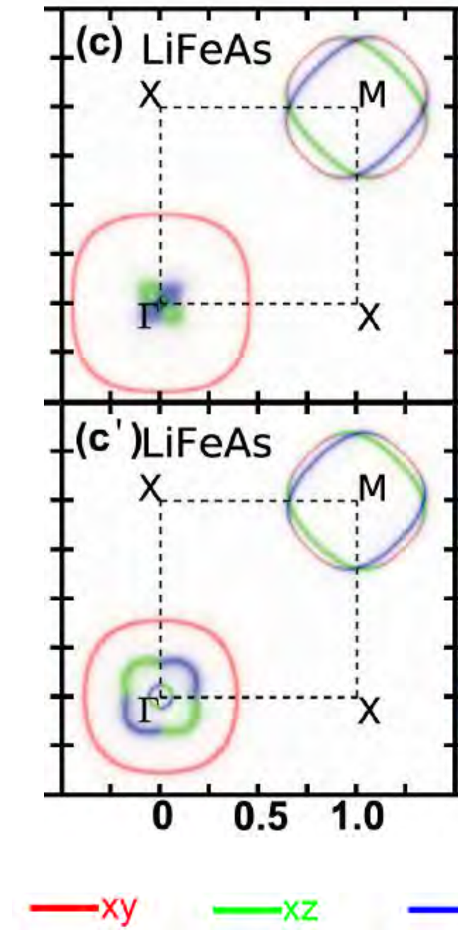
Borisenko et al. PRL (2010)

Good agreement with calculations if correlations are taken into account

Two hole bands

Two electron bands

$n_e \approx n_h \approx 0.2$ *carriers*/Fe



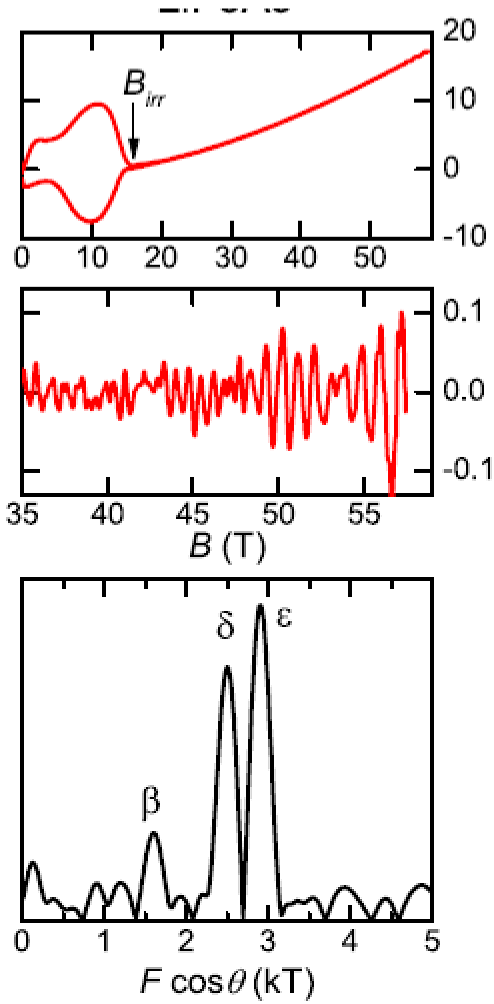
LDA +DMFT

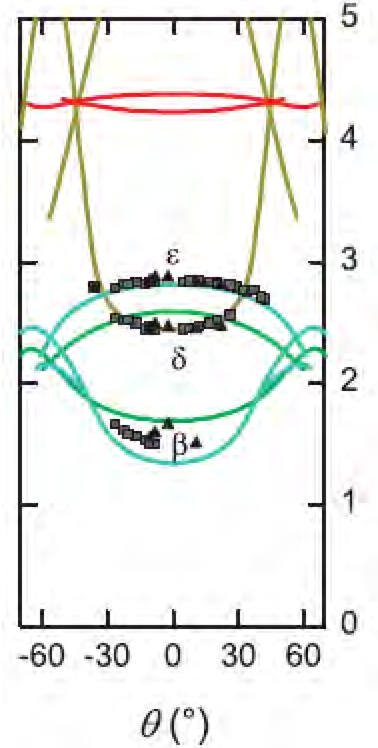
LDA

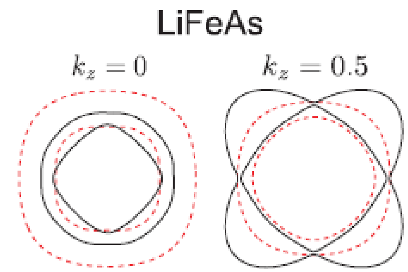
Yin et al., Nature materials

De Haas van Alphen experiments on LiFeAs

C. Putzke et al., PRL (2011)







3 different frequencies

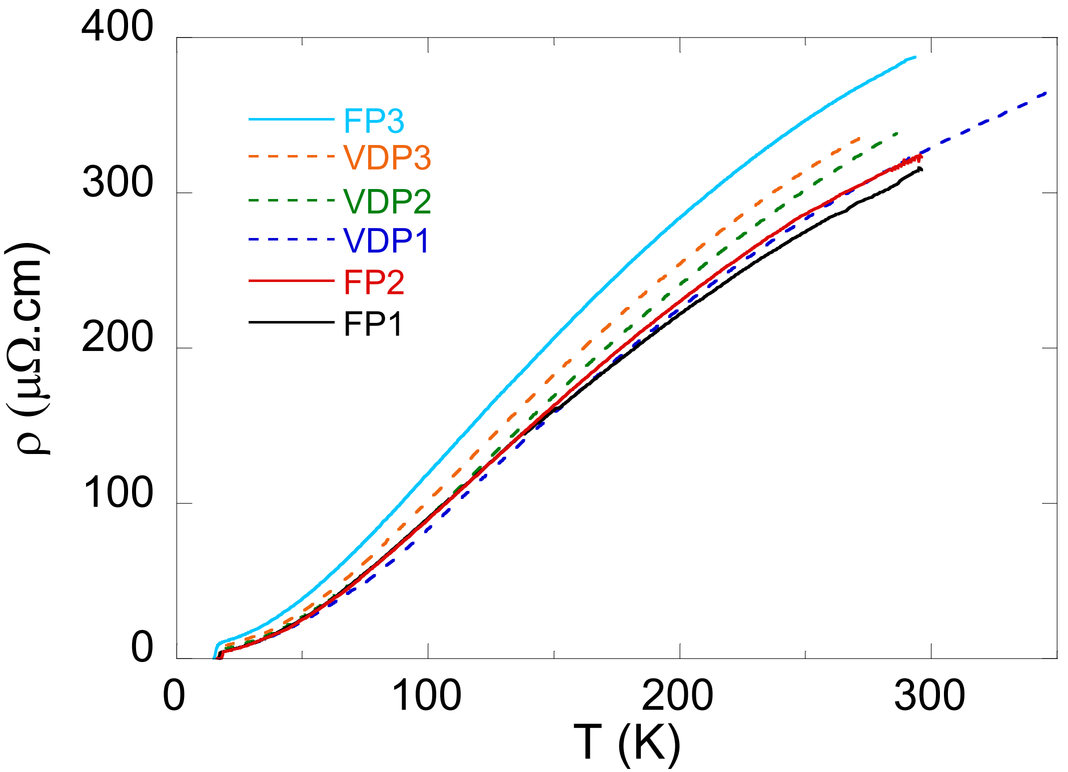
area of the FS sheets

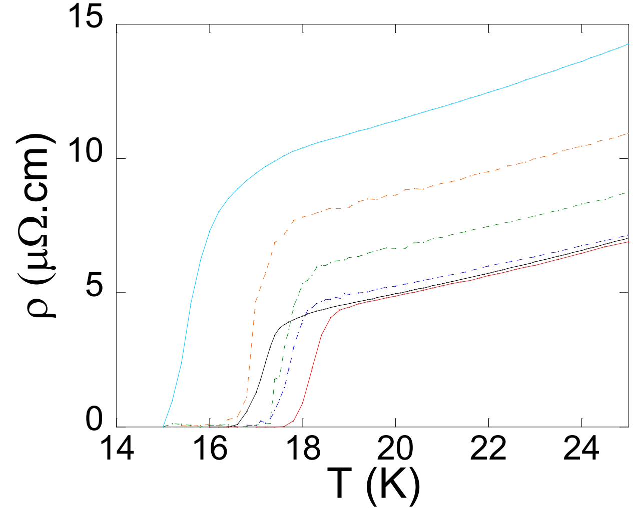
Electron bands

Inner band : ~ 0.08 el/Fe

Outer band: ~ 0.11 el/Fe

Transport properties of LiFeAs : resistivity





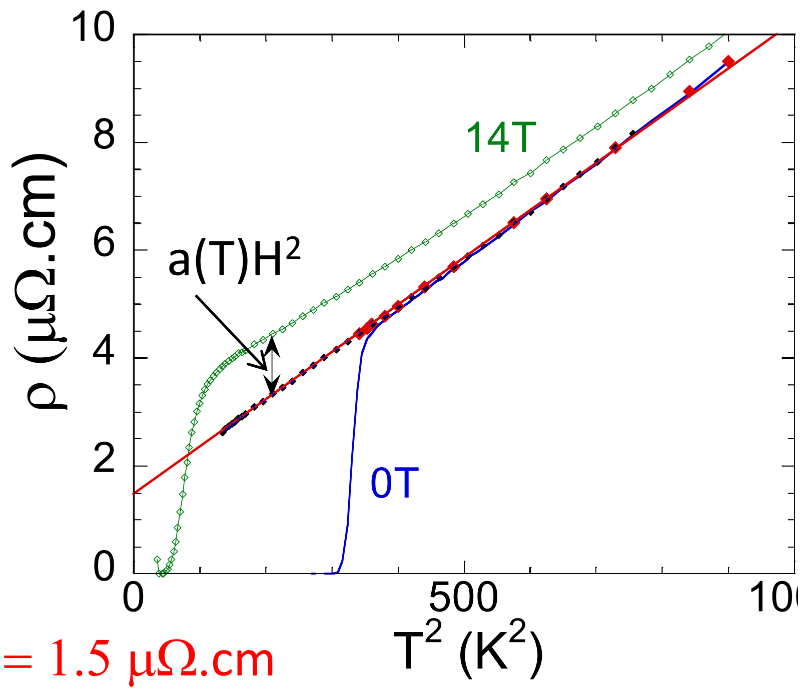
Correlation between T_c and resistivity at T_c

Compared to previous reports

Lower residual resistivity

larger RRR = $\rho(300K)/\rho_0 \sim 250$

LiFeAs : a Fermi liquid compound?



$\rho_0 = 1.5\ \mu\Omega.cm$

$$\rho(T) = \rho_0 + AT^2$$

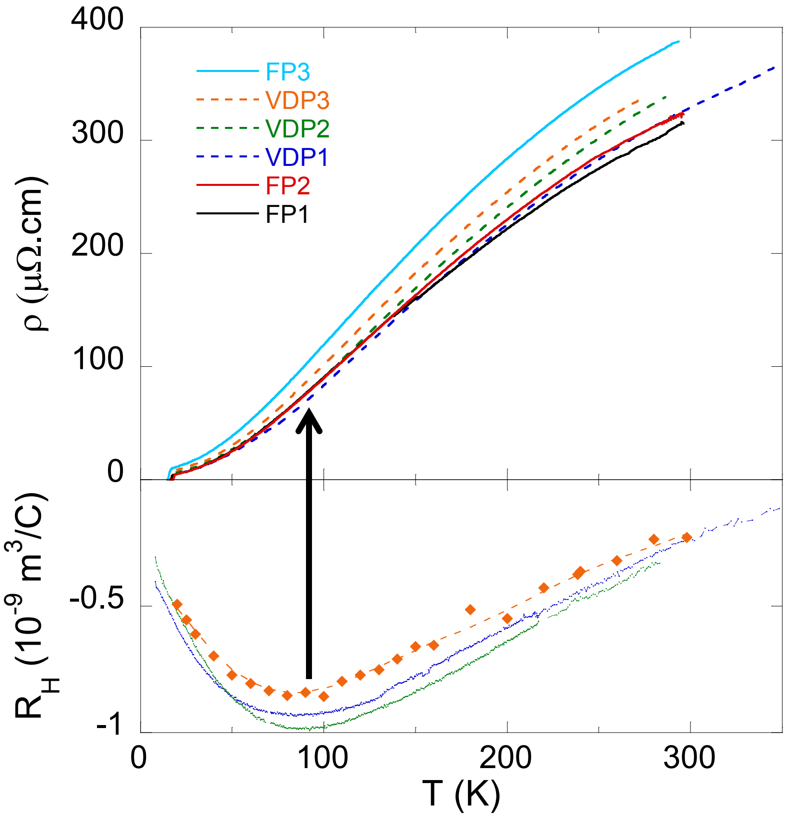
$$A \approx 9\, n\Omega.cm / K^2$$

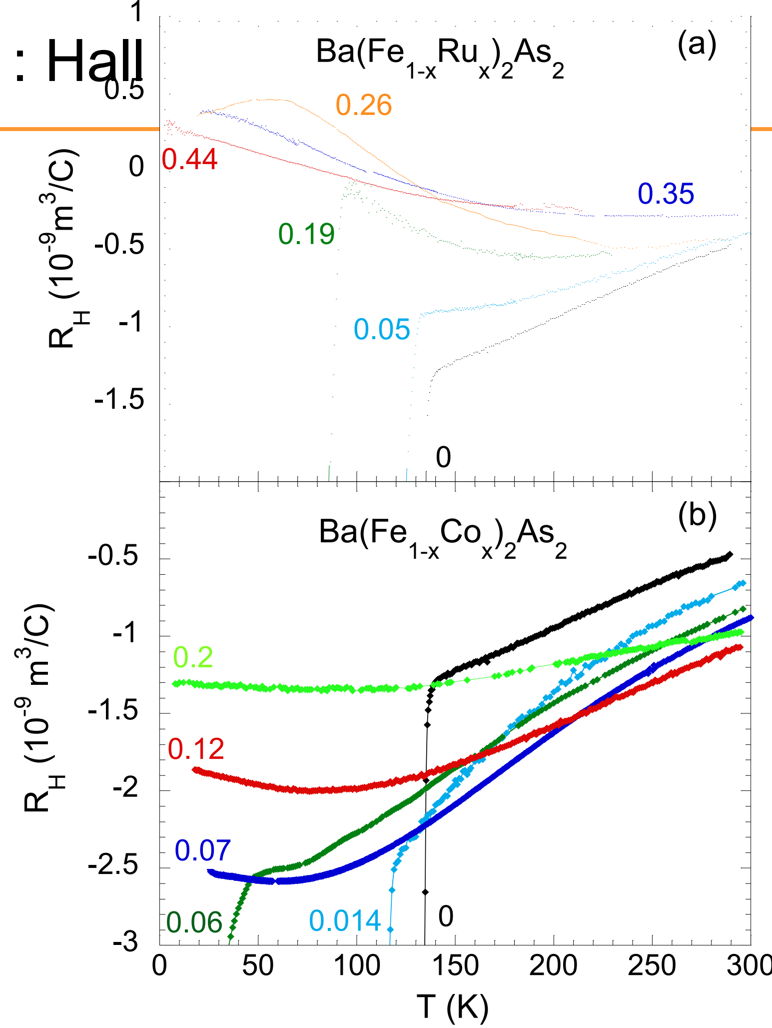
Sample	T_c (K)	ρ_0 ($\mu\Omega.cm$)	RRR	A ($n\Omega.cm/K^2$)
VDP1	17.75	4.15	80	9.7
VDP2	17.6	2.93	119	9.3
VDP3	17	4.55	79	9.5
FP1	18.2	1.47	225	8.8
FP2	17.15	1.21	263	9.3
FP3	15.6	6.34	62	12.7
Ref.[2]	17.75	15.2	38	22
Ref.[3]	17.3	13	53	20

A increases with ρ_0 ➡ Matthiessen's rule is not obeyed

Multiband material

Transport properties of LiFeAs : Hall



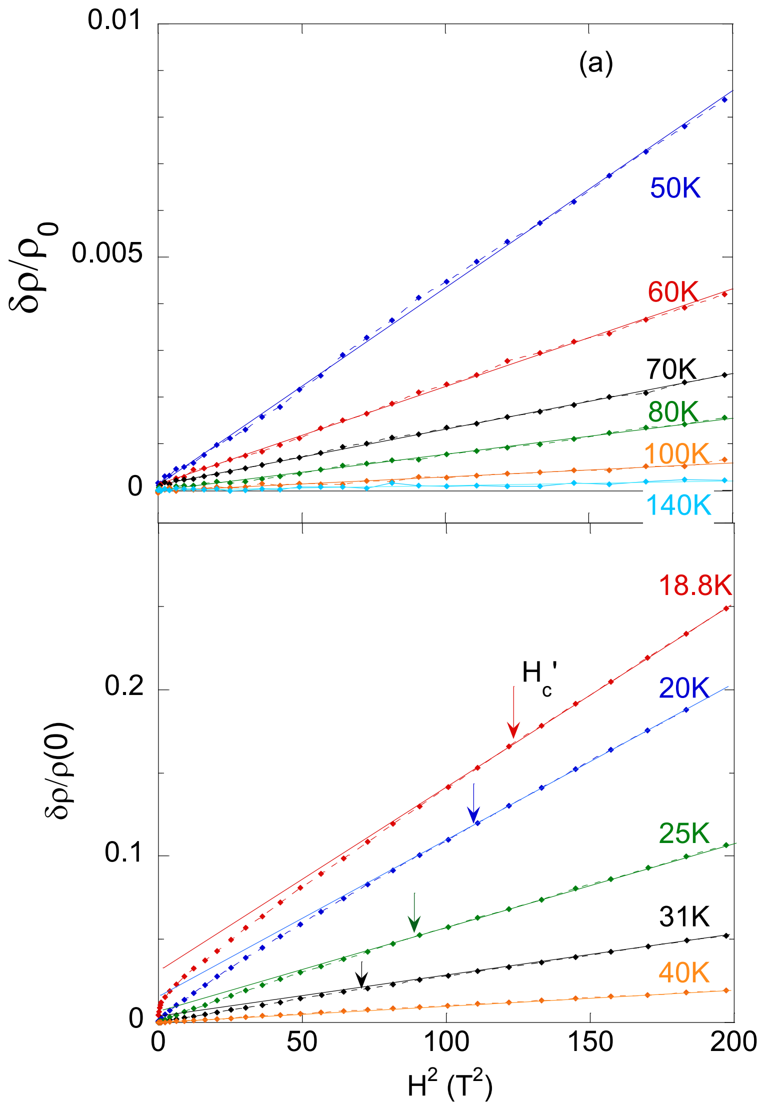


The Hall coefficient is negative

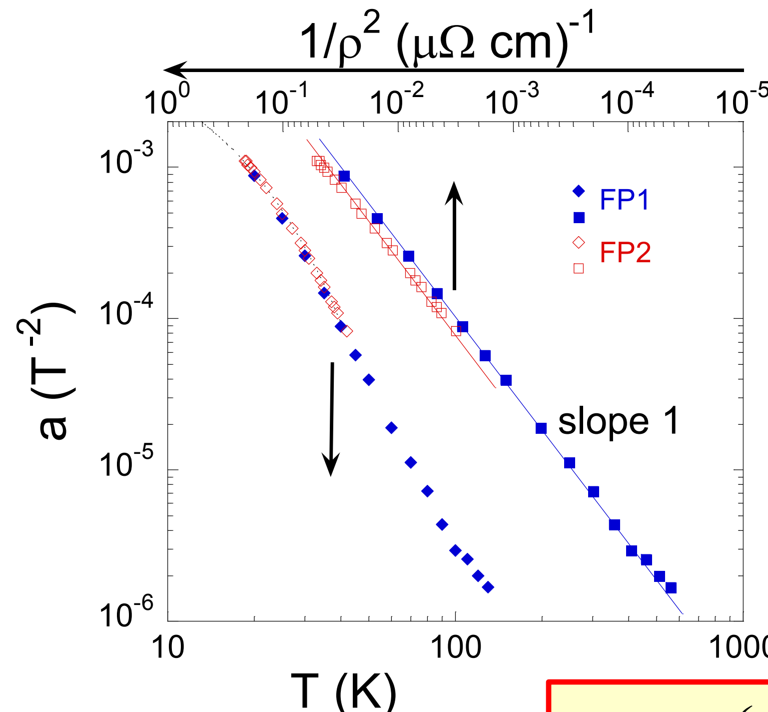
Transport dominated by the electrons as in $BaFe_2As_2$

Small minimum in R_H : corresponds to the change in curvature of $\rho(T)$

Transport properties of LiFeAs : Magnetoresistance



$$\frac{\delta\rho}{\rho(0)} = \frac{\rho(H) - \rho(0)}{\rho(0)} = a(T)H^2$$

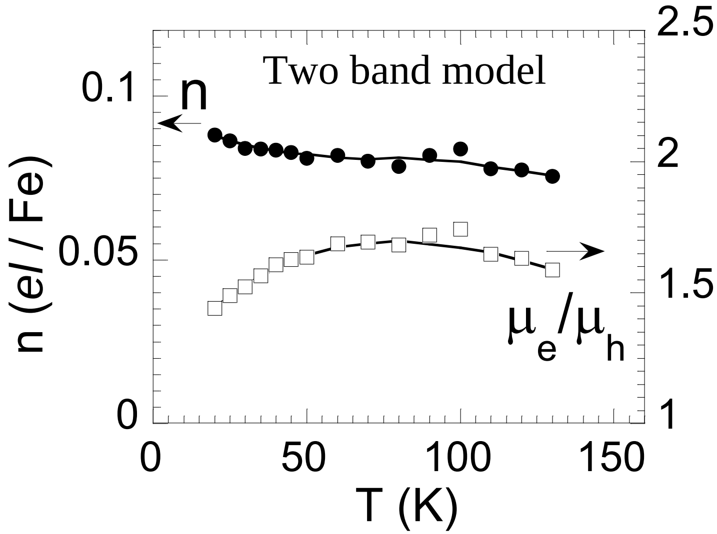


$$\frac{\delta\rho}{\rho(0)} \propto \left(\frac{H}{\rho}\right)^2$$

Kohler's rule

In a single band metal : $\delta\rho / \rho(0) \approx (\mu H)^2 \propto (H / \rho)^2$

Interpretation of the transport data in a two-band model



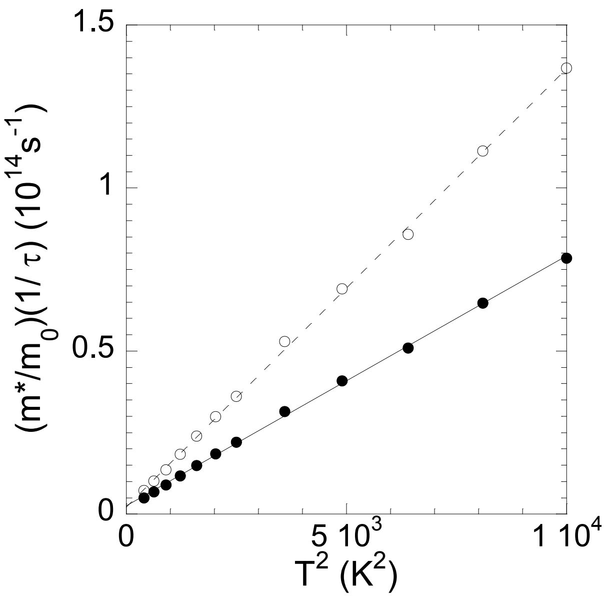
$$R_H / \rho = \mu_h - \mu_e$$

$$\frac{\delta\rho}{\rho(0)} = \mu_e \mu_h H^2$$

Ratio $\mu_e / \mu_h \approx 1.5$

Scattering rates $1/\tau \propto T^2$

➡ Fermi liquid behavior for both carriers

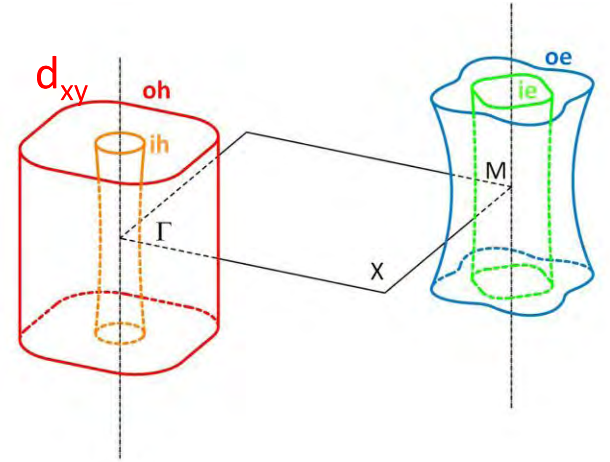


BUT : n ≈ 0.08 *carriers/Fe*

More than twice less than given by ARPES or Quantum oscillations experiments

Beyond the two band-model - 1

4 electronic bands with 4 different mobilities



Number of carriers taken from ARPES and dHvA data

$$\frac{1}{H^2}\frac{\delta\rho}{\rho(0)} = a(T) = \frac{\sigma_e\sigma_h(\mu_e+\mu_h)^2}{(\sigma_e+\sigma_h)^2} + \frac{\sigma_h}{(\sigma_e+\sigma_h)}A_h + \frac{\sigma_e}{(\sigma_e+\sigma_h)}A_e \qquad A_h = \frac{\sigma_{ih}\sigma_{oh}(\mu_{ih}-\mu_{oh})^2}{\sigma_h^{\ 2}}$$

Effective hole band

Effective mobility

$$\mu_h = \frac{\sigma_{ih}}{\sigma_h}\mu_{ih} + \frac{\sigma_{oh}}{\sigma_h}\mu_{oh}$$

Effective number of carriers

$$\sigma_h = n_h^{eff} e\mu_h$$

Can vary with temperature

Effective electron band

→ Two-band model with a Hall coefficient

$$R_H = \frac{\left(-n_e^{eff}\mu_e^2 + n_h^{eff}\mu_h^2\right)e}{(\sigma_e+\sigma_h)^2}$$

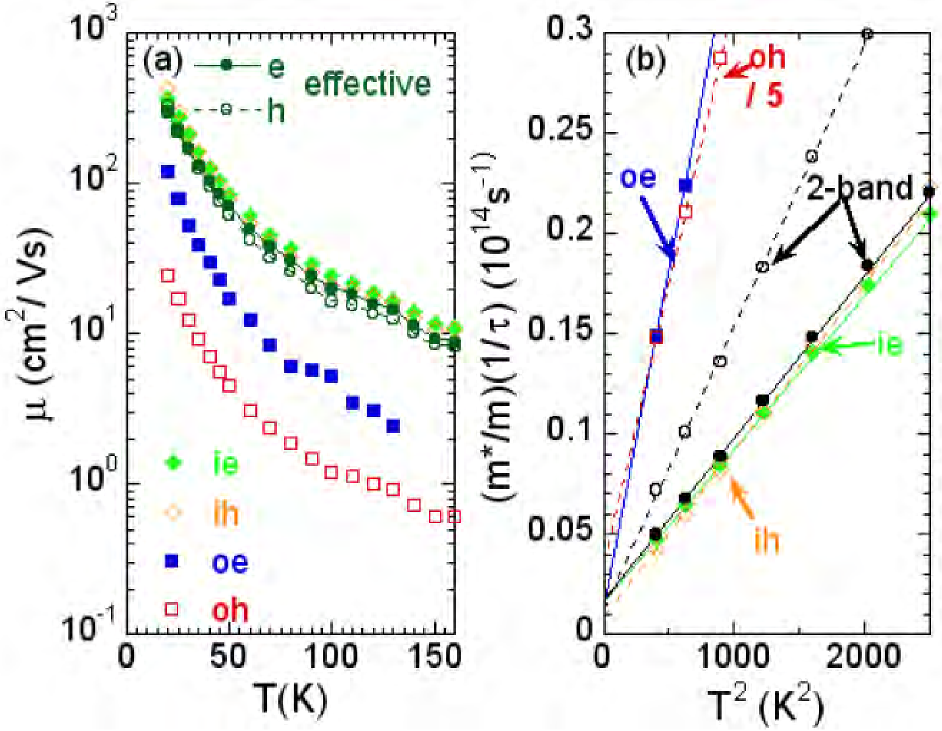
Beyond the two band-model - 2

Four different unknown parameters and only three experimental equations

➡ A unique solution cannot be acquired

Good solution must be such as $\mu_{ie} \geq \mu_{oe}$ and $0.02\, h/Fe \leq n_h^{eff} \leq 0.06\, h/Fe$

For instance : $n_h^{eff} = 0.05\, h/Fe$ independent of *T*



$\mu_{ie} \cong \mu_{ih}$

electrons $\mu_{ie} / \mu_{oe} \cong 3-6$

holes $\mu_{ih} / \mu_{oh} \cong 17$

$n_e^{eff} = 0.13\, e/Fe$

$\mu_e^{eff} \cong \mu_h^{eff}$ ➡ Kohler's rule

For all the carriers :

$1/\tau \propto T^2$

For the outer hole band

ARPES measurements give a MDC half width: δk = 18 meV (*A.A. Kordyuk et al. PRB 2011*)

$(m^*/m_0)(1/\tau) \sim 8\ 10^{13}\ s^{-1}$ comparable with $\sim 2\ 10^{13}\ s^{-1}$ found here by transport

Measurements of the lifetimes for the other pockets should be very interesting

Conclusion

- Multiband description of the transport properties

- For the compounds with isovalent substitution Ru/Fe -
  Description in a two band model seems reasonable
    - Number of carriers compatible with ARPES (Ru/Fe)
    - Fermi liquid behavior for both the holes and the electrons
    - Mobilities of holes and electrons comparable

- LiFeAs: low defect content
    - Comparison with ARPES and quantum oscillation measurements
    - Description more realistic of the transport properties by taking into account four different bands.

- Co substitution in $BaFe_2As_2$
    - Strong electron-hole asymmetry in the scattering rates: holes not visible in the transport properties
    - Difficult to reconcile with the ARPES data on the different lifetimes
    - Many theoretical questions….

Collaborators

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P. Bonville (Mössbauer)

LPS Véronique Brouet (ARPES)
H. Alloul
J. Bobroff , Y. Laplace, Y. Texier (RMN)

Co : Transport: FRA et al., Phys. Rev. Lett. **103** (2009).
ARPES: V. Brouet et al., Phys. Rev. B **80**, (2009).
RMN: Y. Laplace et al., PRB **80** (2009).
Mössbauer: P. Bonville, FRA et al. Europhys. Lett. **89** (2010)

Ni : Transport: A. Olariu, FRA et al.,Phys. Rev. B **83** (2011).
Mössbauer: A. Olariu et al. arXiv 1106.1332.

Ru : Transport: FRA et al., Phys. Rev. B **81** (2010).
ARPES: V. Brouet, FRA et al., Phys. Rev. Lett. **105** (2010)

LiFeAs: Transport: FRA et al, submitted (2012).

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