Nouveaux Supraconducteurs :

2008 : les « oxypnictides » de fer

P. Toulemonde

Institut Néel, Grenoble.

PLAN

- Introduction: Historique

- Cristallographie des différentes familles de composés supraconducteurs à base de tétraèdre de fer
    - LnFeAs(O,F) avec Ln = La, Ce, Pr, Nd, Sm
    - (AE, A)Fe_2As_2 avec AE = Ca, Sr, Ba et A = Li, K, Cs
    - A_xFeAs avec A = Li, Na
    - $FeSe_{1-x}$
- Facteurs structuraux contrôlant la supra (différences & similitudes avec les cuprates)

- Elaboration : poudres & monocristaux
    - tube scellé
    - haute pression – haute température

- Propriétés électroniques & paramètres fondamentaux supra
    - structure électronique
    - existence d'une onde de densité de spins (non supra)
    - transition structurale (non supra)
    - diagramme de phase
    - gap supra, paramètre d'ordre

- Contribution de l'Institut Néel @ Grenoble: élaboration & études sous HP

Arsenic heats up iron superconductors

Every week, scientists are posting papers on the preprint server arXiv with new proclamations of the material's properties. "It's phenomenal, because we've broken the tyranny of copper," says Paul Canfield, a physicist at the Ames Laboratory in Iowa.

The iron-based family might provide a fresh opportunity to engineer superconductors that operate at practical temperatures. It also offers chemists a chance to finally figure out how high-temperature superconductors work.

Much work remains. The researchers have so far worked only with superconducting powders and need to grow crystals, which are more useful for experiments. Copper-based superconductors are easy to work with, but the new family involves a trickier chemistry, and there is the toxicity and volatility of arsenic to consider. Last month, a sealed tube of arsenic exploded at the Argonne National Laboratory in Illinois, when a research group started to synthesize the new material for the first time. No one was hurt, but some academics won't work with arsenic because they don't want their graduate students to take risks.

Plus de 450 preprints depuis mars 2008 sur ArXiv/condmat !

Introduction :Historique

Groupe d'Hosono (Japon)

2006: LaFePO T_c = 3.2 K

J|A|C|S COMMUNICATIONS

Published on Web 07/15/2006

Iron-Based Layered Superconductor: LaOFeP

Yoichi Kamihara,† Hidenori Hiramatsu,† Masahiro Hirano,†,‡ Ryuto Kawamura,§ Hiroshi Yanagi,§ Toshio Kamiya,†,§ and Hideo Hosono*,†,‡

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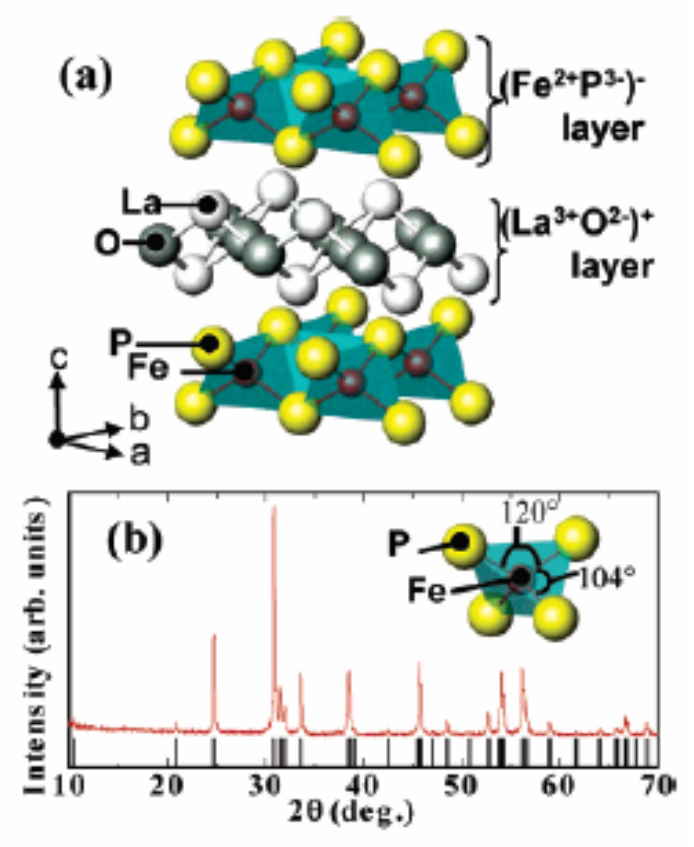
Received May 15, 2006; E-mail: hosono@msl.titech.ac.jp



2007: LaNiPO T_c= 3-7K

Inorg. Chem. **2007**, *46*, 7719–7721

Inorganic Chemistry Communication

Nickel-Based Oxyphosphide Superconductor with a Layered Crystal Structure, LaNiOP

Takumi Watanabe,† Hiroshi Yanagi,† Toshio Kamiya,†,‡ Yoichi Kamihara,‡ Hidenori Hiramatsu,‡ Masahiro Hirano,‡,§ and Hideo Hosono*,†,‡,§

Materials and Structures Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta, Yokohama, Japan, ERATO-SORST, JST, in the Frontier Collaborative Research Center, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama, Japan, and Frontier Collaborative Research Center, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama, Japan

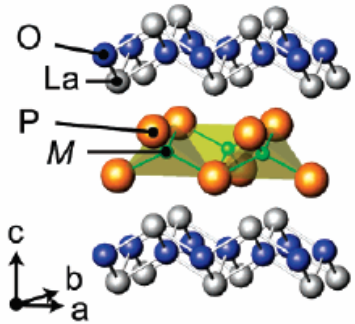


Figure 1. Crystal structure of LaMOP (M = divalent transition-metal cation). The yellow polyhedron indicates the MP_4 tetrahedron. LaO and MP layers are alternately stacked along the *c* axis.

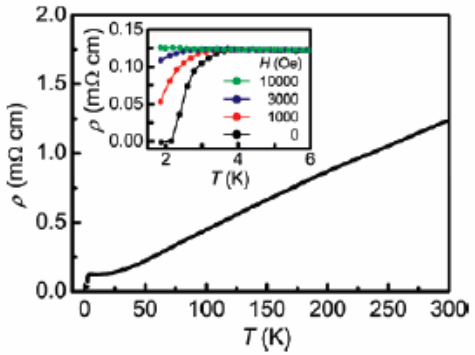


Figure 3. Temperature (T) dependence of the electrical resistivity (ρ) at 0 Oe. The inset shows the $\rho-T$ curves as a function of the magnetic field magnified in the temperature range of 1.9−10 K.

2008: Supraconductivité à T_c= 26 K dans LaFeAs($O_{1-x}F_x$) !!!
Groupe d'Hosono, J. Am. Chem. Soc. 130.

Iron-Based Layered Superconductor La[$O_{1-x}F_x$]FeAs (x = 0.05−0.12) with T_c = 26 K

Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

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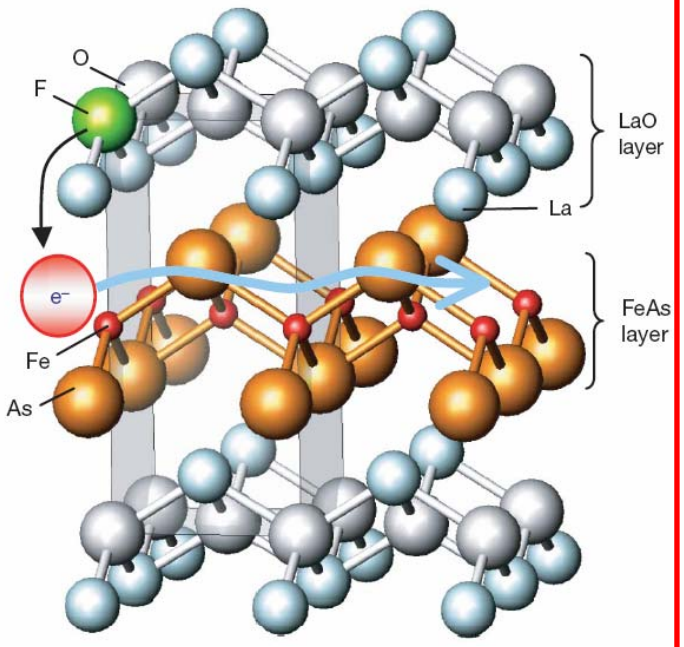


P4/nmm
structure type « ZrCuSiAs »

JOURNAL OF SOLID STATE CHEMISTRY 11, 161–166 (1974)

1974

ZrCuSiAs: A "Filled" PbFCl Type

V. JOHNSON AND W. JEITSCHKO

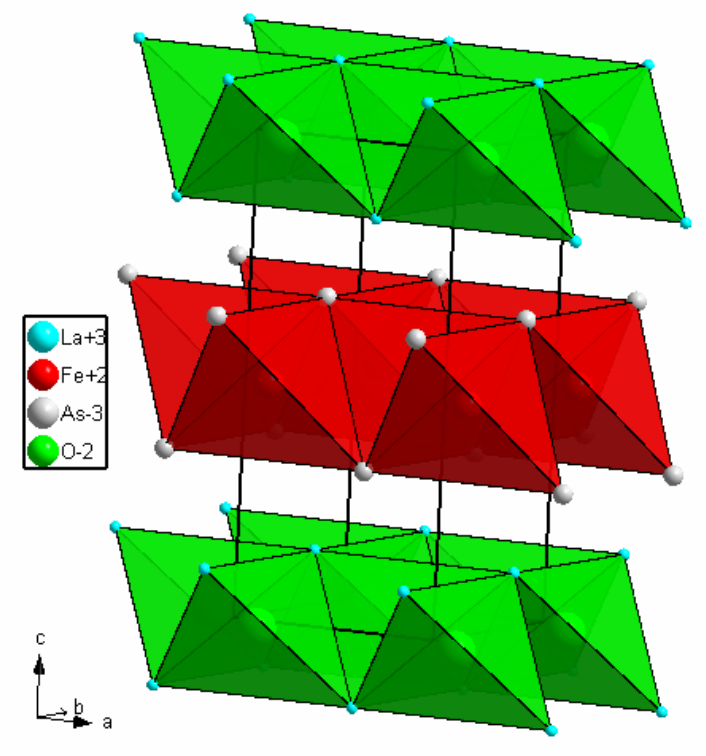
Central Research Department, E. I. du Pont de Nemours and Company, Wilmington Delaware 19898*

Received December 27, 1973

ZrCuSiAs is tetragonal, space group $P4/nmm$, $a = 3.6736$, $c = 9.5712$ Å, $Z = 2$. The structure is a "filled" PbFCl type, or it may alternatively be regarded as a tetragonally distorted $MnCu_2Al$ (Heusler) structure. HfCuSiAs is iso-structural. Bonding in PbFCl-related structures is discussed.

- **Supra** à base de **fer** !
- Structure « lamellaire » ↔ plans CuO_2 des **cuprates**!
- $(La^{3+}O^{2-})(Fe^{2+}As^{3-})$: **transfert de charges** réservoir de charges vers bloc supra

LaFeAsO



OLa_4

$FeAs_4$

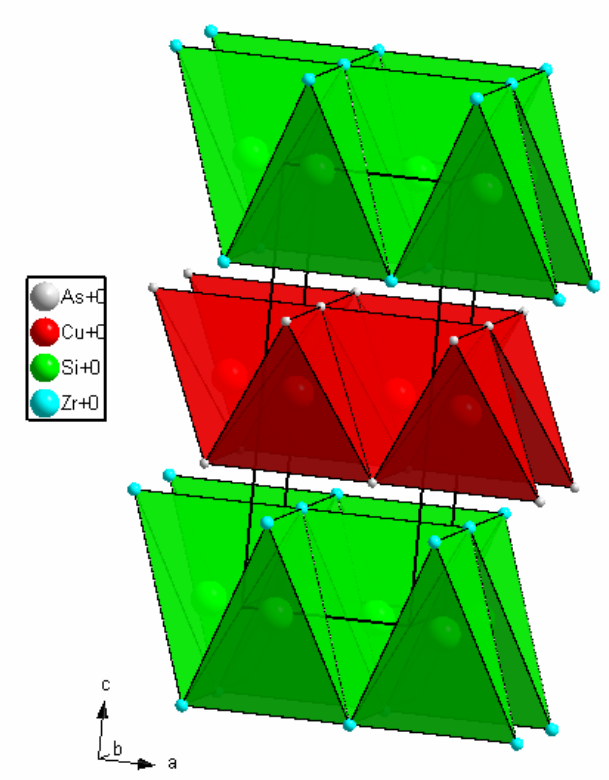
Crystal data

Crystal system	tetragonal
Space group	*P* 4/n m m (no. 129)
Unit cell dimensions	*a* = 4.03 Å *c* = 8.74 Å

Atomic coordinates

Atom	Wyck.	x	y	z
La1	2*c*	1/4	1/4	0.1399(2)
Fe1	2*b*	3/4	1/4	1/2
As1	2*c*	1/4	1/4	0.6565(3)
O1	2*a*	3/4	1/4	0

ZrCuAsSi



$SiZr_4$

$CuAs_4$

Crystal data

Crystal system	tetragonal
Space group	*P* 4/n m m (no. 129)
Unit cell dimensions	*a* = 3.6736(2) Å *c* = 9.5712(9) Å

Atomic coordinates

Atom	Wyck.	x	y	z
Zr	2*c*	1/4	1/4	0.2246(6)
Cu	2*b*	1/4	3/4	1/2
As	2*c*	1/4	1/4	0.6793(8)
Si	2*a*	1/4	3/4	0

1995	Familles LnO**FeP** (Ln = La-Nd, Sm, Gd) LnO**RuP** (Ln = La-Nd, Sm, Gd) LnO**CoP** (Ln = La-Nd, Sm)	flux d'étain structure type ZrCuSiAs P4/nmm	B.I. Zimmer, W. Jeitschko et al. J. Alloy Comp., 229 (1995) 238 **[Münster]**
1998	RO**ZnP** (R = Y, La-Nd, Sm, Gd-Tm) RO**ZnAs** (R) Y, La-Nd, Sm, Gd-Dy)	flux NaCl/KCl **R -3m** ou P4/nmm	A.T. Nientiedt and W. Jeitschko, Inorg. Chem. 37 (1998) 386-389 **[Münster]**
2000	RO**FeAs** (R = La–Nd, Sm, Gd) RO**RuAs** (R = La–Nd, Sm, Gd–Dy) RO**CoAs** (R = La–Nd)	flux NaCl/KCl P4/nmm	P. Quebe, L.J. Terbüchte, W. Jeitschko, Journal of Alloys and Compounds 302 (2000) 70–74 **[Münster]**
2006	CeO**ZnP** PrO**ZnP**	flux NaCl/KCl R -3m ou P4/nmm	H. Lincke, T. Nilges, and R. Pöttgen, Z. Anorg. Allg. Chem. 632 (2006) 1804-1808 **[Münster]**

Plus de 150 composés de structure du type « ZrCuSiAs » !

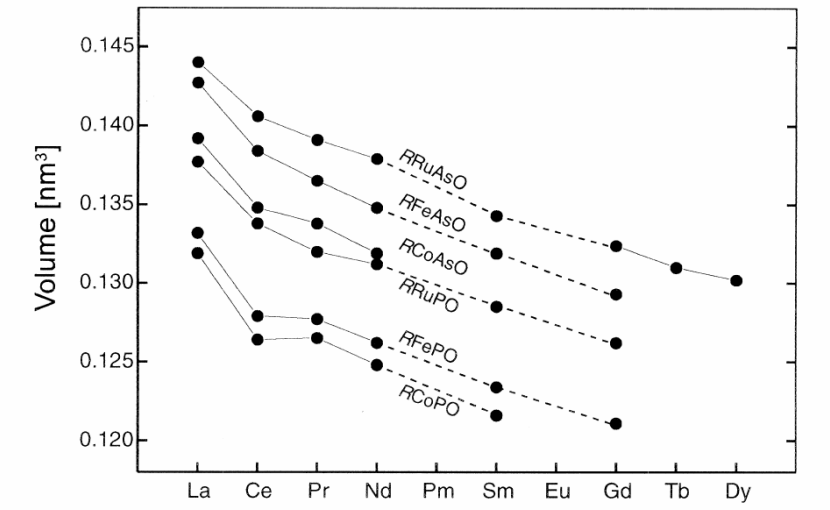


Fig. 1. Cell volumes of compounds *RTPn*O (*T*=Fe, Ru, Co; *Pn*=P, As) with ZrCuSiAs type structure.

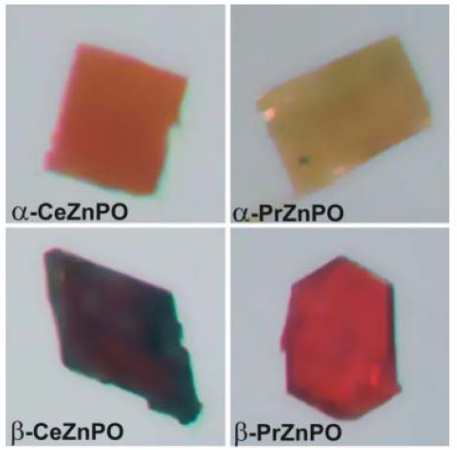


Fig. 1 Photographs of flux grown single crystals of the α- and β-modifications of CeZnPO and PrZnPO. The edge lengths of the crystals are ca. 50 µm.

Famille LnFeAsO
[Ln = La, Ce, Pr, Nd,n Sm, Gd, Tb]
= Ln-1111

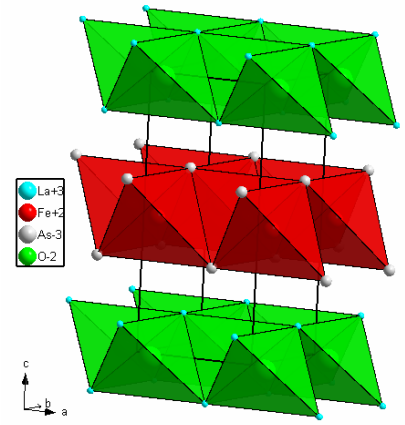
Existe aussi la supra dans
$(Sr_{1-x}La_x)FeAsF$ à T_c = 36K
et dans $Ca(Fe_{1-x}Co_x)AsF$
à T_c = 20K

2006	LaFeP(O,F)	T_c = 4 – 7K	3.964 Å	8.512 Å	
2007	LaNiPO	T_c = 3 – 4 K			
2008	LaFeAs(O,F) **(dopage électrons)**	T_c = 26 K **(41K?)**	4.032 Å	8.726 Å	1150°C / 48h **6 GPa 1250°C / 2h ($O_{0.4}F_{0.6}$)**
	(La,Sr^{2+})FeAsO **(dopage trous)**	T_c = 25 K	4.035 Å	8.771 Å	
	(La,Sr^{2+})NiAsO	T_c = 2.7–3.7K			1150°C / 48h
	CeFeAs(O,F)	T_c = 41 K	3.989 Å	8.631 Å	1150 °C / 50h
	PrFeAs(O,F)	T_c = 50-52 K	3.967 Å	8.561 Å	6 GPa 1250°C / 2h
	NdFeAs(O,F)	T_c = 51 K			3.3 à 6GPa 1300 à 1400°C 2-8h
	SmFeAs(O,F)	T_c = 43 – 54K	3.943 Å	8.514 Å	
	GdFeAs(O,F)	T_c = 10 – 36K	4.001 Å	8.650 Å	
	(Gd,Th^{4+})FeAsO	T_c = 56 K	3.917 Å	8.440 Å	1150°C / 48h
	GdFeAs($O_{1-\delta}$)	T_c = 53 K	3.890 Å	8.383 Å	6 GPa 1350°C 2h
	EuFeAs(O,F), TmFeAs(O,F)	Phase non formée			1150 °C /24-50 h
	LaRuAs(O,F), CeRuAs(O,F)	Métallique			1150 °C /24-50 h
	LaNiAsO	T_c = 4 K	4.123 Å	8.188 Å	1000°C / 24 h
	LaNiBi($O_{1-\delta}$)	T_c = 4 K	4.073 Å	9.301 Å	800°C / 10 h

Famille (AE,A)Fe_2As_2 [AE = Ba,Sr,Ca et A=Cs,Rb,K] = AE-122

LnFeAsO

(dopé: $T_{c\,max}$ = 55 K pour Sm)

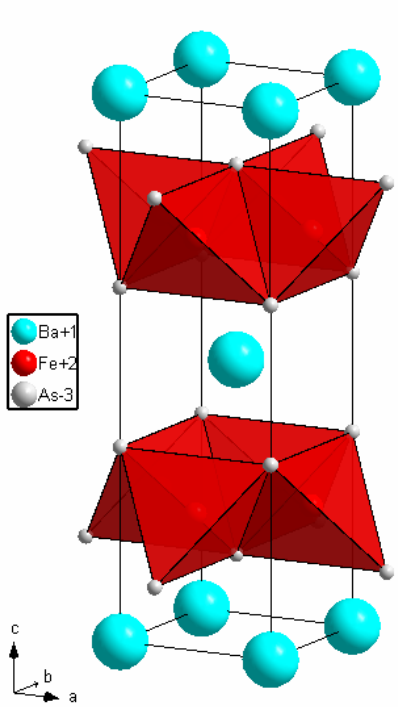


Ln-As: 3.36Å
Fe-As: 2.435Å
Fe-Fe: 2.85Å et 8.74Å

As-Fe-As:
111.6° et 108.4°

$BaFe_2As_2$

(dopé: $T_{c\,max}$=38K)



Ba-As: 3.38Å
Fe-As: 2.40Å
Fe-Fe: 2.80Å et 6.51Å

As-Fe-As:
111.1° et 108.7°

Crystal data

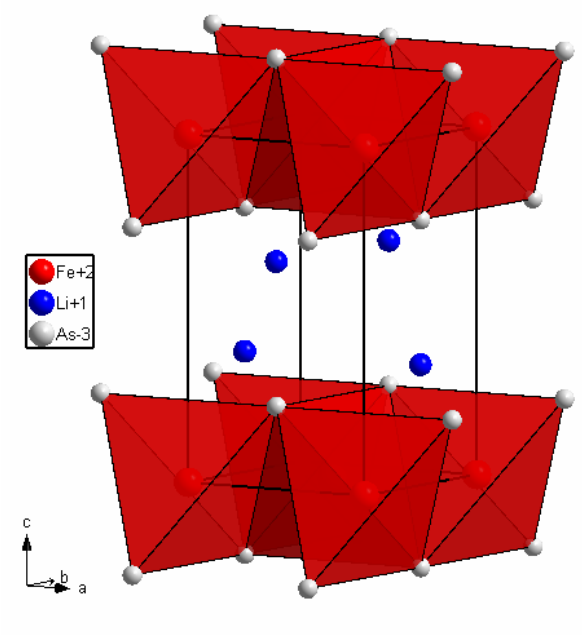
Crystal system	tetragonal
Space group	*I* 4/m m m (no. 139)
Unit cell dimensions	*a* = 3.9625(1) Å *c* = 13.0168(3) Å

Atomic coordinates

Atom	Wyck.	x	y	z
Ba	2*a*	0	0	0
Fe	4*d*	0	1/2	1/4
As	4*e*	0	0	0.3545(1)

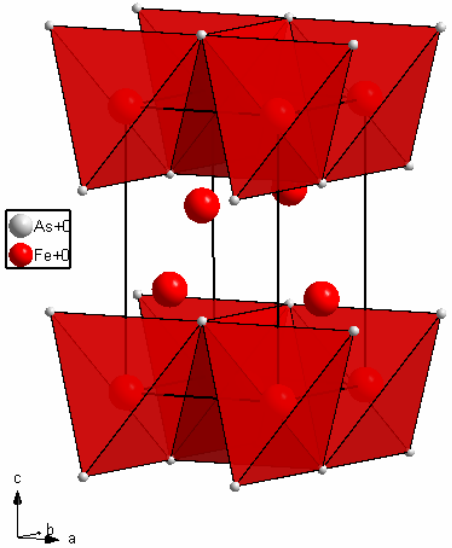
Famille AFeAs [A = Na,Li] = A-111

NaFeAs et LiFeAs (Oxford)



AFeAs	Li	Na
M-As (Å)	2.76	2.99
Fe-As (Å)	2.41	2.437
Fe-Fe (Å)	2.775 et 6.35	2.793 et 7.04
As-Fe-As (°)	112.9 et 102.9	108.3 et 110.1
T_c (K)	18 K	9 K

Fe_2As = FeFeAs



Crystal data

Crystal system	tetragonal
Space group	*P* 4/n m m (no. 129)
Unit cell dimensions	*a* = 3.7754 Å *c* = 6.3534 Å

Atomic coordinates

Atom	Wyck.	x	y	z
Fe1	2*a*	0	0	0
Li1	2*c*	1/2	0	0.65380
As1	2*c*	1/2	0	0.23685

Crystal data

Crystal system	tetragonal
Space group	*P* 4/n m m (no. 129)
Unit cell dimensions	*a* = 3.6300 Å *c* = 5.9800 Å

Atomic coordinates

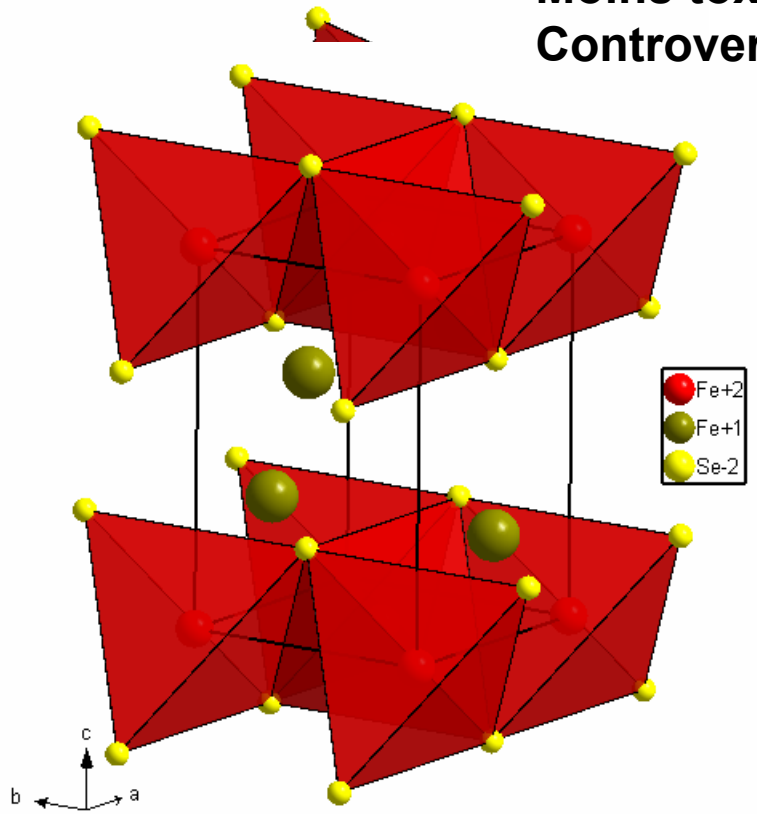
Atom	Wyck.	x	y	z
As1	2*c*	0	1/2	0.73500
Fe1	2*a*	0	0	0
Fe2	2*c*	0	1/2	0.33000

Famille $Fe_yFe(Se_{1-x}Ch_x)$ [Ch = S, Te] = Fe-111

$FeSe_{1-x}$ (tétragonal):

Fe_yFeSe (tétragonal)

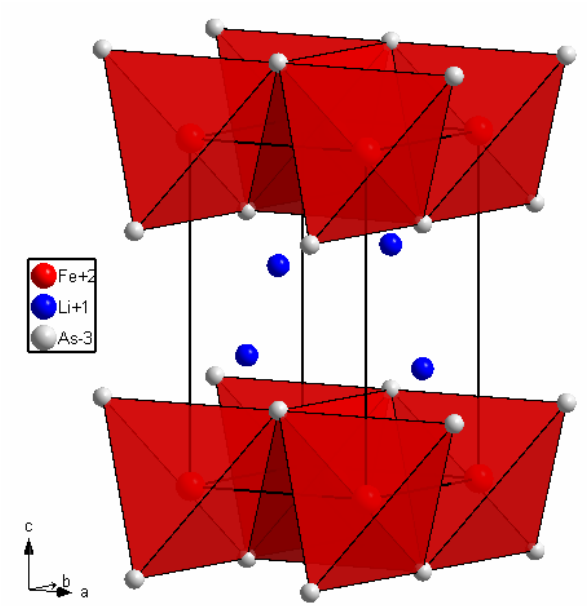
Fe en site tétraédrique!
Moins toxique que As?
Controverse: lacunes de Se?



Fe_y-Se: 2.66 Å
Fe-Se: 2.367 Å
Fe-Fe: 2.66 Å et 5.52 Å

As-Fe-As:
111.6° et 105.4°

LiFeAs



$FeSe_{1-x}$ *F.-C. Hsu et al. Condmat #0807.2369 T_c max = 8 K*
$FeSe_{1-x}$ *Y. Mizuguchi et al. condmat #0807.4315 $T_{c\ onset}$ max = 27K @ 1.5GPa*
$Na_{0.1}FeSe$ $Fe_{0.92}Co_{0.08}Se$ *Z.Liu et al.condmat #08081784 Tc = 8.3-8.4K*
$Fe(Se_{1-x}S_x$ ou $Te_x)$ *Y. Mizuguchi et al. condmat #0811.1123 T_c max = 15K*

condmat #0807.4315

Superconductivity at 27 K in tetragonal FeSe under high pressure

Yoshikazu Mizuguchi[1,2], Fumiaki Tomioka[1], Shunsuke Tsuda[1,3],
Takahide Yamaguchi1 and Yoshihiko Takano1,2
1. National Institute for Materials Science, 1-2-1, Sengen, Tsukuba, 305-0047, Japan
2. University of Tsukuba, 1-1-1, Tennodai, Tsukuba, 305-8577, Japan
3. WPI-MANA-NIMS, 1-1, Namiki, Tsukuba, 305-0044, Japan

Abstract
A huge enhancement of the superconducting transition temperature *T*c was observed in tetragonal FeSe superconductor under high pressure. The onset temperature became as high as 27 K at 1.48 GPa and the pressure coefficient showed a huge value of 9.1 K/GPa. The upper critical field **H_{c2} was estimated to be ~ 72 T** at 1.48 GPa. Because of the high H_{c2}, FeSe system may be a candidate for application as superconducting wire rods. Moreover, the investigation of superconductivity on simple structured FeSe may provide important clues to the mechanism of superconductivity in iron-based superconductors.

D’autres familles ?

Chemistry of layered *d*-metal pnictide oxides and their potential as candidates for new superconductors

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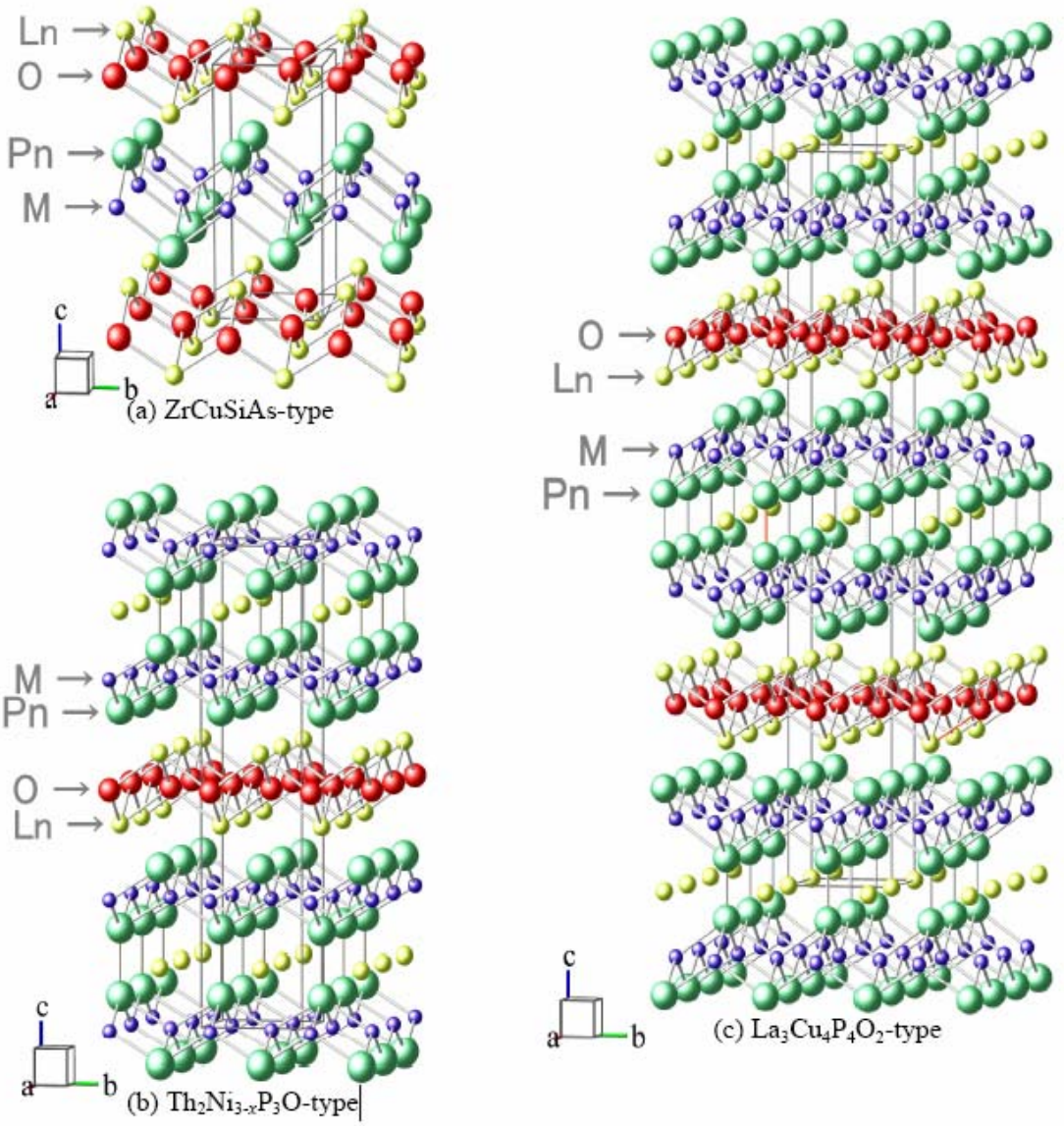
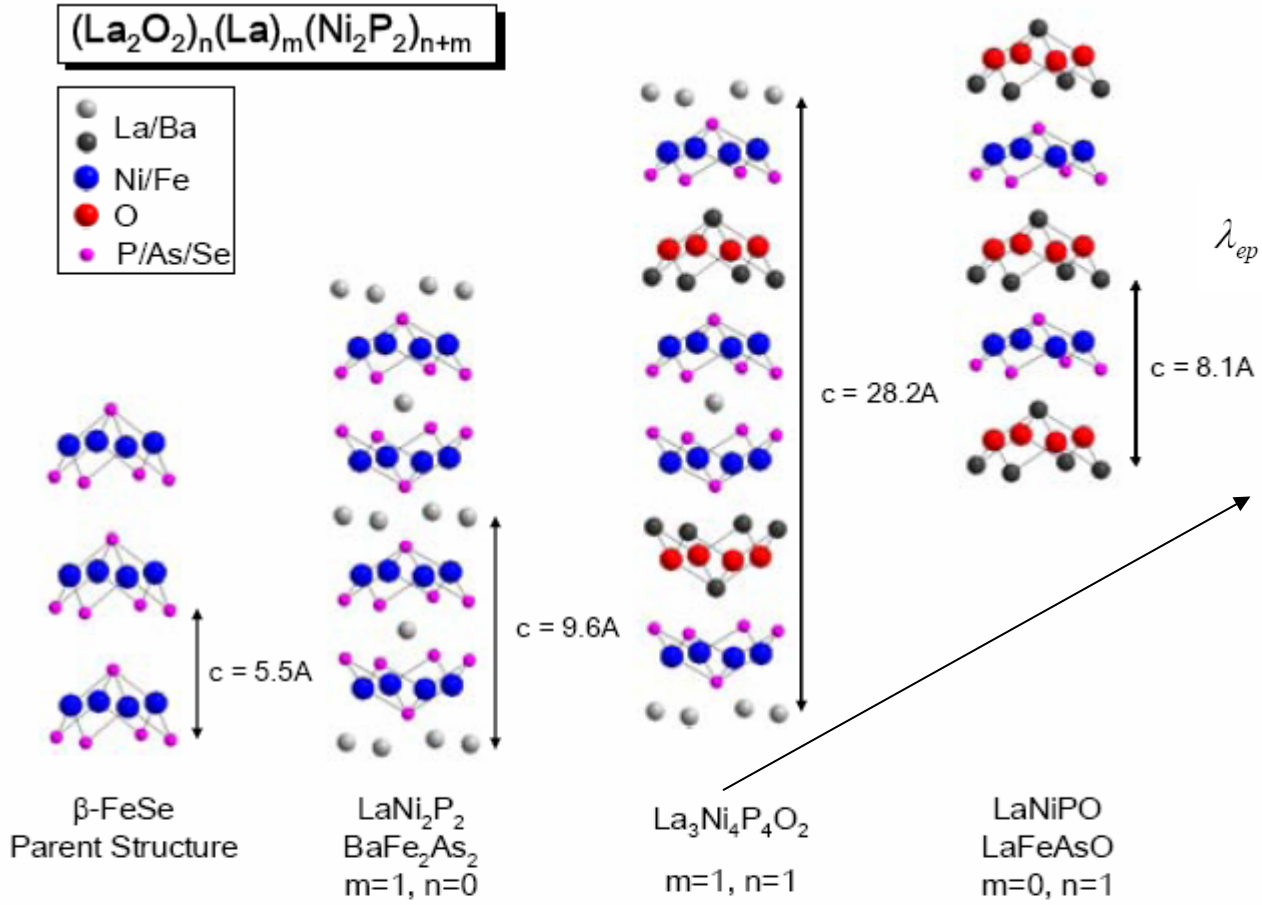
Condmat #0808.1158



D'autres familles ?

Intercroissances: approche du groupe de R.J.Cava (USA)



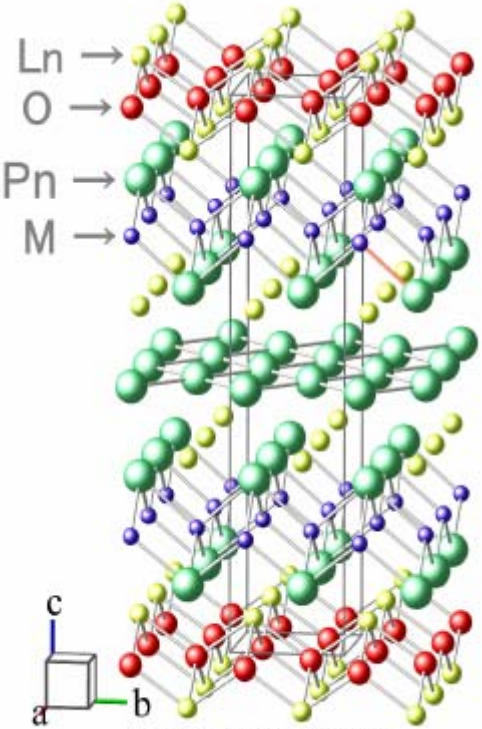
$$\lambda_{ep} = \frac{1.04 + \mu^* \ln(\Theta_D / 1.45T_c)}{(1 - 0.62\mu^*)\ln(\Theta_D / 1.45T_c) - 1.04}$$

$La_3Ni_4P_4O_2$: T_c = 2.2K

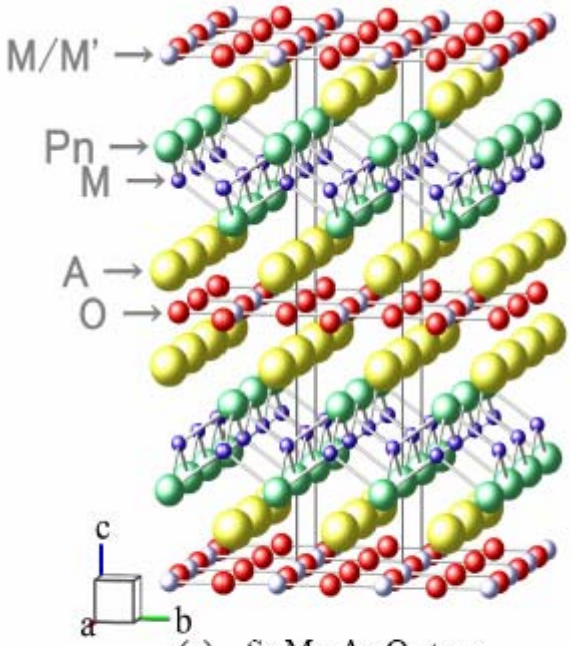
Supra type BCS
avec couplage e-ph faible
à modéré
$\lambda_{e\text{-}ph}$ = 0.46

Figure 1. (color on line) $La_3Ni_4P_4O_2$ is a member of a series of compounds built by inserting charged ions or layers between M_2X_2 sheets of the parent β-FeSe structure. All of the new, known Fe- and Ni- based superconductors are members of this family. The La^{3+} and O^{-2} ions are drawn with ionic radii and the M and X atoms are drawn using covalent radii.

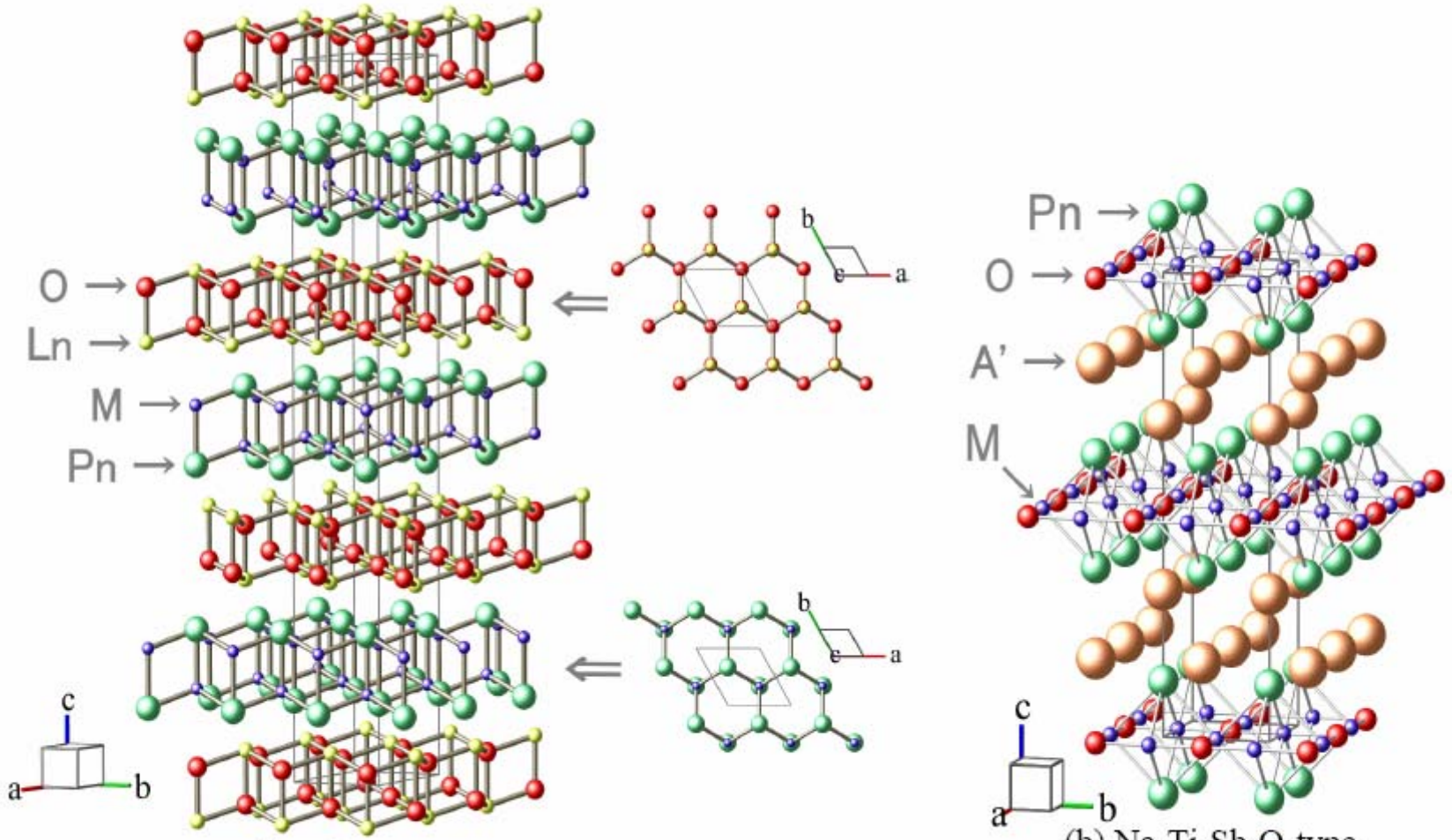
Condmat 0808.1557



(d) $U_2Cu_2As_3O$-type

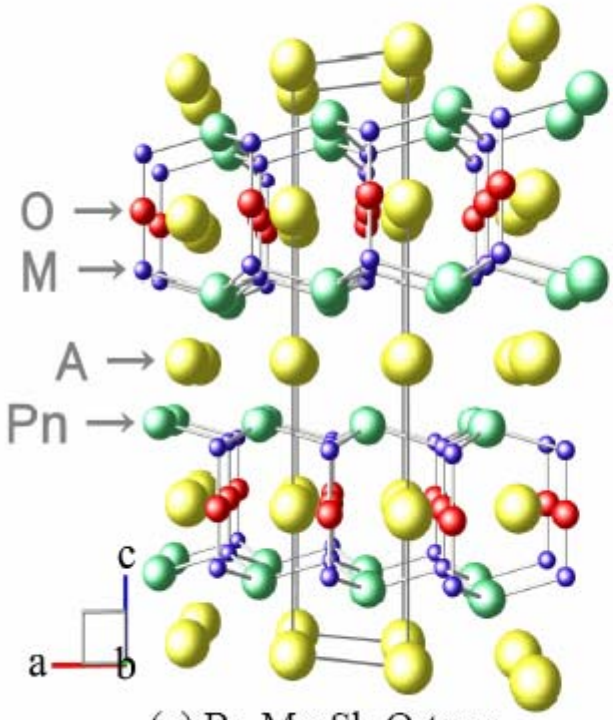


(e) $Sr_2Mn_3As_2O_2$-type

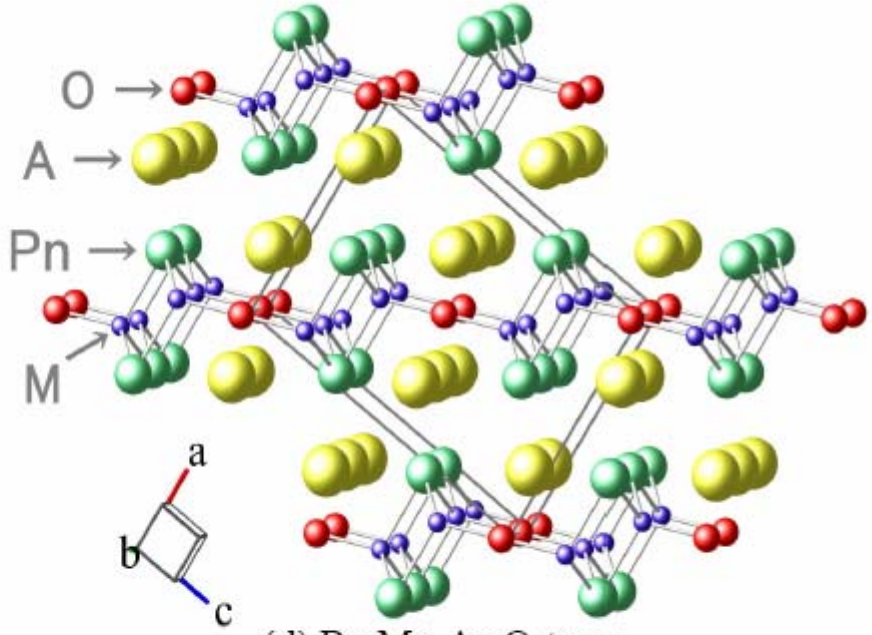


(a) NdZnPO-type

(b) $Na_2Ti_2Sb_2O$-type



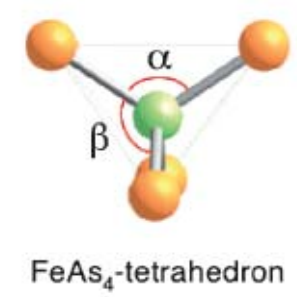
(c) $Ba_2Mn_2Sb_2O$-type



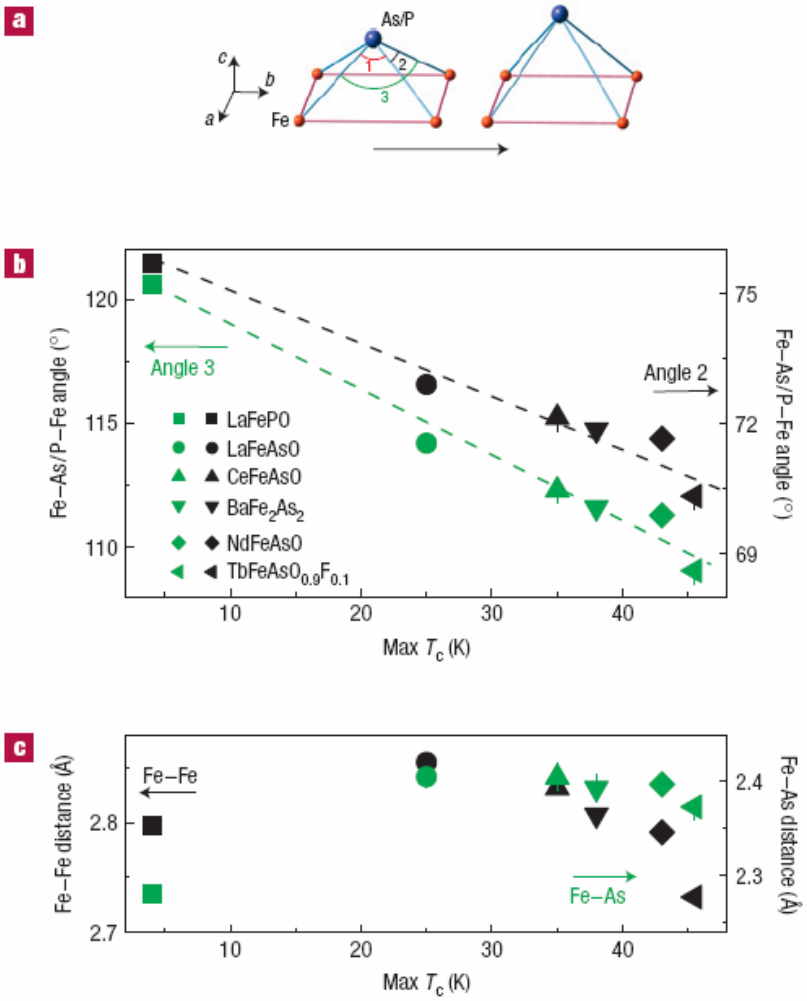
(d) $Ba_2Mn_2As_2O$-type

Bilan: facteurs structuraux contrôlant la supraconductivité:

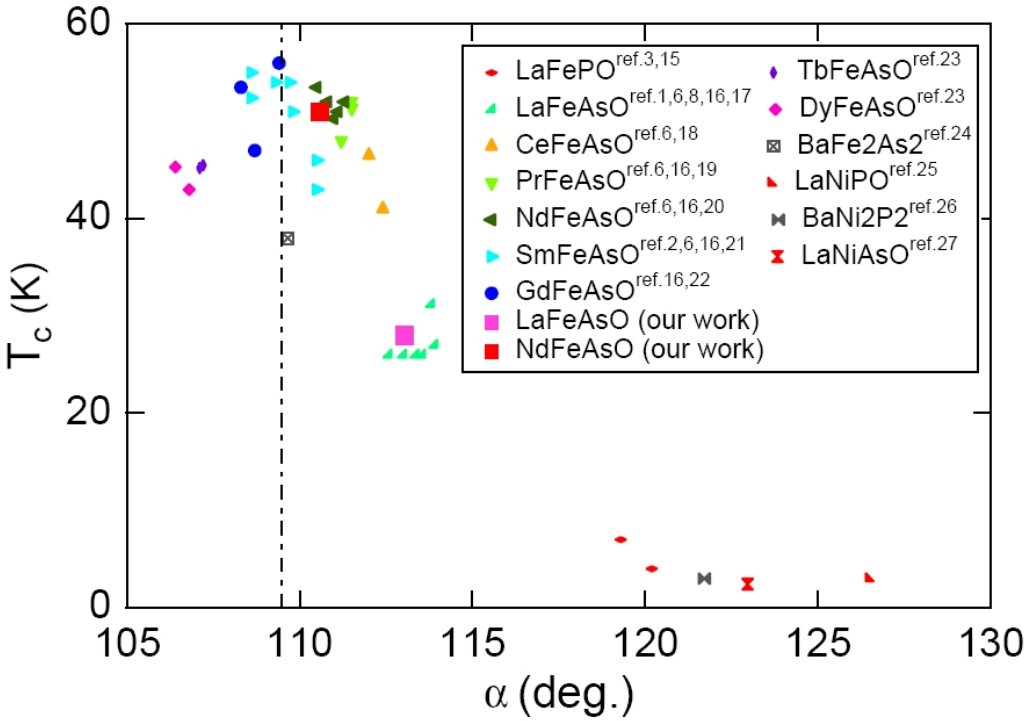
(1) T_c MAX lorsque tétraèdre $FeAs_4$ régulier



$FeAs_4$-tetrahedron



J. Zhao et al. Nature Déc. 2008



C-H. Lee et al. Journal of the Physical Society of Japan Vol. 77, No. 8, August, 2008, 083704

Rappelle les cuprates… lorsque le « buckling » dans plans CuO_2 détériorait la supra

Bilan: facteurs structuraux contrôlant la supraconductivité:

Empiriquement:

(2) T_c augmente lorsque les plans supra Fe_2As_2 sont plus distants les uns des autres:

$T_{c\ max}$	d Fe-Fe	famille
…	…	…
55 K	8.7 Å	Ln-1111
38 K	6.5 Å	(AE,A)-122
18 K	6.35 Å	A-111
8 K	5.5 Å	$Fe_{1+y}Se$ (Fe-111)

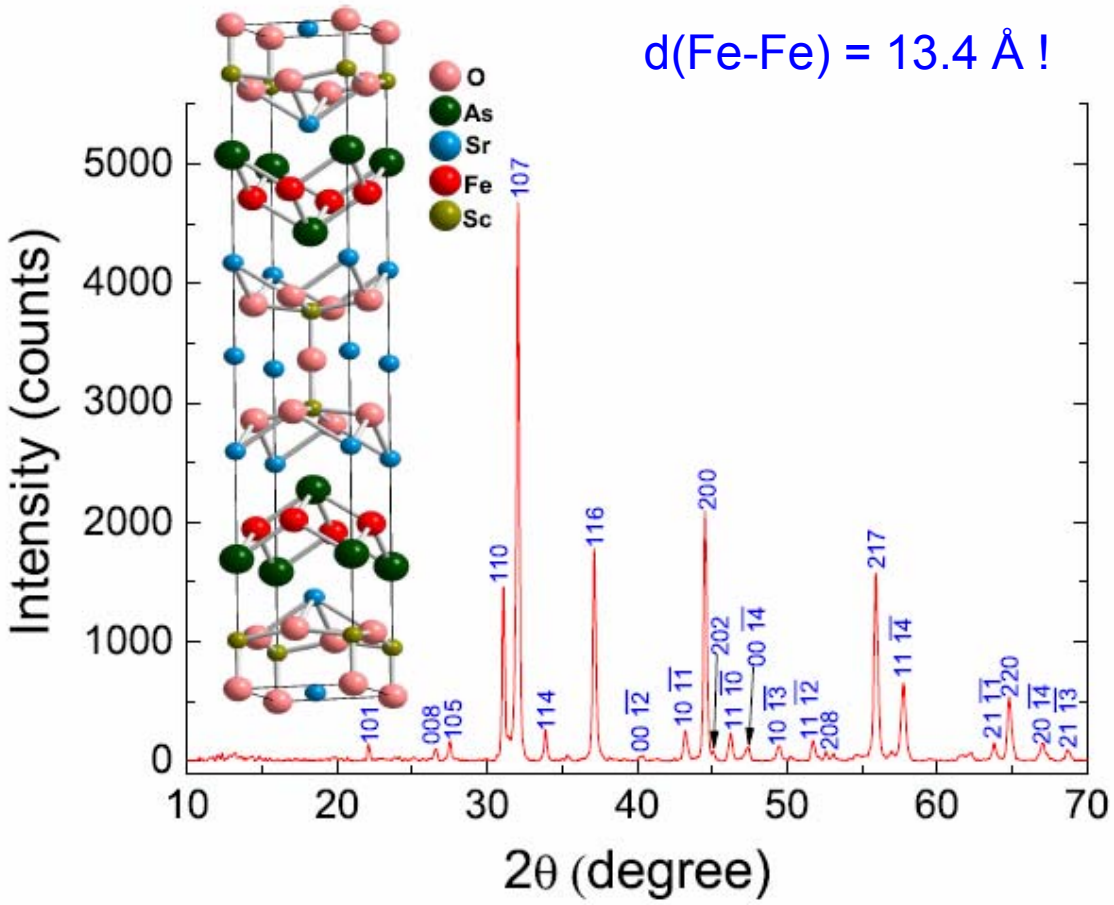
Rappelle les cuprates dont la T_c augmentait avec la distance séparant les blocs supra…

Augmenter d(Fe-Fe) pour améliorer T_c?

Condmat #0811.2205

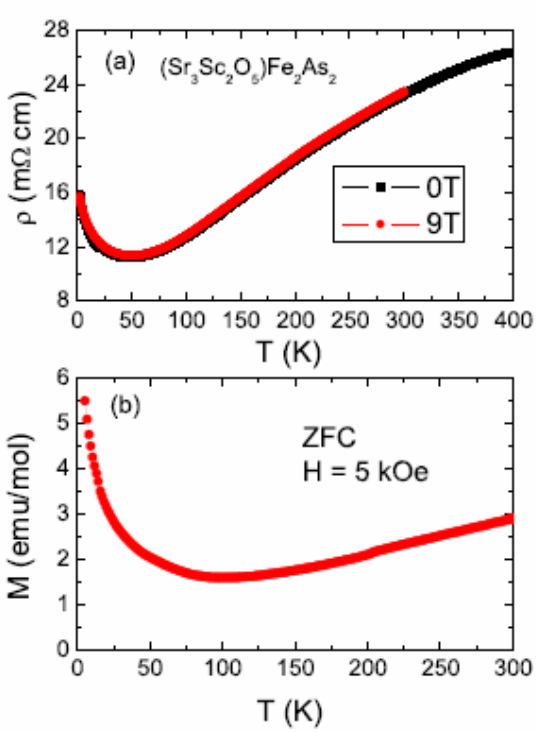
$(Sr_3Sc_2O_5)Fe_2As_2$ as a possible parent compound for the FeAs-based superconductors

Xiyu Zhu, Fei Han, Gang Mu, Peng Cheng, Bing Shen, Bin Zeng, and Hai-Hu Wen*
National Laboratory for Superconductivity, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100190, China



d(Fe-Fe) = 13.4 Å !

Dopage
→ supra haute T_c ?



Famille $(Cu_2S_2)(Sr_{n+1}M_nO_{3n-1})$ avec M=Sc, Ti, Cu...
Otzschi et al. J. of Low Temp. Phys. 117, 729-733 (1999).

Chimie des supra au fer:

- **Elaboration difficile**:
    - utilisation de produits toxiques!
    - Ln-1111 dopé: 5 éléments chimiques!
    - Ln-1111: peu d'oxygène dans la maille, nécessite un contrôle fin!
    - Ln-1111 dopé fluor: différence entre taux (Fluor) nominal et réel!
    - diagramme de phases parfois très compliqué avec polytypes (ex: Fe-Se)

- Propriétés physiques très sensibles à la **stœchiométrie** des échantillons: résultats parfois opposés dans la littérature

- Plus généralement: **composition exacte** des échantillons produits pas toujours bien connus avant études physiques fines → résultats contradictoires dans la littérature

Toxicité des nouveaux supra à base de Fe-As ?

In Vitro Studies of Cells Grown on the Superconductor PrO_xFeAs

Condmat #0809.2169

Shaoguang Yang[1*], Yuxuan Xie[2], Wenrong Yang[2], Rongkun Zheng[2], Frankie Stevens[2], Emine Korkmaz[2], Anthony S. Weiss[3], Simon P. Ringer[2], Filip Braet[2*]

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1 National Laboratory of Microstructures, Nanjing University, Nanjing, China

2 Australian Key Centre for Microscopy and Microanalysis, The University of Sydney

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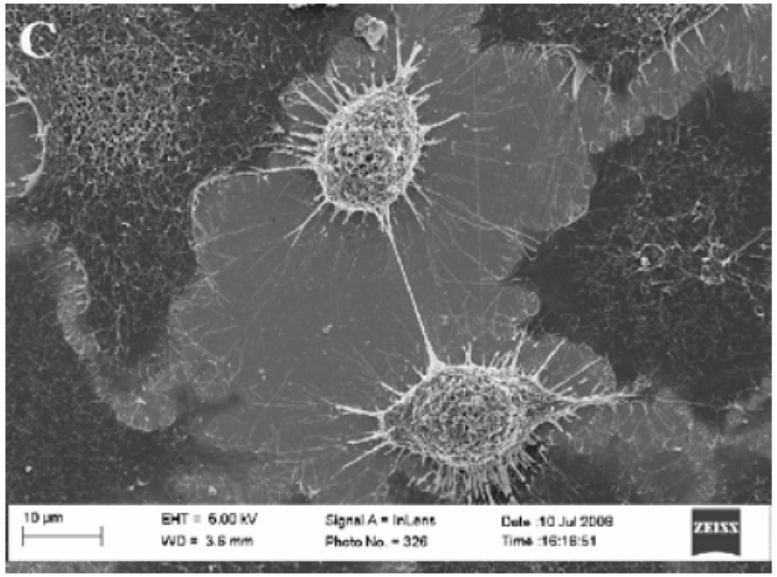
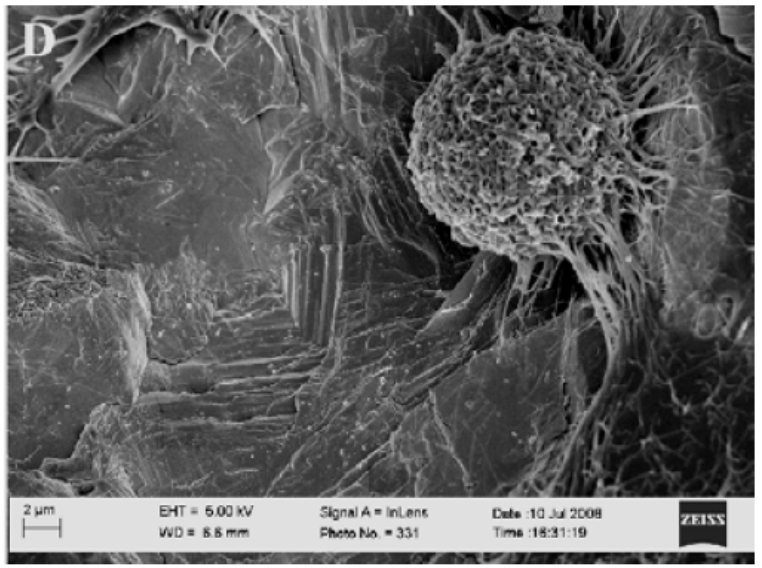


Abstract

The recent discovery of arsenic-based high temperature superconductors has reignited interest in the study of superconductor : biological interfaces. However, the new superconductor materials involve the chemistry of arsenic, their toxicity remain unclear [Nature, 2008, 452(24):922]. In this study the possible adverse effects of this new family of superconductors on cells have been examined. Cell culture studies in conjunction with microscopy and viability assays were employed to examine the influence of arsenic-based superconductor PrO_xFeAs (x=0.75) material *in vitro*. Imaging data revealed that cells were well adhered and spread on the surface of the superconductor. Furthermore, cytotoxicity studies showed that cells were unaffected during the time-course of the experiments, providing support for the biocompatibility aspects of PrO_xFeAs-based superconductor material.



Chimie des supra au fer: exemple de controverse: LaFePO

Résultats contradictoires: importance de la non stœchiométrie!

Electromagnetic properties and electronic structure of iron-based layered superconductor LaOFeP

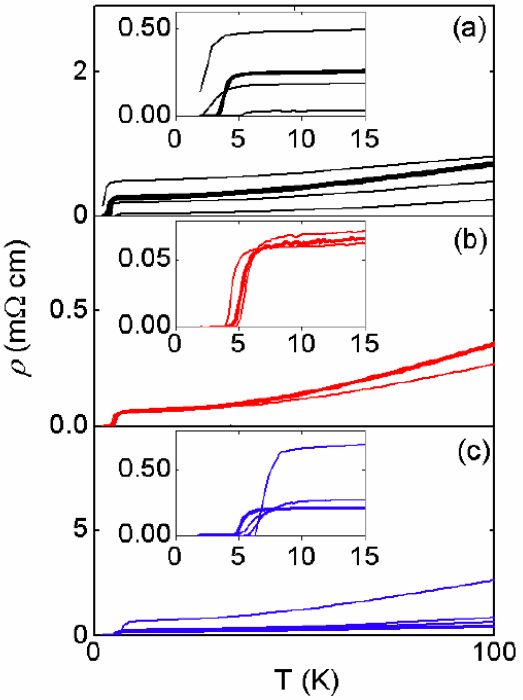
Yoichi Kamihara,[1] Masahiro Hirano,[1,2] Hiroshi Yanagi,[3] Toshio Kamiya,[1,3] Yuji Saitoh,[4] Eiji Ikenaga,[5] Keisuke Kobayashi,[5,6] and Hideo Hosono[1–3]

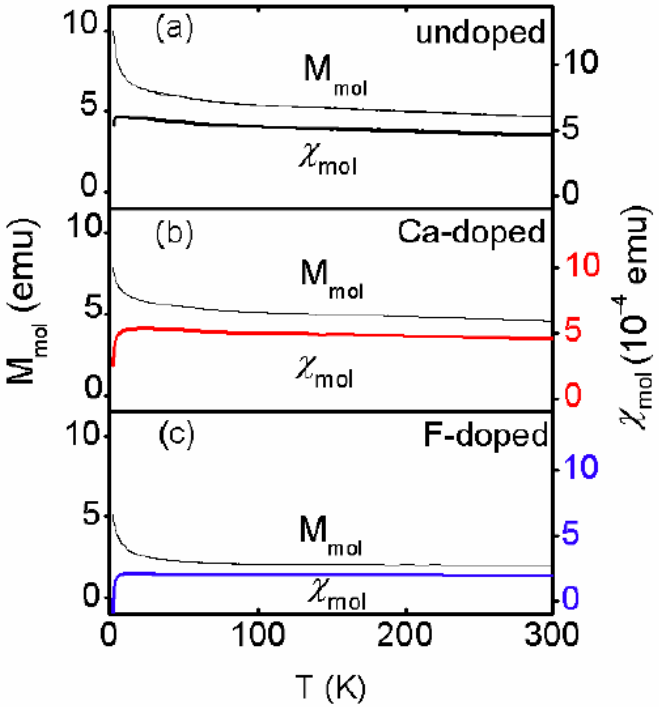
Supra !

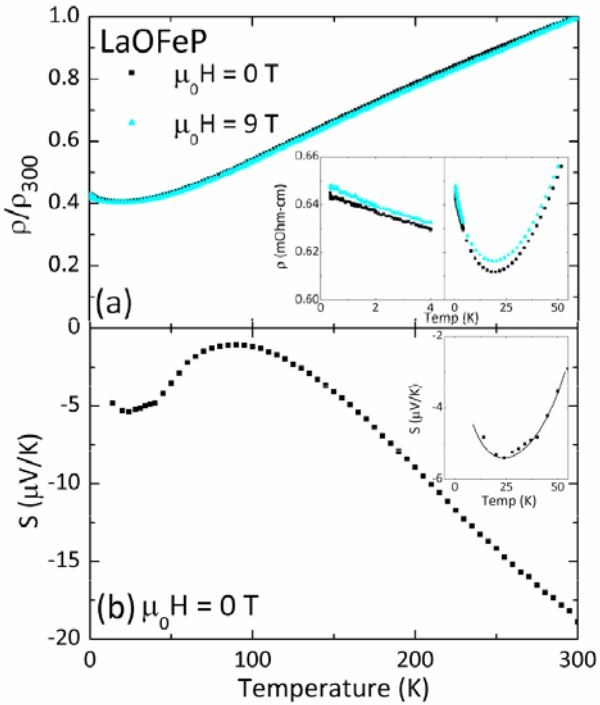
Intrinsic Properties of Stoichiometric LaOFeP

T. M. McQueen[1], M. Regulacio[1], A. J. Williams[1], Q. Huang[2], J. W. Lynn[2], Y. S. Hor[1], D.V. West[1], M. A. Green[2,3], and R. J. Cava[1]

Non supra!







Chimie des supra au fer: exemple de controverse: Fe-Se

Condmat #0811.1613

Extreme Sensitivity of Superconductivity to Stoichiometry in $Fe_{1+\delta}Se$

T. M. McQueen[1], Q. Huang[2], V. Ksenofontov[3], C. Felser[3], Q. Xu[4], H. Zandbergen[4], Y. S. Hor[1], J. Allred[1], A. J. Williams[1], D. Qu[5], J. Checkelsky[5], N. P. Ong[5] and R. J. Cava[1]

Abstract

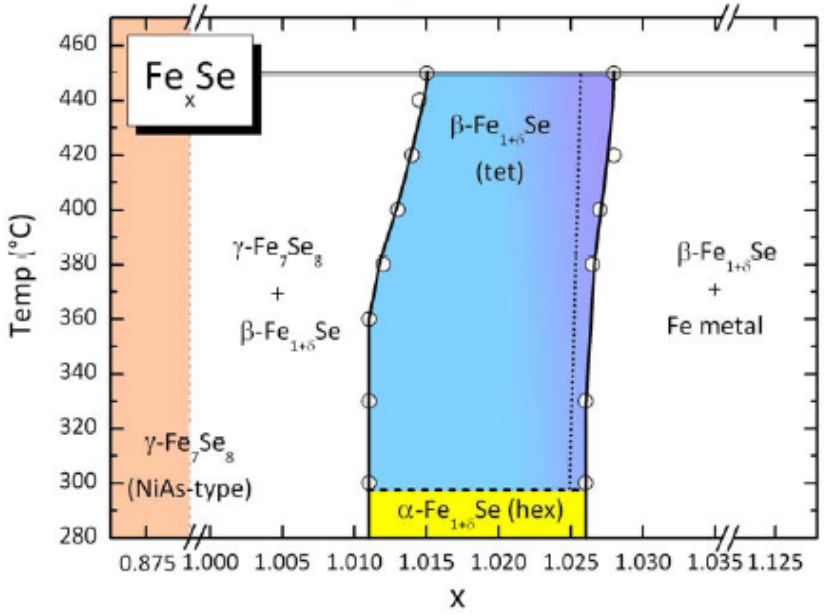
The recently discovered iron arsenide superconductors, which display superconducting transition temperatures as high as 55 *K*, appear to share a number of general features with high-T_c cuprates, including proximity to a magnetically ordered state and robustness of the superconductivity in the presence of disorder. Here we show that superconductivity in $Fe_{1+\delta}Se$, the parent compound of the superconducting arsenide family, is destroyed by very small changes in stoichiometry. Further, we show that non-superconducting $Fe_{1+\delta}Se$ is not magnetically ordered down to low temperatures. These results suggest that robust superconductivity and immediate instability against an ordered magnetic state should not be considered as intrinsic characteristics of iron-based superconducting systems, and that $Fe_{1+\delta}Se$ may present a unique opportunity for determining which materials characteristics are critical to the existence of superconductivity in high T_c iron arsenide superconductors and which are not.

Condmat #0811.1613

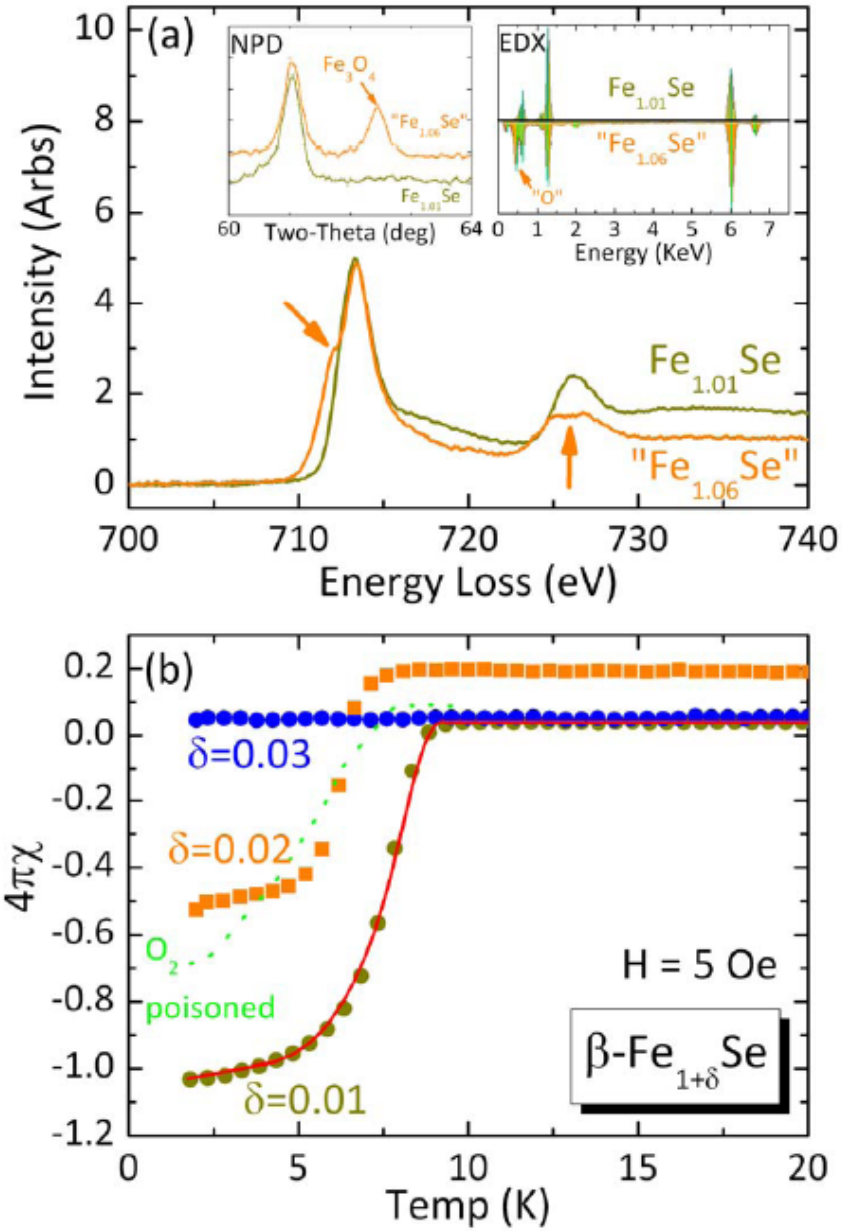
Extreme Sensitivity of Superconductivity to Stoichiometry in $Fe_{1+\delta}Se$

T. M. McQueen[1], Q. Huang[2], V. Ksenofontov[3], C. Felser[3], Q. Xu[4], H. Zandbergen[4], Y. S. Hor[1], J. Allred[1], A. J. Williams[1], D. Qu[5], J. Checkelsky[5], N. P. Ong[5] and R. J. Cava[1]

- Complexité du diagramme de phase Compo-T !

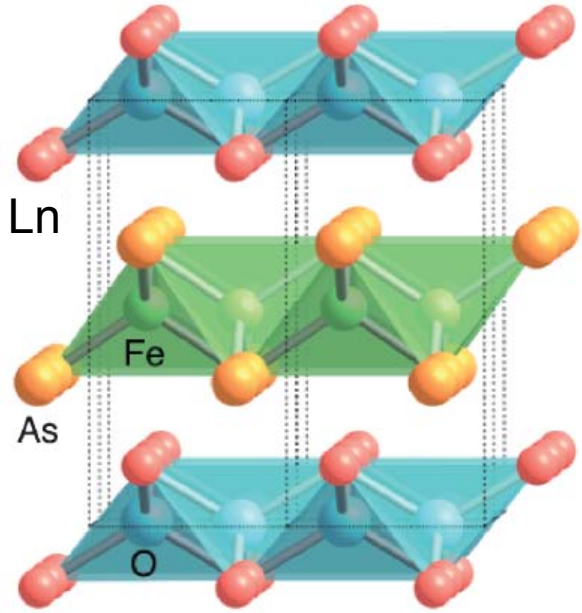


-impuretés Fe_3O_4 (non visibles en DRX!)
- vieillissement et contamination de l'échantillon avec O
- composé supra proche de $Fe_{1.01}Se_{1.0}$



Elaboration de poudres: (1) tube scellé

La(O,F)FeAs



Iron-Based Layered Superconductor La[$O_{1-x}F_x$]FeAs (x = 0.05−0.12) with T_c = 26 K

Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

Received January 9, 2008; E-mail: hosono@msl.titech.ac.jp

Polycrystalline LaOFeAs was synthesized by heating a mixture of lanthanum arsenide, iron arsenide, and dehydrated La_2O_3 powders in a silica tube filled with Ar gas at 1250 °C for 40 h, a procedure similar to that employed for LaOFeP.[8] Ca^{2+} and F^- ion doping was performed by adding CaO and a 1:1 mixture of LaF_3 and La, respectively, to the starting material. The crystal structure, phase

Superconducting properties of Fe-based layered superconductor $LaO_{0.9}F_{0.1-\delta}FeAs$

G. F. Chen, Z. Li, G. Li, J. Zhou, D. Wu, J. Dong, W. Z. Hu, P. Zheng, Z. J. Chen, J. L. Luo, and N. L. Wang

Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, People's Republic of China

We have employed a new route to synthesize single phase F-doped LaOFeAs compound and confirmed the superconductivity above 20 K in this Fe-based system. We show that the new superconductor has a rather high upper critical field of about 54 T. A clear signature of superconducting gap opening below T_c was observed in the far-infrared reflectance spectra, with $2\Delta/kT_c \approx 3.5$-4.2. Furthermore, we show that the new superconductor has electron-type conducting carrier with a rather low carrier density.

The polycrystalline samples were prepared by the solid state reaction using LaAs, Fe_2O_3, Fe and LaF_3 as starting materials. Different from the synthesis method reported by Kamihara et al. [6], we use Fe_2O_3 as a source of oxygen instead of La_2O_3 due to the high stability of Lanthanum oxide. Lanthanum arsenide (LaAs) was obtained by reacting La chips and As pieces at 500 °C for 12 h then at 850 °C for 2h. Mixtures of four components were ground thoroughly and cold-pressed into pellets. The pellets were placed into Ta crucible and sealed in quartz tube under argon atmosphere. They were then annealed for 50 h at a temperature of 1150 °C.

Elaboration de poudres: (1) tube scellé

doi:10.1038/nature07045 nature

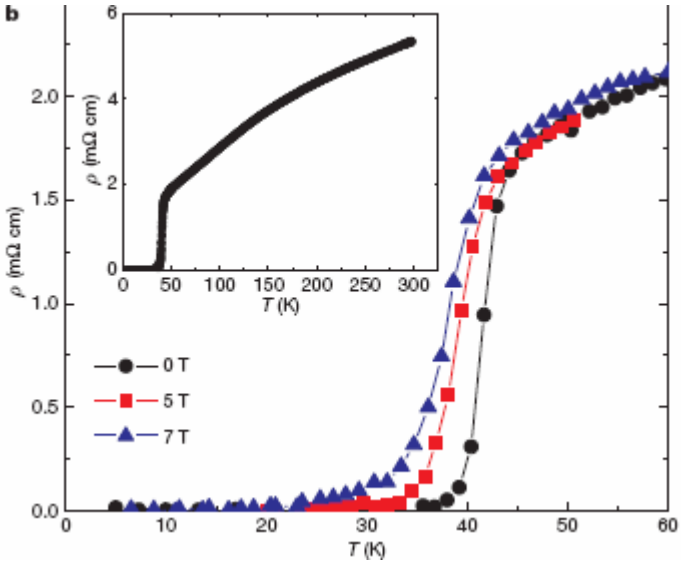
LETTERS

[1]Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, China.

Superconductivity at 43 K in $SmFeAsO_{1-x}F_x$

X. H. Chen[1], T. Wu[1], G. Wu[1], R. H. Liu[1], H. Chen[1] & D. F. Fang[1]

Polycrystalline samples with nominal composition $SmFeAsO_{1-x}F_x$ ($x = 0.15$) were synthesized by conventional solid state reaction using high-purity SmAs, SmF_3, Fe and Fe_2O_3 as starting materials. SmAs was obtained by reacting Sm chips and As pieces at 600 °C for 3 h and then 900 °C for 5 h. The raw materials were thoroughly ground and pressed into pellets. The pellets were wrapped in Ta foil, sealed in an evacuated quartz tube, and finally annealed at either 1,160 °C or 1,200 °C for 40 h.



Elaboration de poudres: (2) haute pression – haute température

EPL, 82 (2008) 57002 www.epljournal.org
doi: 10.1209/0295-5075/82/57002

Superconductivity in the iron-based F-doped layered quaternary compound $Nd[O_{1-x}F_x]FeAs$

ZHI-AN REN[a], JIE YANG, WEI LU, WEI YI, XIAO-LI SHEN, ZHENG-CAI LI, GUANG-CAN CHE, XIAO-LI DONG, LI-LING SUN, FANG ZHOU and ZHONG-XIAN ZHAO[b]

National Laboratory for Superconductivity, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences - P. O. Box 603, Beijing 100190, PRC

received 1 April 2008; accepted in final form 7 April 2008
published online 19 May 2008

PACS 74.10.+v – Occurrence, potential candidates
PACS 74.70.Dd – Ternary, quaternary, and multinary compounds (including Chevrel phases, borocarbides, etc.)

Abstract – Here we report a new quaternary iron-arsenide superconductor $Nd[O_{1-x}F_x]FeAs$, with the onset resistivity transition at 51.9 K and Meissner transition at 51 K. This compound has the same crystal structure as LaOFeAs, and becomes the second superconductor after $Pr[O_{1-x}F_x]FeAs$ that superconducts above 50 K.

The superconducting $Nd[O_{1-x}F_x]FeAs$ samples were prepared by a high pressure synthesis method directly. Nd pieces, As, Fe, Fe_2O_3, FeF_3 powders (the purities of all starting chemicals are better than 99.99%) were mixed together according to the nominal stoichiometric ratio of $Nd[O_{0.89}F_{0.11}]FeAs$, then ground thoroughly and pressed into small pellets. The pellets were sealed in boron nitride crucibles and sintered in a high-pressure synthesis apparatus under the pressure of 6 GPa and temperature of 1300 °C for 2 hours. Here the adoption of high pressure

Élaboration HP-HT:

- Contrôle plus précis du taux de fluor
- Composés lacunaires en O type $LnFeAsO_{1-delta}$
- Compo avec petites terre rares
- Nouvelles compositions/surstructures?

Monocristaux de supra au fer ?

Famille Ln-1111

Condmat #0806.0337, J. Phys. Cond. Mat. 20 (2008)

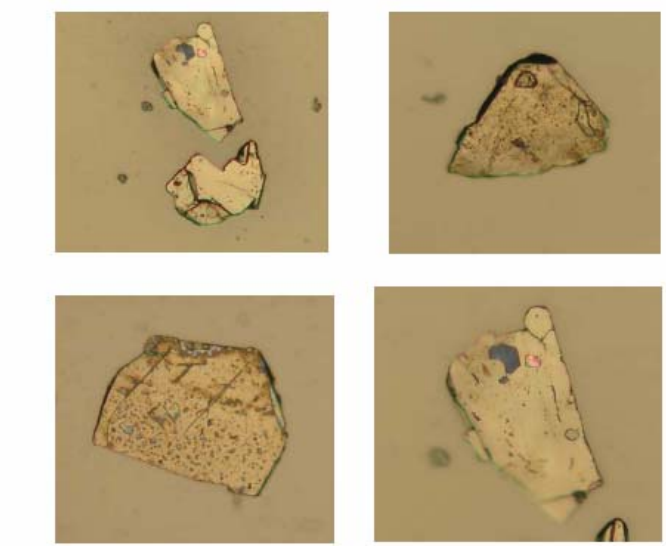


Figure 3. $SmFeAsO_{1-x}F_y$ single crystals grown from NaCl/KCl flux at high pressure. The length of crystals is about 100 μm.

Single crystals of superconducting $SmFeAsO_{1-x}F_y$ grown at high pressure

N D Zhigadlo, S Katrych, Z Bukowski, and J Karpinski

Laboratory for Solid State Physics, ETH, 8093 Zurich, Switzerland

E-mail: karpinski@phys.ethz.ch and zhigadlo@phys.ethz.ch

Abstract. Single crystals of $SmFeAsO_{1-x}F_y$ of a size up to 100x100 μm^2 have been grown from NaCl/KCl flux at pressure of 30 kbar and temperature of 1350-1450 °C using cubic anvil high-pressure technique. Superconducting transition temperature of the obtained single crystals varies between 45 and 53 K. Structure refinement has been performed on single crystal. Differential thermal analysis investigations at 1 bar Ar pressure show decomposition of $SmFeAsO_{1-x}F_y$ at 1302 °C.

- Elaboration HP-HT
- Flux NaCl/KCl

Famille AE-122

Condmat #0806.1874

Anisotropic thermodynamic and transport properties of single crystalline $(Ba_{1-x}K_x)Fe_2As_2$ ($x = 0$ and 0.45).

N. Ni[1,2], S. L. Bud'ko[1,2], A. Kreyssig[1,2], S. Nandi[1,2], G. E. Rustan[1,2], A. I. Goldman[1,2], S. Gupta[1,3], J. D. Corbett[1,3], A. Kracher[1], and P. C. Canfield[1,2]

[1]*Ames Laboratory US DOE, Iowa State University, Ames, Iowa 50011*

[2]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011 and*

[3]*Department of Chemistry, Iowa State University, Ames, Iowa 50011*

(Dated: June 11, 2008)

Flux Sn !

Abstract

Single crystals of $BaFe_2As_2$ and $(Ba_{0.55}K_{0.45})Fe_2As_2$ have been grown out of excess Sn with 1% or less incorporation of solvent. The crystals are exceptionally micaceous, are easily exfoliated and can have dimensions as large as 3 x 3 x 0.2 mm^3. The $BaFe_2As_2$ single crystals manifest a structural phase transition from a high temperature tetragonal phase to a low temperature orthorhombic phase near 85 K and do not show any sign of superconductivity down to 1.8 K. This transition can be detected in the electrical resistivity, specific heat and the anisotropic magnetic susceptibility. In the $(Ba_{0.55}K_{0.45})Fe_2As_2$ single crystals this transition is suppressed and instead superconductivity occurs with a transition temperature near 30 K. Whereas the superconducting transition is easily detected in resistivity and magnetization measurements, the change in specific heat near T_c is small, but resolvable, giving $\Delta C_p/\gamma T_c \approx 1$. The application of a 140 kOe magnetic field suppresses T_c by only ~ 4 K when applied along the c-axis and by ~ 2 K when applied perpendicular to the c-axis. The ratio of the anisotropic upper critical fields, $\gamma = H_{c2}^{\perp c}/H_{c2}^{\parallel c}$, varies between 2.5 and 3.5 for temperatures down to ~ 2 K below T_c.

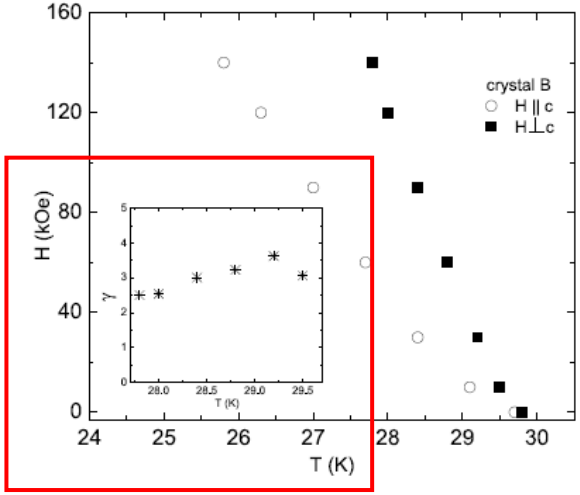


FIG. 14: Anisotropic $H_{c2}(T)$ plot for $H \leq 140$ kOe. Inset: $\gamma = H_{c2}^{\perp c}/H_{c2}^{\parallel c}$ as a function of temperature just below T_c.

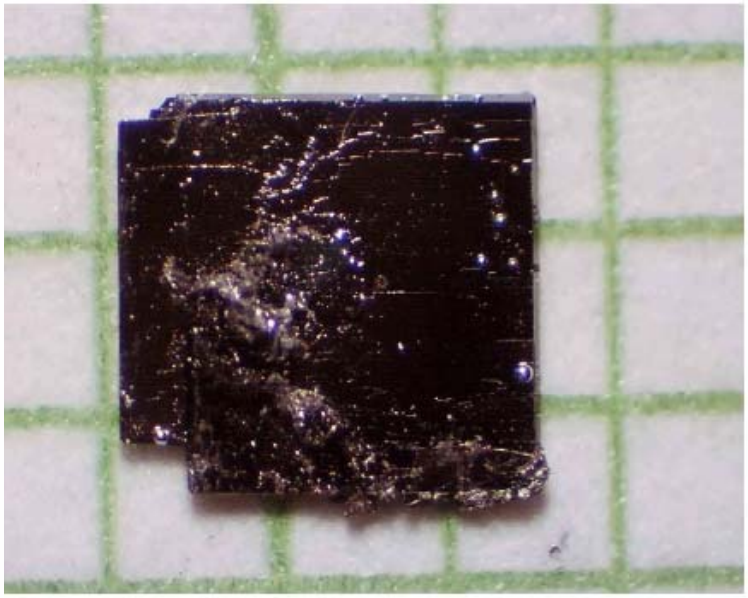
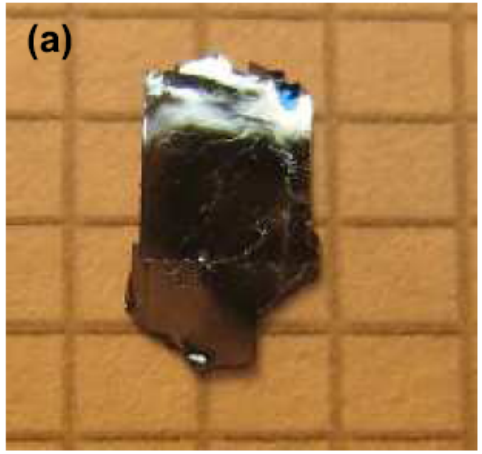
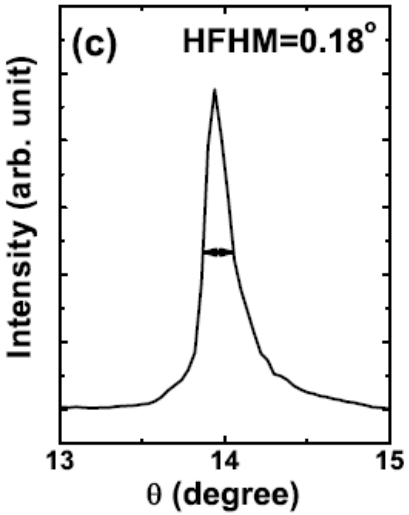


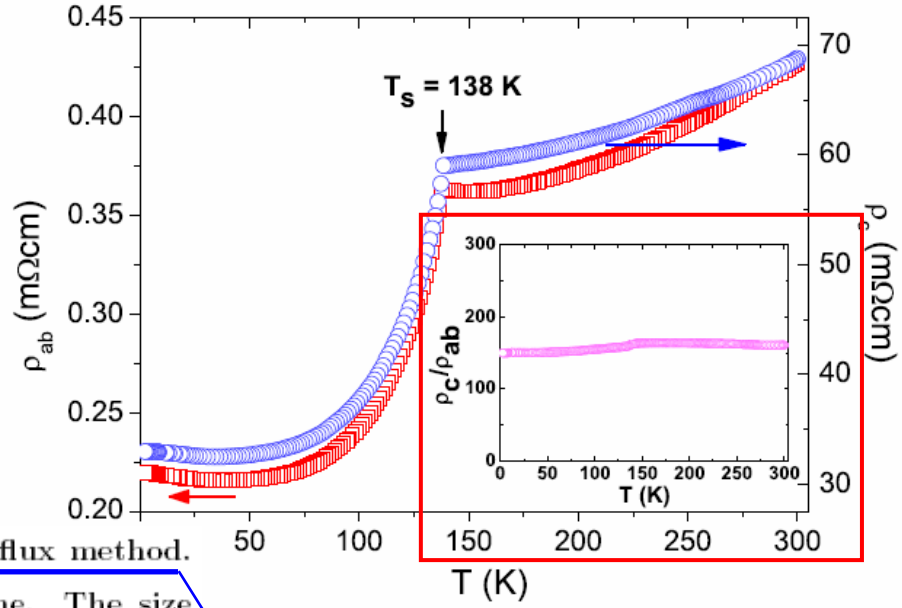
FIG. 1: Photograph of a single crystal of $(Ba_{0.55}K_{0.45})Fe_2As_2$ on a mm grid. The crystallographic c-axis is perpendicular to the plane of the plate. Droplets of Sn flux can be seen on the surface.

Famille AE-122

Wang et al. condmat #0806.2452







Sizable single crystals of $BaFe_2As_2$ have been grown with self-flux method. The crystals are plate-like with c-axis perpendicular to the plane. The size can be as large as 3 x 5 x 0.2 mm^3. The resistivity anisotropy (ρ_c/ρ_{ab}) is as large as about 150, and independent of temperature. The transport in ab plane and along c-axis direction shares the same scattering mechanism. In contrast to the magnetic behavior of polycrystalline samples, no Curie-Weiss behavior are observed, a temperature linear dependent susceptibility occurs above spin-density-wave (SDW) transition. The susceptibility behavior is very similar to that of antiferromagnetic SDW chromium. Magnetic behavior of single crystal definitely gives evidence for existence of local moment except for the contribution to susceptibility from itinerant electrons. A resistivity minimum strongly dependent on magnetic field is observed. A log(1/T) divergency, similar to that of the underdoped cuprates, happens at low temperature. Here we first present intrinsic transport and magnetic properties, and their anisotropy from high quality single crystal.

Flux FeAs

A propos de l'anisotropie dans ces supra à base de fer:

Diminishing superconducting anisotropy in a layered iron arsenic $PrFeAsO_{1-y}$ single crystal

Daichi Kubota [1] and Takekazu Ishida [1,2*]
[1] *Department of Physics and Electronics, Osaka Prefecture University, 1-1 Gakuen-cho, Naka-ku, Sakai, Osaka 599-8531, Japan and*
[2] *Institute for Nanofabrication Research, Osaka Prefecture University, 1-1 Gakuen-cho, Naka-ku, Sakai, Osaka 599-8531, Japan*

Motoyuki Ishikado and Shin-ichi Shamoto
Quantum Beam Science Directorate, Japan Atomic Energy Agency (JAEA), Tokai, Naka, Ibaraki 319-1195, Japan

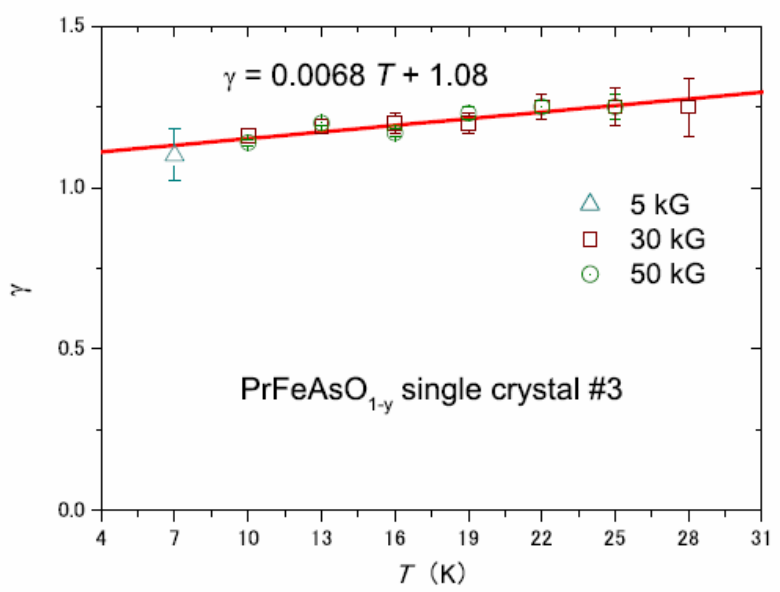
Hiroshi Eisaki, Hijiri Kito, and Akira Iyo
Nanoelectronics Research Institute (NeRI), National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Central 2, Umezono, Tsukuba, Ibaraki 305-8568, Japan

(Dated: October 30, 2008)

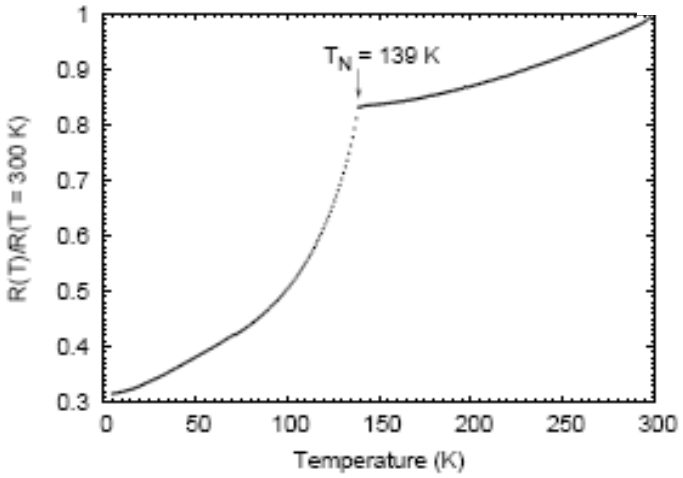
The magnetic torque of a high-quality $PrFeAsO_{1-y}$ single crystal has been investigated at temperatures from 10 K to 45 K in magnetic fields from 5 kG and 50 kG. We find that the superconducting anisotropy γ in $PrFeAsO_{1-y}$ can be approximated by $\gamma = 1.08 + 0.0068T$ in all fields by employing the Kogan model. The reduced superconducting anisotropy in the $PrFeAsO_{1-y}$ crystal seems to be very promising in considering various high-J_c applications.

γ	Method	Material	Carrier	Reference
1.2	torque	$PrFeAsO_{1-y}$	electron	this work
1.2	transport	$Sr(Fe_{1-x}Co_x)_2As_2$	electron	[4]
1.5	transport	$Ba(Fe_{1-x}Co_x)_2As_2$	electron	[34]
6	transport	$NdFeAsO_{0.82}F_{0.18}$	electron	[35]
9	torque	$SmFeAsO_{0.8}F_{0.2}$	electron	[36]
15	transport	$LaFeAsO_{0.89}F_{0.11}$	electron	[37]
65	transport	$SmFeAsO_{0.85}$	electron	[22]

TABLE I: Comparison of the γ values reported in the literature [4, 22, 34, 35, 36, 37]. The anisotropy γ varies very widely from 1.2 to 65. The experimental means and the type of superconducting carriers are also listed.



Famille AE-122



Bridgman

Single-crystal growth of the ternary $BaFe_2As_2$ phase using the vertical technique

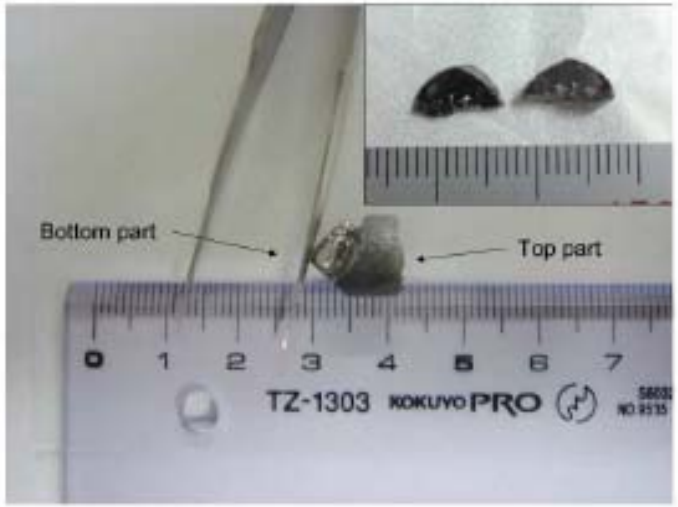
Rei MORINAGA[1], Kittiwit MATAN[1], Hiroyuki S. SUZUKI[2] and Taku J. SATO[1*]

[1] *Neutron Science Laboratory, Institute for Solid State Physics, University of Tokyo, 106-1 Shirakata, Tokai, Ibaraki 319-1106, Japan*

[2] *National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan*

Ternary Ba-Fe-As system has been studied to determine a primary solidification field of the $BaFe_2As_2$ phase. We found that the $BaFe_2As_2$ phase most likely melts congruently and primarily solidifies either in the FeAs excess or $BaAs_2$ excess liquid. Knowing the primary solidification field, we have performed the vertical Bridgman growth using the starting liquid composition of $Ba_{15}Fe_{42.5}As_{42.5}$. Large single crystals of the typical size 10x4x2 mm^3 were obtained and their quality was confirmed by X-ray Laue and neutron diffraction.

Condmat #0809.3084



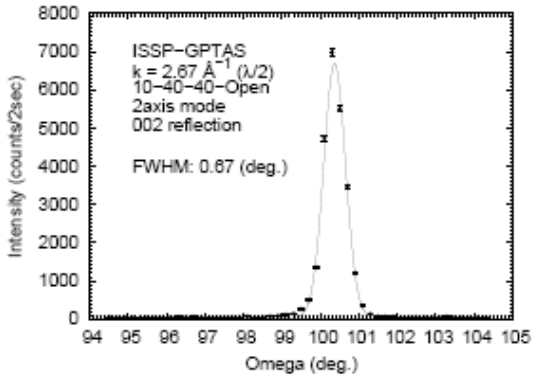


Fig. 5. A photograph of the resulting Bridgman-grown ingot. The bottom part, where the growth of the single grains was confirmed, was broken into pieces on removal from the crucible. Inset: the two pieces of the single grains obtained from the bottom part of the ingot. Indeed, the two pieces came from the same grain, but were torn in parts when they were removed. The thickness of each piece is about 2 mm.

Famille « FeSe »

Zhang et al.
condmat 0809.1905

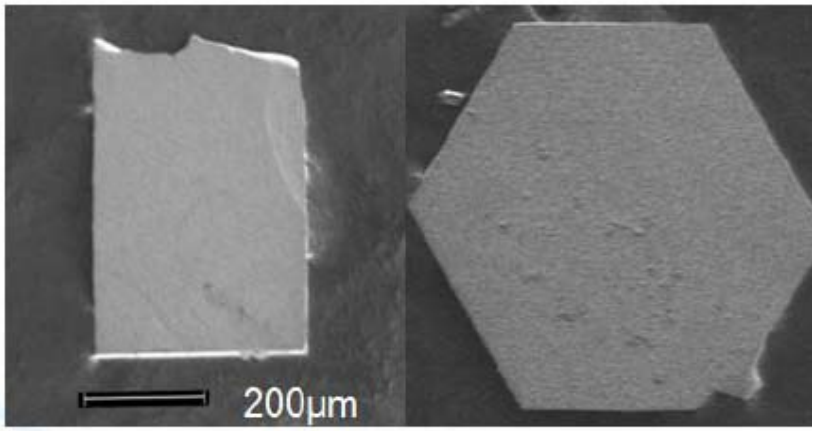


Fig. 1 S. B. Zhang

Crystal growth and superconductivity of $FeSe_x$

S. B. Zhang, Y. P. Sun*, X. D. Zhu, X. B. Zhu, B. S. Wang, G. Li, H. C. Lei, X. Luo, Z. R. Yang, W.H.Song and J.M. Dai

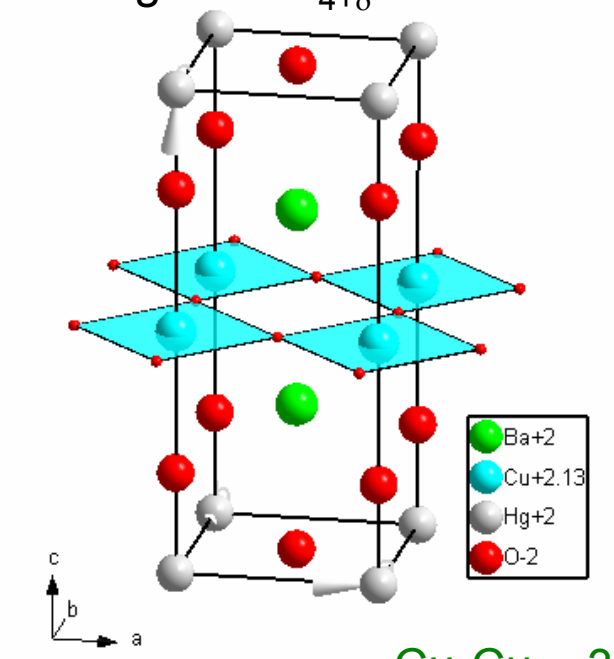
Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, High Magnetic Field Laboratory, Chinese Academy of Sciences, Hefei 230031, China

ABSTRACT

Single crystals $FeSe_x$ have been grown in evacuated sealed quartz tube using a NaCl/KCl flux. The products include two crystal structures of tetragon and hexagon. The electronic transport and magnetic properties measurements of $FeSe_x$ single crystal exhibits a superconducting transition at about 10K.

Propriétés physiques: comparaison avec les cuprates

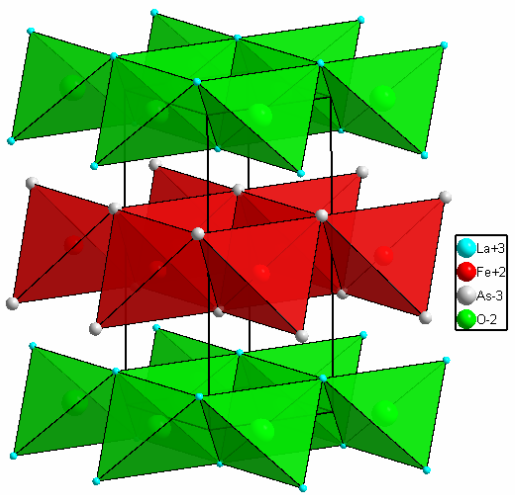
$HgBaCuO_{4+\delta}$



- Cuprate: pas d'interaction direct entre atomes de Cu

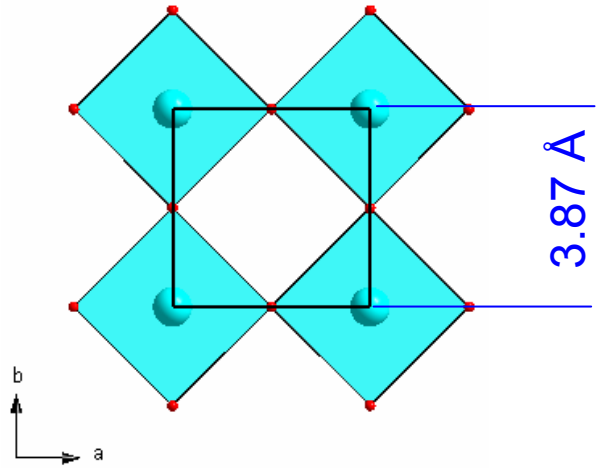
-Composés Fe-As: overlap des orbitales *3d* des Fe!
→ conducteurs à Tamb.

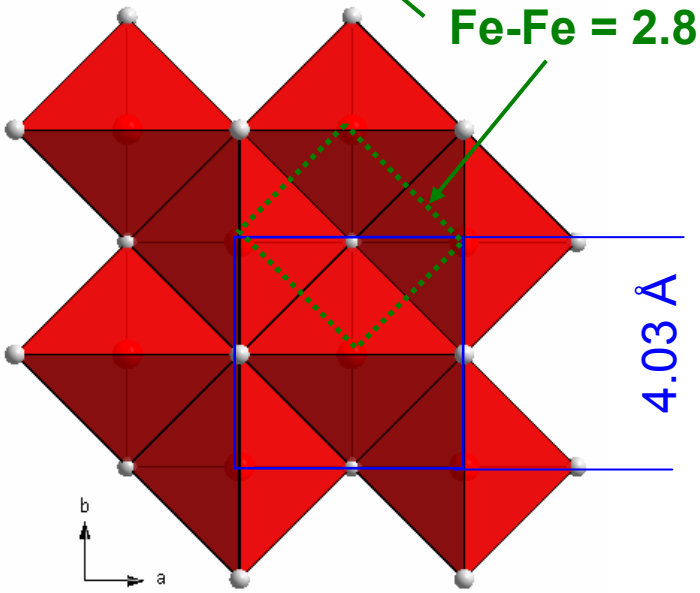
LaFeAsO



Cu-Cu = 3.87Å
Cu-O = 1.935Å

Fe-As = 2.435Å
Fe-Fe = 2.85Å





Les composés au Nickel Ln-1111:

Condmat #0805.4340

Nickel-based layered superconductor, LaNiOAs

Takumi Watanabe[a], Hiroshi Yanagi[a], Yoichi Kamihara[b], Toshio Kamiya[a,b], Masahiro Hirano[b,c], and Hideo Hosono[a,b,c,*]

Abstract

Rietveld analysis of the powder X-ray diffraction of a new layered oxyarsenide, LaNiOAs, which was synthesized by solid-state reactions, revealed that LaNiOAs belongs to the tetragonal ZrCuSiAs-type structure (*P*4/*nmm*) and is composed of alternating stacks of La-O and Ni-As layers. The electrical and magnetic measurements demonstrated that LaNiOAs exhibits a superconducting transition at 2.4 K, and above this, LaNiOAs shows metallic conduction and Pauli paramagnetism. The diamagnetic susceptibility measured at 1.8 K corresponded to ~20% of perfect diamagnetic susceptibility, substantiating that LaNiOAs is a bulk superconductor.

Supra expliqué par couplage e-phonon conventionnel

PHYSICAL REVIEW B **78**, 060506(R) (2008)

Electron-phonon superconductivity in LaNiPO

Alaska Subedi
Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996-1200, USA
and Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114, USA

David J. Singh and Mao-Hua Du
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114, USA
(Received 23 June 2008; published 20 August 2008)

We report first-principles calculations of the electronic structure, phonon dispersions, and electron-phonon coupling of LaNiPO. These calculations show that this material can be explained as a conventional electron-phonon superconductor in contrast to the FeAs based high-temperature superconductors.

Les composés au Nickel Ba-122:

T_c = 0.8 K
Ronning et al.
Condmat #0807.3788

Density functional study of $BaNi_2As_2$: Electronic structure, phonons and electron-phonon superconductivity

Condmat #0809.0499

Alaska Subedi
Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996 and Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6032, USA

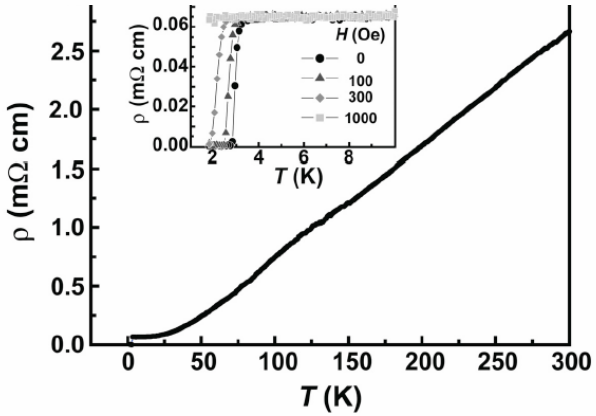
David J. Singh
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6032, USA

(Dated: September 2, 2008)

We investigate the properties of $BaNi_2As_2$ using first principles calculations. The band structure has a similar shape to that of the $BaFe_2As_2$, and in particular shows a pseudogap between a manifold of six heavy d electron bands and four lighter d bands, i.e. at an electron count of six d electrons per Ni. However, unlike $BaFe_2As_2$, where the Fermi energy occurs at the bottom of the pseudogap, the two additional electrons per Ni in the Ni compound place the Fermi energy in the upper manifold. Thus $BaNi_2As_2$ has large Fermi surfaces very distinct from $BaFe_2As_2$. Results for the phonon spectrum and electron-phonon coupling are consistent with a classification of this material as a conventional phonon mediated superconductor although spin fluctuations and nearness to magnetism may be anticipated based on the value of $N(E_F)$.

Nickel-based phosphide superconductor with infinite-layer structure, $BaNi_2P_2$

Takashi Mine [1], Hiroshi Yanagi [1], Toshio Kamiya [1,2], Yoichi Kamihara [2], Masahiro Hirano [2,3], and Hideo Hosono [1,2,3,*]



Supra expliqué par couplage e-phonon conventionnel

Les composés au **Fer** Ln-1111:

PRL **101,** 026403 (2008) PHYSICAL REVIEW LETTERS week ending 11 JULY 2008

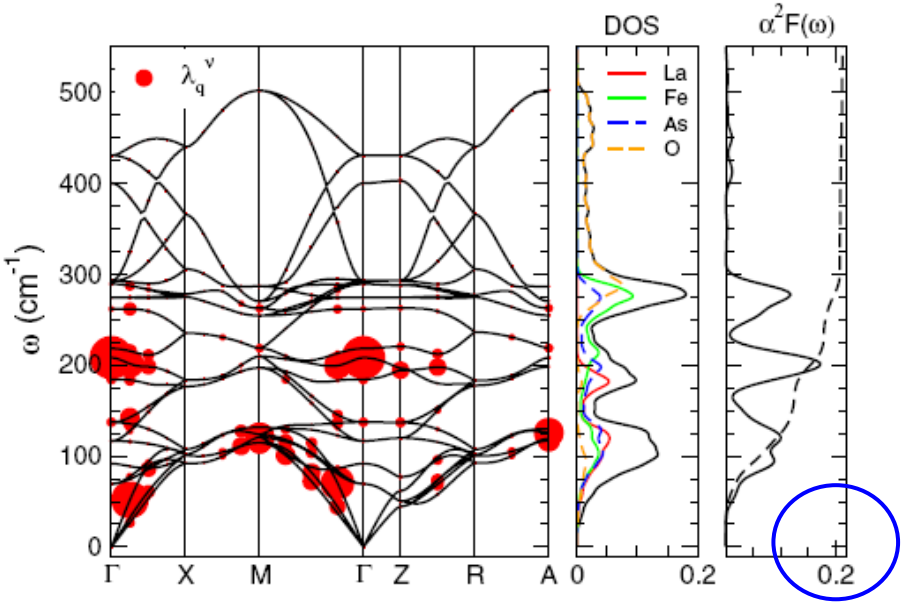
Is $LaFeAsO_{1-x}F_x$ an Electron-Phonon Superconductor?

L. Boeri,[1] O. V. Dolgov,[1] and A. A. Golubov[2]

[1]*Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany*
[2]*Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands*

(Received 18 March 2008; published 8 July 2008)

In this Letter, we calculate the electron-phonon coupling of the newly discovered superconductor $LaFeAsO_{1-x}F_x$ using linear response. For pure LaFeAsO, the calculated electron-phonon coupling constant $\lambda = 0.21$ and logarithmic-averaged frequency $\omega_{\ln} = 206$ K give a maximum T_c of 0.8 K, using the standard Migdal-Eliashberg theory. For the F-doped compounds, we predict even smaller coupling constants. To reproduce the experimental T_c, a 5–6 times larger coupling constant would be needed. Our results indicate that electron-phonon coupling is not sufficient to explain superconductivity in the whole family of Fe-As-based superconductors, probably due to the importance of strong-correlation effects.



Propriétés physiques fondamentales

(1) Faible densité de porteurs !

$LaFeAsO_{1-x}F_x$: A low carrier density superconductor near itinerant magnetism

Condmat 0803.0429

D.J. Singh and M.-H. Du
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114
(Dated: March 5, 2008)

The density functional electronic structure, phonons and magnetic properties of 26K superconducting LaFeAsO are reported. We find that this material is a low carrier density but high density of states near 2D ionic metal near itinerant magnetism. We find competing ferromagnetic and antiferromagnetic fluctuations. The balance between these is controlled by the doping level. This provides a new window into the interplay between magnetism and superconductivity.

PHYSICAL REVIEW B 77, 174503 (2008)

Electronic correlations in the superconductor $LaFeAsO_{0.89}F_{0.11}$ with low carrier density

$\approx 10^{21} cm^{-3}$

Athena S. Sefat, Michael A. McGuire, Brian C. Sales, Rongying Jin, Jane Y. Howe, and David Mandrus
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
(Received 13 March 2008; revised manuscript received 3 April 2008; published 5 May 2008)

The crystal structure and numerous normal and superconducting state properties of layered tetragonal ($P4/nmm$) LaFeAsO, with F doping of $\approx 11\%$, are reported. Resistivity measurements give an onset transition temperature T_c=28.2 K, and low field magnetic susceptibility data indicate bulk superconductivity. In applied magnetic field, analysis of the resistive transition results in a critical field $H_{c2} \approx 30$ T and a coherence length $\xi_{GL} \approx 35$ Å. An upper limit for the electron carrier concentration of 1×10^{21} cm^{-3} is inferred from the Hall data just above T_c. Strong electron-electron correlations are suggested from temperature-dependent resistivity, Seebeck coefficient, and thermal conductivity data. Anomalies near T_c are observed in both Seebeck coefficient and thermal conductivity data.

$H_{c2} \approx 30$ T
$\xi_{GL} \approx 35$ Å

Structure électronique, Surface de Fermi
LaFePO

S. Lebègue (Nancy)
PRB 75 (2007)

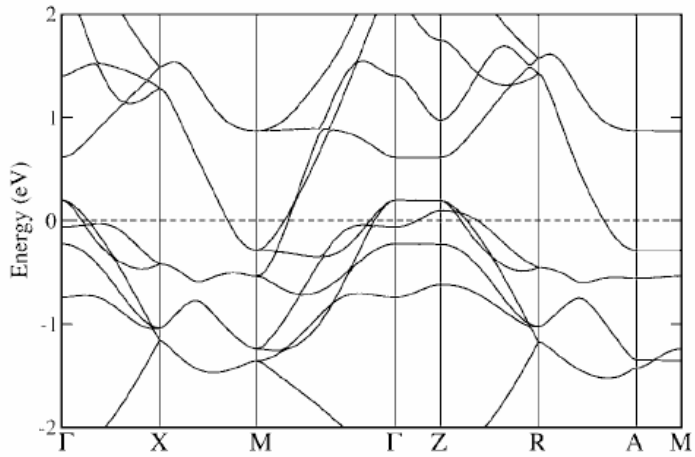


FIG. 5. Calculated band structure of LaOFeP. The Fermi level is at zero energy and is marked by a horizontal dashed line.

5 bandes traversent le niveau de Fermi, donc:

Surface de Fermi composée de 5 contributions:
- 4 surfaces quasi cylindriques (caractère 2D de la structure) de direction k_z centrée sur les directions Γ-Z et X-R
- 1 surface de sphère distordue centrée sur le point de haute symétrie Z

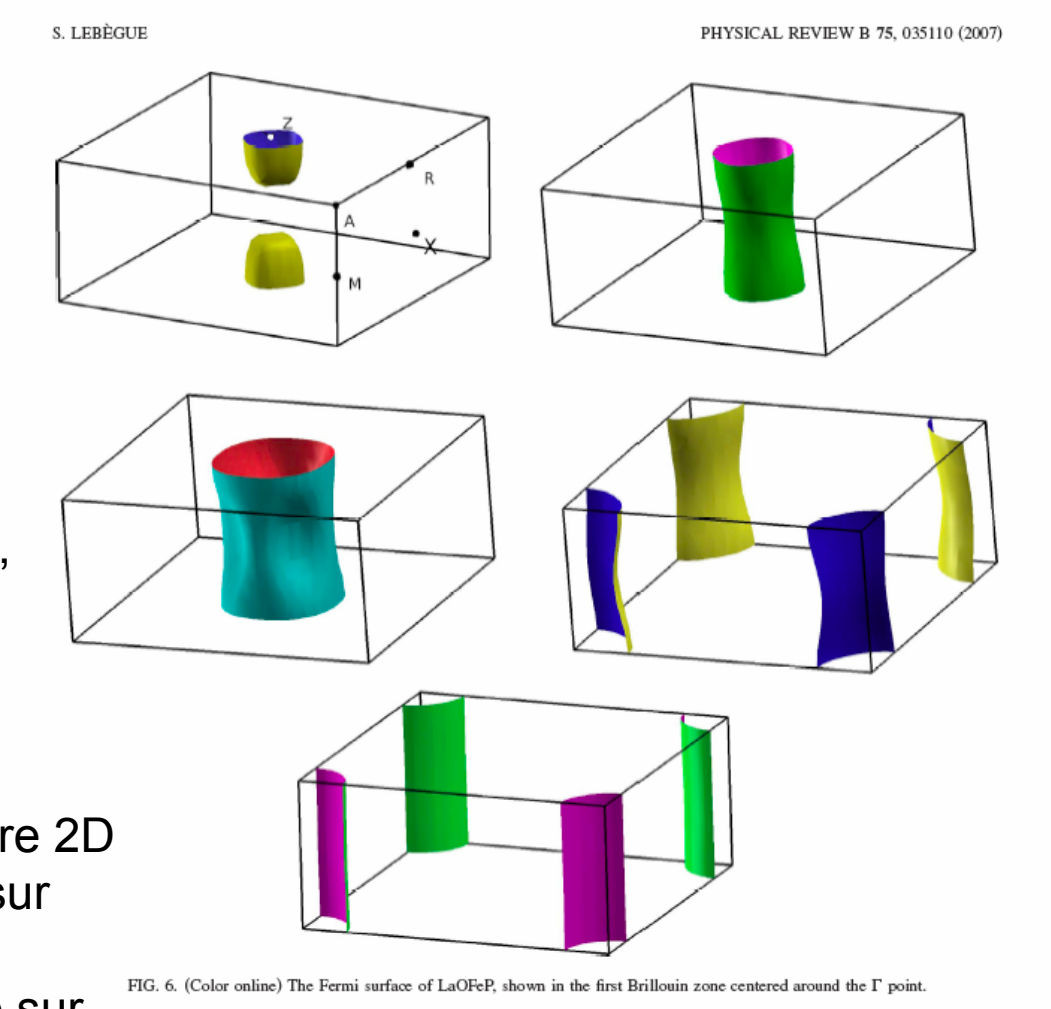


FIG. 6. (Color online) The Fermi surface of LaOFeP, shown in the first Brillouin zone centered around the Γ point.

Structure électronique, Surface de Fermi

$LaFeAsO_{1-x}F_x$

Iron-based layered superconductor $LaO_{1-x}F_xFeAs$: an antiferromagnetic semimetal

Fengjie Ma[1] and Zhong-Yi Lu[2*]
[1]Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, China and
[2]Department ofPhysics, Renmin University of China, Beijing 100872, China

Condmat #0803.3286

DOS:

E<-2eV bandes formées par les liaisons entre les orbitales du La et O + celles des orbitales atomiques du Fe et As

-2eV<E<2eV orbitales du **3d** de Fe centrées sur le niveau de Fermi

(effet du champ cristallin beaucoup moins fort que dans les oxydes de métaux de transition [électronégativité de As << O])

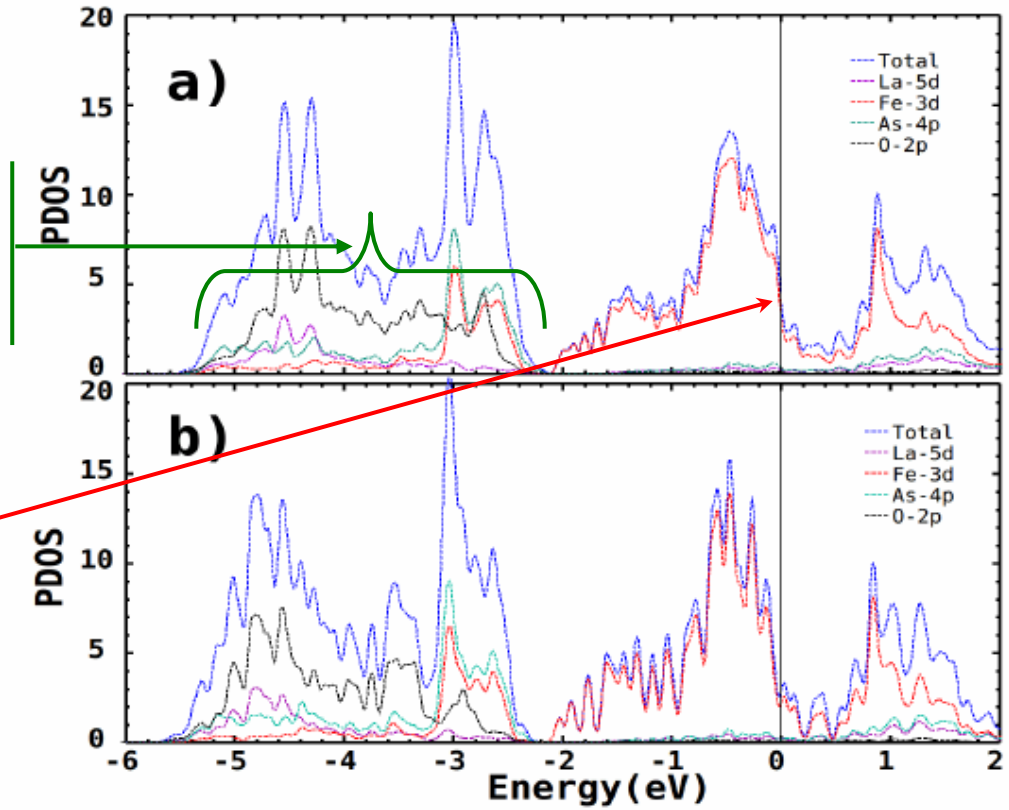


FIG. 1: (Color online) Calculated atomic orbital-resolved partial density of states of $LaO_{1-x}F_xFeAs$ in nonmagnetic state. (a) parent compound LaOFeAs; (b) $LaO_{0.95}F_{0.05}FeAs$ (5% F-doping). The Fermi energy sets to zero.

Structure électronique, Surface de Fermi

$LaFeAsO_{1-x}F_x$

Iron-based layered superconductor $LaO_{1-x}F_xFeAs$: an antiferromagnetic semimetal

Fengjie Ma[1] and Zhong-Yi Lu[2*]
[1]Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, China and
[2]Department ofPhysics, Renmin University of China, Beijing 100872, China

degrés de spin non inclus

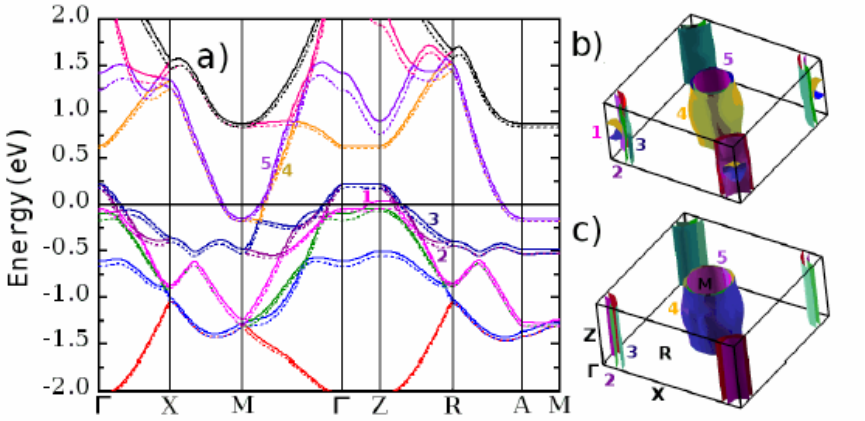


FIG. 2: (Color online) Calculated nonmagnetic electronic structures of $LaO_{1-x}F_xFeAs$. (a) energy band structures: the solid lines for the undoping while the dotted lines for the 5% F-doping (the Fermi energy sets to zero); (b) undoping: Fermi surface; (c) 5% F-doping: Fermi surface.

avec degrés de spin

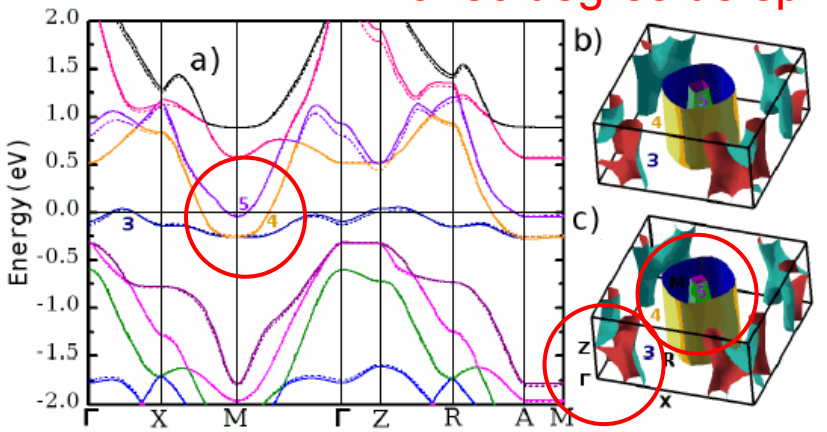
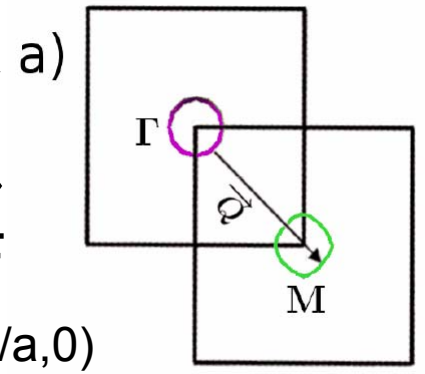


FIG. 3: (Color online) Calculated antiferromagnetic electronic structures of $LaO_{1-x}F_xFeAs$. (a) energy band structures: the solid lines for to the undoping while the dotted lines for 5% F-doping (the Fermi energy sets to zero); (b) undoping: Fermi surface; (c) 5% F-doping: Fermi surface. Note that here only the spin-up part is shown.

SF composée de 5 contributions:
- 2 surfaces quasi cylindriques dues à deux bandes d'e$^-$ (4,5) centrées autour de M-A
- 3 autres surfaces dues à trois bandes de trous (1,2,3) formées de 2 cylindres autour de Γ-Z et d'une poche 3D autour de Z

« Nesting » de SF



Q = (π/a,π/a,0)
qui stabilise l'état AFM (type SDW)

Structure électronique, Surface de Fermi: calculs analogues (DFT)

$LaFeAsO_{1-x}F_x$

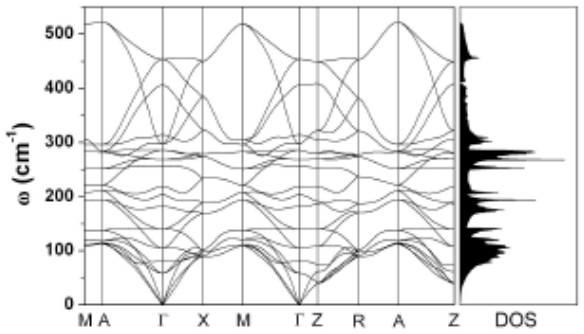


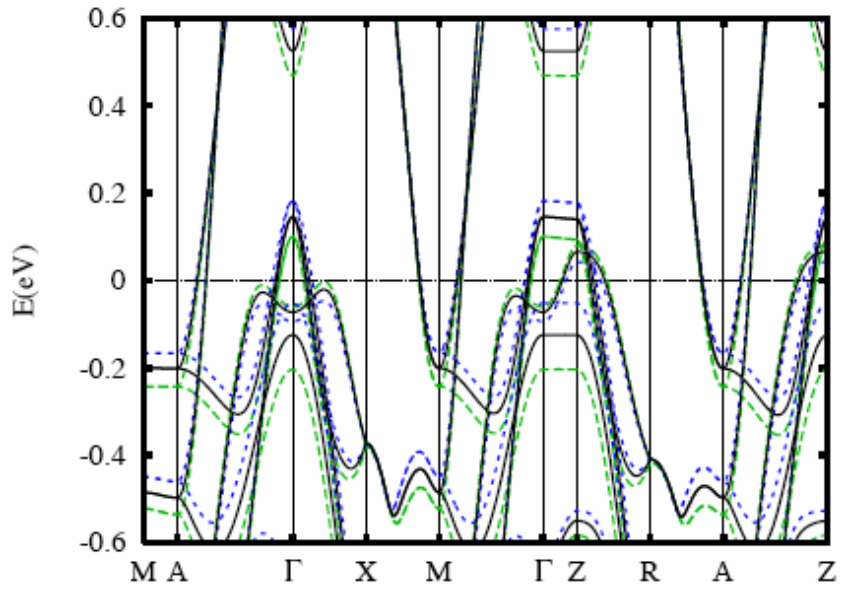
FIG. 5: Calculated phonon dispersions and phonon density of states of LaFeAsO.

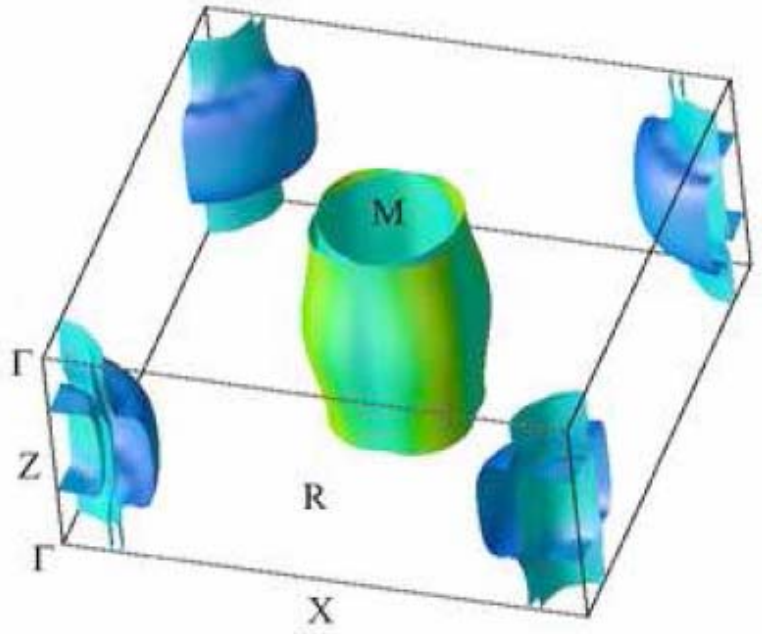
$LaFeAsO_{1-x}F_x$: A low carrier density superconductor near itinerant magnetism

D.J. Singh and M.-H. Du
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114
(Dated: March 5, 2008)

The density functional electronic structure, phonons and magnetic properties of 26K superconducting LaFeAsO are reported. We find that this material is a low carrier density but high density of states near 2D ionic metal near itinerant magnetism. We find competing ferromagnetic and antiferromagnetic fluctuations. The balance between these is controlled by the doping level. This provides a new window into the interplay between magnetism and superconductivity.

Condmat 0803.0429



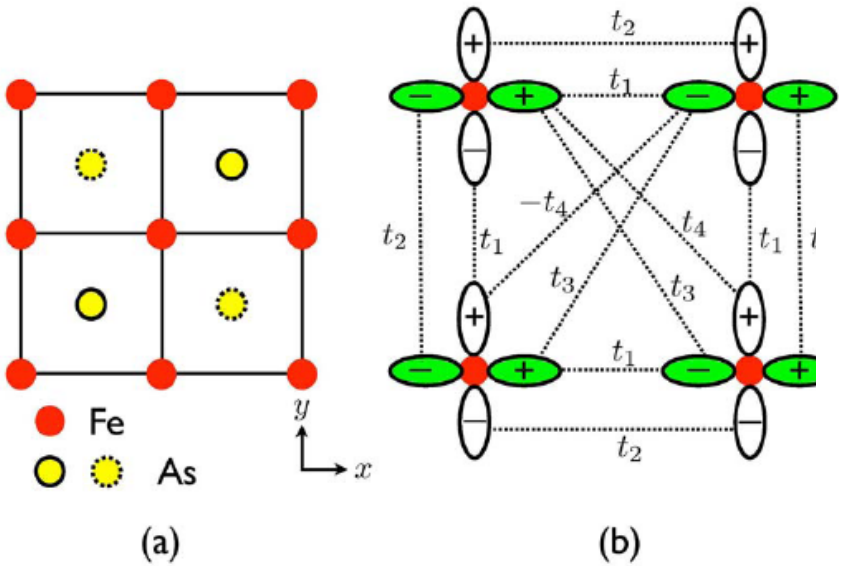


Surface de Fermi cylindriques séparés par un vecteur compatible avec la période de la structure magnétique conduisant à un scénario avec « nesting » pour l'origine du magnétisme (comme dans Cr).

Autres modèles pour rendre compte de la SF et du magnétisme: $LaFeAsO_{1-x}F_x$

Condmat #0803.3286

Model: 2 orbitals per site on a 2D square lattice. By adjusting the one-electron hopping parameters and the chemical potential, one can obtain a Fermi surface which has the same topology as found from the band structure calculations.

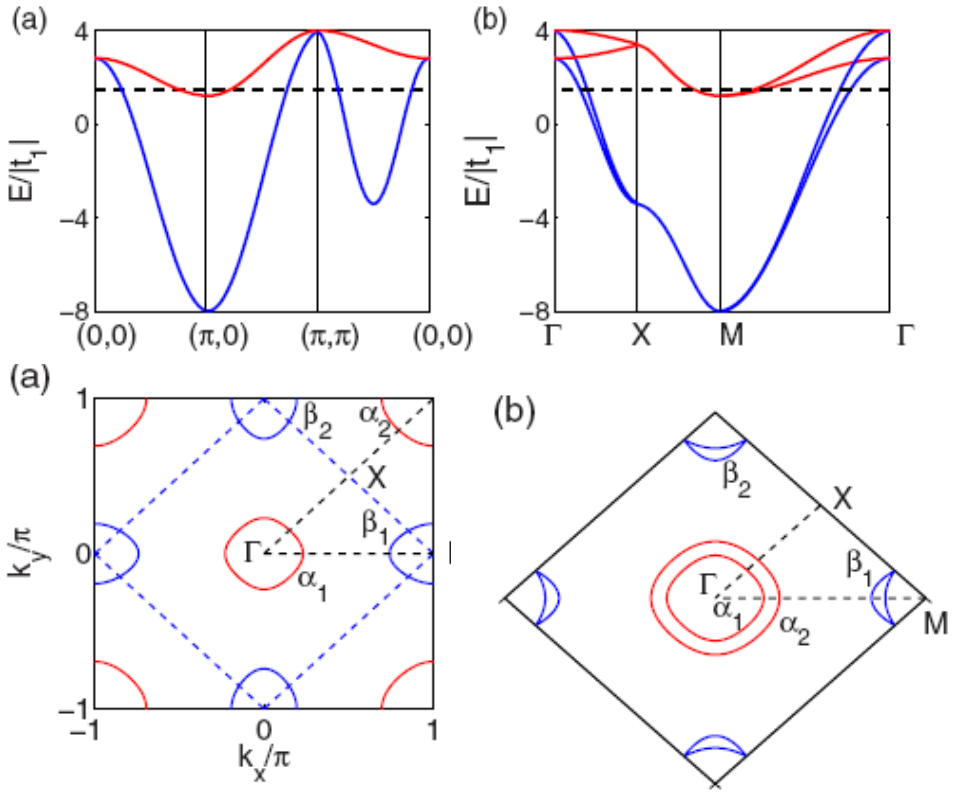


PHYSICAL REVIEW B 77, 220503(R) (2008)

Minimal two-band model of the superconducting iron oxypnictides

S. Raghu,[1] Xiao-Liang Qi,[1] Chao-Xing Liu,[2,1] D. J. Scalapino,[3] and Shou-Cheng Zhang[1]
[1]*Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA*
[2]*Center for Advanced Study, Tsinghua University, Beijing 100084, People's Republic of China*
[3]*Department of Physics, University of California, Santa Barbara, California 93106-9530, USA*
(Received 15 April 2008; revised manuscript received 8 May 2008; published 11 June 2008)

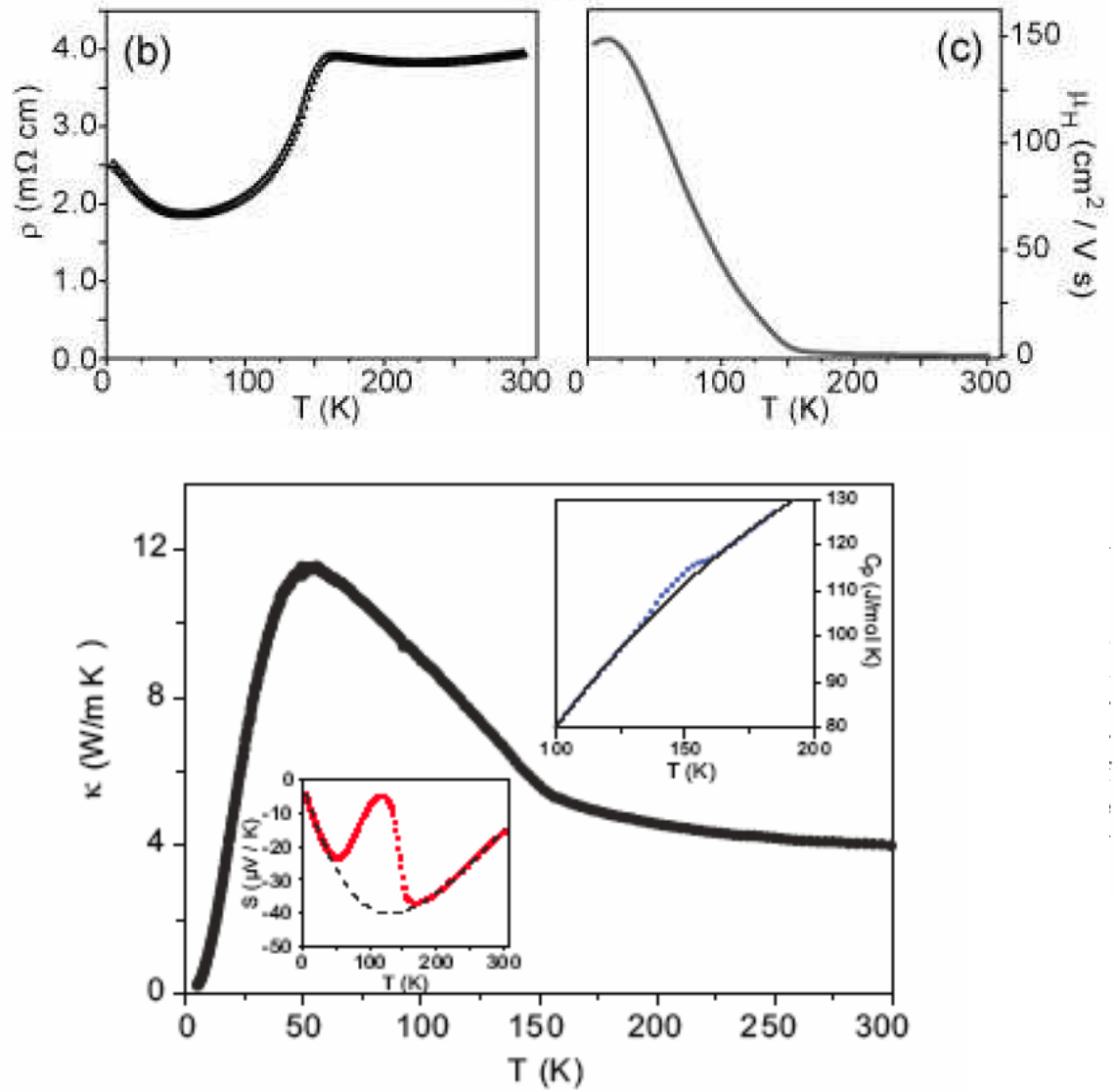
Following the discovery of the Fe-pnictide superconductors, local-density approximation (LDA) band structure calculations showed that the dominant contributions to the spectral weight near the Fermi energy came from the Fe 3*d* orbitals. The Fermi surface is characterized by two hole surfaces around the Γ point and two electron surfaces around the *M* point of the two Fe/cell Brillouin zone. Here, we describe a two-band model that reproduces the topology of the LDA Fermi surface and exhibits both ferromagnetic and $q=(\pi,0)$ spin-density wave fluctuations. We argue that this minimal model contains the essential low energy physics of these materials.



Onde de densité de spins (SDW) dans le composé non supra

LaFeAsO

Mc. Guire et al. (Oak Ridge) condmat #0804.0796



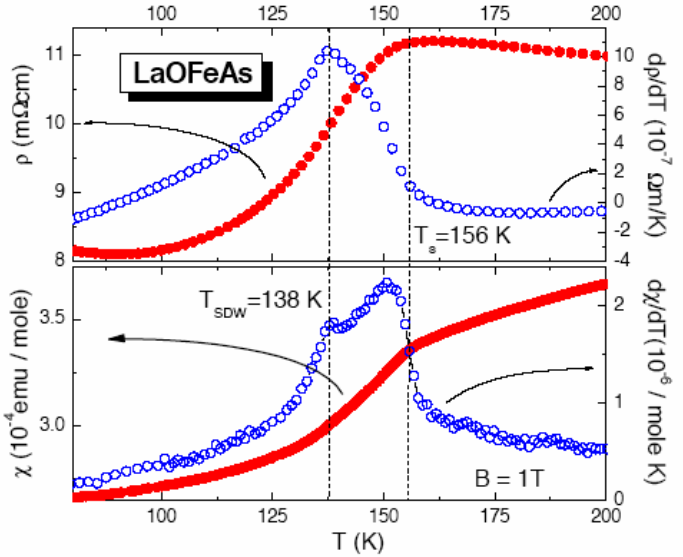
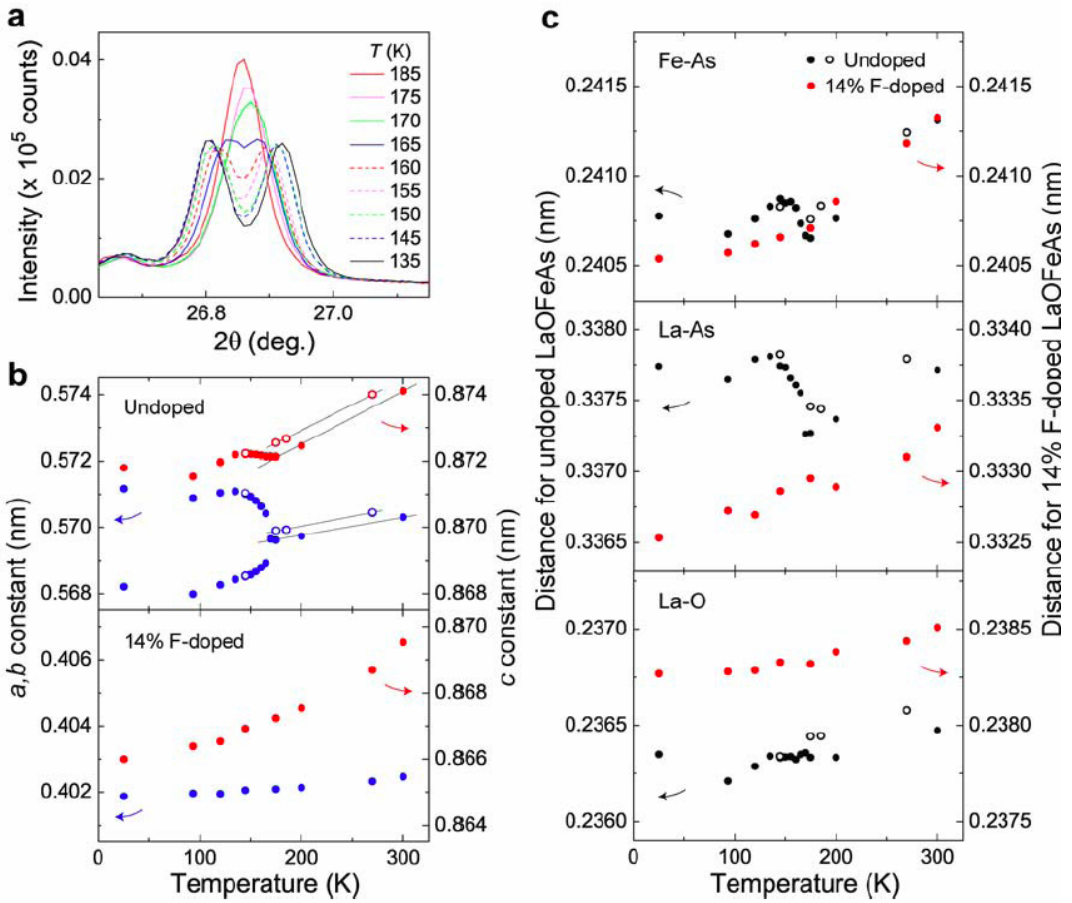


FIG. 4: Temperature dependence of (top) the electrical resistivity and (bottom) the magnetisation vs. temperature and the respective derivatives $\partial\chi/\partial T$ and $\partial\rho/\partial T$. T_S and T_N mark the structural phase transition at 156 K and the SDW-formation at 138 K.

Transition structurale dans le composé non supra LaFeAsO

Crystallographic Phase Transition and High-T_c Superconductivity in LaOFeAs:F

Takatoshi Nomura[1], Sung Wng Kim[2], Yoichi Kamihara[3], Masahiro Hirano[3], Peter V. Sushko[4], Kenichi Kato[5], Masaki Takata[5], Alexander L. Shluger[4], and Hideo Hosono[1,3,6]*



Origine? Mis-Match entre couches LaO & FeAs ?
comme dans $La_{2-x}Sr_xCuO_4$?

Onde de densité de spins (SDW) dans le composé non supra

$LaFeAsO_{1-x}F_x$
Diffraction de neutrons @ BT

nature

LETTERS

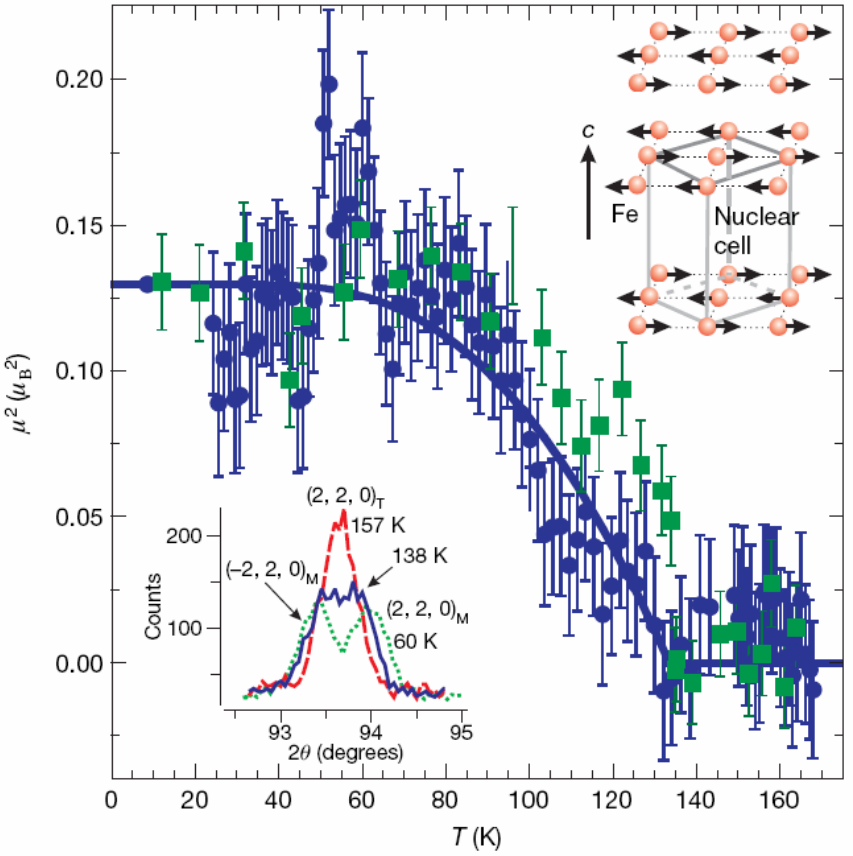
Magnetic order close to superconductivity in the iron-based layered $LaO_{1-x}F_xFeAs$ systems

Clarina de la Cruz[1,2], Q. Huang[3], J. W. Lynn[3], Jiying Li[3,4], W. Ratcliff II[3], J. L. Zarestky[5], H. A. Mook[2], G. F. Chen[6], J. L. Luo[6], N. L. Wang[6] & Pengcheng Dai[1,2]

Composé mère LaFeAsO non supra:
- distorsion structurale brutale à T=155 K tétragonale (P4/nmm) à monoclinique (P112/n) ou orthorhombique (Cmma) @BT

- puis à 137 K, développe un ordre AFM à longue portée de type onde de densité de spins (SDW) avec un moment magnétique réduit à **0.4μB/Fe** et une structure magnétique en « stripes » dans le plan (a,b) et doublée par rapport à la maille cristallographique suivant l'axe c

- structure magnétique confirmée par calculs théoriques (LDA) mais moment sur-estimé



Onde de densité de spins (SDW) dans le composé non supra

PHYSICAL REVIEW B 78, 020503(R) (2008)

Spin-density-wave anomaly at 140 K in the ternary iron arsenide $BaFe_2As_2$

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Department Chemie und Biochemie, Ludwig-Maximilians-Universität München, Butenandtstrasse 5-13, Haus D, München 81377, Germany

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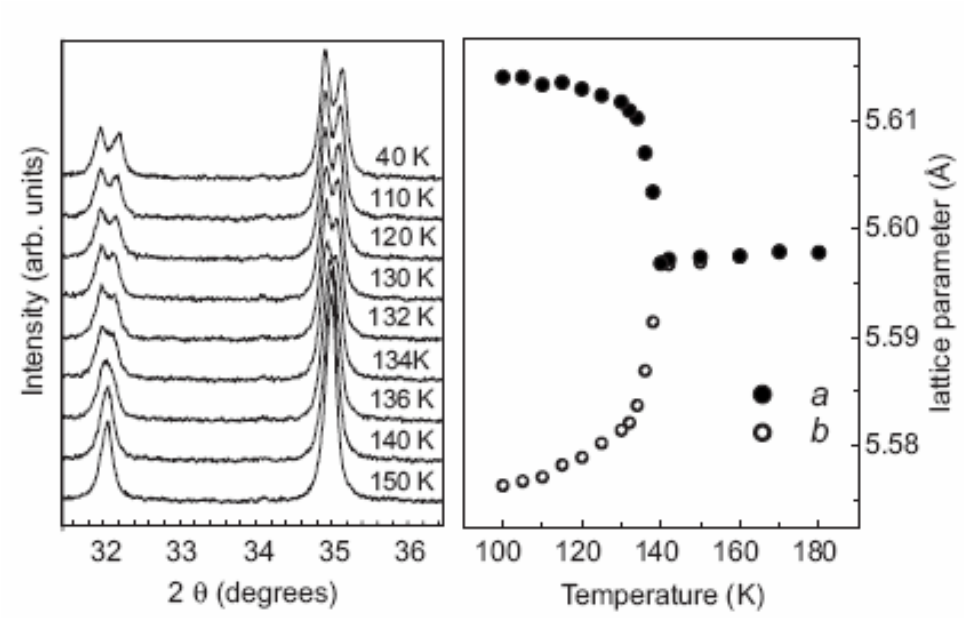
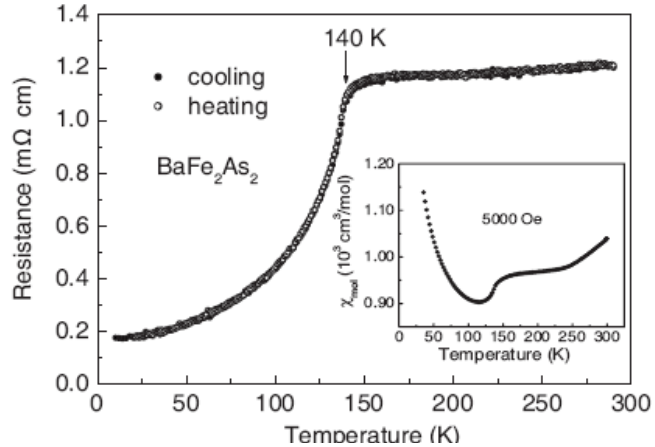
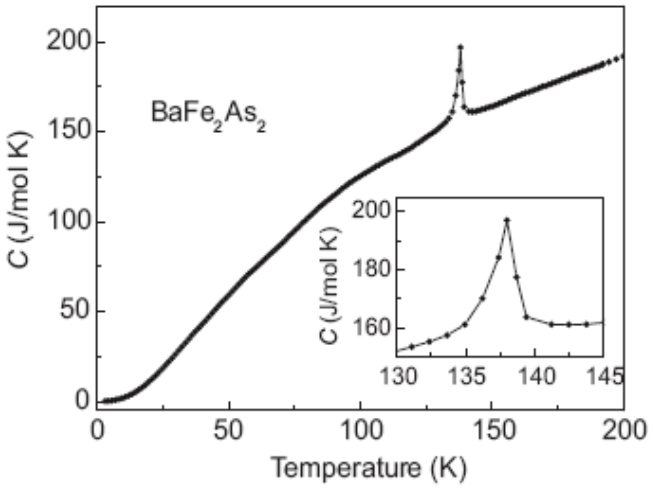
(Received 26 May 2008; published 8 July 2008)







Transition magnétique ET transition cristallographique tétragonale (I4/mmm) → orthorhombique (Fmmm)

Onde de densité de spins (SDW) dans le composé non supra

Magnetic order in $BaFe_2As_2$, the parent compound of the FeAs based superconductors in a new structural family

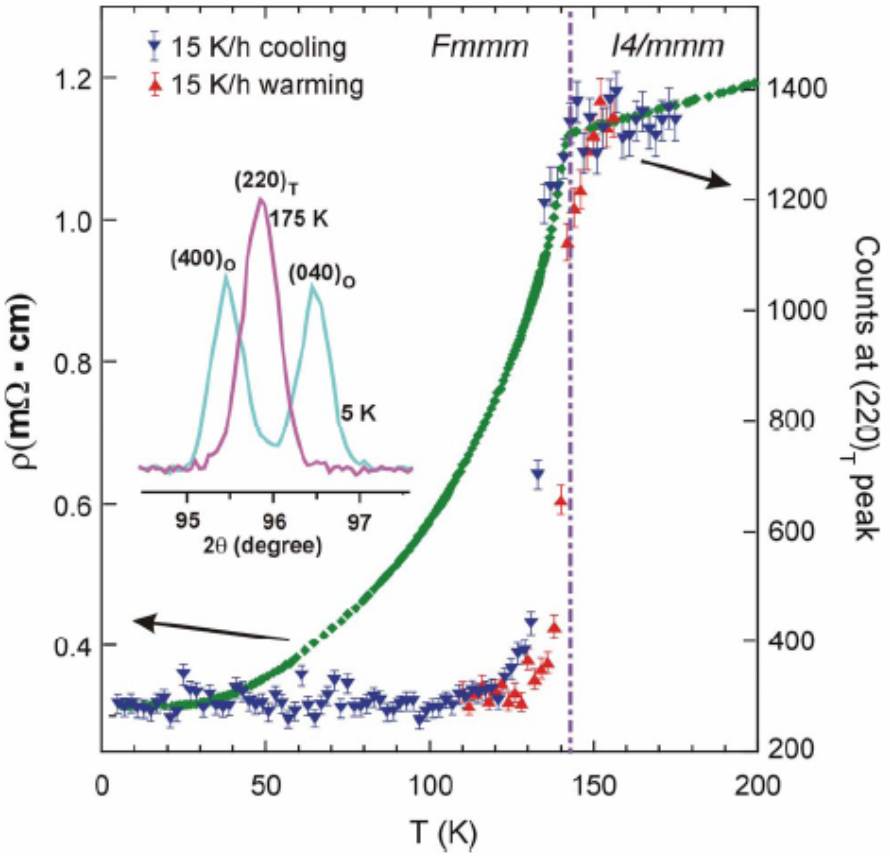
$BaFe_2As_2$
Diffraction de neutrons @ BT

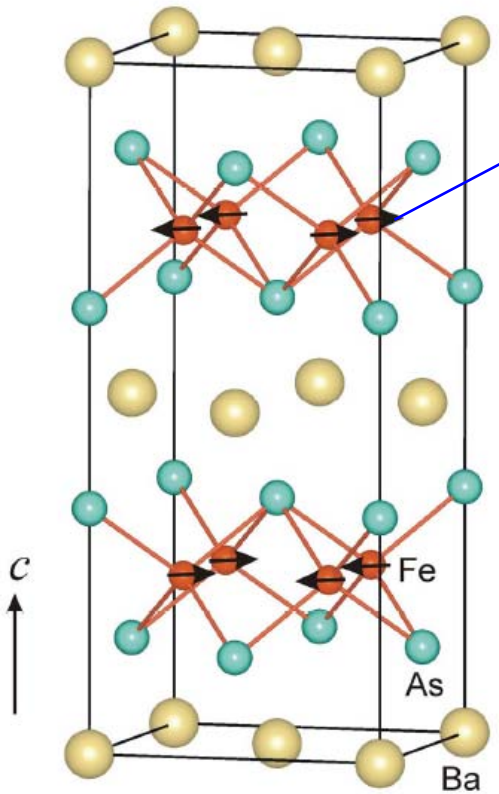
Q. Huang[1], Y. Qiu[1,2], Wei Bao[3], J.W. Lynn[1], M.A. Green[1,2], Y.C. Gasparovic[1,2], T. Wu[4], G. Wu[4] & X. H. Chen[4]

Condmat #0806.2776

[1]*NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg,*

Transition structurale





0.87μB (5K)

Résultats similaires dans SrFe2As2 (*condmat #0807.1077*)

Onde de densité de spins (SDW) dans le composé non supra

Crystal structure of the new $FeSe_{1-x}$ superconductor

S. Margadonna…
E. Suard and K. Prassides
Condmat #0807.4610

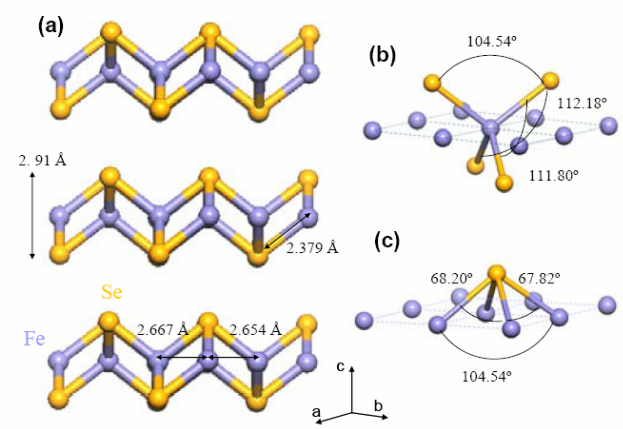
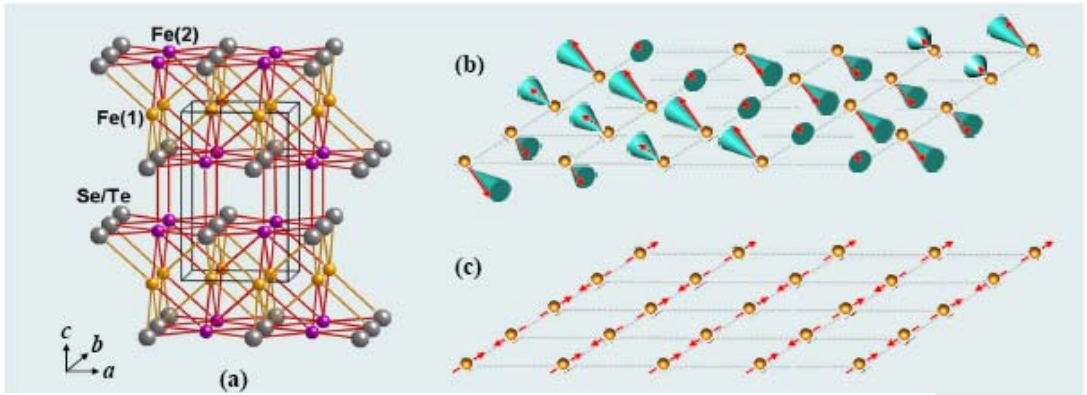


Fig. 1 (a) Schematic diagram of the low-temperature orthorhombic crystal structure of α-$FeSe_{0.92}$. Fe and Se ions are depicted as blue and yellow spheres, respectively. **(b)** and **(c)** Geometry of the $FeSe_4$ tetrahedra and the $SeFe_4$ pyramids with the three distinct Se-Fe-Se and Fe-Se-Fe bond angles indicated.

Incommensurate magnetic order in the $Fe(Te_{1-x}Se_x)$ superconductor systems

Wei Bao, … Z.Q. Mao condmat #0809.2058

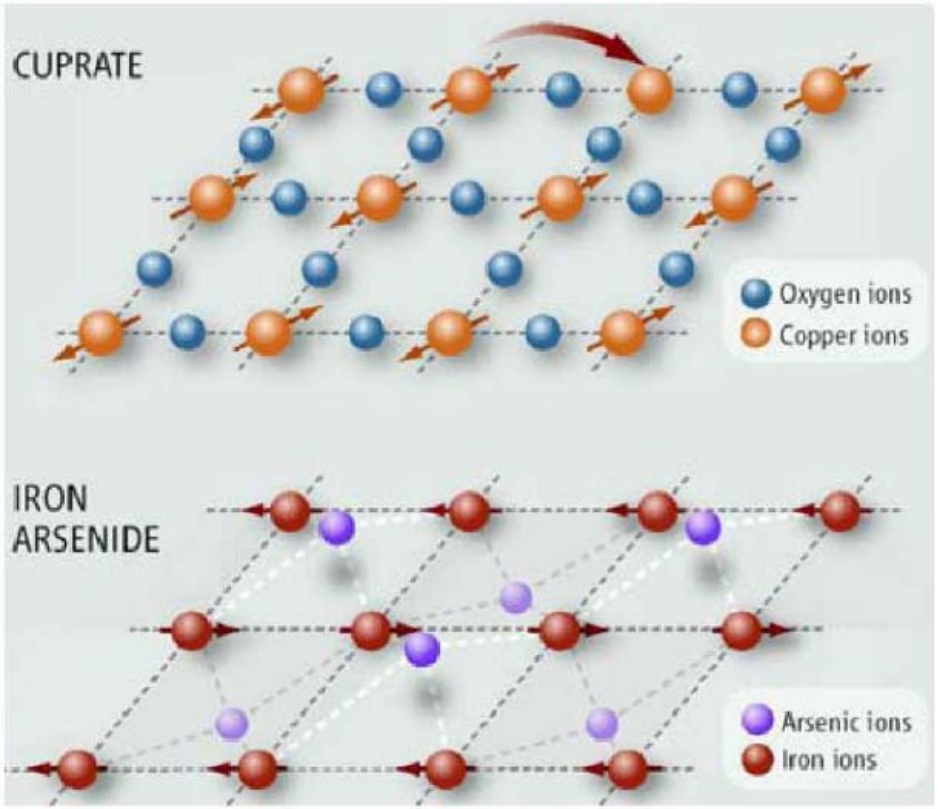


Onde de densité de spins incommensurable!

Figure 1 **Crystal and magnetic structures of α-iron-chalcogen.** **a**, The Fe(1) and Te/Se are fully occupied sites of the tetragonal PbO structure. The excessive Fe of $Fe_{1+y}(Te_{1-x}Se_x)$ is located on the partially occupied Fe(2) site. Magnetic structures of **b**, α-FeTe and **c**, $BaFe_2As_2$ are shown in a Fe layer for comparison. The dashed lines denotes the Fe "square" sublattice. Each row of magnetic moments along the diagonal direction (the b-axis of the crystal structure) are identical in **b**. They modulate incommensurately with the lattice along the other diagonal (the a-axis), with both a linear sinusoid component pointing in the b-direction and a spiral component in the ac-plane. In contrast, in the commensurate antiferromagnetic order of $BaFe_2As_2$, the row of identical magnetic moments line along one edge of the Fe square lattice (the a-axis of the orthorhombic unit cell) and alternate along the other edge (the b-axis)[6].

Onde de densité de spins (SDW) dans le composé non supra

Analogie avec les cuprates: ordre AFM et distorsion structurale supprimés par dopage



MAIS: dans les composés Fe-As, la phase AFM reste métallique alors que les cuprates celle-ci est isolante

Diagramme de phase

Expériences µSR

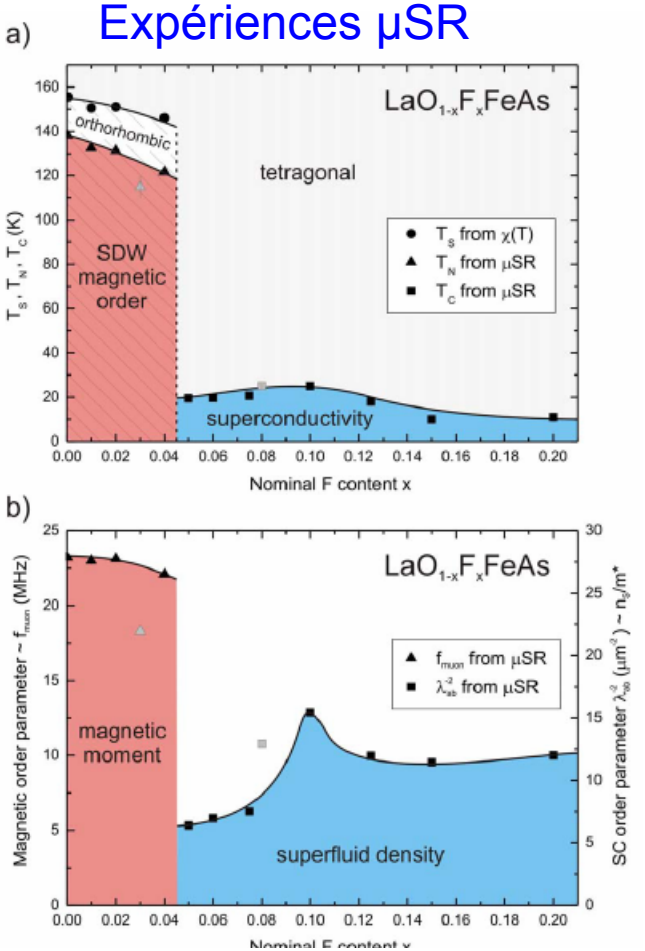


Figure 3. Electronic phase diagram of $LaO_{1-x}F_xFeAs$. (a) The doping dependence of the magnetic and superconducting transition temperatures determined from the µSR experiments. Also shown are the tetragonal to orthorhombic structural transition temperatures T_S determined from resistivity measurements which show a king and subsequent strong reduction below T_S [10,26]. **(b)** The doping dependence of the low temperature saturation value of the magnetic order parameter (the spontaneous muon spin precession frequency f_{muon} (T→ 0)) and of the superfluid density n_s/m^* measured via $1/\lambda_{ab}^2$ (T→ 0) in TF µSR experiments. The grey data points at x=0.03 and x=0.08 are taken from Carlo et al [17]

$LaFeAs(O_{1-x}F_x)$

H. Luetkens et al. condmat0806.3533

The competition of magnetic order and superconductivity is a key element in the electronic phase diagram of all unconventional superconductors as e.g. the high-transition-temperature (high-T_c) cuprates [1], heavy fermions [2] and organic superconductors[3]. In these systems superconductivity is often found close to a quantum critical point where long-range antiferromagnetic order is gradually suppressed as a function of a control parameter, e.g. charge carrier doping or pressure. It is widely believed that dynamic spin fluctuations associated with this quantum critical behaviour are crucial for the mechanism of superconductivity. Recently high-temperature superconductivity has been discovered in iron-pnictides providing a new class of unconventional superconductors[4,5,6]. Similar as in the unconventional superconductors mentioned above superconductivity in the pnictides occurs in close proximity to a magnetic instability. Several experiments yield that the undoped compound LaOFeAs shows a metallic spin-density-wave (SDW) state with a small ordered moment below ~134 K[7,8]. In contrast, highly sensitive muon spin relaxation (µSR) experiments on superconducting $LaO_{1-x}F_xFeAs$ with optimally doped x~0.10 show the absence of static magnetic correlations[9]. In this Letter we determine the electronic phase diagram and, in particular, the exact nature of the change from the magnetically ordered to the superconducting state by means of µSR and Mössbauer spectroscopy on the series $LaO_{1-x}F_xFeAs$. Our experiments yield information on both, the doping dependence of the transition temperatures and the respective order parameters. In strong contrast to cuprates and heavy fermions we find a discontinuous first-order-like change of the Néel temperature, the superconducting transition temperature, the sublattice magnetisation and the superfluid density. While these results strongly question the relevance of quantum critical behaviour in iron pnictides they suggest an important role of the structural orthorhombic distortion disappearing exactly at the phase boundary between the magnetic SDW and the superconducting state.

Diagramme de phase

Diffraction de neutrons

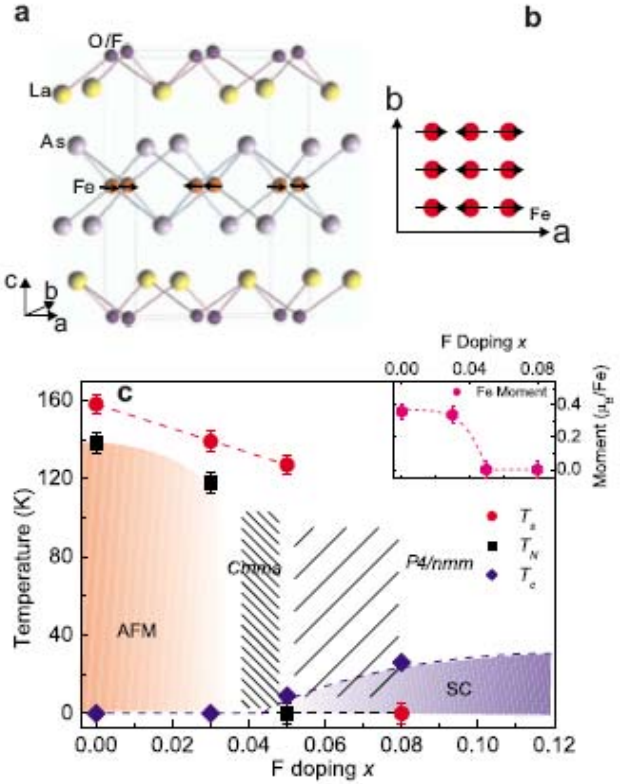


FIG. 1. (Color online) (a) The Fe spin ordering in the LaFeAsO chemical unit cell. (b) The Fe magnetic unit cell of LaFeAsO in the Fe-As plane. The Fe moments lie in the a-b plane along the a axis and form an antiferromagnetic collinear spin structure similar to $BaFe_2As_2$, $SrFe_2As_2$, and $CaFe_2As_2$ (Refs. 7–10) (c) The structural and magnetic phase diagram determined from our neutron measurements on $LaFeAsO_{1-x}F_x$ with x=0,0.03,0.05,0.08. The red circles indicate the onset temperature of the $P4/nmm$ to $Cmma$ phase transition. The black squares designate the Néel temperatures of Fe as determined from neutron measurements in Fig. 3. The superconducting transition temperatures T_c for x=0.05,0.08 are determined from susceptibility measurements. The AFM to superconducting phase transition happens between x=0.03 and 0.05. The inset in (d) shows the F doping dependence of the Fe moment as determined from the intensity of the $(1,0,3)_M$ magnetic peak at 4 K.

$LaFeAs(O_{1-x}F_x)$

Q. Huang et al. PRB 78, août 2008.

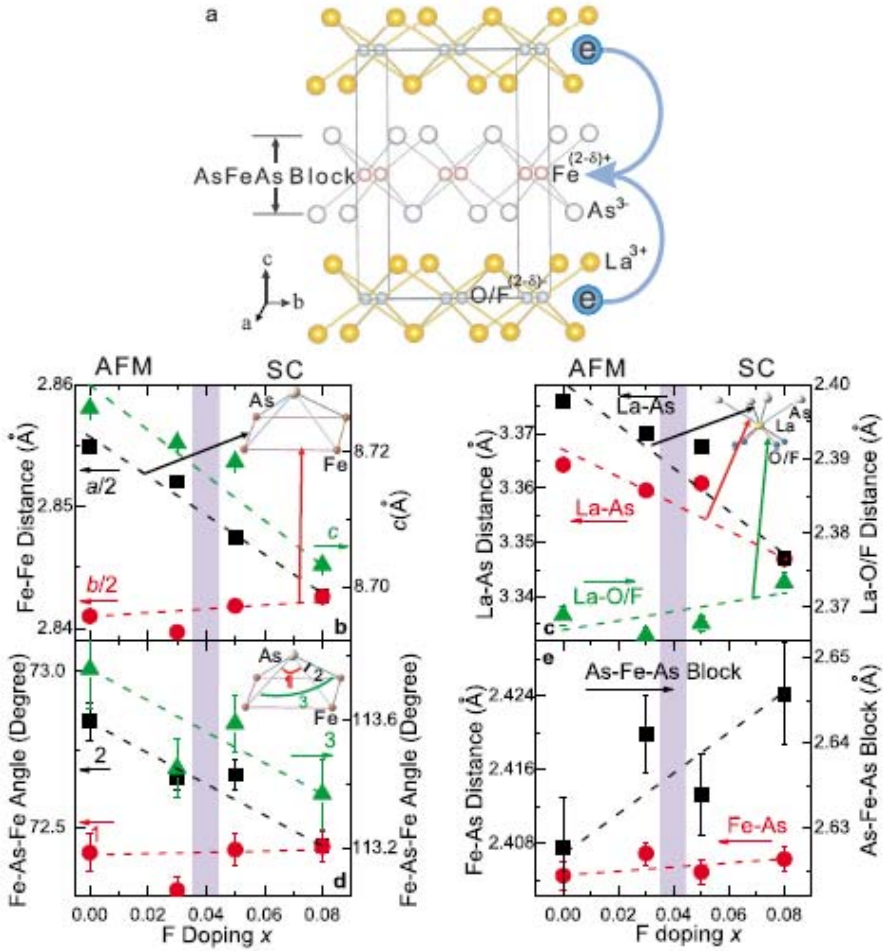
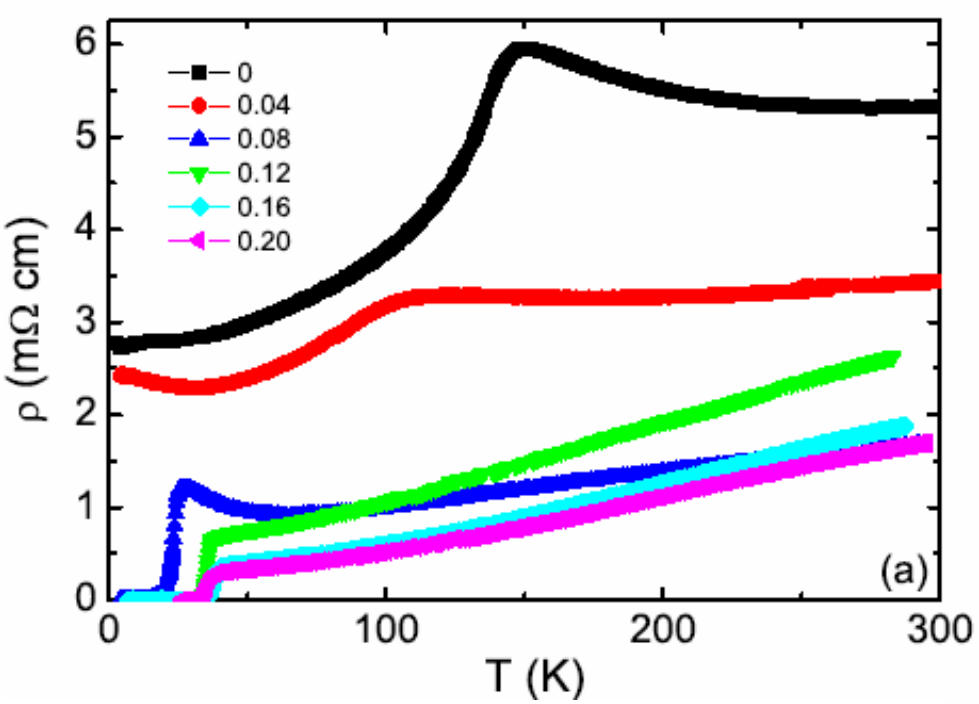


FIG. 4. (Color online) Low temperature structural evolution of $LaFeAsO_{1-x}F_x$ as a function of F doping obtained from analysis of the BT-1 data. There is no sudden structural transition as the AFM order is replaced by the superconducting phase. The atomic positions of $LaFeAsO_{1-x}F_x$ and their temperature dependence are shown in Tables I and II. (a) schematic defining the As-Fe-As block and illustrating the process of electron doping. (b) a, b, c lattice constants of the orthorhombic unit cell and the two Fe-Fe nearest-neighbor distances as a function of F doping. Similar to $CeFeAsO_{1-x}F_x$, F doping only suppresses the long axis of the orthorhombic structure. (c) La-O/F and La-As distances as a function of F doping. The slight increase in the La-O/F block size is compensated by a much larger reduction in the La-As distance, resulting in an overall c-axis lattice contraction as shown in (b). (d) Fe-As-Fe bond angles as defined in the inset versus F doping. While angle 1 hardly changes with doping, angles 2 and 3 decrease substantially with increasing F doping. (e) The Fe-As bond distance and As-Fe-As block size versus F doping. The Fe-As distance is independent of F doping.

Onde de densité de spins (SDW) et compétition avec l'ordre supra

Superconductivity at 41 K and its competition with spin-density-wave instability in layered $CeO_{1-x}F_xFeAs$

G. F. Chen, Z. Li, D. Wu, G. Li, W. Z. Hu, J. Dong, P. Zheng, J. L. Luo, and N. L. Wang
Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, Peoples Republic of China



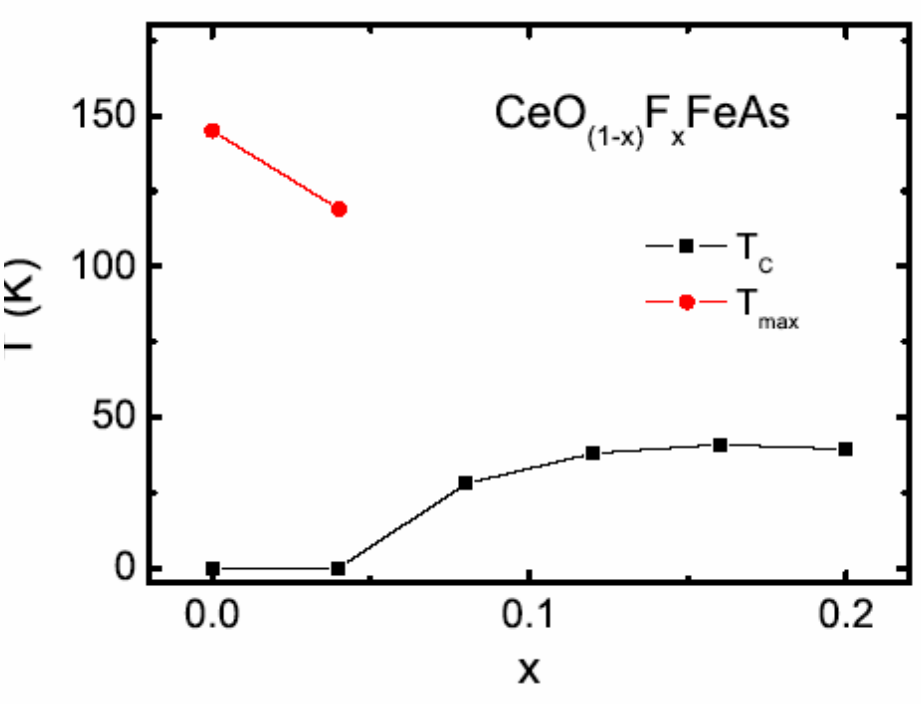
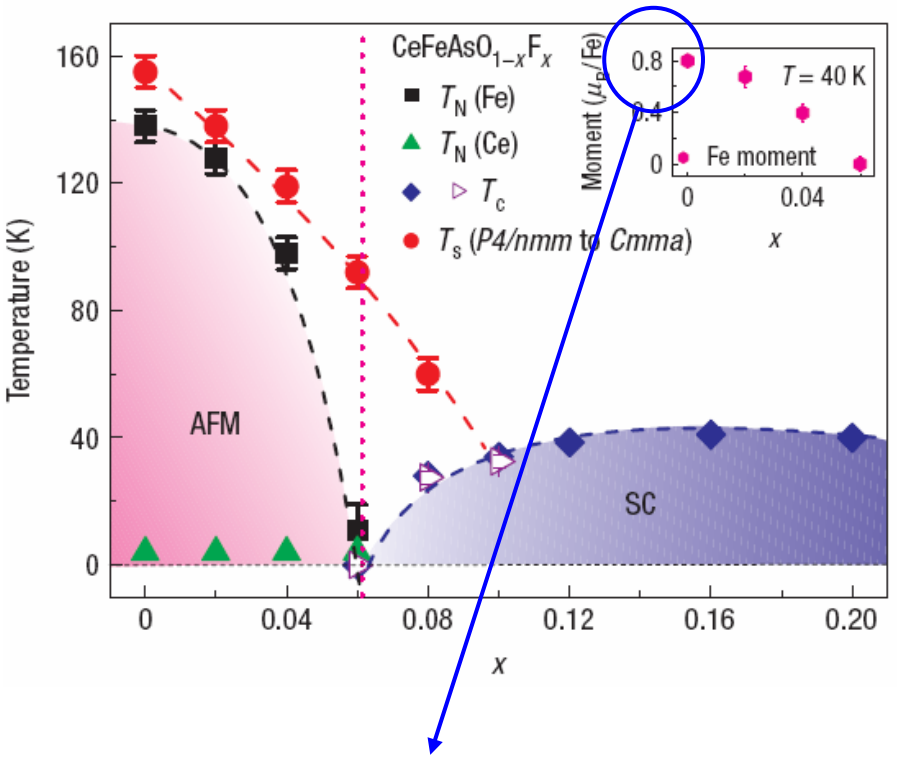


Diagramme de phase

$CeFeAsO_{1-x}F_x$

J. Zhao et al. Nat.Mat. Dec 2008

Diffraction de neutrons



0.8μB/Fe à x=0

$SmFeAs(O_{1-x}F_x)$ résistivité

R. H. Liu et al.

PRL **101,** 087001 (2008)

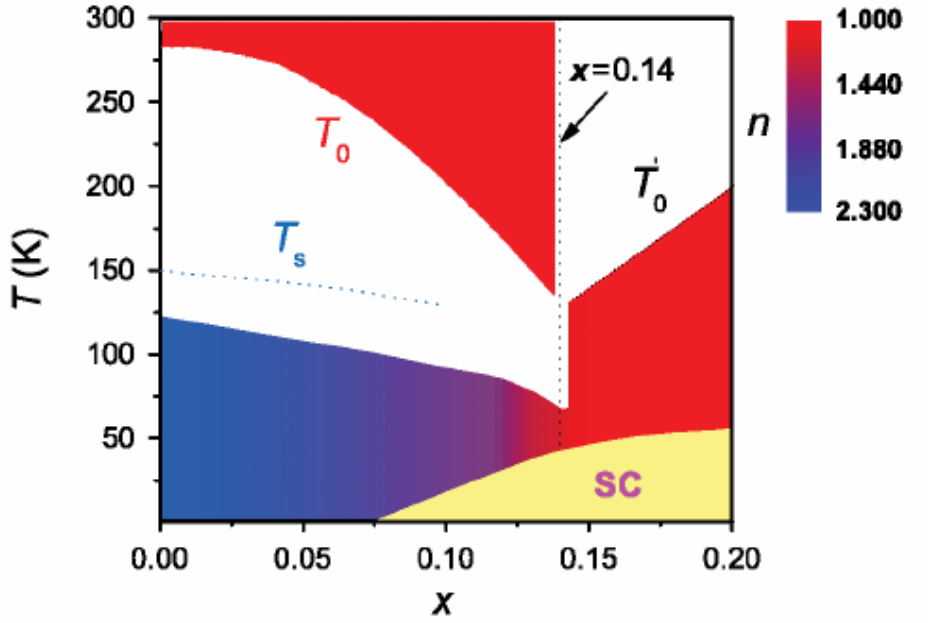


FIG. 4 (color). Electronic phase diagram for a $SmFeAsO_{1-x}F_x$ system. T_s indicates the temperature of the anomaly peak in resistivity. T_0 and T_0' represent the deviating temperature from a T-linear dependence of resistivity in low and high temperatures, respectively. The different color regions represent different n in the formula $\rho = a + bT^n$ shown in Fig. 2. The dotted line of $x = 0.14$ clearly shows a boundary for different behavior of T-dependent resistivity below and above $x = 0.14$, suggesting a QCP around $x \sim 0.14$. The superconductivity is abbreviated as SC.

Coexistence of the spin-density-wave and superconductivity in the $Ba_{1-x}K_xFe_2As_2$

?

H. Chen,[1] Y. Ren,[2] Y. Qiu,[3,4] Wei Bao,[5,*] R. H. Liu,[1] G. Wu,[1]
T. Wu,[1] Y. L. Xie,[1] X. F. Wang,[1] Q. Huang,[3] and X. H. Chen[1,†]

Condmat #0807.3950

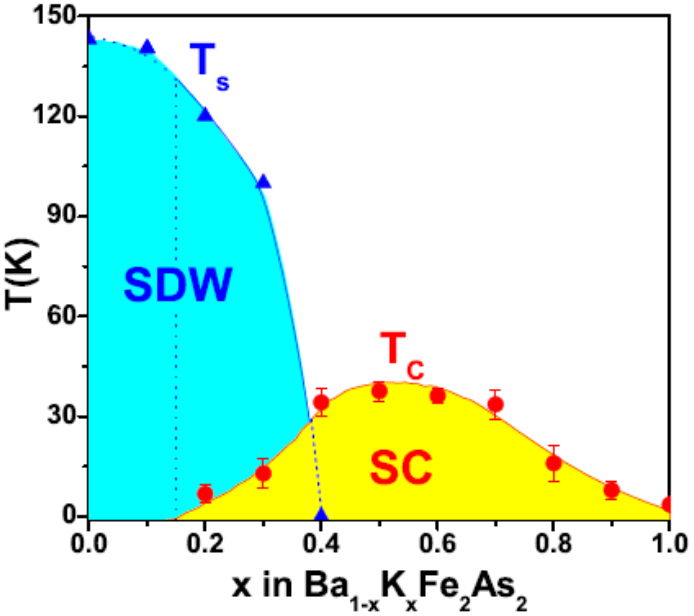


FIG. 3: The composition-temperature phase-diagram, showing the structural, magnetic and superconducting transitions. The T_S denotes the temperature of the simultaneous structural and magnetic transition, and T_C the superconducting one. The spin-density-wave (SDW) and superconducting (SC) orders coexist at low temperature in $0.2 \leq x < 0.4$.

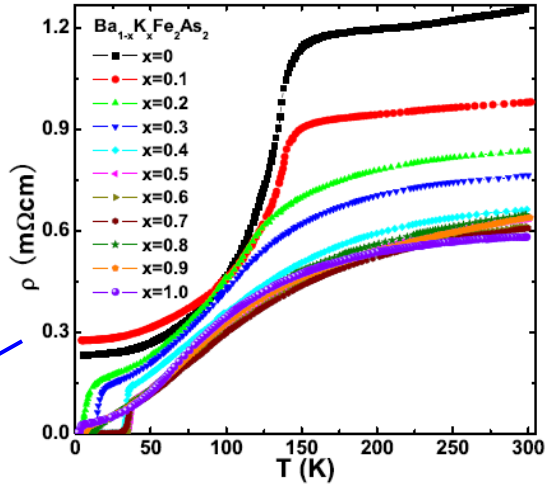
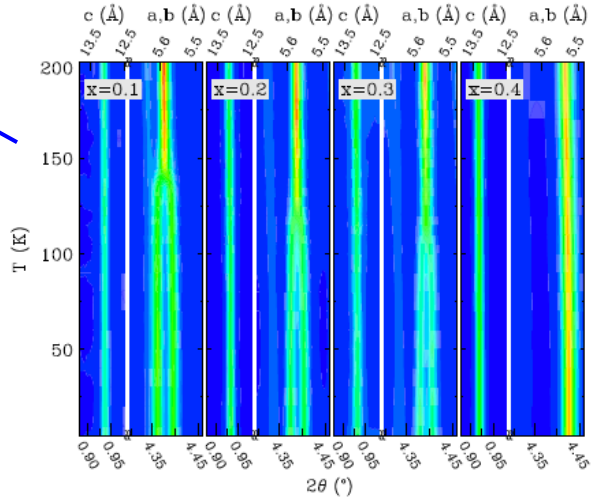


FIG. 2: Temperature dependence of the resistivity.



Gap supra, paramètre d'ordre supra

La-1111

Mesure de C_p

CHIN.PHYS.LETT. Vol. 25, No. 6 (2008) 2221

Nodal Gap in Fe-Based Layered Superconductor $LaO_{0.9}F_{0.1-\delta}FeAs$ Probed by Specific Heat Measurements *

MU Gang(牟刚), ZHU Xi-Yu(祝熙宇), FANG Lei(方磊), SHAN Lei(单磊), REN Cong(任聪), WEN Hai-Hu(闻海虎)**

National Laboratory for Superconductivity, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, PO Box 603, Beijing 100190

(Received 30 April 2008)

We report the specific heat measurements on the newly discovered Fe-based layered $LaO_{0.9}F_{0.1-\delta}FeAs$ superconductor with the onset transition temperature $T_c \approx 28\,K$. A nonlinear magnetic field dependence of the electronic specific heat coefficient $\gamma(H)$ has been found in the low temperature limit, which is consistent with the prediction for a nodal superconductor. The maximum gap value $\Delta_0 \approx 3.4 \pm 0.5\,meV$ is derived by analysing $\gamma(H)$ based on the d-wave model. We also detected the electronic specific heat difference between $9\,T$ and $0\,T$ in a wide temperature range, a specific heat anomaly can be clearly observed near T_c. The Debye temperature of our sample is determined to be about $315.7\,K$. Our results suggest an unconventional mechanism for this new superconductor.

Gap nodal

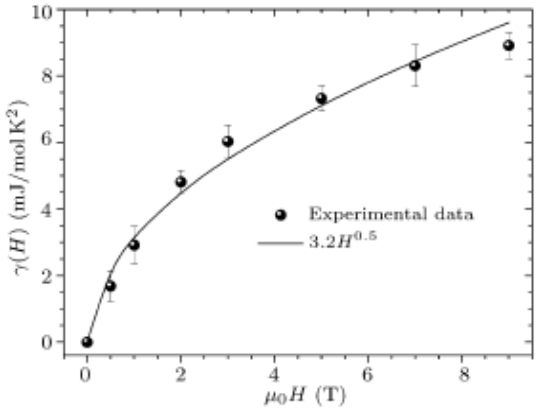


Fig. 3. Field dependence of the field-induced term $\gamma(H)$ at $T = 0\,K$ (symbols). The solid line is the fit to $\gamma(H) = A\sqrt{H}$.

Gap supra, paramètre d'ordre supra

nature Vol 453|26 June 2008|doi:10.1038/nature07081

LETTERS

Sm-1111

A BCS-like gap in the superconductor $SmFeAsO_{0.85}F_{0.15}$

T. Y. Chen[1], Z. Tesanovic[1], R. H. Liu[2], X. H. Chen[2] & C. L. Chien[1]

Since the discovery of superconductivity in the high-transition-temperature (high-T_c) copper oxides two decades ago, it has been firmly established that the CuO_2 plane is essential for superconductivity and gives rise to a host of other very unusual properties. A new family of superconductors with the general composition of $LaFeAsO_{1-x}F_x$ has recently been discovered[1–8] and the conspicuous lack of the CuO_2 planes raises the tantalizing question of a different pairing mechanism in these oxypnictides. The superconducting gap (its magnitude, structure, and temperature dependence) is intimately related to pairing. Here we report the observation of a single gap in the superconductor $SmFeAsO_{0.85}F_{0.15}$ with $T_c = 42$ K as measured by Andreev spectroscopy. The gap value of $2\Delta = 13.34 \pm 0.3$ meV gives $2\Delta/k_BT_c = 3.68$ (where k_B is the Boltzmann constant), close to the Bardeen–Cooper–Schrieffer (BCS) prediction of 3.53. The gap decreases with temperature and vanishes at T_c in a manner consistent with the BCS prediction, but dramatically different from that of the pseudogap behaviour in the copper oxide superconductors. Our results clearly indicate a nodeless gap order parameter, which is nearly isotropic in size across different sections of the Fermi surface, and are not compatible with models involving antiferromagnetic fluctuations, strong correlations, the t-J model, and the like, originally designed for the high-T_c copper oxides.

- Single Gap « BCS-like » Δ = 6.6meV

- Paramètre d'ordre sans node, quasi isotrope en amplitude à travers les différentes sections de la surface de Fermi

Andreev spectroscopy

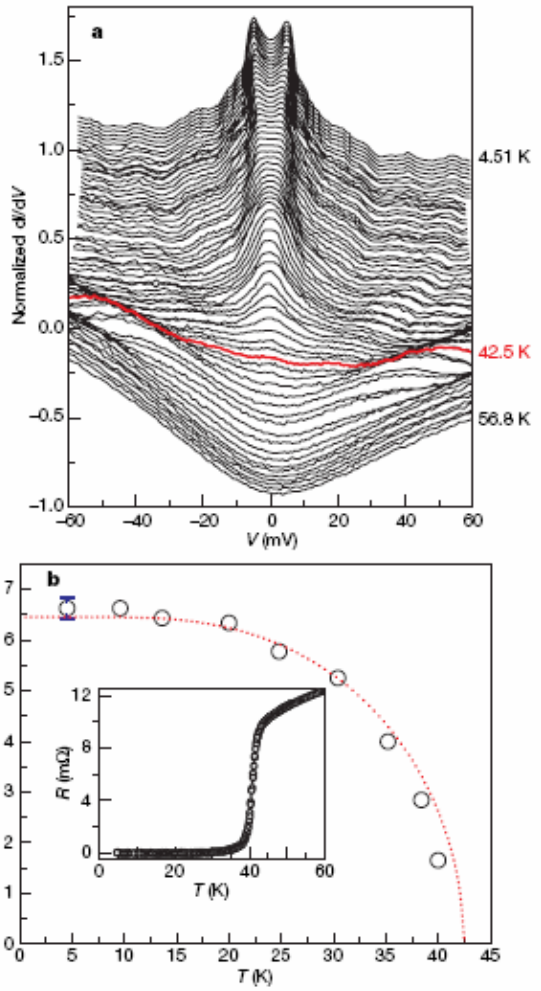


Figure 3 | Temperature dependence of the gap. **a**, Andreev spectra from 4.51 K to 56.8 K of an Au/$SmFeAsO_{0.85}F_{0.15}$ contact taken every ~0.8 K, showing the decrease of the gap value and the eventual disappearance of the gap structure at $T_c \approx 42$ K. **b**, Main panel, temperature dependence of the gap value (open circles) obtained from the modified BTK fit of $SmFeAsO_{0.85}F_{0.15}$ is close to the BCS theory prediction (dotted curve). Error bars at 4.51 K show ±1 s.e.m. from the average of 15 spectra for different contacts. Inset, the resistive transition at T_c.

isplays two gaps with values

Gap supra, paramètre d'ordre supra

Nd-1111

ARPES

PRL 101, 147003 (2008) PHYSICAL REVIEW LETTERS week ending 3 OCTOBER 2008

Momentum Dependence of the Superconducting Gap in $NdFeAsO_{0.9}F_{0.1}$ Single Crystals Measured by Angle Resolved Photoemission Spectroscopy

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[2]*Laboratoire Photons Et Matière, UPR-5 CNRS, ESPCI, 10 rue Vauquelin, 75231 Paris cedex 5, France*
[3]*Labratoire de Physique des Solides, UMR-8502 CNRS, Université Paris-Sud, Bâtiment 510, 91405 Orsay, France*
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(Received 6 July 2008; published 2 October 2008)

We use angle resolved photoemission spectroscopy to study the momentum dependence of the superconducting gap in $NdFeAsO_{0.9}F_{0.1}$ single crystals. We find that the Γ hole pocket is fully gapped below the superconducting transition temperature. The value of the superconducting gap is 15 ± 1.5 meV and its anisotropy around the hole pocket is smaller than 20% of this value—consistent with an isotropic or anisotropic *s*-wave symmetry of the order parameter. This is a significant departure from the situation in the cuprates, pointing to the possibility that the superconductivity in the iron arsenic based system arises from a different mechanism.

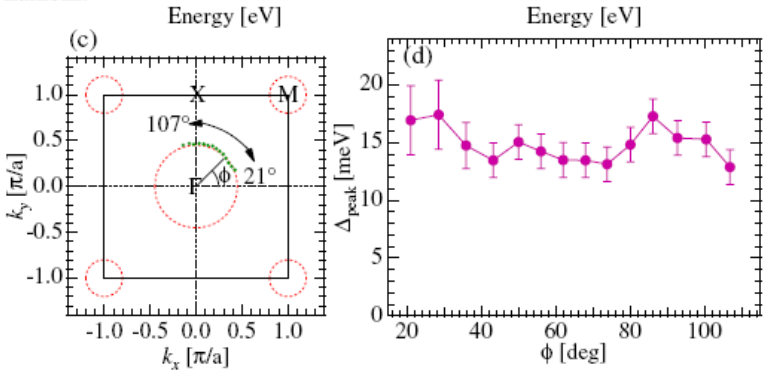

FIG. 2 (color online). The magnitude of the superconducting gap along the Γ hole pocket. (a) Raw- and (b) symmetrized-EDCs at the Fermi crossing momenta marked by green (or gray) dots in panel (c), where the definition of the ϕ angle is shown. (d) The value of the superconducting gap extracted from the data in panel (b) using the coherent peak position method. Peak positions are indicated by arrows.

Gap supra, paramètre d'ordre supra

La-1111

^{75}As NQR

Condmat #0810.1818

Two-gaps feature in $LaFeAsO_{0.92}F_{0.08}$ superconductor revealed by nuclear quadrupole resonance

S. Kawasaki[1], K. Shimada[1], G. F. Chen[2], J. L. Luo[2], N. L. Wang[2], and Guo-qing Zheng[1]
[1]*Department of Physics, Okayama University, Okayama 700-8530, Japan and*
[2]*Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
(Dated: October 10, 2008)

We report ^{75}As nuclear quadrupole resonance (NQR) studies on superconducting oxypnictide $LaFeAsO_{0.92}F_{0.08}$ ($T_c = 23$ K). The temperature dependence of the spin lattice relaxation rate ($1/T_1$) decreases below T_c without a coherence (Hebel-Slichter) peak and shows a temperature dependence that is not simple power-law nor exponential. We show that the result can be understood in terms of two superconducting gaps of either d- or $\pm s$-wave symmetry, with the larger gap $\Delta_1 \sim 4k_BT_c$ and the smaller one $\Delta_2 \sim 1.5k_BT_c$. Our result suggests that the multiple-gaps feature is universal in the oxypnictides superconductors, which is probably associated with the multiple electronic bands structure in this new class of materials. We also find that $1/T_1T$ above T_c increases with decreasing temperature, which suggests weak magnetic fluctuations in the normal state.

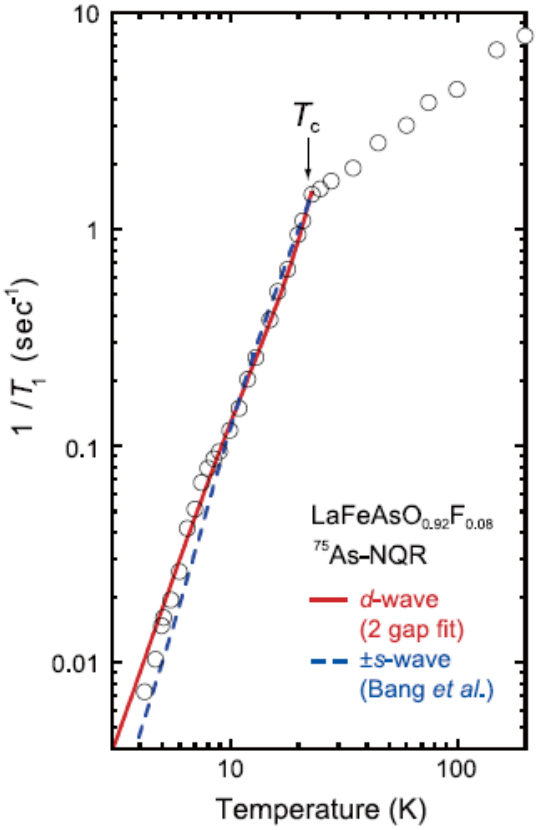

FIG. 3: (color online) The temperature dependence of $^{75}(1/T_1)$ in $LaFeAsO_{0.92}F_{0.08}$ measured at zero magnetic field. The solid curve is a two gap fit assuming a d-wave symmetry with parameters, $\Delta_1(0) = 4.2k_BT_c$, $\Delta_2(0) = 1.6k_BT_c$, and $\alpha = 0.6$ (see text). The dotted curve is a simulation assuming two s-wave gaps that change signs with parameters, $\Delta_1(0) = 3.75k_BT_c$, $\Delta_2(0) = 1.5k_BT_c$, and $\alpha = 0.38$ referred from literature.[30,31] The solid arrow indicates T_c.

Gap supra, paramètre d'ordre supra

ARPES

$Ba_{0.6}K_{0.4}Fe_2As_2$ (Ba,K)-122:

Observation of Fermi-surface–dependent nodeless superconducting gaps

H. Ding et al. EPL 83, Juillet 2008

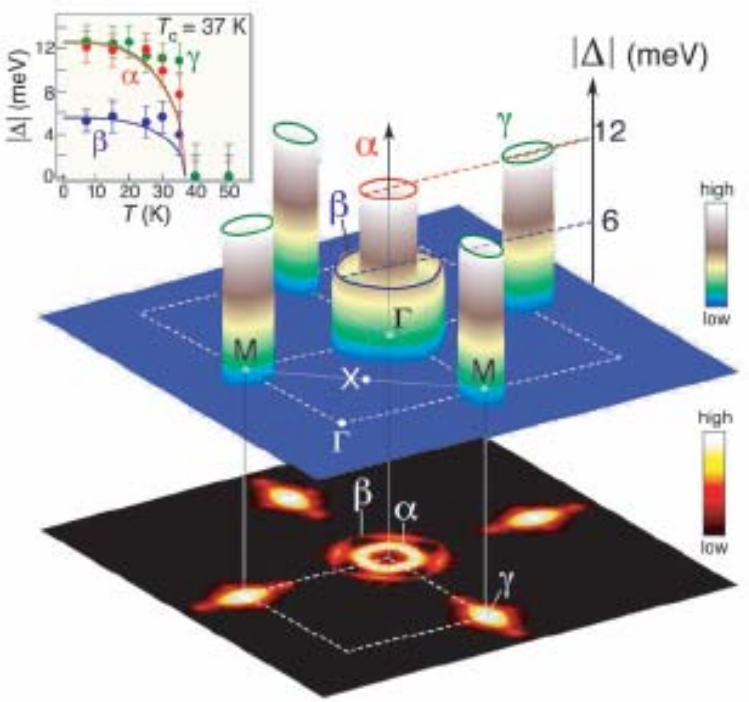

Fig. 4: (Colour on-line) Three-dimensional plot of the superconducting-gap size (Δ) measured at 15 K on the three observed FS sheets (shown at the bottom as an intensity plot) and their temperature evolutions (inset).

Abstract – We have performed a high-resolution angle-resolved photoelectron spectroscopy study on the newly discovered superconductor $Ba_{0.6}K_{0.4}Fe_2As_2$ ($T_c = 37$ K). We have observed two superconducting gaps with different values: a large gap ($\Delta \sim 12$ meV) on the two small hole-like and electron-like Fermi surface (FS) sheets, and a small gap (~ 6 meV) on the large hole-like FS. Both gaps, closing simultaneously at the bulk transition temperature (T_c), are nodeless and nearly isotropic around their respective FS sheets. The isotropic pairing interactions are strongly orbital dependent, as the ratio $2\Delta/k_BT_c$ switches from weak to strong coupling on different bands. The same and surprisingly large superconducting gap due to strong pairing on the two small FSs, which are connected by the (π, 0) spin-density-wave vector in the parent compound, strongly suggests that the pairing mechanism originates from the inter-band interactions between these two nested FS sheets.

Gap supra, paramètre d'ordre supra

PRL 101, 057003 (2008) PHYSICAL REVIEW LETTERS week ending 1 AUGUST 2008

La-1111
Calculs DFT

Unconventional Superconductivity with a Sign Reversal in the Order Parameter of $LaFeAsO_{1-x}F_x$

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[2]*Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114, USA*
(Received 18 March 2008; published 29 July 2008)

We argue that the newly discovered superconductivity in a nearly magnetic, Fe-based layered compound is unconventional and mediated by antiferromagnetic spin fluctuations, though different from the usual superexchange and specific to this compound. This resulting state is an example of extended *s*-wave pairing with a sign reversal of the order parameter between different Fermi surface sheets. The main role of doping in this scenario is to lower the density of states and suppress the pair-breaking ferromagnetic fluctuations.

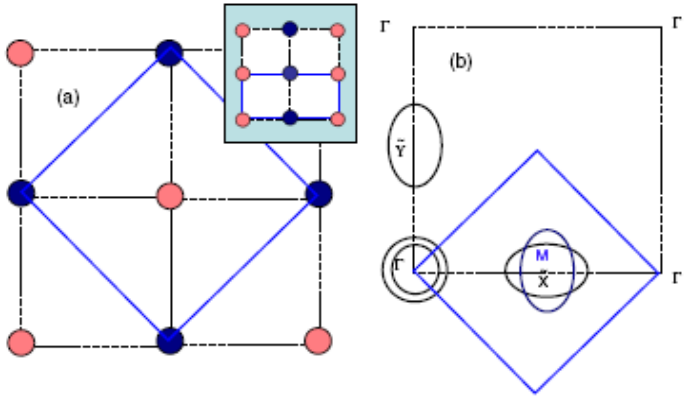


FIG. 2 (color online). Fermi surface formation upon backfolding of the large BZ corresponding to a simple Fe square lattice. (a) Real space: the four small unit cells of the Fe-only sublattice (dashed lines) with the larger solid diamond of actual two-Fe unit cell. Dark and light circles indicate superexchange (checkerboard) ordering. The inset shows the spin-density wave corresponding to $\tilde{X}$ point SFs. (b) Reciprocal space: the dashed black square is the unfolded BZ, the solid blue diamond is the downfolded zone, and the blue ellipse is the electron pocket from the $\tilde{Y}$ point downfolded onto the $\tilde{X}$ point (which is M in the small BZ).

Paramètres d'ordre de signe opposé sur les poches de trous et d'électrons de la surface de Fermi

À l'Institut Néel @ Grenoble ?

Depuis avril 08: Elaboration et expériences sous haute pression

- Élaboration HP-HT + études structurales : **P. Toulemonde** et al. (Institut Néel)
- Etude du transport par résistivité sous HP : **M. Nuñez-Regueiro** et al. (Institut Néel)
- Etude structurale sous HP par XRD sur ID27 : **G. Garbarino** (ESRF)

Mais entre temps, déjà: mesure de T_c de LnOFeAs sous HP

nature Vol 453|15 April 2008|doi:10.1038/nature06972

LETTERS

Superconductivity at 43 K in an iron-based layered compound $LaO_{1-x}F_xFeAs$

Hiroki Takahashi[1], Kazumi Igawa[1], Kazunobu Arii[1], Yoichi Kamihara[2], Masahiro Hirano[2,3] & Hideo Hosono[2,3]

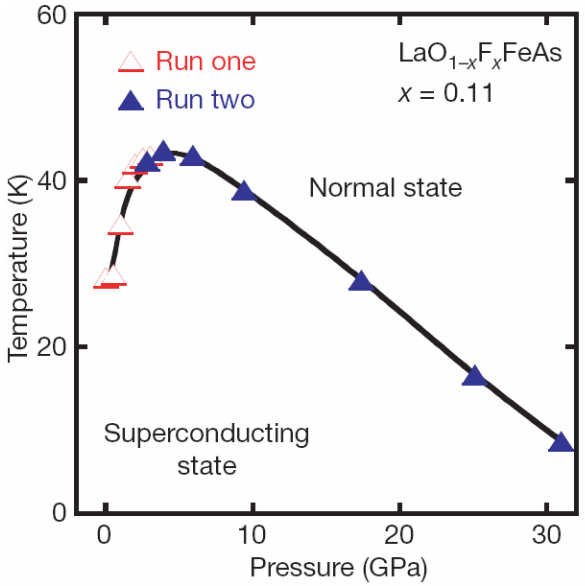
Pressure Effects on the Superconducting and Spin-Density-Wave States of the Newly Discovered $Sm(O_{1-x}F_x)FeAs$

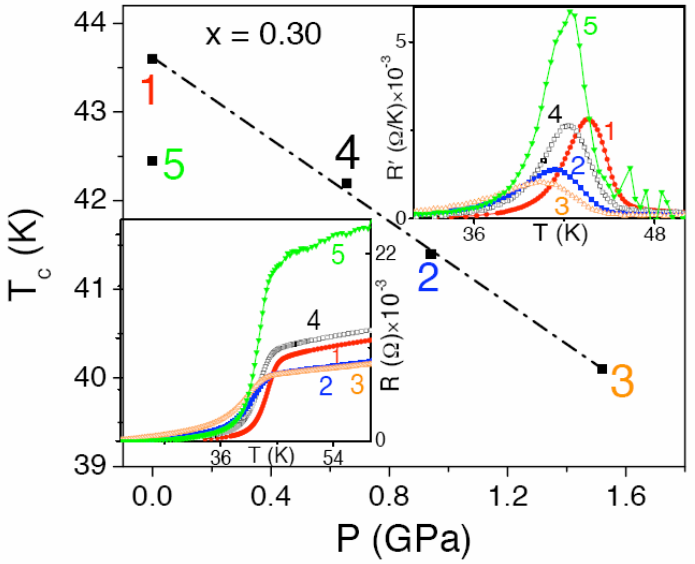
B. Lorenz,[1] K. Sasmal,[1] R. P. Chaudhury,[1] X. H. Chen,[2] R. H. Liu,[2] T. Wu,[2] and C. W. Chu[1,3,4]

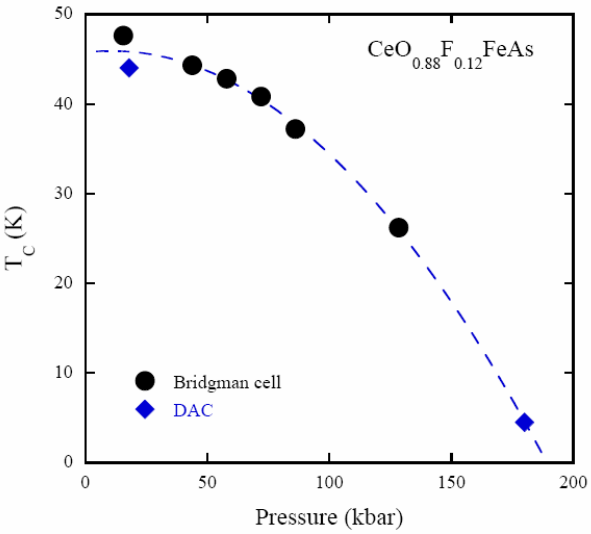
Effect of pressure on the superconducting critical temperature of $La[O_{0.89}F_{0.11}]FeAs$ and $Ce[O_{0.88}F_{0.12}]FeAs$

D. A. Zocco[a] J. J. Hamlin[a] R. E. Baumbach[a] M. B. Maple[a,*] M. A. McGuire[b] A. S. Sefat[b] B. C. Sales[b] R. Jin[b] D. Mandrus[b] J. R. Jeffries[c] S. T. Weir[c] Y. K. Vohra[d]

[a]*Department of Physics and Institute for Pure and Applied Physical Sciences, University of California at San Diego, La Jolla, CA 92093, USA*





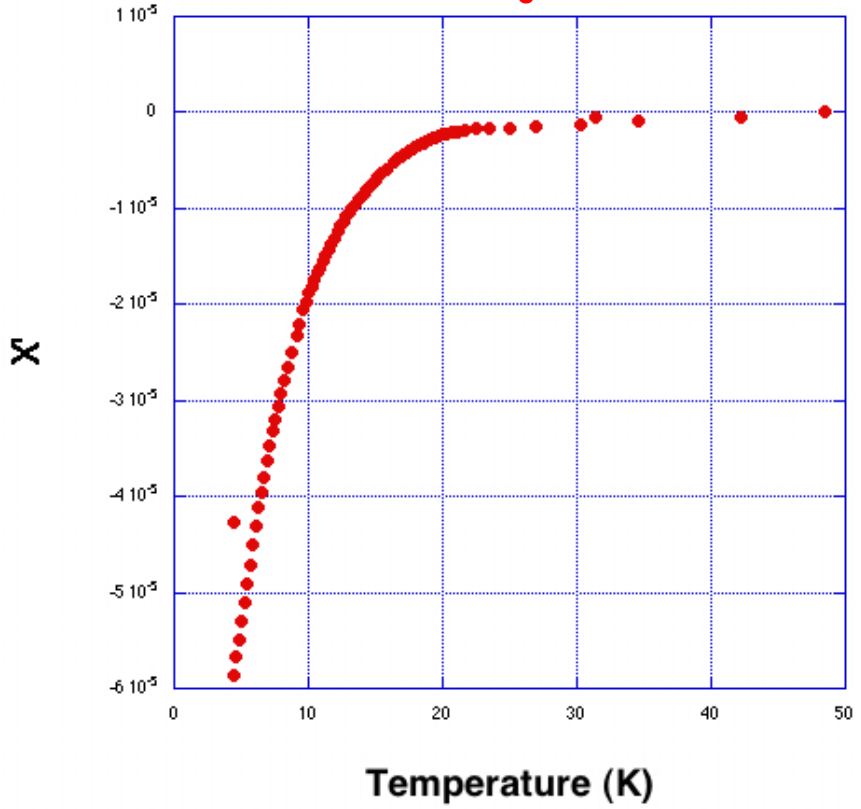


Synthèses de poudres en presse belt à l'Institut Néel [avril 08] :

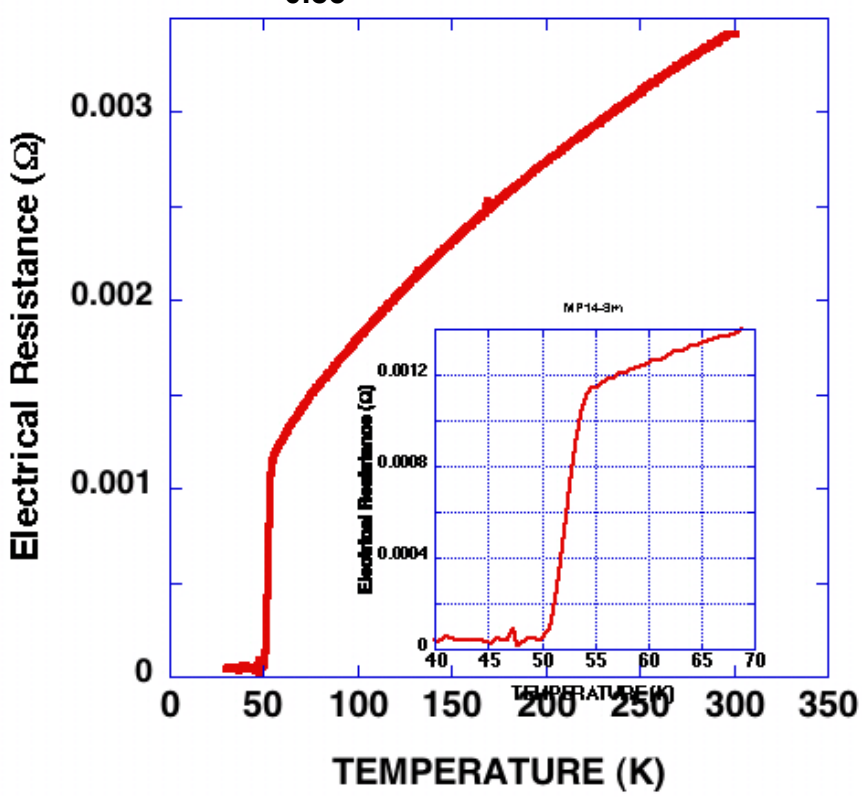
- A partir de mélange de: La (Sm), LaAs (SmAs), Fe, Fe_2O_3, FeAs, LnF_3, As
- Conditions: 3-6 GPa – 1000-1400°C

en creuset de BN (hexagonal) : LaFeAs(O,F) (a = 4.01 Å, c=8.69Å) + LaAs, LaOF
SmFeAs(O,F), $SmFeAsO_{1-delta}$ + SmAs + FeAs

LaFeAs(O,F) **supra (T_c = 20K)**

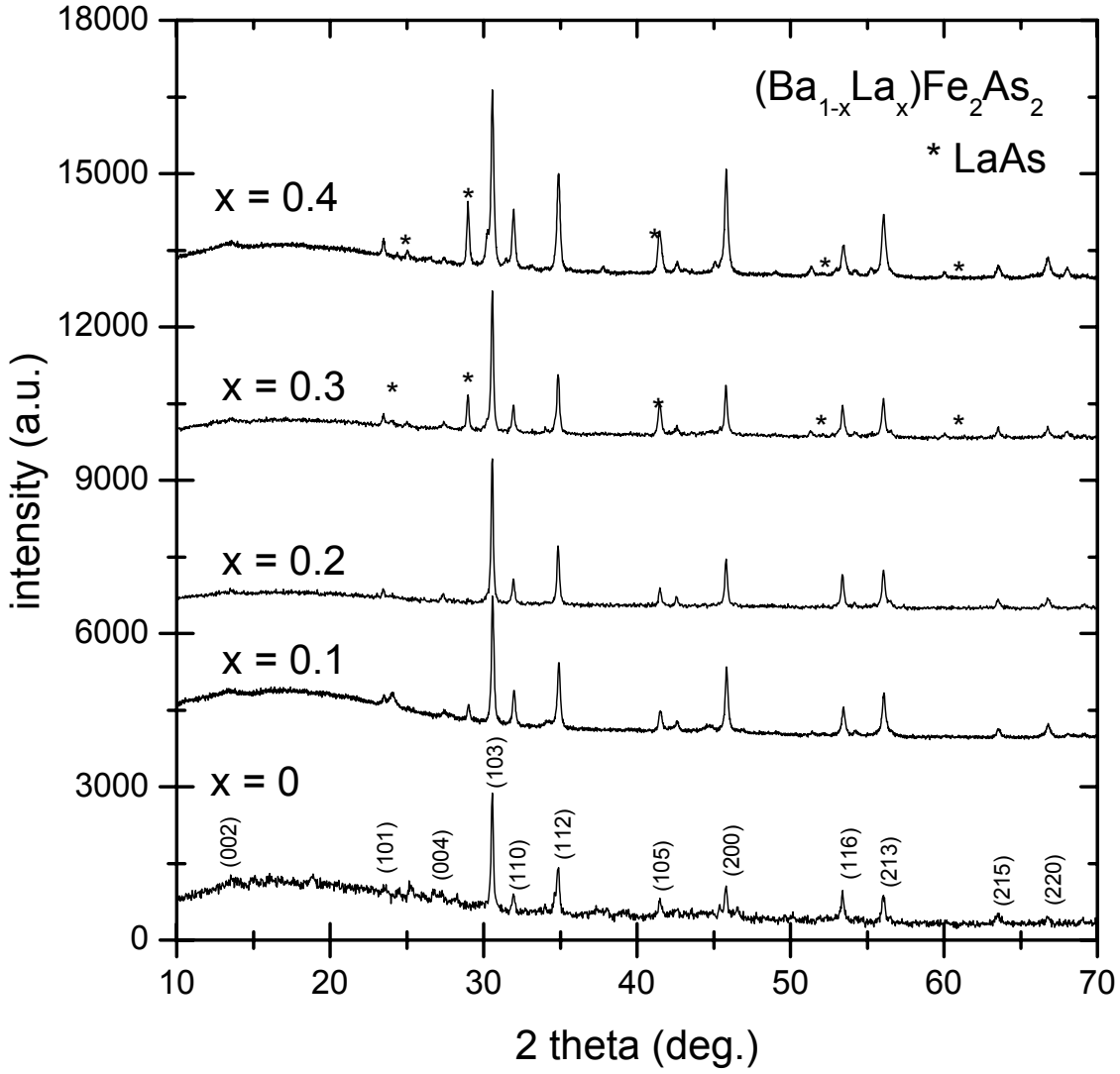


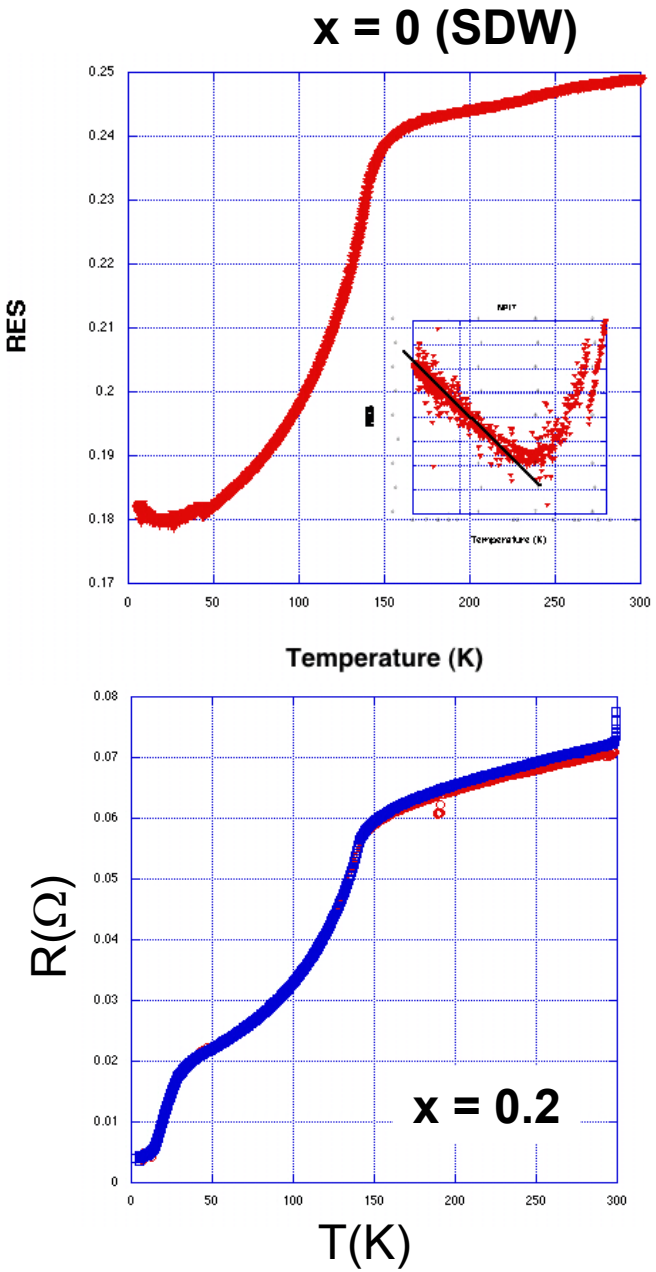
$SmFeAsO_{0.85}$ **supra ($T_{c\ onset}$ = 55K)**



Polycristaux obtenus @ HP-HT

- **Série $(Ba_{1-x}La_x)Fe_2As_2$**



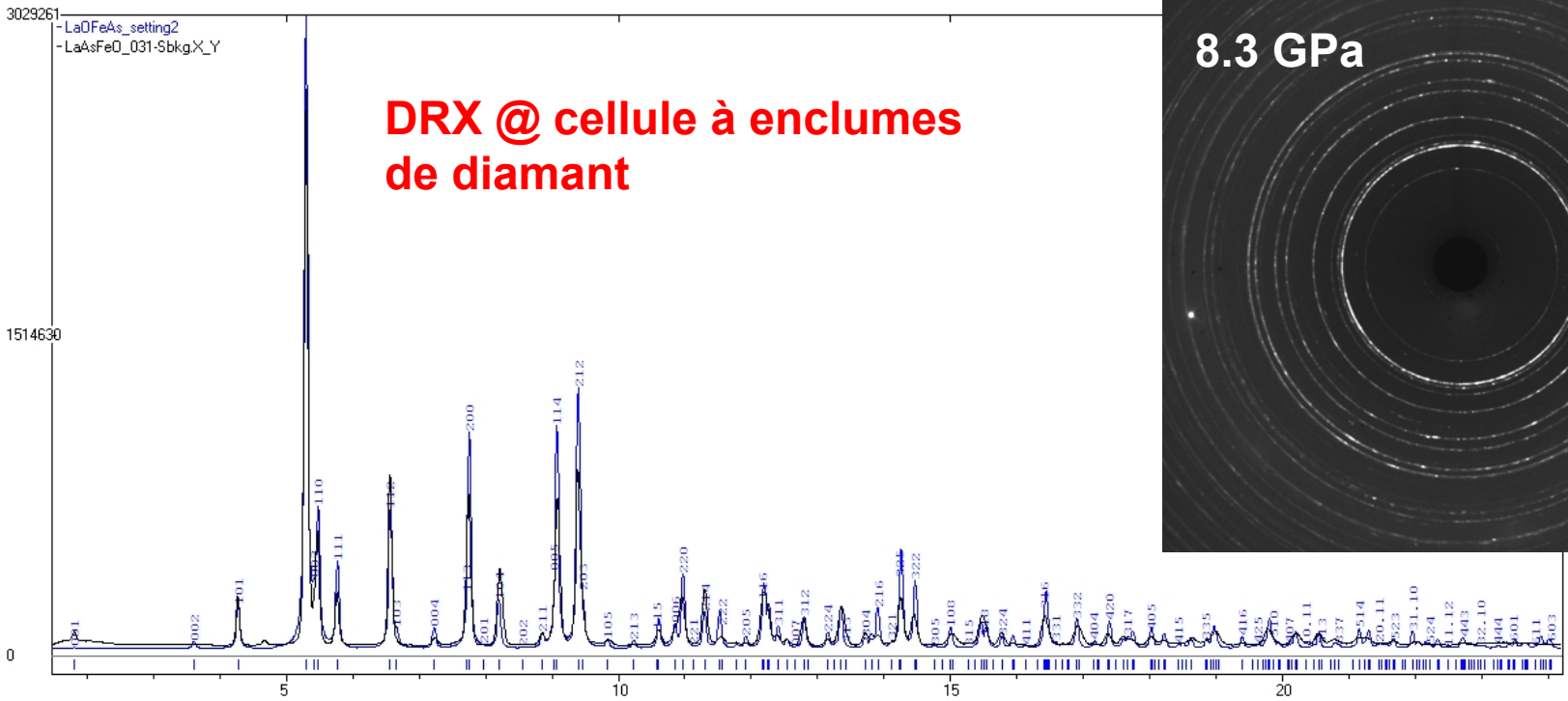


- **composés Fe-Se + substitutions**

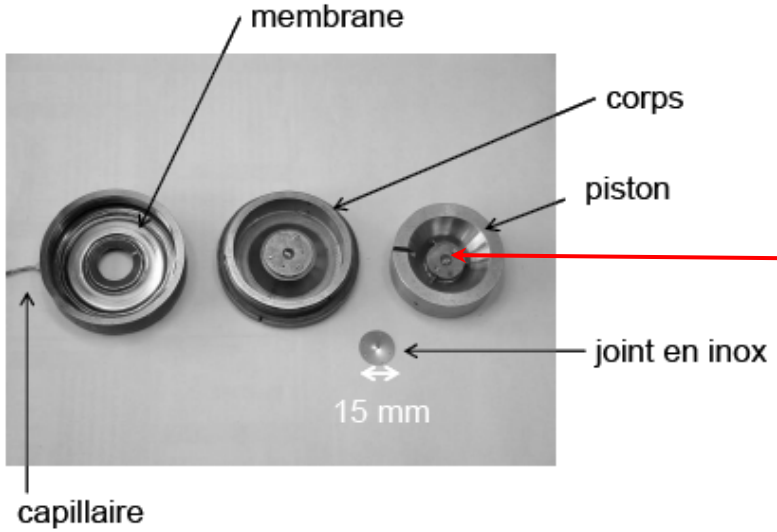
(non publié)

Etude structurale sous haute pression

ESRF
Gaston Garbarino



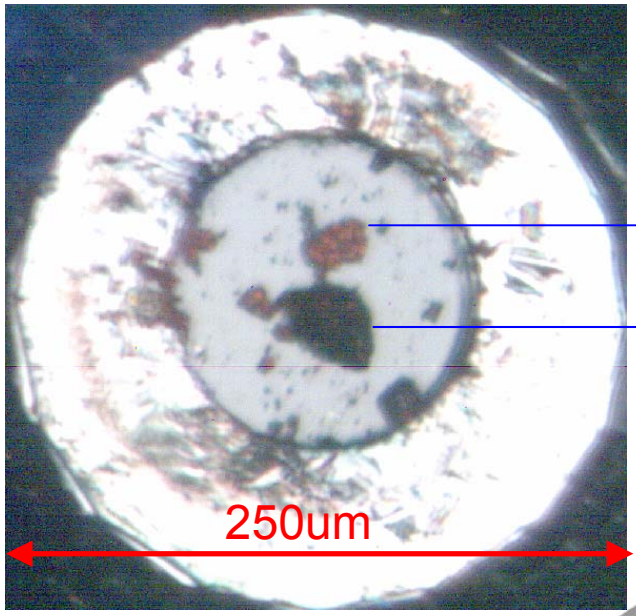
DRX @ cellule à enclumes de diamant



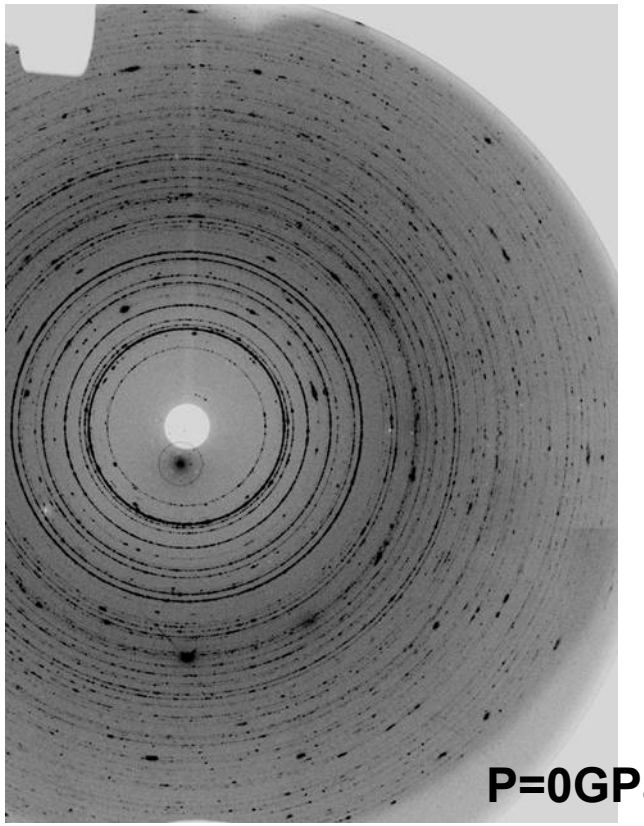
VOIR POSTER de Gaston!

LaFeAs(O,F)

Structural studies P<35GPa

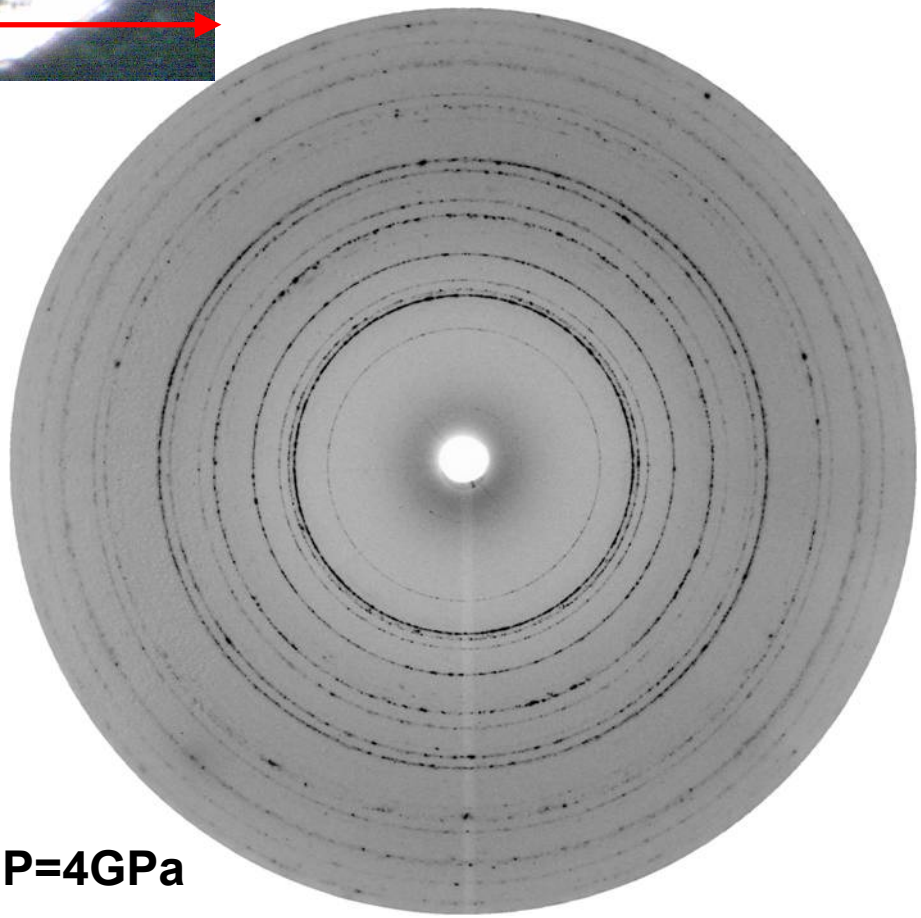


ESRF
Gaston Garbarino



P=0GPa

VOIR POSTER de Gaston!



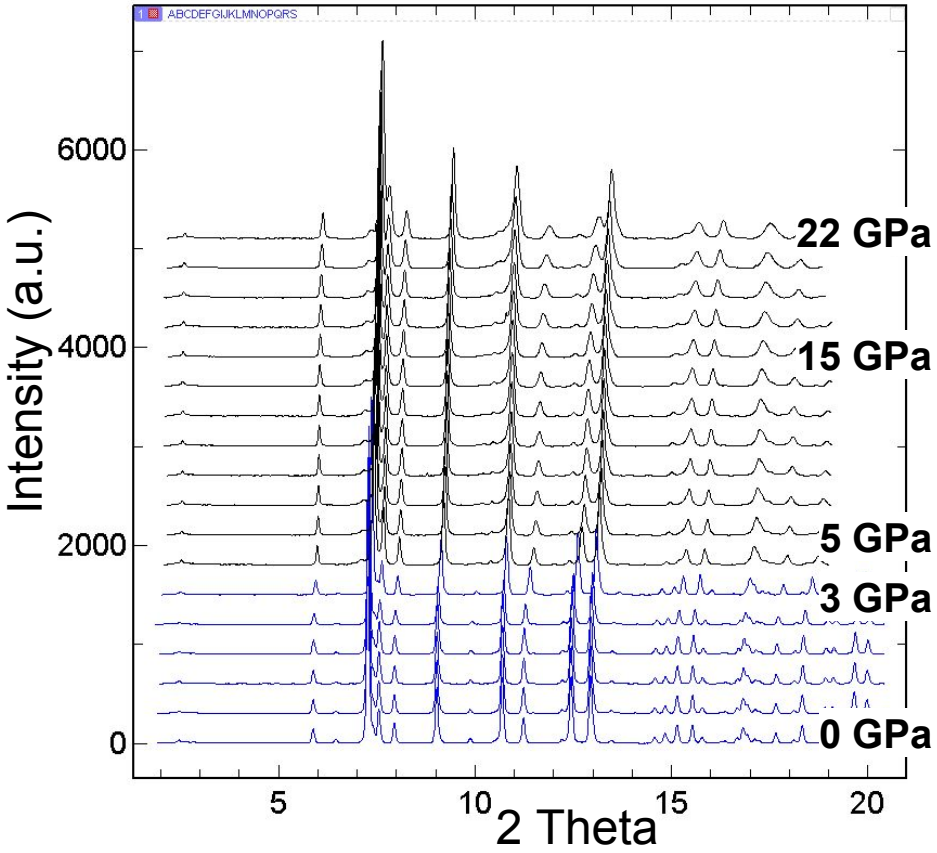
P=4GPa

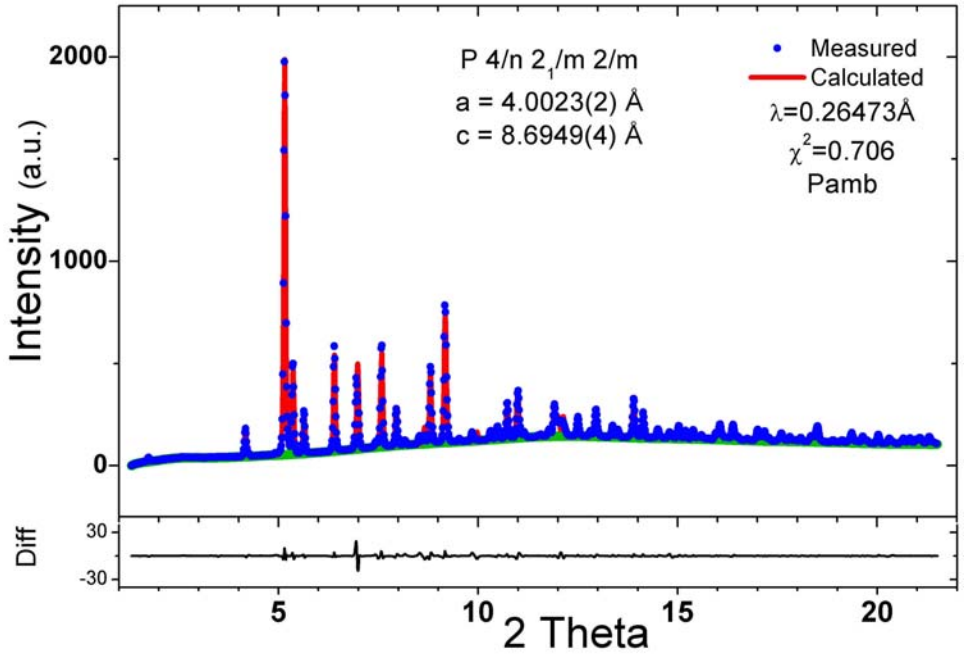
LaFeAs(O,F)

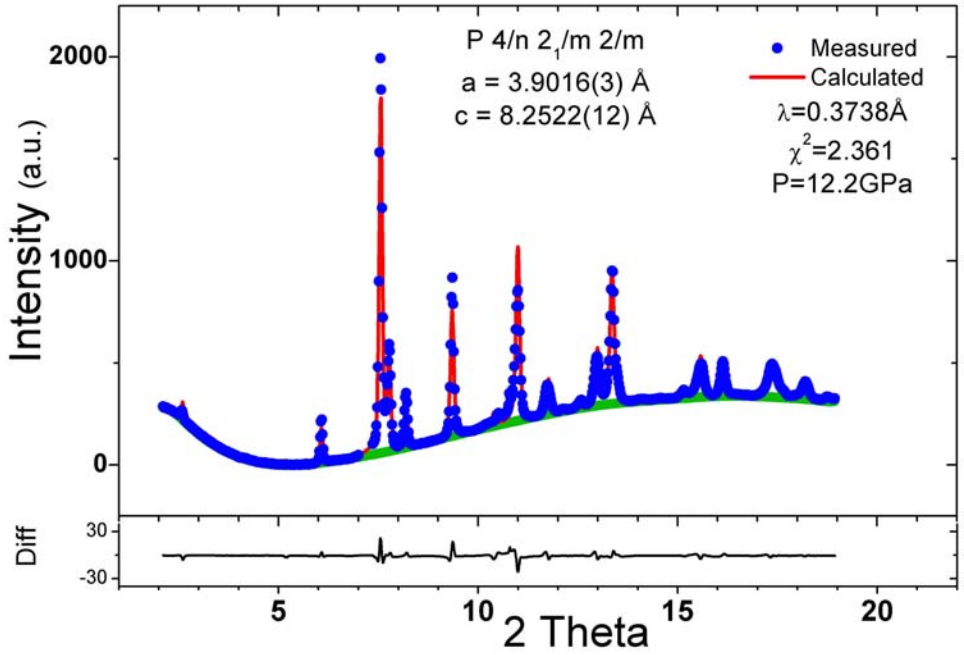
P ambiante
a = 4.002 Å
c = 8.695 Å
surdopé

Structural studies P<35GPa

Il n'y a pas de transition de phase jusqu'à 30GPa.



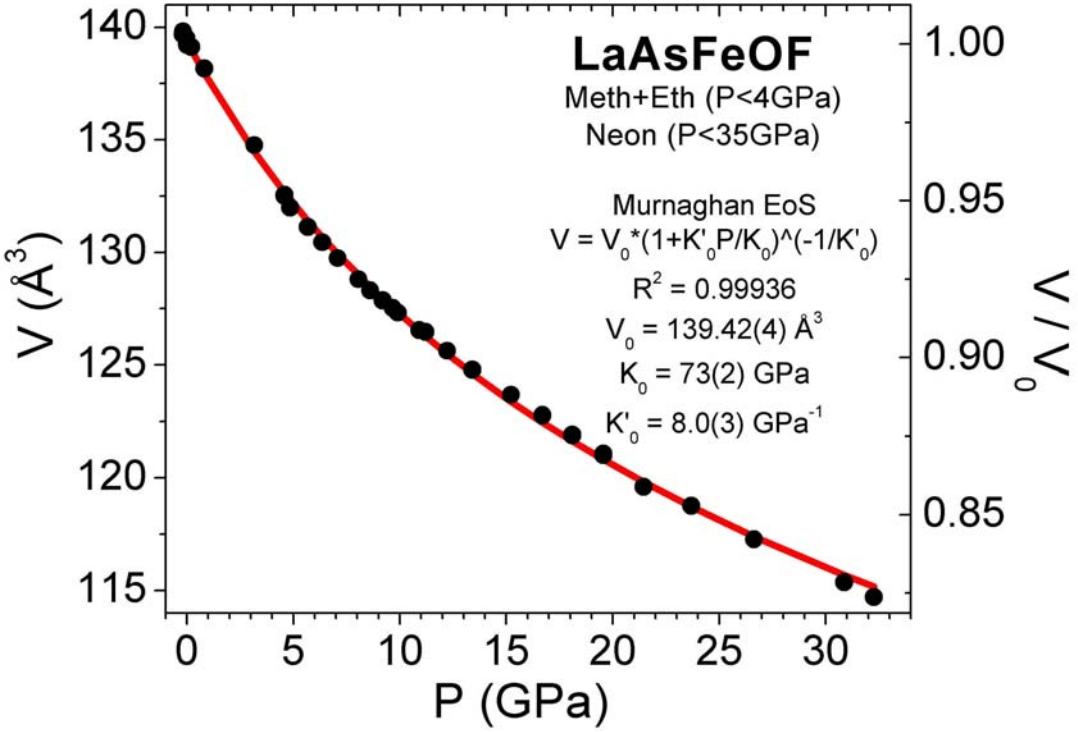


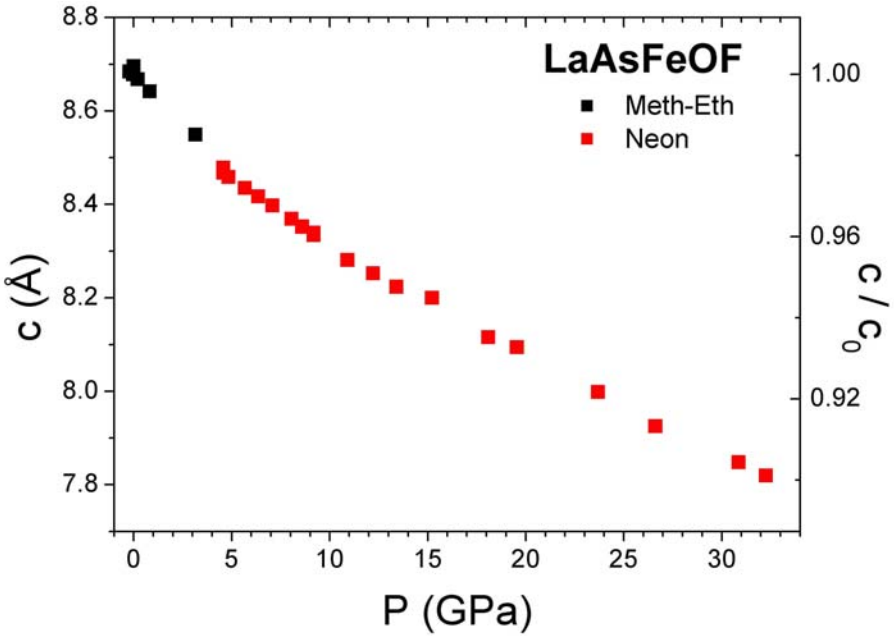


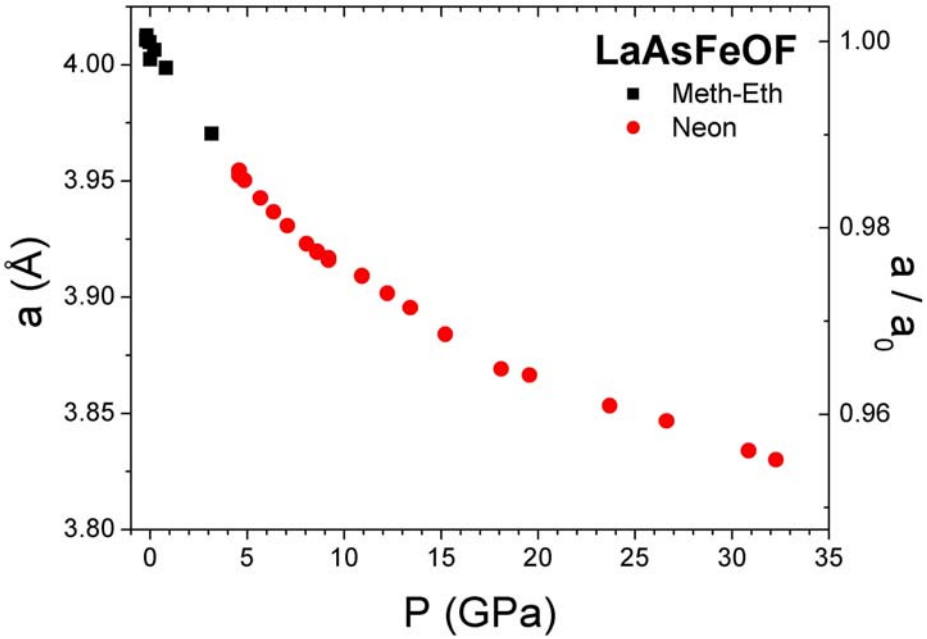
LaFeAs(O,F)

Structural studies P<35GPa

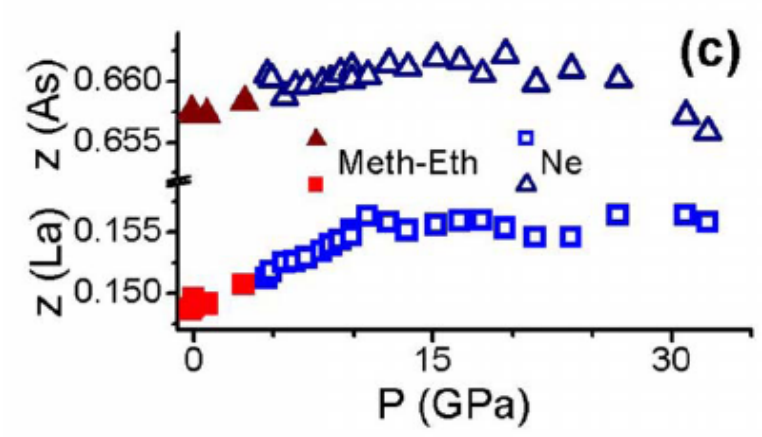
VOIR POSTER de Gaston!

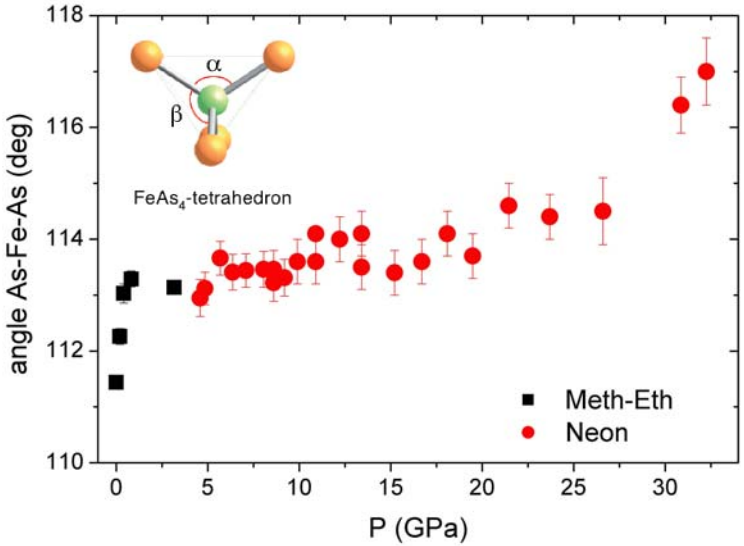


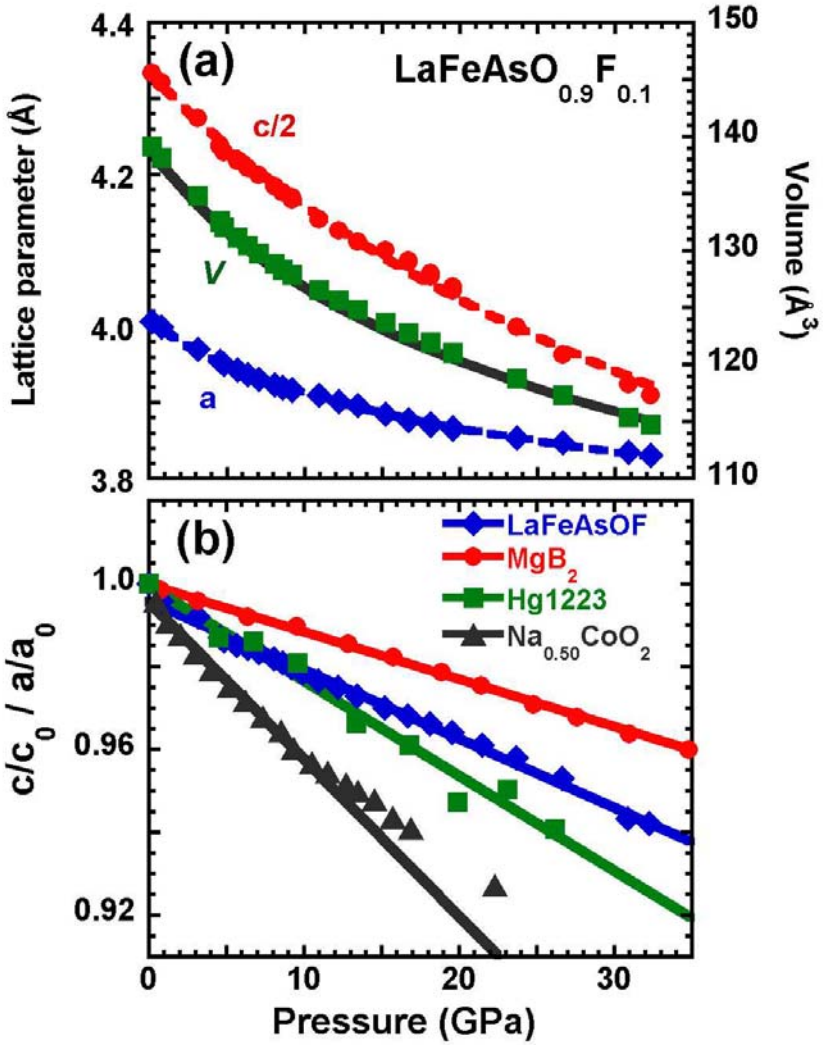




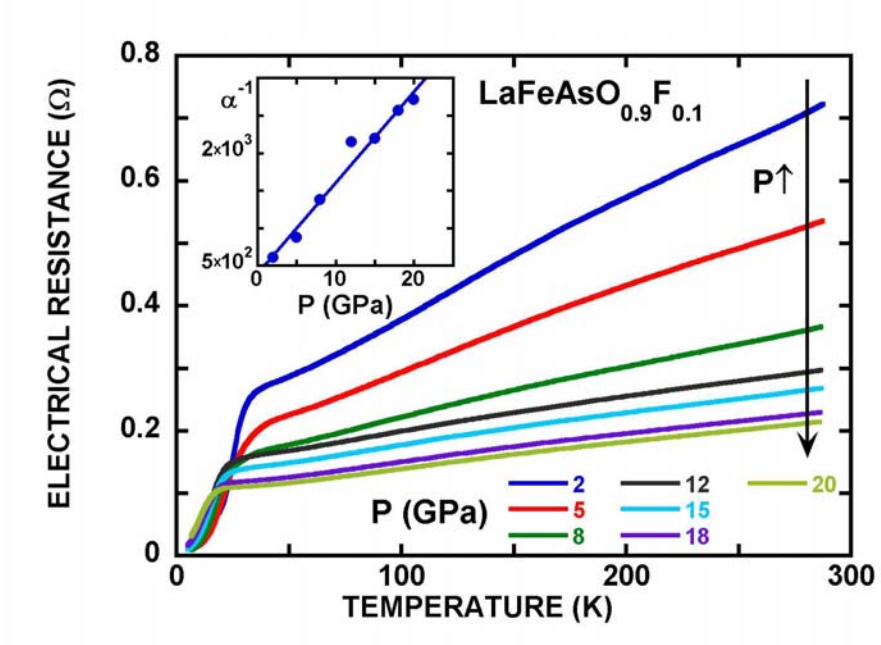
Paramètres structuraux versus P : LAFeAs(O,F)

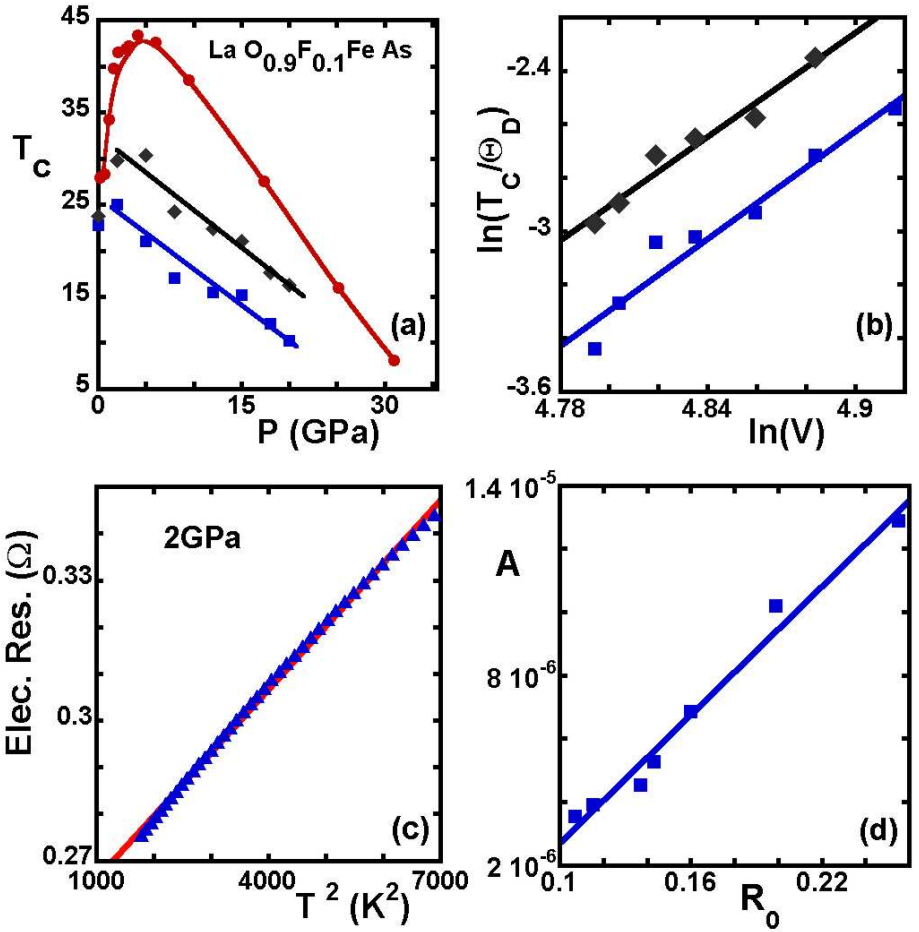






Etude du transport par résistivité sous haute pression (M. Nuñez-Regueiro)





Levy and Olsen

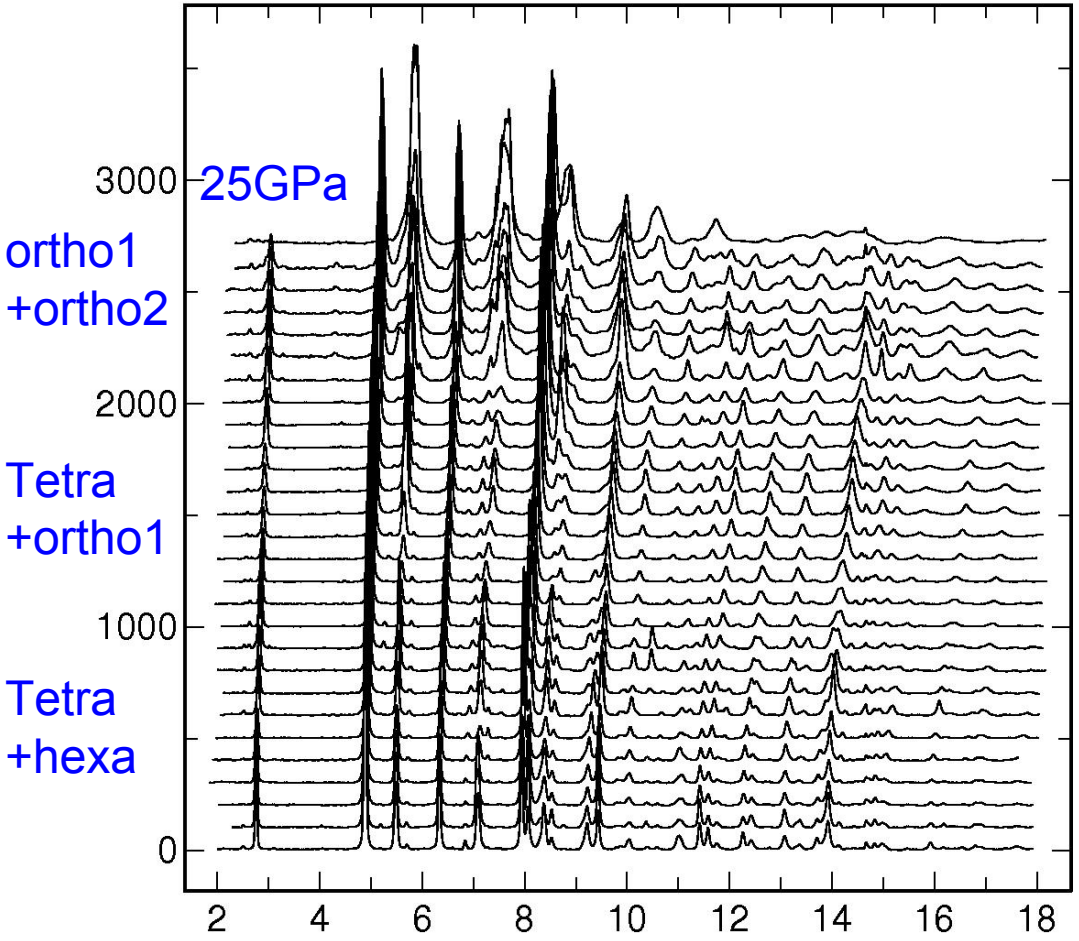
$$\frac{d\ln(T_c/\Theta_D)}{d\ln V} = \ln\left(\frac{\Theta_D}{T_c}\right)\frac{d\ln(\lambda)}{d\ln V} \equiv \ln\left(\frac{\Theta_D}{T_c}\right)\varphi$$

Avec θ_D=316K, on obtient φ=2.75, compatible avec un **couplage e-ph**

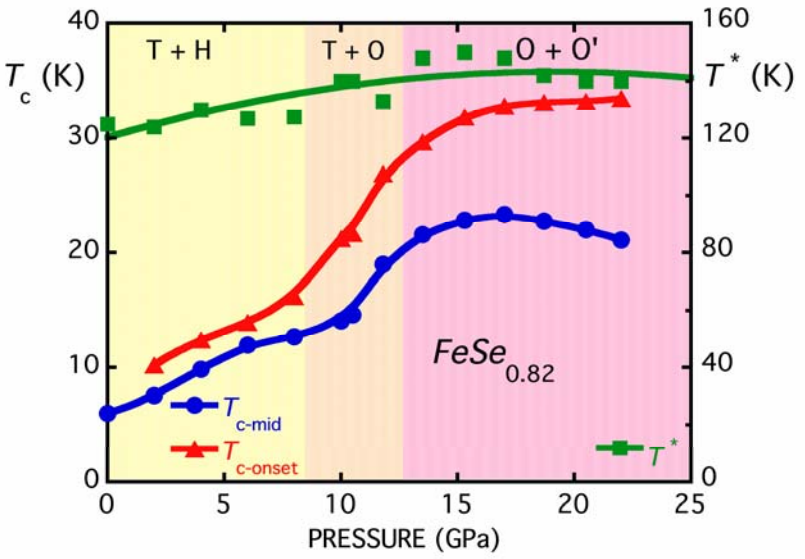
VOIR POSTER de Gaston!

$FeSe_{0.82}$ (P.Lejay) sous HP

DRX sous HP (ESRF, id27)



T_c max ~ 30 K @ 15 GPa



VOIR POSTER de Gaston!

Conclusion

Paramètres structuraux contrôlant la supra:

- régularité du tétraèdre $FeAs_4$
- distance entre blocs FeAs supra
- distance Fe-As intra-bloc supra optimale

Similarités & différences avec les cuprates à haute T_c :

- Composé mère non dopé: ordonné **AFM**: **métallique** avec cependant **faible conductivité** (Fe-As) // isolant (cuprates)
- ordre **AFM colinéaire** dans les 2 cas (doublement de la maille)
- **moment magnétique** sur-estimé par calculs: **0.5 à 1.5 celui des cuprates**
- avec le dopage, **T(AFM) diminue et s'annule près de la transition supra**
- **avec le dopage, T_S (transition structurale) diminue aussi**
- T_c max lorsque T_S = 0 K dans $LnFeAs(O_{1-x}F_x)$ avec Ln = La, Ce
- **diagramme de phase** similaire à celui du cuprate $La_{2-x}Sr_xCuO_4$
- **symétrie de l'ordre supra?**
  - certains: node dans les excitations des quasiparticules @ LT suggérant une symétrie « d-wave », comme dans les cuprates
  - d'autres: « full gap », suggérant une symétrie plus + conventionnelle « s-wave »
  - ou encore symétrie « s-wave » non conventionnnelle, i.e. avec un paramètre d'ordre changeant de signe d'une surface de Fermi à une autre

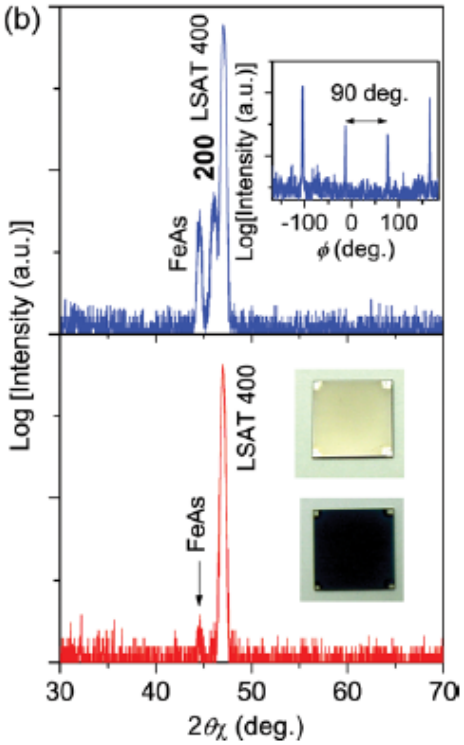
Perspectives (nombreuses!):

- Nouvelles compositions/empilements
- Applications (fort H_{c2}, plus faible anisotropie que les cuprates): déjà des papiers sur **filaments** produits par PIT « Powder In Tube »
- **films** existent déjà!

-**Questions ouvertes:**

- le gap avec/sans nodes?
- mécanisme d'appariement des paires de Cooper?
- rôle des fluctuations de spins
- effet de la substitution Cobalt/Fer: pourquoi ne détruit-elle pas la supra?
- …

Donc encore **beaucoup de travail** pour comprendre ces nouveaux supraconducteurs prometteurs… et les cuprates!



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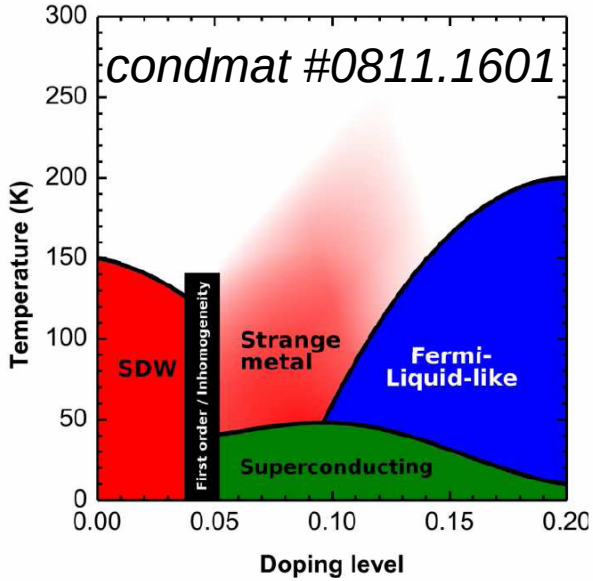

Condmat #0806.2751

Large Seebeck coefficients in Iron-oxypnictides : a new route towards n-type thermoelectric materials

Loreynne Pinsard-Gaudart[1], David Berardan[1], Julien Bobroff[2], Nita Dragoe[*,1]

[1] Institut de Chimie Moléculaire et des Matériaux d'Orsay (UMR CNRS 8182), Bât. 410, Univ. Paris-Sud 11, F-91405 Orsay, France.
2 Laboratoire de Physique des Solides (UMR 8502), Bât. 510, Univ. Paris-Sud 11, F-91405 Orsay, France.

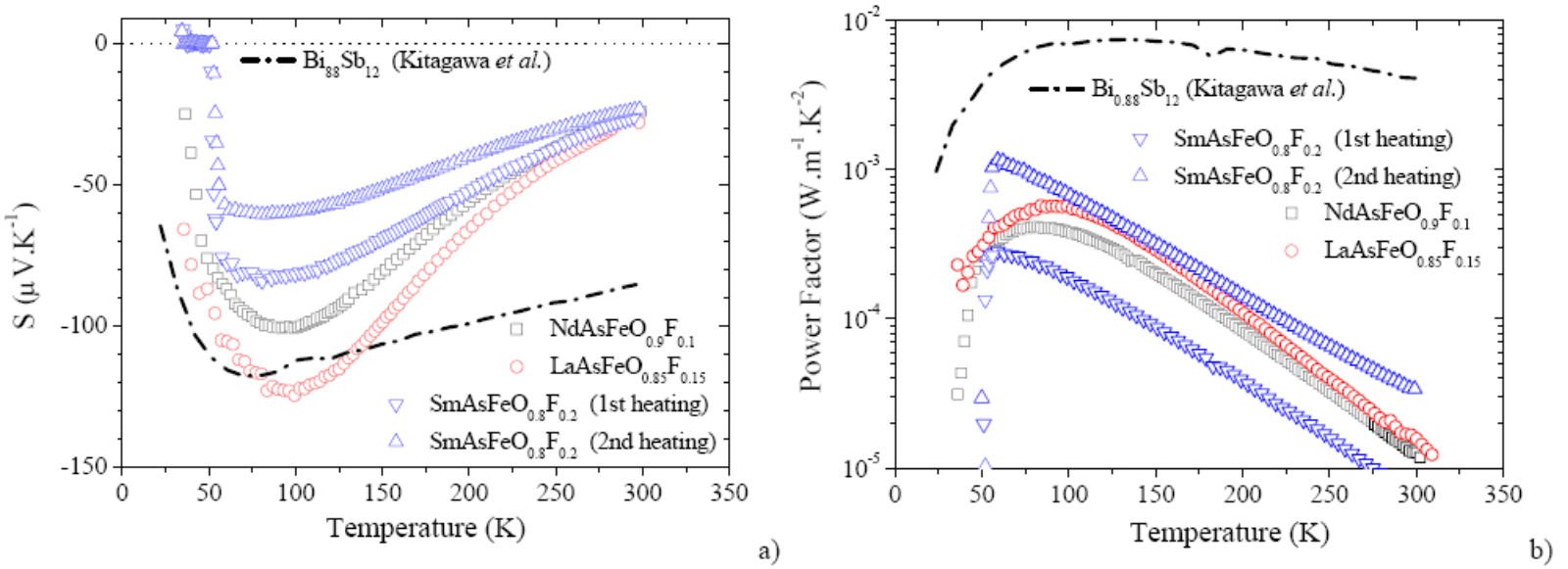

Figure 2 Temperature dependence of a) the Seebeck coefficient and b) thermoelectric power factor of some $REFeAsO_{1-x}F_x$ compounds. The dashed-dotted lines correspond to the data of $Bi_{88}Sb_{12}$ reported in ref 9.