Neutron scattering study on the Fe-based superconductor systems

WEI BAO
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RENMIN UNIVERSITY OF CHINA
BEIJING, CHINA

collaborators:

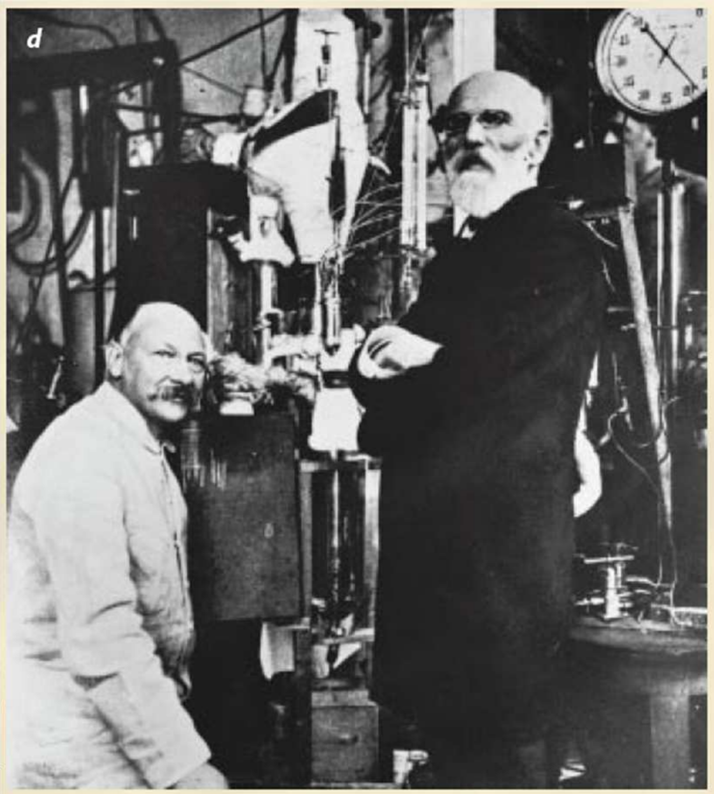
- Samples of the 1111 and 122 systems (CUST) : X.H. Chen, T. Wu, G. Wu, H. Chen, R.H. Liu, Y.L. Xie, X.F. Wang
- Samples of the 11 system (Tulane U.) : Z-Q. Mao, J. Hu , J. Yang, B. Qian, M-H. Fang (ZheDa)
- Samples of the 245 system (RenMin U.): G.F. Chen, D.M. Wang, J.B. He

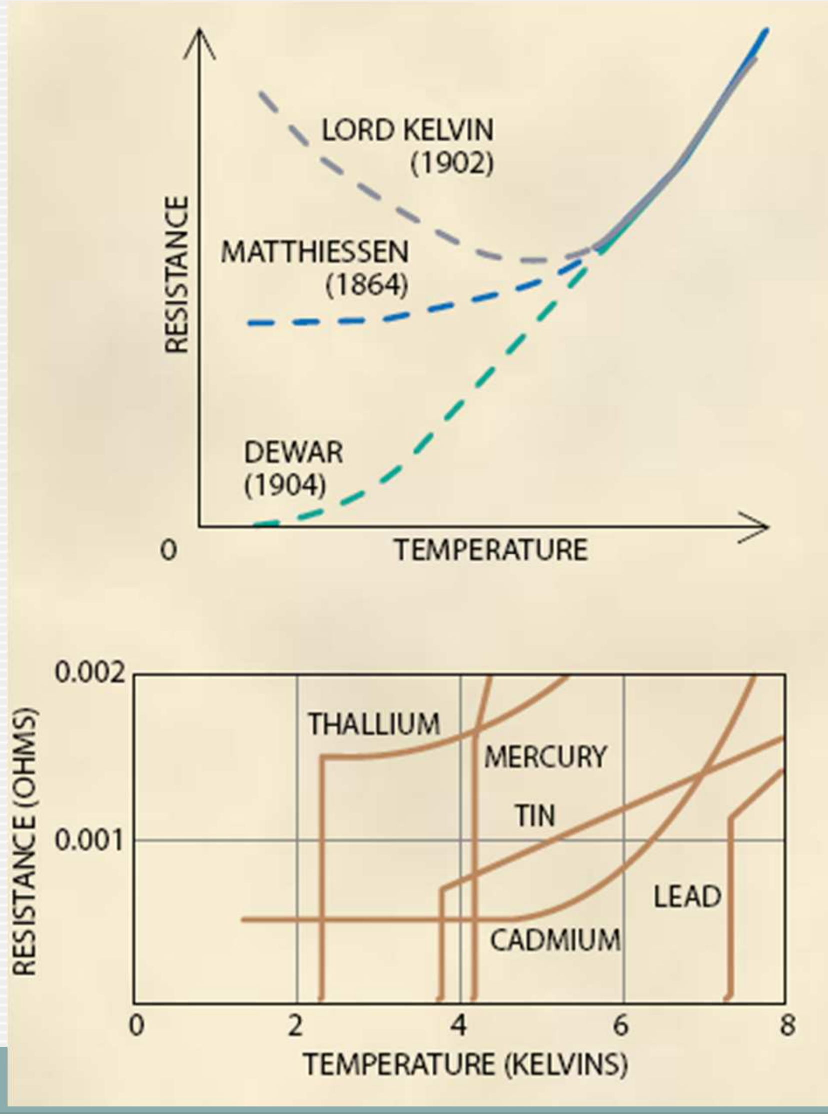
- Neutron and x-ray diffraction: Y. Qiu, Q. Huang, M.A. Green, P. Zajdel, J.W. Lynn, J.R.D. Copley, S. Chang (NIST), M. Kofu, S.-H. Lee (UVirginia), Y. Ren (ANL), M.R. Fitzsimmons, M. Zhernenkov (Lujan)

- Inelastic neutron scattering: Y. Qiu (NIST), C. Broholm, V. Thampy, Y. Zhao (JHU), A. Savici, G. Granroth, A. Zheludev, T. Hong (ORNL), K. Habicht, D. Argyriou (HZB), A. Hiess (ILL)

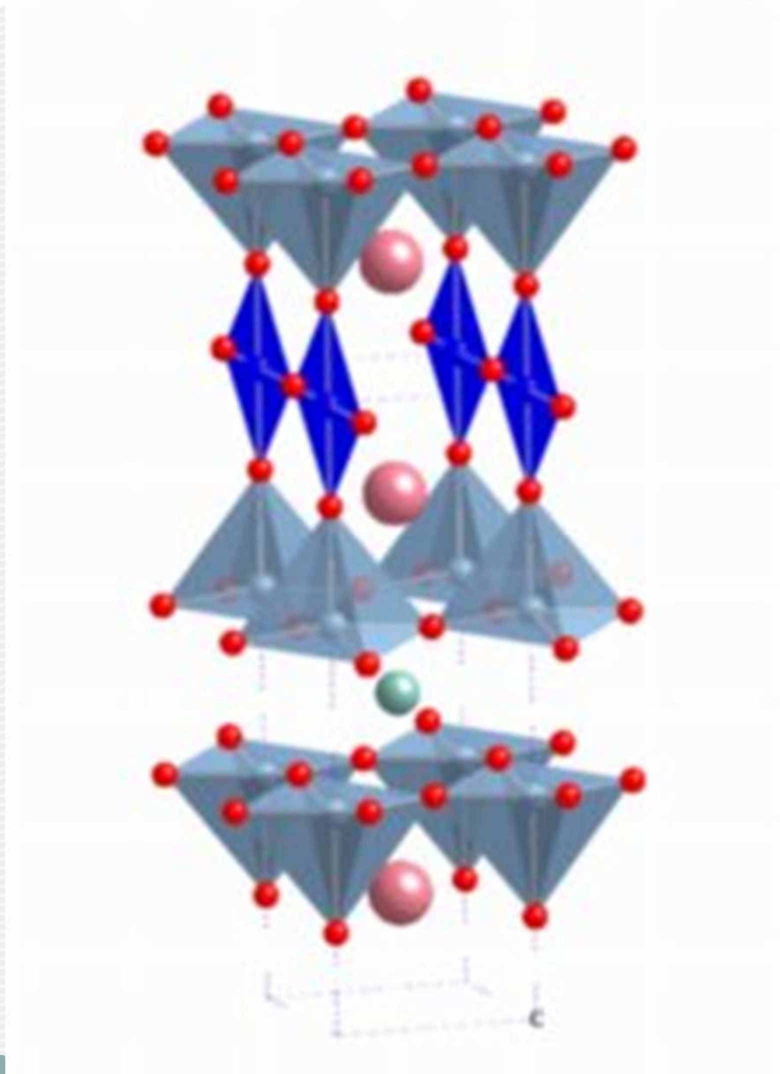
Unexpected Discovery of Superconductivity

- 1911: Onnes
  - ➢ No electric resistance
  - ➢ Complete diamagnetism



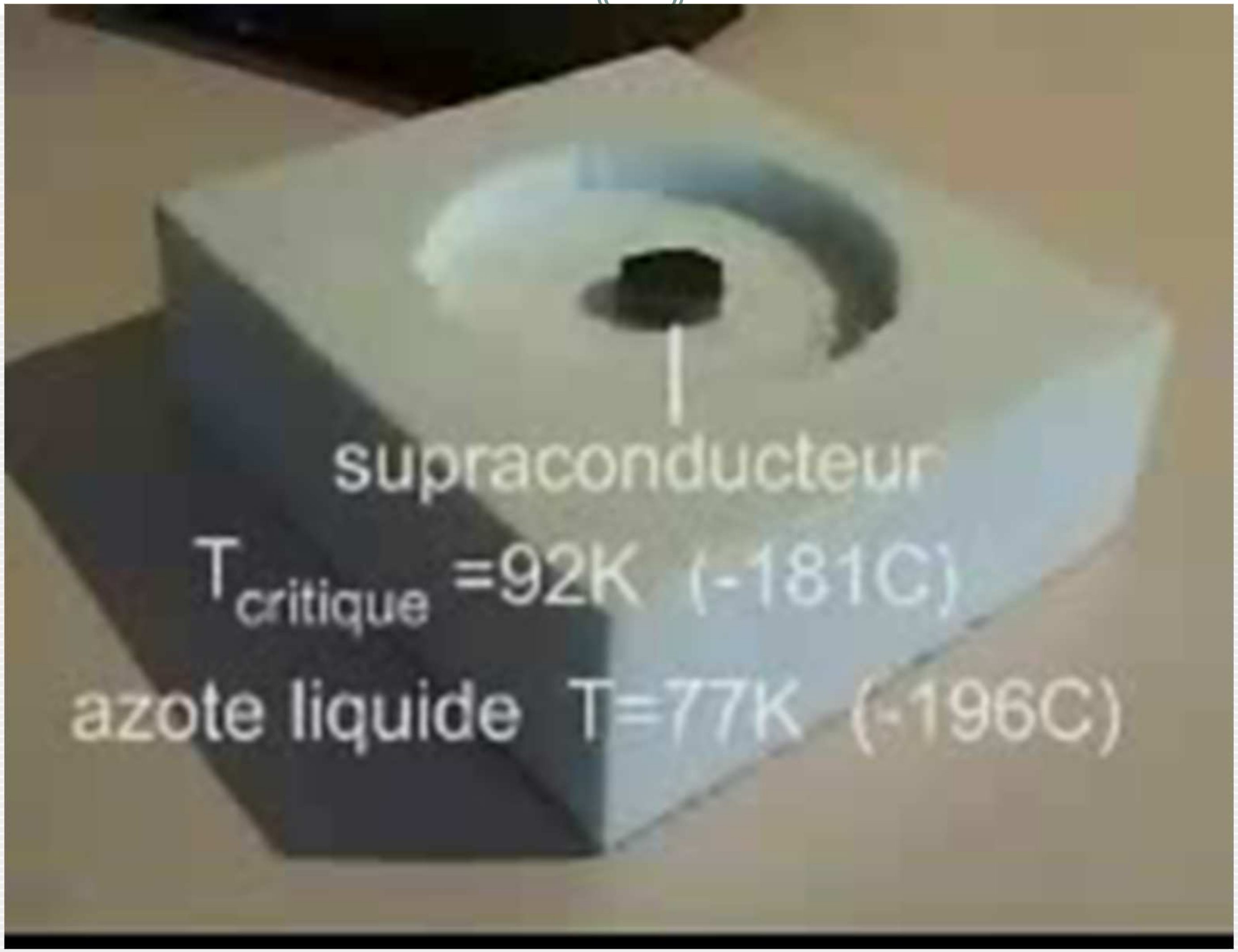


YBCO: the first superconductor at liquid nitrogen T



吴茂昆先生及太太

Magnetic suspension of superconductor



Mechanism of Superconductivity

- Conventional superconductors: BCS
- Unconventional magnetic superconductors ?
  - Heavy fermion superconductors
  - Copper oxide superconductors

B.C.S.

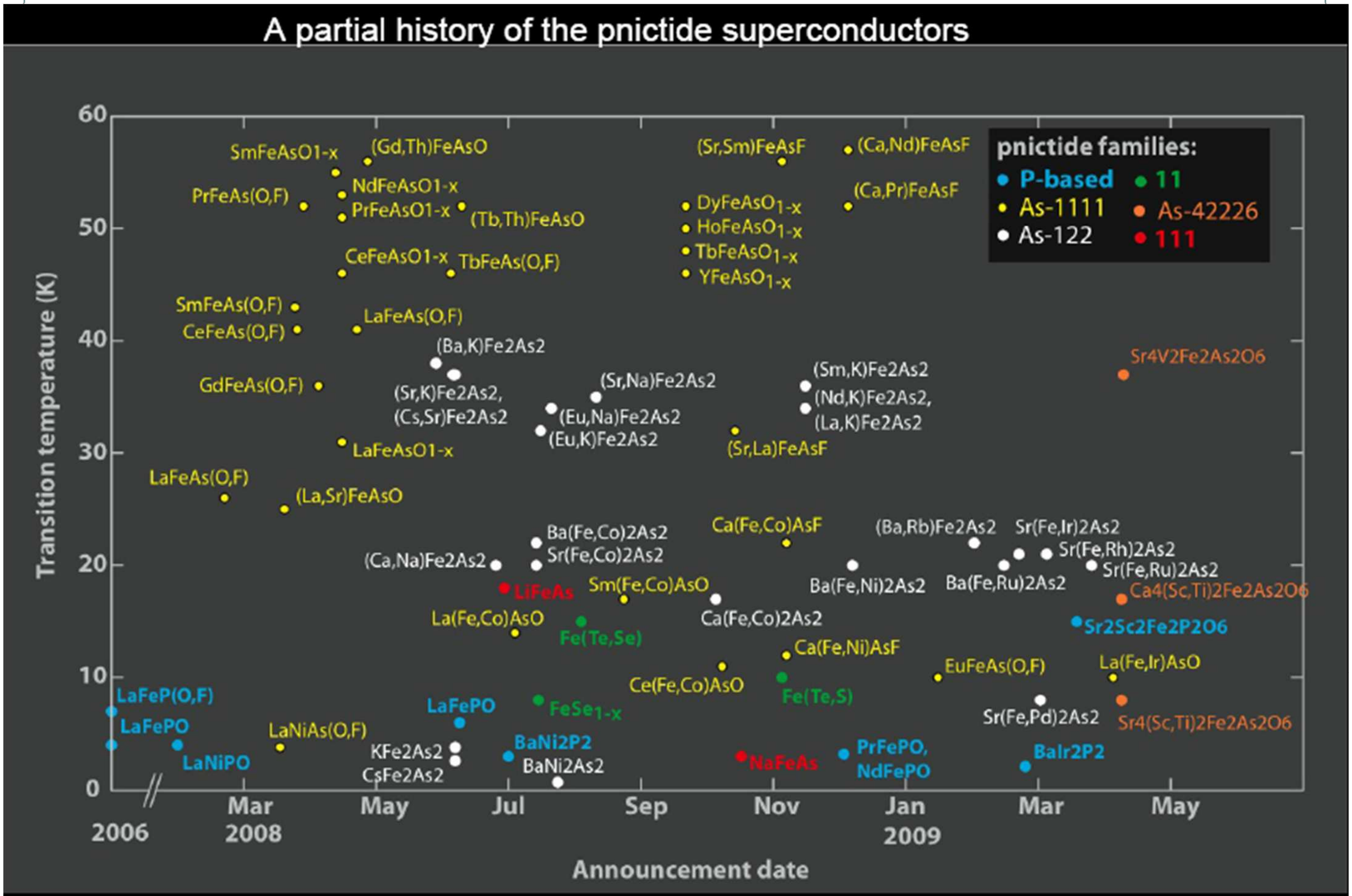
Grand Challenge in Physics

- What is the mechanism for cuprate, heavy fermion unconventional superconductors

  unresolved physics of Mott system, Kondo lattice system

- Where to find superconductors of higher transition temperature

  applications limited by expansive cryogenic requirement


A partial history of the pnictide superconductors
pnictide families:
P-based
11
As-1111
As-42226
As-122
111
Transition temperature (K)
Announcement date
2006
Mar 2008
May
Jul
Sep
Nov
Jan 2009
Mar
May
SmFeAsO1-x
(Gd,Th)FeAsO
PrFeAs(O,F)
NdFeAsO1-x
PrFeAsO1-x
(Tb,Th)FeAsO
CeFeAsO1-x
TbFeAs(O,F)
SmFeAs(O,F)
CeFeAs(O,F)
LaFeAs(O,F)
GdFeAs(O,F)
LaFeAsO1-x
(La,Sr)FeAsO
(Ba,K)Fe2As2
(Sr,K)Fe2As2,
(Cs,Sr)Fe2As2
(Sr,Na)Fe2As2
(Eu,Na)Fe2As2
(Eu,K)Fe2As2
(Sr,Sm)FeAsF
(Ca,Nd)FeAsF
(Ca,Pr)FeAsF
DyFeAsO1-x
HoFeAsO1-x
TbFeAsO1-x
YFeAsO1-x
(Sm,K)Fe2As2
(Nd,K)Fe2As2,
(La,K)Fe2As2
(Sr,La)FeAsF
Sr4V2Fe2As2O6
Ba(Fe,Co)2As2
Sr(Fe,Co)2As2
(Ca,Na)Fe2As2
LiFeAs
Sm(Fe,Co)AsO
La(Fe,Co)AsO
Fe(Te,Se)
Ca(Fe,Co)AsF
Ca(Fe,Co)2As2
(Ba,Rb)Fe2As2
Sr(Fe,Ir)2As2
Sr(Fe,Rh)2As2
Sr(Fe,Ru)2As2
Ba(Fe,Ni)2As2
Ba(Fe,Ru)2As2
Ca4(Sc,Ti)2Fe2As2O6
Sr2Sc2Fe2P2O6
Ca(Fe,Ni)AsF
Ce(Fe,Co)AsO
Fe(Te,S)
EuFeAs(O,F)
La(Fe,Ir)AsO
Sr(Fe,Pd)2As2
Sr4(Sc,Ti)2Fe2As2O6
LaFeP(O,F)
LaFePO
LaNiPO
LaNiAs(O,F)
LaFePO
FeSe1-x
KFe2As2
CsFe2As2
BaNi2P2
BaNi2As2
NaFeAs
PrFePO,
NdFePO
BaIr2P2

Four types: 1111, 122, 111 and 11 & three structure families of superconductors

J|A|C|S COMMUNICATIONS

Published on Web 02/23/2008

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

PRL **101,** 107006 (2008) PHYSICAL REVIEW LETTERS week ending 5 SEPTEMBER 2008

Superconductivity at 38 K in the Iron Arsenide ($Ba_{1-x}K_x$)Fe_2As_2

Marianne Rotter, Marcus Tegel, and Dirk Johrendt*

Contents lists available at ScienceDirect

ELSEVIER Solid State Communications

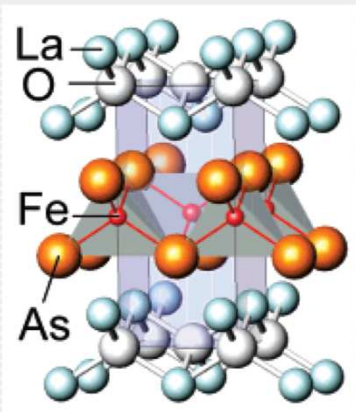
journal homepage: www.elsevier.com/locate/ssc

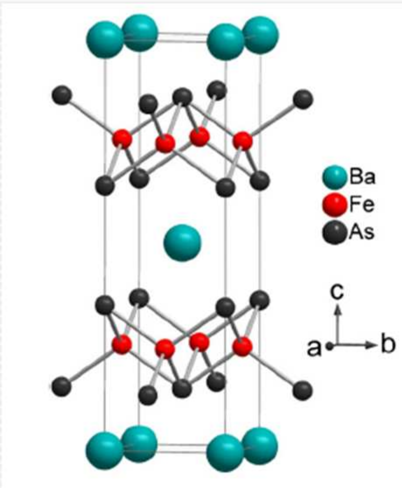
Superconductivity in the PbO-type structure α-FeSe

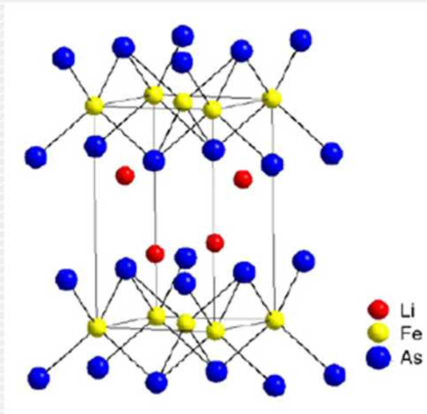
Fong-Chi Hsu*†, Jiu-Yong Luo*, Kuo-Wei Yeh*, Ta-Kun Chen*, Tzu-Wen Huang*, Phillip M. Wu‡, Yong-Chi Lee*, Yi-Lin Huang*, Yan-Yi Chu*†, Der-Chung Yan*, and Maw-Kuen Wu*§

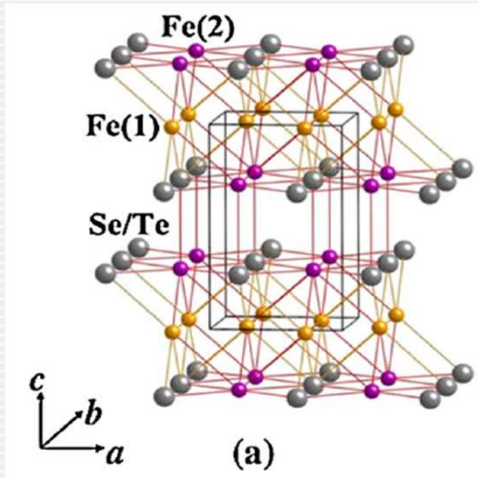
The superconductivity at 18 K in LiFeAs system

X.C. Wang, Q.Q. Liu, Y.X. Lv, W.B. Gao, L.X. Yang, R.C. Yu, F.Y. Li, C.Q. Jin*









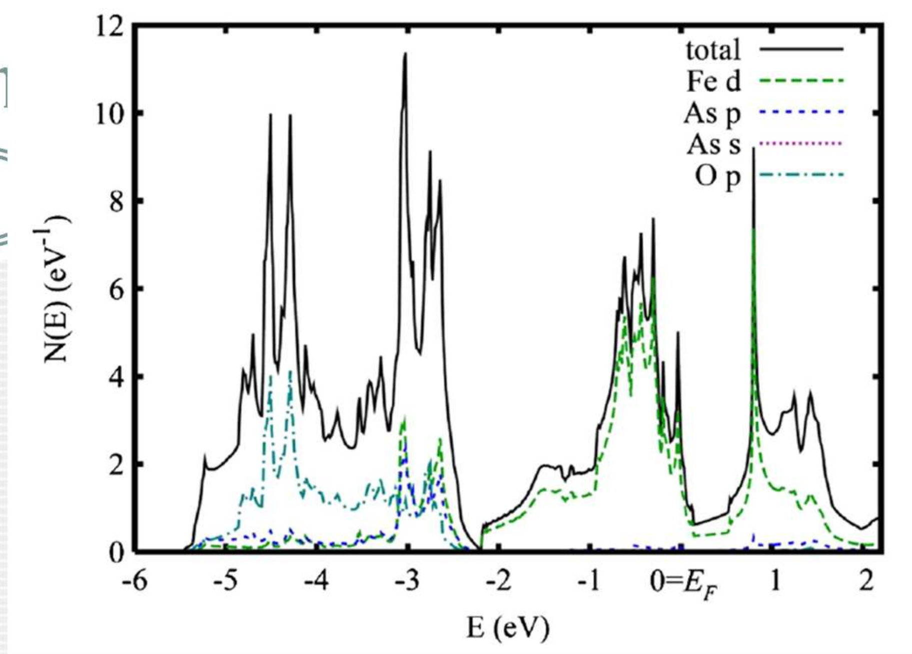
Bao et al.,PRL 102, 247001 (2009)

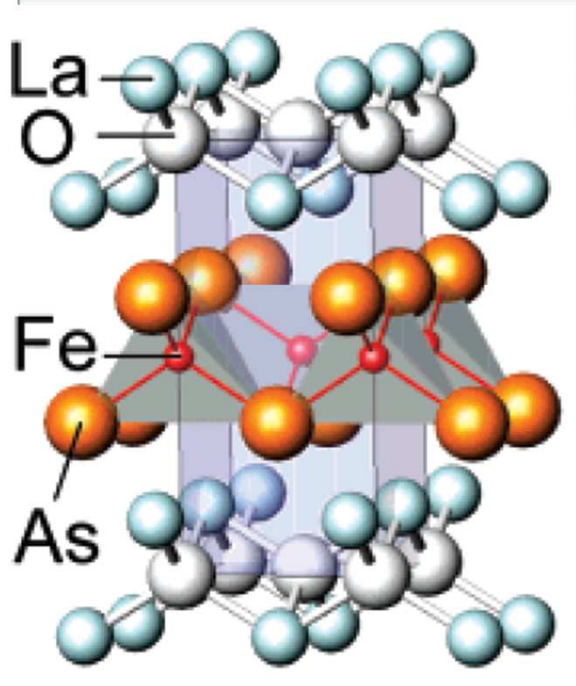
Important ingredien

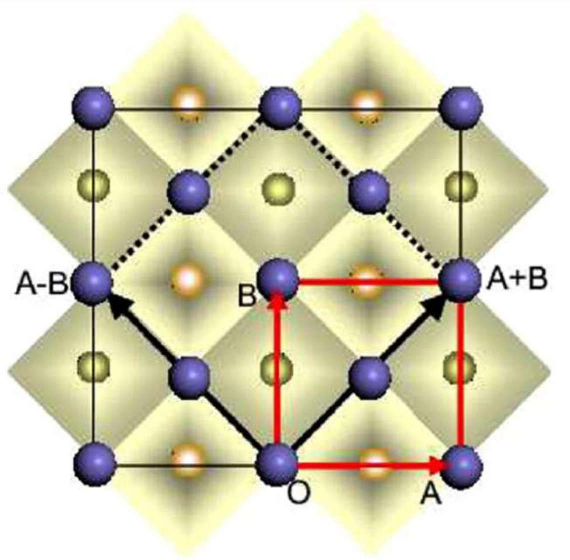
IOP Publishing SUPERCONDUCTOR SCIENCE AND TECHNOLOGY
Supercond. Sci. Technol. **21** (2008) 125028 (9pp) doi:10.1088/0953-2048/21/12/125028

Crystallographic phase transition and high-T_c superconductivity in LaFeAsO:F

T Nomura[1], S W Kim[2], Y Kamihara[3], M Hirano[3], P V Sushko[4,5], K Kato[6], M Takata[6], A L Shluger[4,5] and H Hosono[1,3,7,8]







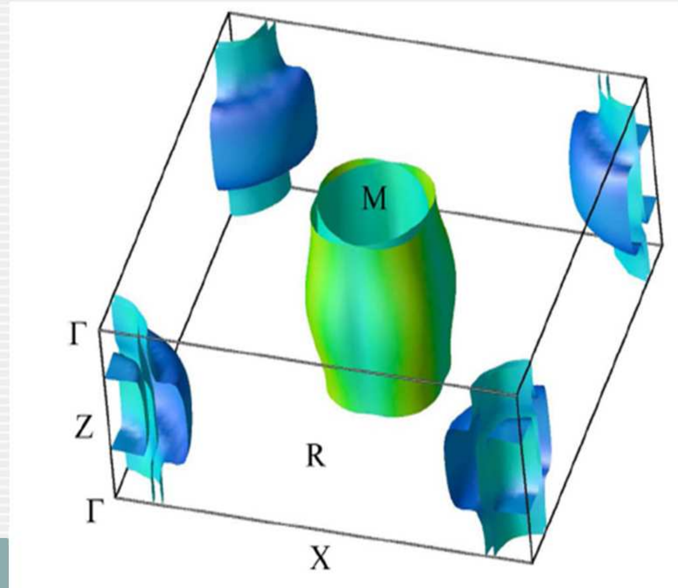


FIG. 3 (color online). LDA Fermi surface of LaFeAsO shaded

VOLUME 72, NUMBER 2 PHYSICAL REVIEW LETTERS 10 JANUARY 1994

Bulk Superconductivity at an Elevated Temperature ($T_c \approx 12$ K) in a Nickel Containing Alloy System Y-Ni-B-C

LETTERS TO NATURE

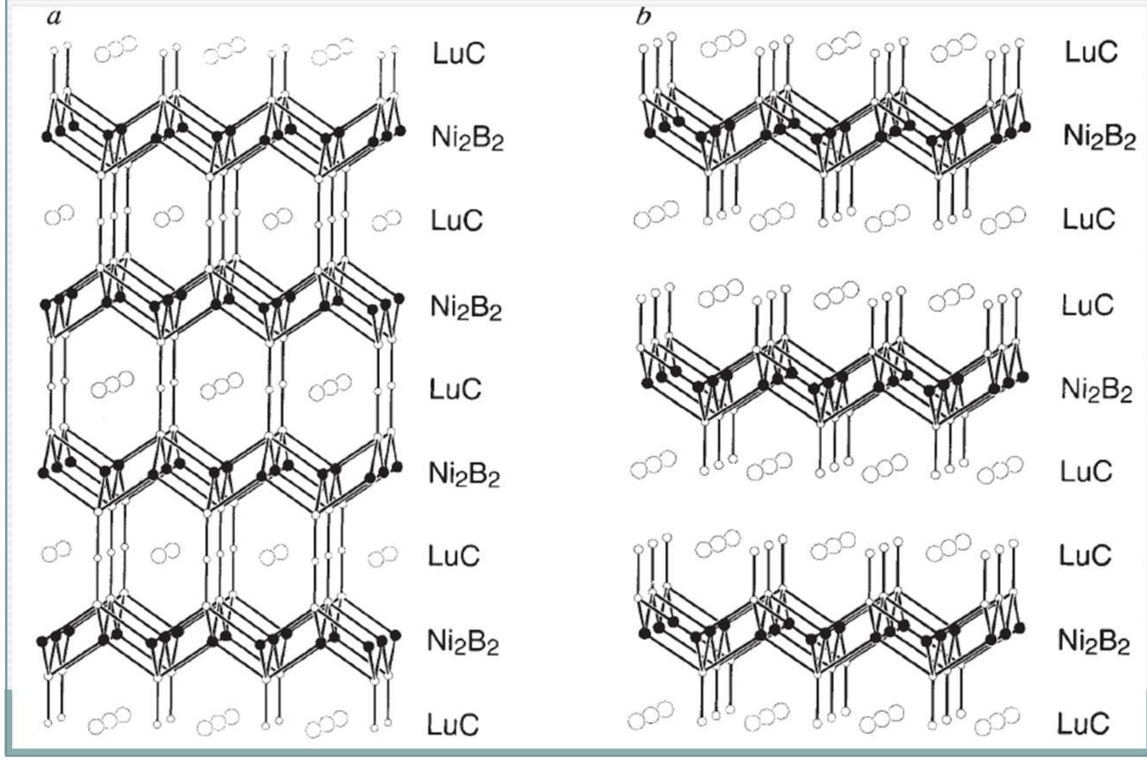
The crystal structure of superconducting $LuNi_2B_2C$ and the related phase LuNiBC

T. Siegrist, H. W. Zandbergen*, R. J. Cava, J. J. Krajewski & W. F. Peck Jr

LETTERS TO NATURE

Superconductivity in the quaternary intermetallic compounds $LnNi_2B_2C$

R. J. Cava, H. Takagi*, H. W. Zandbergen†, J. J. Krajewski, W. F. Peck Jr, T. Siegrist, B. Batlogg, R. B. van Dover, R. J. Felder, K. Mizuhashi*, J. O. Lee*, H. Eisaki* & S. Uchida*

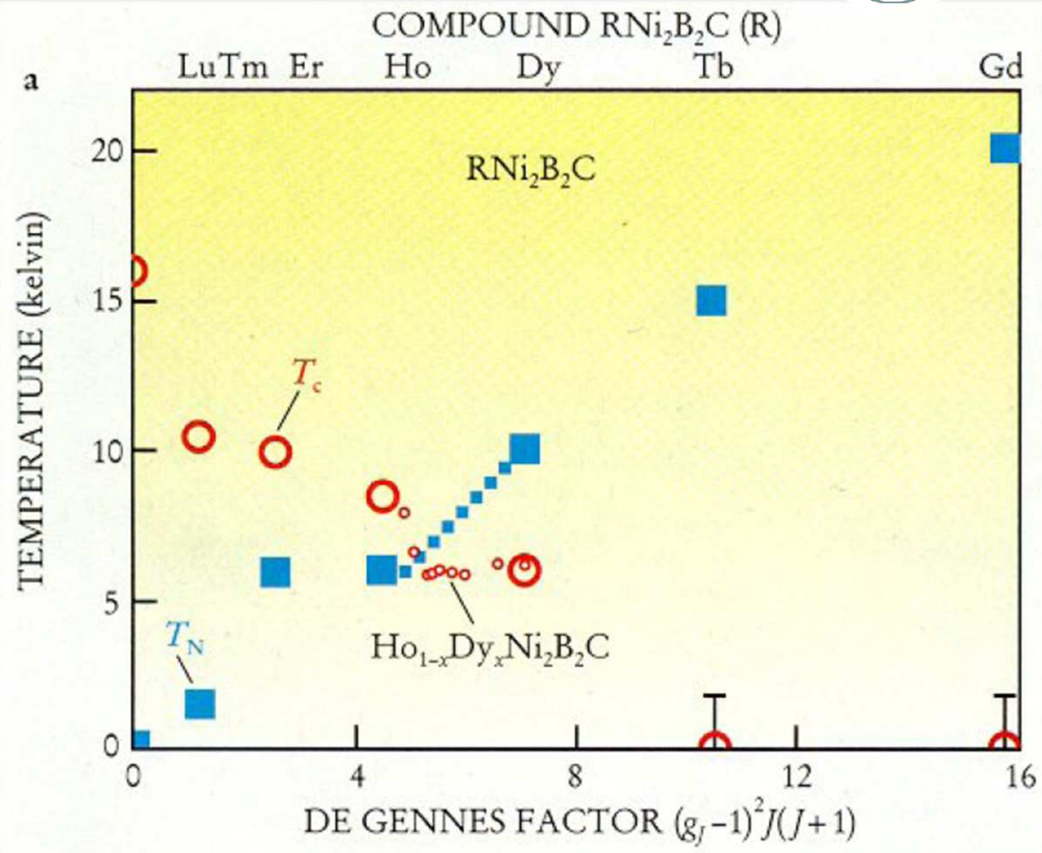


LETTERS TO NATURE

Superconductivity at 23 K in yttrium palladium boride carbide

R. J. Cava*, H. Takagi†, B. Batlogg*, H. W. Zandbergen‡, J. J. Krajewski*, W. F. Peck Jr*, R. B. van Dover*, R. J. Felder*, T. Siegrist*, K. Mizuhashi†, J. O. Lee†, H. Eisaki†, S. A. Carter* & S. Uchida†

Magnetic RE suppresses s-wave superconductivity



A. A. Abrikosov and L. P. Gorkov, Zh. Eksp. Teor. Fiz. **39**, 1781 (1960) [Sov. Phys. JETP **12**, 1243 (1961).

Magnetic RE replacement enhances Tc: unconventional superconductivity!

PRL 100, 247002 (2008) PHYSICAL REVIEW LETTERS week ending 20 JUNE 2008

Superconductivity at 41 K and Its Competition with Spin-Density-Wave Instability in Layered $CeO_{1-x}F_xFeAs$

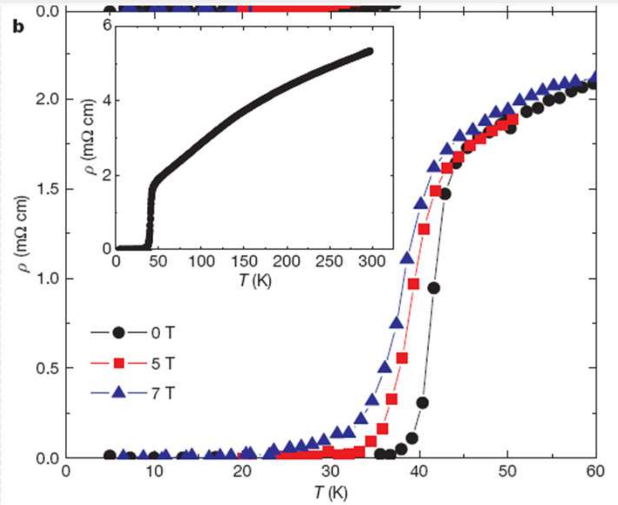
G. F. Chen, Z. Li, D. Wu, G. Li, W. Z. Hu, J. Dong, P. Zheng, J. L. Luo, and N. L. Wang

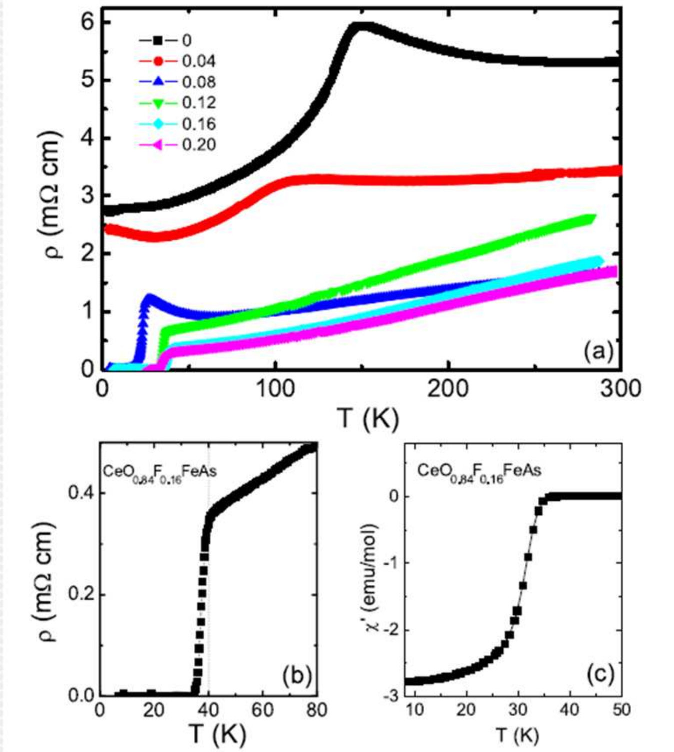
Vol 453|5 June 2008|**doi:10.1038/nature07045**

LETTERS

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]





Outline

1. What is the symmetry of the superconducting order parameter? $S^{+/-}$
2. Which material parameter (s) control Tc? Shape of the FeAs tetrahedron
3. Can the superconducting state coexist with AFM state? Yes
4. Is the antiferromagnetic order really caused by a SDW instability due to the Fermi surface nesting? Orbital ordering transition
5. Itinerant or localized spins for normal state of superconductors? Itinerant
6. How to destroy the superconductivity? Diffusive spin fluctuations

7. A new different family of Fe-based superconductors? Yes

What is the superconducting symmetry for the Fe-based superconductors? S-wave or $S^{+/-}$

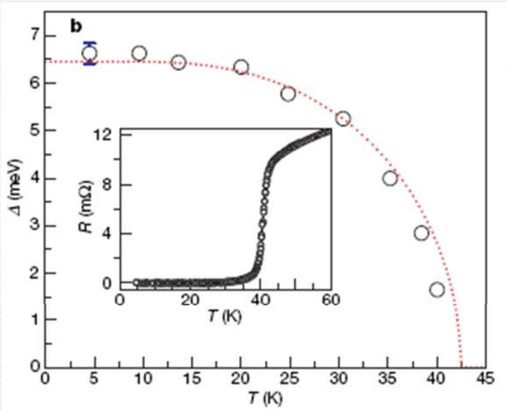
ARPES: $|\Delta(q)|$

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

LETTERS

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]



CHIN.PHYS.LETT. Vol. 25, No. 12 (2008) 4402

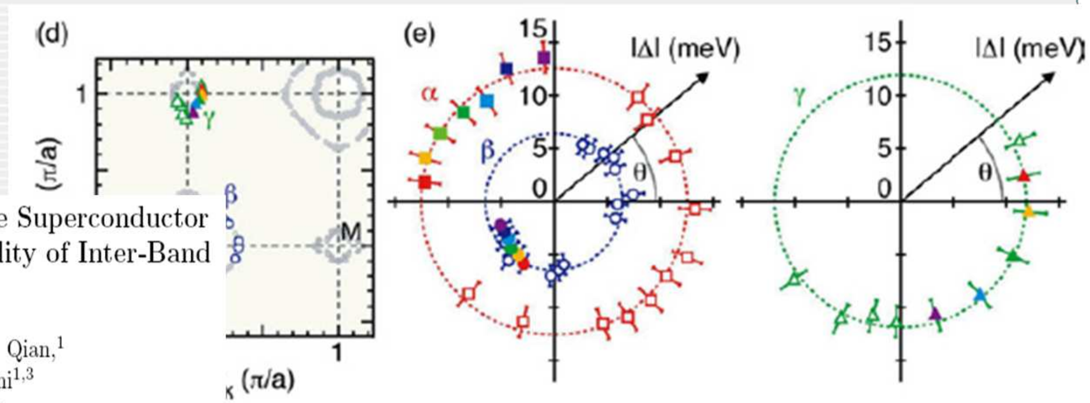
Multiple Nodeless Superconducting Gaps in $(Ba_{0.6}K_{0.4})Fe_2As_2$ Superconductor from Angle-Resolved Photoemission Spectroscopy *

ZHAO Lin(赵林)[1**], LIU Hai-Yun(刘海云)[1], ZHANG Wen-Tao(张文涛)[1], MENG Jian-Qiao(孟建桥)[1], JIA Xiao-Wen(贾小文)[1], LIU Guo-Dong(刘国东)[1], DONG Xiao-Li(董晓莉)[1], CHEN Gen-Fu(陈根富)[2], LUO Jian-Lin(雒建林)[2], WANG Nan-Lin(王楠林)[2], LU Wei(陆伟)[1], WANG Gui-Ling(王桂玲)[3], ZHOU Yong(周永)[3], ZHU Yong(朱镛)[4], WANG Xiao-Yang(王晓洋)[4], XU Zu-Yan(许祖彦)[3], CHEN Chuang-Tian(陈创天)[4], ZHOU Xing-Jiang(周兴江)[1***]

epl A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS August 2008
EPL, 83 (2008) 47001 www.epljournal.org
doi: 10.1209/0295-5075/83/47001

Observation of Fermi-surface–dependent nodeless superconducting gaps in $Ba_{0.6}K_{0.4}Fe_2As_2$

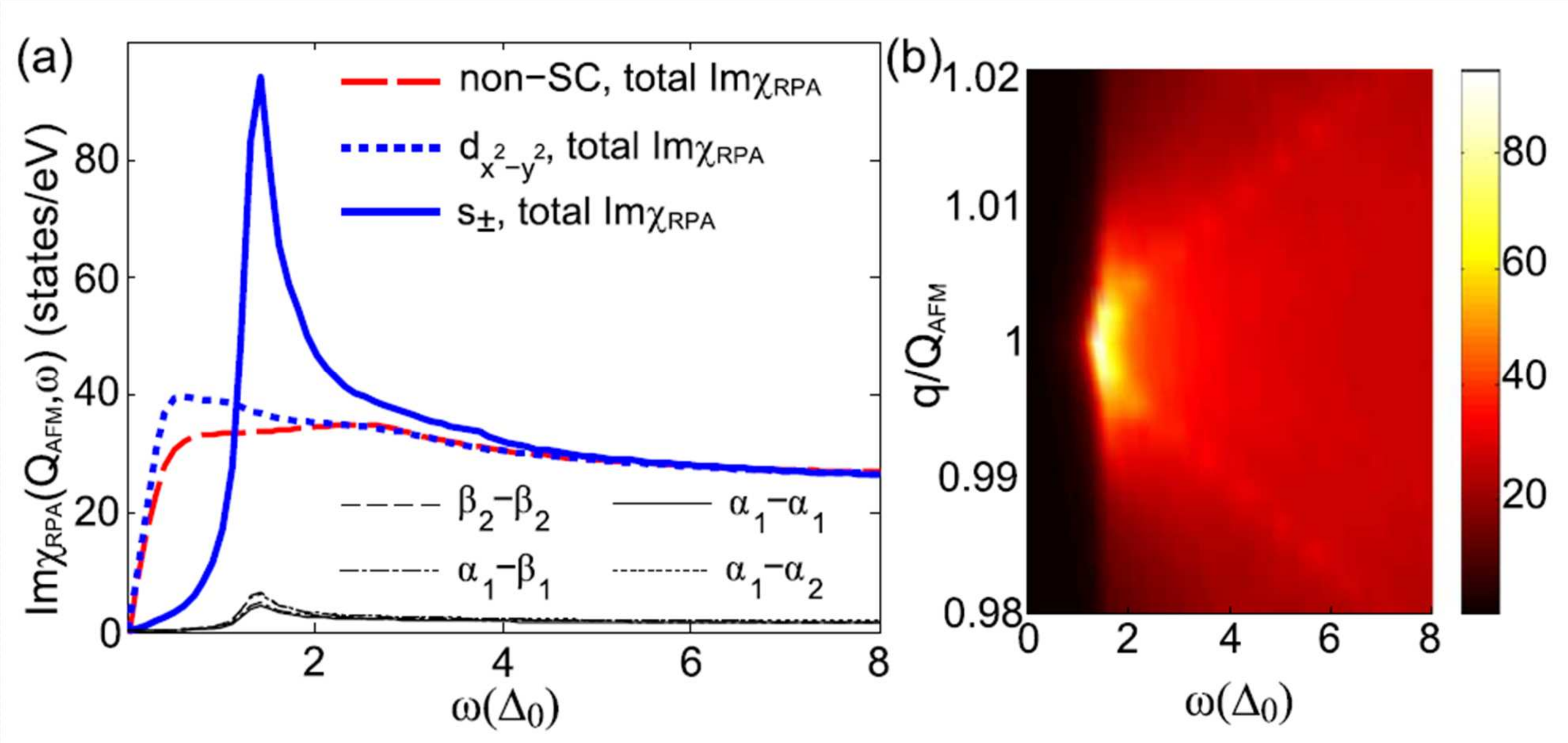
H. Ding[1(a)], P. Richard[2], K. Nakayama[3], K. Sugawara[3], T. Arakane[3], Y. Sekiba[3], A. Takayama[3], S. Souma[2], T. Sato[3], T. Takahashi[2,3], Z. Wang[4], X. Dai[1], Z. Fang[1], G. F. Chen[1], J. L. Luo[1] and N. L. Wang[1]



Angle-Resolved Photoemission Spectroscopy of Iron-Chalcogenide Superconductor $Fe_{1.03}Te_{0.7}Se_{0.3}$: Strong-Coupling Superconductivity and Universality of Inter-Band Scattering

K. Nakayama,[1] T. Sato,[1,2] P. Richard,[3] T. Kawahara,[1] Y. Sekiba,[1] T. Qian,[1] G. F. Chen,[4] J. L. Luo,[4] N. L. Wang,[4] H. Ding,[4] and T. Takahashi[1,3]
[1]Department of Physics, Tohoku University, Sendai 980-8578, Japan
[2]TRiP, Japan Science and Technology Agency (JST), Kawaguchi 332-0012, Japan
[3]WPI Research Center, Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan and
[4]Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Neutron scattering measures spin-pair excitations



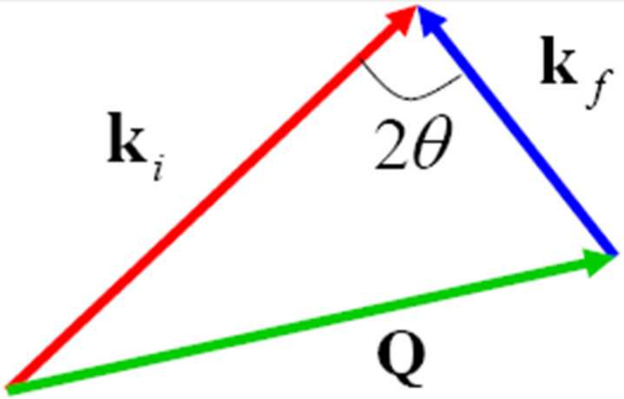
PHYSICAL REVIEW B **78**, 140509(R) (2008)

Theory of magnetic excitations in iron-based layered superconductors

M. M. Korshunov[1,2,*] and I. Eremin[1,3,†]
[1]*Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany*

Maier, T. A., Graser, S., Scalapino, D. J. & Hirschfeld, P. Neutron scattering resonance and the iron-pnictide superconducting gap. *Phys. Rev. B* **79**, 134520 (2009).

Neutron scattering



$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

$$\hbar\omega = E_i - E_f$$

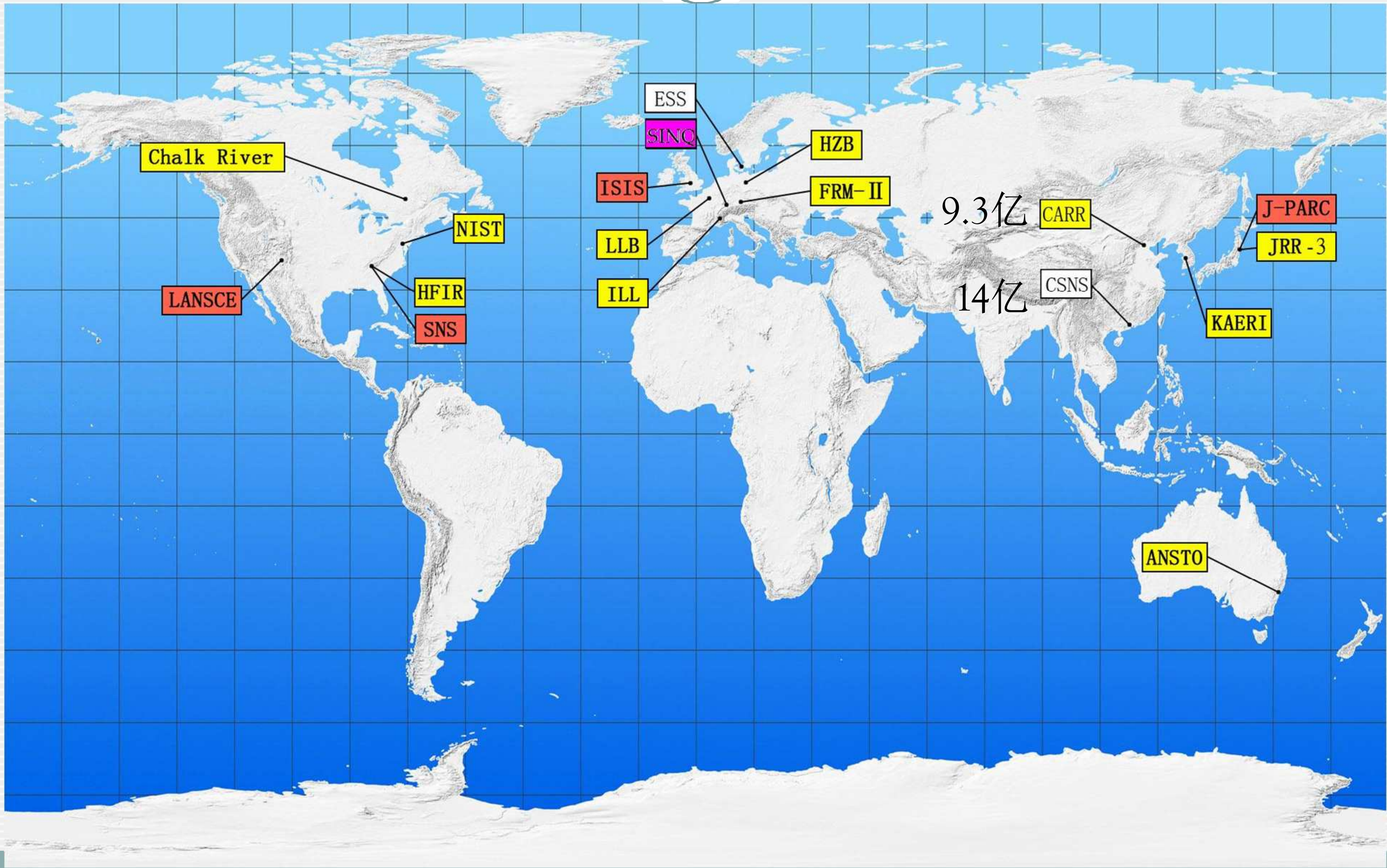
Nuclear scattering

$$\mathrm{S}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t}\,\frac{1}{N}\left\langle \rho_{\mathbf{Q}}(0)\rho_{-\mathbf{Q}}(t)\right\rangle$$

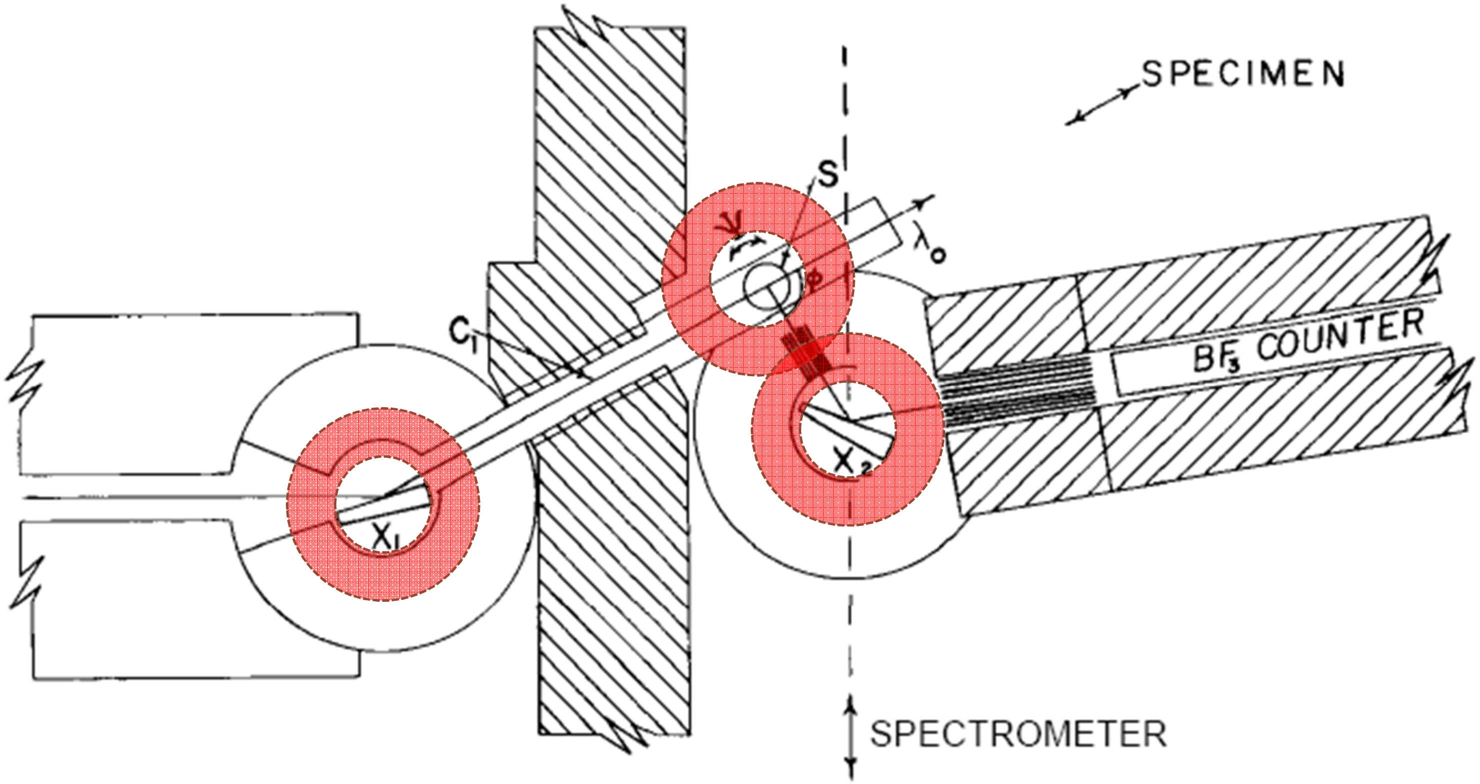
Magnetic scattering

$$\mathrm{S}^{\alpha\beta}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t}\,\frac{1}{N}\sum_{\mathbf{RR'}} e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{R'})} < S^{\alpha}_{\mathbf{R}}(0)\, S^{\beta}_{\mathbf{R'}}(t) >$$

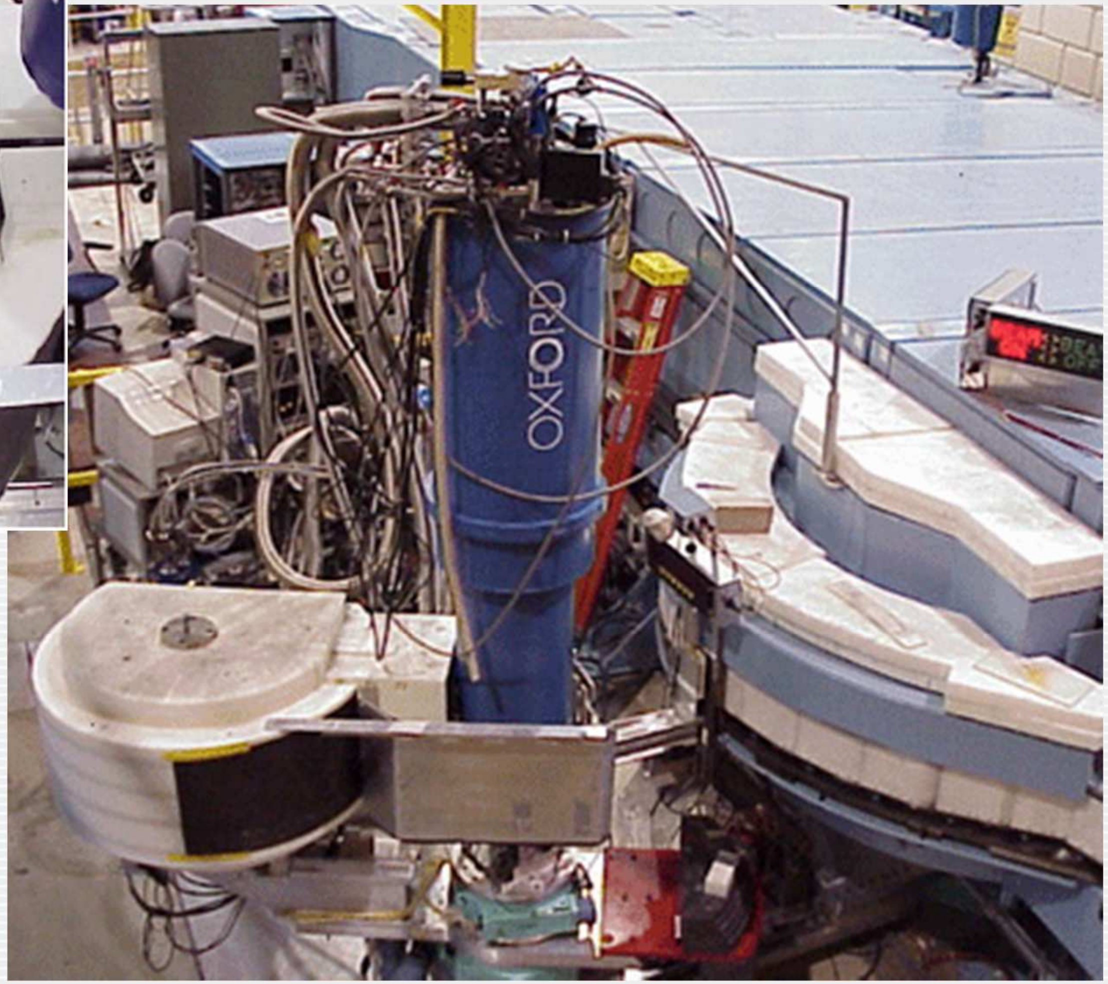
Reactor and spallation neutron user facilities



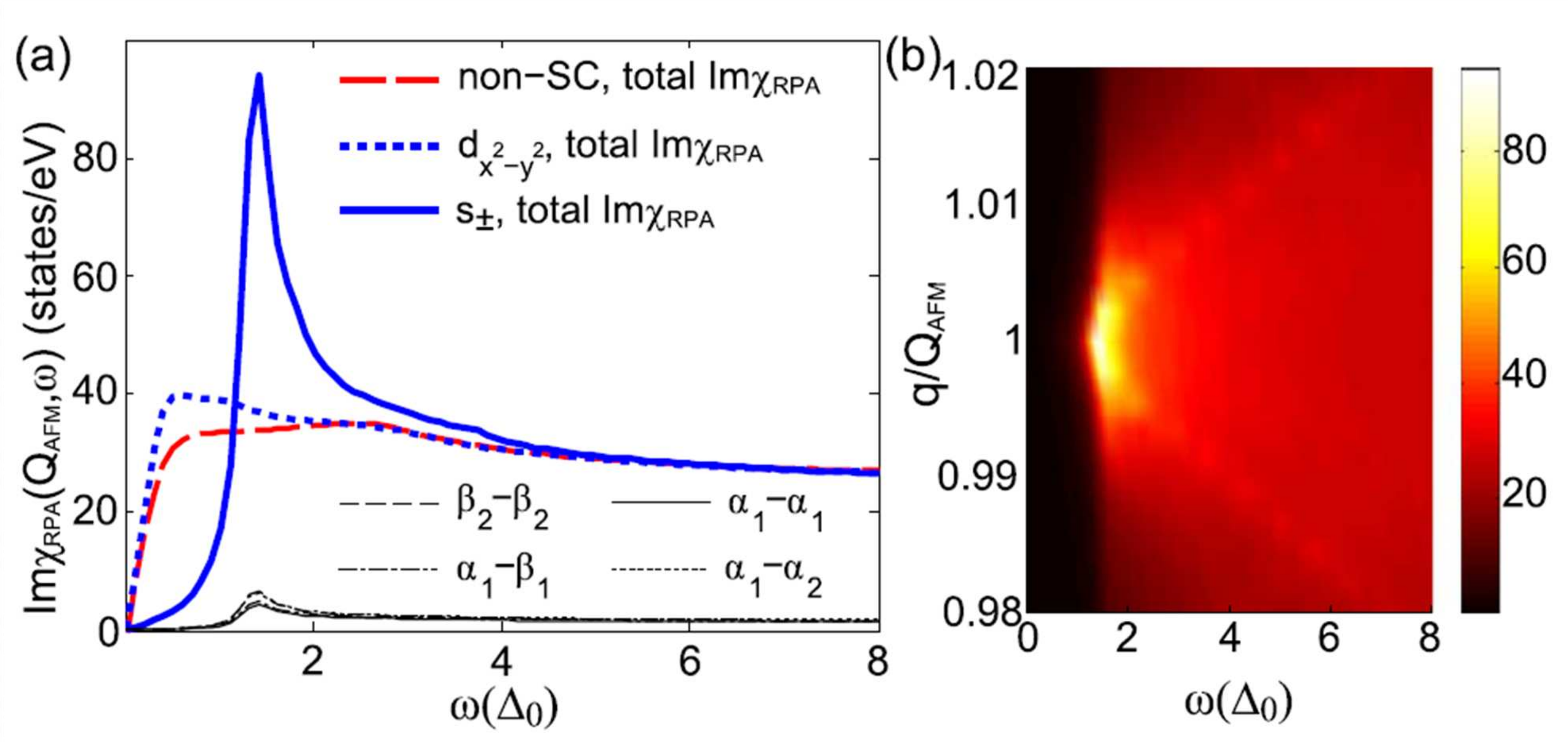
Triple-axis spectrometer



SPINS @ NIST



Neutron scattering measures spin-pair excitations



PHYSICAL REVIEW B **78**, 140509(R) (2008)

Theory of magnetic excitations in iron-based layered superconductors

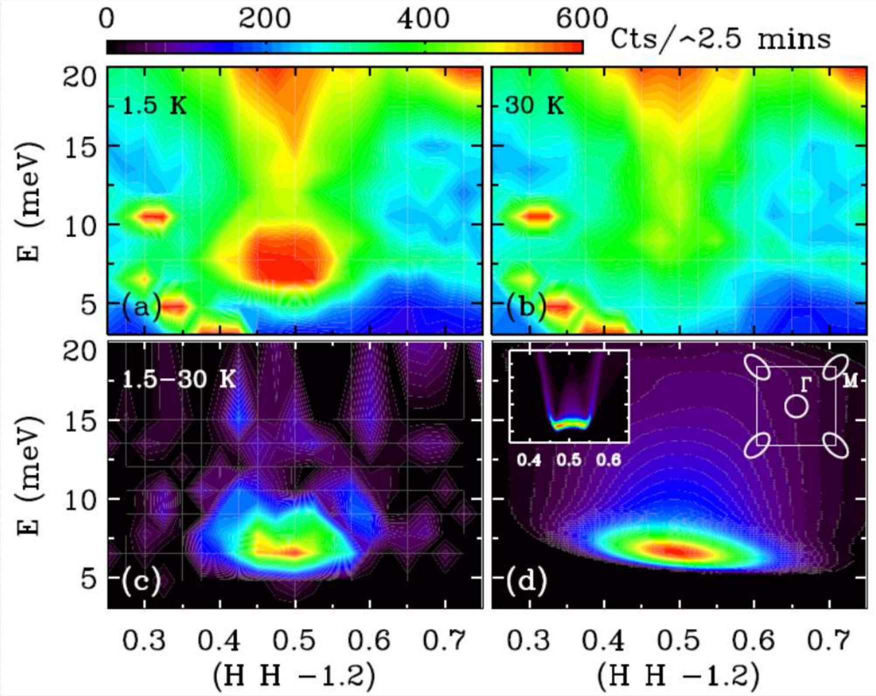
M. M. Korshunov[1,2,*] and I. Eremin[1,3,†]
[1]*Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany*

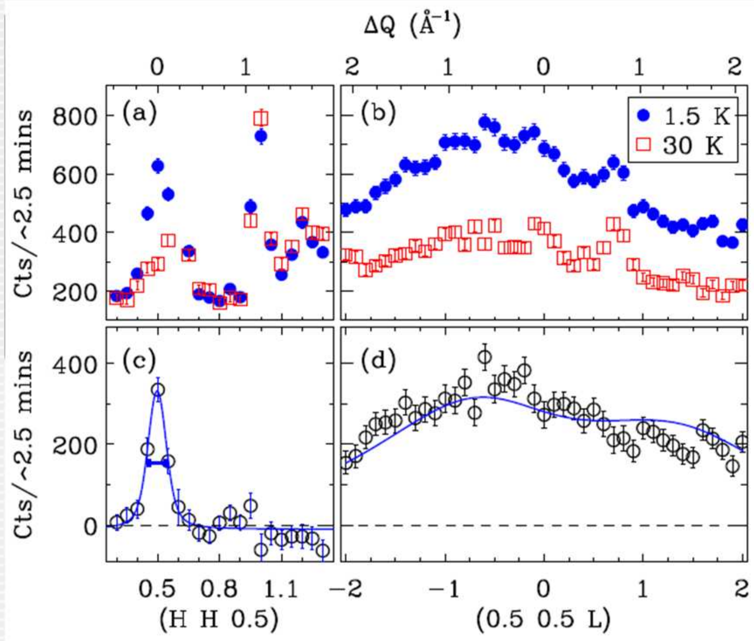
Maier, T. A., Graser, S., Scalapino, D. J. & Hirschfeld, P. Neutron scattering resonance and the iron-pnictide superconducting gap. *Phys. Rev. B* **79**, 134520 (2009).

PRL 103, 067008 (2009) PHYSICAL REVIEW LETTERS week ending 7 AUGUST 2009

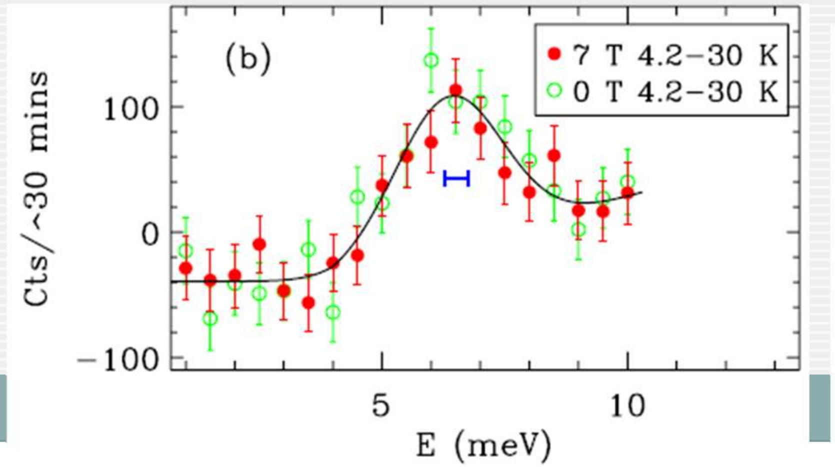
Spin Gap and Resonance at the Nesting Wave Vector in Superconducting $FeSe_{0.4}Te_{0.6}$

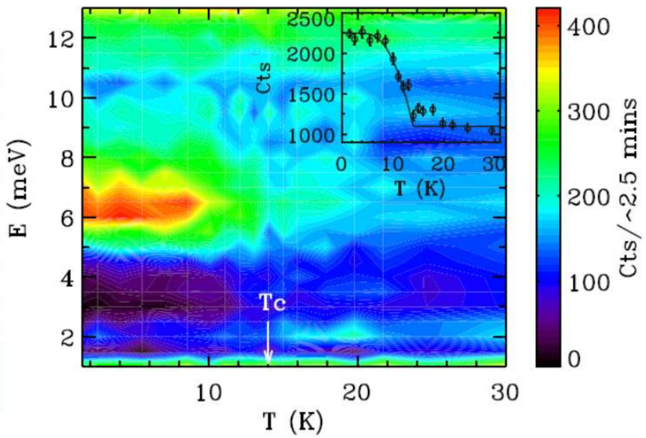
Yiming Qiu,[1,2] Wei Bao,[3,*] Y. Zhao,[4] Collin Broholm,[4,1] V. Stanev,[4] Z. Tesanovic,[4] Y. C. Gasparovic,[1,2] S. Chang,[1]
Jin Hu,[5] Bin Qian,[5] Minghu Fang,[5,6] and Zhiqiang Mao[5]

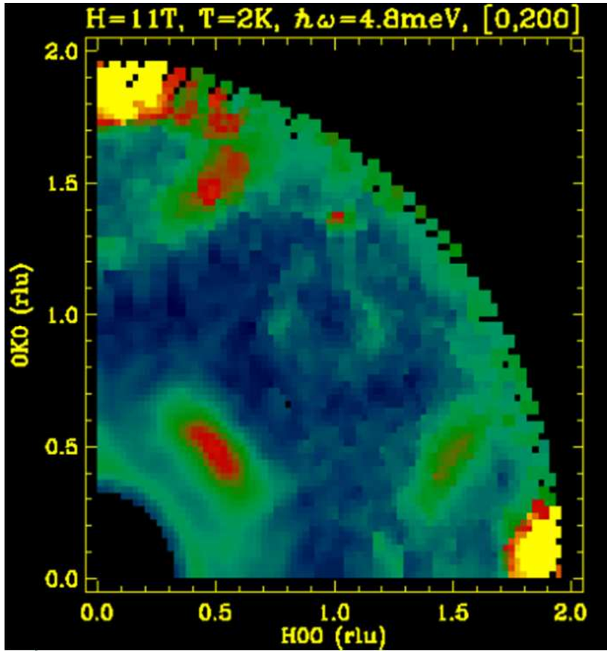




$E_0/k_BTc=5.3$



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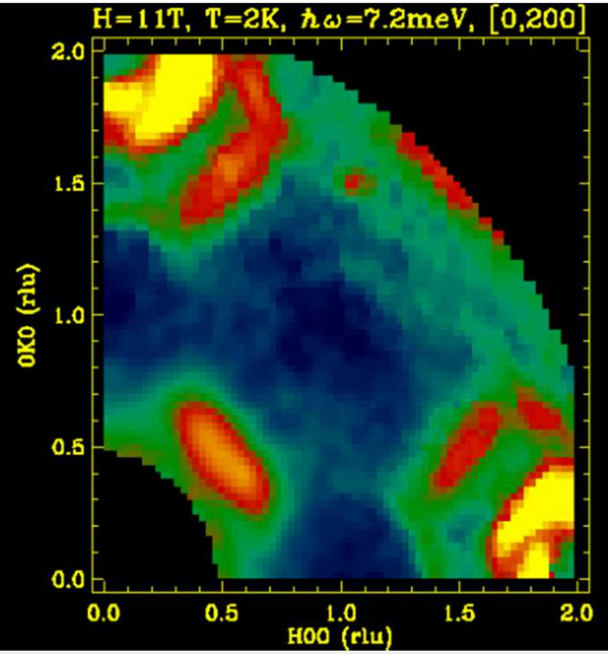
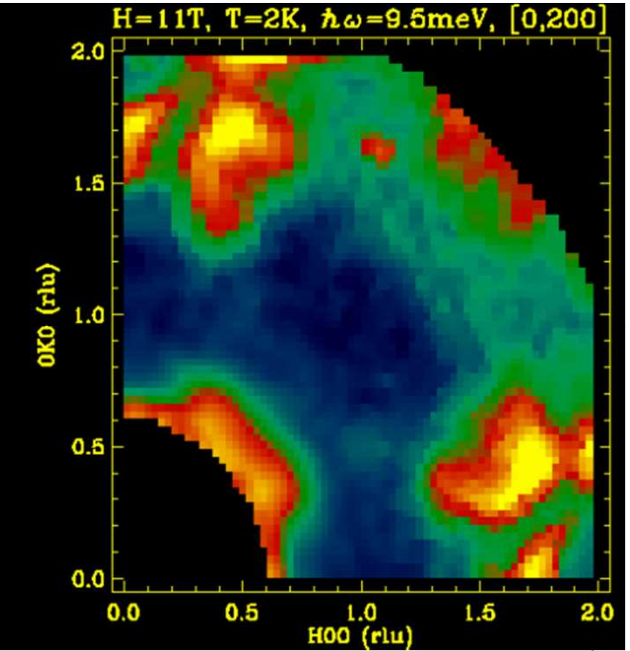
0K0 (rlu)
H00 (rlu)
0.0
0.5
1.0
1.5
2.0


H=11T, T=2K, ℏω=7.2meV, [0,200]
0K0 (rlu)
H00 (rlu)
0.0
0.5
1.0
1.5
2.0


H=11T, T=2K, ℏω=9.5meV, [0,200]
0K0 (rlu)
H00 (rlu)
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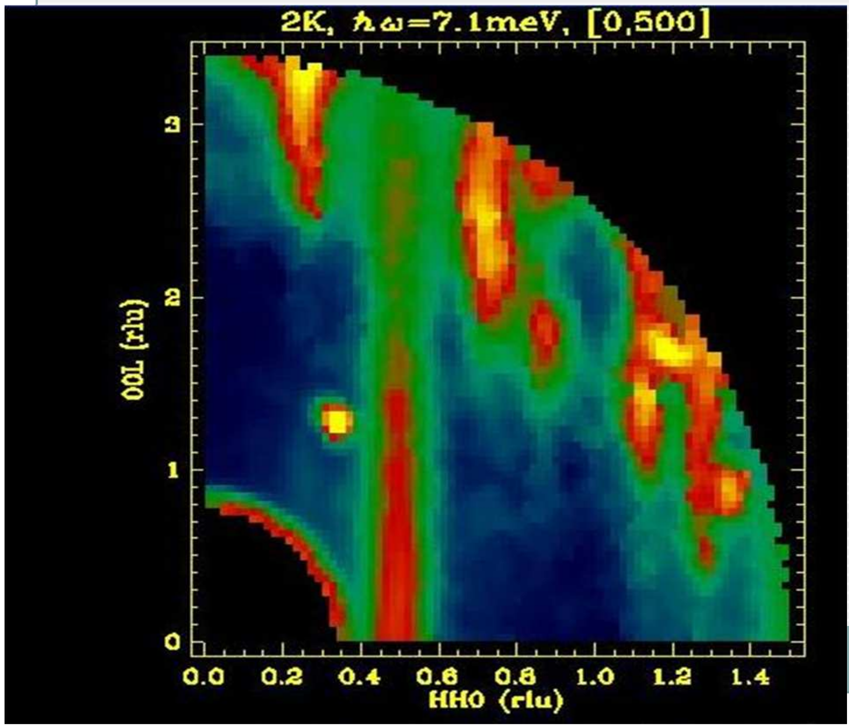
0.5
1.0
1.5
2.0


2K, ℏω=7.1meV, [0,500]
00L (rlu)
HH0 (rlu)
0
1
2
3
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4

Symmetry of superconducting order

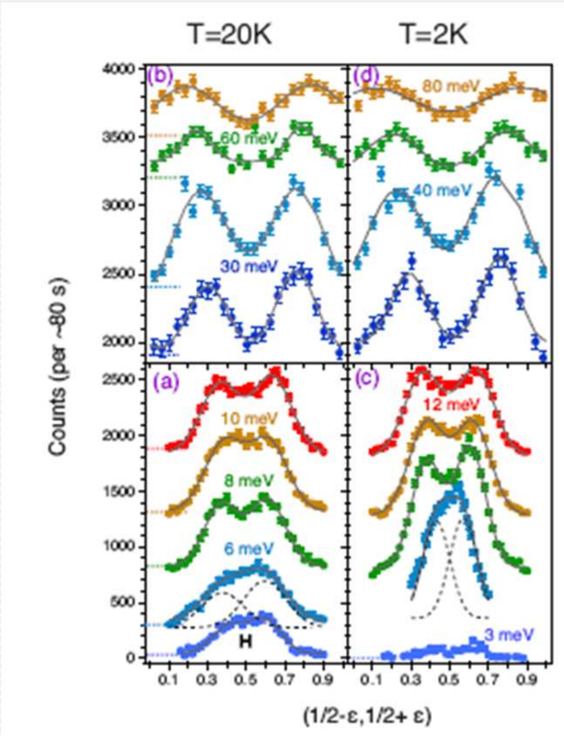
- ARPES: nodeless gap of 2Δ
- Inelastic neutron scattering: resonance peak at $Q \approx (\pi,0)$ & $E_0 < 2\Delta$
  - $S^{+/-}$ symmetry
  - The Cooper pairs formed of quasi-2D electrons

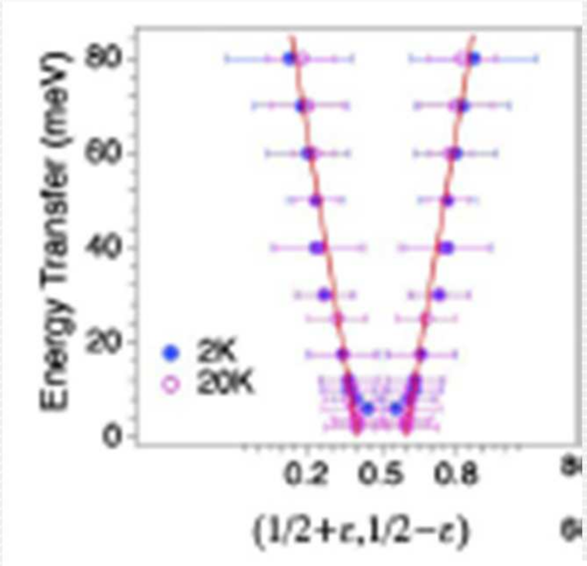
RAPID COMMUNICATIONS

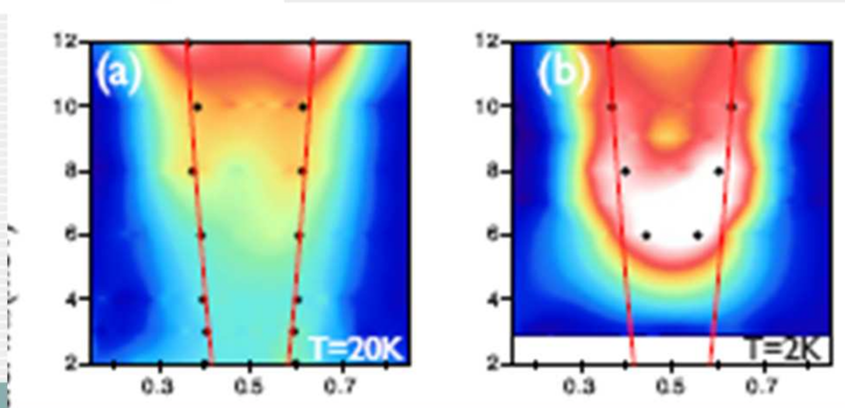
PHYSICAL REVIEW B 81, 220503(R) (2010)

Incommensurate itinerant antiferromagnetic excitations and spin resonance in the $FeTe_{0.6}Se_{0.4}$ superconductor

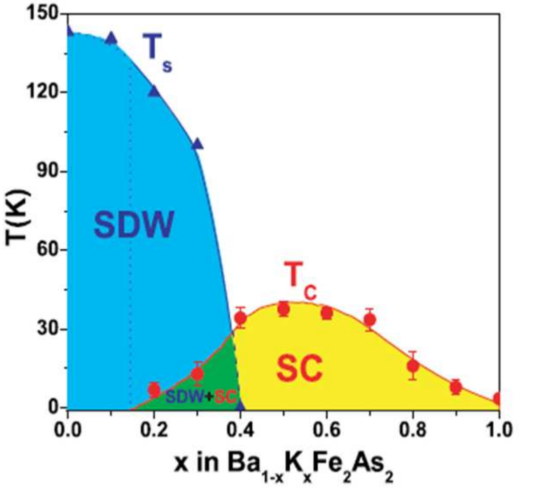
D. N. Argyriou,[1,*] A. Hiess,[2] A. Akbari,[3] I. Eremin,[3,4,†] M. M. Korshunov,[3,5,‡] Jin Hu,[6] Bin Qian,[6] Zhiqiang Mao,[6] Yiming Qiu,[7,8] Collin Broholm,[9] and W. Bao[10,§]



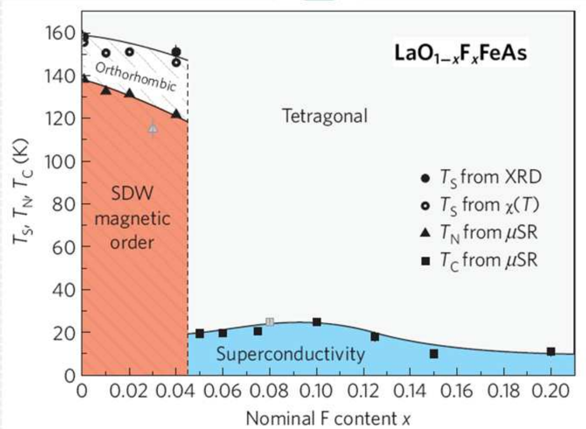




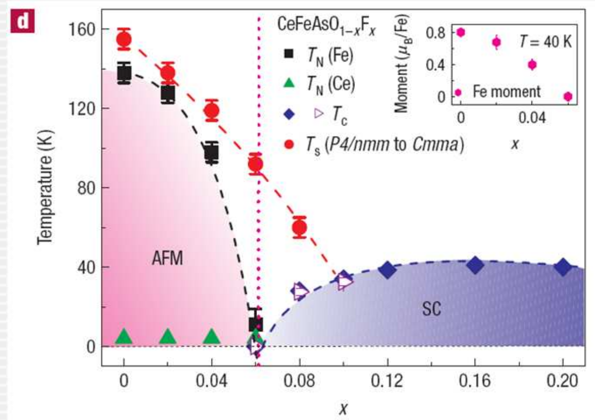
Physical nature of the antiferromagnetic transition?



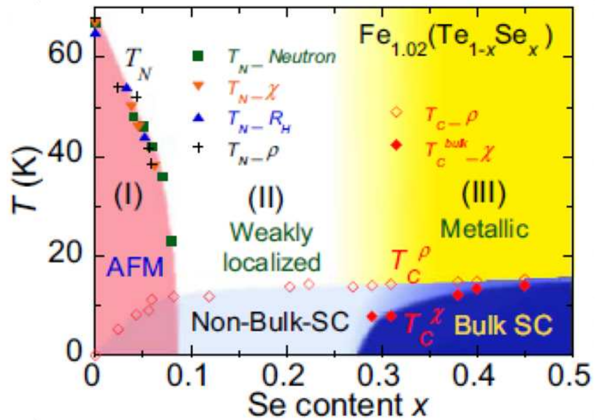
H. Chen et al., EPL **85**, 17006 (2009)



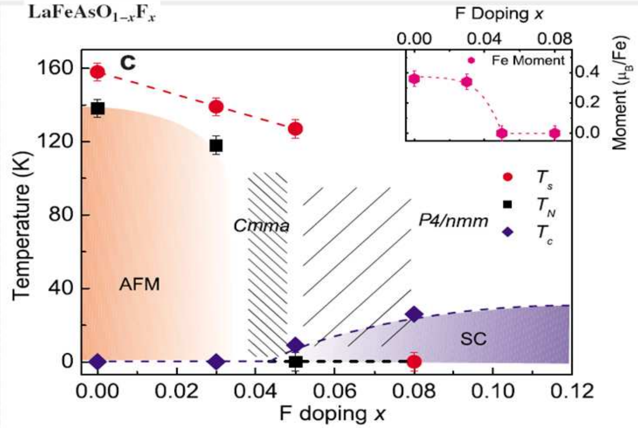
Luetkens et al. Nature Mat. 8, 305 (2009)



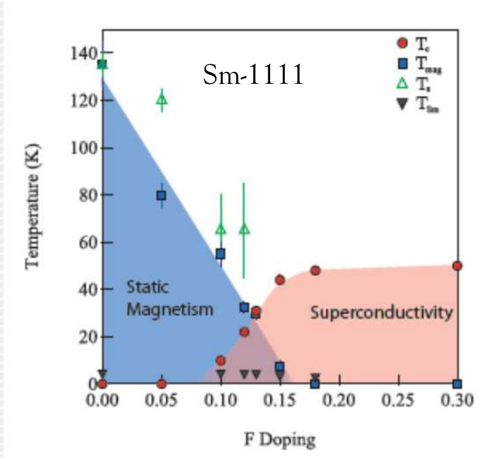
Zhao et al. Nature Mat. 7, 953 (2008)



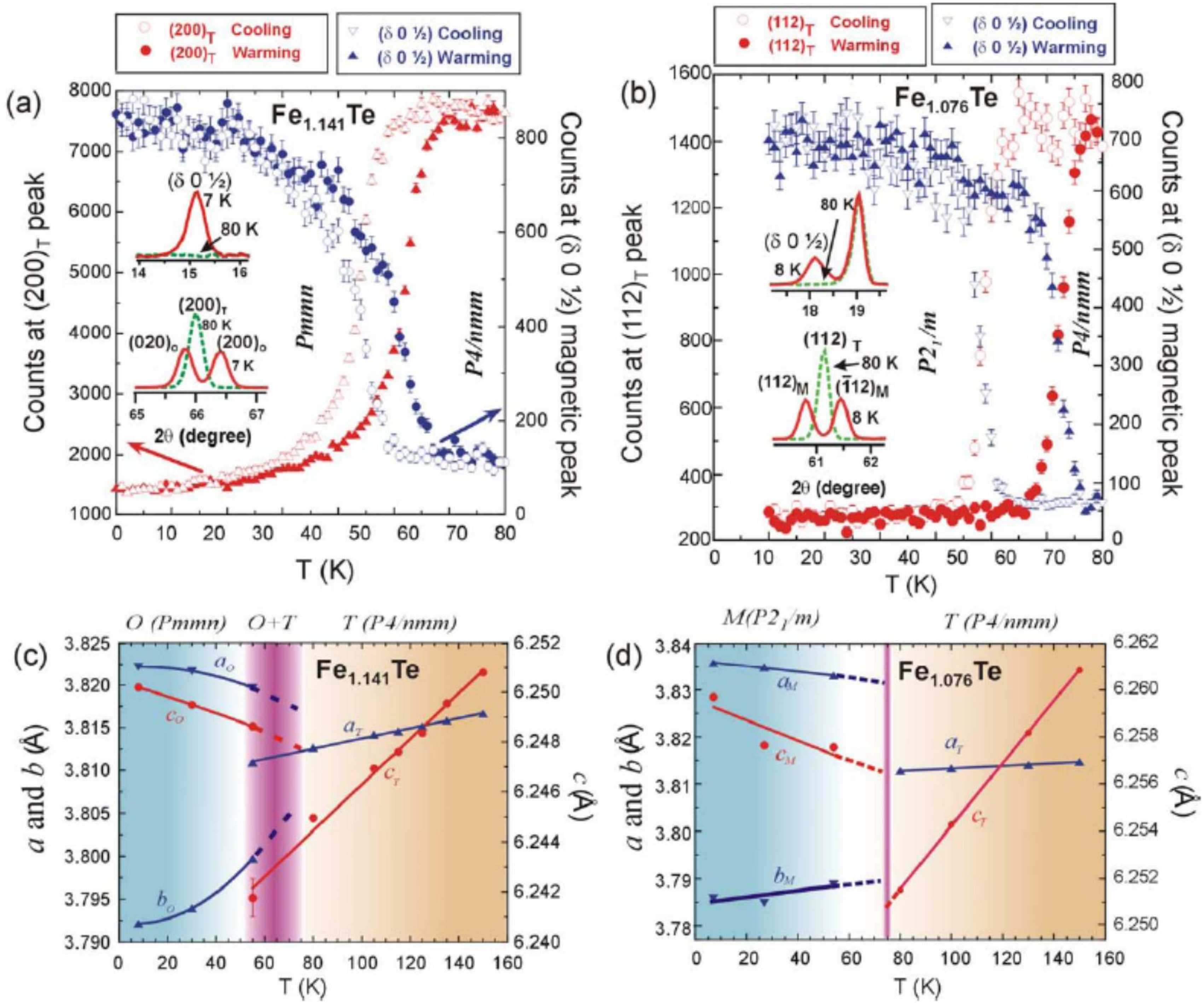
T.J. Liu et al., Nature Materials **9**, 718 (2010)



Q. Huang et al., PRB 78, 054529 (2008)



Drew et al., Nature Mat. **8**, 310 (2009)



(200)T Cooling
(200)T Warming
(δ 0 ½) Cooling
(δ 0 ½) Warming
(a)
Fe1.141Te
Counts at (200)T peak
Counts at (δ 0 ½) magnetic peak
Pmmn
P4/nmm
2θ (degree)
T (K)
(112)T Cooling
(112)T Warming
(b)
Fe1.076Te
Counts at (112)T peak
P21/m
(c)
O (Pmmn)
O+T
T (P4/nmm)
a and b (Å)
c (Å)
(d)
M(P21/m)

Spin-density-wave (SDW) order of a Fermi gas/liquid: (W.M. Lomer, 1962)
divergent Lindhard function $\chi_0(\mathbf{Q},\omega)$ at nesting vector $\mathbf{Q}_{sdw}$

PRL **100**, 237003 (2008) PHYSICAL REVIEW LETTERS week ending 13 JUNE 2008

Density Functional Study of $LaFeAsO_{1-x}F_x$: A Low Carrier Density Superconductor Near Itinerant Magnetism

D. J. Singh and M.-H. Du

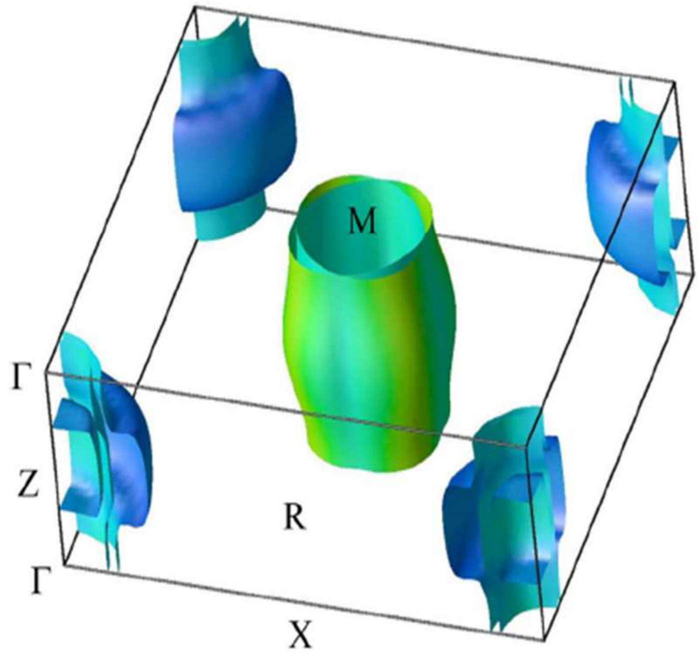
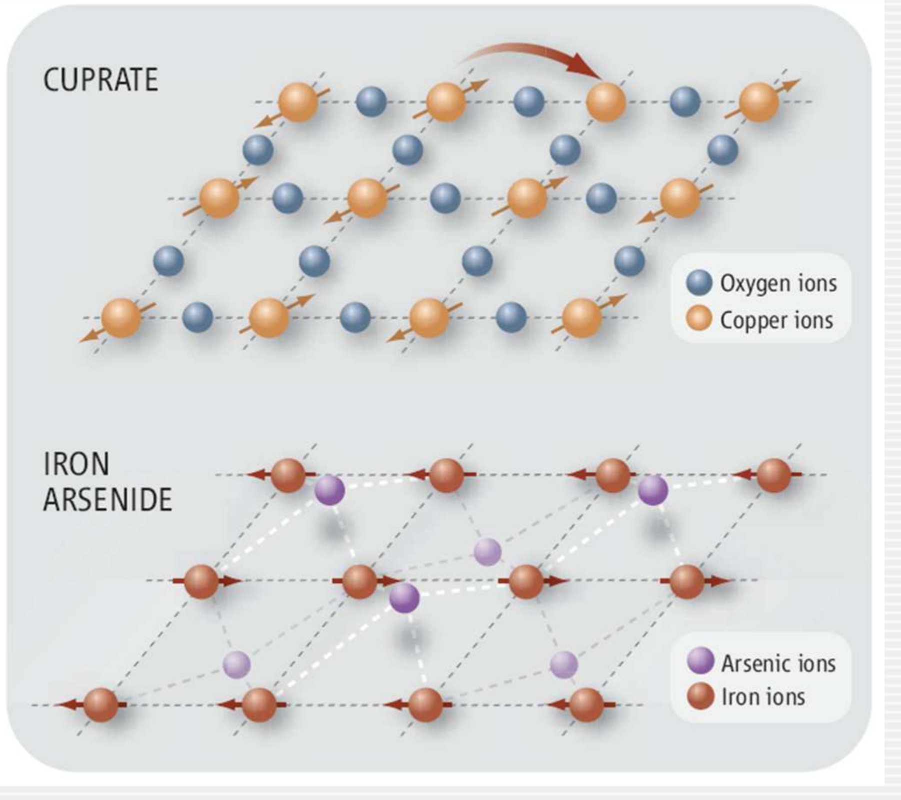


FIG. 3 (color online). LDA Fermi surface of LaFeAsO shaded

SDW: Dong et al., EPL ‘08
Ma and Lu, PRB ’08
Kuroki et al, PRL ’08
Cao et al., PRB ‘08
……

PHYSICS

The Hot Question: How New Are The New Superconductors?

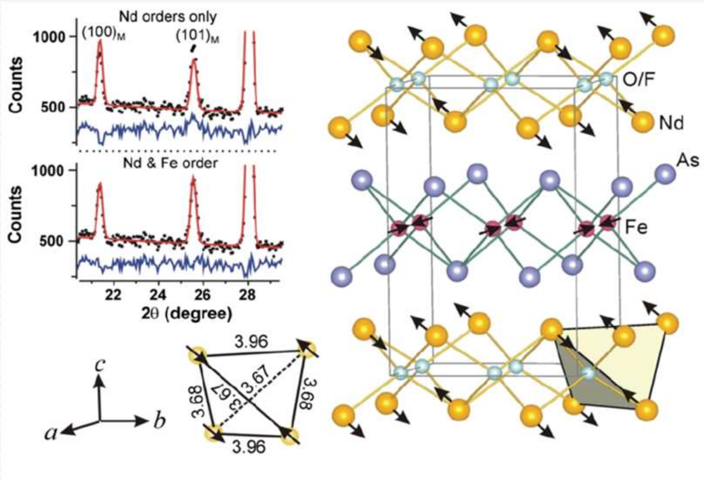


Orthorhombic not tetragonal structure: direction of M and Q?

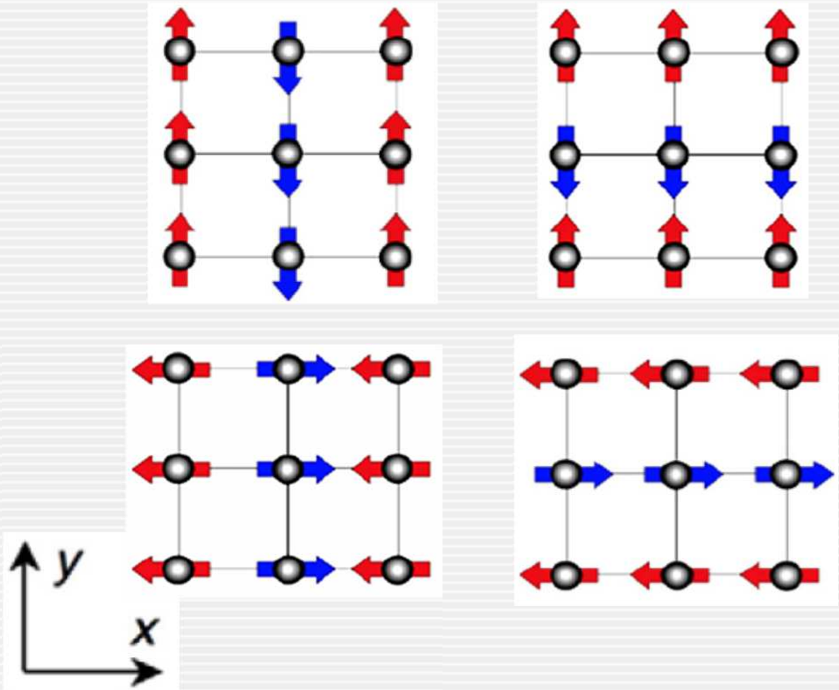
PRL 101, 257002 (2008) PHYSICAL REVIEW LETTERS week ending 19 DECEMBER 2008

Crystal Structure and Antiferromagnetic Order in $NdFeAsO_{1-x}F_x$ ($x = 0.0$ and 0.2) Superconducting Compounds from Neutron Diffraction Measurements

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



The Fe moments are orientated along the longer of the two axes, a, the direction where Nd also has a component. While the antiferromagnetic alignment for Nd is along the b axis, it is along the a axis for the Fe moments, which is consistent with previous first-principles calculations [22]. The total staggered magnetic moments are $1.55(4)\mu_B$ per Nd and $0.9(1)\mu_B$ per Fe at 0.3 K.



(pi,0) and (0,pi) not equivalent in orthorhombic lattice

arXiv:0806.2195

PRL 101, 257002 (2008) PHYSICAL REVIEW LETTERS week ending 19 DECEMBER 2008

Crystal Structure and Antiferromagnetic Order in $NdFeAsO_{1-x}F_x$ ($x = 0.0$ and 0.2) Superconducting Compounds from Neutron Diffraction Measurements

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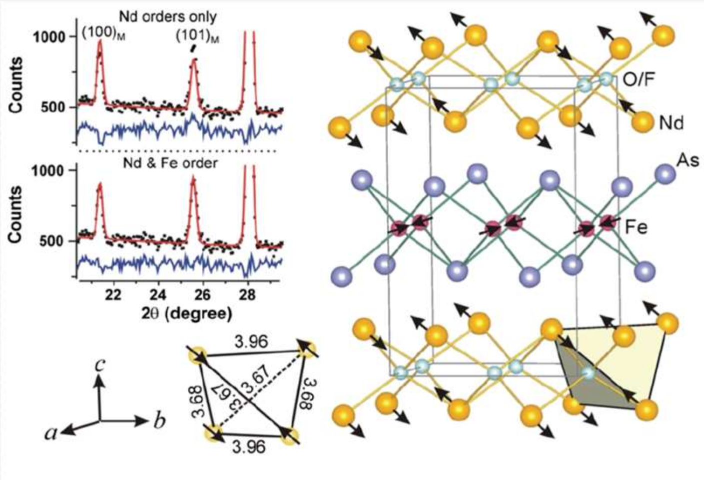
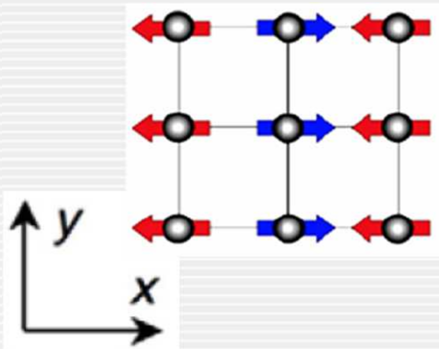


The Fe moments are orientated along the longer of the two axes, a, the direction where Nd also has a component. While the antiferromagnetic alignment for Nd is along the b axis, it is along the a axis for the Fe moments, which is consistent with previous first-principles calculations [22]. The total staggered magnetic moments are $1.55(4)\mu_B$ per Nd and $0.9(1)\mu_B$ per Fe at 0.3 K.



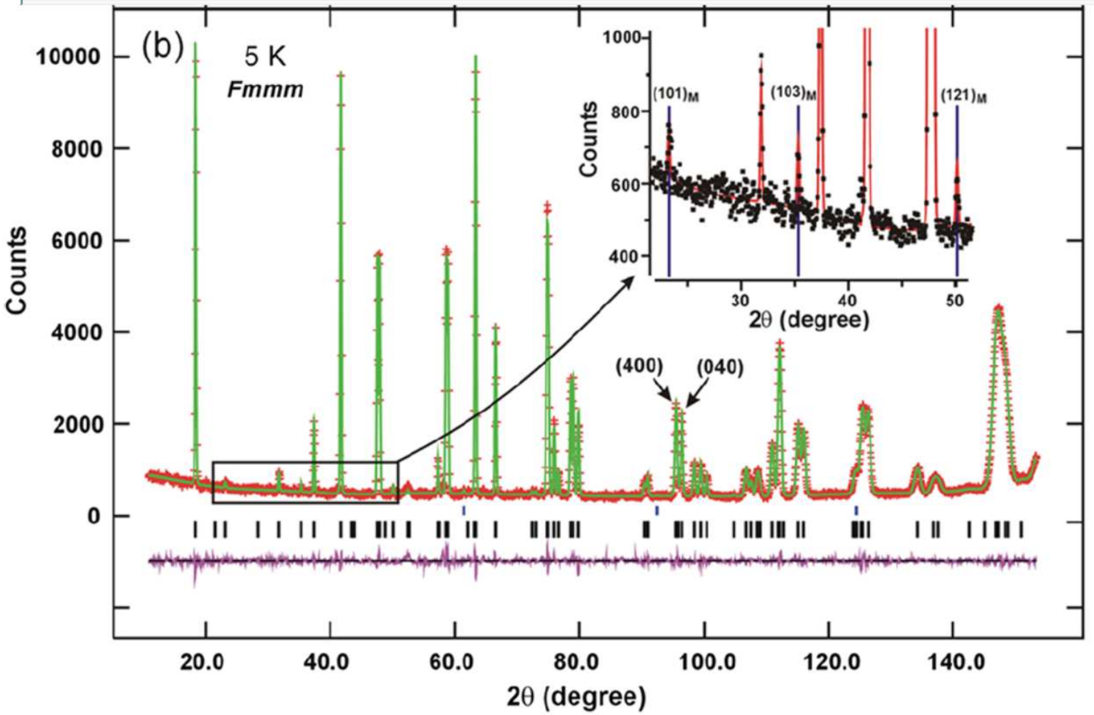
The first correct determination of the **Q/M** direction of magnetic order of 1111 in term of the orthorhombic unit cell

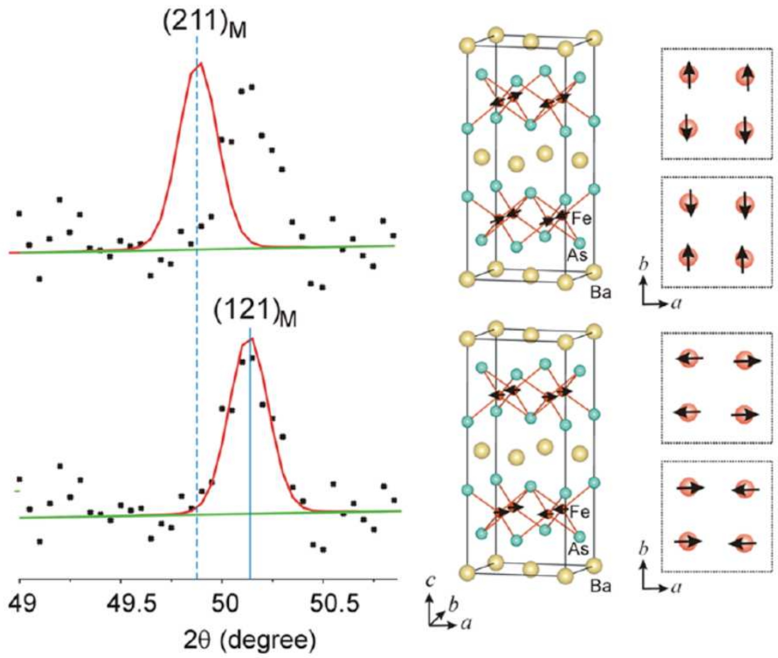
arXiv:0806.2195

PRL **101,** 257003 (2008) PHYSICAL REVIEW LETTERS week ending 19 DECEMBER 2008

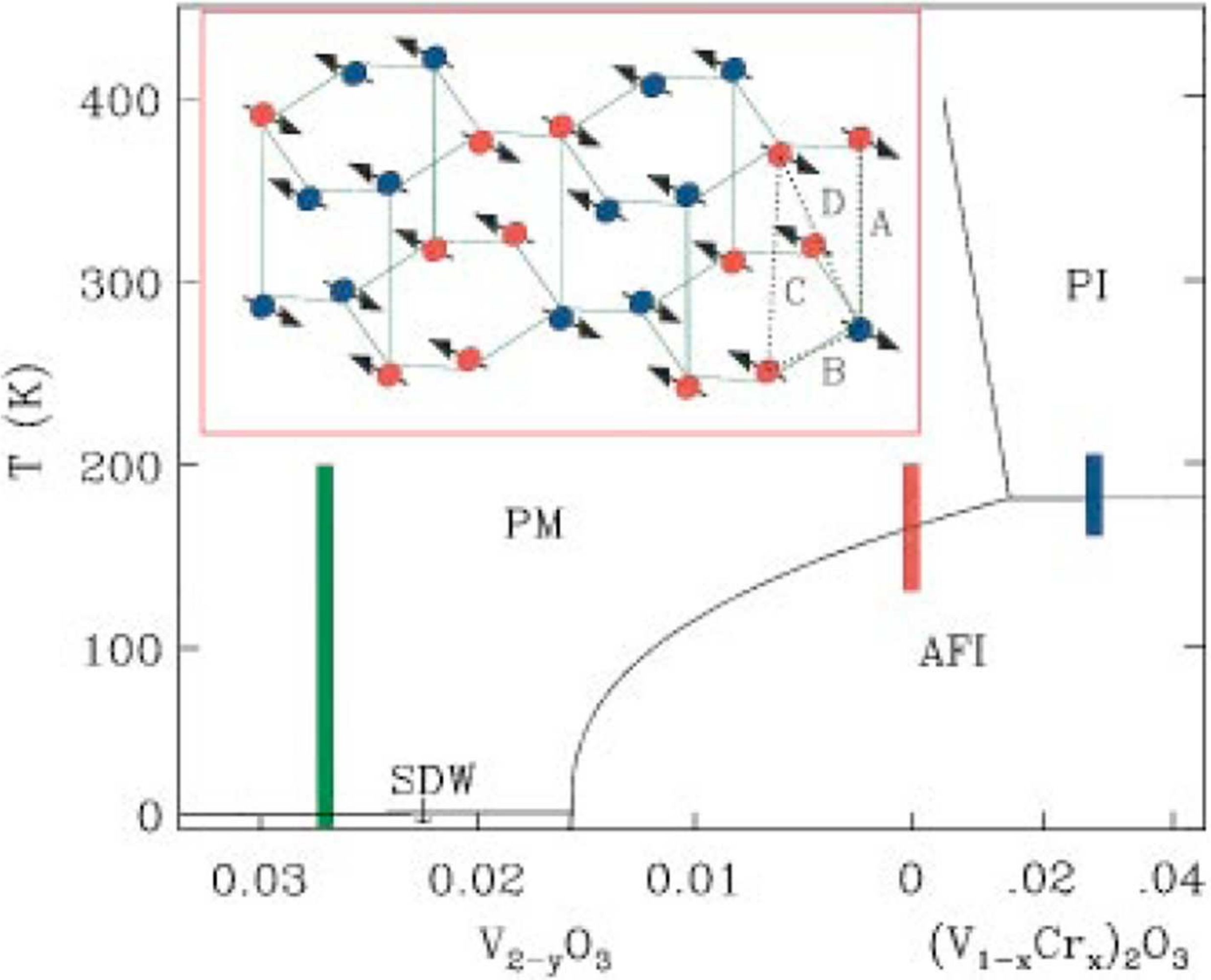
Neutron-Diffraction Measurements of Magnetic Order and a Structural Transition in the Parent $BaFe_2As_2$ Compound of FeAs-Based High-Temperature Superconductors

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





arXiv:0806.2776 The 1st magnetic structure determination of the 122 system



week ending
19 DECEMBER 2008

ral Transition
uperconductors

. Wu,[4] and X. H. Chen[4]

T.M. Rice, F.C. Zhang '95
Pen et al. '97
Castellani, Natoli, Ranninger '78
Kugel, Khomskii '73
Cyrot, Lyon-Caen '73
.....

VOLUME 78, NUMBER 3 PHYSICAL REVIEW LETTERS 20 JANUARY 1997

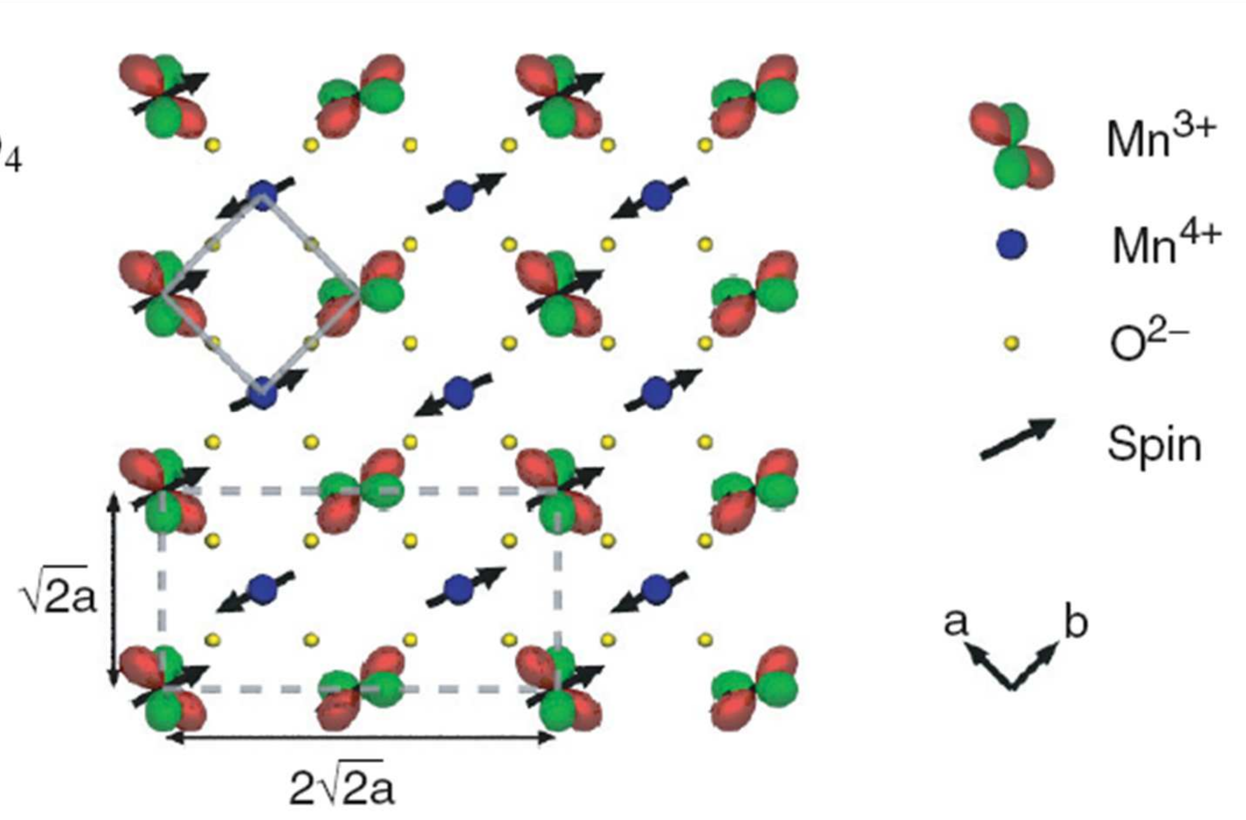
Dramatic Switching of Magnetic Exchange in a Classic Transition Metal Oxide: Evidence for Orbital Ordering

Wei Bao,[1,2] C. Broholm,[1,3] G. Aeppli,[4] P. Dai,[5] J. M. Honig,[6] and P. Metcalf[6]

Magnetic exchange J determined by orbital overlap

Goodenough.

$La_{0.5}Sr_{1.5}MnO_4$



Ordered pattern of J comes from ordered pattern of orbital occupation

The same SDW state predicted for the 11 system

PRL **100**, 237003 (2008) PHYSICAL REVIEW LETTERS week ending 13 JUNE 2008

Density Functional Study of LaFeAsO$_{1-x}$F$_x$: A Low Carrier Density Superconductor Near Itinerant Magnetism

D. J. Singh and M.-H. Du

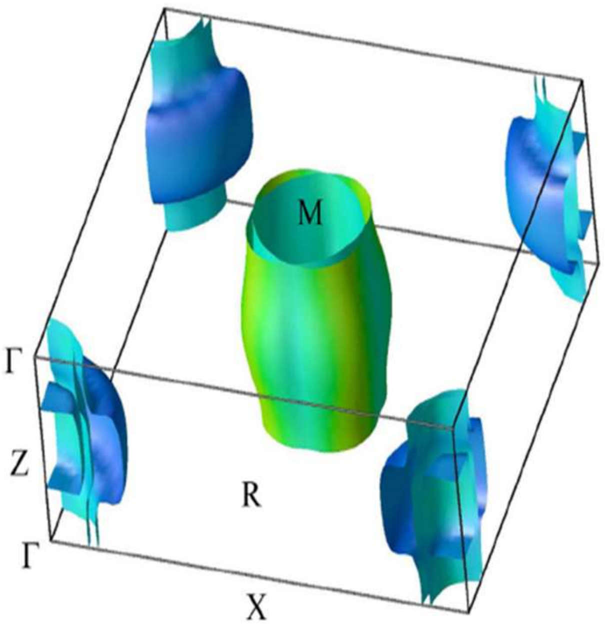
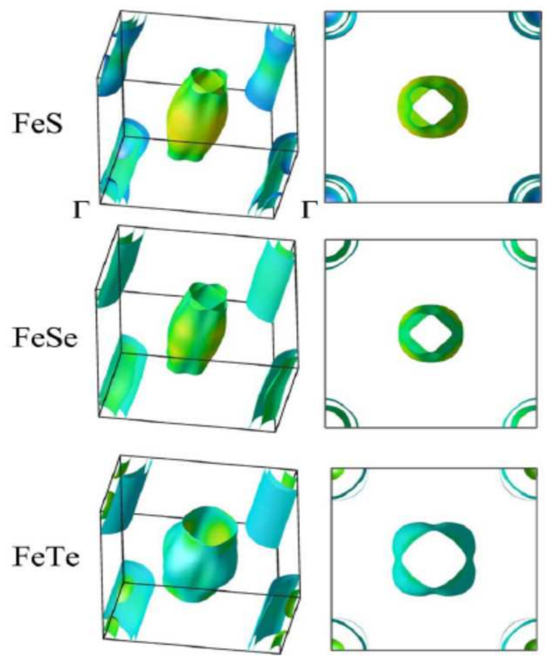


FIG. 3 (color online). LDA Fermi surface of LaFeAsO shaded

Selected for a Viewpoint in *Physics*
PHYSICAL REVIEW B **78**, 134514 (2008)

Density functional study of FeS, FeSe, and FeTe: Electronic structure, magnetism, phonons, and superconductivity

Alaska Subedi



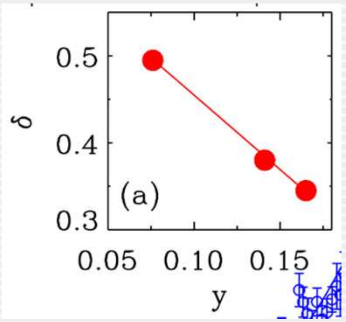
PRL **102**, 247001 (2009) PHYSICAL REVIEW LETTERS week ending 19 JUNE 2009

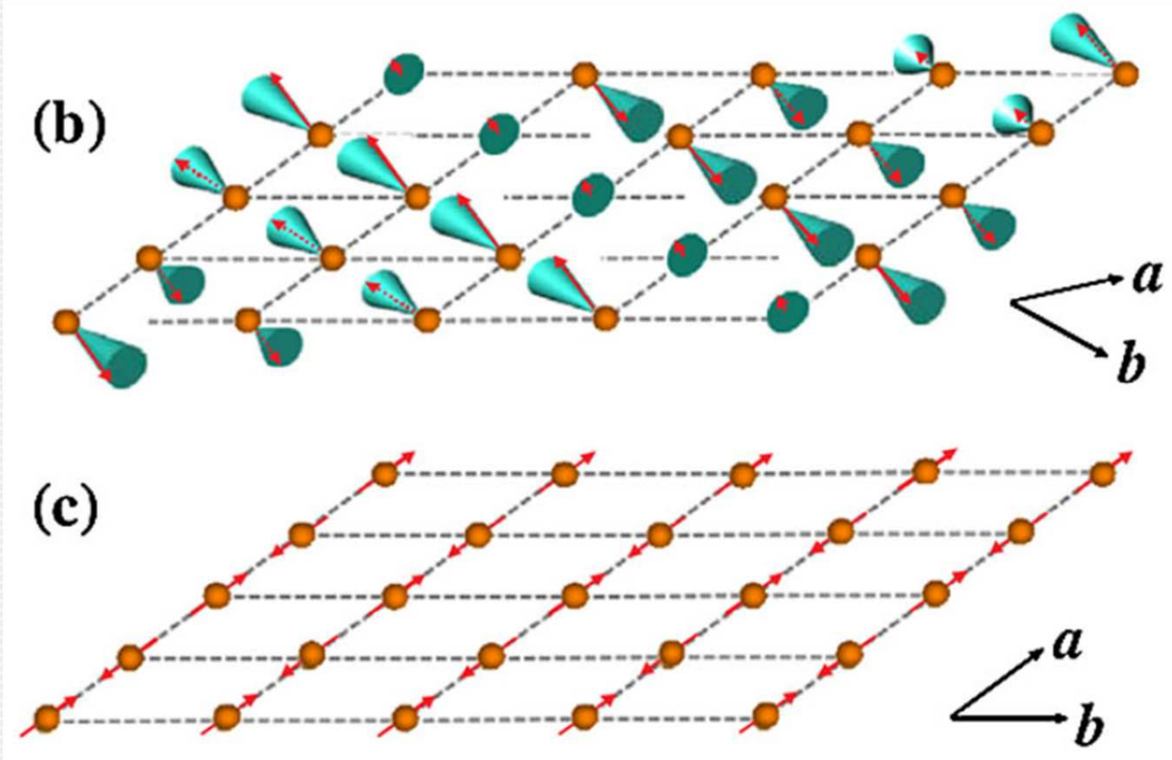
Tunable $(\delta\pi, \delta\pi)$-Type Antiferromagnetic Order in α-Fe(Te,Se) Superconductors

Wei Bao,[1,2,*] Y. Qiu,[3,4] Q. Huang,[3] M. A. Green,[3,4] P. Zajdel,[3,5] M. R. Fitzsimmons,[2] M. Zhernenkov,[2] S. Chang,[3] Minghu Fang,[6,7] B. Qian,[6] E. K. Vehstedt,[6] Jinhu Yang,[7] H. M. Pham,[8] L. Spinu,[8] and Z. Q. Mao[6]

Not $FeTe_{1-x}$ but $Fe_{1+y}Te$

The 11 system:





The 1111 or 122 systems:

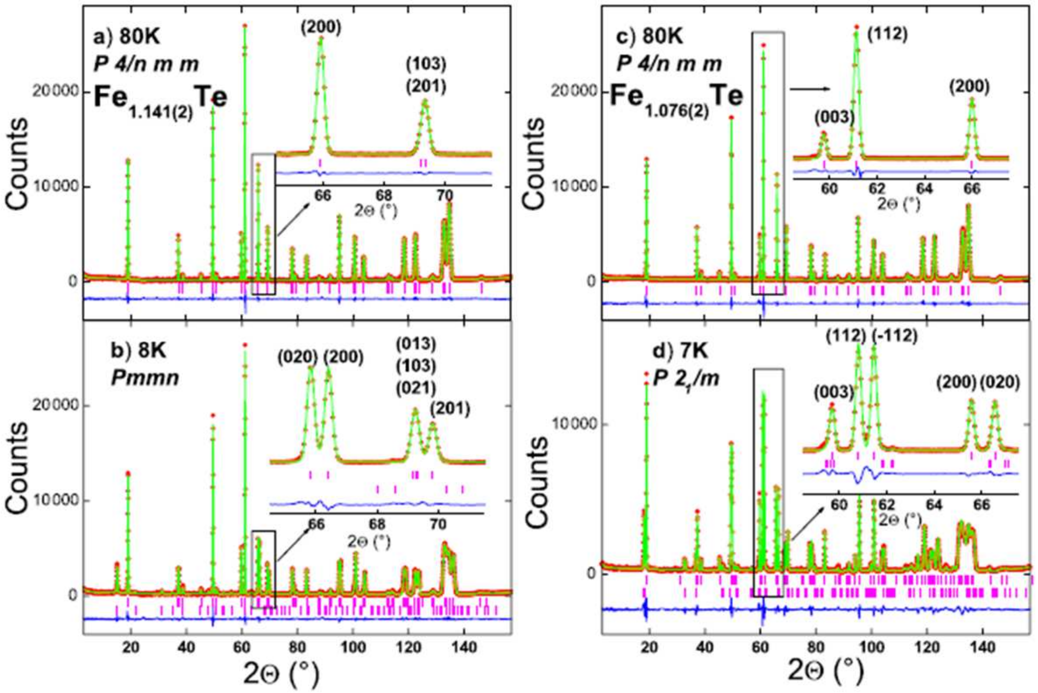
$$\chi(\mathbf{Q},\omega) = \frac{\chi_0(\mathbf{Q},\omega)}{1 - J(\mathbf{Q})\chi_0(\mathbf{Q},\omega)}$$

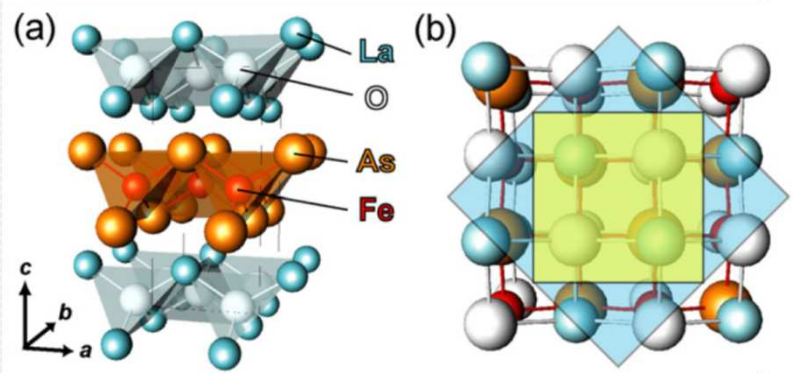
arXiv:0809.2058 (2008)

(Received 29 September 2008; published 17 June 2009)

Orthorhombic distortion of the 11 system differs from that in either 1111 or 122 system

No unit cell doubling in the 11 system





Bao et al., PRL **102**, 247001 (2009)

$Fe_{1+y}Te$: tetragonal at room T

- $y>0.076$
- weak first-order
- Metallic
- Orthorhombic (a>b)
- Q incommensurate

- $y\leq0.076$
- strong first-order
- semiconducting
- Monoclinic (a>b)
- Q commensurate

Empirical rules for relating the sign of magnetic interaction J and lattice distortion

- From experimental results of combined crystalline and magnetic structure study of 1111, 122 and 11 systems
  - Rule 1: Lattice spacing expands: Antiferromagnetic J
  - Rule 2: Lattice spacing contracts: Ferromagnetic J

Structural transition is a manifest of orbital occupation ordering transition

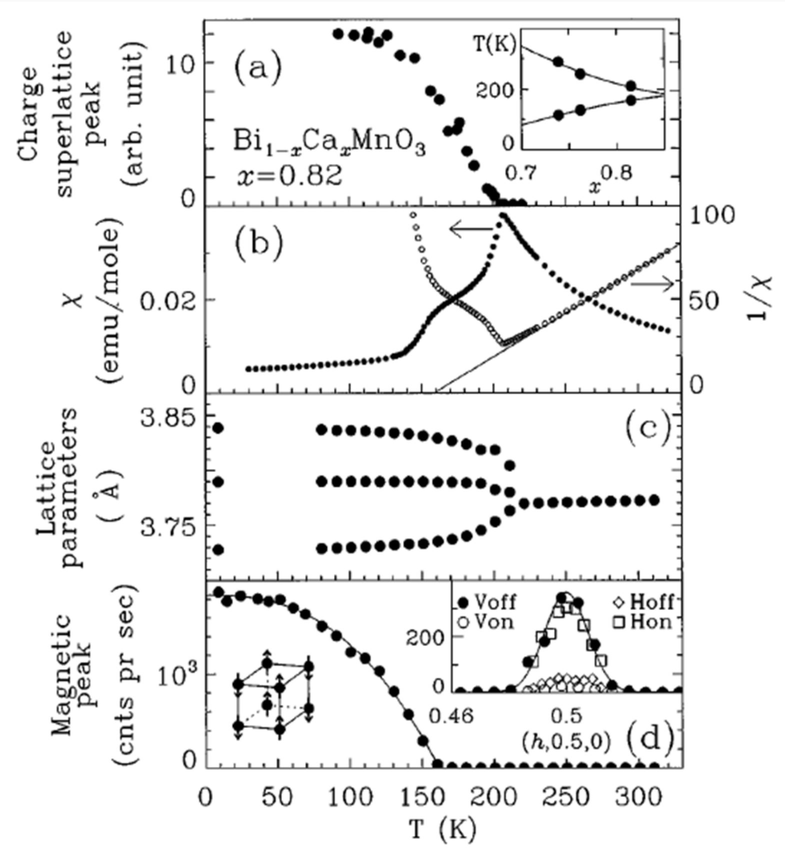
Type I: structure transition followed by mag. transition

Type II: simultaneous 1st order Magnetostructural transition

VOLUME 78, NUMBER 3 PHYSICAL REVIEW LETTERS 20 JANUARY 1997

Impact of Charge Ordering on Magnetic Correlations in Perovskite (Bi, Ca)MnO_3

Wei Bao,[1] J. D. Axe,[1] C. H. Chen,[2] and S-W. Cheong[2]
[1] *Brookhaven National Laboratory, Upton, New York 11973*
[2] *Bell Laboratories, Lucent Technologies, Murray Hill, New Jersey 07974*
(Received 29 May 1996)

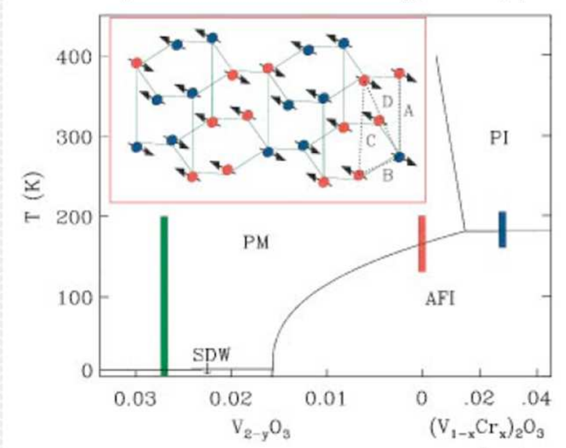


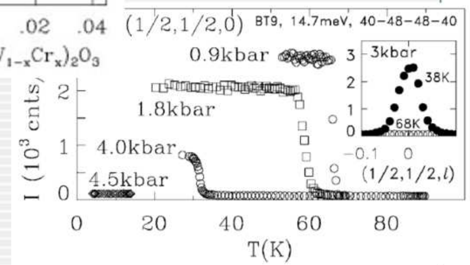
VOLUME 78, NUMBER 3 PHYSICAL REVIEW LETTERS 20 JANURY 1997

Dramatic Switching of Magnetic Exchange in a Classic Transition Metal Oxide: Evidence for Orbital Ordering

Wei Bao,[1,2] C. Broholm,[1,3] G. Aeppli,[4] P. Dai,[5] J. M. Honig,[6] and P. Metcalf[6]
[1] *Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218*
[2] *Physics Department, Brookhaven National Laboratory, Upton, New York 11973*
[3] *National Institute of Standards and Technology, Gaithersburg, Maryland 20899*
[4] *NEC, 4 Independence Way, Princeton, New Jersey 08540*
[5] *Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831*
[6] *Purdue University, West Lafayette, Indiana 47907*
(Received 26 August 1996)

Spin correlations in metallic and insulating phases of V_2O_3 and its derivatives are investigated using





122: Q. Huang et al. PRL **101**, 257003 (2008)

11: W. Bao et al., PRL **102**, 247001 (2008)

1111: de la Cruz et al. Nature (2008)

Physics process of the structural-magnetic transition(s) in the parent compounds

1. Geometry of the Fermi surface leads to an enhanced Lindhard function near (pi,0), but may not divergent
2. Orbital order leads to a set of $\{J_{ij}\}$ which makes $J(\mathbf{Q})\,\chi_0(\mathbf{Q},0) = 1$ at antiferromagnetic vector
3. Meanwhile also reflected by structural distortion
4. When $T_N\{J_{ij}\} > T_s$: first-order magnetostructural transition
5. When $T_N\{J_{ij}\} < T_s$: separated structural and magnetic transitions

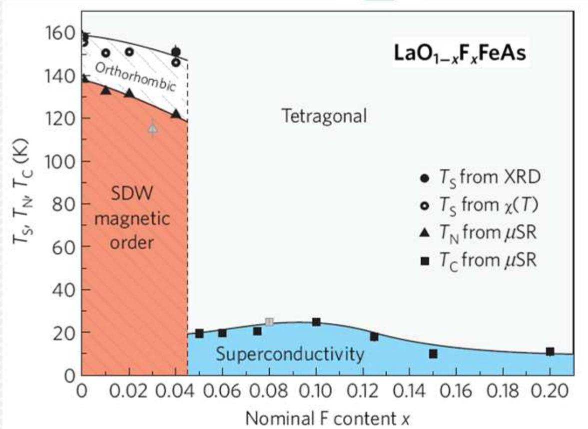
Reviews of orbital physics:

- Imada, Fujimori & Tokura, RMP 1998
- Tokura & Nagaosa, Science 2000

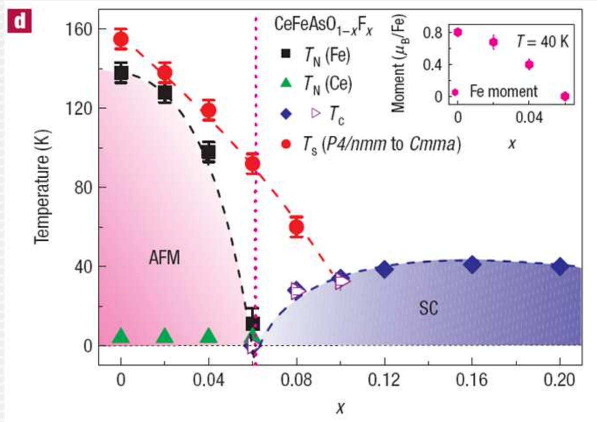
Corroborated by Uchida et al.; Chu et al., arXiv:1002.3364; Tanatar et al., arXiv:1002.3801

Separated Structural and magnetic transition

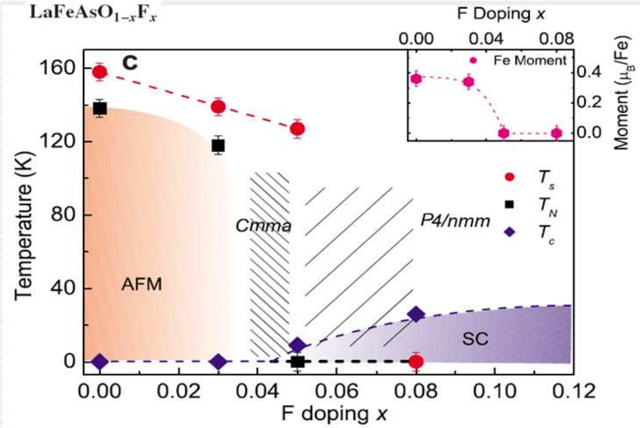
1111 systems



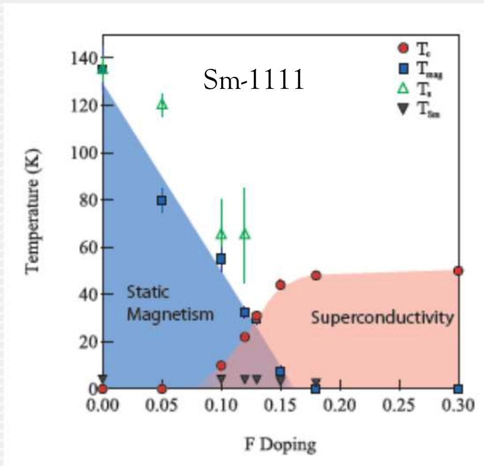
Luetkens et al. Nature Mat. 8, 305 (2009)



Zhao et al. Nature Mat. 7, 953 (2008)



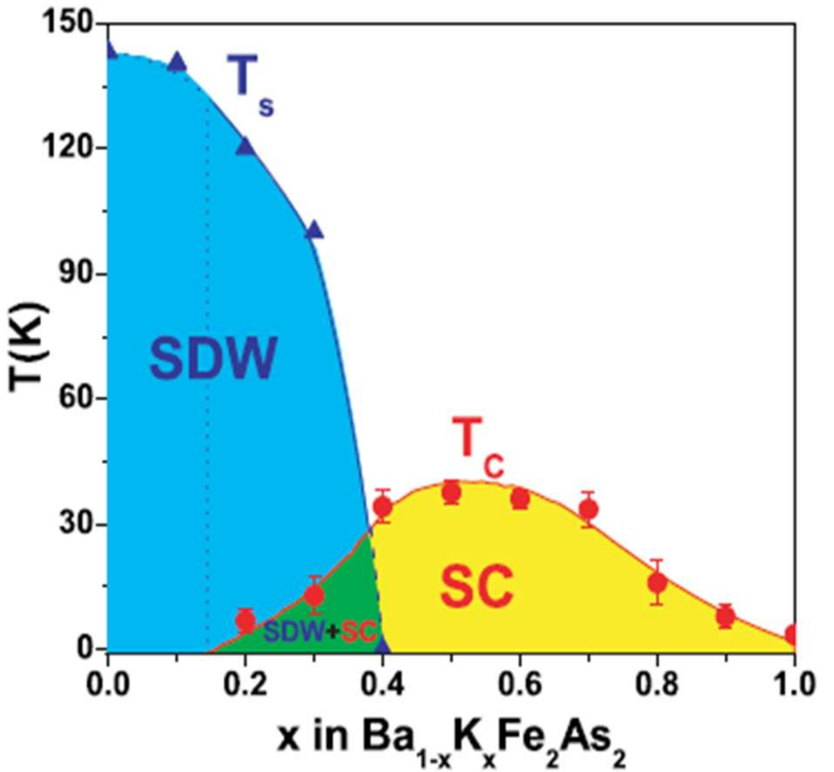
Q. Huang et al., PRB 78, 054529 (2008)



Drew et al., Nature Mat. 8, 310 (2009)

Simultaneous structural and magnetic transition

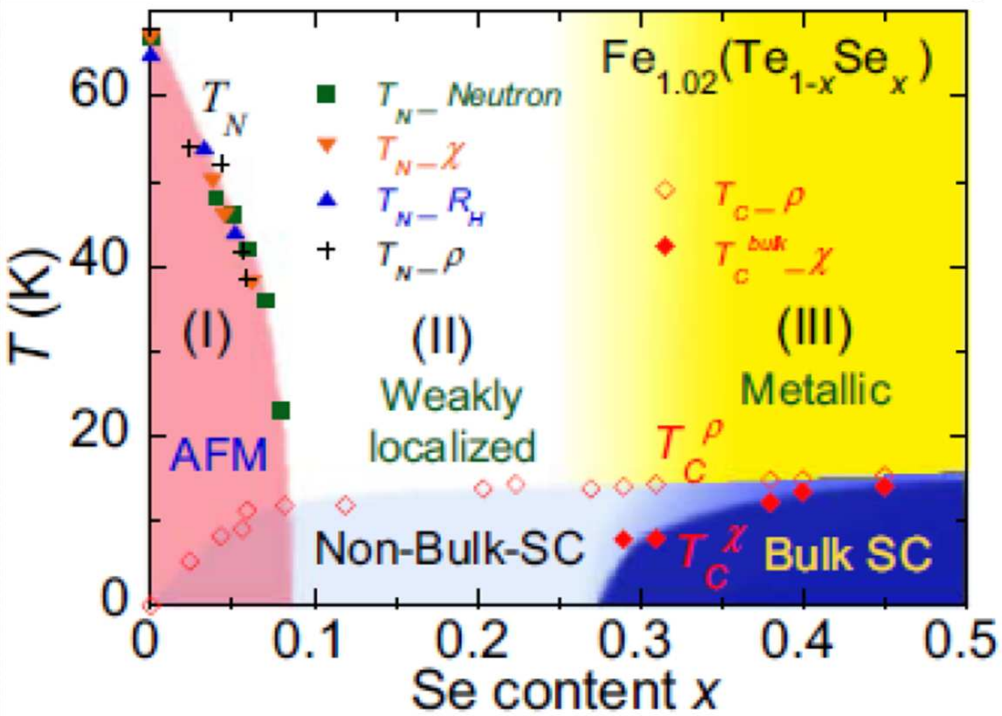
122



H. Chen et al., EPL **85**, 17006 (2009)

The 1st report of coexistence of AF & SC orders in 122 systems: no macroscopic phase separation

11



T.J. Liu et al., Nature Materials **9**, 718 (2010)

The sole phase diagram similar to cuprates

Orbital order

- Magnetic transition and structural transition, whether separated or simultaneous, are naturally accounted for by the occupational order of d-electron orbitals.

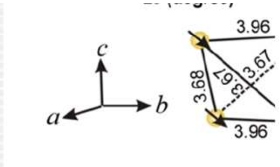
Journal of the Physical Society of Japan
Vol. 77, No. 8, August, 2008, 083704

LETTERS

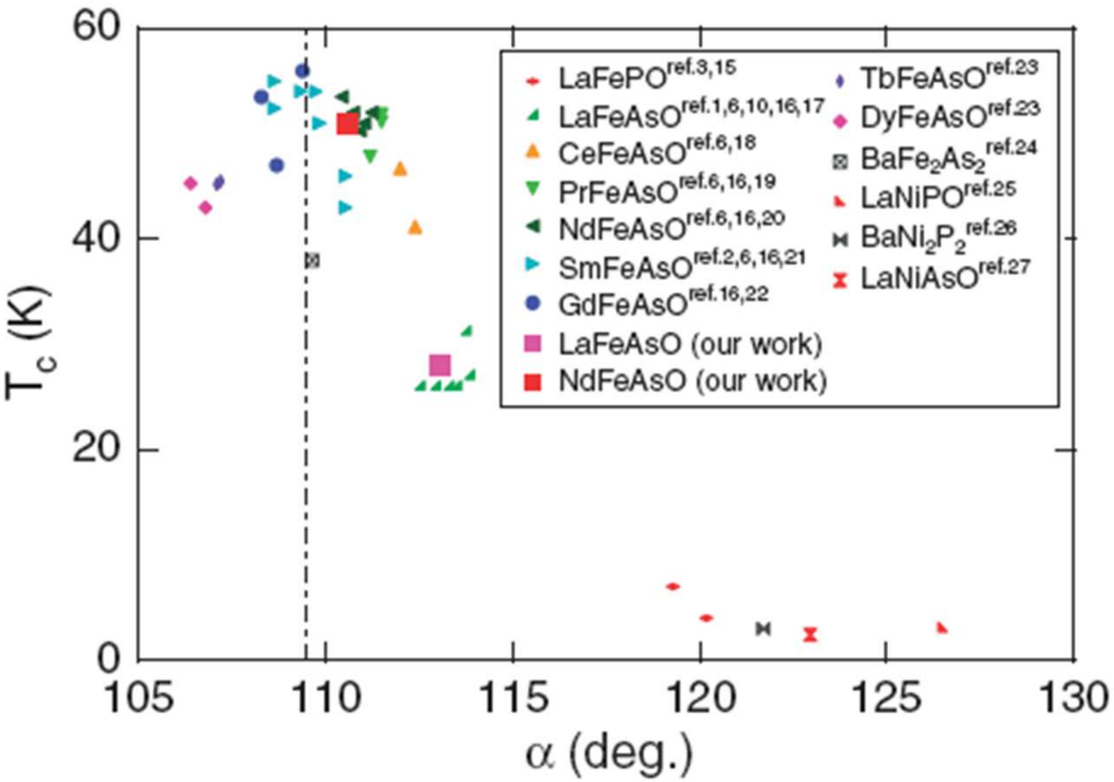
Effect of Structural Parameters on Superconductivity in Fluorine-Free $LnFeAsO_{1-y}$ (Ln = La, Nd)

Chul-Ho LEE, Akira IYO, Hiroshi EISAKI, Hijiri KITO, Maria Teresa FERNANDEZ-DIAZ[1], Toshimitsu ITO, Kunihiro KIHOU, Hirofumi MATSUHATA, Markus BRADEN[2], and Kazuyoshi YAMADA[3]

National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568
[1]Institut Laue-Langevin, BP 156, F-38042 Grenoble Cedex 9, France
[2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany
[3]Institute for Materials Research, Tohoku University, Sendai 980-8577

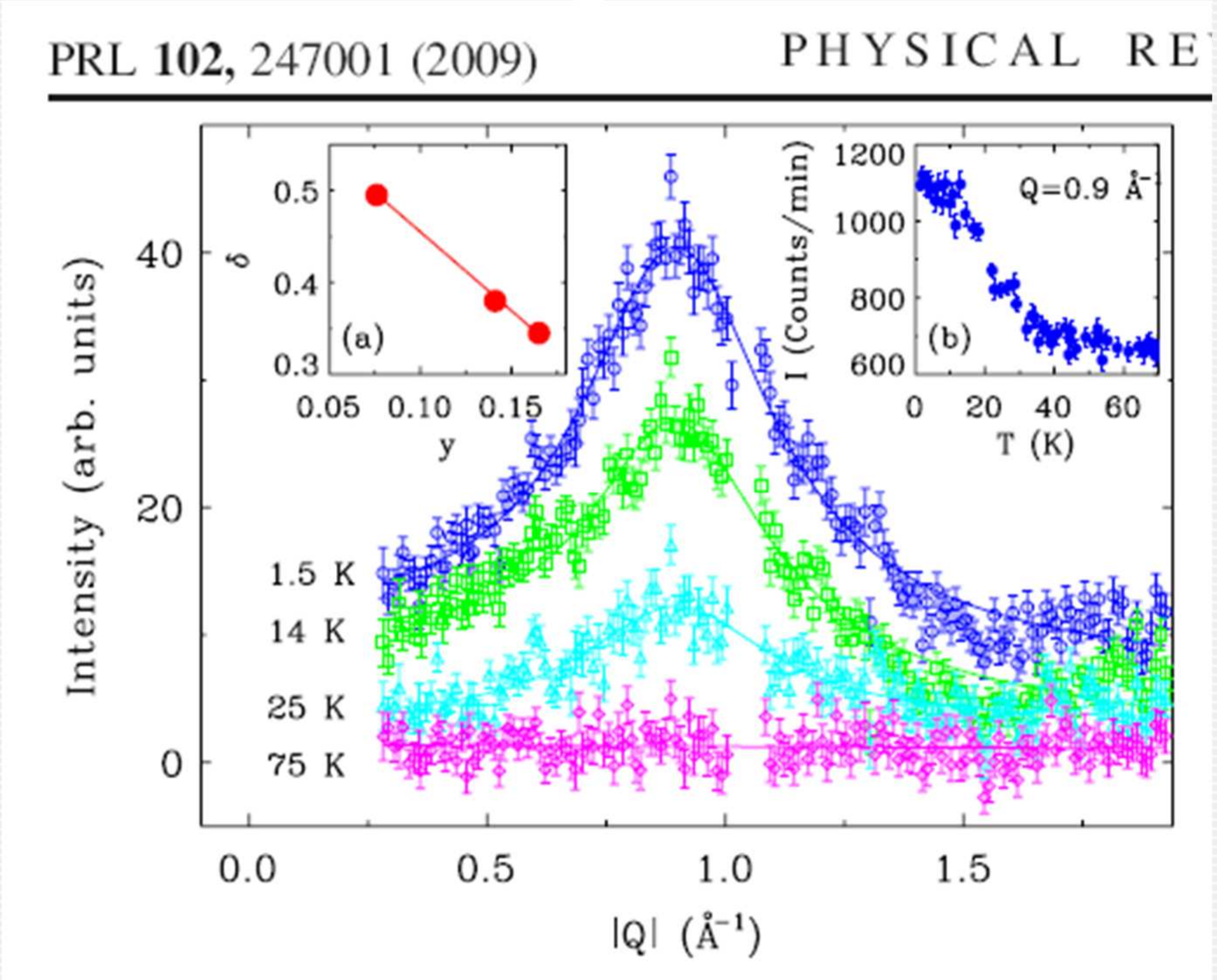


113.99° a ... It seems that the cl ... etrahedral angle arc

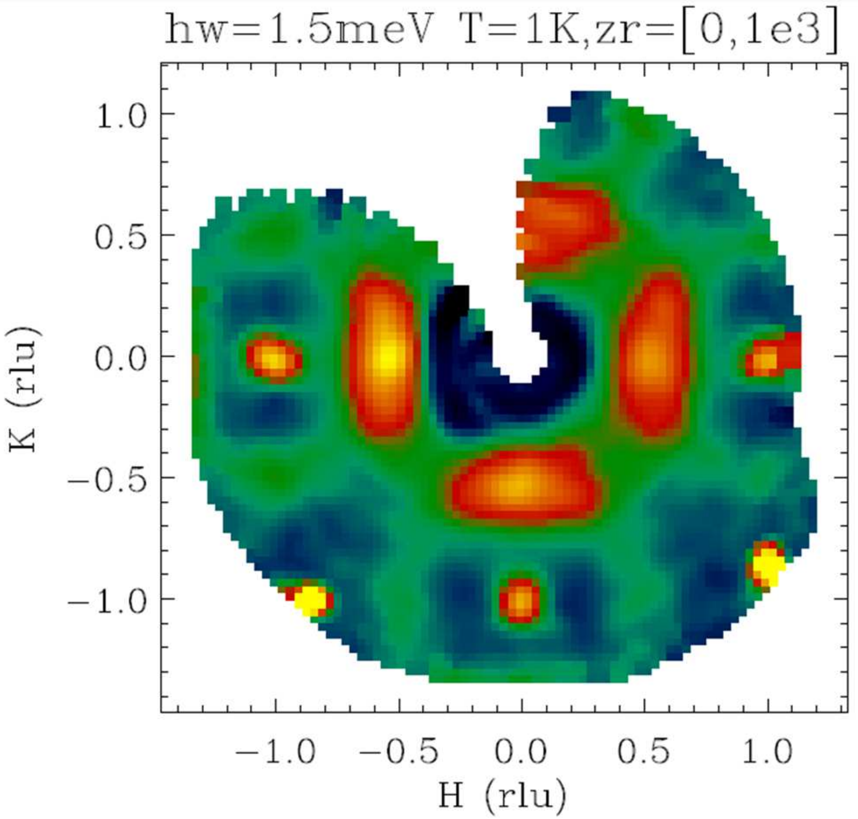


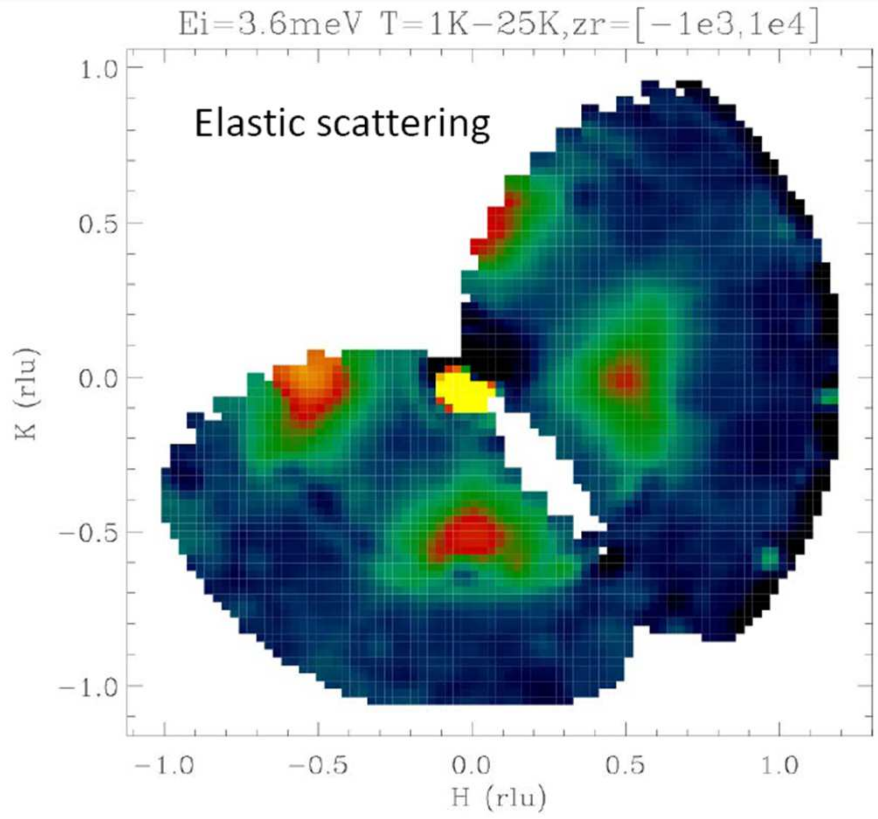
Better illust

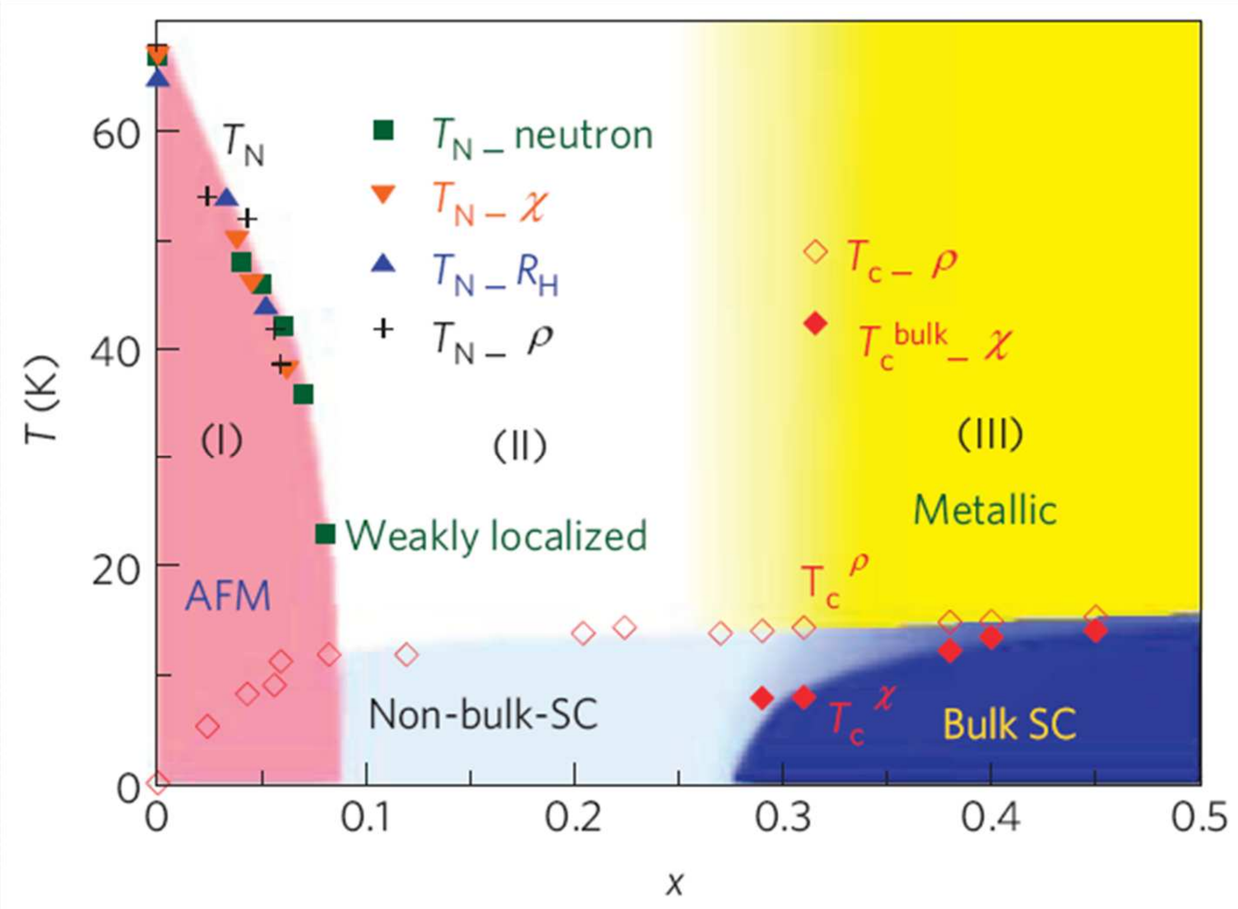
Diffusive (glassy) spin fluctuations



MACS: diffuse magnetic scattering

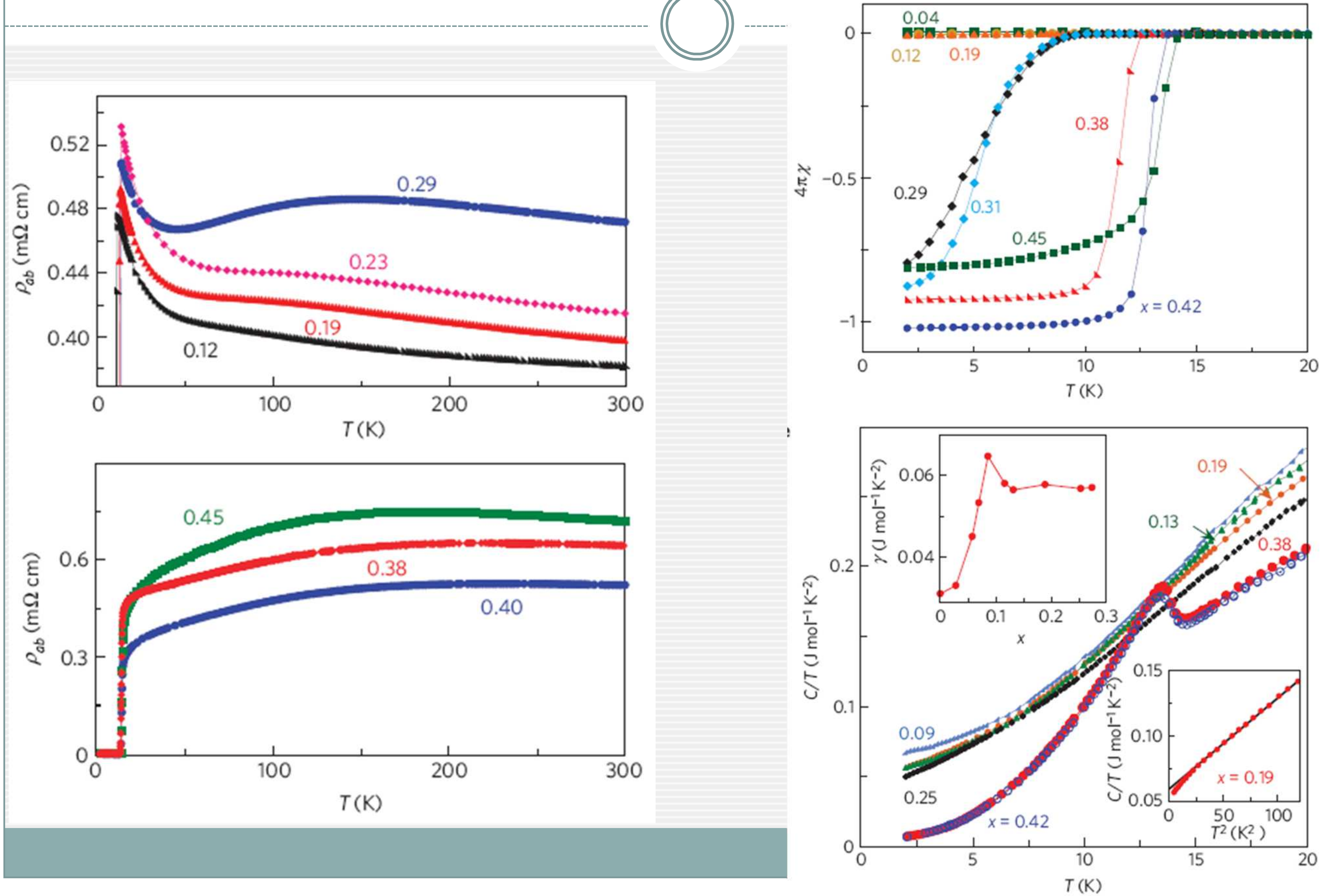






T_N
T_N _ neutron
T_N _ χ
T_N _ R_H
T_N _ ρ
T_c _ ρ
T_c^bulk _ χ
(I)
(II)
(III)
Metallic
Weakly localized
AFM
T_c^ρ
T_c^χ
Non-bulk-SC
Bulk SC
T (K)
x
60
40
20
0
0
0.1
0.2
0.3
0.4
0.5

Weak localization of electrons by diffuse spin fluctuations



RAPID COMMUNICATIONS

PHYSICAL REVIEW B **82**, 180520(R) (2010)

Superconductivity in the iron selenide $K_xFe_2Se_2$ ($0 \le x \le 1.0$)

Jiangang Guo,[1] Shifeng Jin,[1] Gang Wang,[1] Shunchong Wang,[1] Kaixing Zhu,[1] Tingting Zhou,[1] Meng He,[2] and Xiaolong Chen[1]
[1]*Research & Development Center for Functional Crystals, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China*
[2]*National Centre for Nanoscience and Technology, Beijing 100190, China*
(Received 4 October 2010; revised manuscript received 11 November 2010; published 29 November 2010)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **23** (2011) 052203 (4pp) doi:10.1088/0953-8984/23/5/052203

FAST TRACK COMMUNICATION

Synthesis and crystal growth of $Cs_{0.8}(FeSe_{0.98})_2$: a new iron-based superconductor with $T_c = 27$ K

A Krzton-Maziopa[1,5], Z Shermadini[2], E Pomjakushina[1], V Pomjakushin[3], M Bendele[2,4], A Amato[2], R Khasanov[2], H Luetkens[2] and K Conder[1]

[1] Laboratory for Developments and Methods, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **83**, 060512(R) (2011)

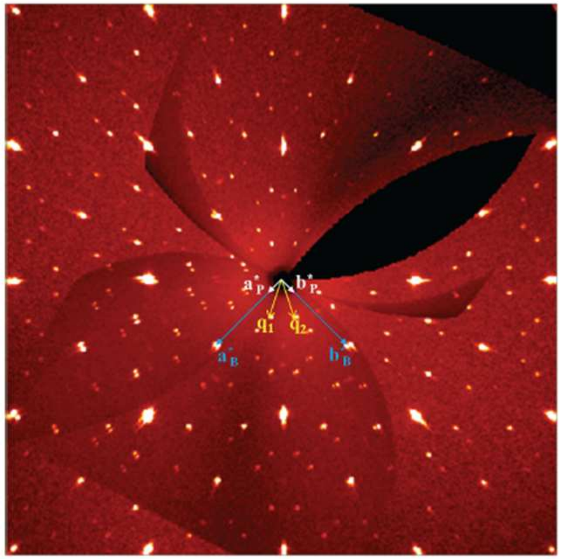
Superconductivity at 32 K in single-crystalline $Rb_xFe_{2-y}Se_2$

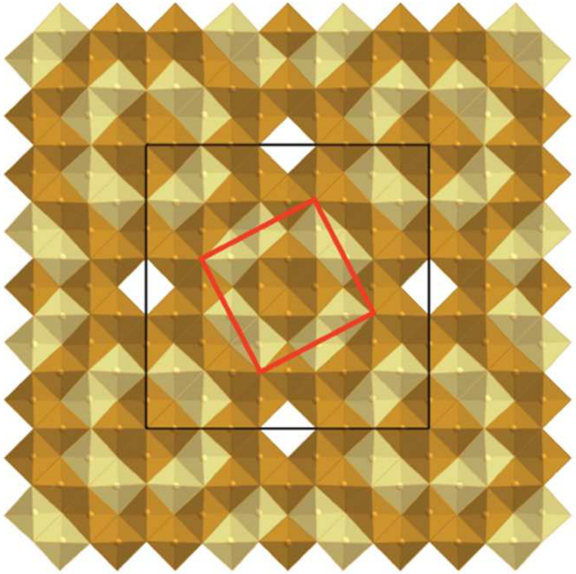
A. F. Wang, J. J. Ying, Y. J. Yan, R. H. Liu, X. G. Luo,* Z. Y. Li, X. F. Wang, M. Zhang, G. J. Ye, P. Cheng, Z. J. Xiang, and X. H. Chen†
Hefei National Laboratory for Physical Science at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China
(Received 26 December 2010; revised manuscript received 29 January 2011; published 28 February 2011)

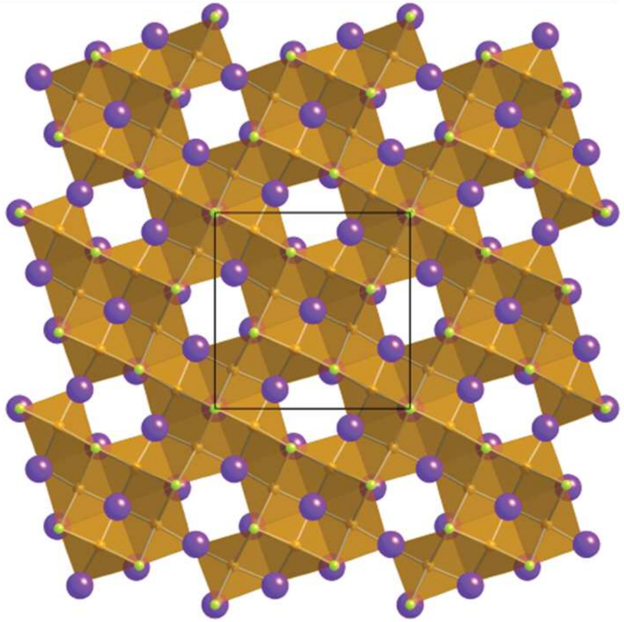
arXiv:1101.4882 PRB Rapid Comm. accepted

On the Structure of Vacancy Ordered Superconducting Alkali Metal Iron Selenide

P. Zavalij[1], Wei Bao[2,*], X. F. Wang[3], J. J. Ying[3], X. H. Chen[3], D. M. Wang[2], J. B. He[2], X. Q. Wang[2], G.F Chen[2], P-Y Hsieh[4], Q. Huang[5] and M. A. Green[4,5,*]





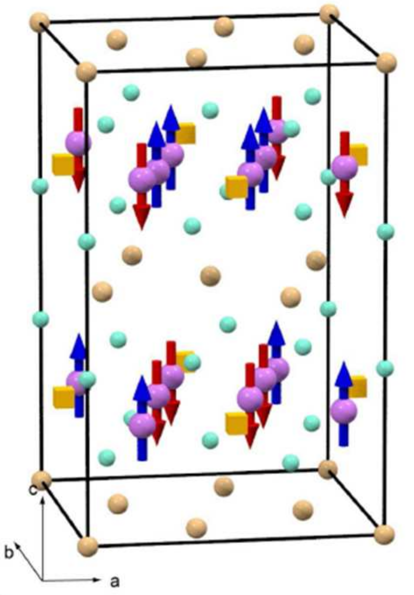


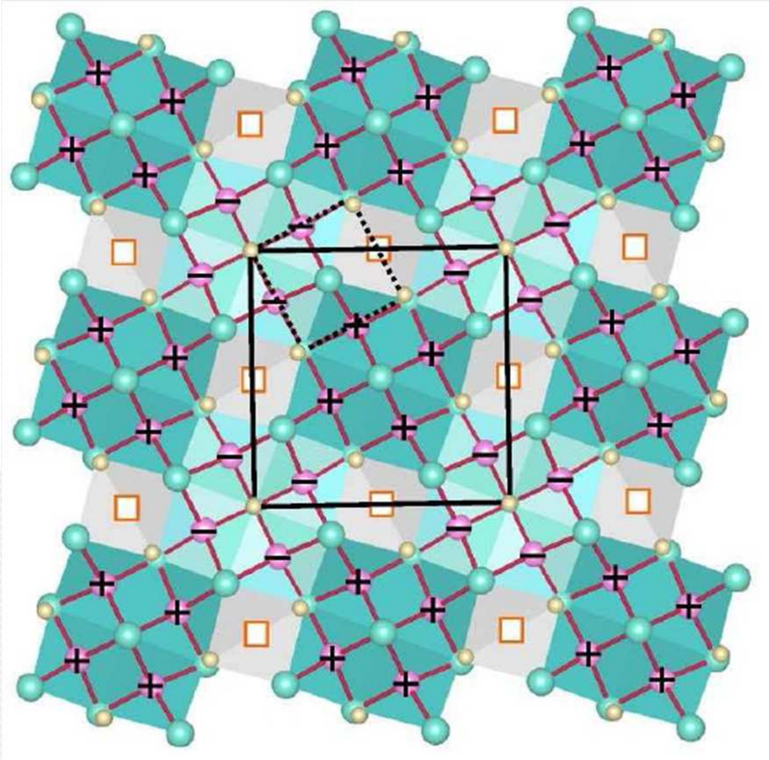
- Chemical composition:
  - close to K0.8Fe1.6Se2,
  - Fe ion 2+
- Unit cell:
  - r5 X r5 X 1,
  - RR or LL interplane stacking

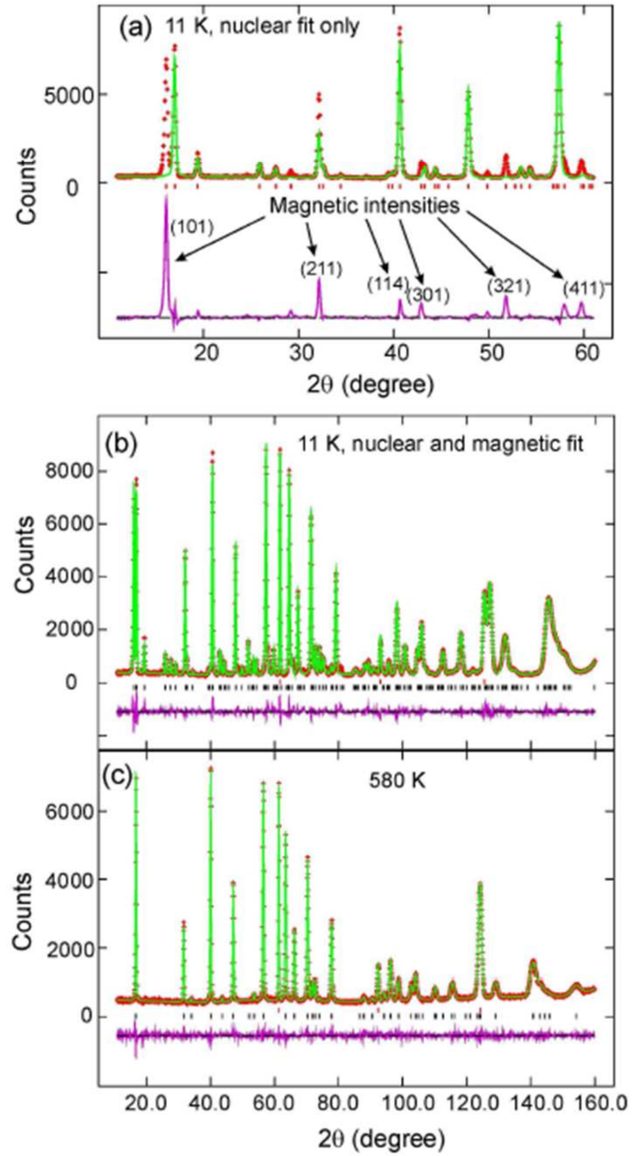
1102.0830

A Novel Large Moment Antiferromagnetic Order in $K_{0.8}Fe_{1.6}Se_2$ Superconductor

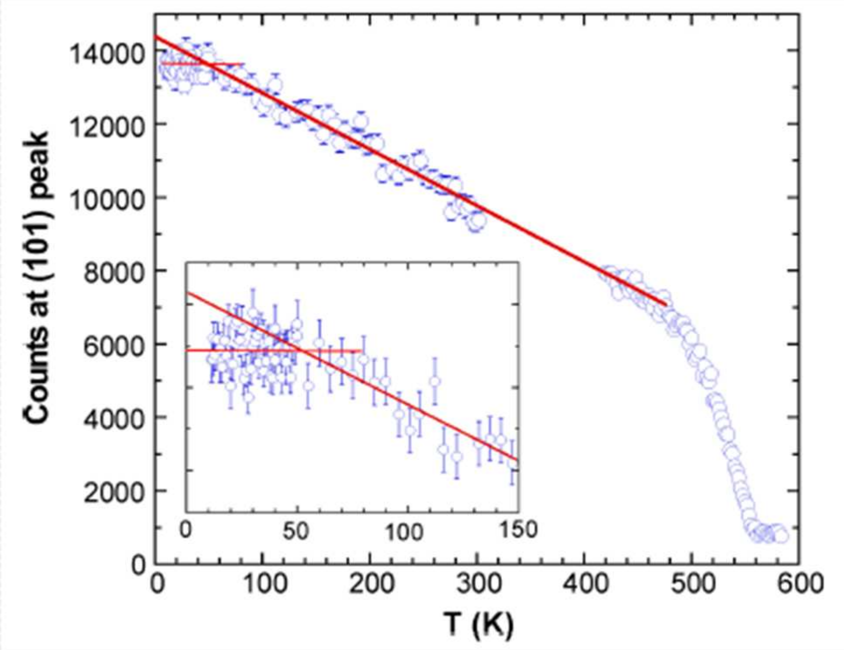
Wei Bao,[1,*] Q. Huang,[2] G. F. Chen,[1] M. A. Green,[2,3] D. M. Wang,[1] J. B. He,[1] X. Q. Wang,[1] and Y. Qiu[2,3]



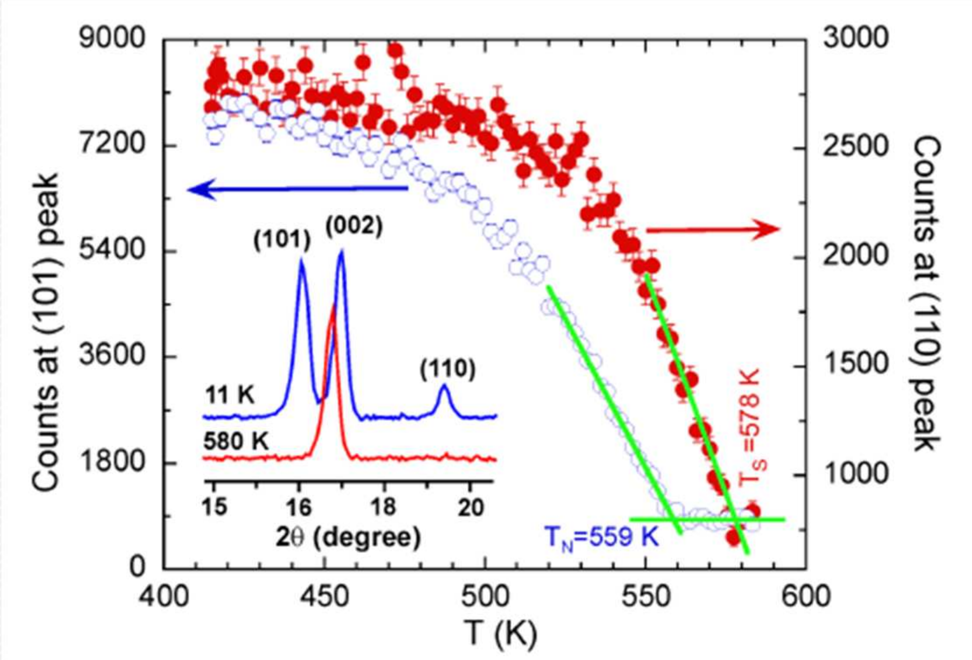




$M=3.3\mu_B/Fe$



Counts at (101) peak
T (K)

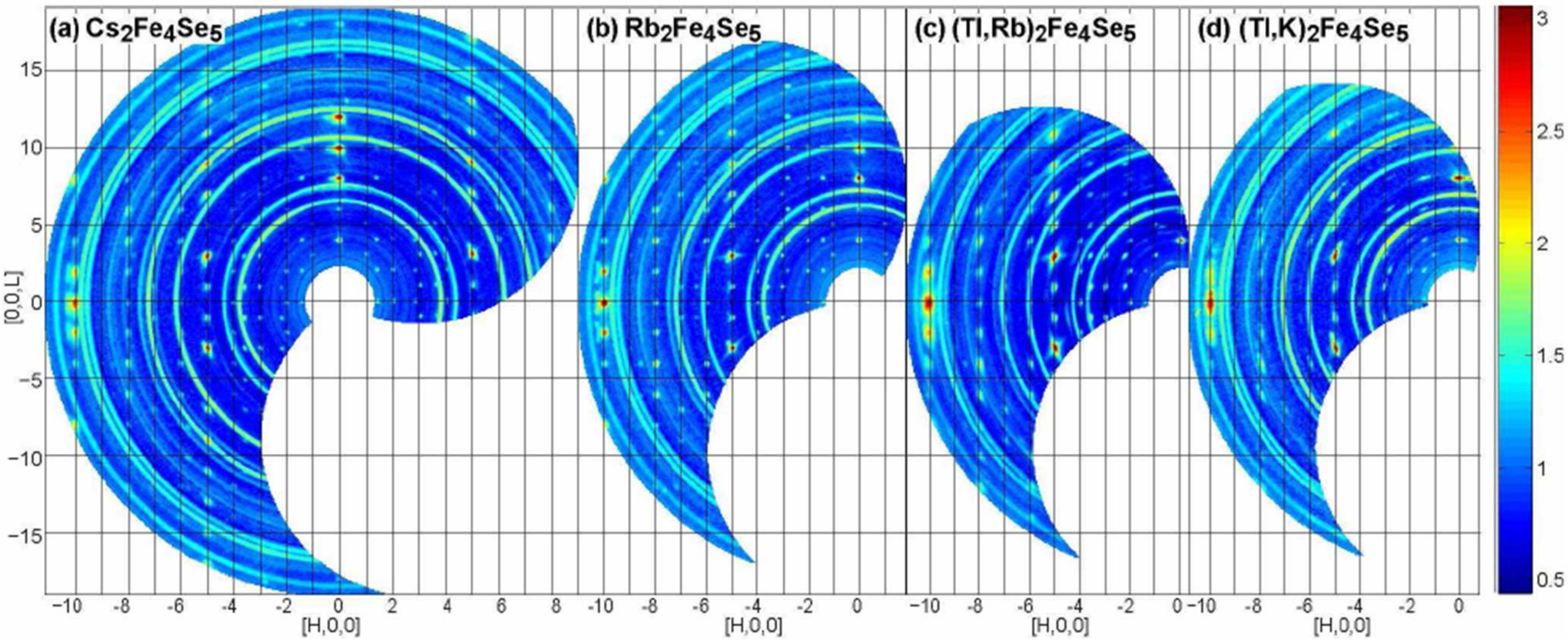


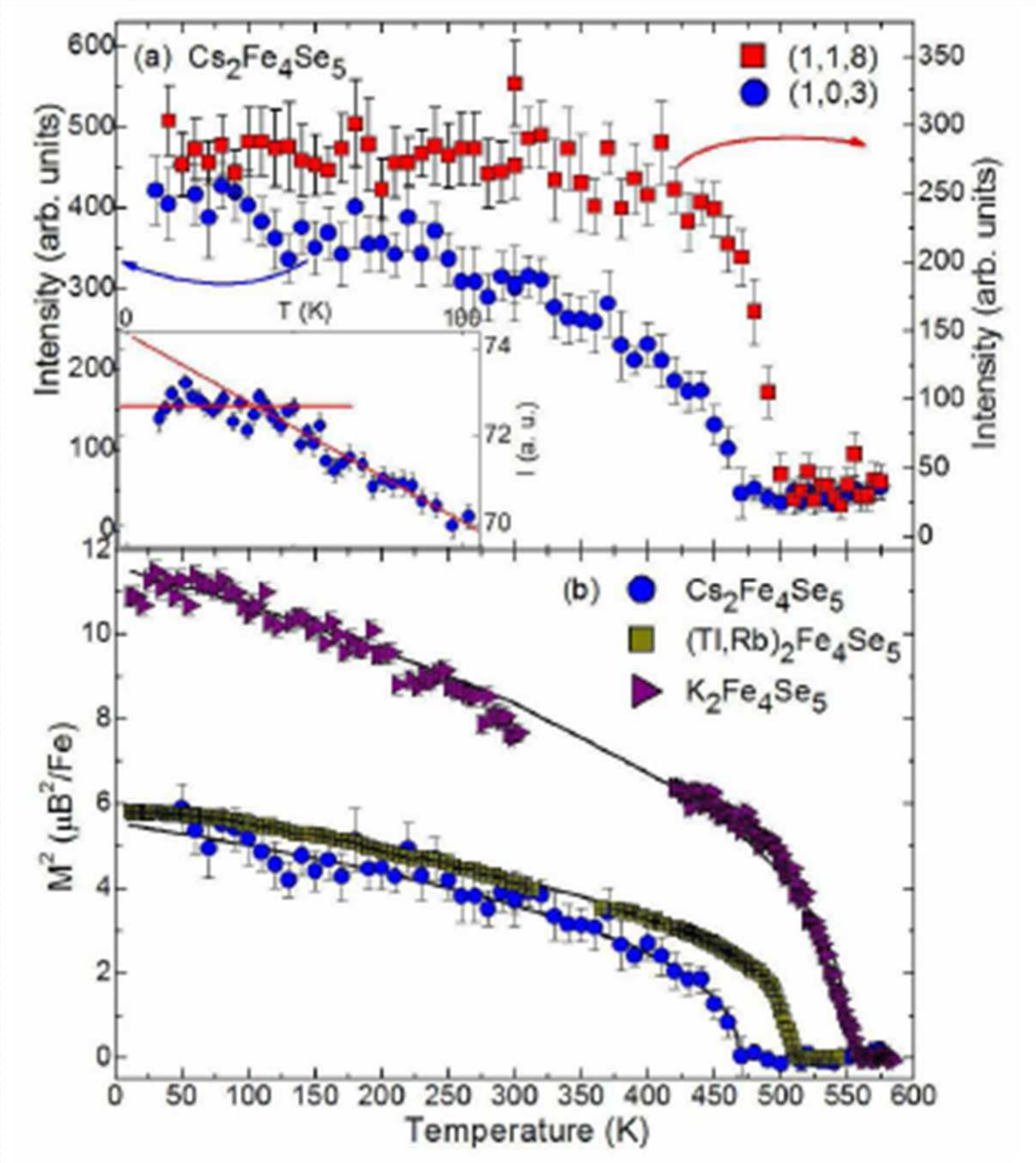
Counts at (101) peak
Counts at (110) peak
T (K)
(101)
(002)
(110)
11 K
580 K
2θ (degree)
T_N=559 K
T_S=578 K

1102.2882

Common Structural and Magnetic Framework in the $A_2Fe_4Se_5$ Superconductors

F. Ye,[1] S. Chi,[1] Wei Bao,[2,*] X. F. Wang,[3] J. J. Ying,[3] X. H. Chen,[3] H. D. Wang,[4] C. H. Dong,[4] and Minghu Fang[4]



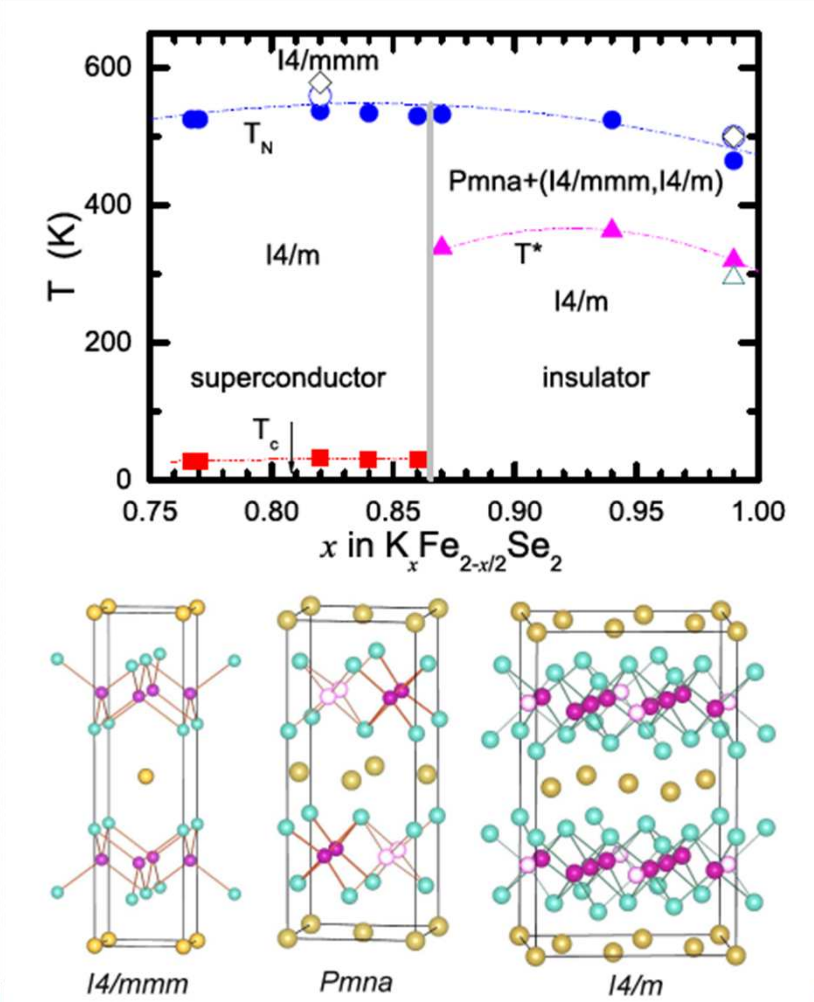


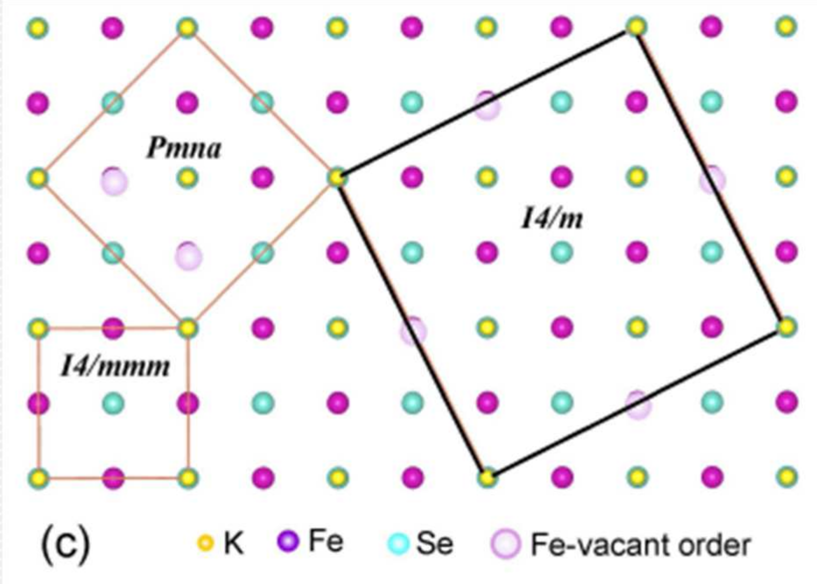
(a) $Cs_2Fe_4Se_5$
(1,1,8)
(1,0,3)
Intensity (arb. units)
T (K)
I (a. u.)
(b)
$Cs_2Fe_4Se_5$
$(Tl,Rb)_2Fe_4Se_5$
$K_2Fe_4Se_5$
M^2 (μB^2/Fe)
Temperature (K)

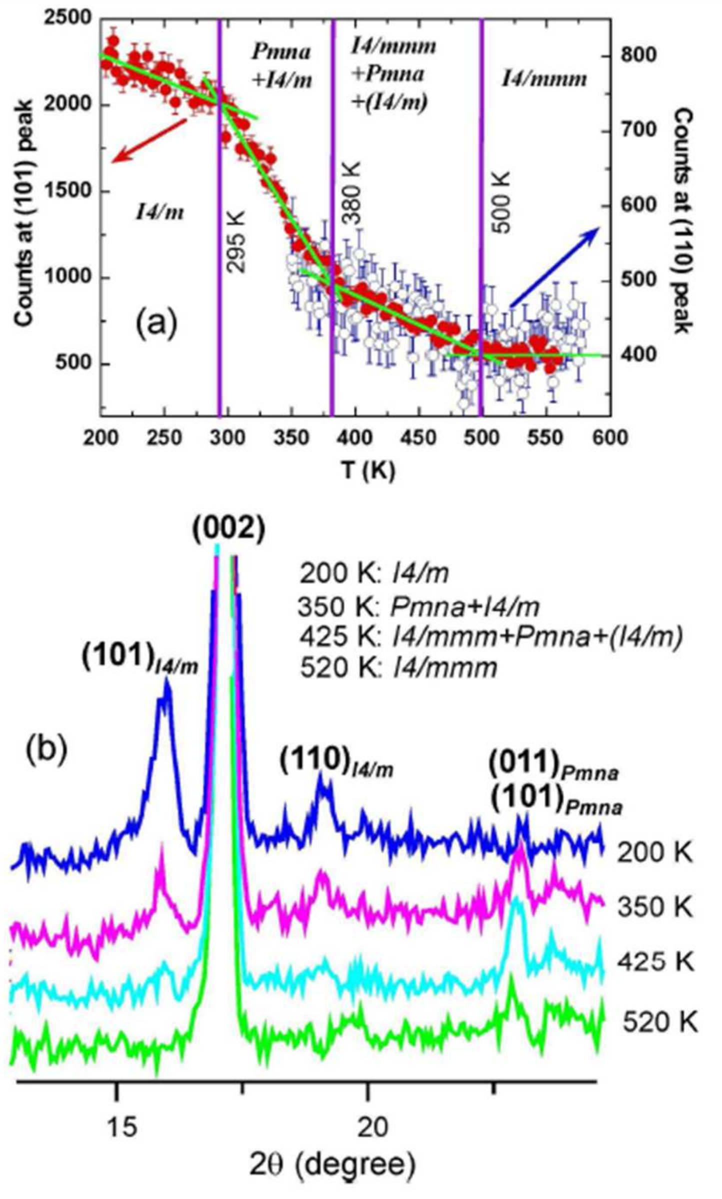
1102.3674

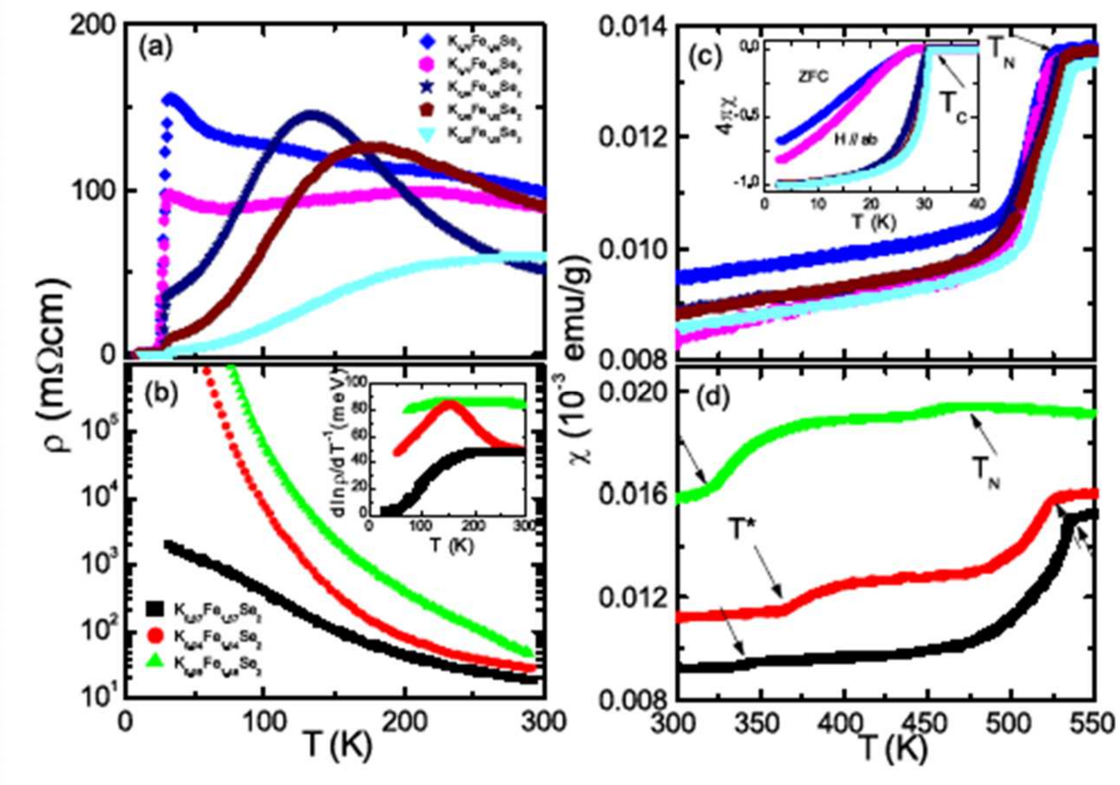
Vacancy tuned magnetic high-T_c superconductor $K_xFe_{2-x/2}Se_2$

Wei Bao,[1,*] G. N. Li,[2,3] Q. Huang,[2] G. F. Chen,[1,†] J. B. He,[1] M. A. Green,[2,4] Y. Qiu,[2,4] D. M. Wang,[1] J. L. Luo,[3] and M. M. Wu[5]





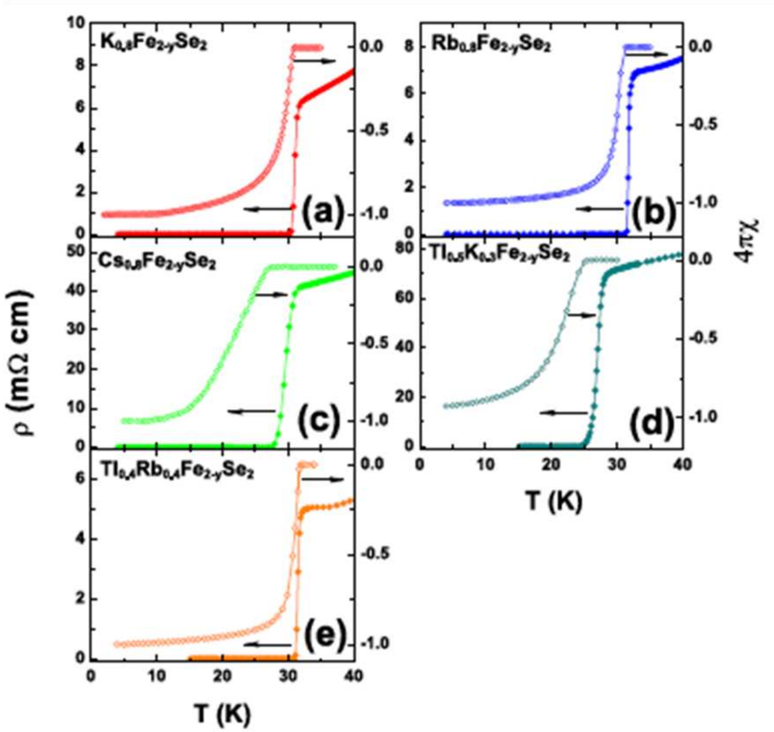

(a)
Counts at (101) peak
Counts at (110) peak
T (K)
I4/m
Pmna
+I4/m
I4/mmm
+Pmna
+(I4/m)
I4/mmm
295 K
380 K
500 K
(b)
(002)
(101)$_{I4/m}$
(110)$_{I4/m}$
(011)$_{Pmna}$
(101)$_{Pmna}$
200 K: I4/m
350 K: Pmna+I4/m
425 K: I4/mmm+Pmna+(I4/m)
520 K: I4/mmm
200 K
350 K
425 K
520 K
2θ (degree)

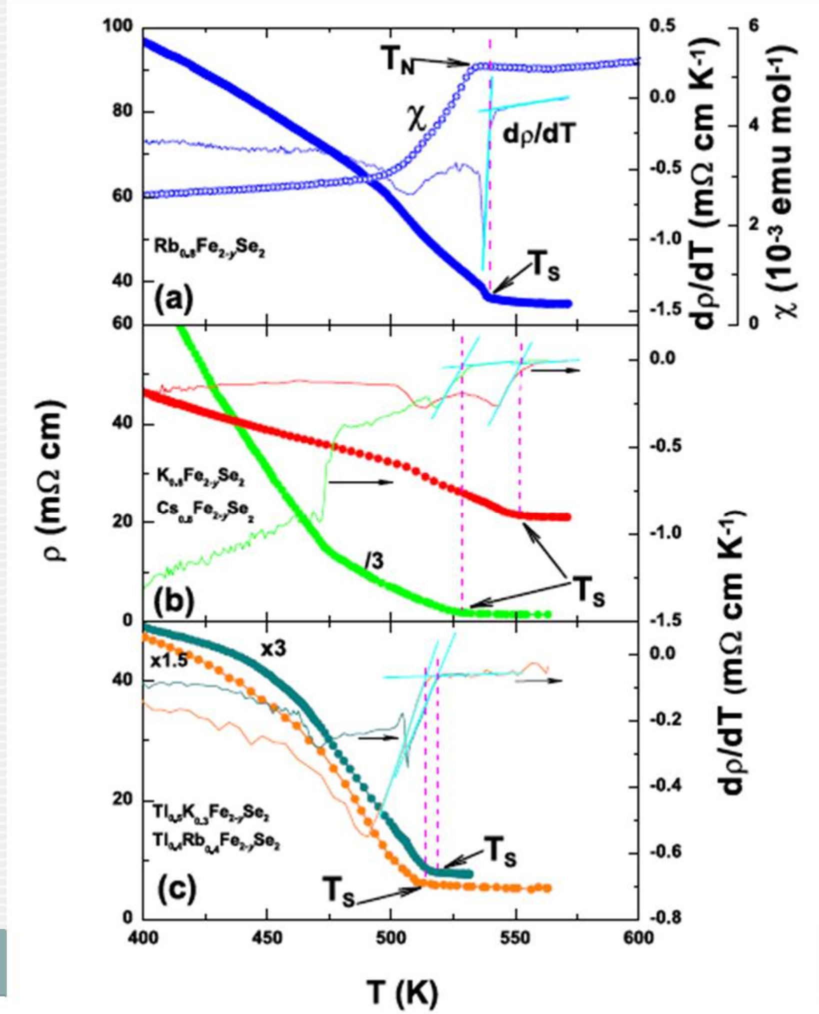

(a)
(b)
ρ (mΩcm)
T (K)
d ln ρ/dT^{-1} (meV)
(c)
ZFC
H // ab
4πχ
T$_N$
T$_C$
(d)
T*
T$_N$
χ (10^{-3} emu/g)
T (K)

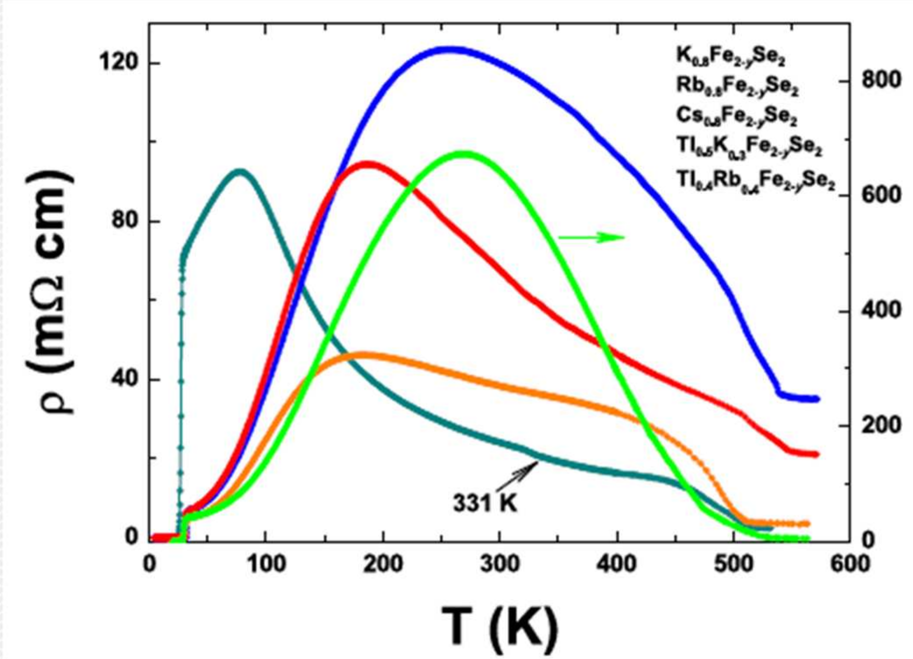
1102.2783

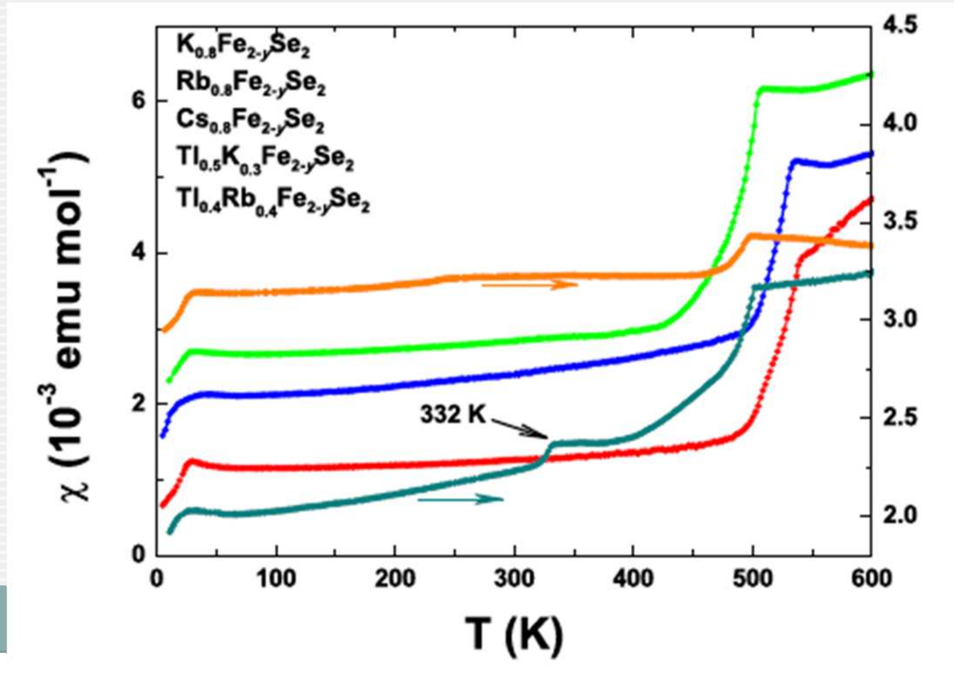
Coexistence of superconductivity and antiferromagnetism in single crystals $A_{0.8}Fe_{2-y}Se_2$ (A= K, Rb, Cs, Tl/K and Tl/Rb): evidence from magnetization and resistivity

R. H. Liu, X. G. Luo, M. Zhang, A. F. Wang, J. J. Ying, X. F. Wang, Y. J. Yan, Z. J. Xiang, P. Cheng, G. J. Ye, Z. Y. Li and X. H. Chen*





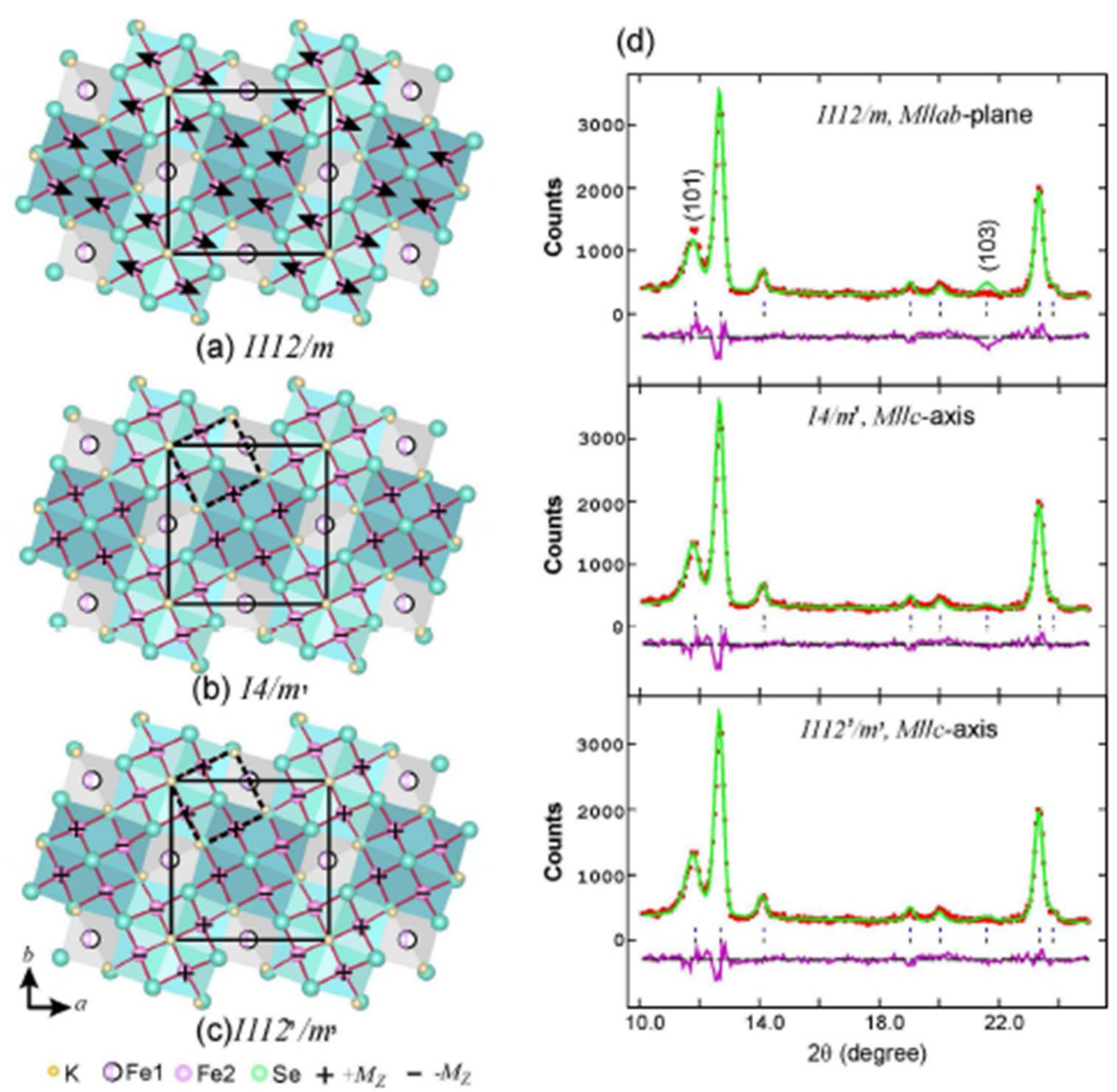

K0.8Fe2-ySe2
Rb0.8Fe2-ySe2
Cs0.8Fe2-ySe2
Tl0.5K0.3Fe2-ySe2
Tl0.4Rb0.4Fe2-ySe2
ρ (mΩ cm)
T (K)
331 K
0
40
80
120
0
100
200
300
400
500
600
0
200
400
600
800


K0.8Fe2-ySe2
Rb0.8Fe2-ySe2
Cs0.8Fe2-ySe2
Tl0.5K0.3Fe2-ySe2
Tl0.4Rb0.4Fe2-ySe2
χ (10^-3 emu mol^-1)
T (K)
332 K
0
2
4
6
0
100
200
300
400
500
600
2.0
2.5
3.0
3.5
4.0
4.5

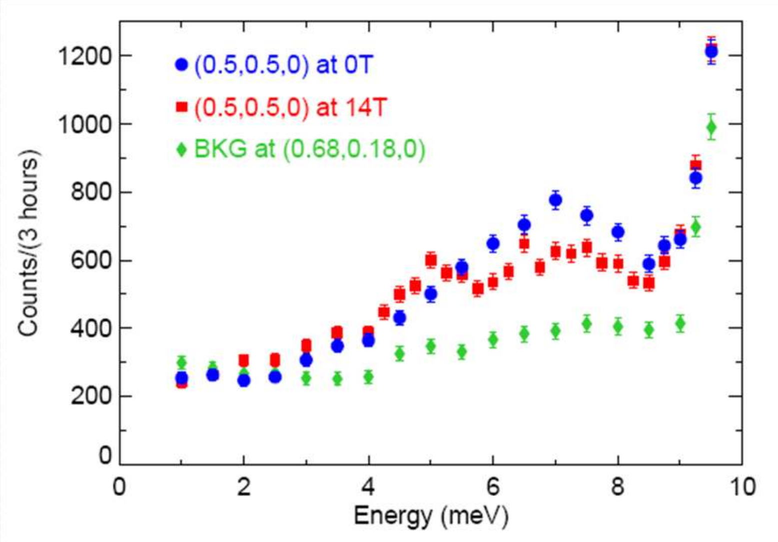
Summary

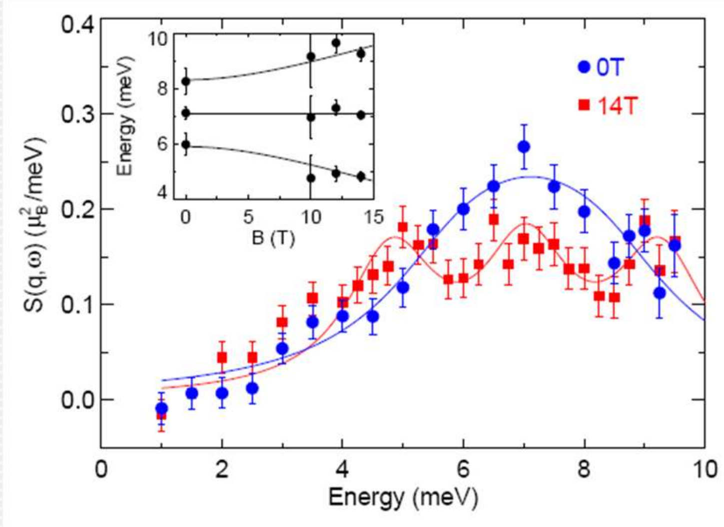
- There exists close relation between magnetic structure and crystalline distortion in the 11, 122 and 1111 systems
- Orbital ordering (structure transition) generates a set of J's, which lead to a J(**Q**), which competes with bare $\chi_0(\mathbf{Q},\omega)$ to determine the antiferromagnetic order in Fe pnictide/chalcogenides.
- Magnetic resonance of $Fe(Se_{0.4}Te_{0.6})$ at E_0/k_BT_c=5.3, below the charge gap $2\Delta/k_BT_c$=7.
- Support the sign change of superconducting order parameter. Support for the $s^{+/-}$ symmetry, in combination with other data.

- Long-range magnetic order can coexists with superconductivity
- Normal state magnetic excitations: itinerant inclined concentrated continuum.
- Diffuse low energy magnetic fluctuations break electronic coherence and destroy superconductivity
- Higher Tc for samples with more perfect FeAs/Se tetrahedron
- Empty site decorated Fe square lattice offers a new route for discovery


(a) I112/m
(b) I4/m'
(c) I112'/m'
K Fe1 Fe2 Se + +M_Z − -M_Z
b
a
(d)
I112/m, M//ab-plane
I4/m', M//c-axis
I112'/m', M//c-axis
(101)
(103)
Counts
2θ (degree)

the resonance in high magnetic field





□Need higher magnetic field at neutron scattering facilities

HZB data 07.2009; arXiv:1002.1617

PRL 101, 257003 (2008) PHYSICAL REVIEW LETTERS week ending 19 DECEMBER 2008

Neutron-Diffraction Measurements of Magnetic Order and a Structural Transition in the Parent $BaFe_2As_2$ Compound of FeAs-Based High-Temperature Superconductors

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

The concurring first-order structural and magnetic transition indicates strong coupling between the structural and magnetic order parameters. A similar previous experimental observation has led to the identification of an orbital ordering among degenerate *d* orbitals as the driving force of a first-order structural transition in the vicinity of a SDW transition [33]. There are degenerate Fermi sheets from the Fe *d* orbitals for the FeAs-based materials in the tetragonal phase [28–30]. The structural transition could in principle break the degeneracy and involve the orbital degree of freedom in the combined magnetic and structural transition.

The 1st experimental suggestion of the orbital ordering

PRL 101, 257003 (2008) PHYSICAL REVIEW LETTERS week ending 19 DECEMBER 2008

Neutron-Diffraction Measurements of Magnetic Order and a Structural Transition in the Parent $BaFe_2As_2$ Compound of FeAs-Based High-Temperature Superconductors

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

(Received 14 July 2008; published 17 December 2008)

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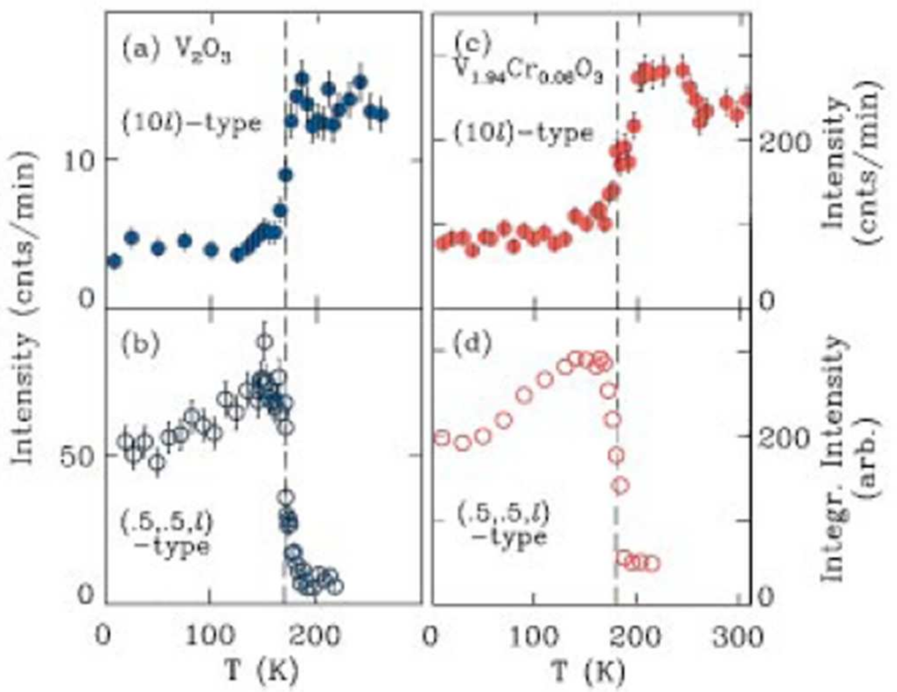
SDW transition [33]. There are degener
from the Fe *d* orbitals for the FeAs-base
tetragonal phase [28–30]. The structural t
principle break the degeneracy and in
degree of freedom in the combined magn
transition.



VOLUME 78, NUMBER 3 PHYSICAL REVIEW LETTERS 20 JANUARY 1997

Dramatic Switching of Magnetic Exchange in a Classic Transition Metal Oxide: Evidence for Orbital Ordering

Wei Bao,[1,2] C. Broholm,[1,3] G. Aeppli,[4] P. Dai,[5] J. M. Honig,[6] and P. Metcalf[6]

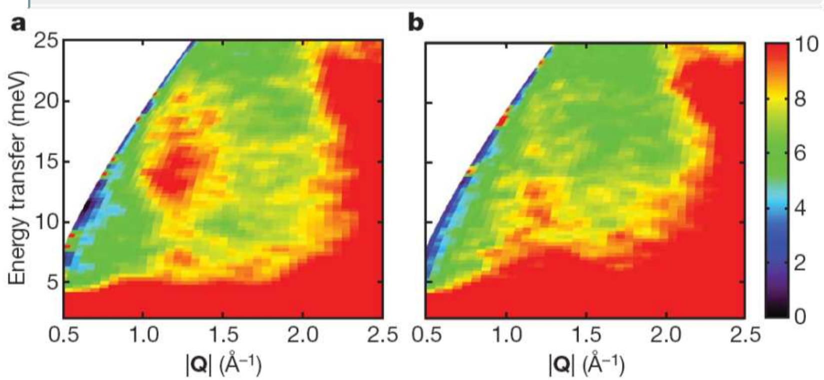
Resonance peak in 122 superconductors

Polycrystalline sample

nature Vol 456|18/25 December 2008|doi:10.1038/nature07625

Unconventional superconductivity in $Ba_{0.6}K_{0.4}Fe_2As_2$ from inelastic neutron scattering

A. D. Christianson[1], E. A. Goremychkin[2,3], R. Osborn[2], S. Rosenkranz[2], M. D. Lumsden[1], C. D. Malliakas[2,4], I. S. Todorov[2], H. Claus[2], D. Y. Chung[2], M. G. Kanatzidis[2,4], R. I. Bewley[3] & T. Guidi[3]

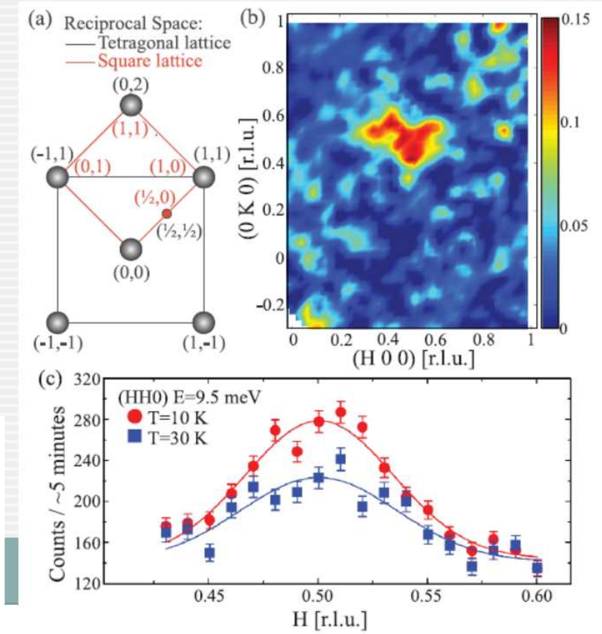


Single crystalline sample

PRL 102, 107005 (2009) PHYSICAL REVIEW LETTERS week ending 13 MARCH 2009

Two-dimensional resonant magnetic excitation in $BaFe_{1.84}Co_{0.16}As_2$

M. D. Lumsden,[1] A. D. Christianson,[1] D. Parshall,[2] M. B. Stone,[1] S. E. Nagler,[1] G. J. MacDougall,[1] H. A. Mook,[1] K. Lokshin,[3] T. Egami,[1,2,3] D. L. Abernathy,[1] E. A. Goremychkin,[4,5] R. Osborn,[4] M. A. McGuire,[1] A. S. Sefat,[1] R. Jin,[1] B. C. Sales,[1] and D. Mandrus[1]



PRL 102, 107006 (2009) PHYSICAL REVIEW LETTERS week ending 13 MARCH 2009

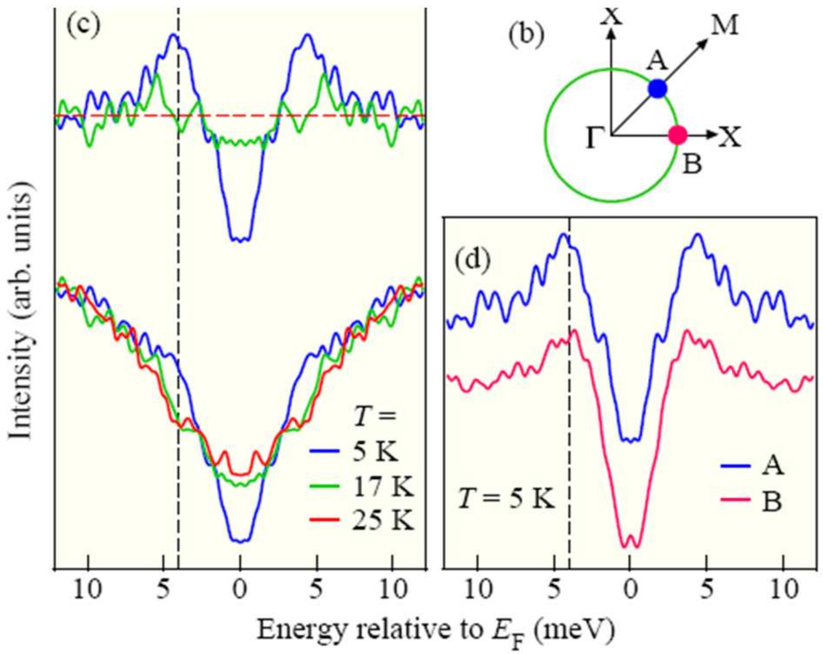
Inelastic Neutron-Scattering Measurements of a Three-Dimensional Spin Resonance in the FeAs-Based $BaFe_{1.9}Ni_{0.1}As_2$ Superconductor

Songxue Chi,[1] Astrid Schneidewind,[2] Jun Zhao,[1] Leland W. Harriger,[1] Linjun Li,[3] Yongkang Luo,[3] Guanghan Cao,[3] Zhu'an Xu,[3] Micheal Loewenhaupt,[2] Jiangping Hu,[4] and Pengcheng Dai[1,5,*]

Angle-Resolved Photoemission Spectroscopy of Iron-Chalcogenide Superconductor $Fe_{1.03}Te_{0.7}Se_{0.3}$: Strong-Coupling Superconductivity and Universality of Inter-Band Scattering

K. Nakayama,[1] T. Sato,[1,2] P. Richard,[3] T. Kawahara,[1] Y. Sekiba,[1] T. Qian,[1]
G. F. Chen,[4] J. L. Luo,[4] N. L. Wang,[4] H. Ding,[4] and T. Takahashi[1,3]
[1] *Department of Physics, Tohoku University, Sendai 980-8578, Japan*
[2] *TRiP, Japan Science and Technology Agency (JST), Kawaguchi 332-0012, Japan*
[3] *WPI Research Center, Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan and*
[4] *Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
(Dated: July 4, 2009)

We have performed high-resolution angle-resolved photoemission spectroscopy of iron-chalcogenide superconductor $Fe_{1.03}Te_{0.7}Se_{0.3}$ (T_c = 13 K) to investigate the electronic structure relevant to superconductivity. We observed a hole- and an electron-like Fermi surfaces at the Brillouin zone center and corner, respectively, which are nearly nested by the $Q\sim(\pi, \pi)$ wave vector. We do not find evidence for the nesting instability with $Q\sim(\pi+\delta, 0)$ reminiscent of the antiferromagnetic order in the parent compound $Fe_{1+y}Te$. We have observed an isotropic superconducting gap along the hole-like Fermi surface with the gap size Δ of $\sim$4 meV ($2\Delta/k_BT_c\sim7$), demonstrating the strong-coupling nature of the superconductivity. The observed similarity of low-energy electronic excitations between iron-chalcogenide and iron-arsenide superconductors strongly suggests that common interactions which involve $Q\sim(\pi, \pi)$ scattering are responsible for the superconducting pairing.



arXiv: 0907.0763

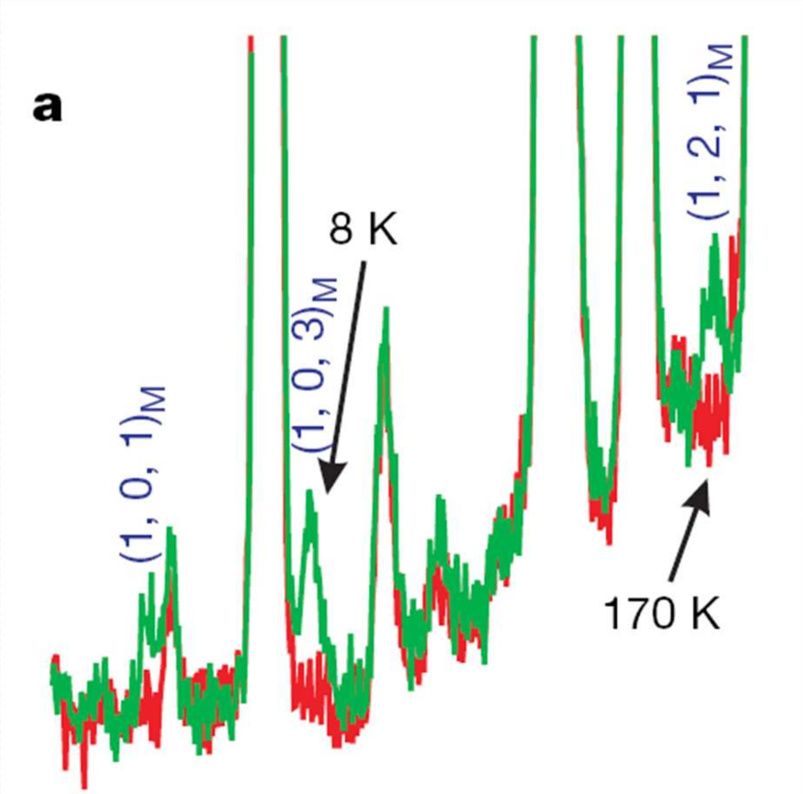
$E_0<2\Delta$

Vol 453|12 June 2008|doi:10.1038/nature07057 nature

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]

- (π,0) in-plane magnetic vector



- Separated structural and magnetic transitions

See also: McGuire et al., PRB '08

Superconductivity and Magnetic Properties of high-quality single crystals of $A_x\mathrm{Fe}_2\mathrm{Se}_2$ (A = K and Cs)

J. J. Ying, X. F. Wang, X. G. Luo†, A. F. Wang, M. Zhang, Y. J. Yan, Z. J. Xiang, R. H. Liu, P. Cheng, G. J. Ye and X. H. Chen*