# $BaFe_2As_2$: A Model Platform for Unconventional Superconductivity

*David Mandrus, Oak Ridge National Lab.*

*"Og discovered fire, and Thorak invented the wheel. There's nothing left for us."*

Oak Ridge National Laboratory

# Correlated Electron Materials Group

David Mandrus

Brian Sales

Rongying Jin
(now at LSU)

Michael McGuire
Wigner Fellow

Athena Sefat
Wigner Fellow

# Collaborators

**ORNL:** A. Christianson, M. Lumsden, S. E. Nagler (neutrons); J. Howe (electron microscopy); A. Payzant (X-rays); D. Christen (flux dynamics); M. Pan (tunneling); D. J. Singh (theory)

**NHML/FSU:** Larbalestier group, Tozer group

**UCSD:** Maple group (pressure), Basov group (IR)

**McMaster:** Imai group (NMR), Y. Mozharivskyj (crystallography)

**Julich/Liege:** R. Hermann (Mossbauer)

**UTK:** Keppens group (elastic properties), Mannella group (X-ray spectroscopy, ARPES), Egami group (PDF), Plummer group (STM)

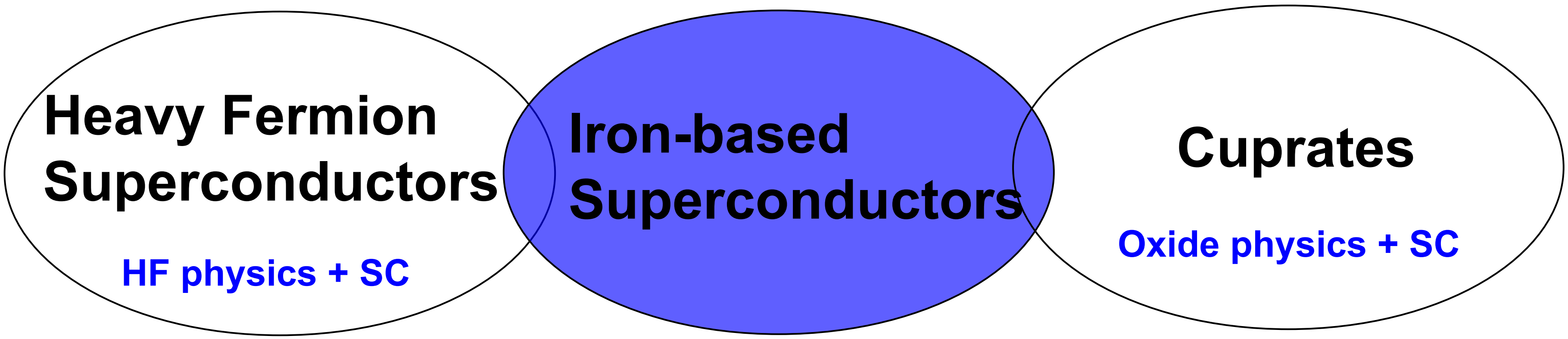
**LANL:** F. Ronning, R. Movshovich, E. D. Bauer, J. D. Thompson

**Houston:** S. Pan group

**LSU:** Plummer Group, Zhang group, Jin group

**UIUC:** L. Greene group

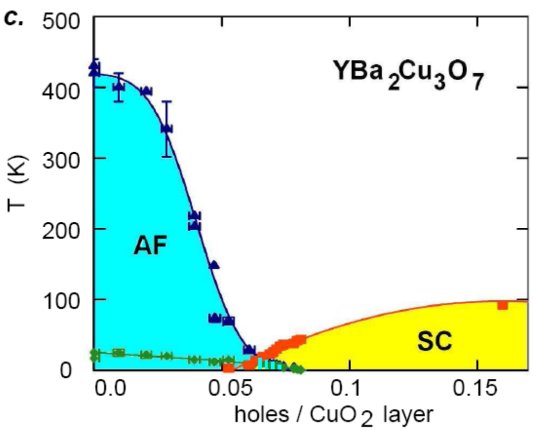
# Pnictides are the Missing Link Between Cuprates and HFs



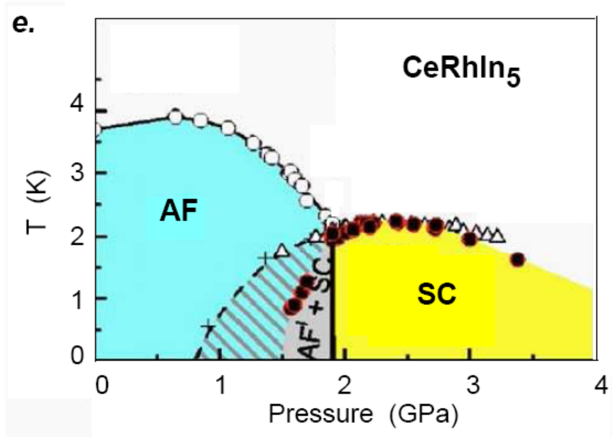

**Chemically very different, but evidence points to similar SC mechanism**

# Great Similarity of Phase Diagrams

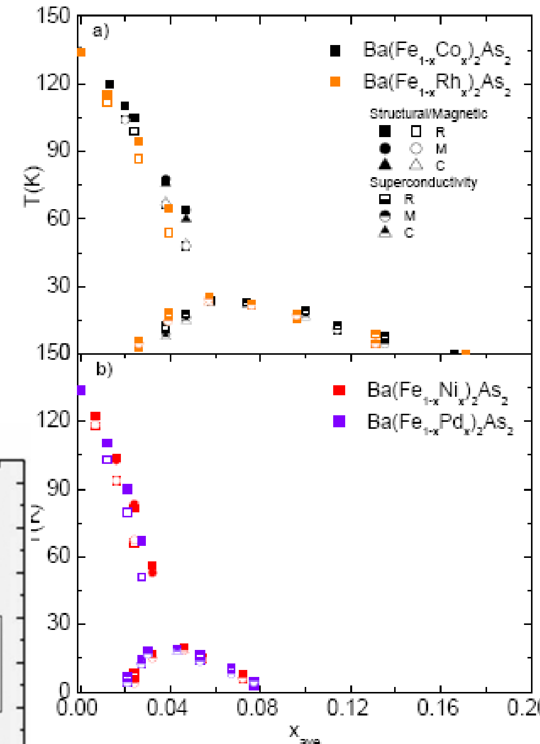
S. Sanna, et al.
PRL 93, 207001

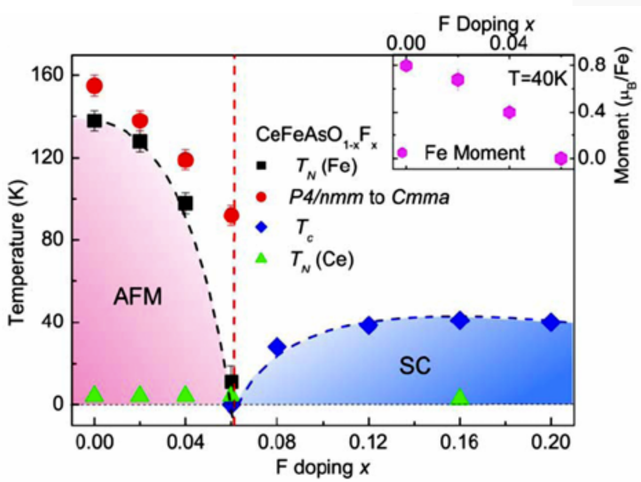



G. Knebel, et al.
PRB 74, 020501 (2006)

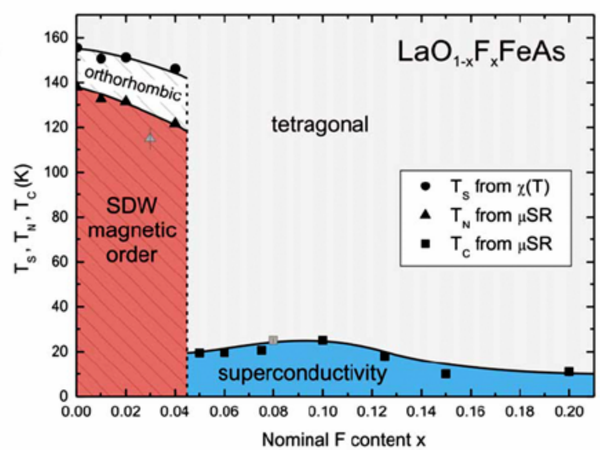



Canfield group,
arXiv: 0905.4894



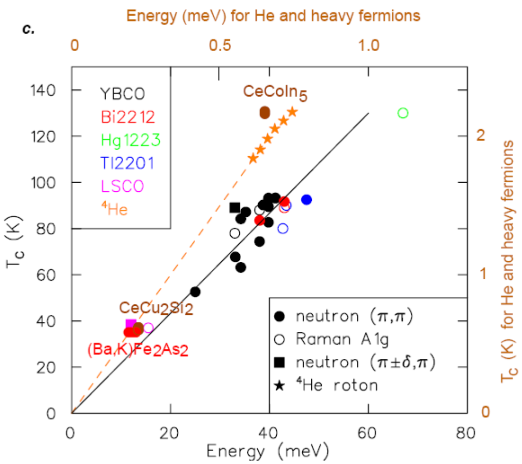




J. Zhao, et al.
Nature Materials **7**, 953 (2008)



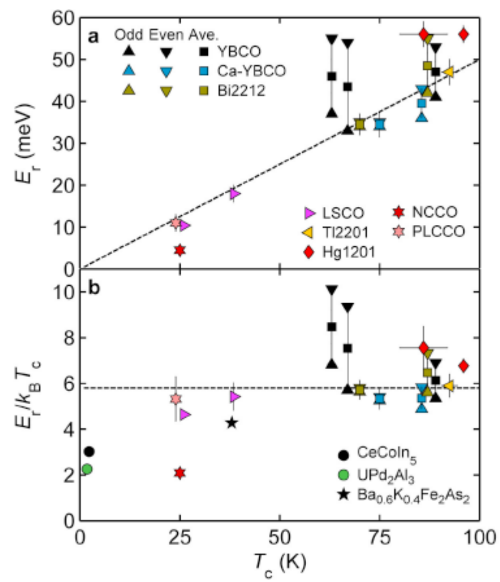

H. Luetkens, et al.
Nature Materials **8**, 305 (2009)

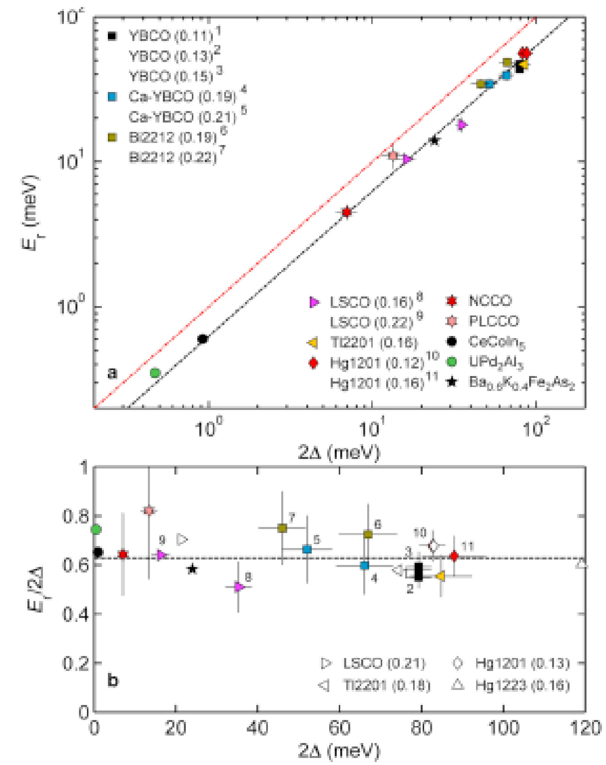
# Universal Behavior of Spin Resonance




Y. J. Uemura,
Cond-mat: 0903.2758

$E_r \sim 4k_BT_c$




Greven group,
Cond-mat: 0903.2291

$E_r/2\Delta \sim 0.64$

# Motivation and Perspective

**Evidence points to a common mechanism underlying HF, Pnictide, and Cuprate SC**

**Focus on materials-specific properties**

**Work toward a *predictive understanding***

**Doping studies are important in this regard**

**122 Materials show great chemical flexibility**

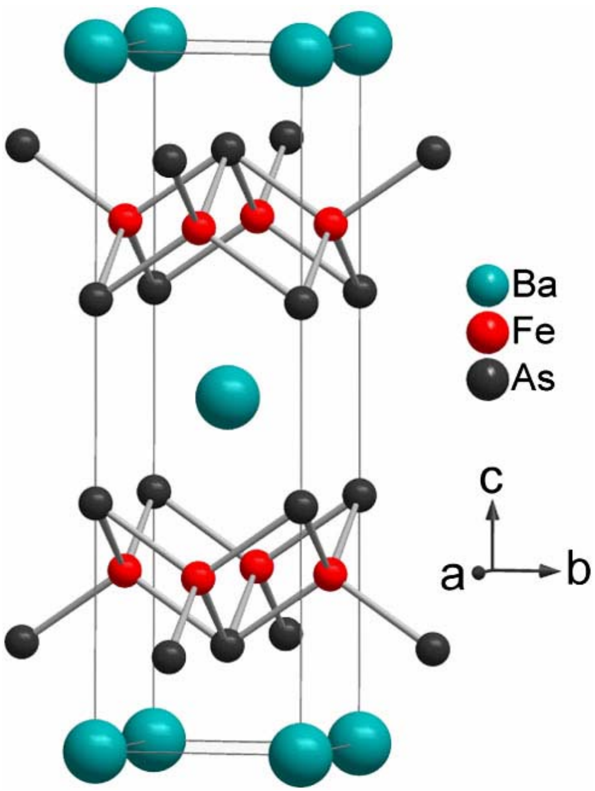
Oak Ridge National Laboratory

# Some of Known Fe compounds (Before 1991) with the $ThCr_2Si_2$ Structure

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $EuFe_2As_2$ | $KFe_2As_2$ | $BaFe_2As_2$ | $SrFe_2As_2$ | $DyFe_2B_2$ | $HoFe_2B_2$ | $TmFe_2B_2$ | $BaFe_2P_2$ |
| $CaFe_2P_2$ | $CeFe_2Ge_2$ | $ErFe_2B_2$ | $LuFe_2B_2$ | $YFe_2B_2$ | $CeFe_2P_2$ | $GdFe_2B_2$ | $TbFe_2B_2$ |
| $CeFe_2Si_2$ | $DyFe_2Si_2$ | $ErFe_2Ge_2$ | $EuFe_2P_2$ | $DyFe_2Ge_2$ | $ErFe_2Si_2$ | $EuFe_2Si_2$ | $LaFe_2Ge_2$ |
| $LaFe_2P_2$ | $SmFe_2Ge_2$ | $UFe_2Ge_2$ | $LaFe_2Si_2$ | $NdFe_2Si_2$ | $TlFe_2Se_2$ | $ThFe_2Si_2$ | $YFe_2Si_2$ |
| $UFe_2P_2$ | $GdFe_2Ge_2$ | $NdFe_2Ge_2$ | $TbFe_2Ge_2$ | $YbFe_2Ge_2$ | $LuFe_2Si_2$ | $PrFe_2Si_2$ | $SmFe_2Si_2$ |
| $TmFe_2Si_2$ | $YbFe_2Si_2$ | $PrFe_2Ge_2$ | $ThFe_2Ge_2$ | $HoFe_2Si_2$ | $SrFe_2P_2$ | $TbFe_2Si_2$ | $TlFe_2S_2$ |
| $UFe_2Si_2$ | $ZrFe_2Si_2$ | | | | | | |

**Crystals with $ThCr_2Si_2$ Structure ($BaFe_{1.84}Co_{0.16}As_2$)**

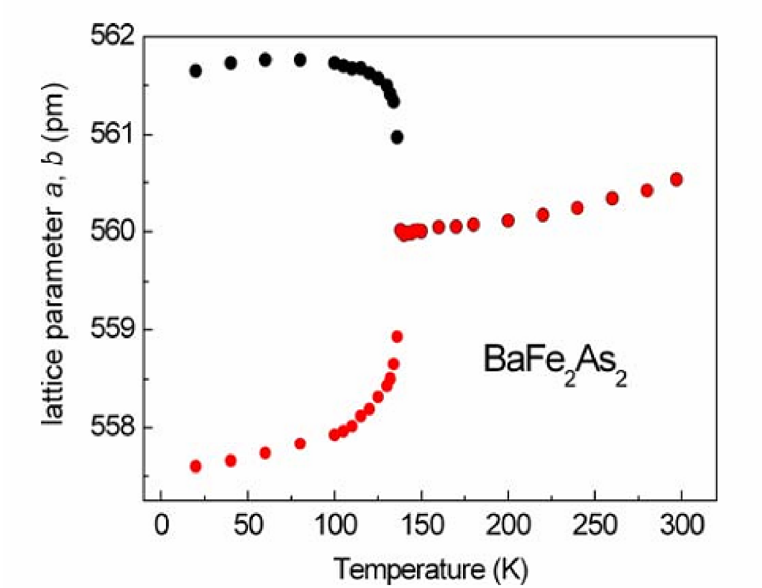
# $BaFe_2As_2$ Basic Properties




**$ThCr_2Si_2$ structure *I4/mmm***

**Layers of edge-sharing $FeAs_4$ tetrahedra**

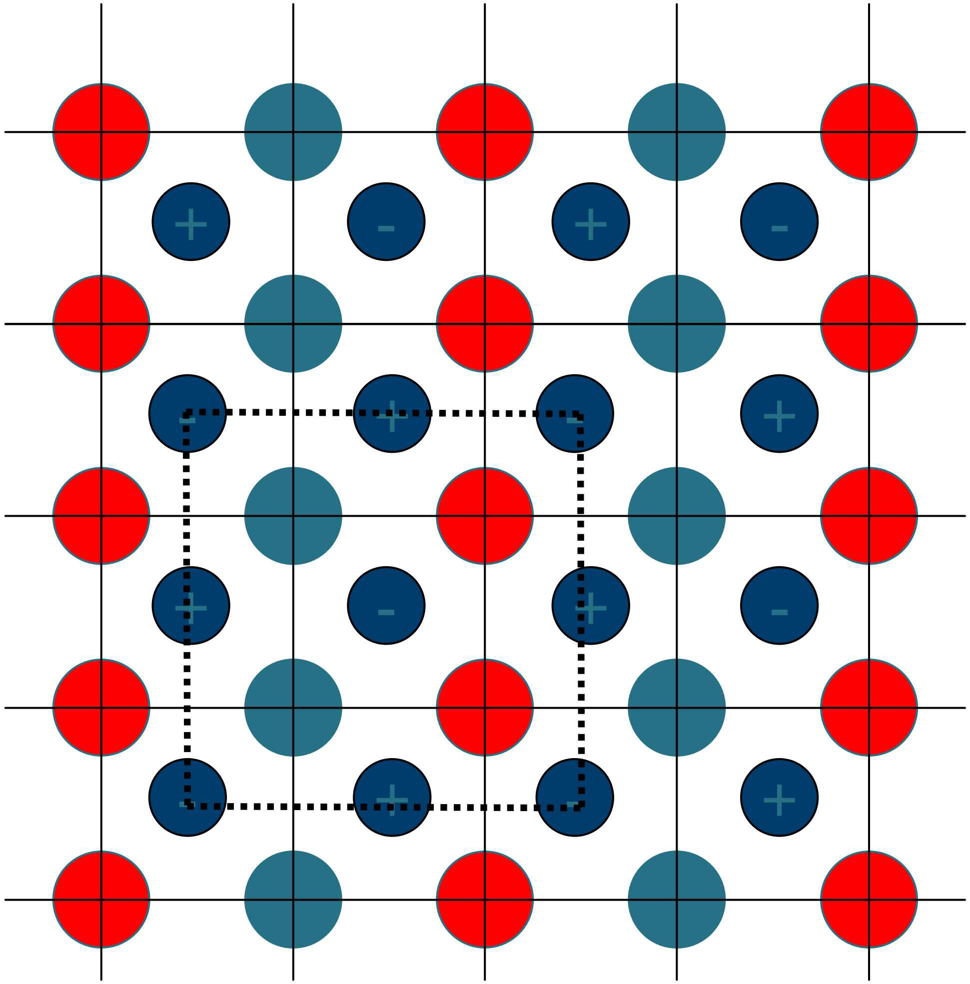
**Coupled SPT-AFM transition ~140 K**

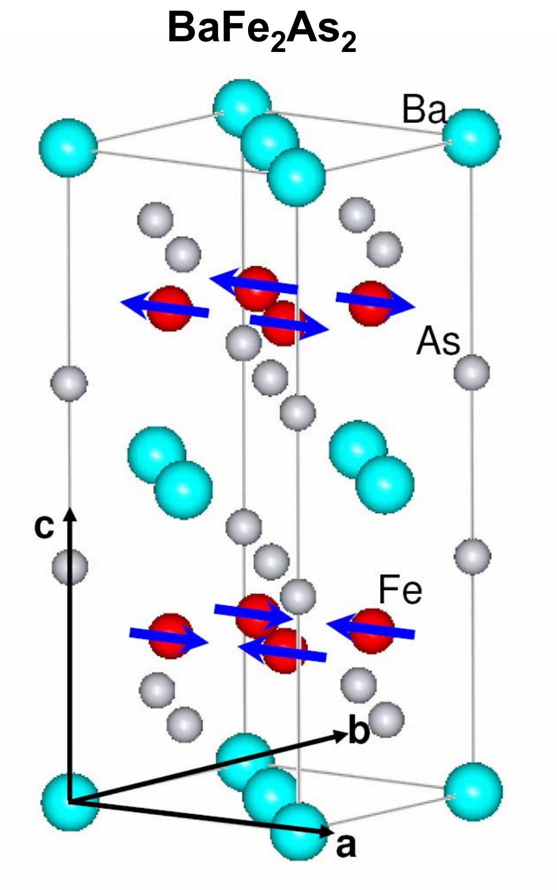



M. Rotter, et al.
PRL 101, 107006 (2008)

**D. Johrendt, R. Poettgen 0902.1085**

# Magnetic Order

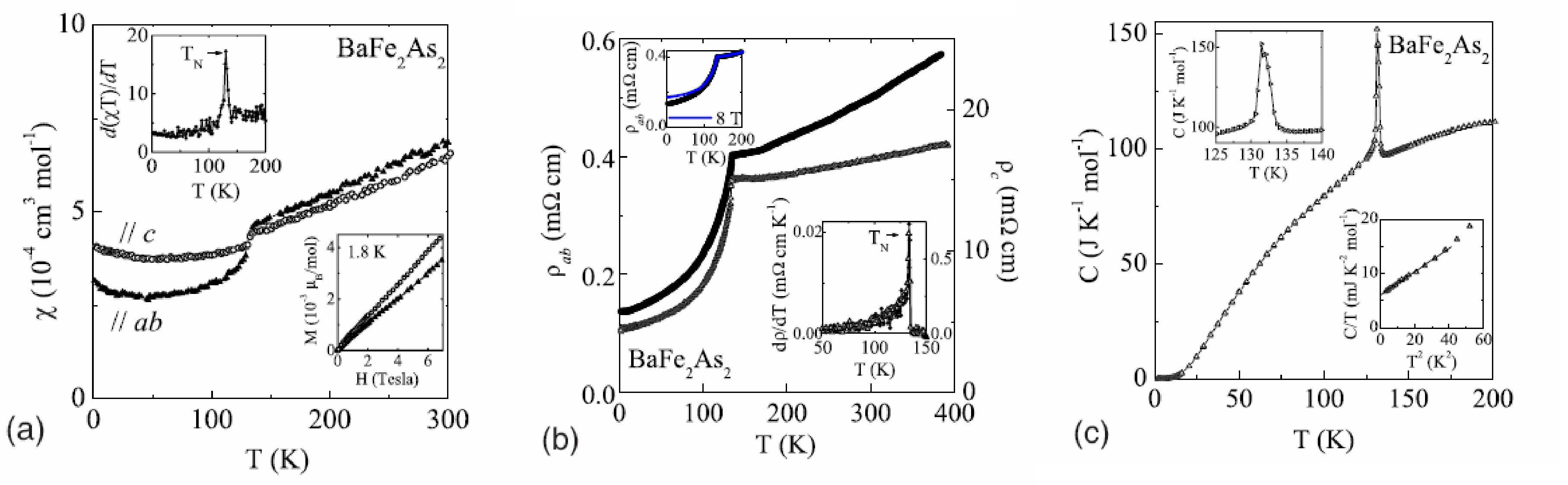



Y. Su, et al. PRB 79, 064504 (2009)

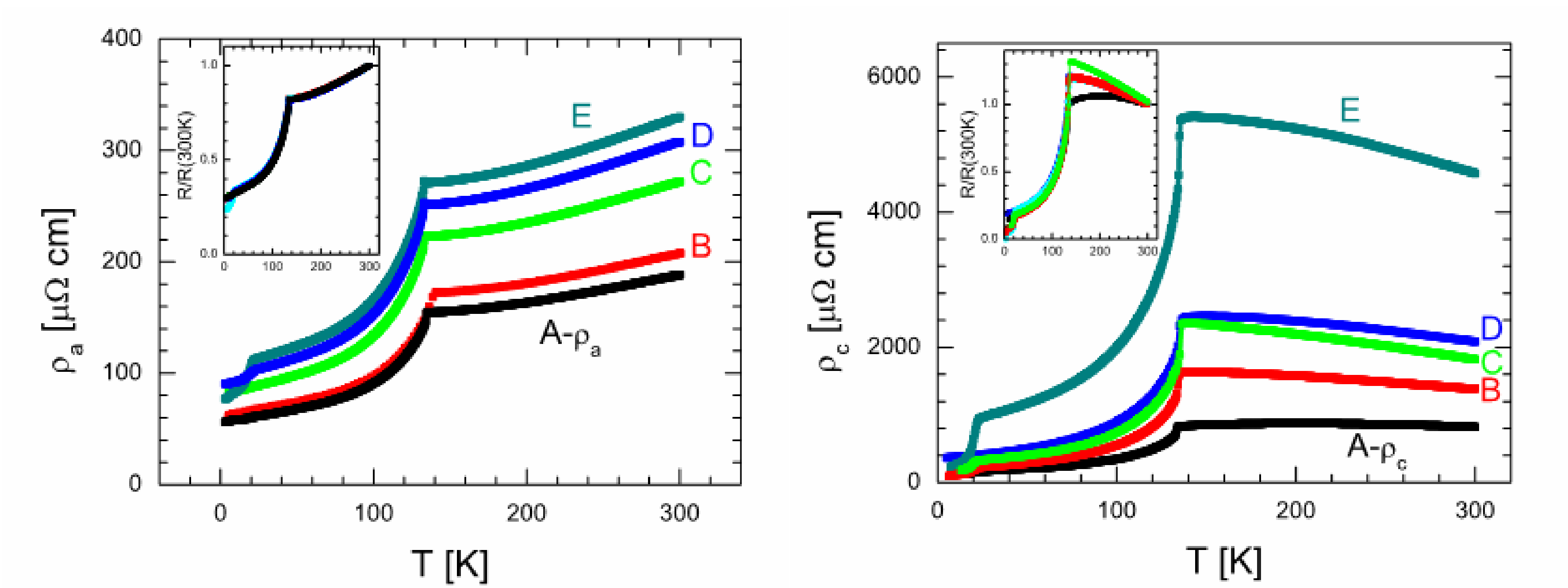
1 D Chains of parallel spin Fe atoms.

# $BaFe_2As_2$ Properties



# $BaFe_2As_2$ is not very anisotropic

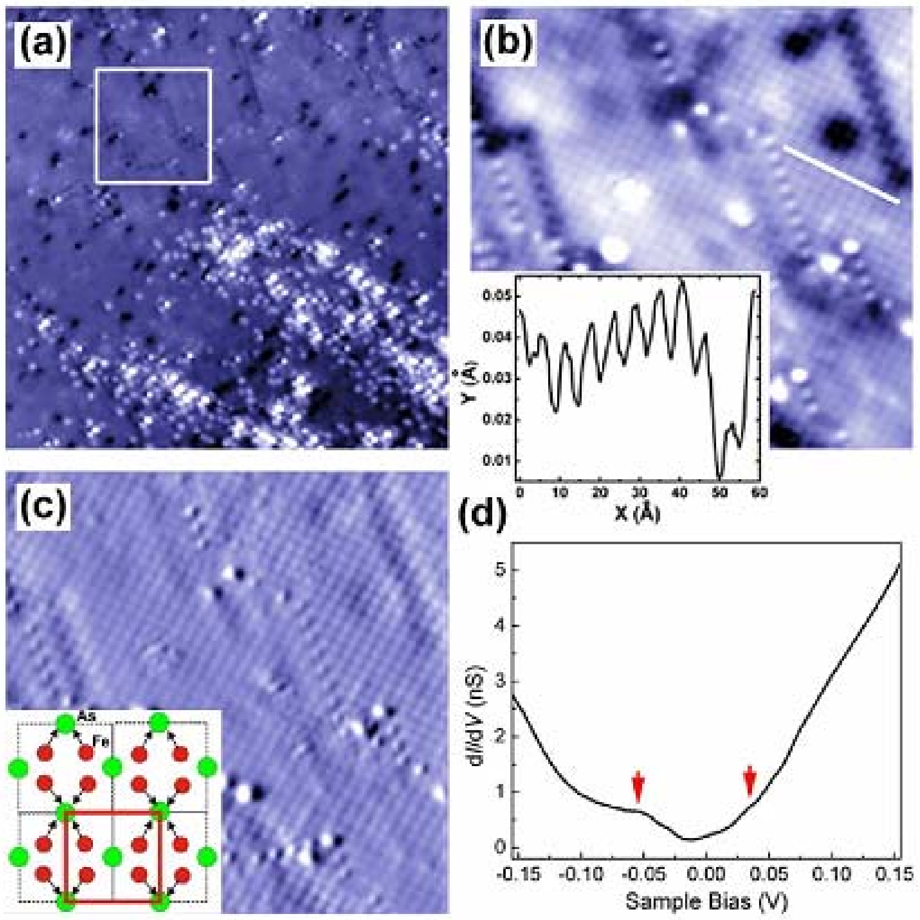
## $\rho_c/\rho_{ab} \approx 5$



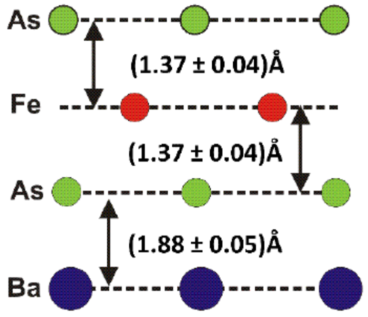

**M. A. Tanatar, et al. PRB 79, 134528 (2009) (Canfield group)**

# Surface of $BaFe_2As_2$

T = 4.3 K




- Cleaved surface of BaFe2As2 is As terminated
- Ba layer destroyed, some random Ba atoms observed on surface
- No surface reconstruction
- Some evidence of orbital order since only one DOS of one type of As was detected




**In collaboration with E. W. Plummer group & S.H. Pan group**

Bulk As-Fe and As-Ba interlayer distances are 1.3437 A and 1.8926 A respectively

# Superconductivity at 38 K in the iron arsenide $(Ba_{1-x}K_x)Fe_2As_2$

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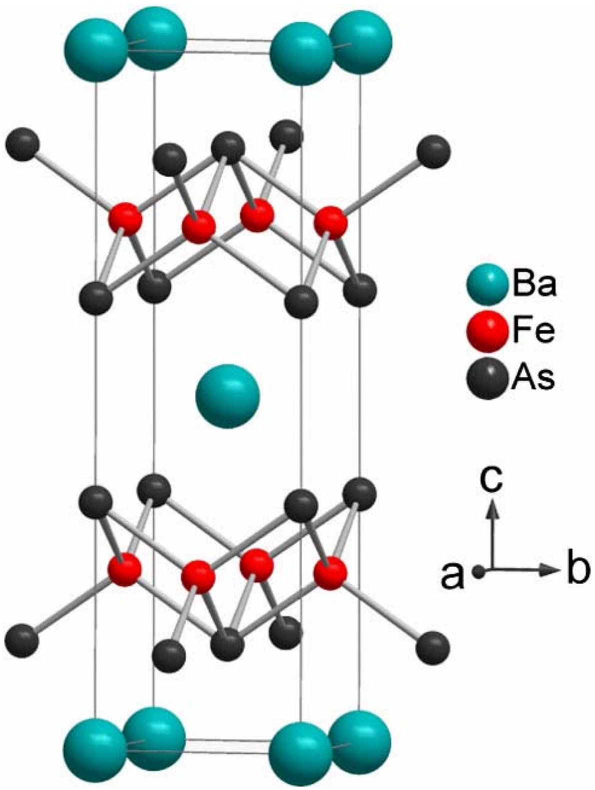
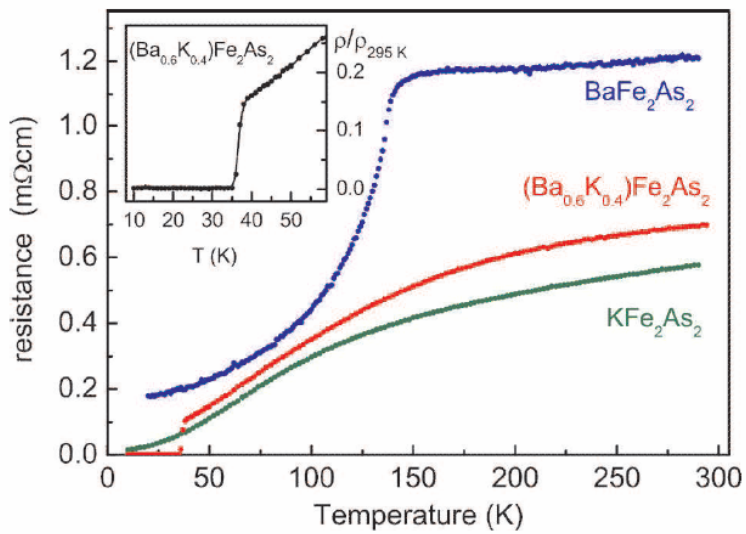
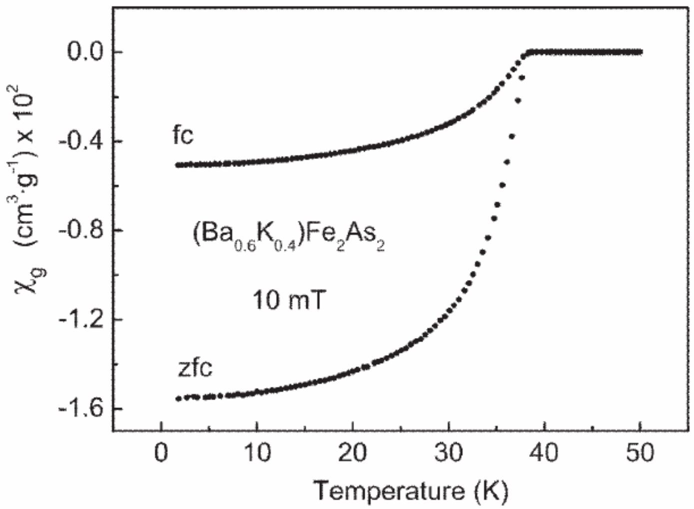
*Department Chemie und Biochemie, Ludwig-Maximilians-Universität München, Butenandtstrasse 5-13 (Haus D), 81377 München, Germany*

(Dated: June 2, 2008)
PRL 101, 107006 (2008)

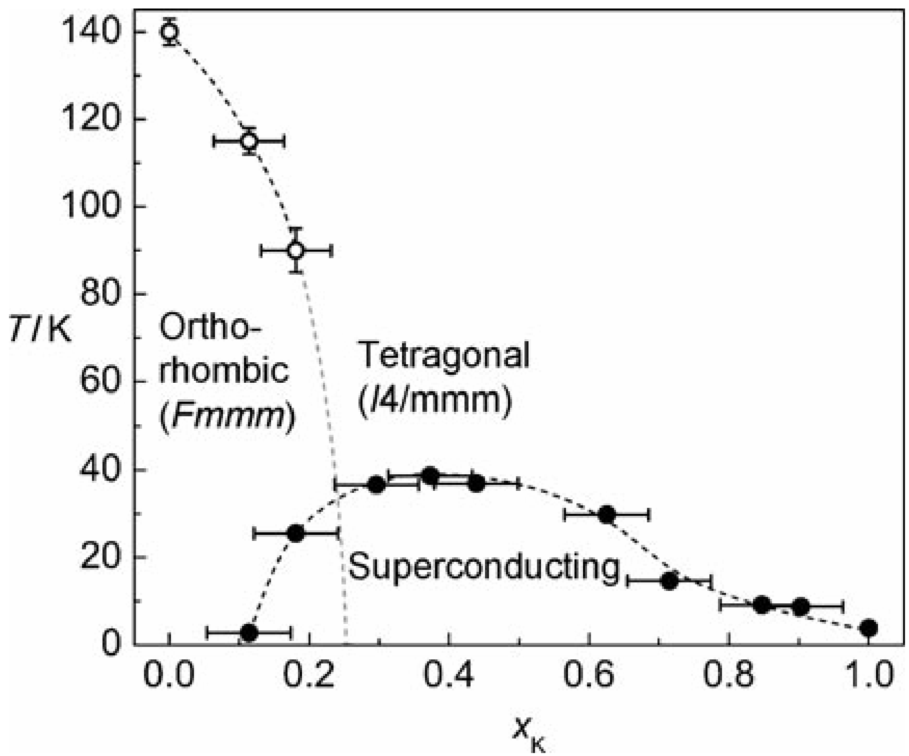


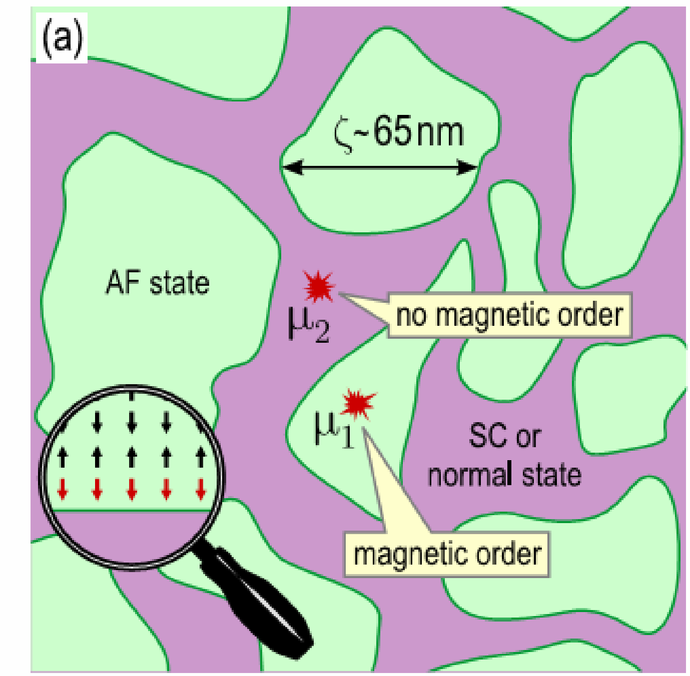



# Phase Diagram

## $Ba_{1-x}K_xFe_2As_2$




M. Rotter, et al. Angew. Chem. I
nt. Ed. 47, 7949 (2008)




J. T. Park, et al. PRL 102, 117006 (2009)
Stuttgart group—Keimer, Hinkov

Electronically phase separated on
a scale of ~65 nm

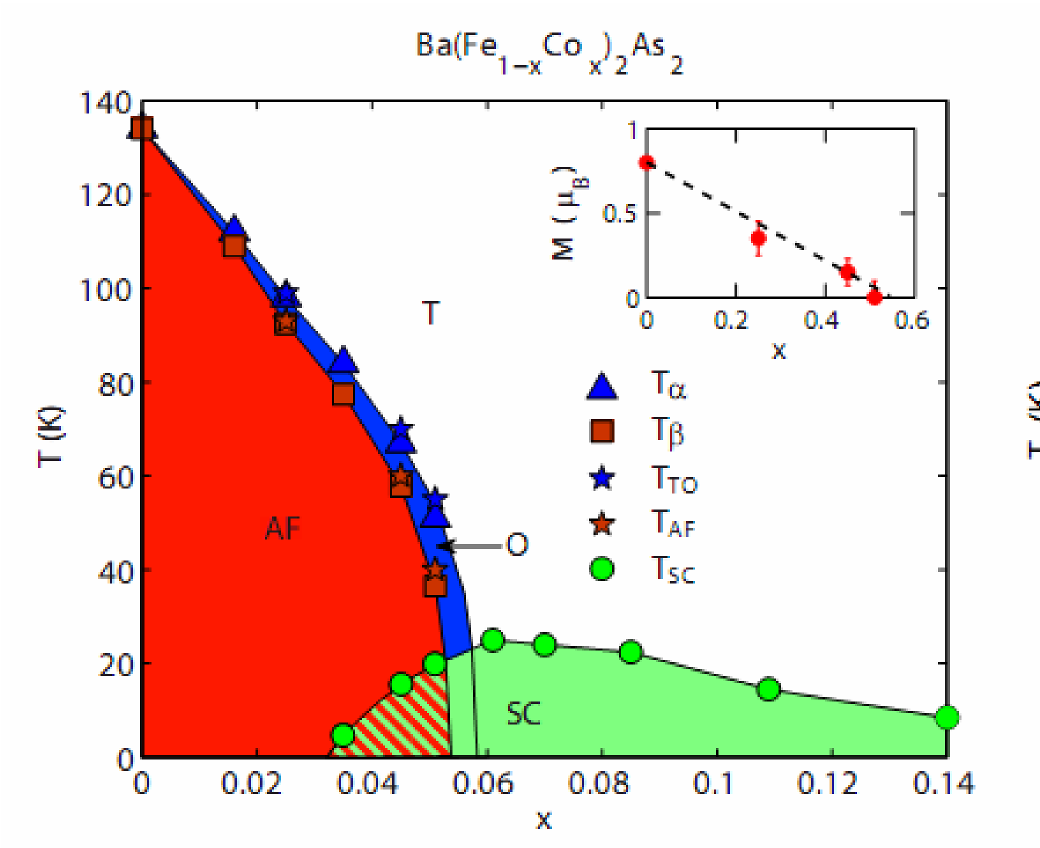
PRL **101,** 117004 (2008) PHYSICAL REVIEW LETTERS week ending 12 SEPTEMBER 2008

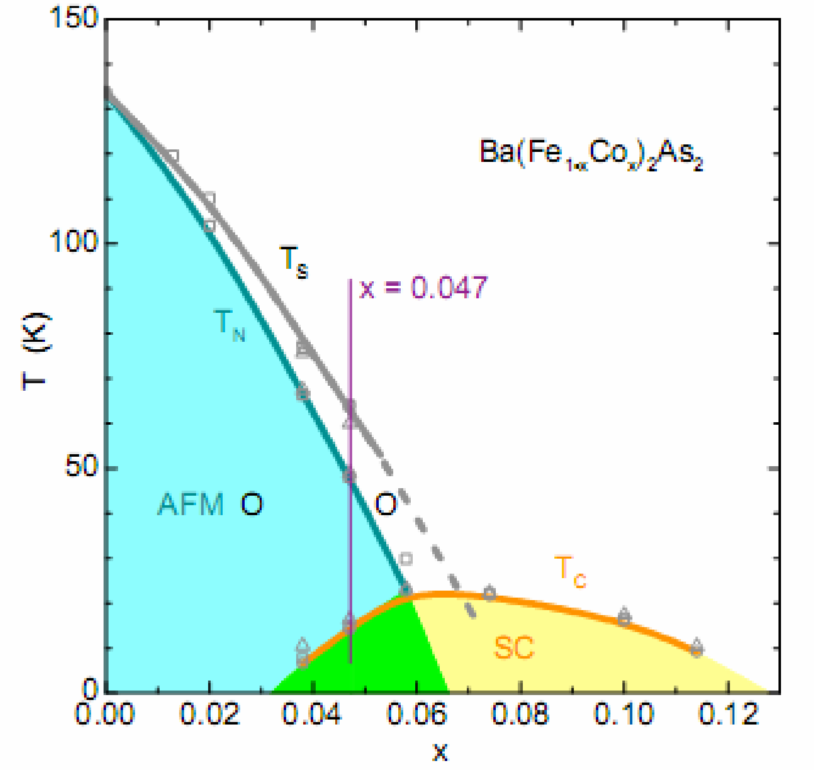
# Superconductivity at 22 K in Co-Doped $BaFe_2As_2$ Crystals

Athena S. Sefat, Rongying Jin, Michael A. McGuire, Brian C. Sales, David J. Singh, and David Mandrus
*Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
(Received 25 July 2008; published 11 September 2008)

- **Electron rather than hole doping**
- **Superconductivity robust to in-plane disorder**
- **Evidence for *s* symmetry superconducting state**
- **Very “clean” system experimentally—crystals quite homogeneous**

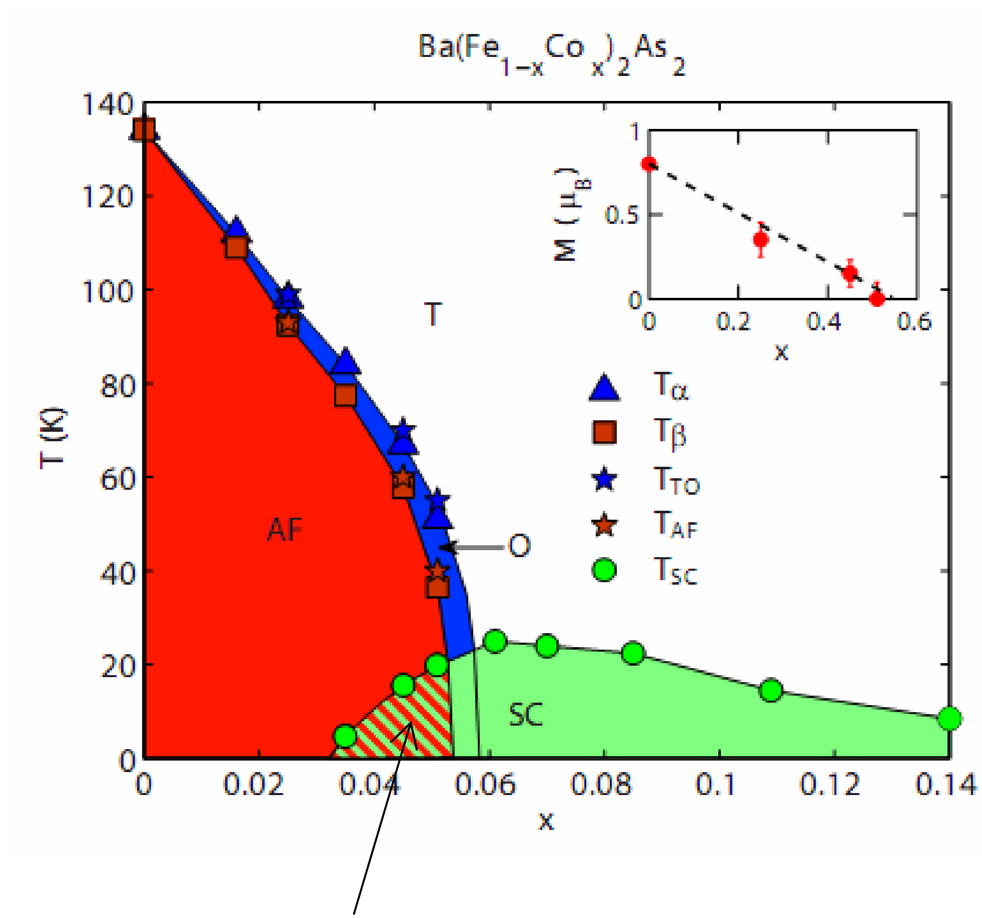
# $Ba(Fe_{1-x}Co_x)_2As_2$ Phase Diagram




C. Lester, et al. PRB 79, 114523 (2009)
I.R. Fisher, S. M. Hayden groups

D. K. Pratt, et al. Cond-mat 0903.2833
P. C. Canfield, R. J. McQueeney groups

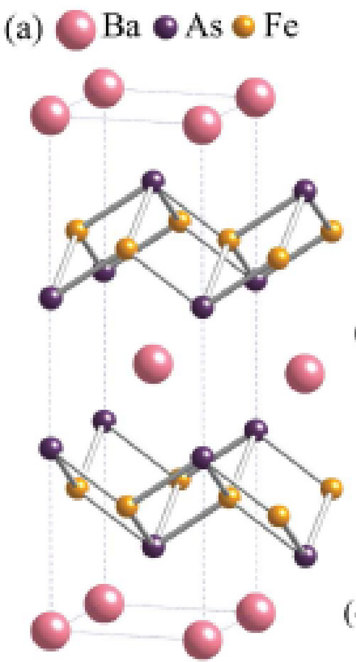


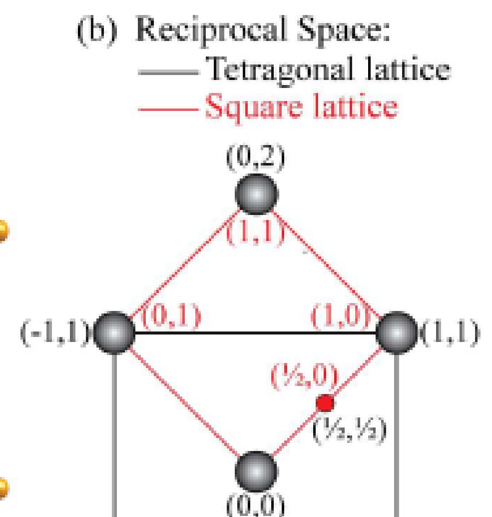

“No superconducting phase separation”
--S.-H. Pan

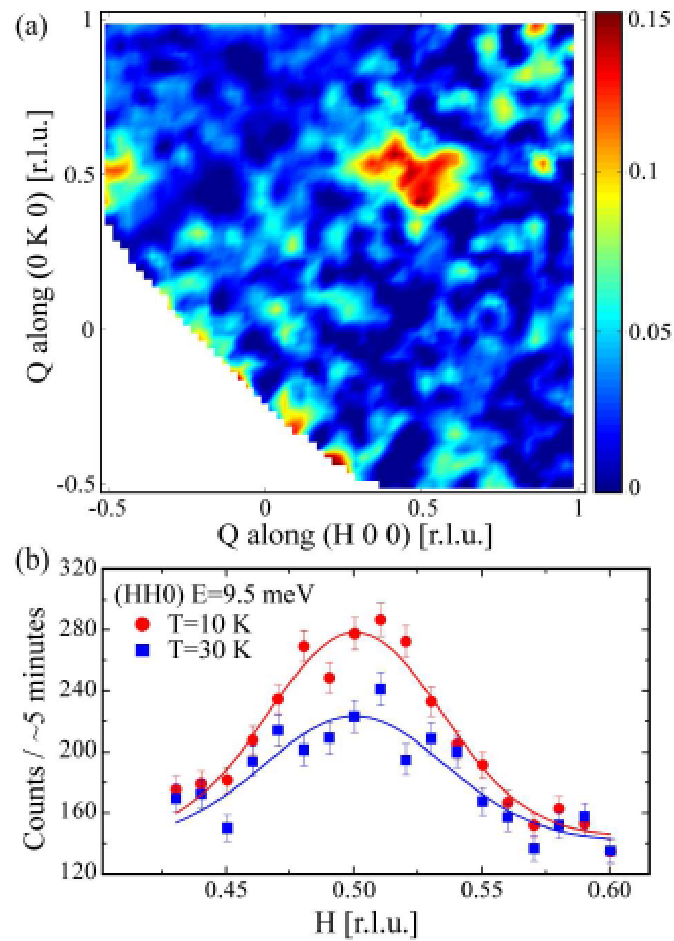
PRL 102, 107005 (2009) PHYSICAL REVIEW LETTERS week ending 13 MARCH 2009

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

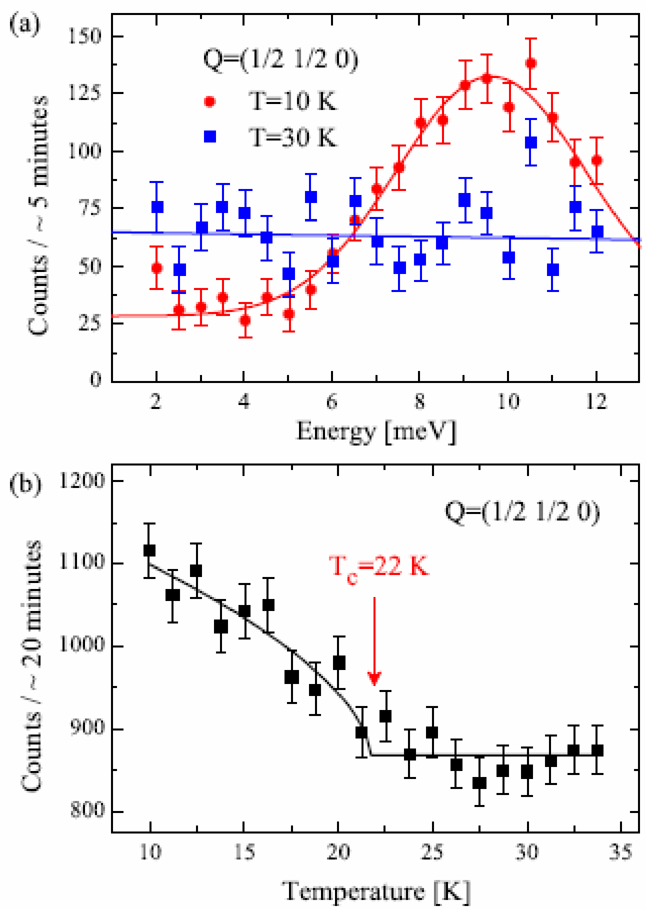
M. D. Lumsden,[1] A. D. Christianson,[1] D. Parshall,[2] M. B. Stone,[1] S. E. Nagler,[1] G. J. MacDougall,[1] H. A. Mook,[1] K. Lokshin,[3] T. Egami,[1,2,3] D. L. Abernathy,[1] E. A. Goremychkin,[4,5] R. Osborn,[4] M. A. McGuire,[1] A. S. Sefat,[1] R. Jin,[1] B. C. Sales,[1] and D. Mandrus[1]

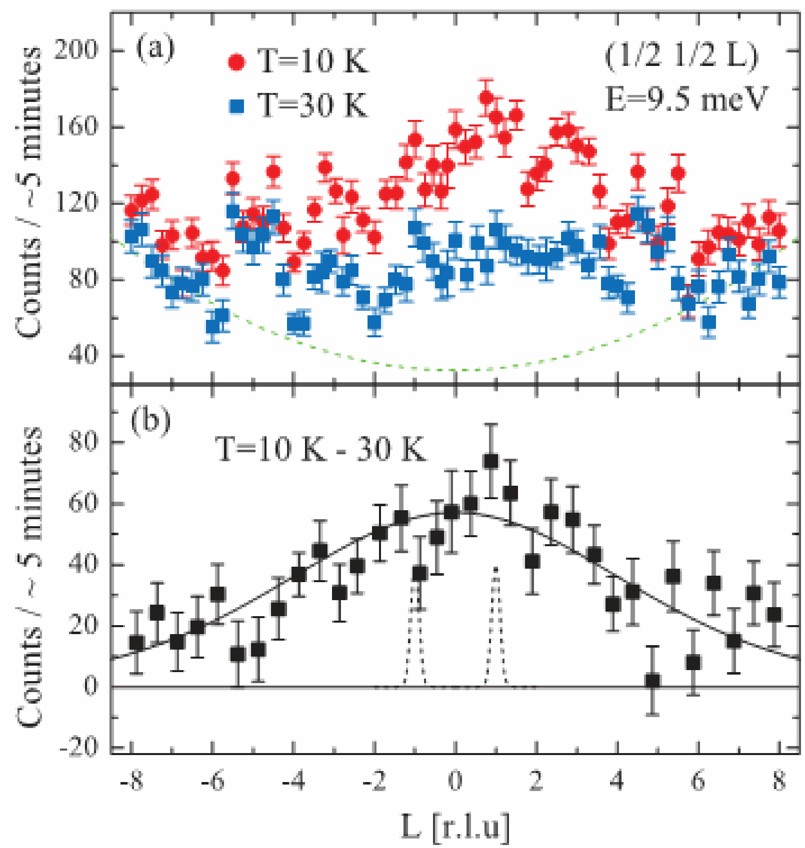


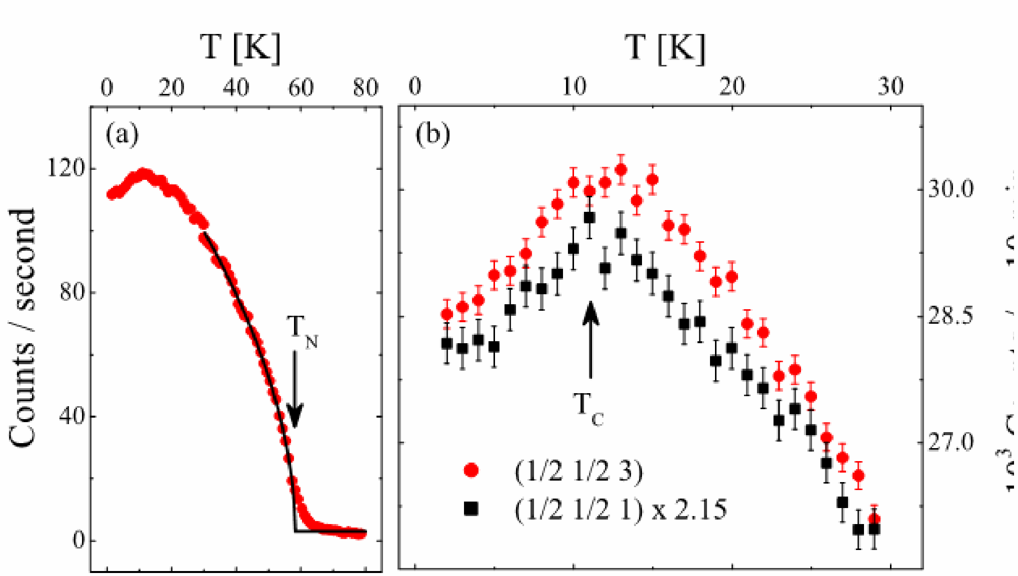



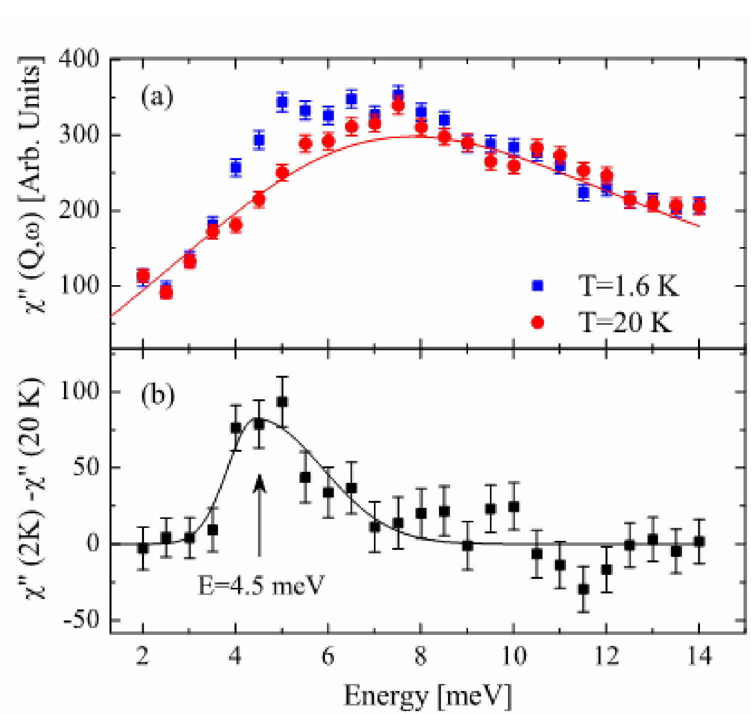
# Resonance in Single Crystal $BaCo_{0.16}Fe_{1.84}As_2$



# Neutron Scattering on Underdoped $BaFe_{1.92}Co_{0.08}As_2$




- $T_c$ = 11 K
- Drop in intensity of Bragg Peak below Tc
- Resonance obeseved at 4.5 meV = 4.7 $k_B T_c$
- Spectral weight transferred from Bragg peaks to resonance?
- Scattering is 3D vs. 2D in optimally doped

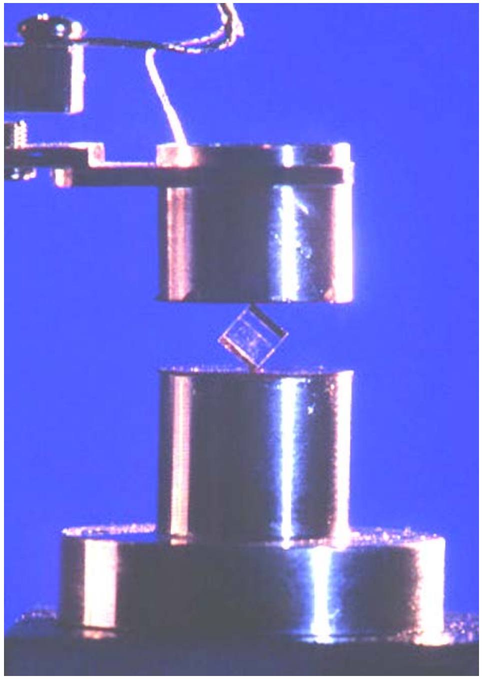
A. D. Christianson, et al. Cond-mat 0904.0767

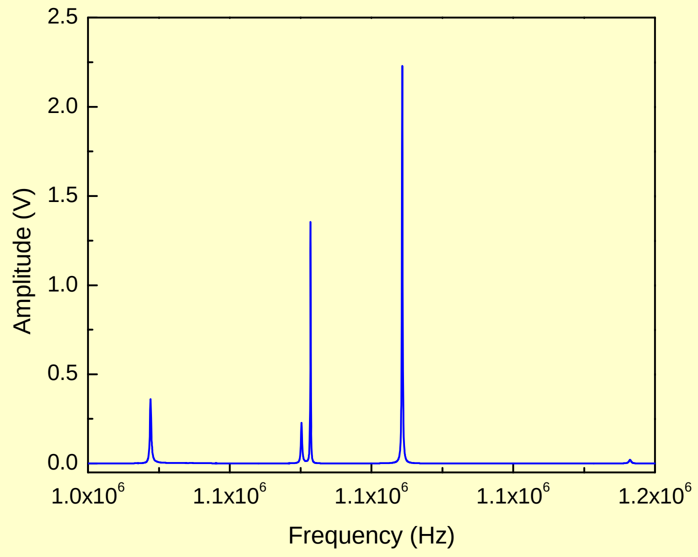
Oak Ridge National Laboratory

Veerle Keppens

advantages of RUS: all elastic constants can be obtained in one measurement

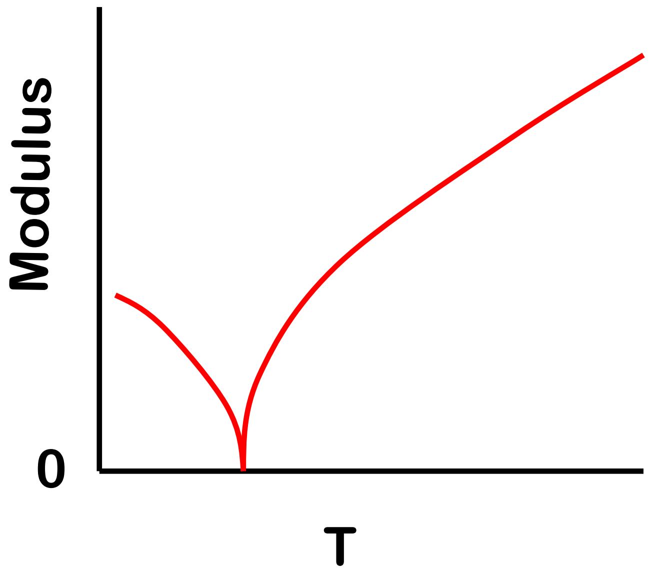
small samples ($mm^3$)





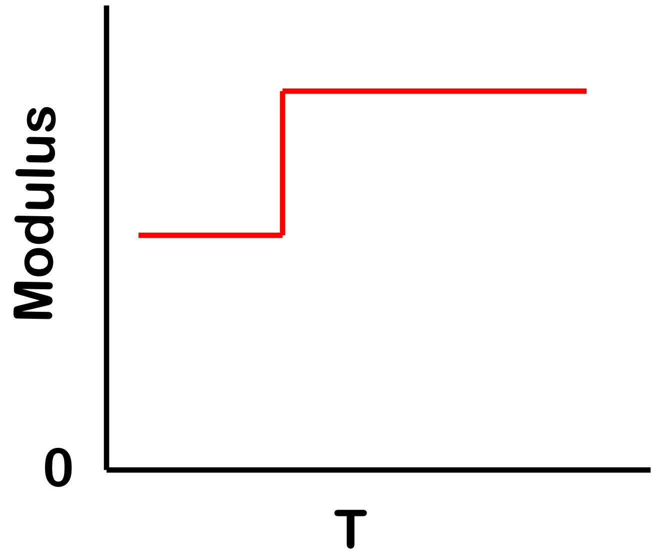

# Strain-Order Parameter Coupling at Phase Transitions

## Bi-Linear coupling:
## $F_c = \beta Q \varepsilon$



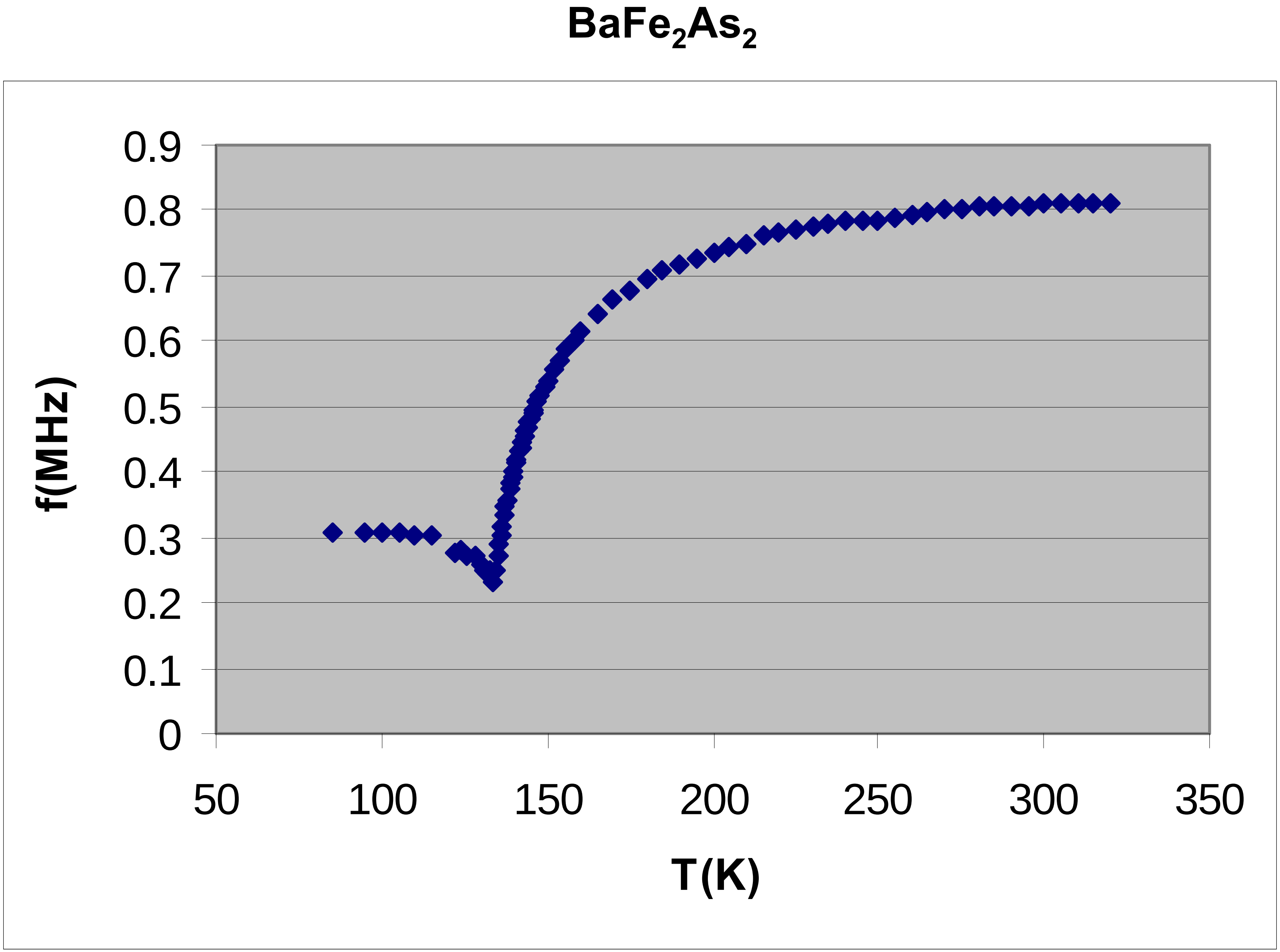

$$c = c^0 - \frac{a}{T - \theta}$$

## Quadratic coupling:
## $F_c = \beta Q^2 \varepsilon$

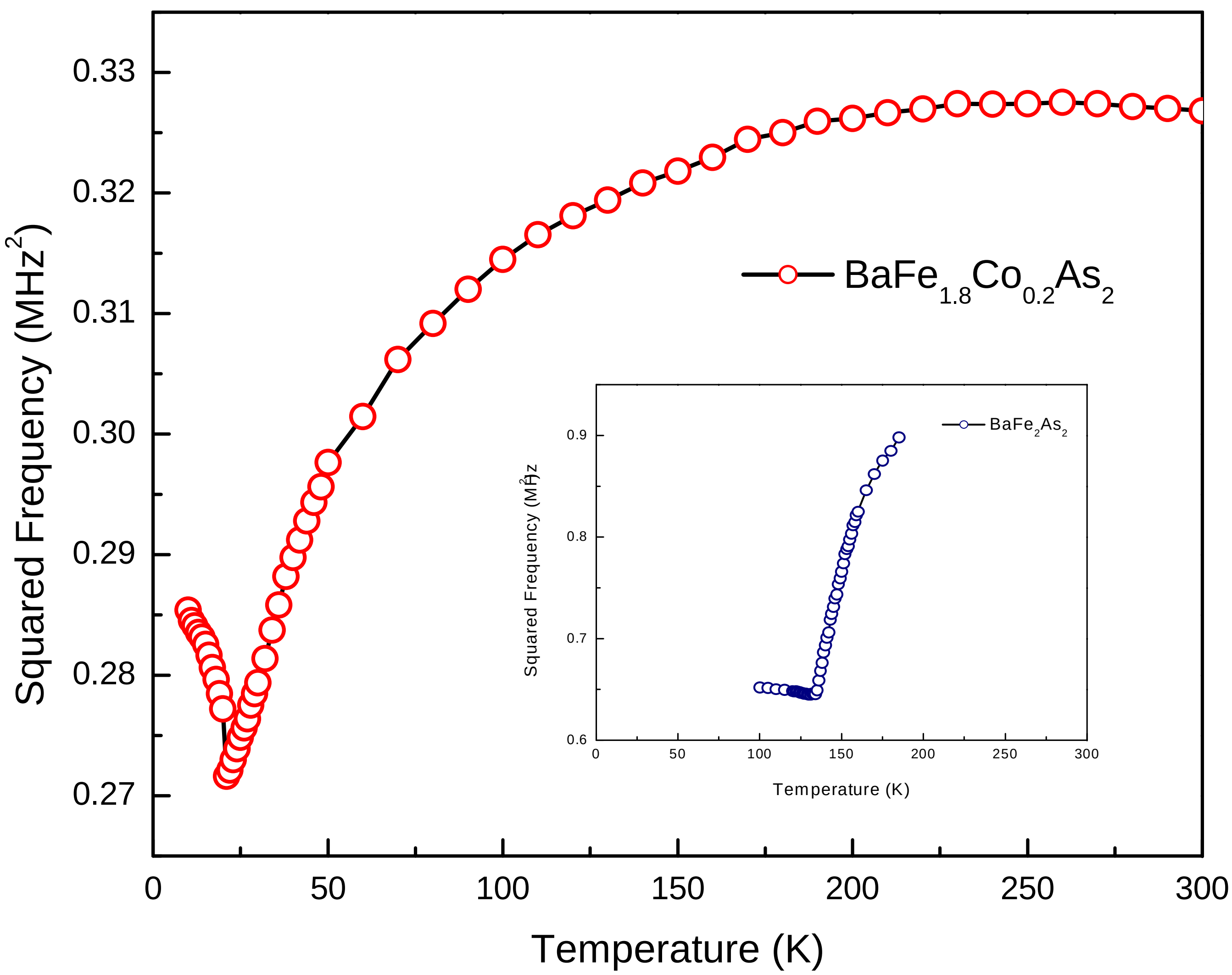



$$c = c^0 \qquad T > T_c$$

$$c = c^0 - \frac{2h^2}{\beta} \qquad T < T_c$$



BaFe2As2
f(MHz)
T(K)
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
50
100
150
200
250
300
350


0.33
0.32
0.31
0.30
0.29
0.28
0.27
Squared Frequency (MHz$^2$)
0
50
100
150
200
250
300
Temperature (K)
BaFe$_{1.8}$Co$_{0.2}$As$_2$
0.9
0.8
0.7
0.6
Squared Frequency (MHz$^2$)
0
50
100
150
200
250
300
Temperature (K)
BaFe$_2$As$_2$

# The role of striction at magnetic and structural transitions in iron-pnictides

Victor Barzykin and Lev P. Gor'kov*
*National High Magnetic Field Laboratory, Florida State University,*
*1800 E. Paul Dirac Dr., Tallahassee, Florida 32310*

We discuss the role of striction in the intertwined magnetic and structural phase transitions in the underdoped iron-pnictides. The magneto-elastic coupling to acoustic modes is then derived and estimated in framework of the multiband spectrum for itinerant electrons with nesting features. We argue that the 1-st order character of the magneto-elastic phase transition originates from the lattice instabilities near the onset of spin-density wave order introducing, thus, a shear acoustic mode as a new order parameter. Taking non-harmonic termis in the lattice energy into account may explain the splitting of the structural and magnetic transitions in some oxypnictides. Fluctuations of the magnetic order parameter show up in the precursory temperature dependence of the elastic moduli.

PHYSICAL REVIEW B 77, 224509 (2008)

# Theory of electron nematic order in LaFeAsO

Chen Fang,[1] Hong Yao,[2] Wei-Feng Tsai,[2,3] JiangPing Hu,[1] and Steven A. Kivelson[2]
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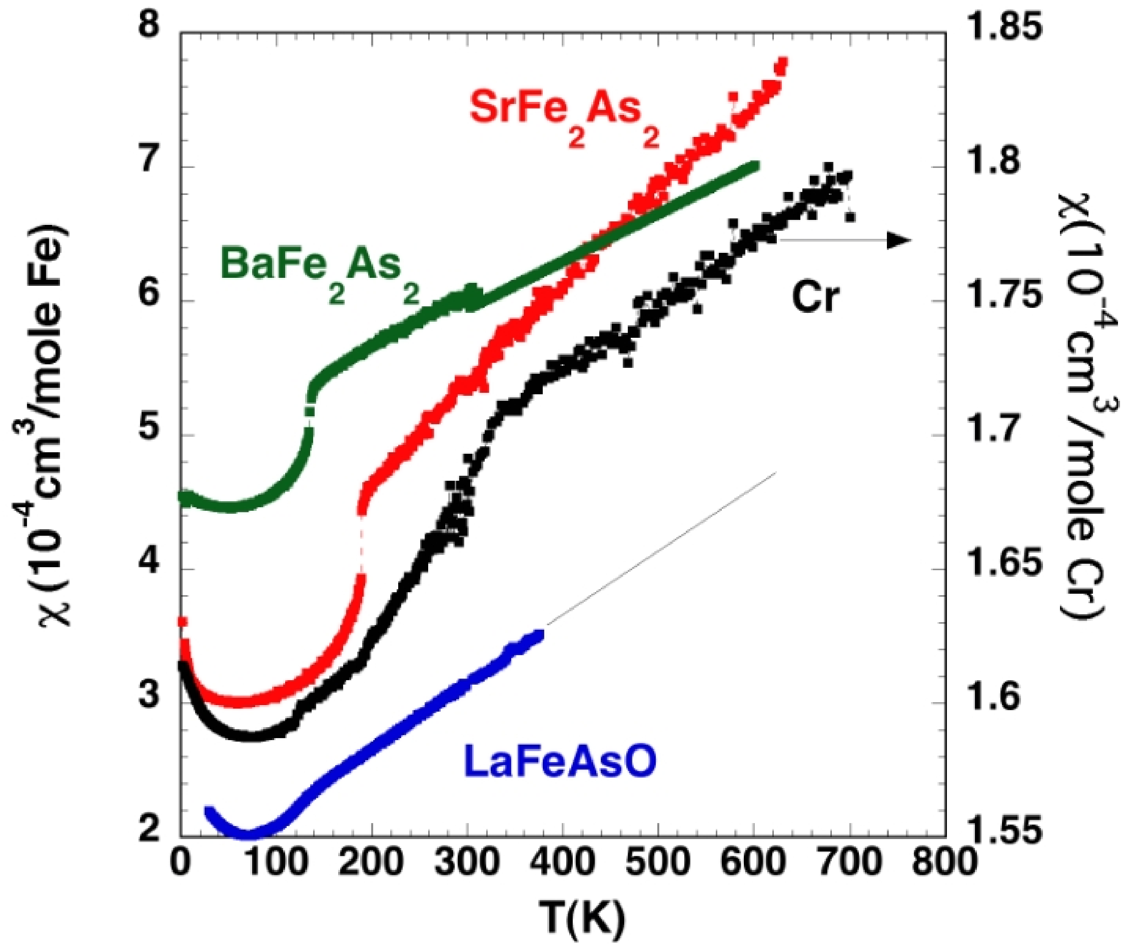
[2]*Department of Physics, Stanford University, Stanford, California 94305, USA*
[3]*Department of Physics and Astronomy, University of California, Los Angeles, California 90095, USA*
(Received 26 April 2008; published 20 June 2008)

We study a spin $S$ quantum Heisenberg model on the Fe lattice of the rare-earth oxypnictide superconductors. Using both large $S$ and large $N$ methods, we show that this model exhibits a sequence of two phase transitions: from a high-temperature symmetric phase to a narrow region of intermediate "nematic" phase, and then to a low-temperature spin ordered phase. Identifying phases by their broken symmetries, these phases correspond precisely to the sequence of structural (tetragonal to monoclinic) and magnetic transitions that have been recently revealed in neutron-scattering studies of LaFeAsO. The structural transition can thus be identified with the existence of incipient ("fluctuating") magnetic order.

DOI: 10.1103/PhysRevB.77.224509 PACS number(s): 71.27.+a, 71.10.−w, 74.25.Ha

# Susceptibility not Curie-Weiss -- looks like Cr



## Hall effect and resistivity study of the magnetic transition, carrier content and Fermi liquid behavior in $Ba(Fe_{1-x}Co_x)_2As_2$

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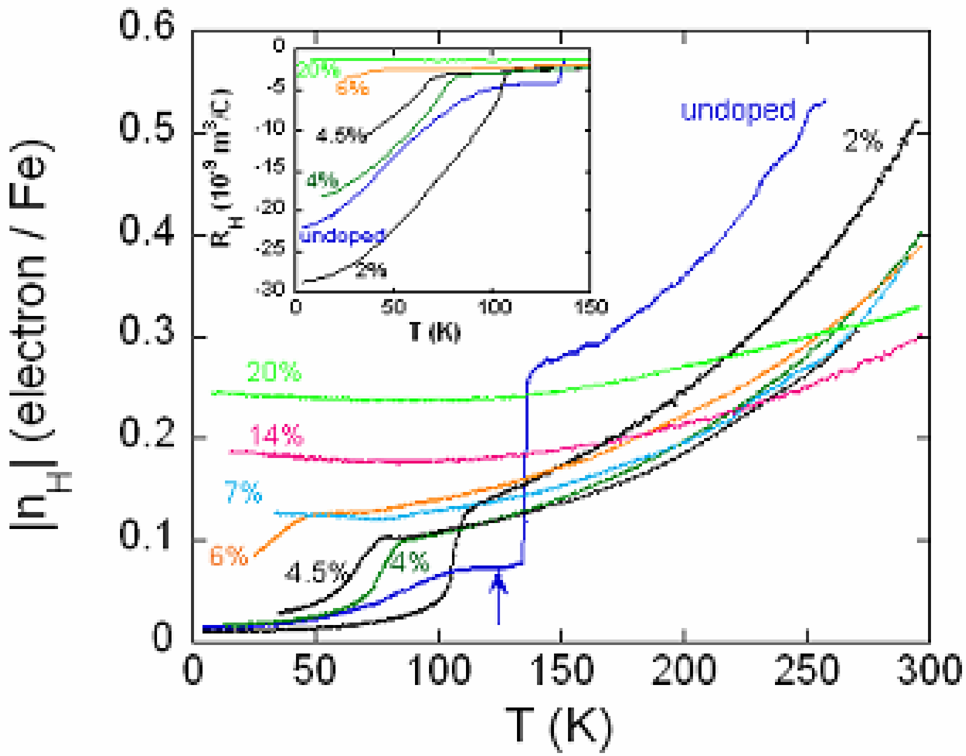
[1] *Service de Physique de l'Etat Condensé, Orme des Merisiers, CEA Saclay (CNRS URA 2464), 91191 Gif sur Yvette cedex, France*

[2] *Laboratoire de Physique des Solides, UMR CNRS 8502, Université Paris Sud, 91405 Orsay, France*

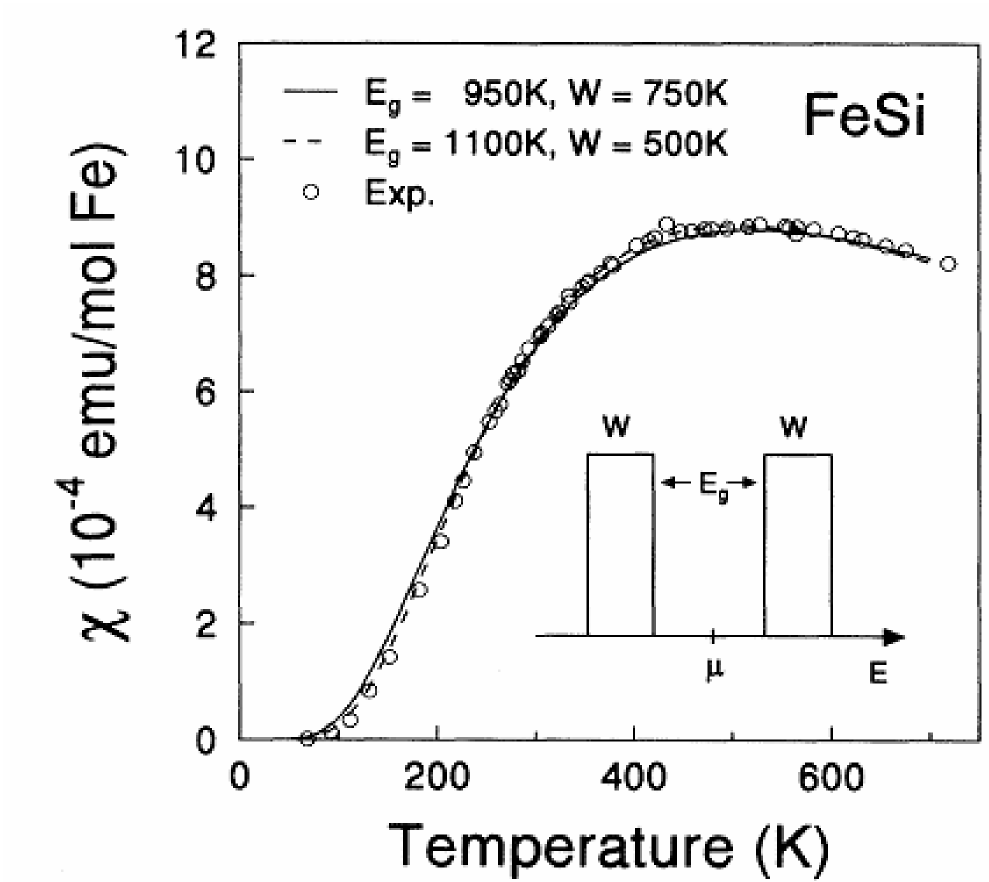
(Dated: march 30th 2009)




**$E_F$ is only 20-40 meV above the bottom of the electron bands**

**Usual assumption that $k_BT << E_F$ is not valid**

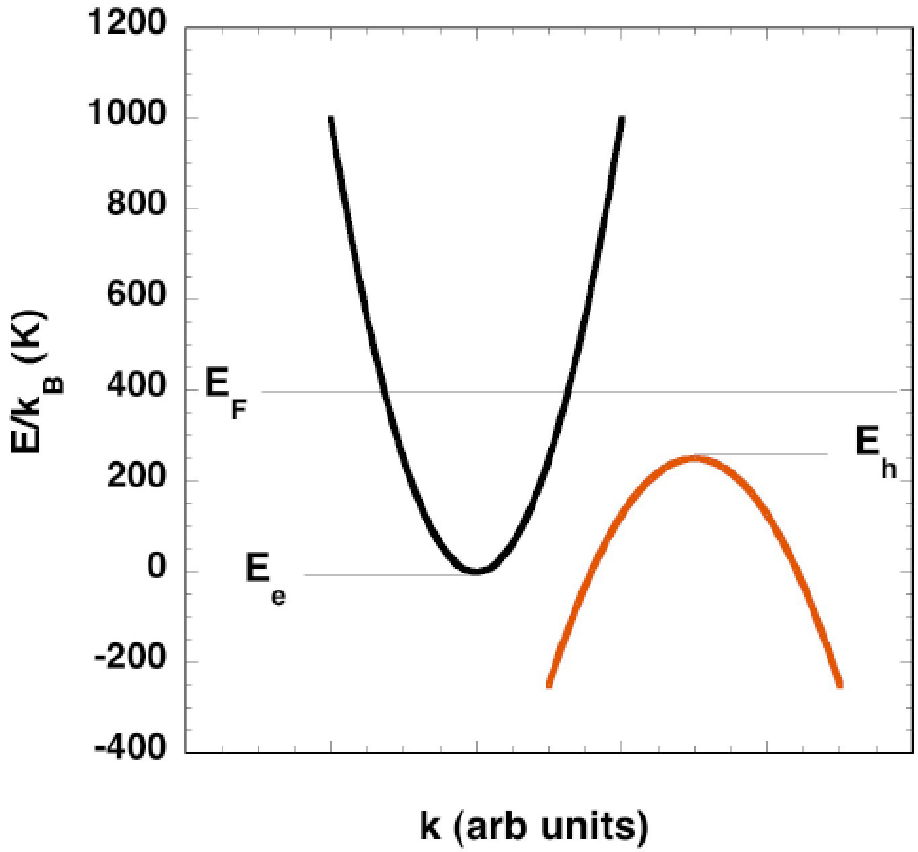
# Sharp Features in the DOS and a variable carrier concentration can give you a susceptibility that increases with T




$$\chi(T) = -2\mu_B^2 \int N(E) \frac{\partial f(E,\mu,T)}{\partial E} dE$$

**D. Mandrus, et al. PRB 51, 4763 (1995)**

**This simple model, with only somewhat unreasonable parameters, can describe Hall, Seebeck coefficient, and susceptibility as a function of T and doping.**




$N_0 = 1.4 \times 10^{21}/cm^3$

$E_H = 250$ K

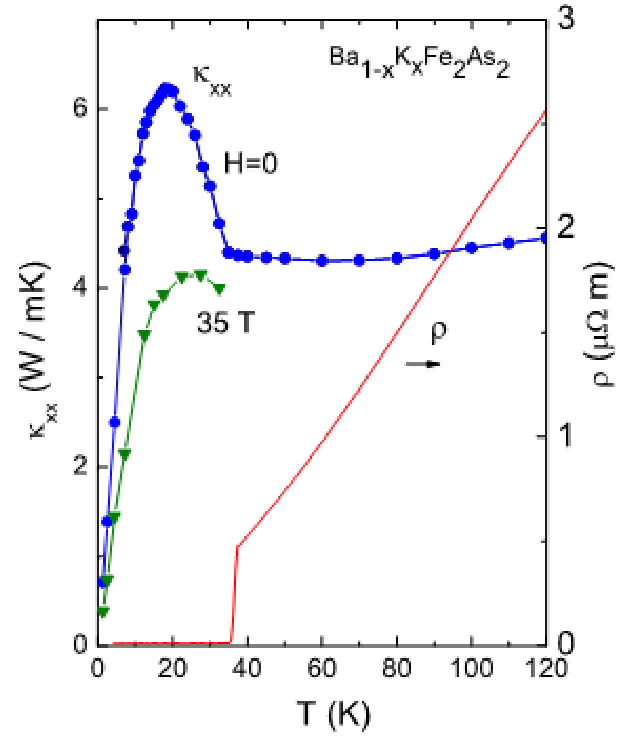
$m_e^* = 17\ m_0$

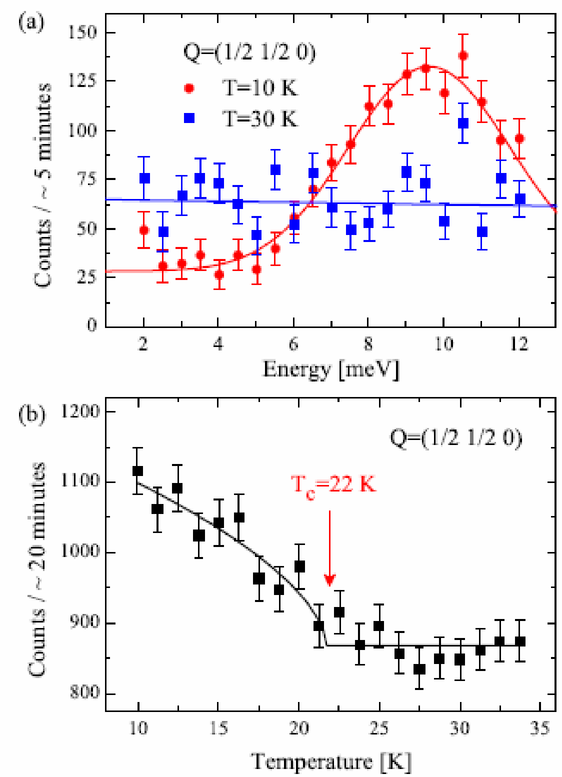
$m_h^* = 30\ m_0$

B. C. Sales, et al.
Cond-mat: 0906.2134

# Concluding Speculation

**Peak in T.C.** **Correlates With** **Resonance**




**J. G. Checkelsky, et al. 0811.4668**
**(Ong group)**

**Lumsden, et al.**
**PRL 102 107005 (2009)**

# Discussion Questions

1) What causes the structural and magnetic transitions to separate in $Ba(Fe_{1-x}Co_x)_2As_2$

2) How do we explain the temperature dependence of the susceptibility?

3) Are spin fluctuations causing the elastic constants to soften?