What we have learned from $Ba(Fe_{1-x}TM_x)_2As_2$ studies: empirical rules to inform theory

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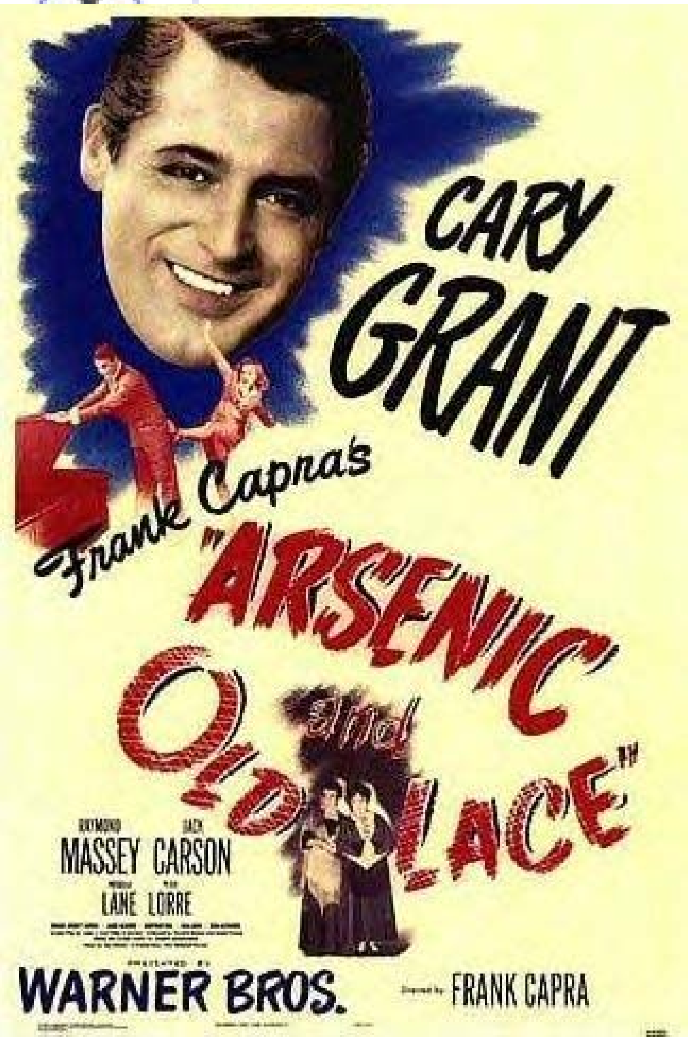
Physics 590 B



Between February and May of 2008 two related classes of FeAs based compounds were found to superconduct.

These compounds have T_c values that span from ~ 30 K to over 55 K; they appear to be part of a diverse and varied set of FeAs based materials and show early promise of being "user friendly" in terms of their superconductivity, although they are unfriendly in terms of arsenic….

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†,‡,§

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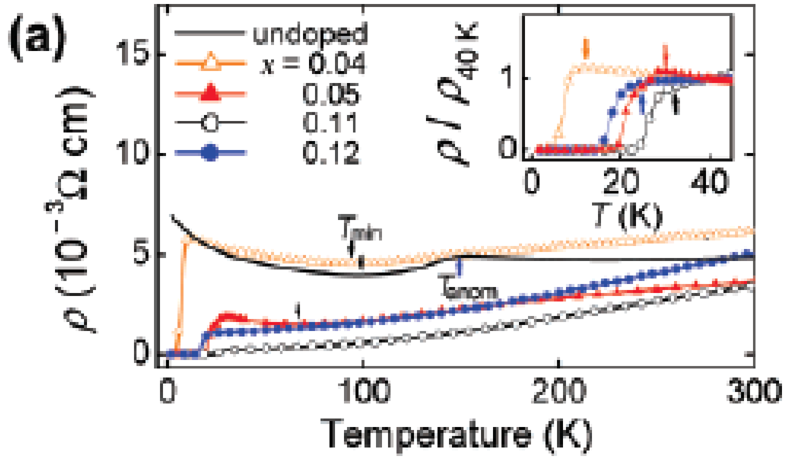
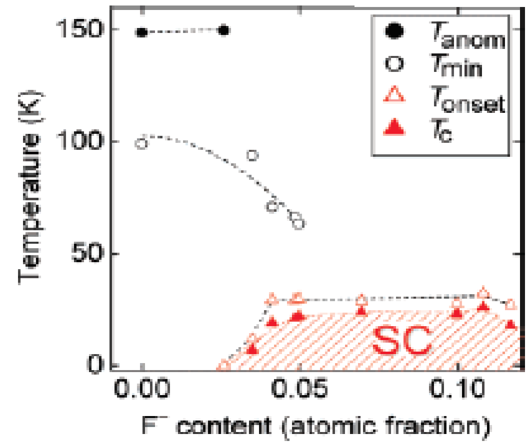
Published on Web 02/23/2008





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

(Received 29 May 2008; published 5 September 2008)

Marianne Rotter, Marcus Tegel, and Dirk Johrendt*

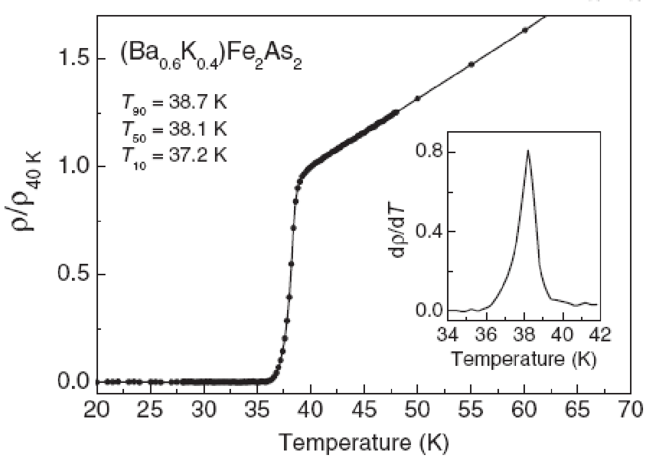
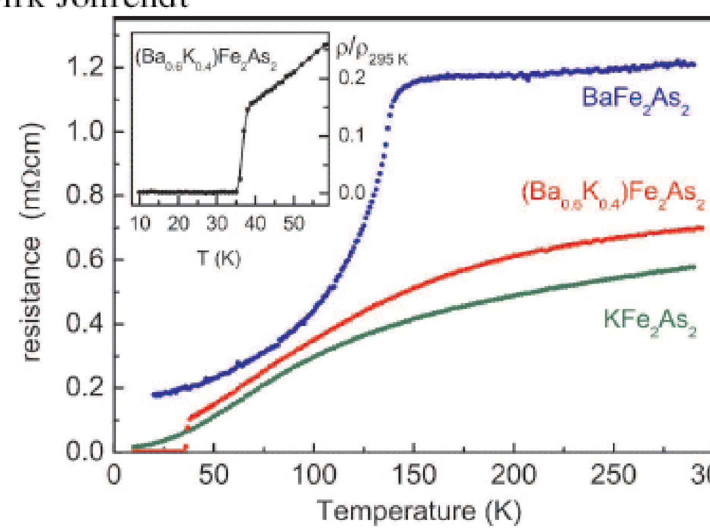


FIG. 4. Resistivity transition of ($Ba_{0.6}K_{0.4}$)Fe_2As_2.



In both of these structures there is a square planar sheet of Fe that is capped top and bottom with As. The AE or R-O layers separate these FeAs units.

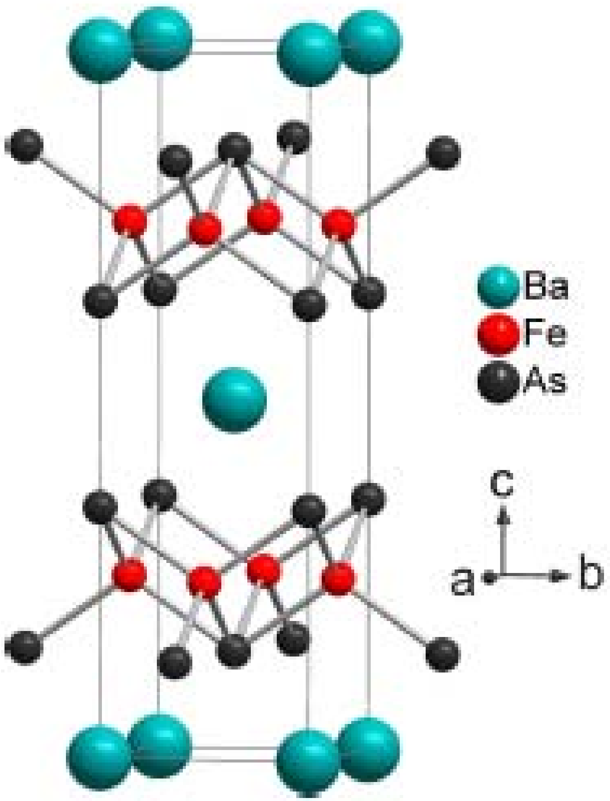
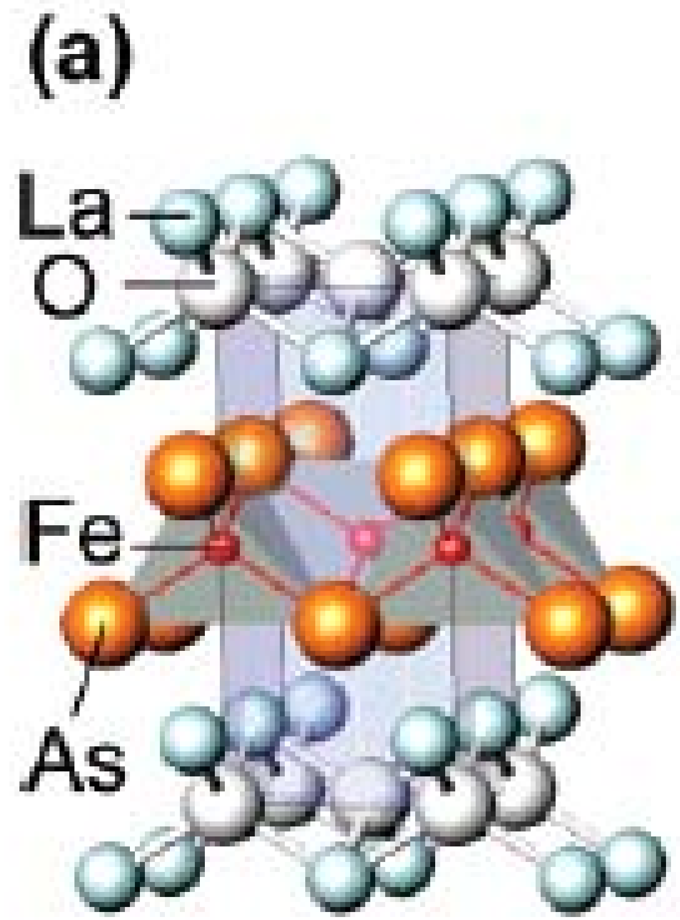


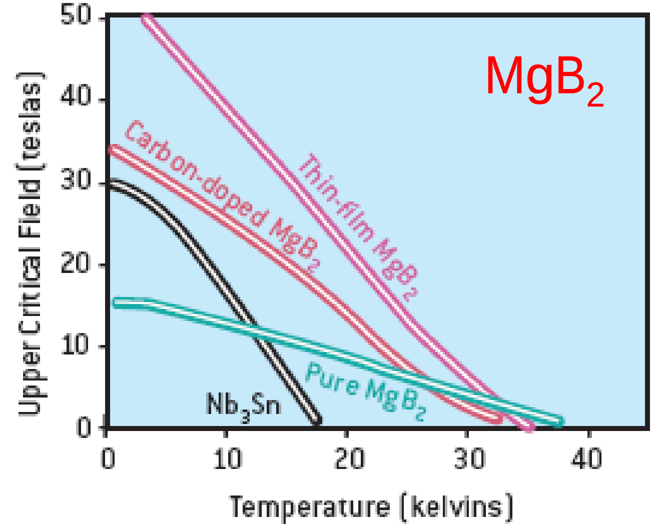
FIG. 1: Crystal structure of $BaFe_2As_2$.

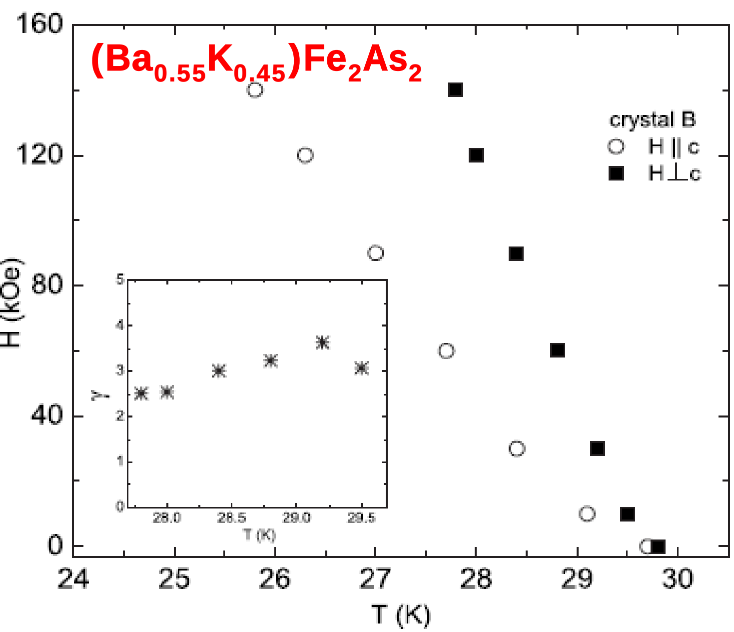


Single crystals of the $AEFe_2As_2$ (AE = Ba, Sr, Ca) compounds can be grown out of Sn and FeAs readily.

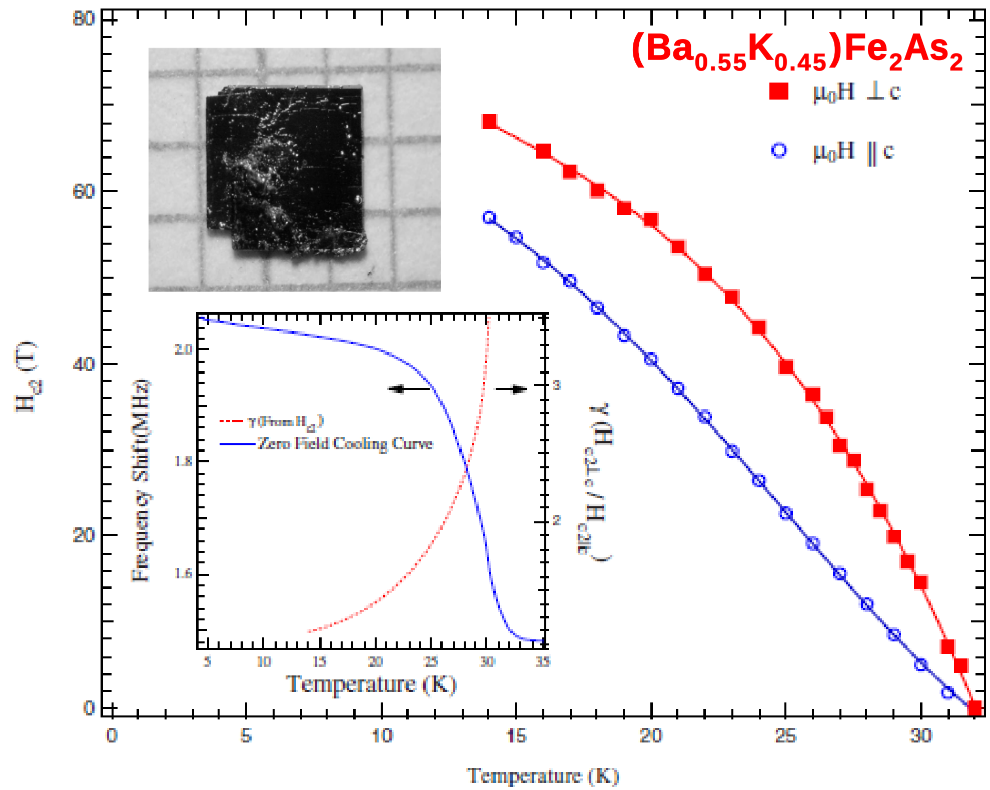
Anisotropic $H_{c2}(T)$ data indicate that FeAs compounds may well be of practical as well as basic interest.

PAUL C. CANFIELD AND SERGEY L. BUD'KO SCIENTIFIC AMERICAN APRIL 2005 81





NI *et al.* PHYSICAL REVIEW B 78, 014507 (2008)



ALTARAWNEH *et al.* PHYSICAL REVIEW B 78, 220505(R) (2008)

PHYSICAL REVIEW B 78, 104505 (2008)

Co-doping can be used to stabilize T_c!!

Superconductivity in $LaFe_{1-x}Co_xAsO$

(Received 6 July 2008; revised manuscript received 4 August 2008; published 10 September 2008)

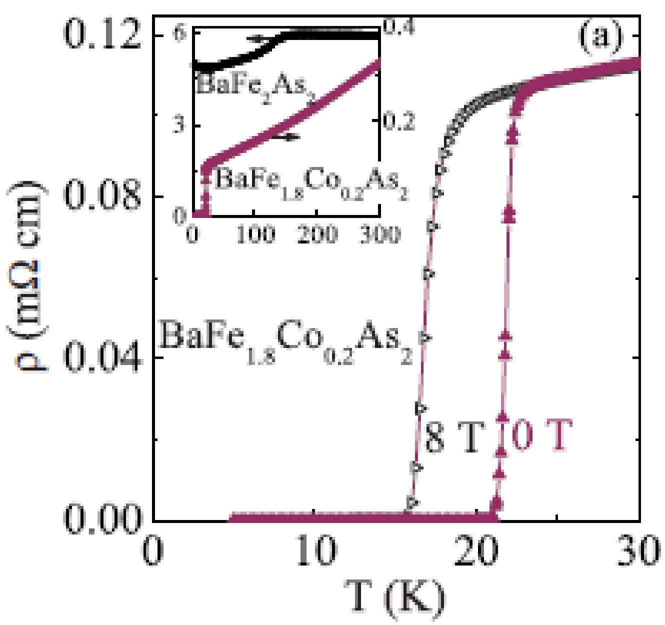
Athena S. Sefat,[1] Ashfia Huq,[2] Michael A. McGuire,[1] Rongying Jin,[1] Brian C. Sales,[1] David Mandrus,[1] Lachlan M. D. Cranswick,[3] Peter W. Stephens,[4] and Kevin H. Stone[4]

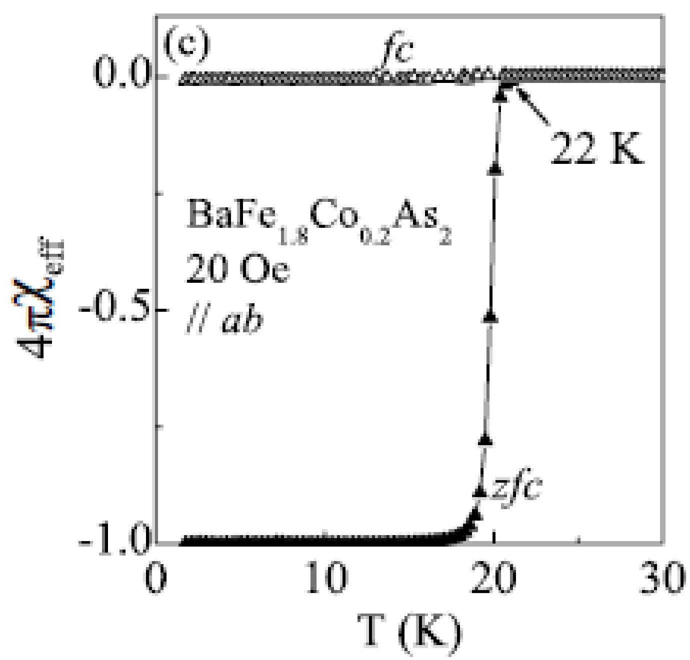
PRL 101, 117004 (2008) PHYSICAL REVIEW LETTERS week ending 12 SEPTEMBER 2008

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

(Received 25 July 2008; published 11 September 2008)



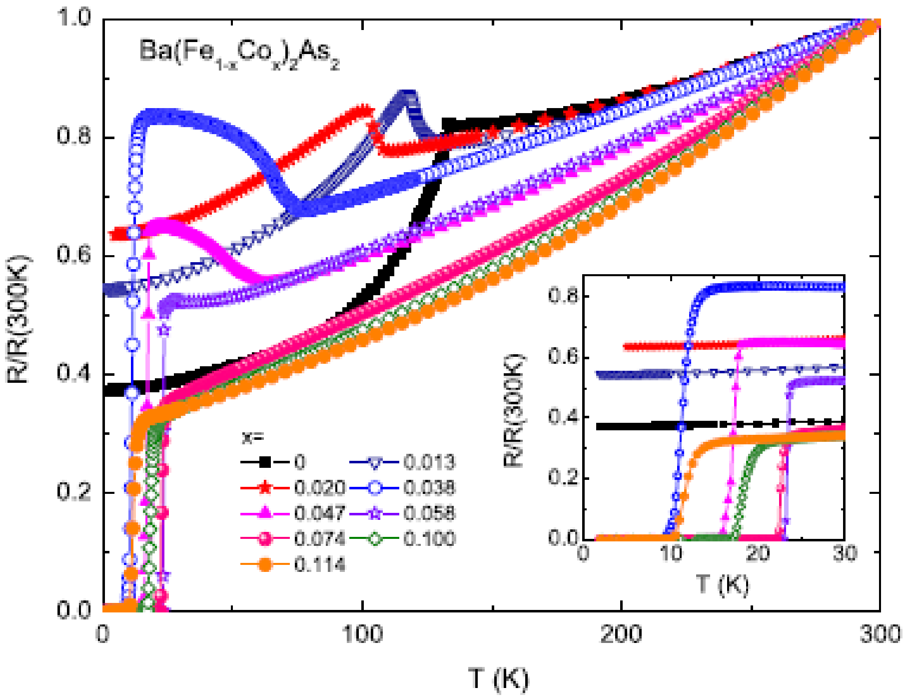


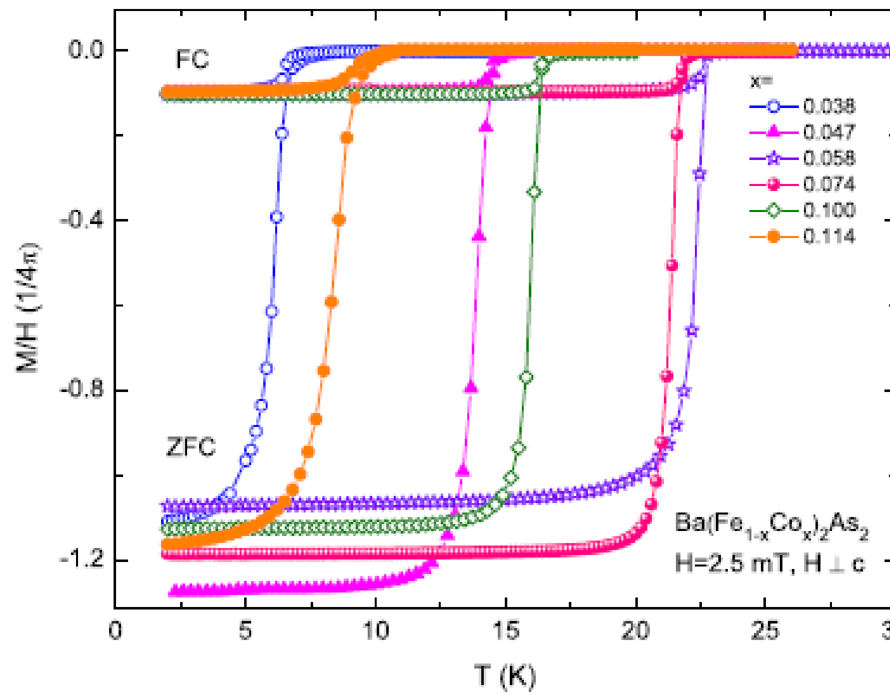
PHYSICAL REVIEW B 78, 214515 (2008)

Effects of Co substitution on thermodynamic and transport properties and anisotropic H_{c2} in $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals

N. Ni,[1] M. E. Tillman,[1] J.-Q. Yan,[1] A. Kracher,[1] S. T. Hannahs,[2] S. L. Bud'ko,[1] and P. C. Canfield[1]

(Received 11 November 2008; published 29 December 2008)

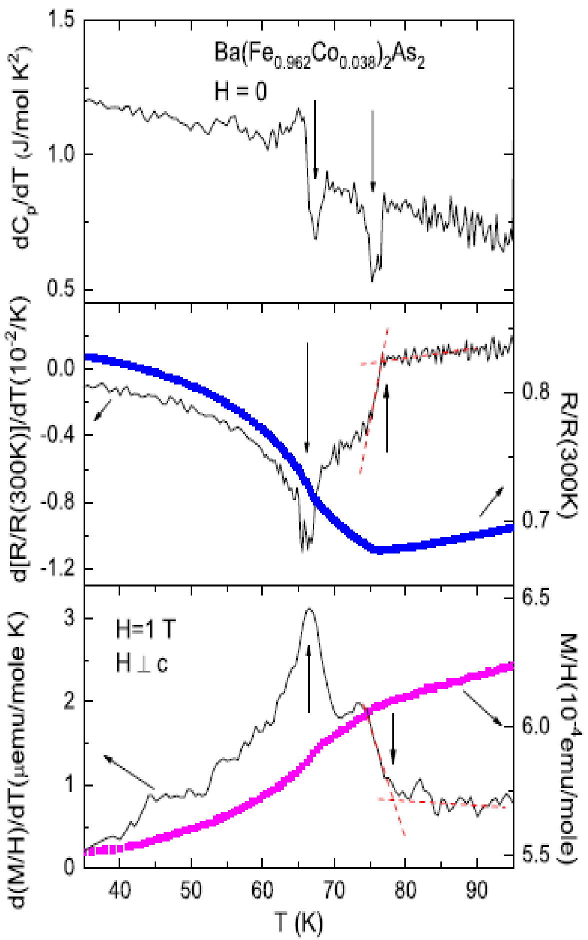


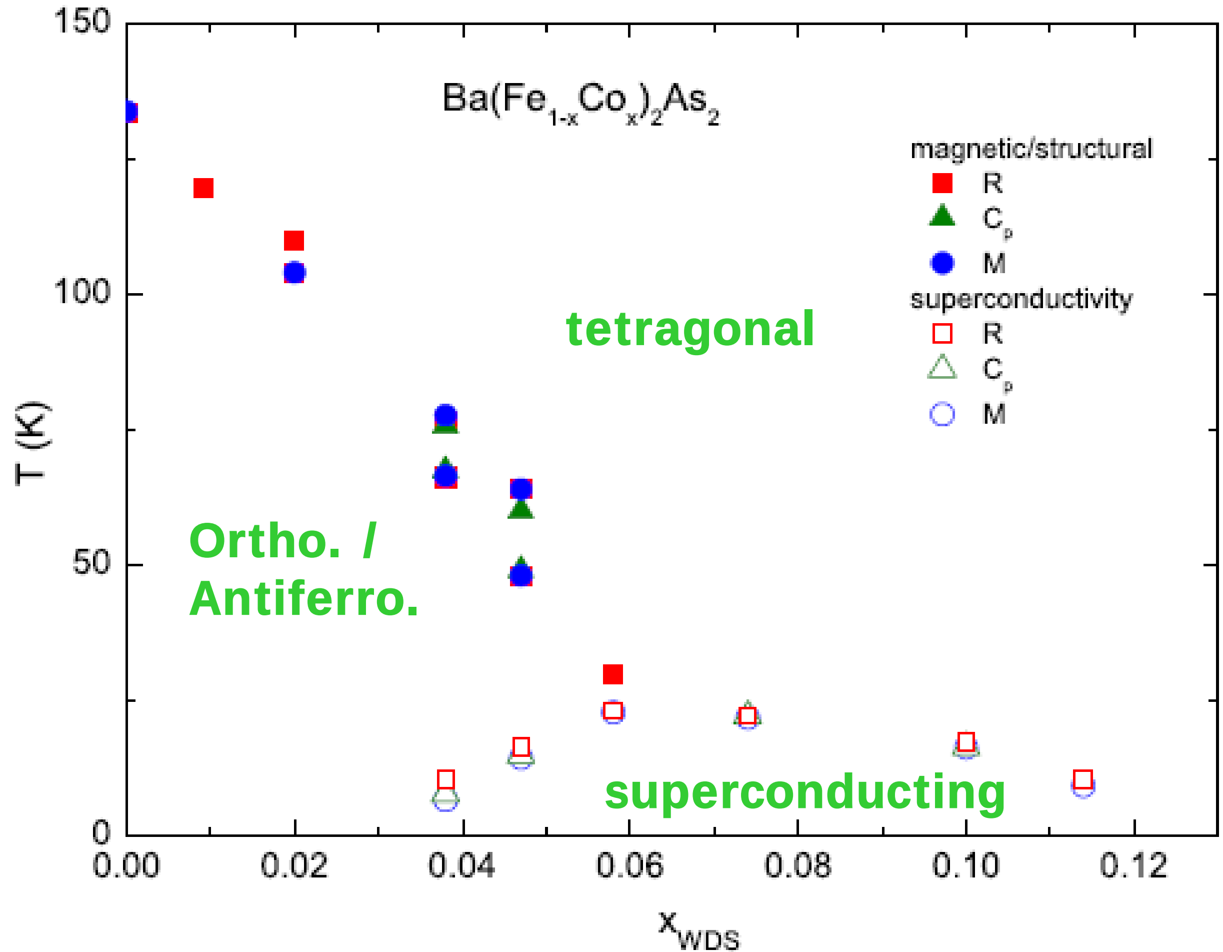


Doping of $AEFe_2As_2$ compounds on the Fe site with transition metals (TM) is important for two basically different reasons: (i) very different from CuO-based superconductors, (ii) offered easier and more homogeneous doping than K- or other alkali-doping.

Using thermodynamic and transport data we could assemble a T-x phase diagram that clearly showed (i) superconducting dome existing in both ortho/AF and tetragonal phases and (ii) a splitting (or broadening) of the x = 0 simultaneous orthorhombic and antiferromagnetic phase transition. Similar results were posted soon after by Fisher's group: Jiun-Haw Chu PHYSICAL REVIEW B 79, 014506 (2009)

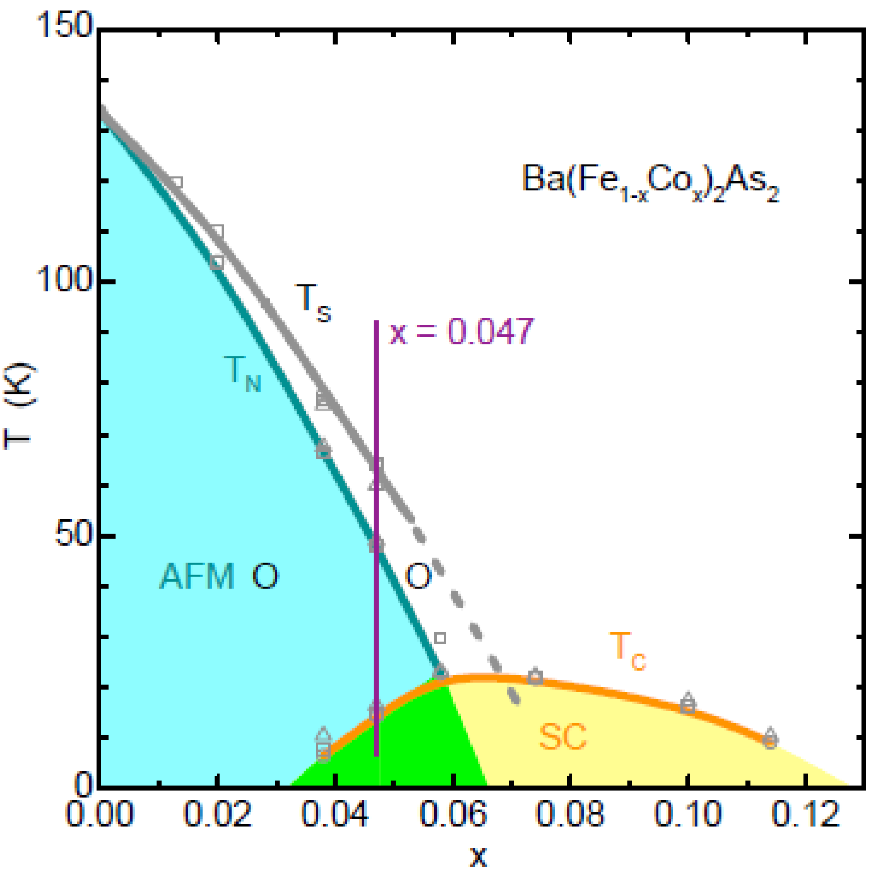
To clarify point (ii) microscopic data was needed....

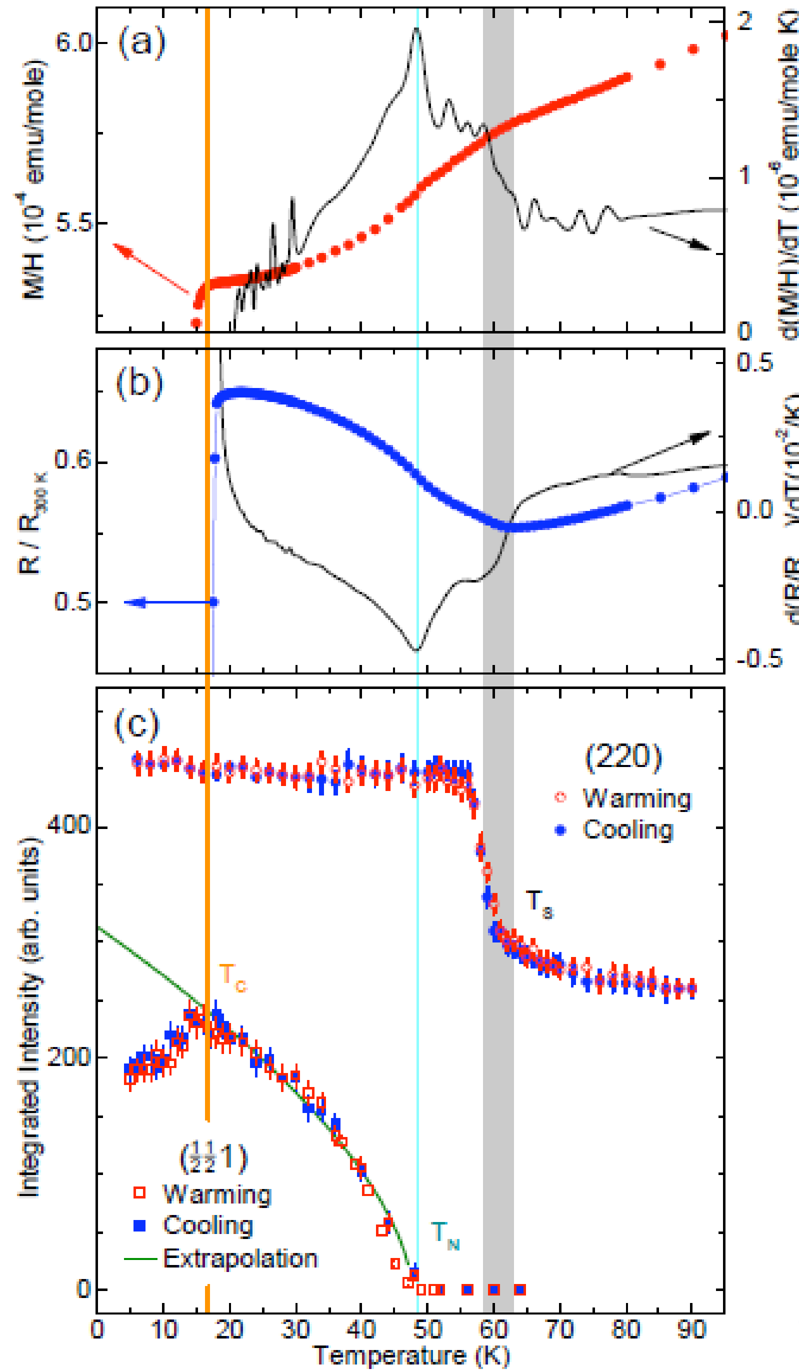




NI et al. PHYSICAL REVIEW B 78, 214515 (2008)

Neutron and X-ray scattering clarified the question of splitting / broadening. There is a clear separation between the structural (upper transition) and magnetic (lower). This confirms the criterion we used to infer them from our bulk measurements.





Pratt et al. ArXiv 0903.2833 PRL in press

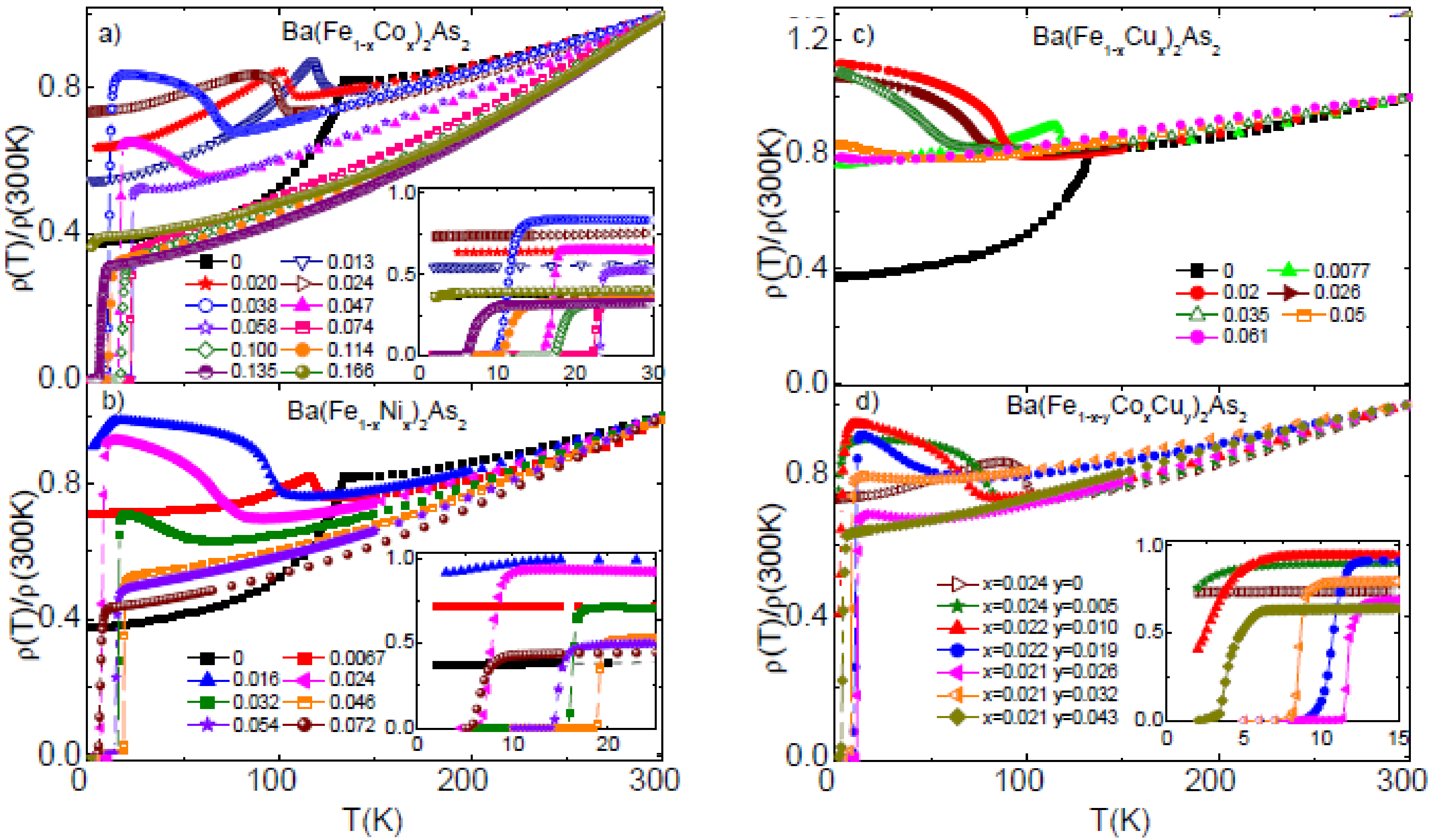
Decoupling of the superconducting and magnetic/structural phase transitions in electron-doped $BaFe_2As_2$

P. C. Canfield, S. L. Bud'ko, Ni Ni, J. Q. Yan, and A. Kracher

Ni- and Cu-doping suppress the upper transitions in a manner similar to Co.

Whereas Ni stabilizes superconductivity, Cu does not (at least above 2 K).

To prove that Cu-doping was not poisonous to S.C. we examined a Co/Cu doping.



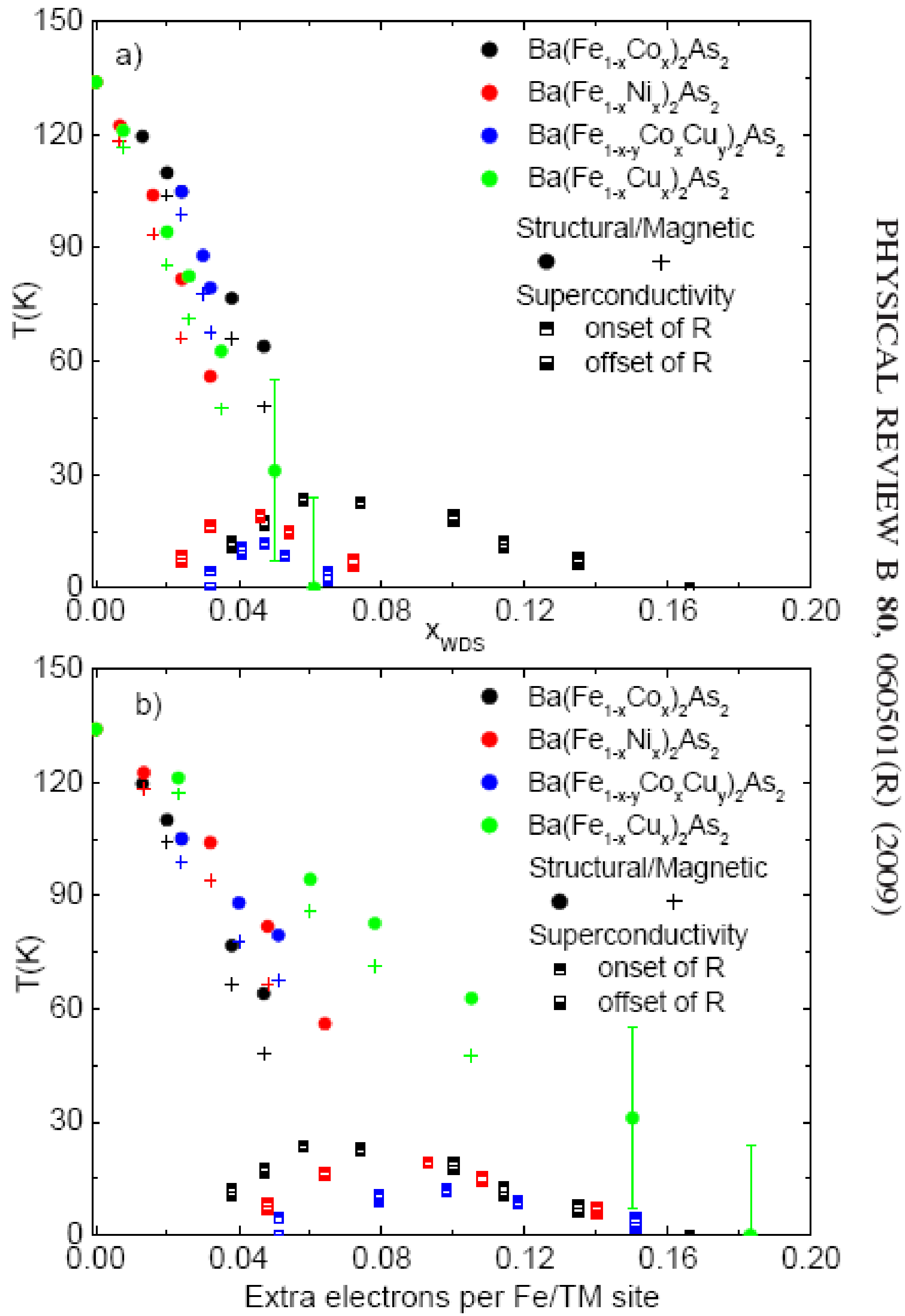
PHYSICAL REVIEW B 80, 060501(R) (2009)

By substituting various TM for Fe in $BaFe_2As_2$ we change vary a number of different, but correlated, parameters.

The two most obvious are the number of impurities (x) and the change in electron count (e).

We directly measure x for each sample via WDS and we infer e as follows: for Co --- e = x, for Ni --- e = 2x, for Cu --- e = 3x.

Whereas the upper, structural and magnetic phases transitions scale better with x, the lower, superconducting phase transition scales with e, especially on the overdoped side of the dome.

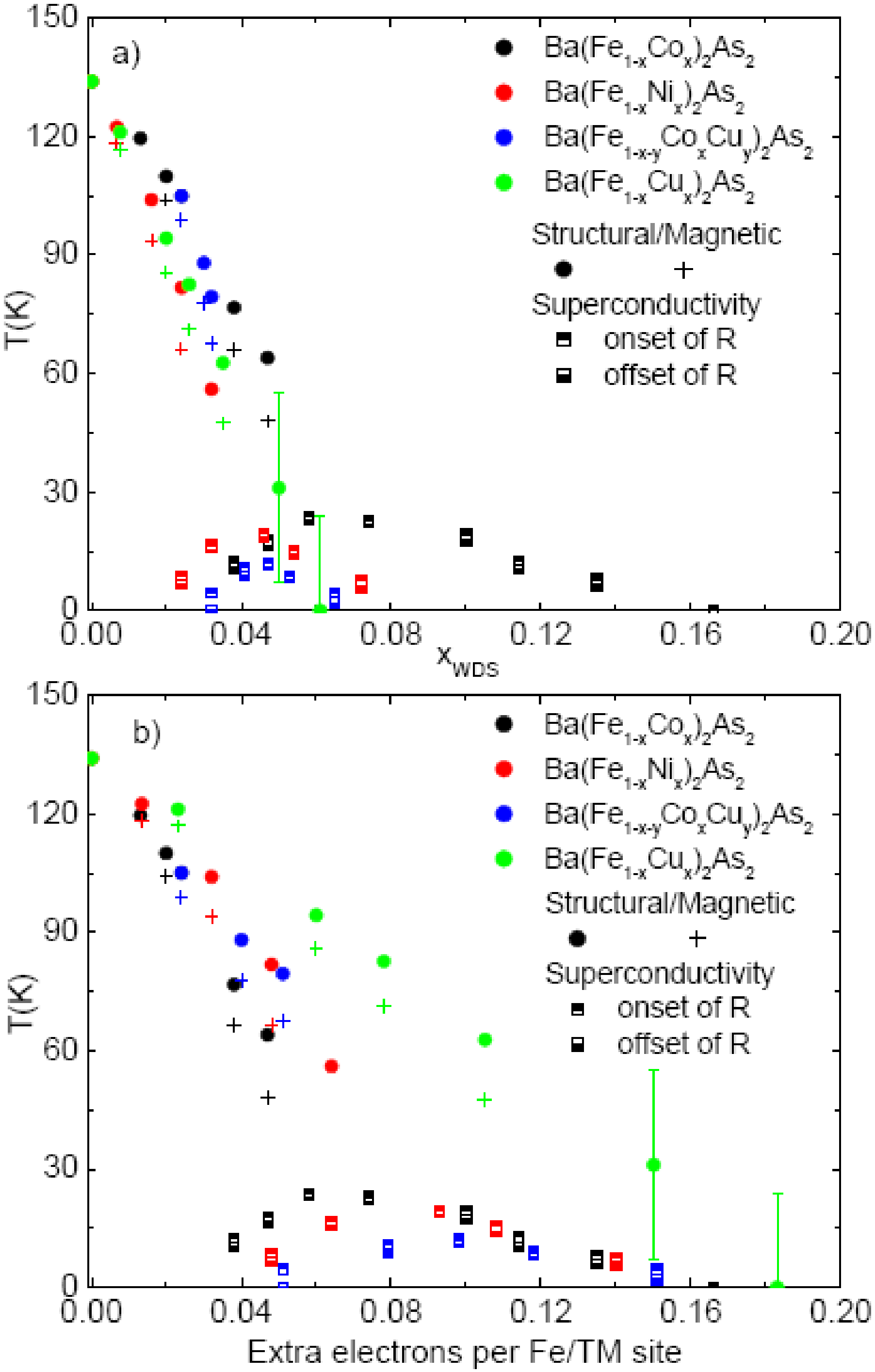


These data show that suppression of the upper, structural / antiferromag transitions is a necessary, but not sufficient condition for superconductivity.

There is a region of e (bandfilling) that can support superconductivity IF the structural / AF transition ($T_{S/M}$) is suppressed sufficiently.

We can hypothesize that if $T_{S/M}$ is suppressed sufficiently, then the low temperature state is sufficiently similar to the tetragonal state that the superconductivity can be stabilized, even in the ordered state. *<u>(E.g. reduce the size of distortion and / or ordered moment or change fluctution spectrum.)</u>*

This can explain poorer scaling of T_c with e on under doped side.



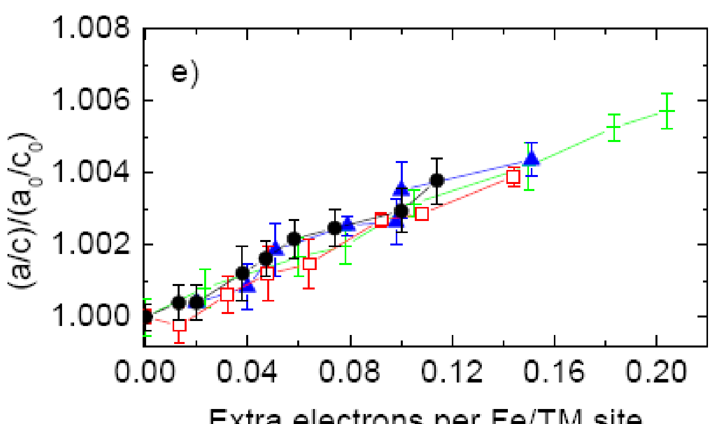
PHYSICAL REVIEW B 80, 060501(R) (2009)

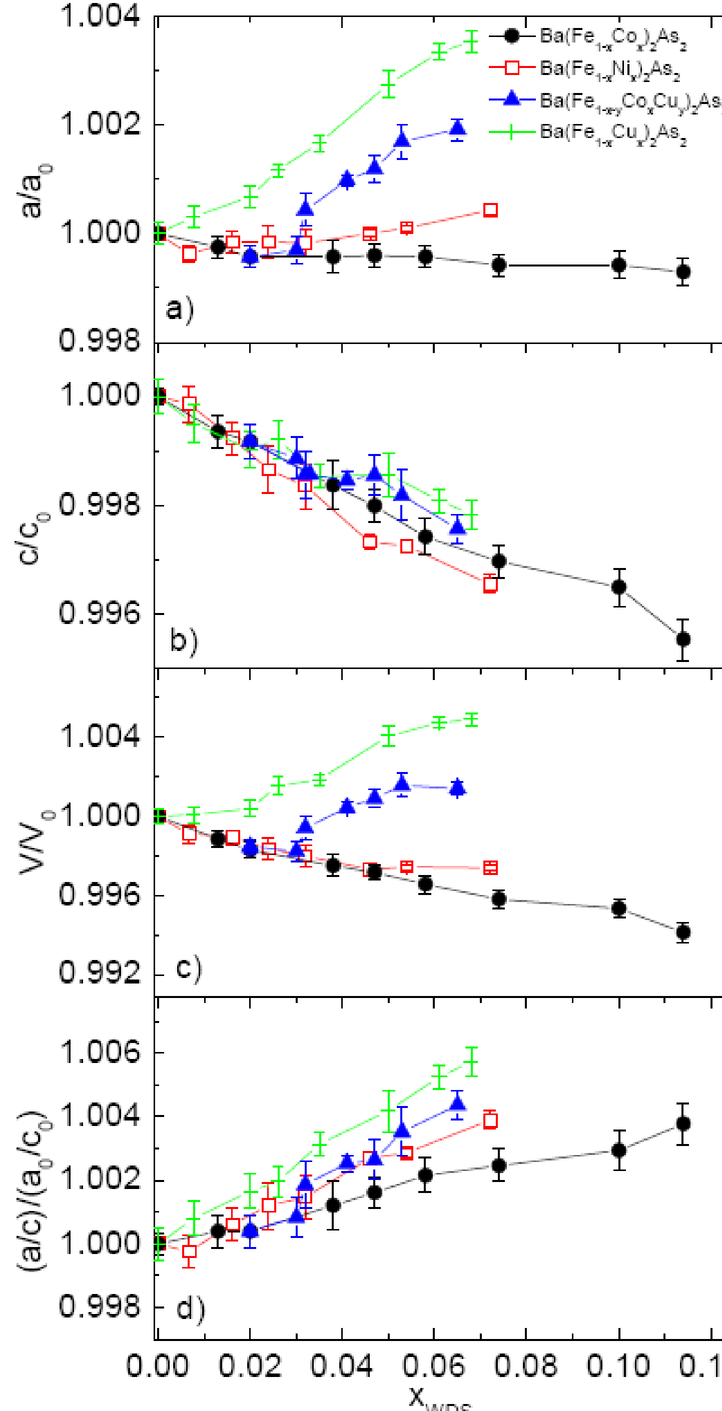
By substituting various TM for Fe in $BaFe_2As_2$ we change vary a number of different, but correlated, parameters.

x and e are not the only parameters that vary with doping: the lattice parameters change as well.

For 3d-TM doping, we find that c/c_0 varies as x and $(a/c)/(a_0/c_0)$ varies as e.

A key question is, “Can we separate x and e from the structural, c and a/c, parameters?





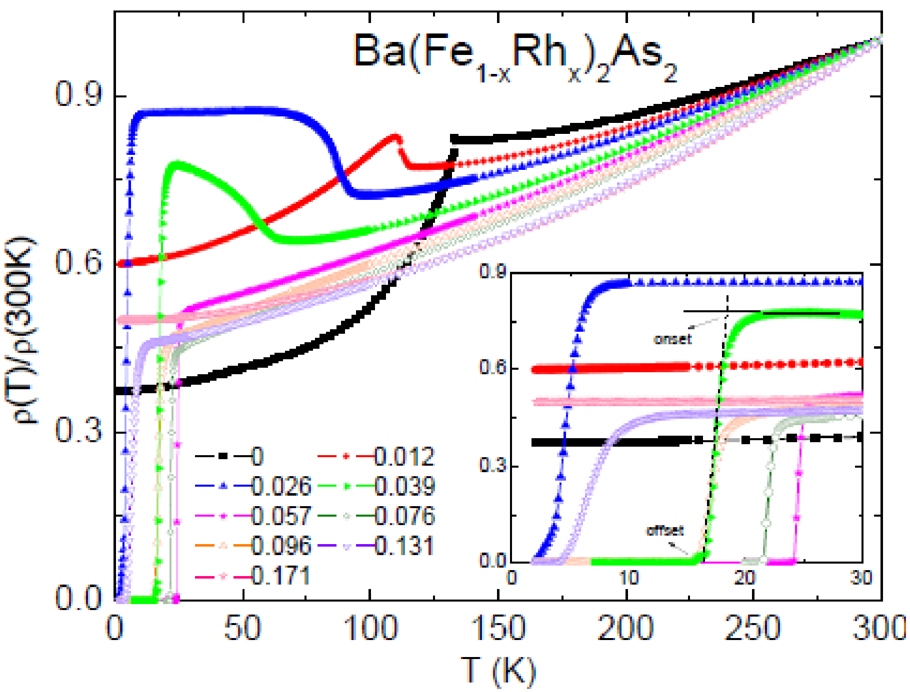
PHYSICAL REVIEW B 80, 060501(R) (2009)

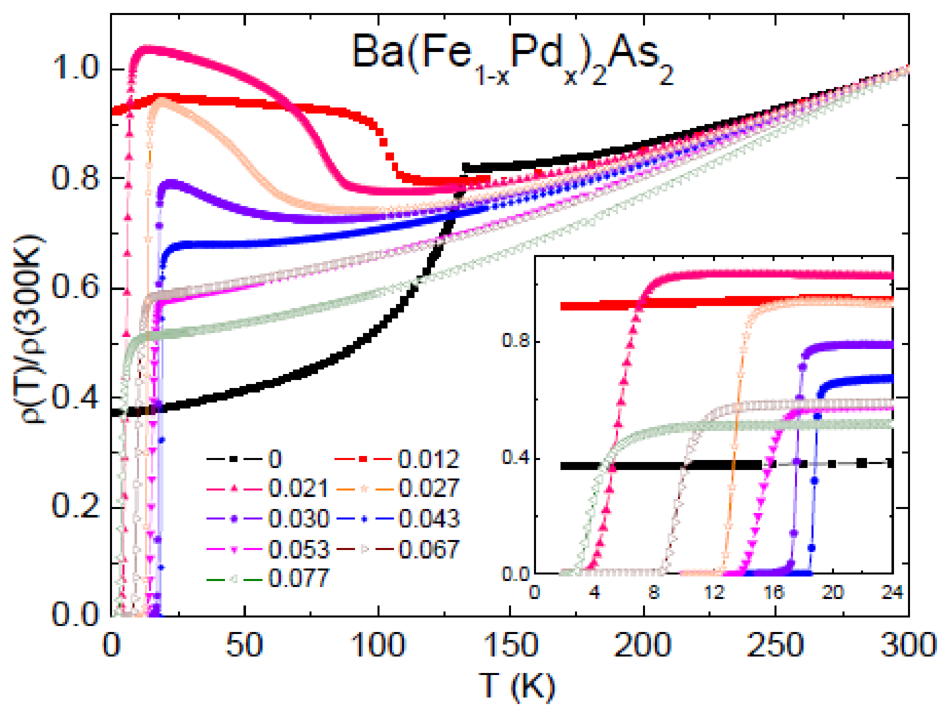
To do this we studied the isoelectronic, 4d-TM doping series.

PHYSICAL REVIEW B **80**, 024511 (2009)

Phase diagrams of $Ba(Fe_{1-x}M_x)_2As_2$ single crystals (M=Rh and Pd)

N. Ni, A. Thaler, A. Kracher, J. Q. Yan, S. L. Bud'ko, and P. C. Canfield



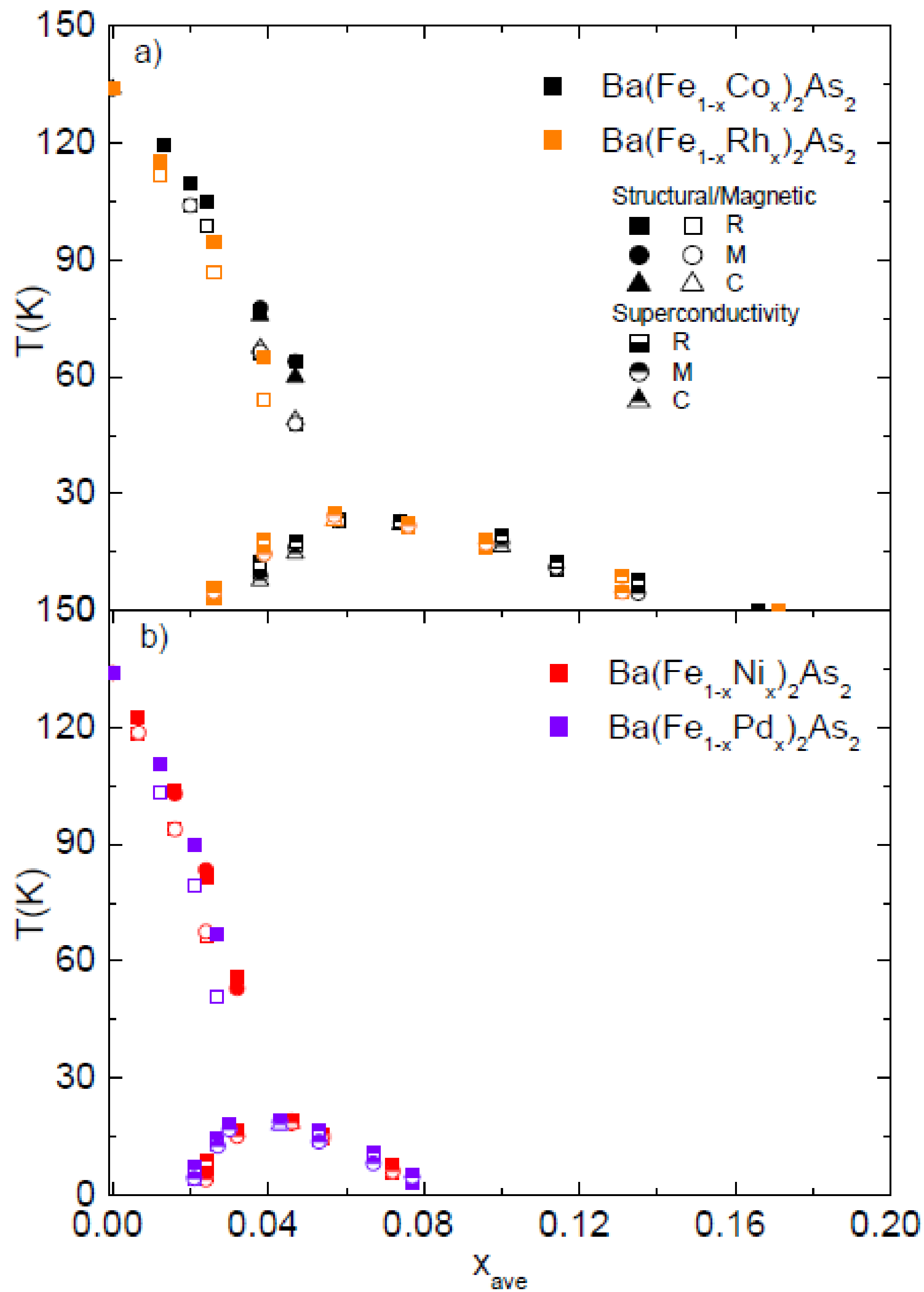


Using our thermodynamic and transport data (as well as the experimentally determined x values) we can construct T-x and T-e phase diagrams.

When we compare the isoelectronic Co- and Rh-doped series we find identical phase diagrams.

When we compare the isoelectronic Ni- and Pd-doped series we again find identical phase diagrams.

This remarkable similarity between the isoelectronic phase diagrams can only be appreciated if the actual x is determined. Nominal x-values differ from TM to TM' series.

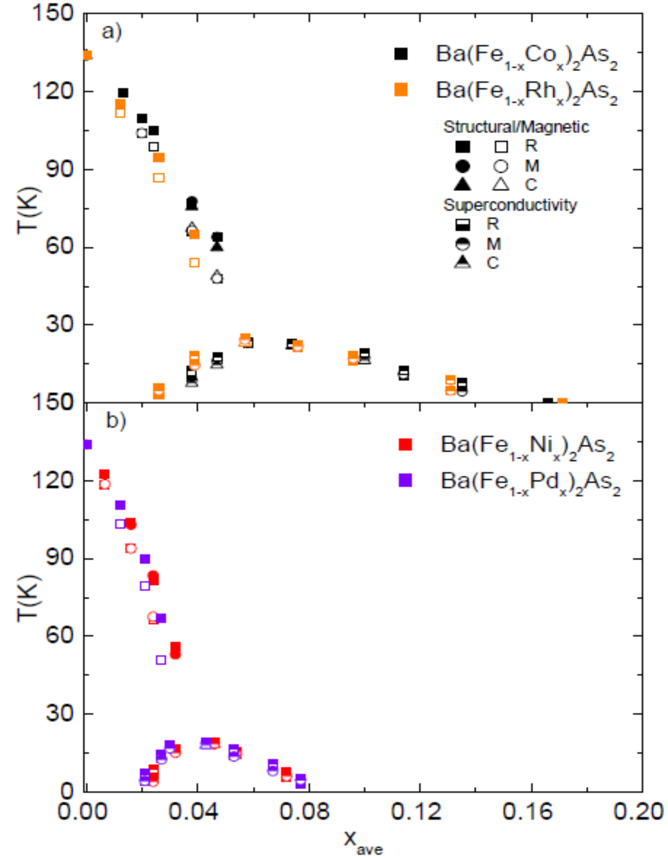


PHYSICAL REVIEW B 80, 024511 (2009)

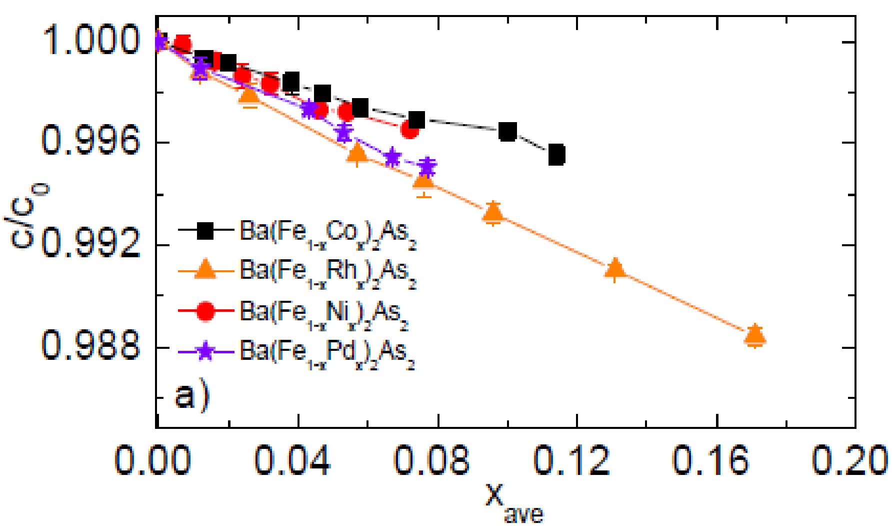
Although we find excellent scaling of the transitions with x and e, the changes in the lattice parameters (and their ratios) no longer parameterize the transitions for the 3d- and 4d-TM dopings. This can be seen in the plots of c/c_0 and $(a/c)/(a_0/c_0)$. The data group into 3d- and 4d- manifolds.

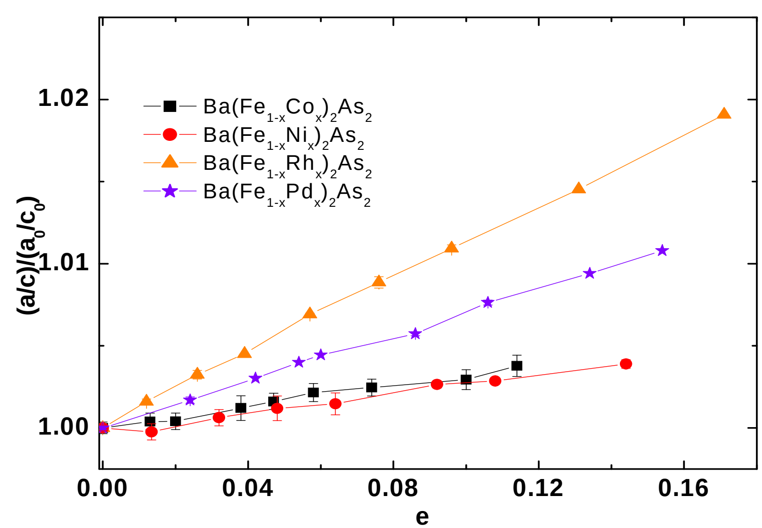
The upper phase transitions scale with a very local parameter: x.

The superconducting transition depends on e (band filling), at least on the over-doped side.

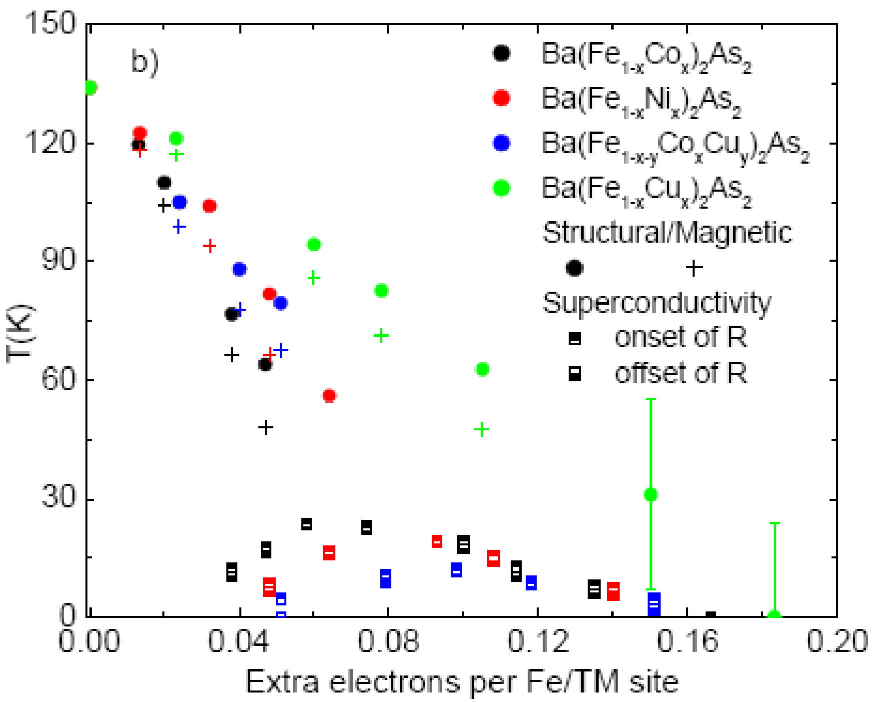


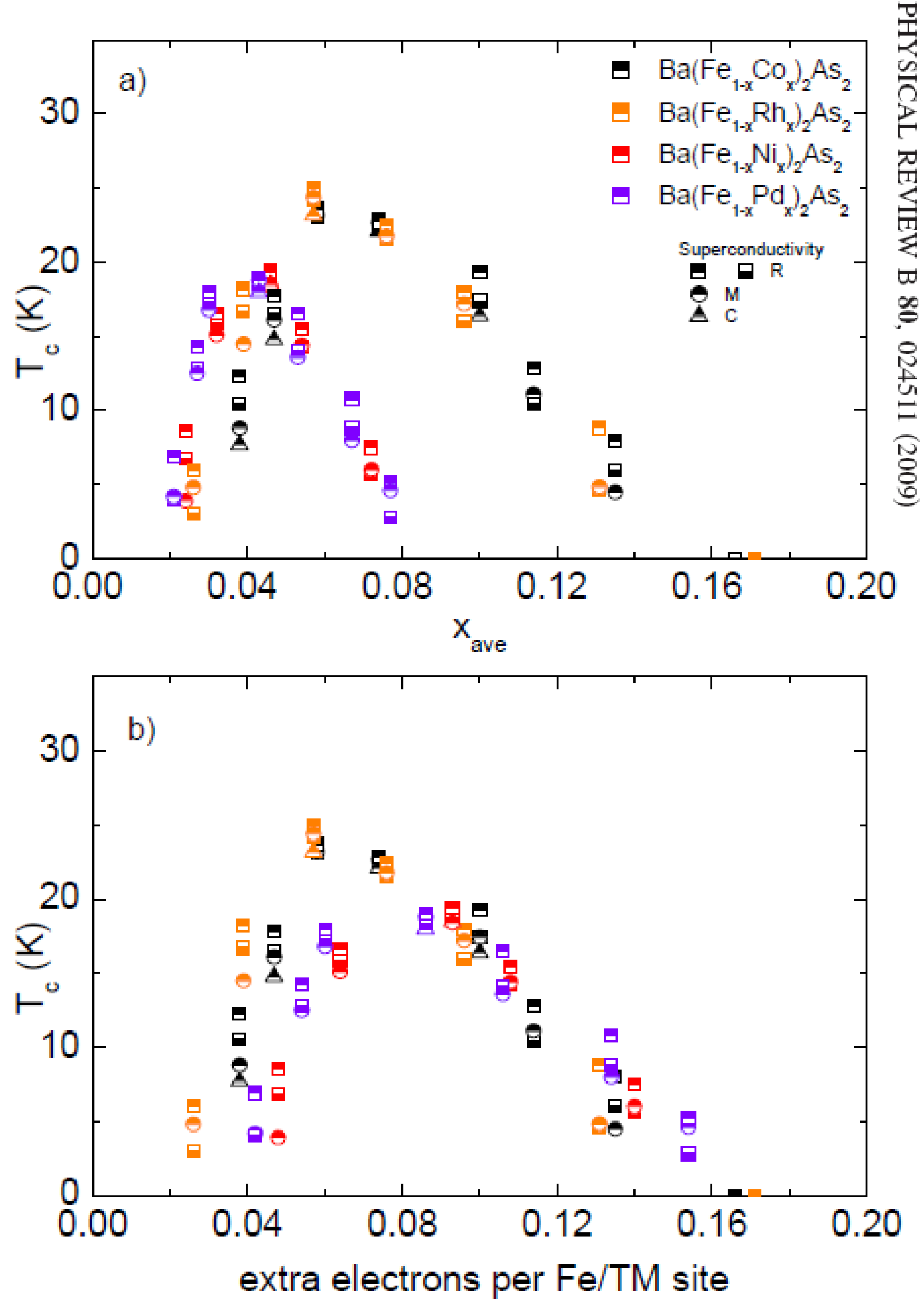
PHYSICAL REVIEW B 80, 024511 (2009)



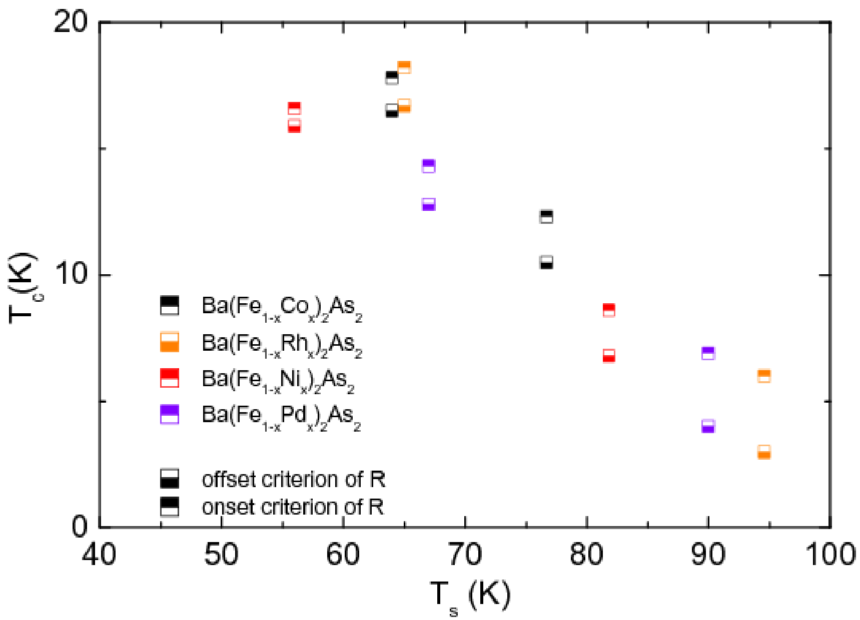


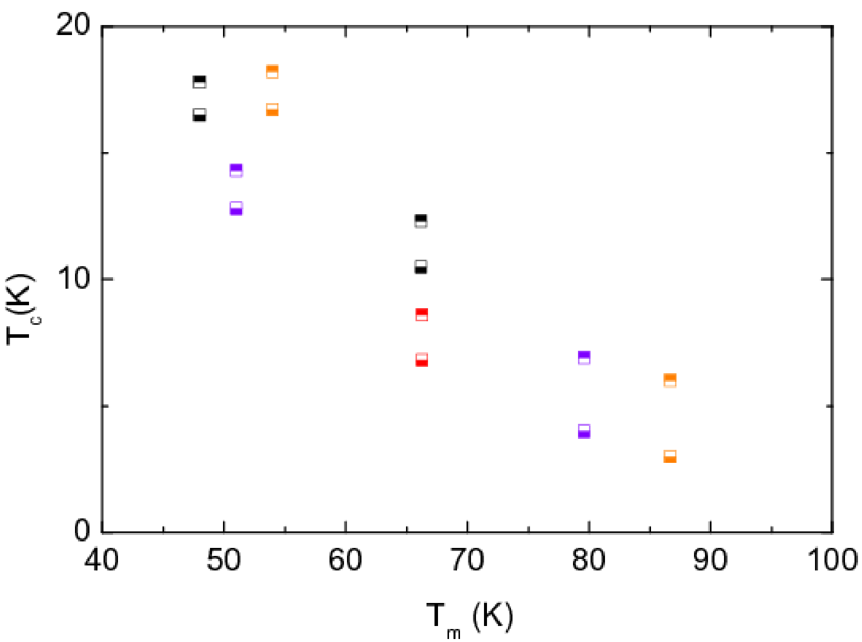
We can now examine the T_c dome is greater detail. There is excellent scaling of T_c with e on the over doped side. On the under-doped side, there is a variation that is associated with how far we have suppressed the upper transitions.



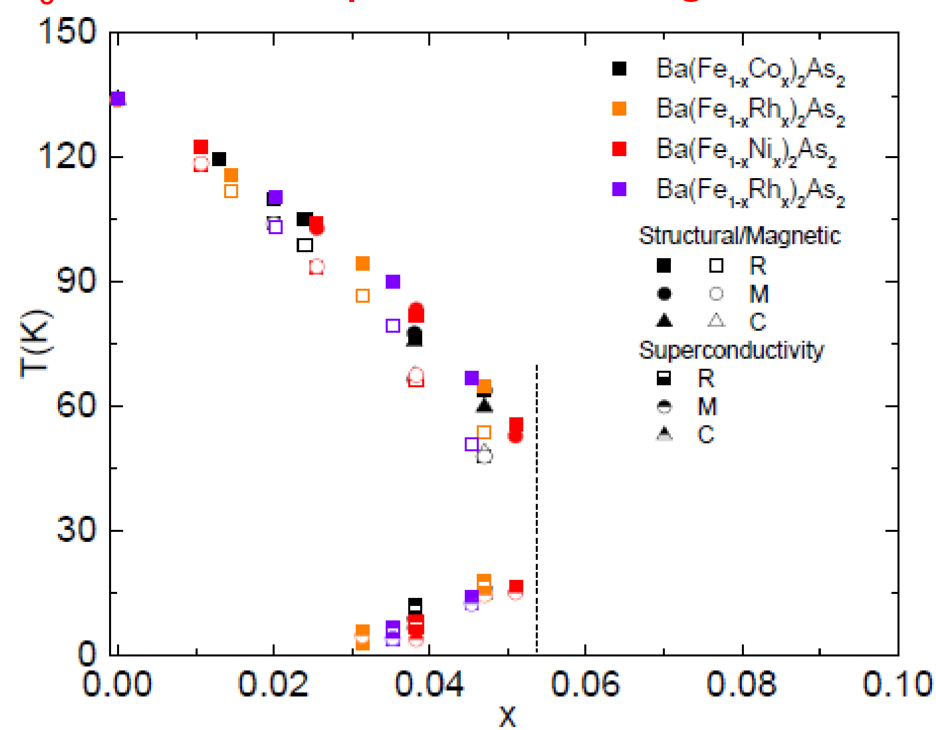


We can test this idea more quantitatively. Since there is a rough scaling between the upper transitions and x, perhaps the $T_c(x)$ scaling simply reflects the dependence of T_c on the value of the upper transition temperatures.





If we normalize the suppression of the upper transitions we see that all of the T_c curves collapse onto a single manifold.

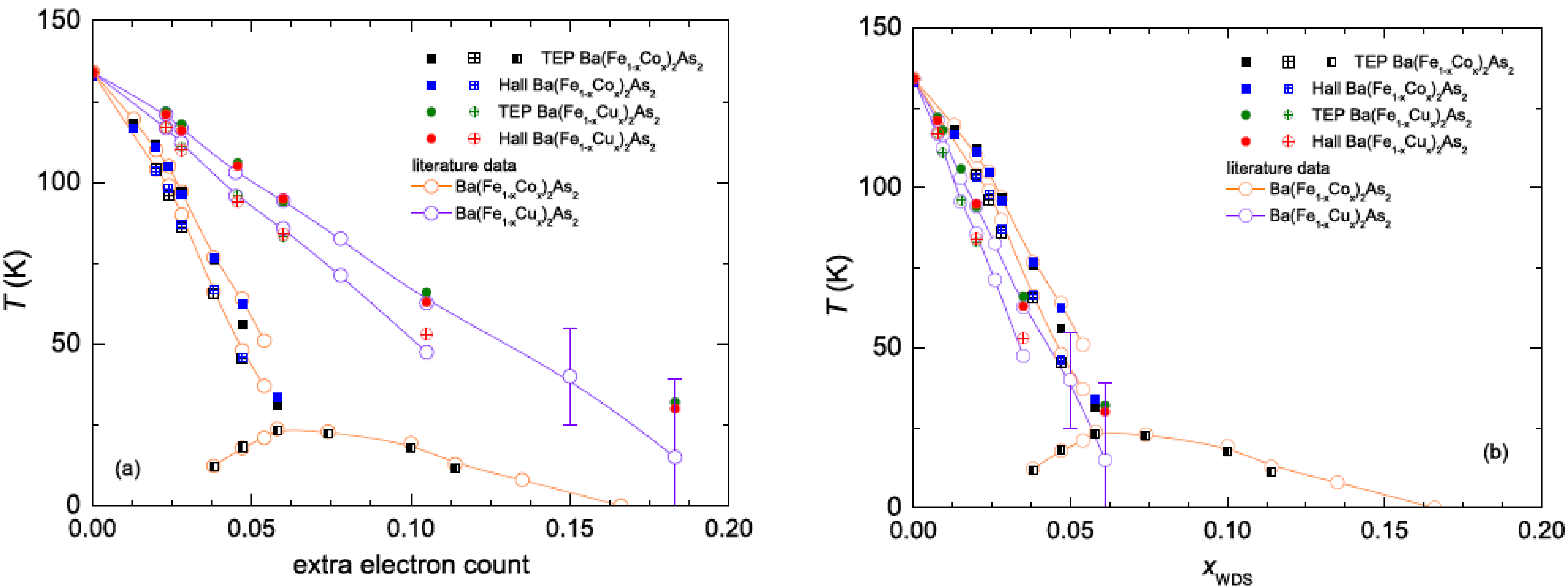


A remaining question is, what determines the low-doping onset of the superconducting dome?

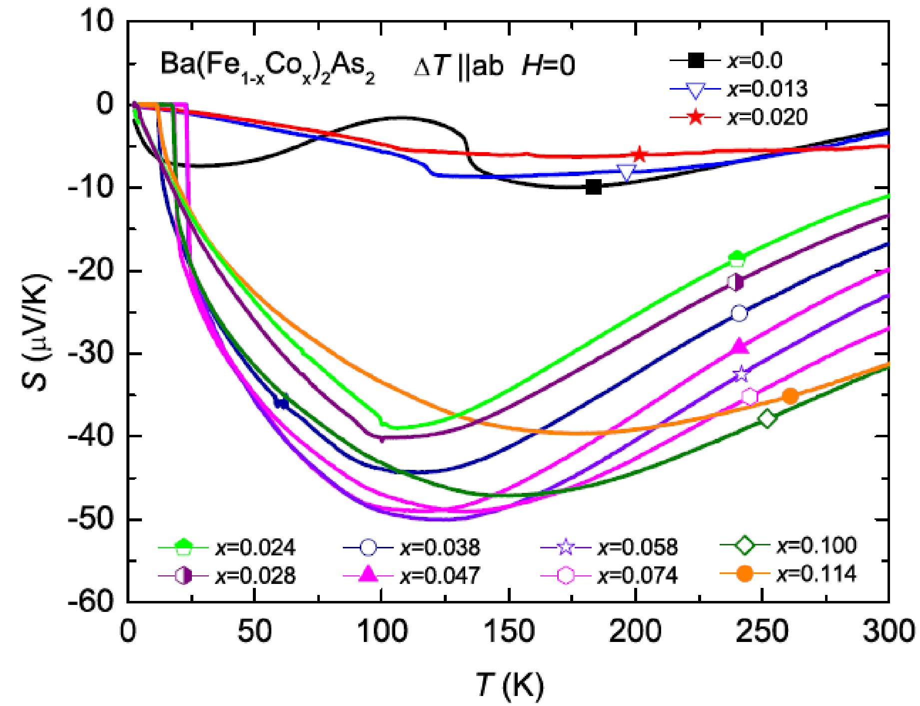
Thermoelectric power and Hall coefficient measurements on $Ba(Fe_{1-x}TM_x)_2As_2$ (TM = Co and Cu)

Eun Deok Mun, Sergey L. Bud'ko, Ni Ni, and Paul C. Canfield

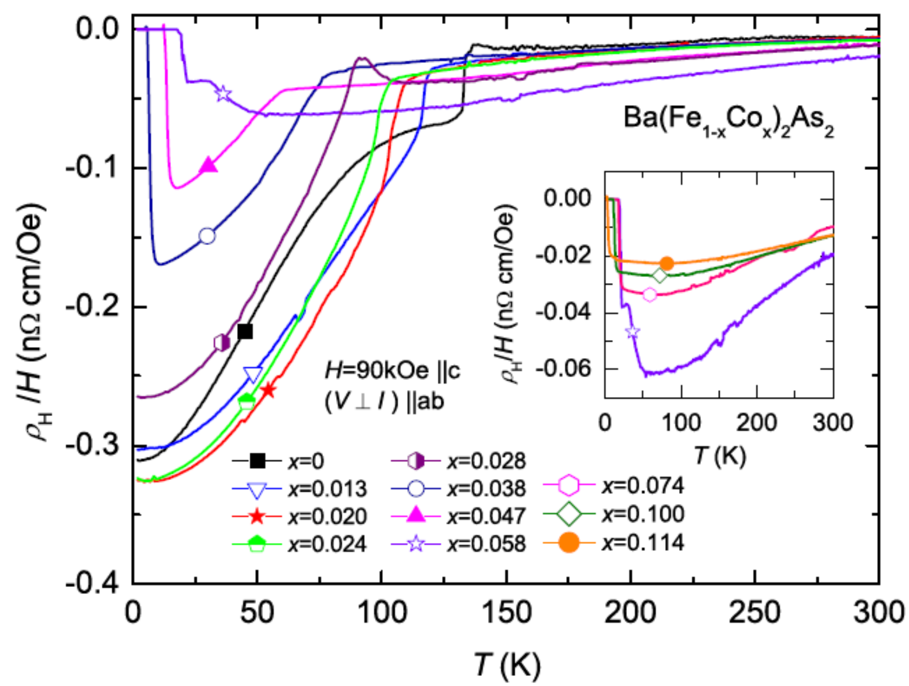
arXiv:0906:1548v2, accepted PRB



We measured the TEP and Hall coefficient for Co doped $BaFe_2As_2$, with specifically high density on the low Co-doped side.

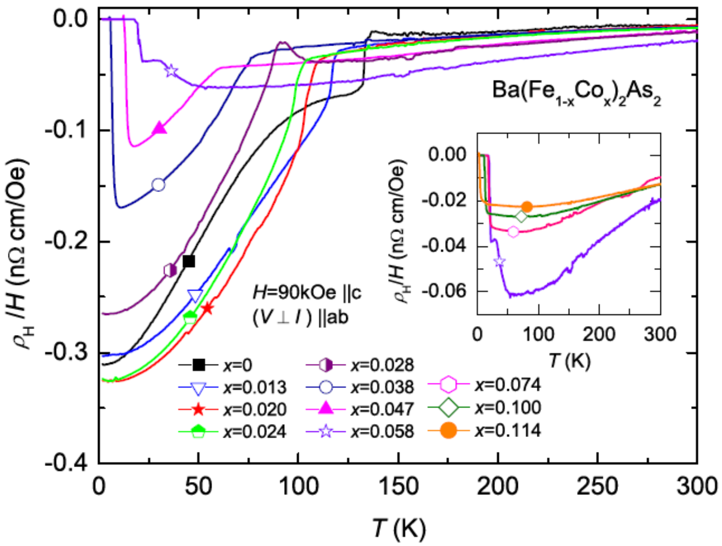


There is a dramatic change in TEP over the whole temperature range measured as x crossed from 0.02 to 0.024

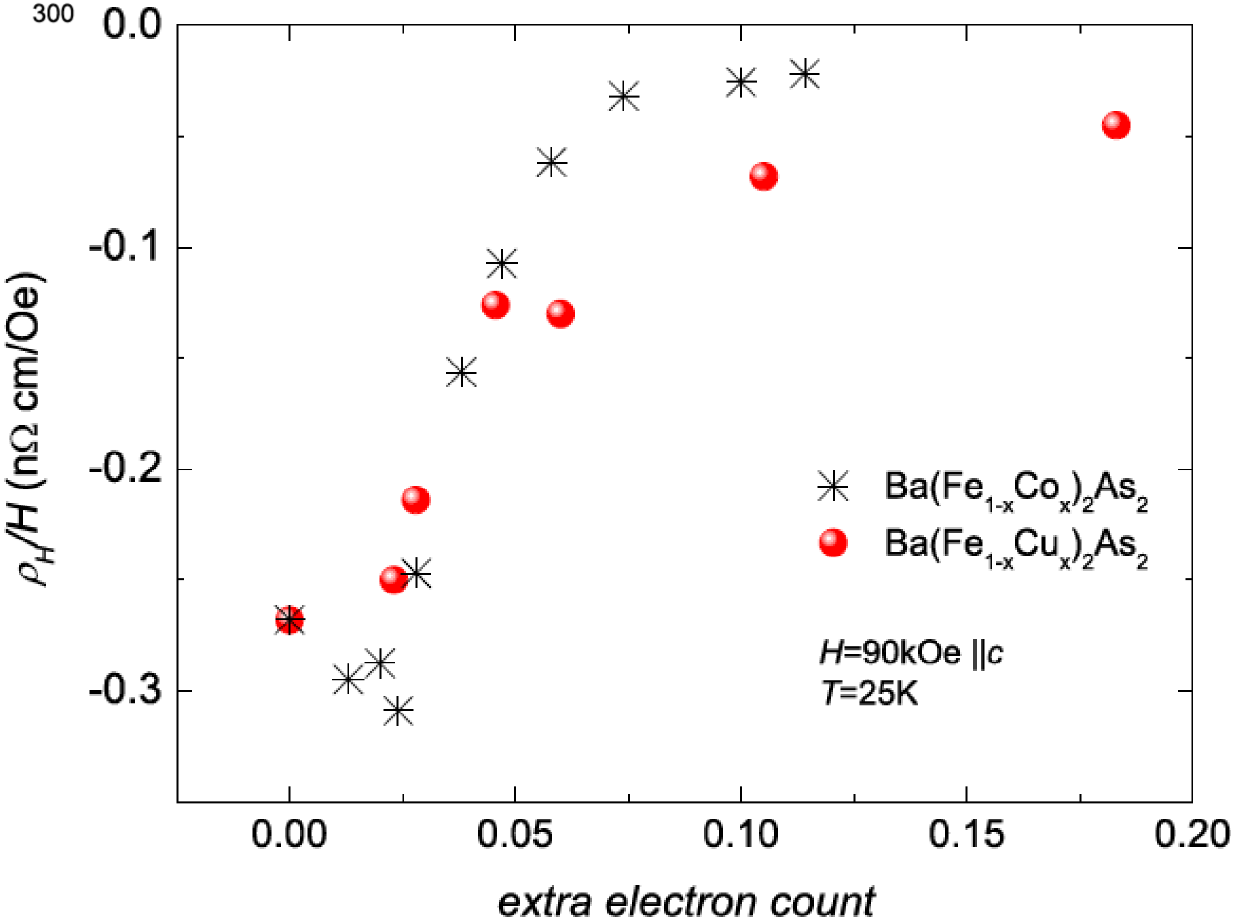


The low temperature Hall coefficient changes for the same x values.

arXiv:0906:1548v2, accepted PRB

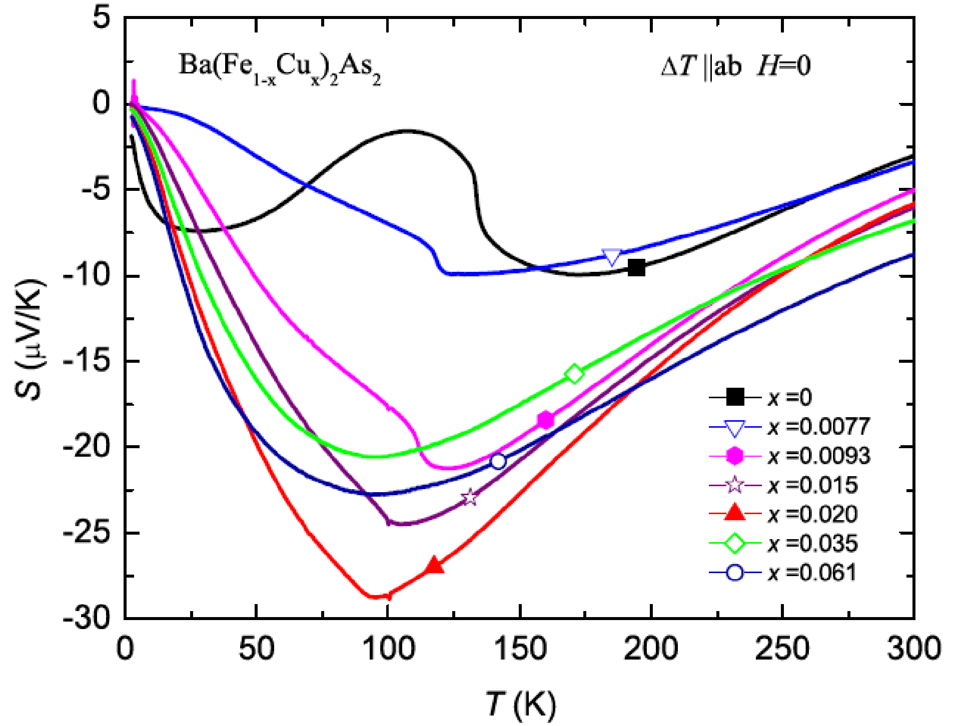


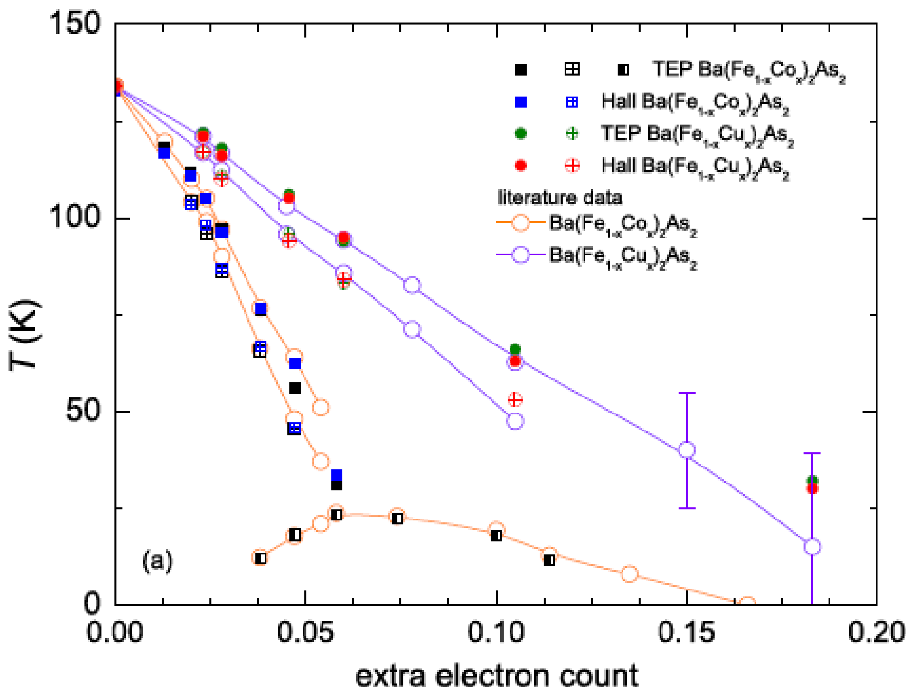
ρ_H/H at 25 K can be plotted and shows this change.

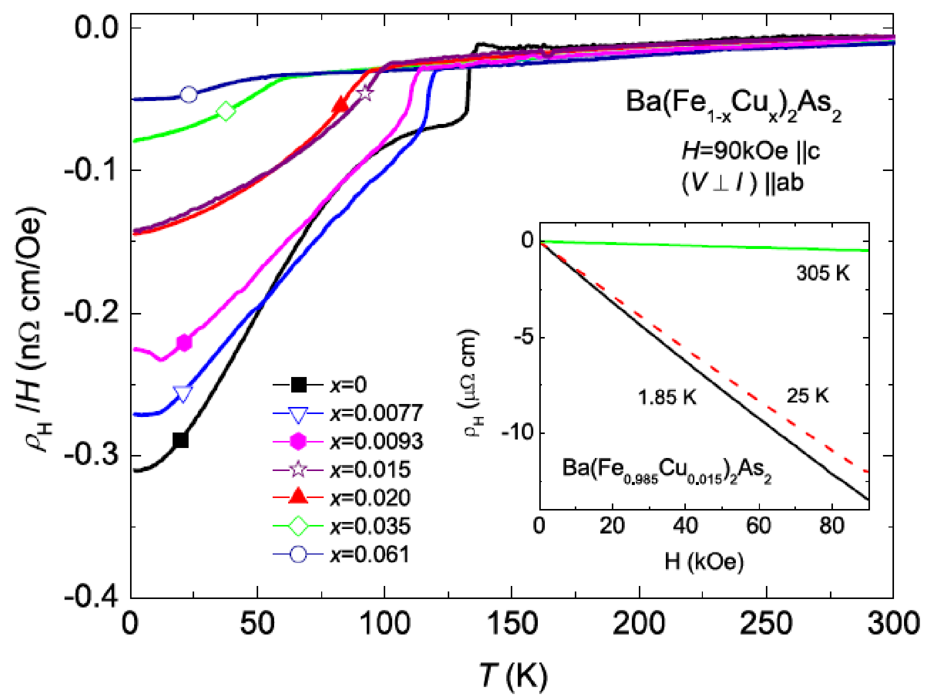


arXiv:0906:1548v2, accepted PRB

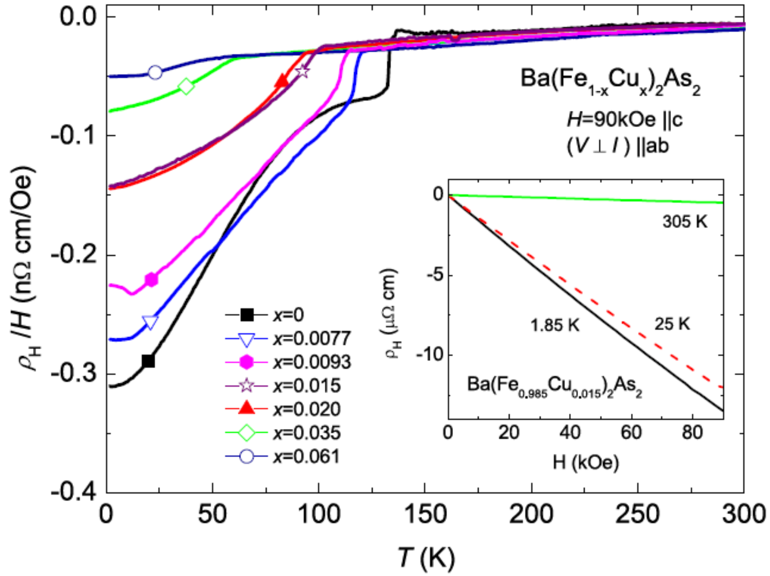
The same changes can be seen in the TEP and Hall data for Cu doping, at the same e-count. This feature appears to be associated with a band filling of e ~ 0.025.





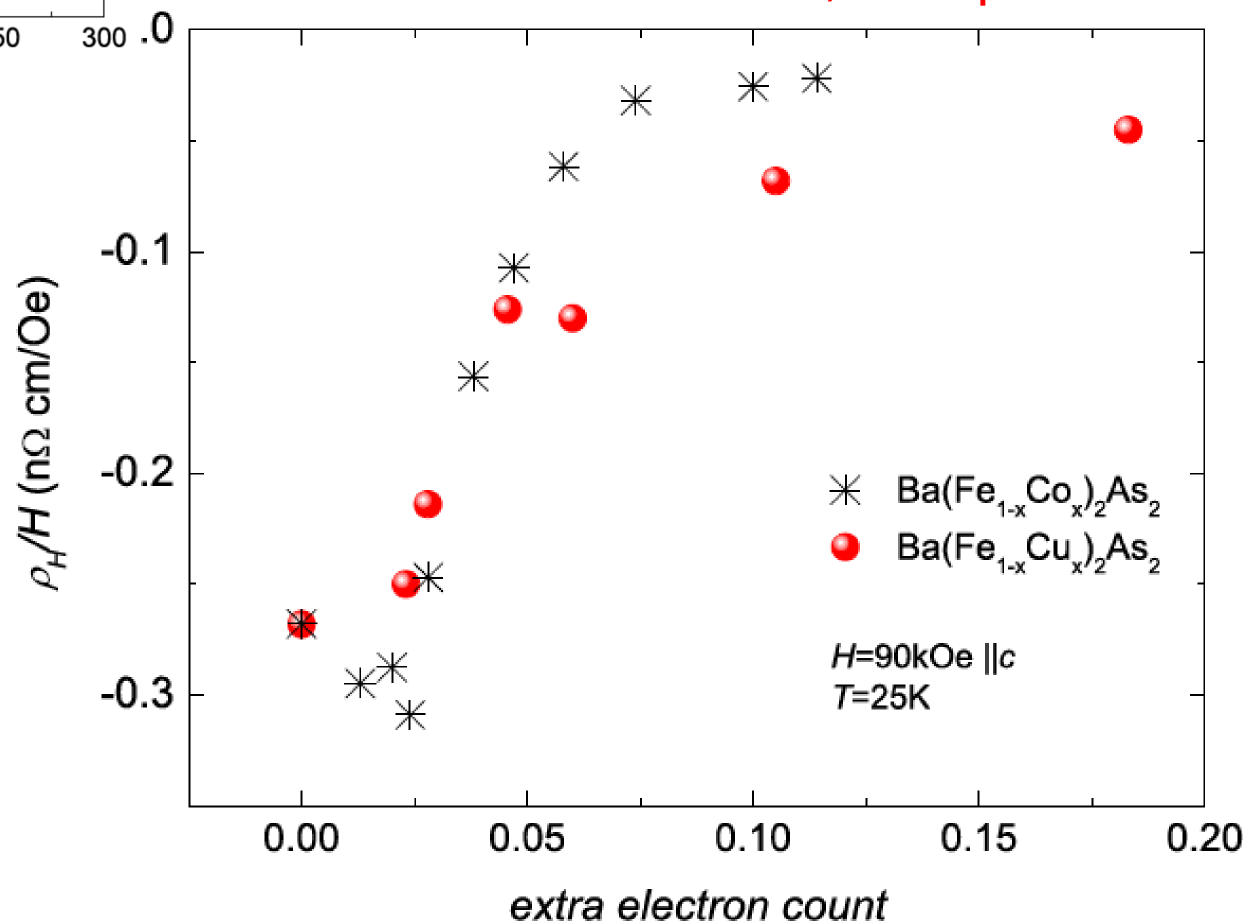


arXiv:0906:1548v2, accepted PRB



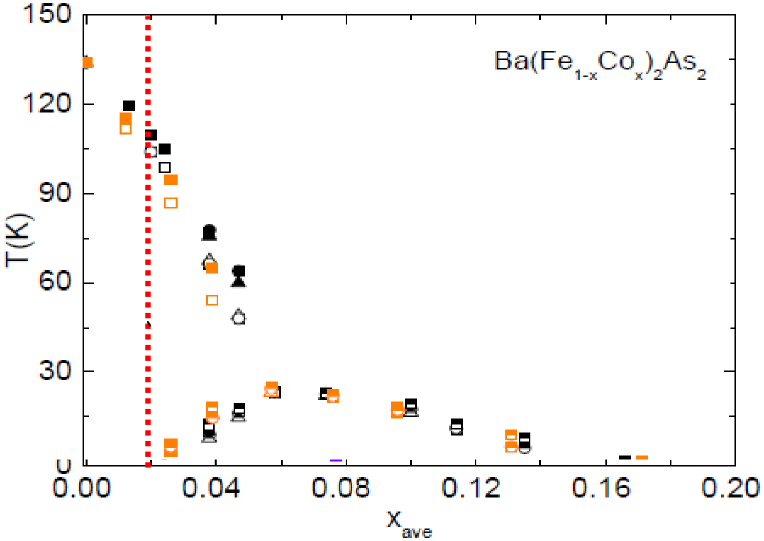
ρ_H/H at 25 K for both the Cu and Co doping show this change at similar e.

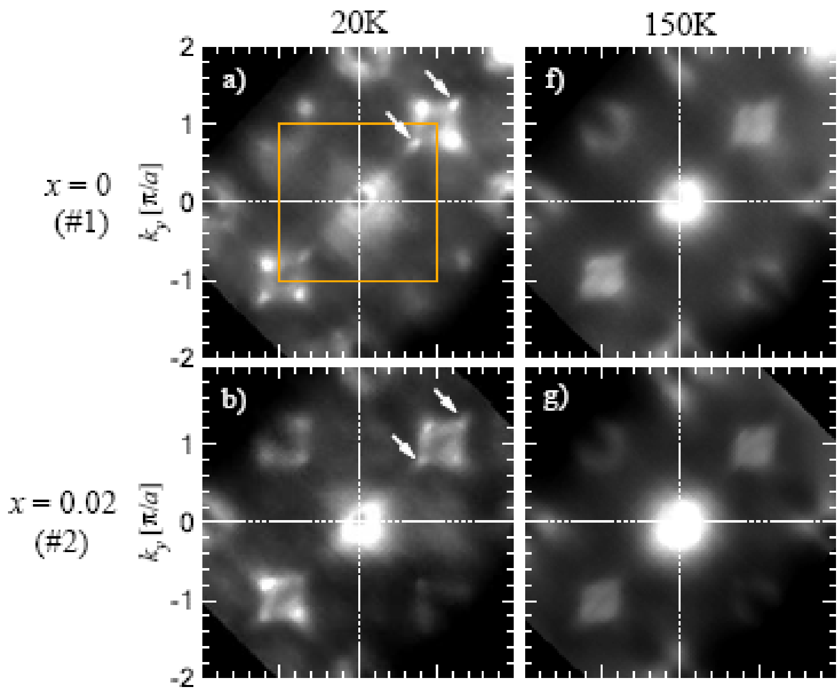
arXiv:0906:1548v2, accepted PRB

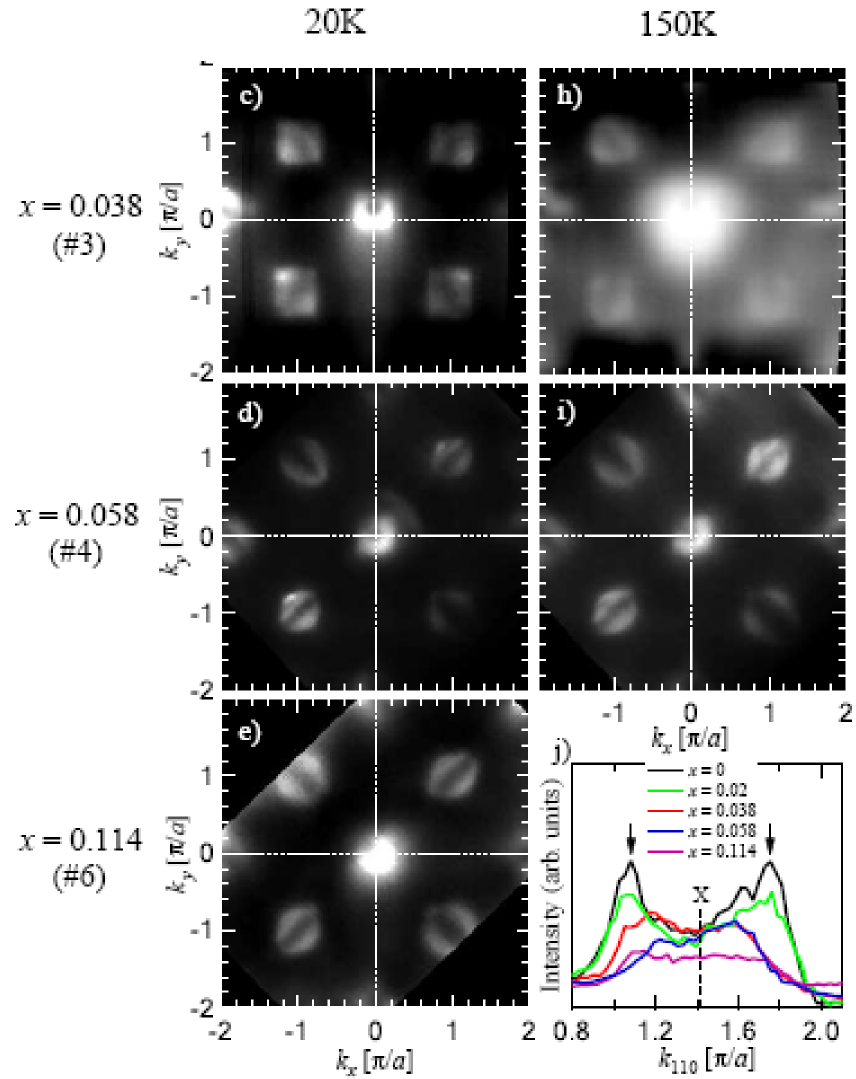


These data indicate that there is a change in the band structure / FS in $BaFe_2As_2$ for small e-doping and it happens independently of the existence of superconductivity.

ARPES on $Ba(Fe_{1-x}Co_x)_2As_2$ show similar changes.







A. Kaminski

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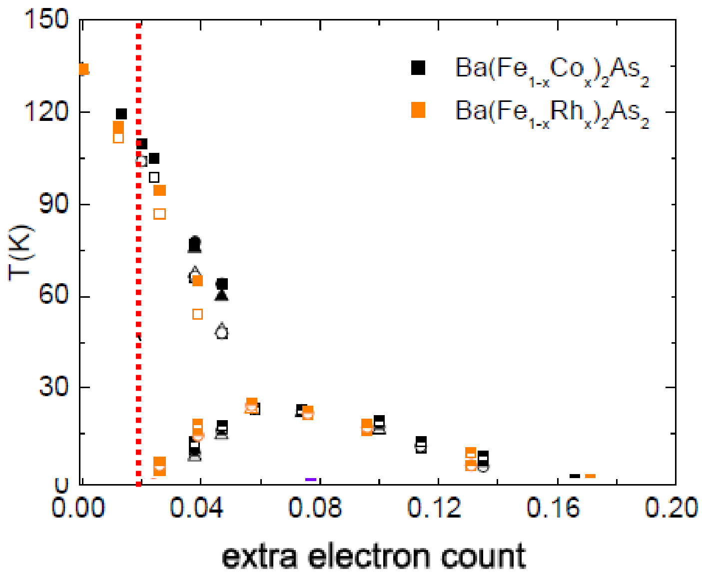
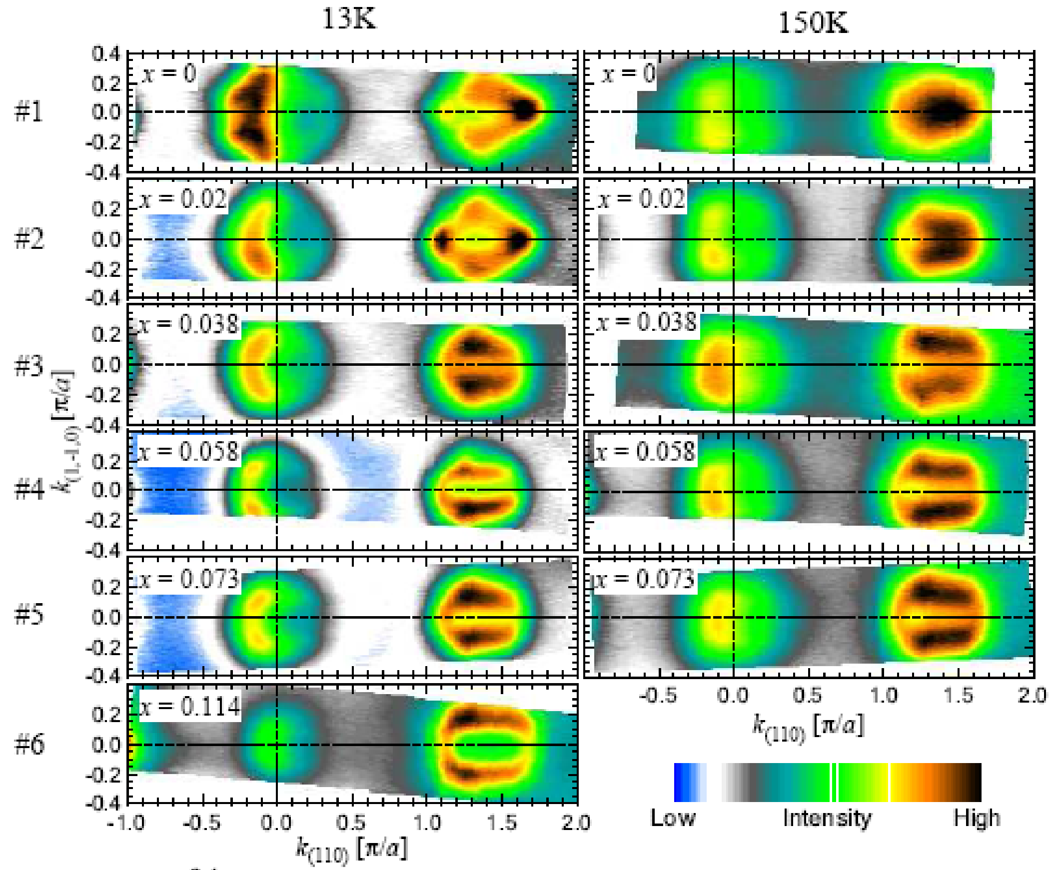
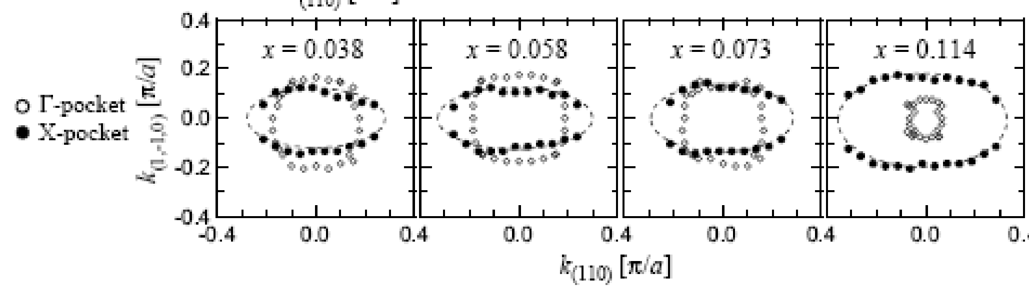
Lab based data also show the suppression of the reconstruction of the FS in the AF state as well as a qualitative change in the 150 K FS for x >~ 0.025







A. Kaminski

Posted soon

By studying $Ba(Fe_{1-x}TM_x)_2As_2$ series for a variety of 3d- and 4d-TM dopants we have found that:

(i) The structural / antiferromagnetic phase transition is suppressed in a similar manner for all TM and scales roughly with x.

(ii) There is a region of e (band filling) that supports superconductivity if the structural / antiferromagnetic phase transition is suppressed sufficiently.

(iii) The superconducting dome scales very well with e on the over-doped, tetragonal phase, side.

(iv) The onset of the superconducting dome on the under-doped, O / AF side depends on how quickly the upper transitions are suppressed. T_c scales well with T_S and / or T_M.

(v) The onset of the region of e-values that supports superconductivity seems to be associated with a change in the Fermi surface / band structure that prevents dramatic reconstruction of the FS in the AF state.