Neutron Scattering Studies of Fe-based Superconductors

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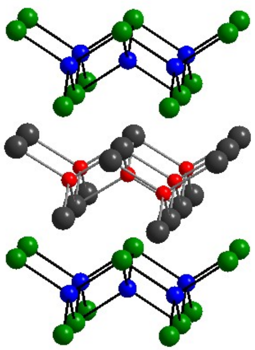
References:

Optimally doped $Ba(Fe_{1-x}Co_x)_2As_2$ Physical Review Letters **102**, 107005 (2009).
Underdoped $Ba(Fe_{1-x}Co_x)_2As_2$ Physical Review Letters **103**, 087002 (2009).
Spin Resonance in $FeTe_{0.5}Se_{0.5}$ Physical Review Letters **104**, 187002 (2010).
High Energy Spin Excitations in $FeTe_{1-x}Se_x$ Nature Physics **6**, 182 (2010).
Magnetism in $Ba(Fe_{1-x}Cr_x)_2As_2$ Phys. Rev. B 83, 060509(R) (2011).

Families of Fe-based Superconductors

LaFeAsO

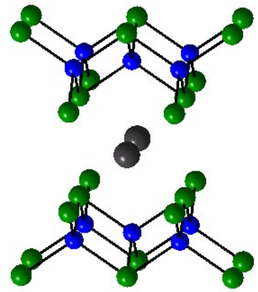


Gd0.8Th0.2FeAsO

TC = 56 K

Wang *et al*., Europhysics Letters 83, 67006 (2008).

BaFe2As2

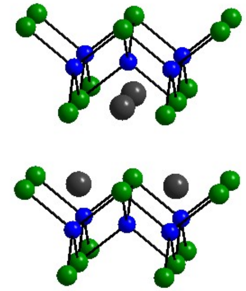


Ba0.6K0.4Fe2As2

TC = 38 K

Rotter *et al*., Angew. Chem. Int. Ed. 47, 7949 (2008).

LiFeAs

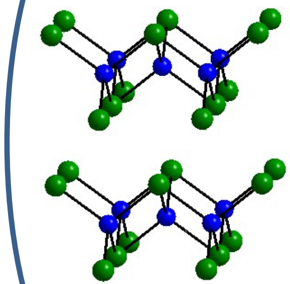


Na1-xFeAs

TC = 25 K

Chu *et al*., Physica C 469 326 (2009).

FeSe



FeSe0.5Te0.5

TC = 15 K

Yeh *et al*., Europhys. Lett. 84 37002.

Common Characteristics:

Suppression of structural and magnetic transitions found in the parent compounds is required for superconductivity.

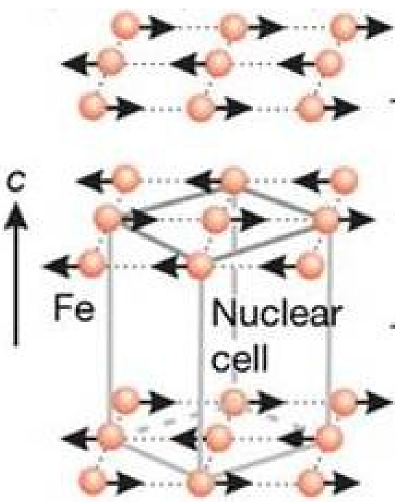
Numerous chemical substitution routes to superconductivity
e.g. in BaFe2As2, substitution on the Fe site surprisingly leads to superconductivity with a large number of transition metals including Co, Ni, Rh, Pd, Ir, Pt, and Ru (Sefat; Li; Ni; Han; Saha; Sharma; Thaler, *etc*.).

Magnetism found throughout the phase diagrams of the Fe-based materials.

Magnetism

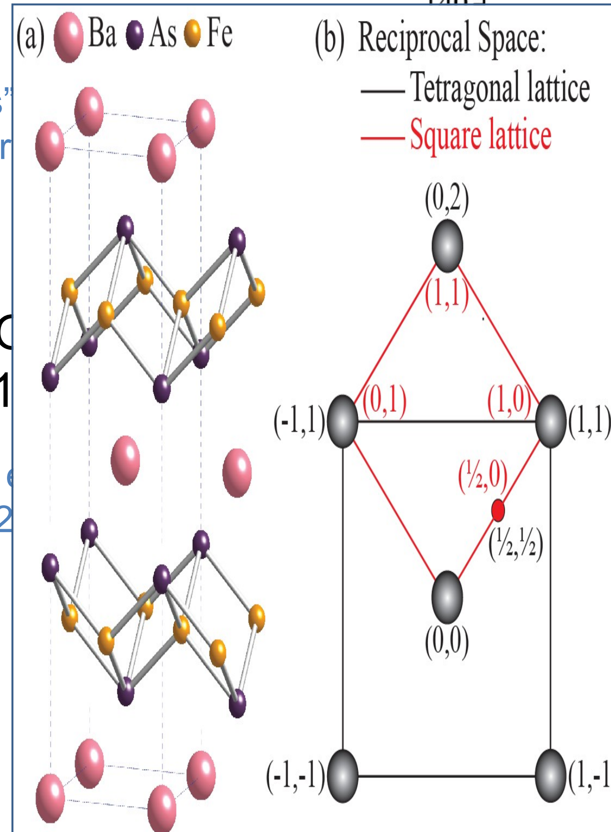
J.-H. Chu *et al.*, Phys. Rev. B **79**, 014506 (2009)

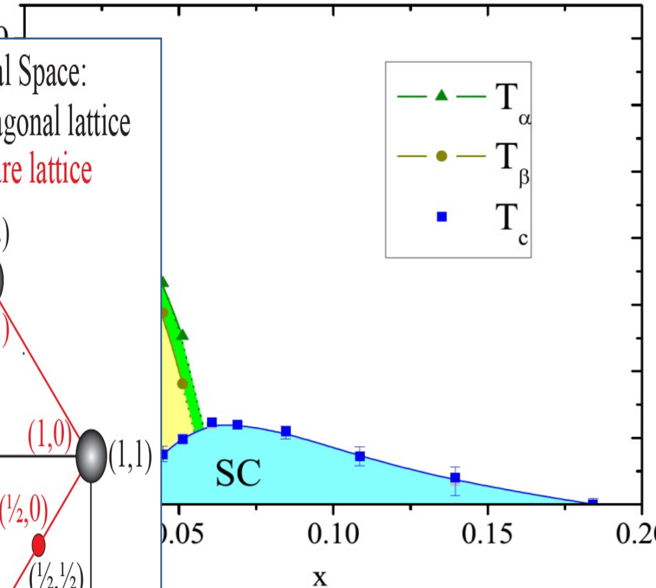
M.D. Lumsden and A.D. Christianson,
"Magnetism in Fe-based superconductors"
Topical review: J. Phys.: Condens. Matter



LaFeAsO
Q=(1/2 1

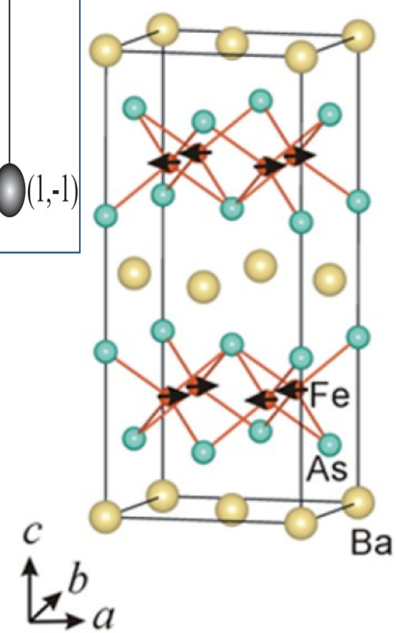
de la Cruz e
453, 899 (2





Q=(1/2 1/2 1)

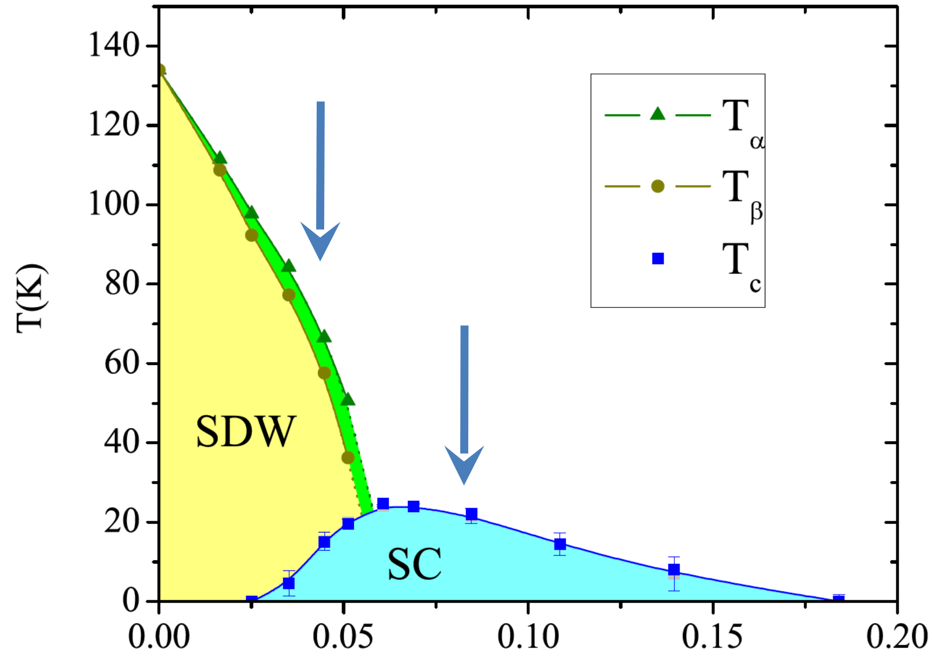
Huang et al., PRL **101**, 257003 (2008)



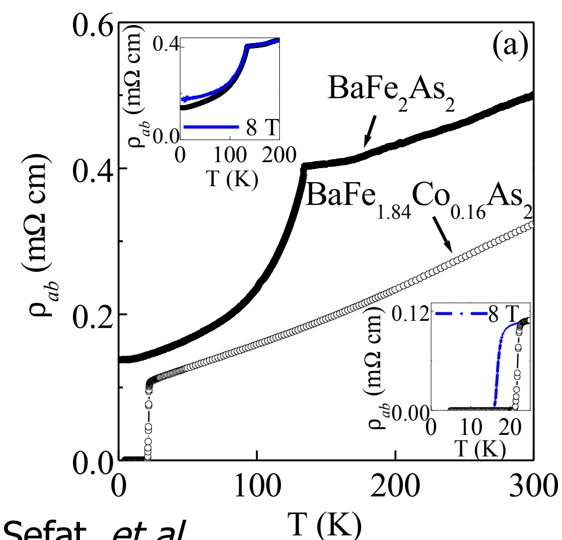
Notation
(1/2 1/2) Tetragonal = (π,π)
(1 0) Orthorhombic
(1/2 0) Square lattice = $(\pi,0)$

Ba(Fe1-xCox)2As2 General Properties

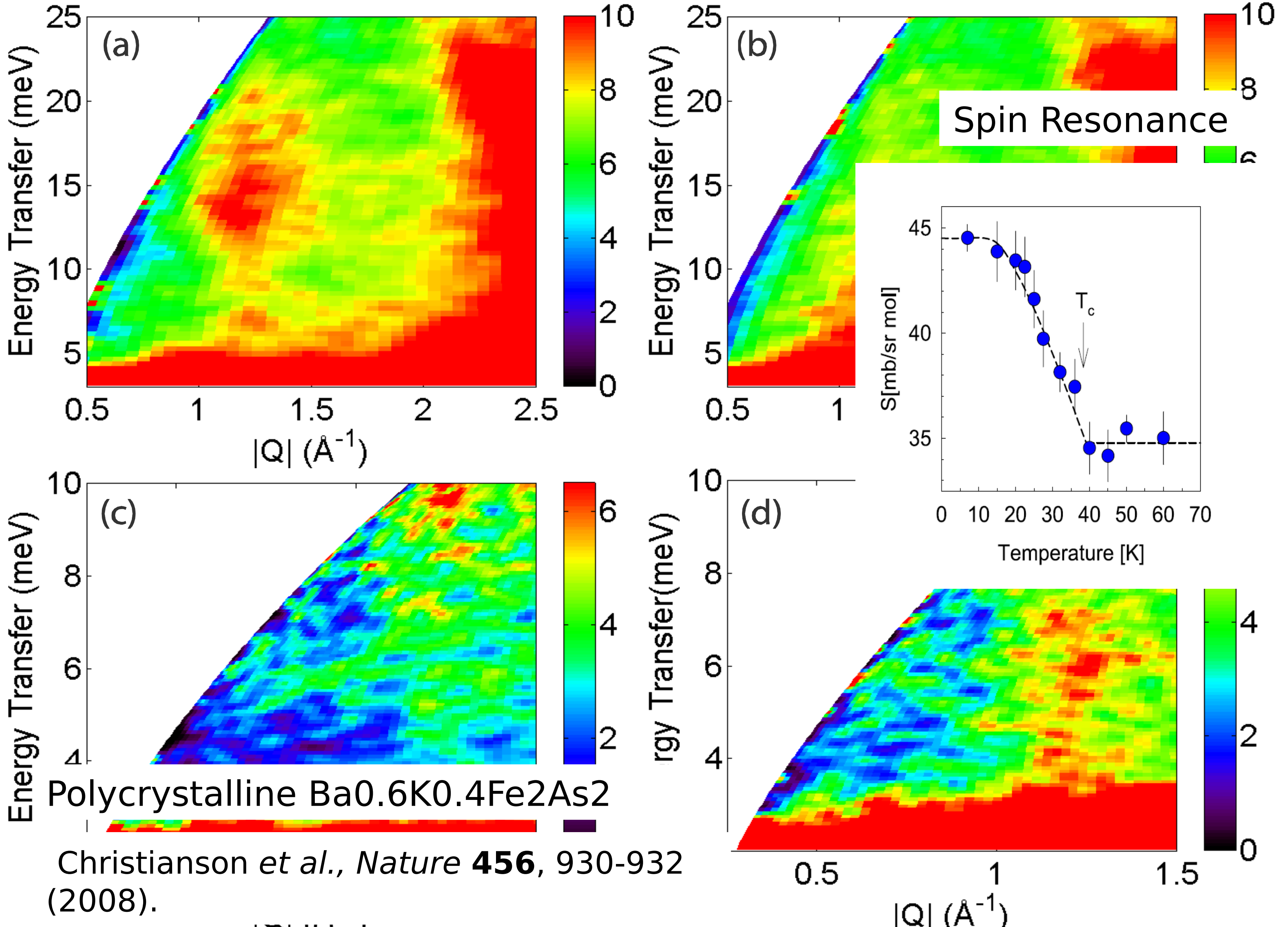
- Route to high quality single crystals, (Sefat *et al.*)
- Optimal doping (x~0.08) – mass=1.8g in 3 crystals (Tc=22K)
- Underdoped sample (x~0.04) – mass=2g in 4 crystals (Tc=11K)



Chu, *et al.*



Sefat, *et al.*

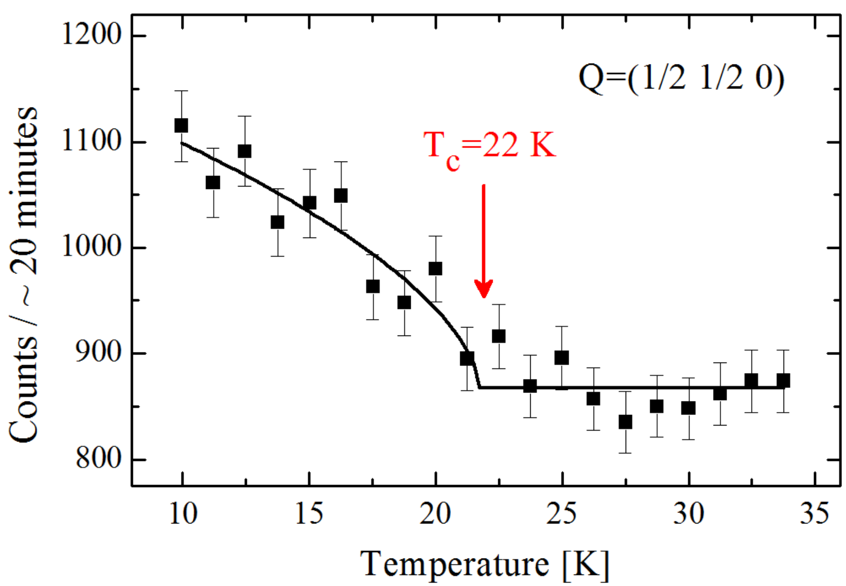


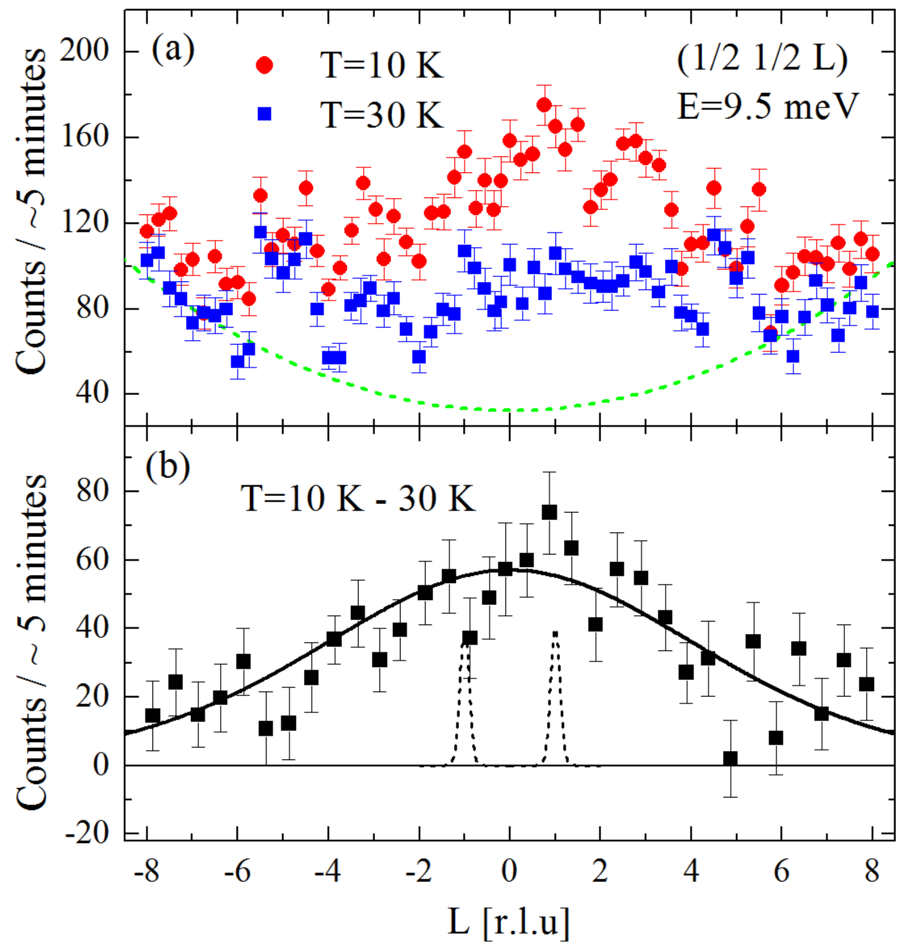
Spin Resonance

Polycrystalline Ba0.6K0.4Fe2As2

Christianson *et al., Nature* **456**, 930-932 (2008).

L-dependence and link to TC



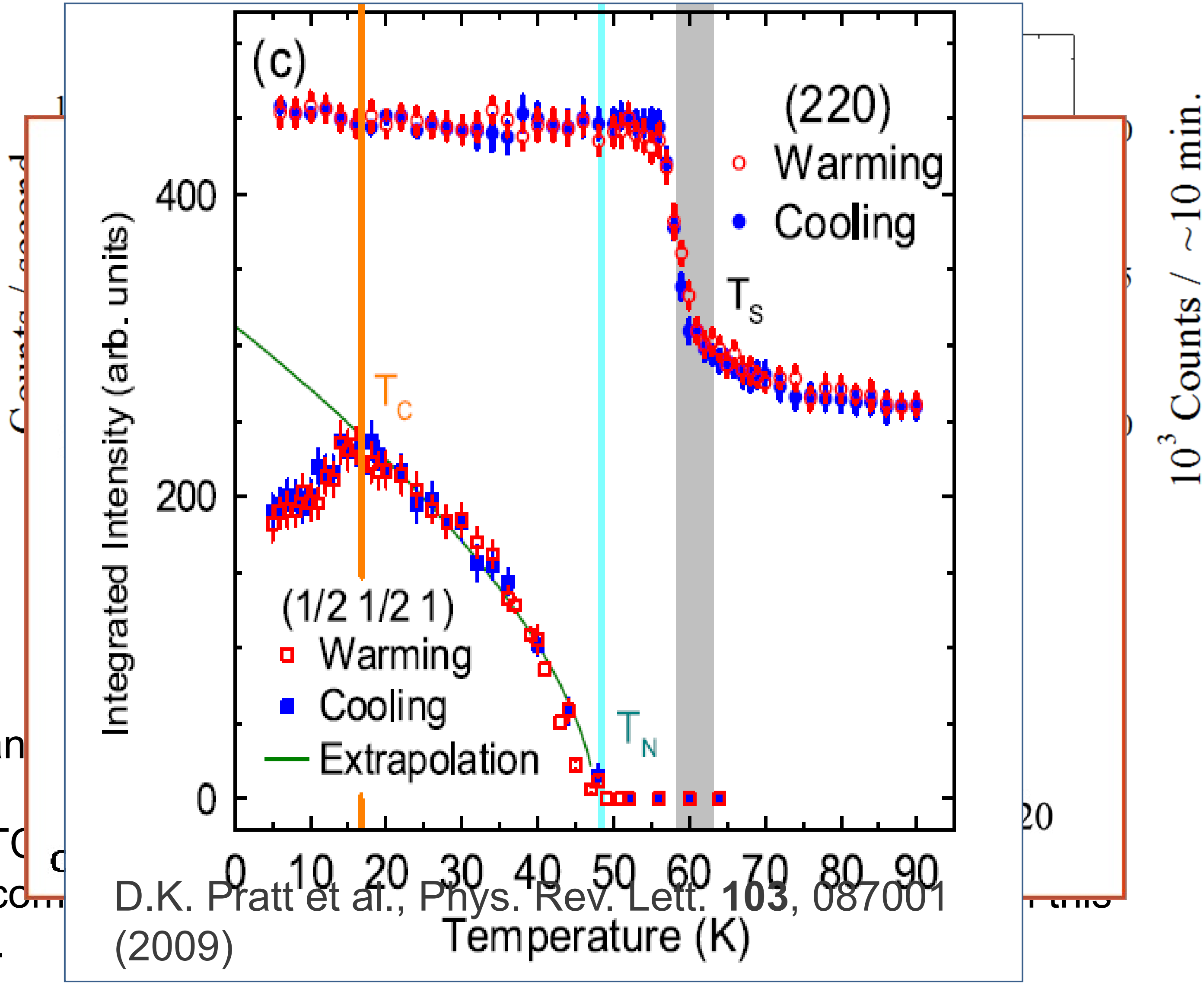


Excitation clearly linked to TC.

Very weak L-dependence indicating a quasi-2d excitation

Difference depends only on the form factor indicating magnetic nature of the resonance.

Underdoped (x~0.04)

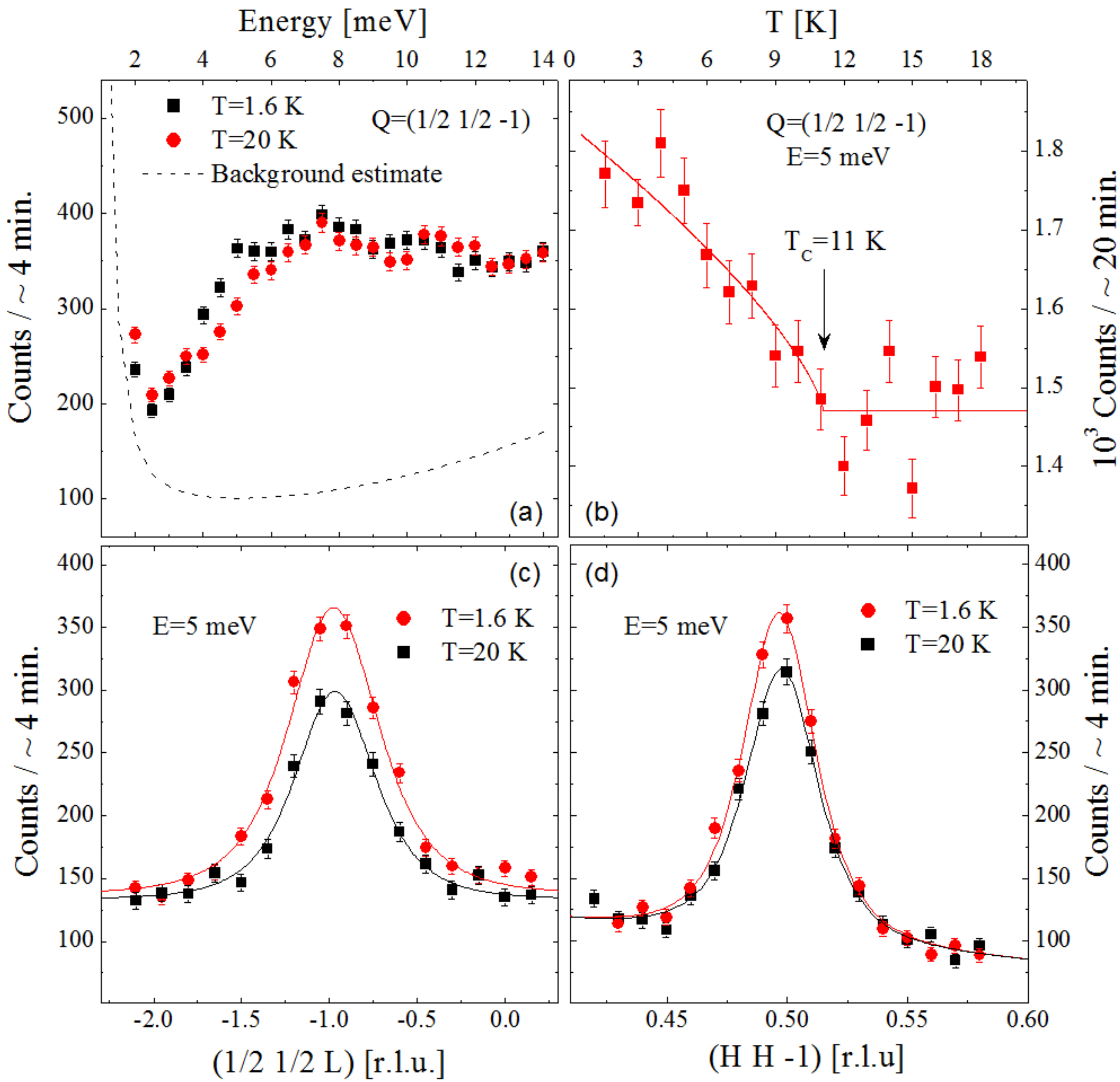


D.K. Pratt et al., Phys. Rev. Lett. **103**, 087001 (2009)

Long-ran

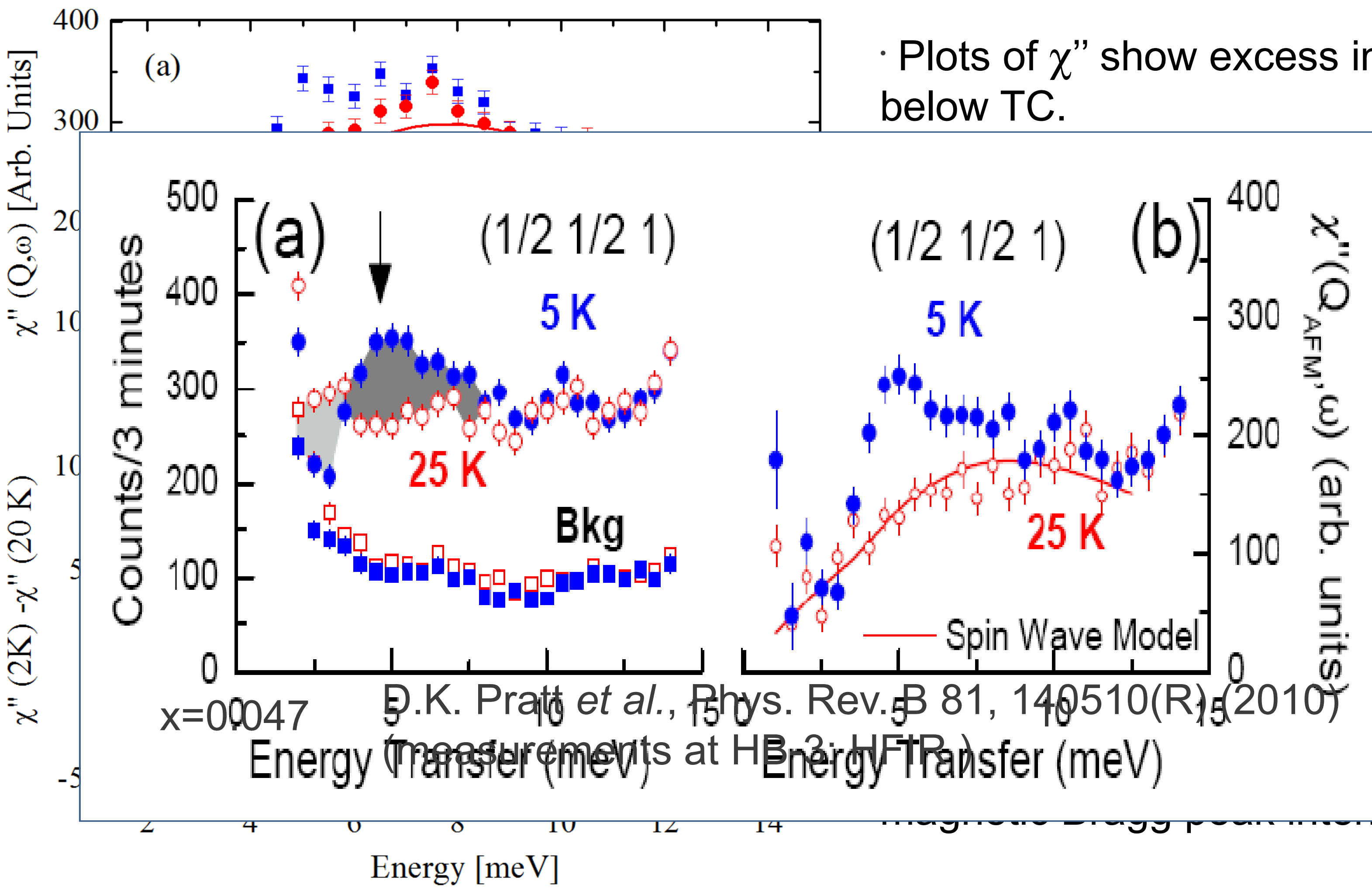
Below TC
strong co
sample.

Resonance in an underdoped sample



- Gapped excitation both above and below TC.
- Excess scattering located only for Q at AFM zone center for E~5 meV.
- Both scattering above TC and excess below TC strongly peaked in H and L indicating 3D correlations.
- Excess intensity strongly coupled to TC (~11K in this sample).

Where does the spectral weight for the resonance come from?



x=0.047

D.K. Pratt *et al.*, Phys. Rev. B 81, 140510(R) (2010)
(measurements at HB-3; HFIR)

- Plots of χ'' show excess intensity below TC.

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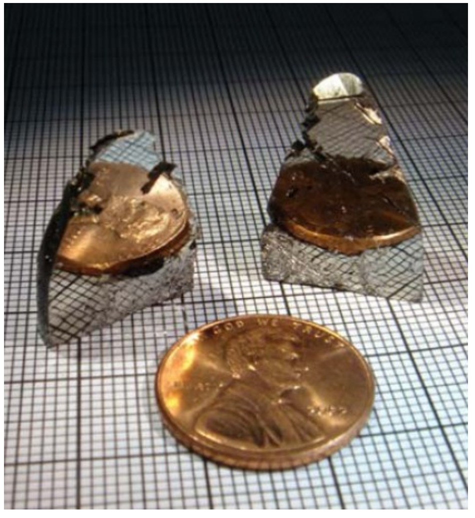
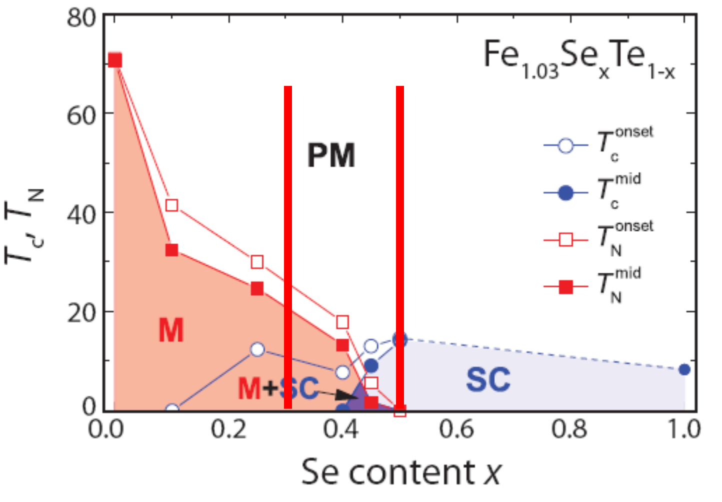
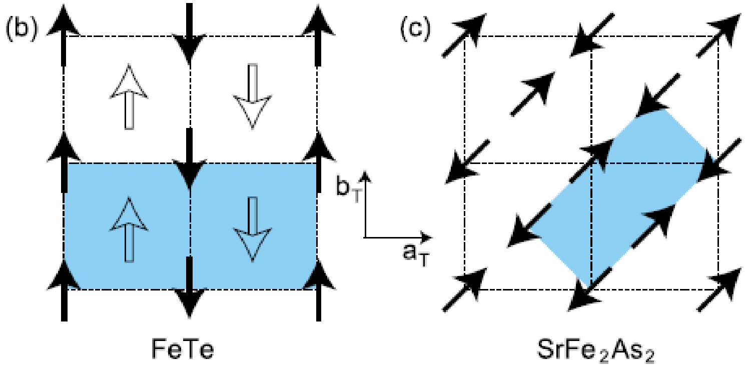
Spin Excitations: FeTe1-xSex



Superconductivity in α-FeSe with TC~8K.
F.-C. Hsu *et al.*, PNAS 105, 14262 (2008)

(e) $Fe_{1.03}Se_xTe_{1-x}$
Kasanov et al., Physical Review B, **80**,140511, 2009.





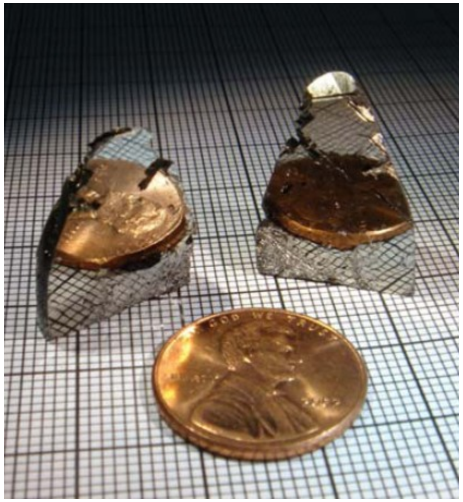
Fe1+yTe orders at (0.5 0 0.5)
Li *et al.*, Phys. Rev. B **79**, 054503 (2009).

Phase diagram with Te doping
Yeh *et al.*, Europhys Lett. **84** (2008) 37002

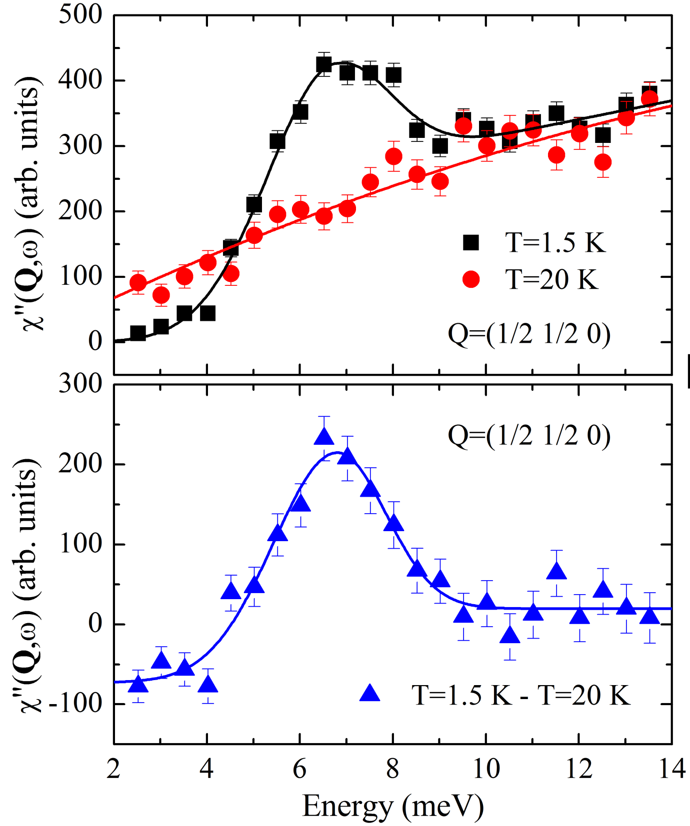
FeTe isn't superconducting

Only samples near 0.5 are bulk superconductors.
Sales et al., Phys. Rev. B **79**, 094521 (2009)

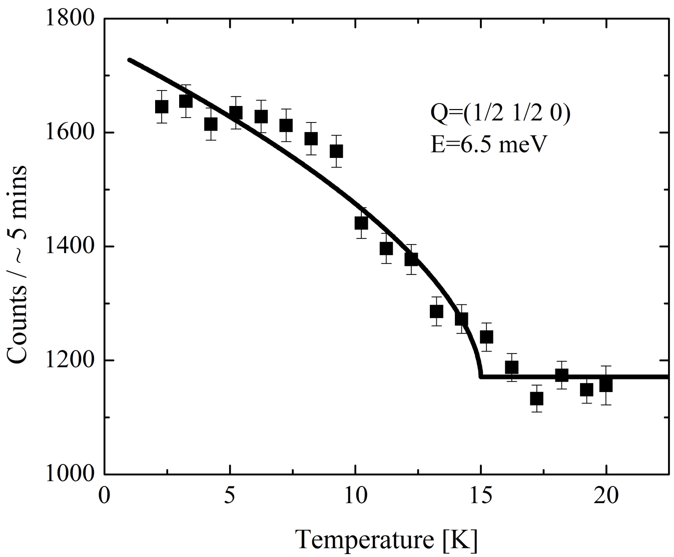
Triple-axis measurements – HB3, HB1



FeSe0.5Te0.5 crystal mounted in (HK0) scattering plane



ER~7 meV≈5 kBTC



Despite magnetic ordering in FeTe with Q=(1/2 0 1/2), inelastic spectrum shows a resonance which is located at Q=(1/2 1/2 0)

Response very similar to other Fe based superconductors.

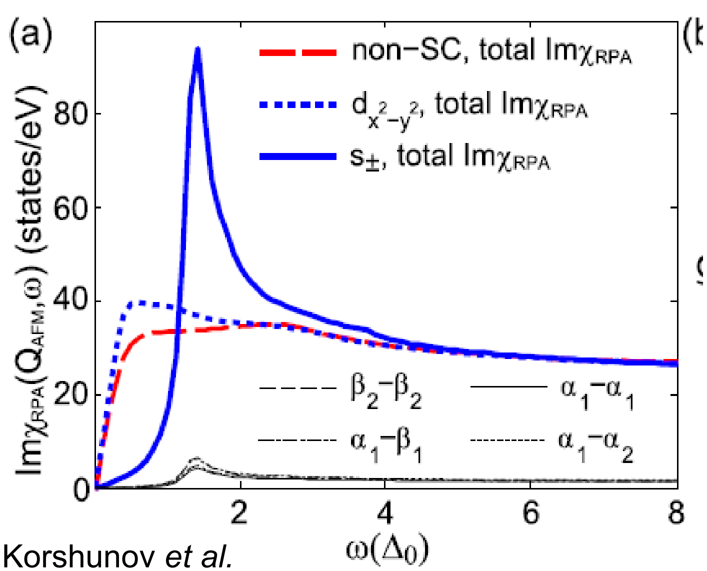
Interpretation of the resonance

Implies phase shift on some portion of Fermi surface and hence an unconventional symmetry of the superconducting gap

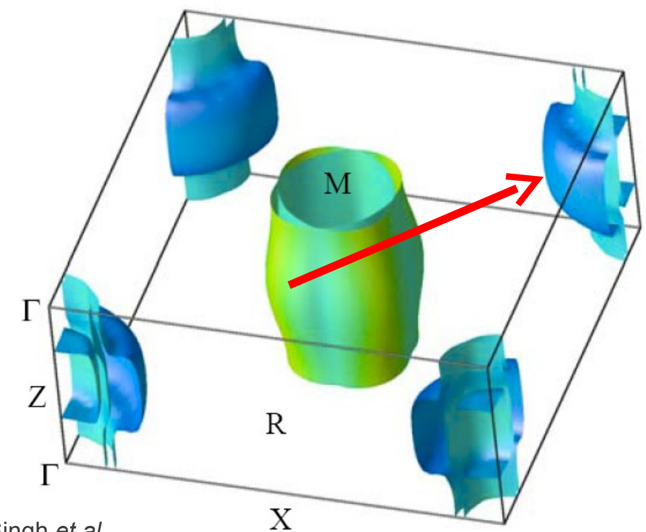
$\Delta K+Q=-\Delta K$; i.e. nodes or Sign reversed s-wave symmetry (Mazin *et al.*)

Theory of a Resonance in FeAs systems

(Maier *et al*., Korshunov *et al.,* etc)



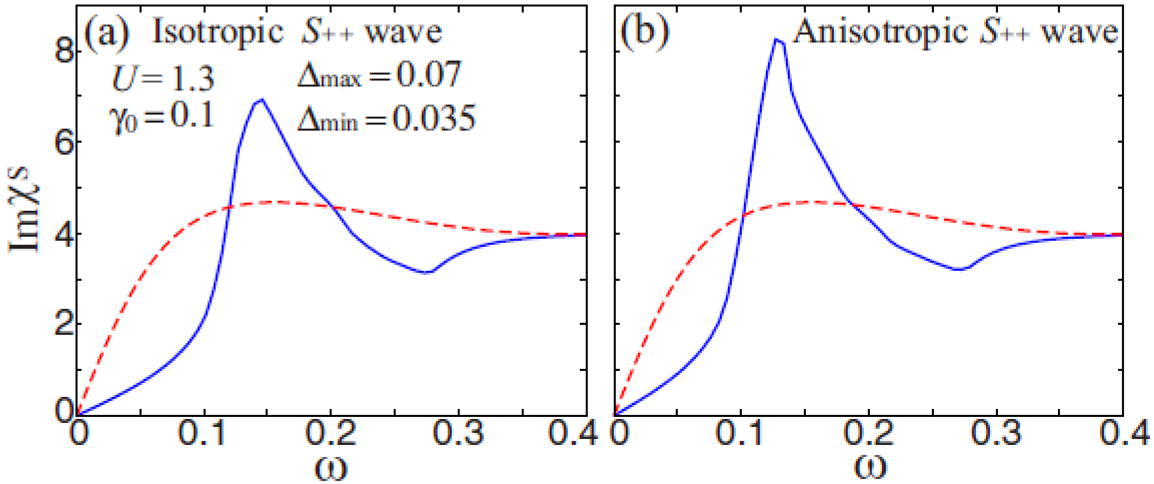
Korshunov *et al.*



Singh *et al.*

Interpretation of the resonance (alt.)

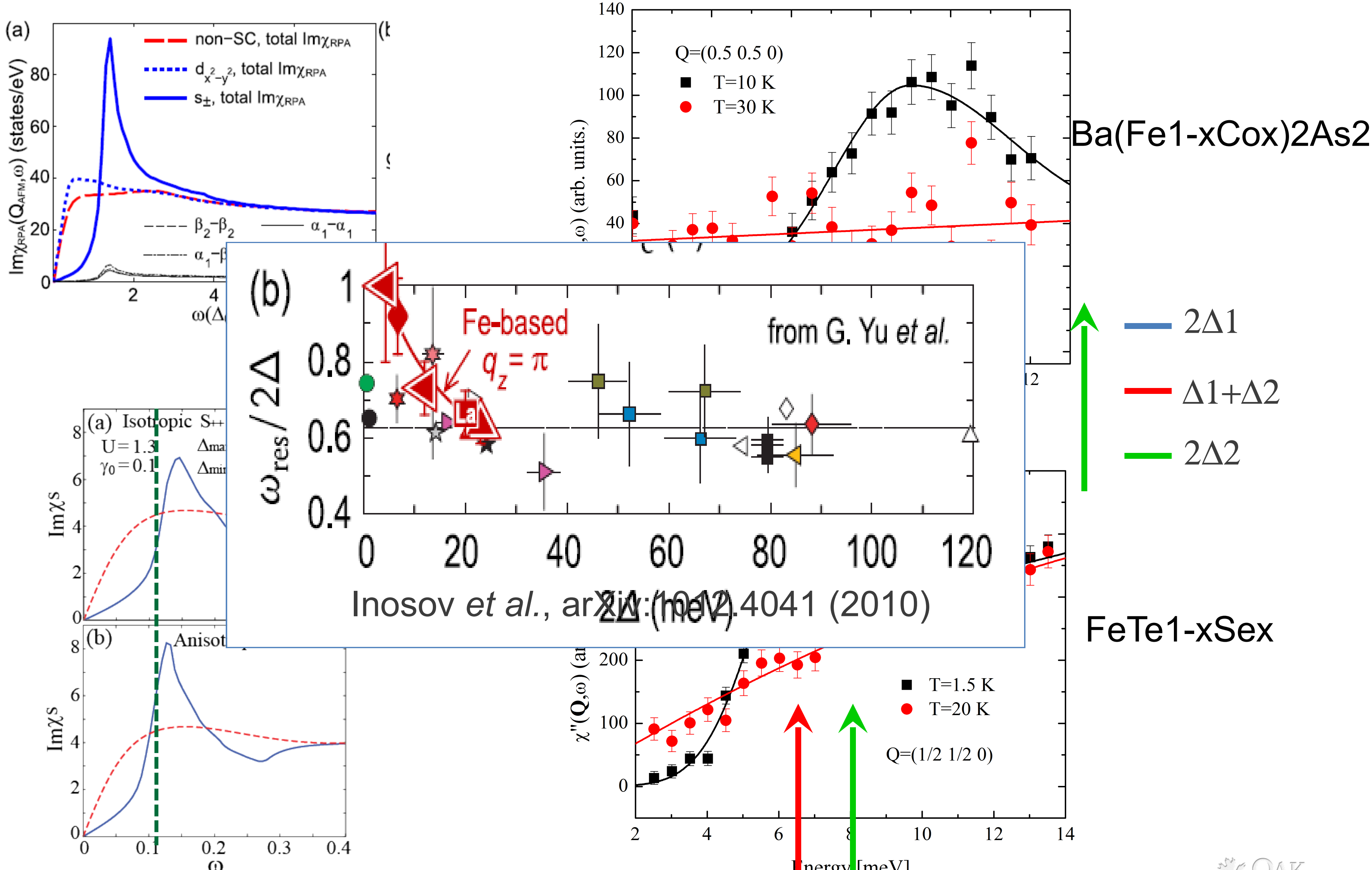
S. Onari, H. Kontani, and M. Sato, Phys. Rev. B 81, 060504(R) (2010):



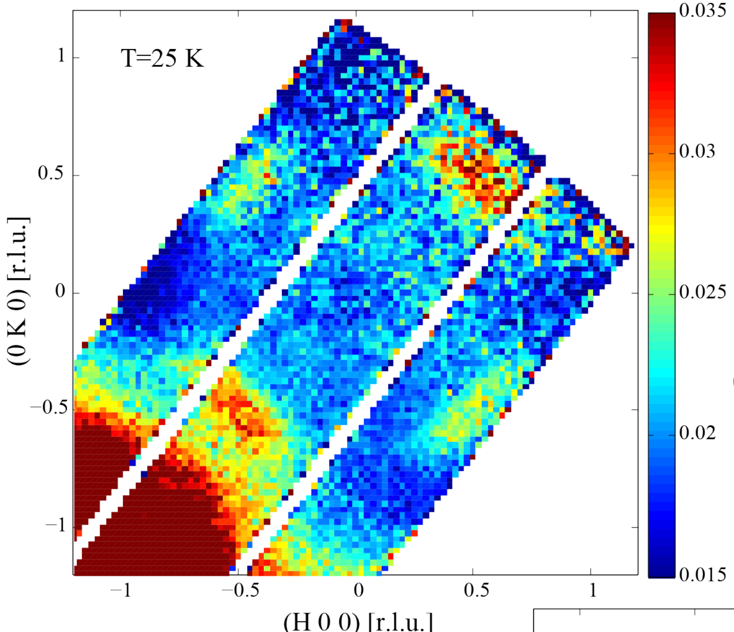
S++ wave

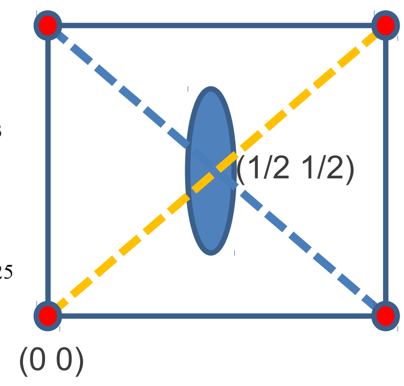
Suppression of quasiparticle damping due to the opening of a superconducting gap results in a “resonance-like” feature.

Comparison with experiment

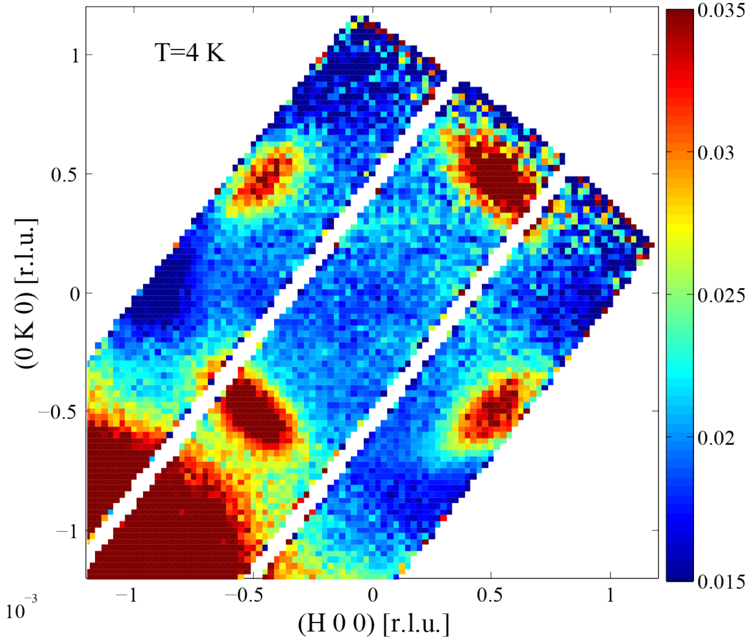


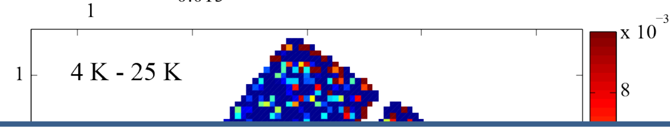
FeTe1-xSex cont.
Symmetry of the Normal State Spin Excitations

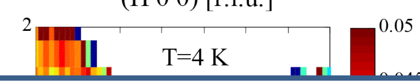




5.5 > E > 7.5







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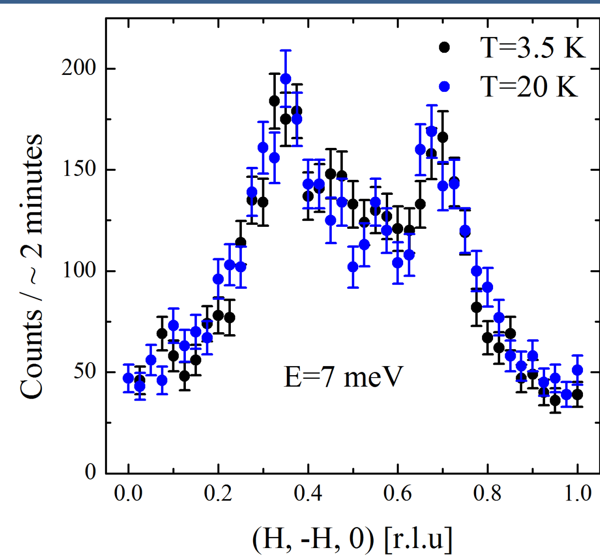
Other concentrations?

Fe1.04Te0.73Se0.27

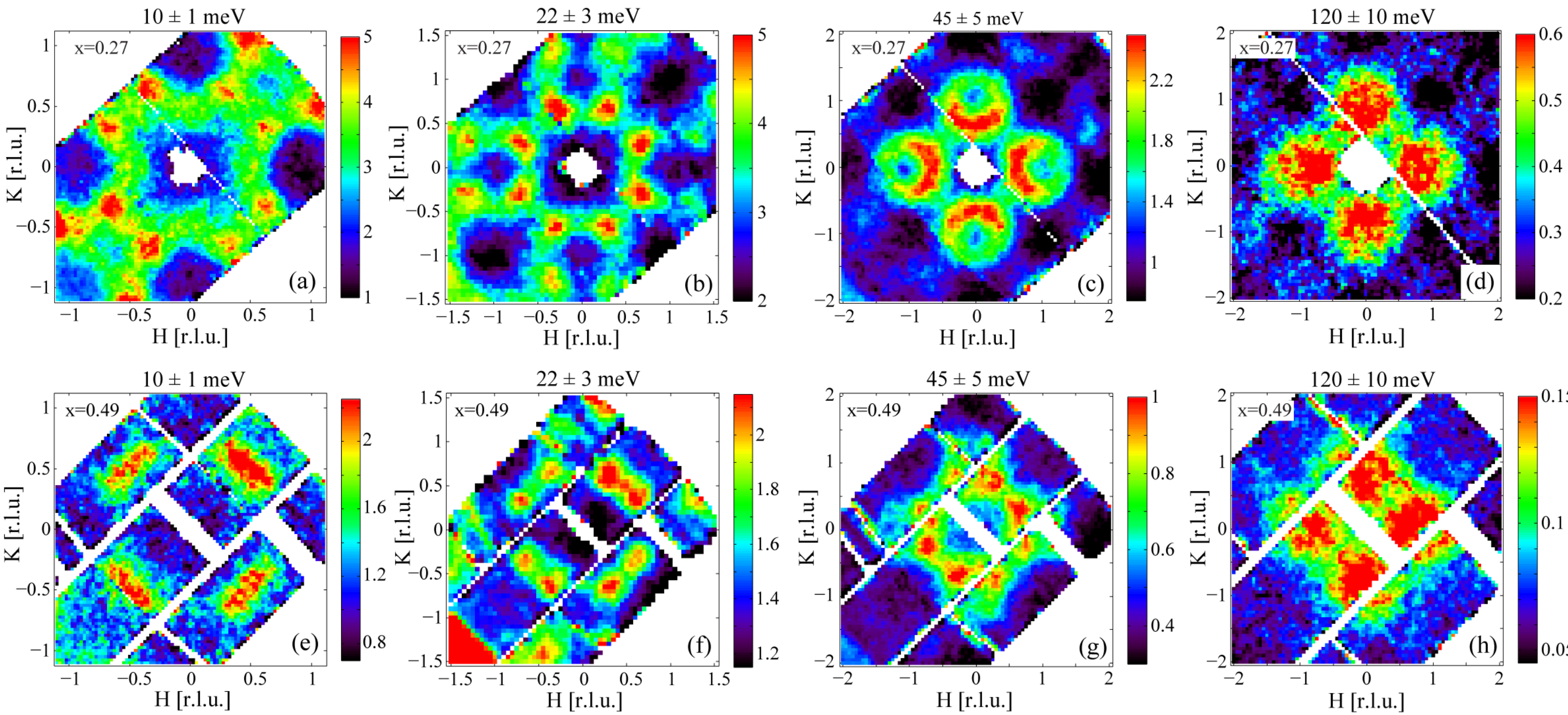


No resonance – not bulk superconductor.

Excitations appear incommensurate

Normal State Spin Excitations:
TOF Measurements – MERLIN, ARCS

$Fe_{1.04}Te_{0.73}Se_{0.27}$ – MERLIN
$FeTe_{0.51}Se_{0.49}$ – ARCS

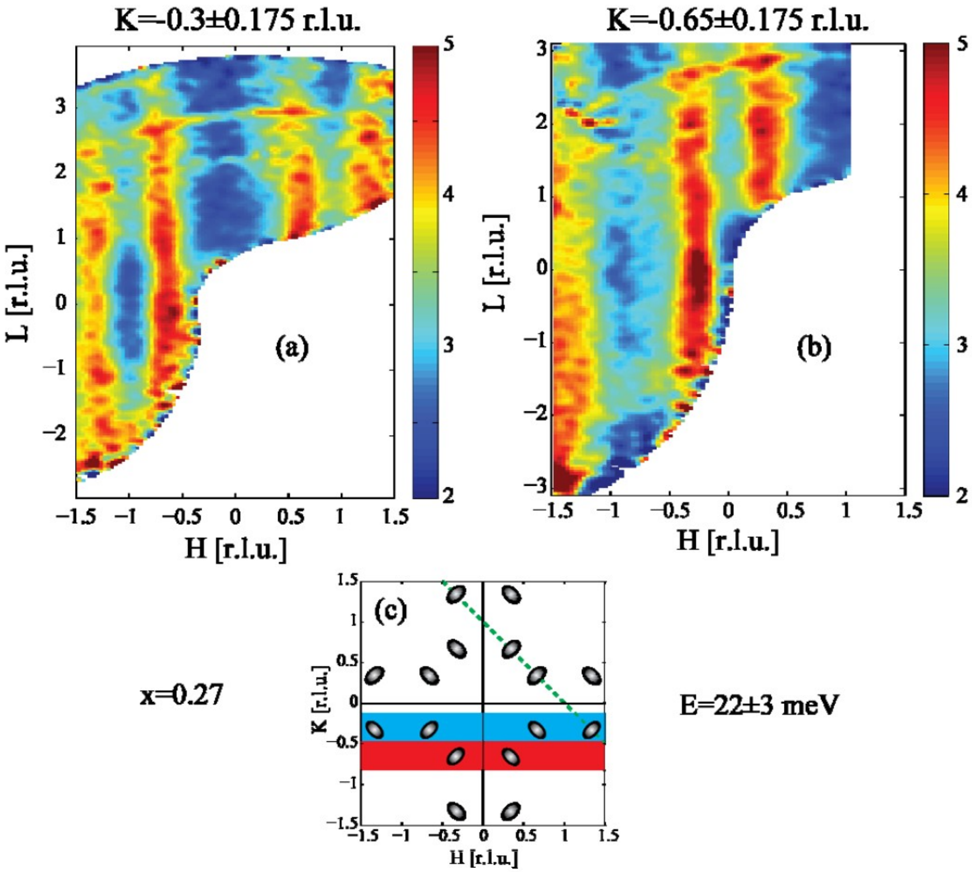


Scattering pattern 4-fold symmetric about (1, 0) wavevector

Wavevectors: $(1\pm\xi, \pm\xi)$ and $(1\pm\xi, \mp\xi)$

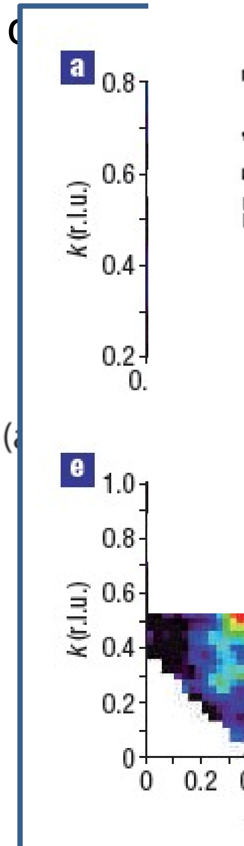
Dimensionality of The Spin Excitations-Power of the New Time of Flight Instruments

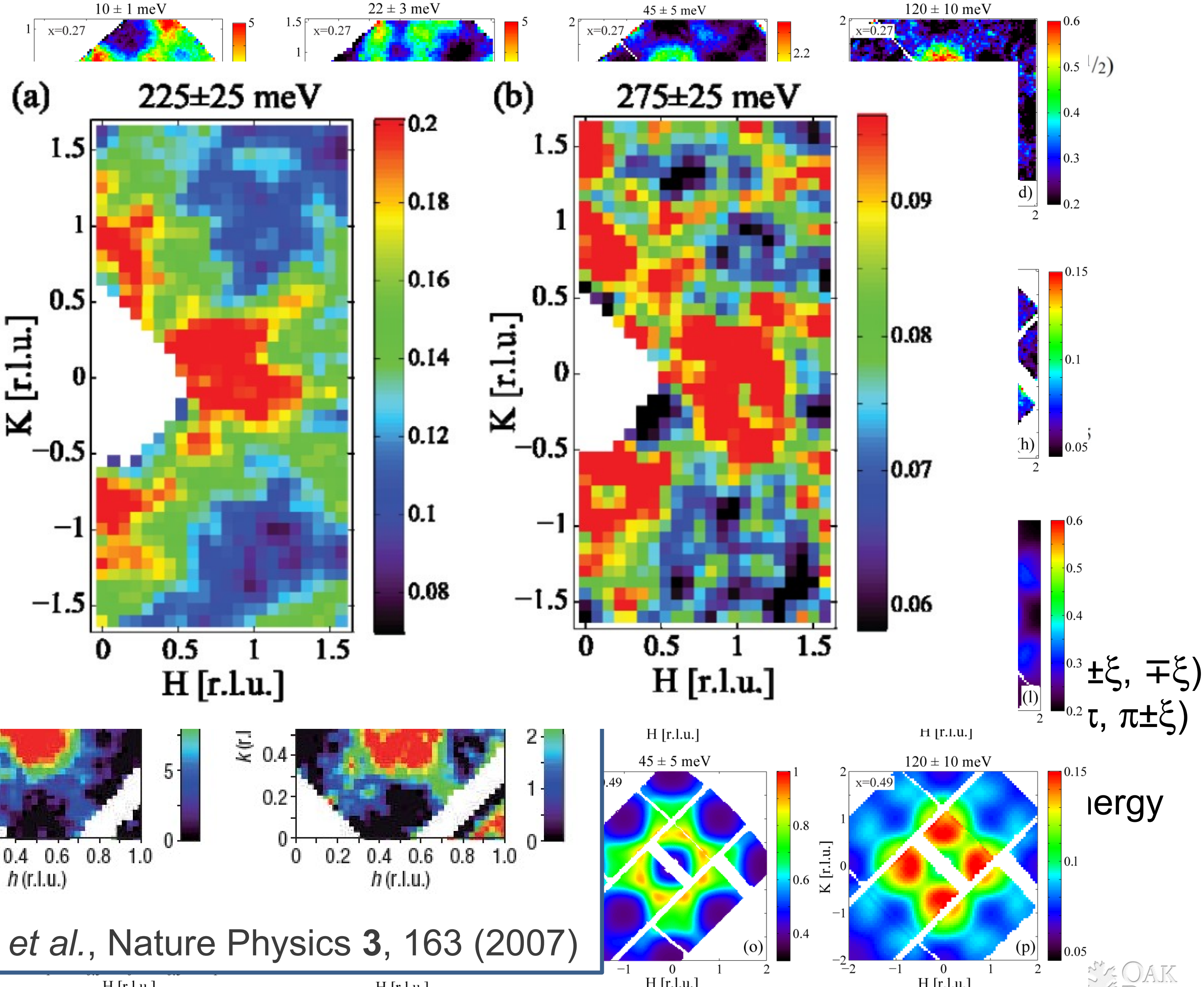
Qiu, *et al.,* (PRL 2009), show over limited energy the spin excitations appear 2D.
Time of Flight measurements where the sample has been rotated show this over a large range (Lumsden, *et al*. Nature Physics 2010)



Dispe

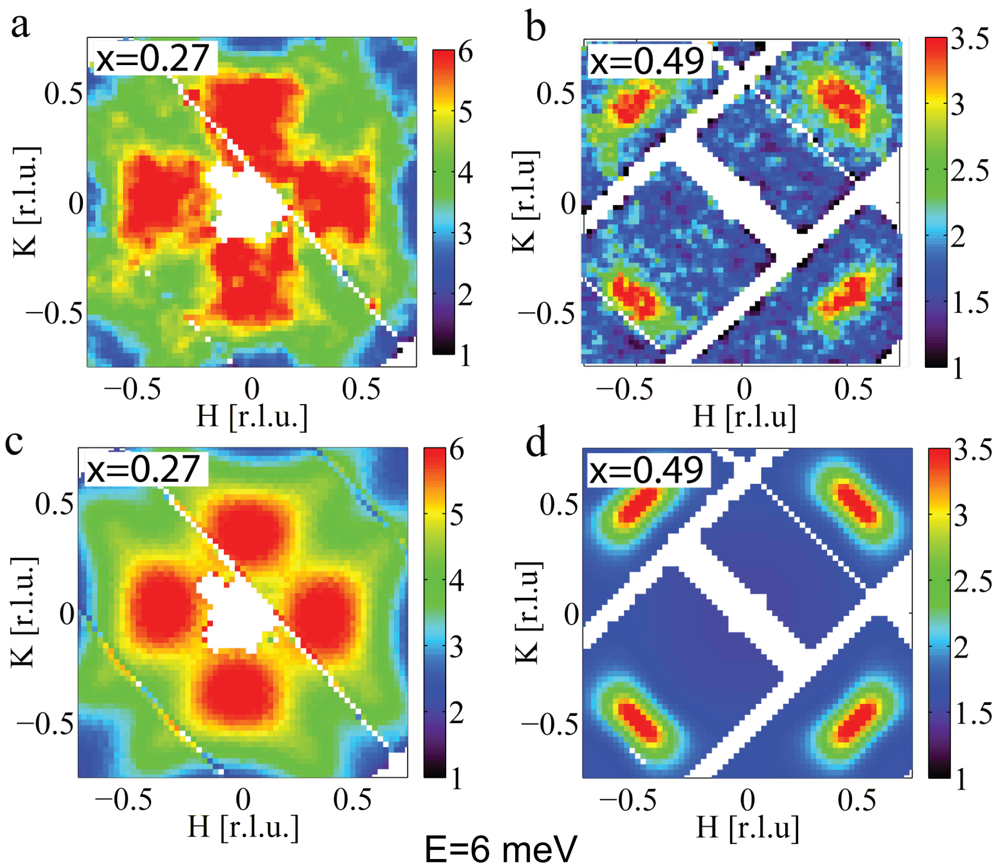
Disper
at low
x=0.49





Vignolle *et al.*, Nature Physics **3**, 163 (2007)

Low energy excitations



For x=0.49, only have the same excitations shown previously.

For x=0.27, we have an additional broad scattering component centered near (1/2 0).

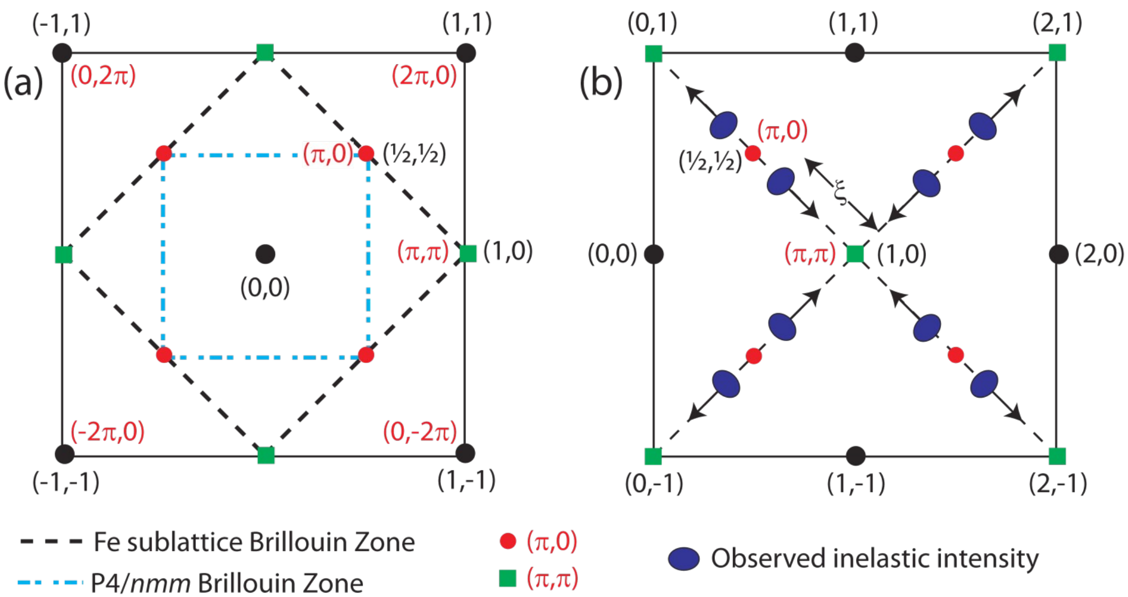
This is consistent with the short range order seen in diffraction.

As it exists at low energies below the gap, it could represent pair breaking scattering which prevents bulk superconductivity in the x=0.27 sample.

Quite possibly the result of excess Fe in x=0.27.

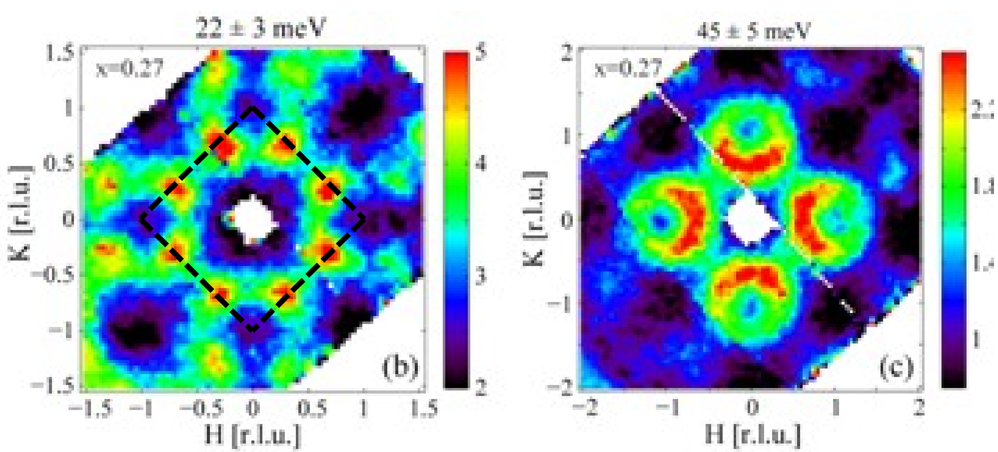
What is driving the competition between (0.5 0 0.5) and (0.5 0.5 0) and are spin fluctuations at (0.5 0.5 0) necessary for superconductivity?

Symmetry of excitations



Similar results seen in:

·Paramagnetic state of CaFe2As2 (Diallo, *et al.*)
·Optimally doped Ba(Fe1-xCox)2As2 (Lester, *et al.* ; Li, *et al.*)
·Optimally doped Ba(Fe1-xNix)2As2 (Park, *et al.*)



Symmetry of excitations is consistent with BZ of square Fe sublattice.

Calculations should be performing in this zone to be compared to experiment.

Summary

Spin resonance appears below Tc in superconducting samples near an in-plane wave vector (1/2 1/2) or (π,0) in $Ba(Fe_{1-x}Co_x)_2As_2$ and $FeSe_xTe_{1-x}$.

Resonance in optimally doped $Ba(Fe_{1-x}Co_x)_2As_2$ is two-dimensional with very weak dispersion along c-axis.

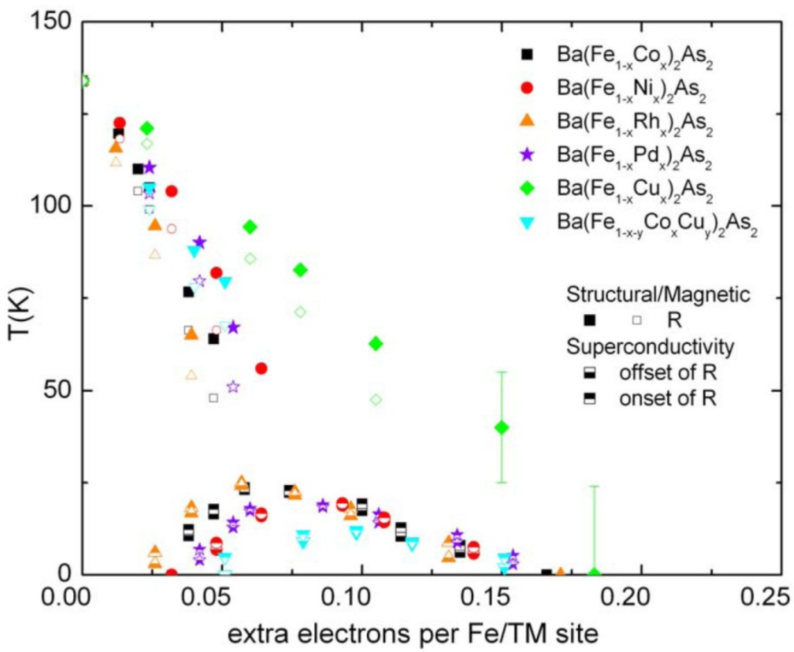
Underdoped sample shows magnetic Bragg peak suppression on entering superconducting state and a resonance co-existing with spin waves.

Normal State Spin Excitations in $FeSe_xTe_{1-x}$

- Overall spin excitation spectrum is two-dimensional and extends to very high energies
- Symmetry of the spin excitations is compatible with Fe square lattice and evolution of the intensity with increasing energy is similar to observations in the cuprates

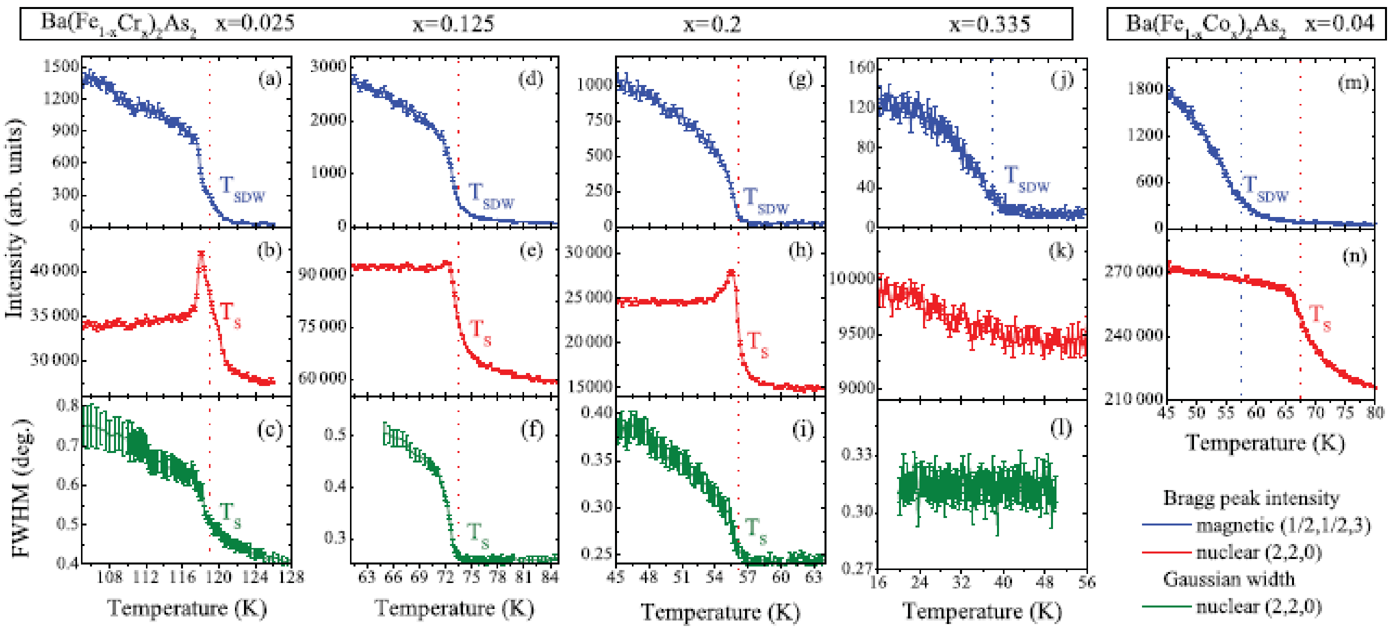
Transition Metal Doping in BaFe2As2

Almost always leads to superconductivity.
"Hole-doping" on the Fe-site seems to be an exception, *e.g.* Cr or Mn.



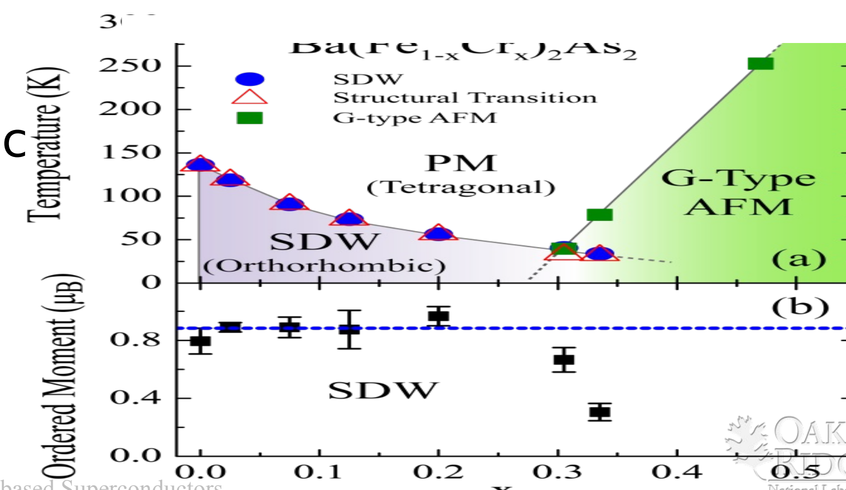
Canfield, et al.

Transition Metal doping induced Superconductivity-a counter example: Ba(Fe1-xCrx)2As2

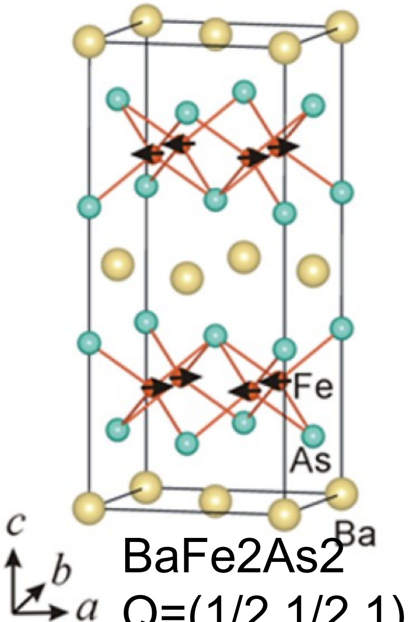


K. Marty

No separation of structural and magnetic transitions.

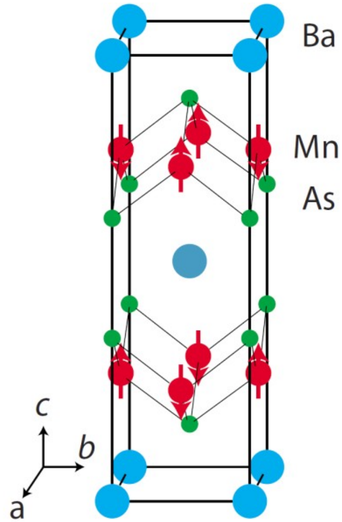


Comparison of Magnetic Structures



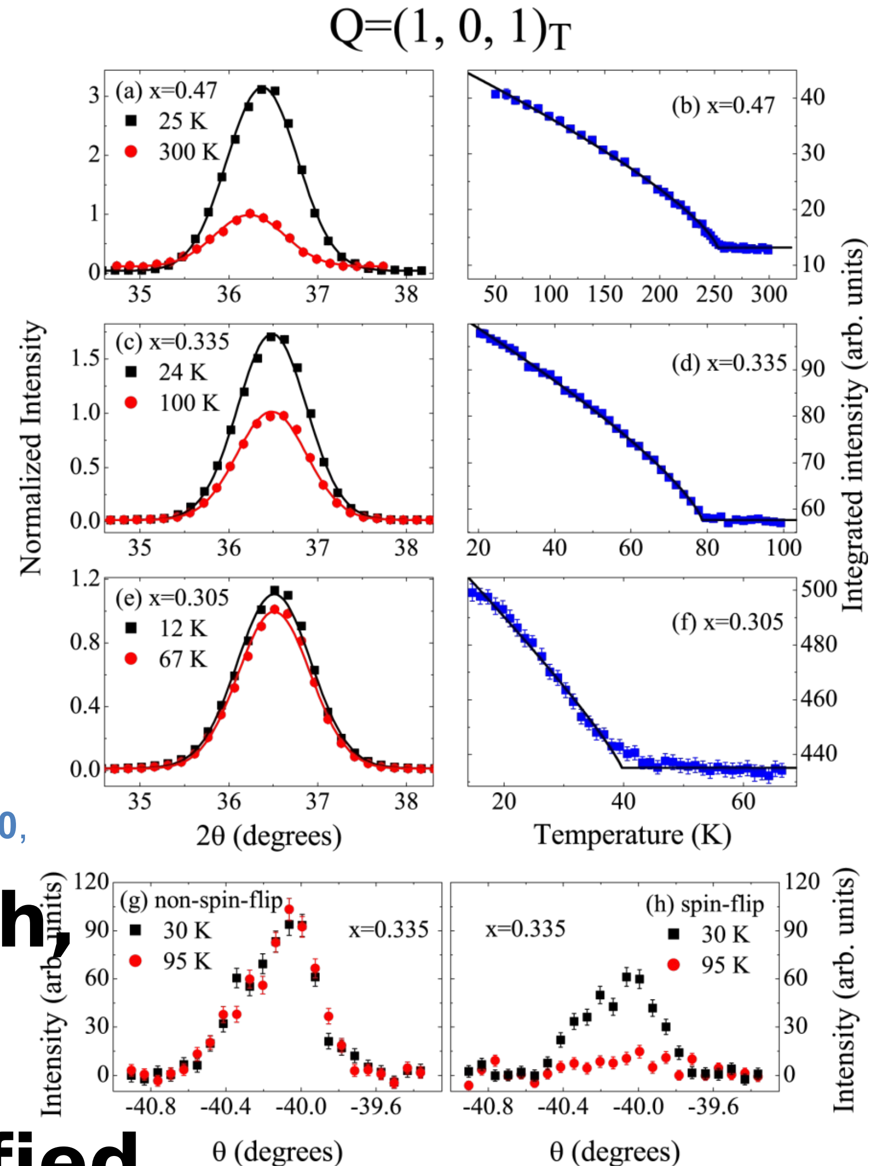
BaFe2As2
Q=(1/2 1/2 1)
TN=143 K
M=0.9 μB

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



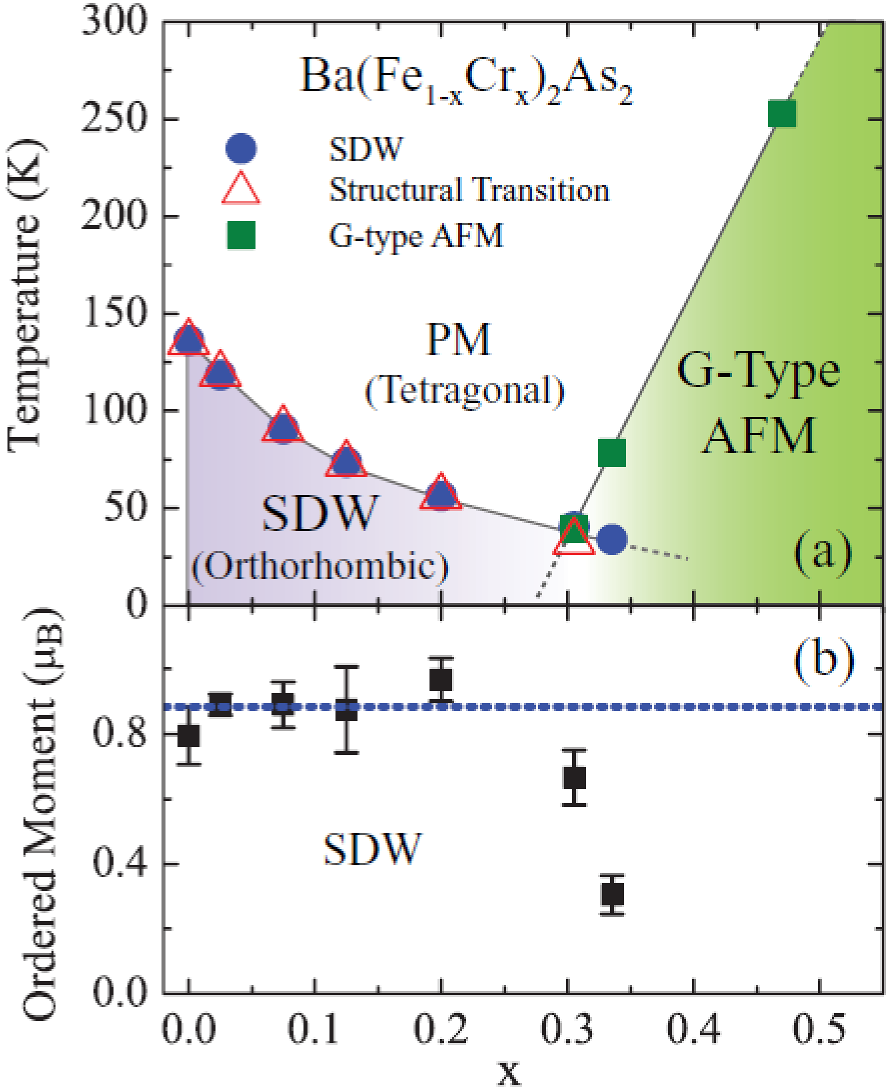
BaMn2As2
Q=(1 0 1)
TN=625 K
M=3.88 μB

Y. Singh *et al*., PRB **80**, 100403 (2009)



- **Calculations by Singh, *et al*. predict a competing G-type magnetic order-verified experimentally.**

Ba(Fe1-xCrx)2As2 Phase Diagram



Phase diagram similarities with Ba(Fe1-xRux)2As2 (Thaler, *et al.*)

- SDW survives to high doping level
- No separation of phase transitions

No superconductivity for Cr-doping

Additional magnetic phase with Cr-doping

Magnetic order seems similar to that found in BaMn2As2 (An, *et al.*)