

Кристаллическая структура, фазовый состав и сверхпроводимость новых соединений на основе FeSe



MAX-PLANCK-GESELLSCHAFT



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Max Planck Institute for Solid State Research



Зеленогорск, 2013



MPI-FKF

Stuttgart

Collaborators



MAX-PLANCK-GESELLSCHAFT



MPI-FKF Stuttgart, Germany

Neutron scattering: J. T. Park, G. Friemel, J.-H. Kim,
Yuan Li, V. Hinkov, B. Keimer;

LDA calculations: A. Yaresko;

Single crystals: C. T. Lin *et al.*

Augsburg University, Germany

Single crystals: V. Tsurkan, J. Deisenhofer,
H.-A. Krug von Nidda, A. Loidl.

Université Paris-Sud

NMR measurements: J. Bobroff, Y. Texier, Y. Laplace.

Institut Laue-Langevin, Grenoble, France

Instrument support: A. Ivanov

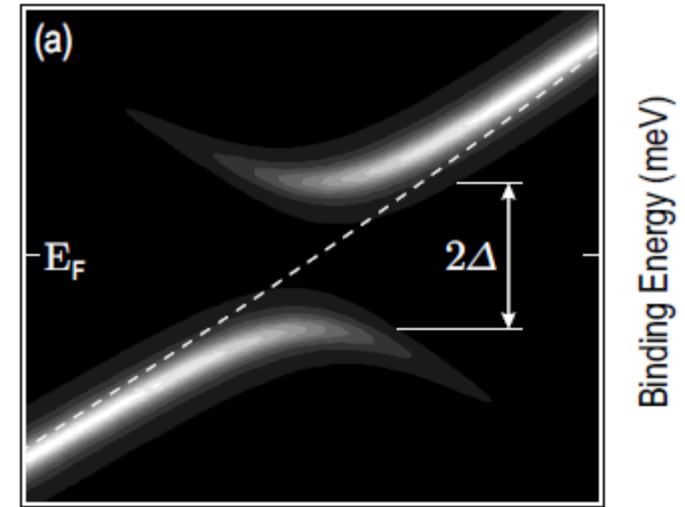
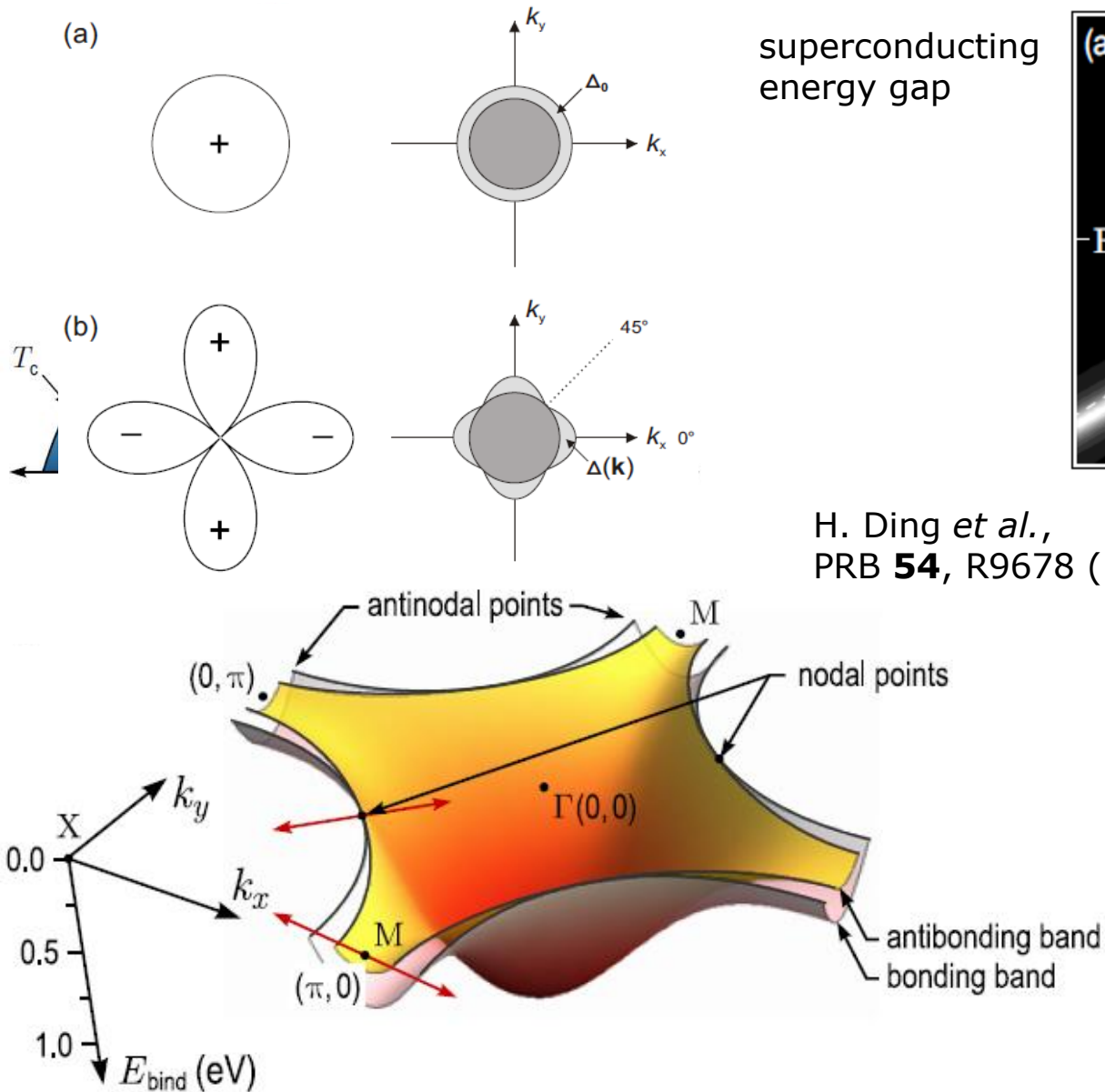
ISIS, Rutherford Appleton Laboratory

Instrument support: E. A. Goremychkin

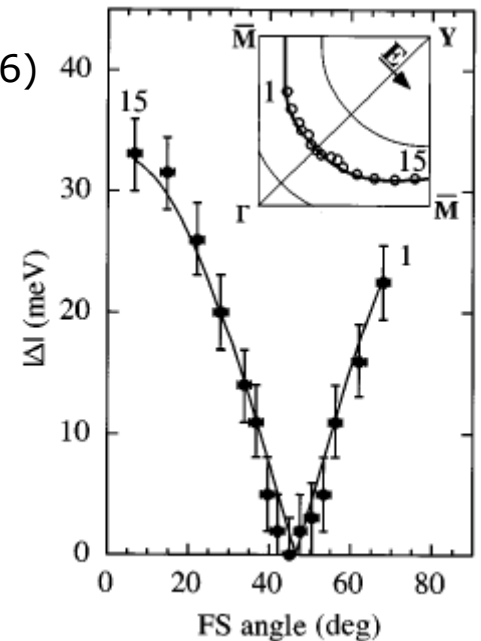
Oak Ridge National Lab

Band structure calculations: T. A. Maier

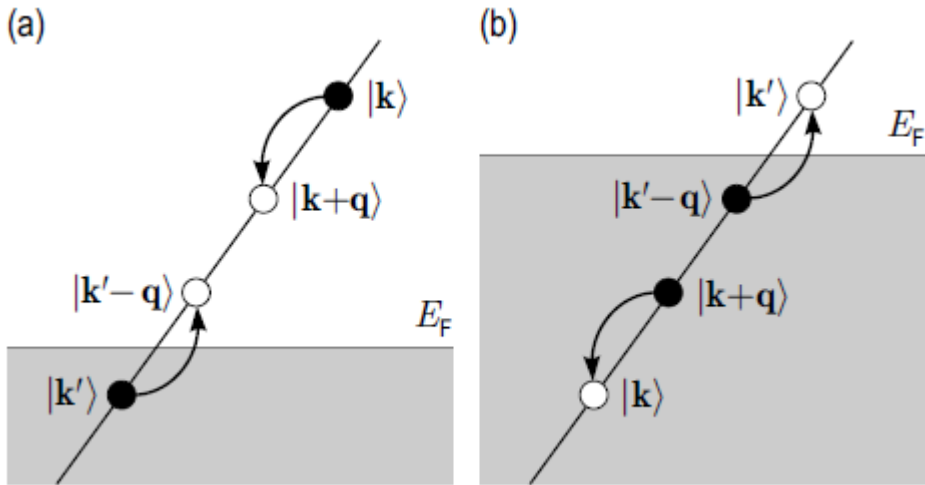
Unconventional superconductors



H. Ding *et al.*,
PRB **54**, R9678 (1996)



Particle-hole scattering

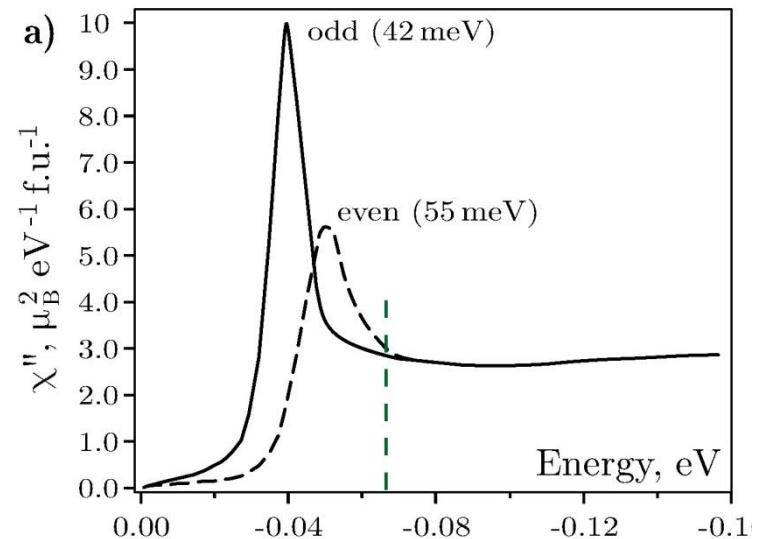
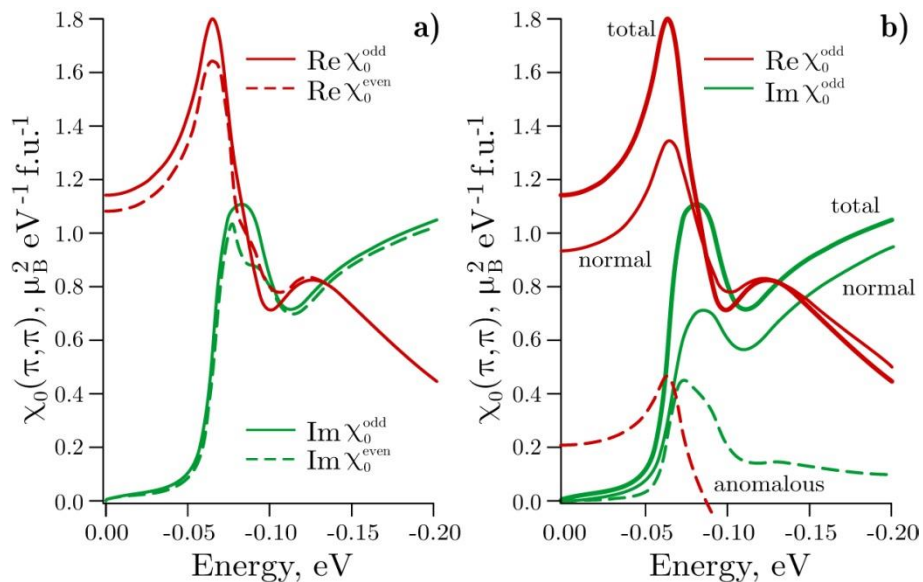


Lindhard susceptibility:

$$\chi_0(\mathbf{q}, \omega) = 2 \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{n_F(\epsilon_{\mathbf{k}}) - n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}} + \omega + i0^+}$$

Spin exciton below the particle-hole continuum:

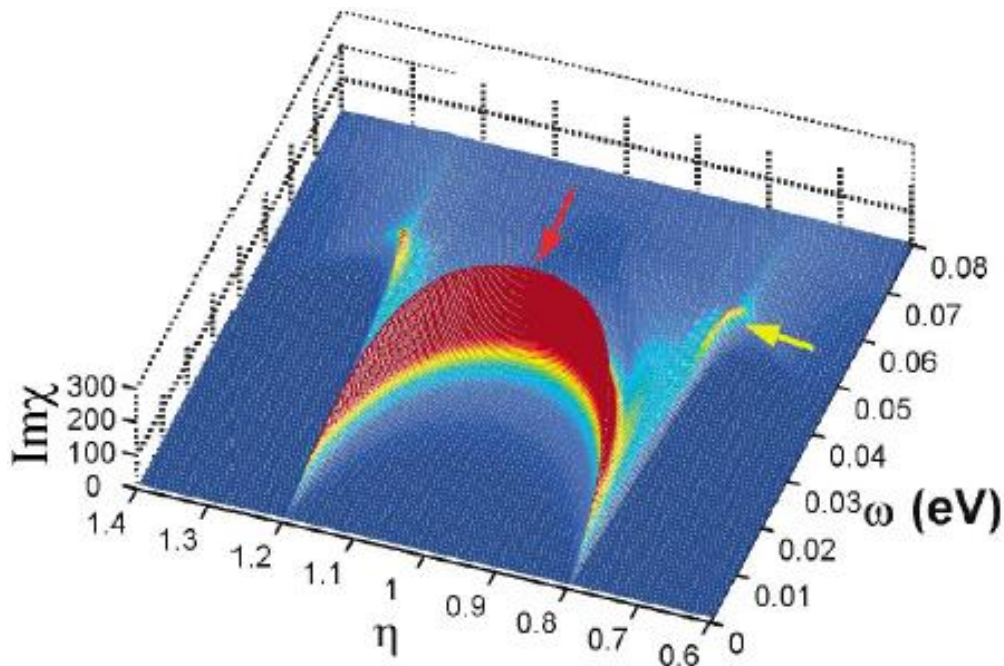
$$\chi(\mathbf{q}, \omega) = \frac{\chi_0(\mathbf{q}, \omega)}{1 - g(\mathbf{q})\chi_0(\mathbf{q}, \omega)}$$



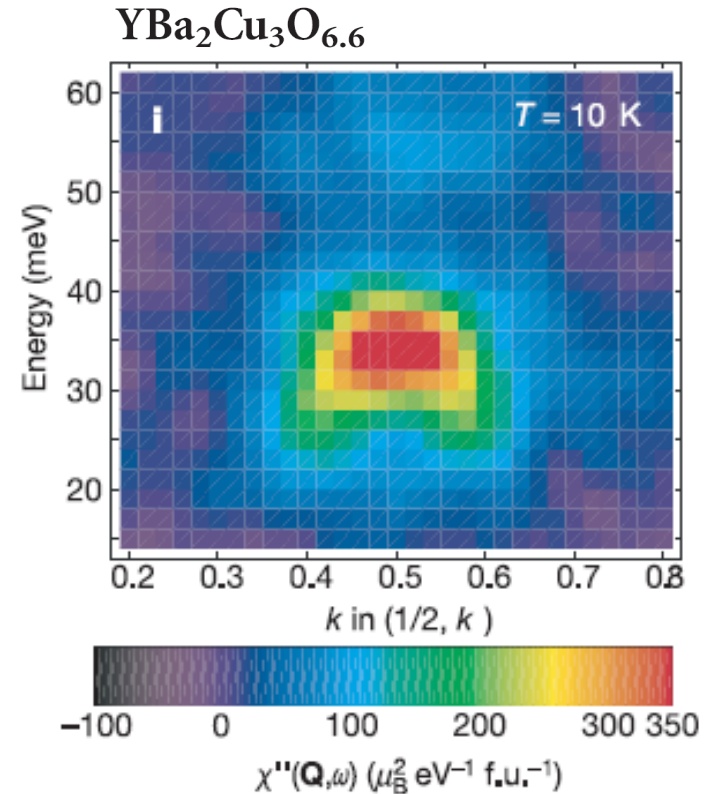
Resonant mode in copper oxides

“Hourglass” dispersion in cuprates:
Fermi-surface + d -wave gap

$$\chi(\mathbf{q}, \omega) = \frac{\chi_0(\mathbf{q}, \omega)}{1 - g(\mathbf{q})\chi_0(\mathbf{q}, \omega)}$$



I. Eremin *et al.*, Phys. Rev. Lett. **94**, 147001 (2005)

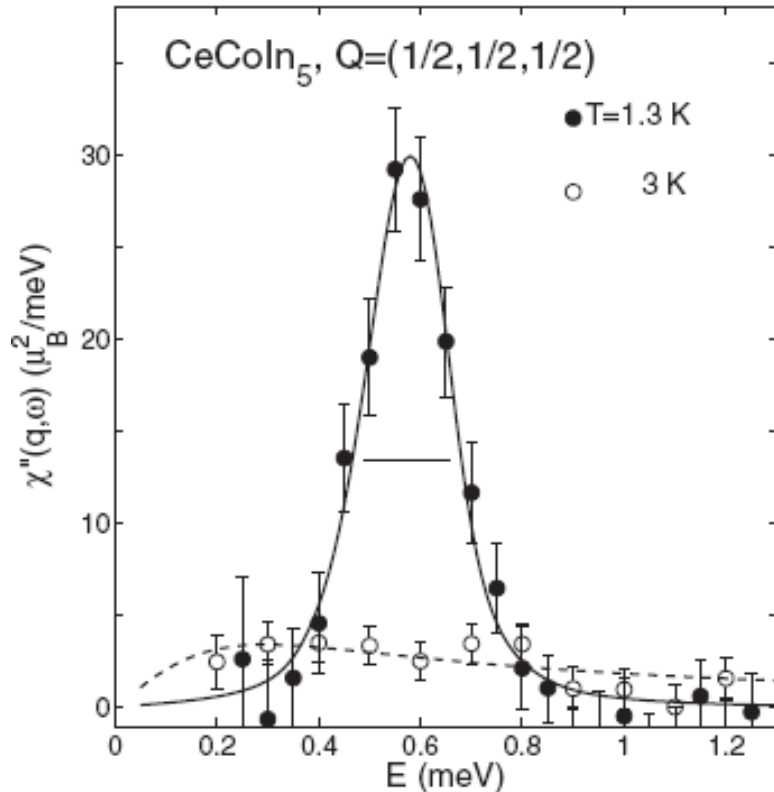


S. M. Hayden *et al.*,
Nature **429**, 531 (2004)

Original discovery:
J. Rossat-Mignod *et al.*,
Physica C **185**, 86 (1991)

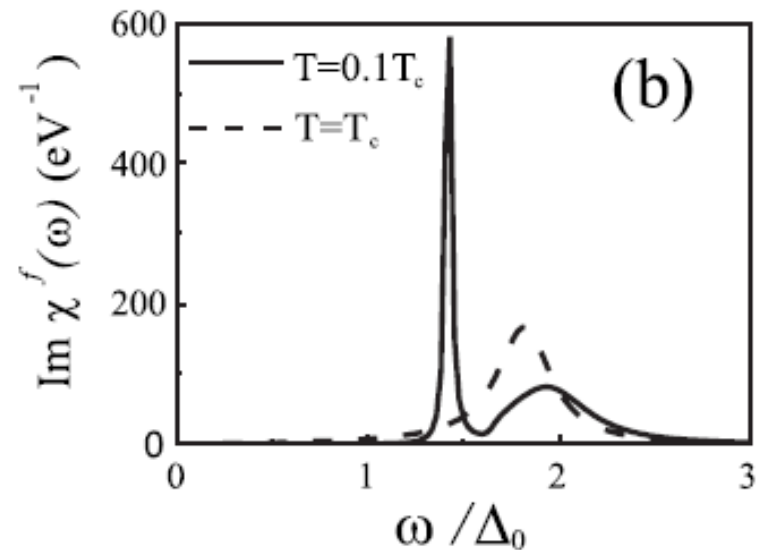
Magnetic resonant mode in CeCoIn₅

Heavy-fermion superconductor



C. Stock *et al.*,
Phys. Rev. Lett. **100**, 087001 (2008)

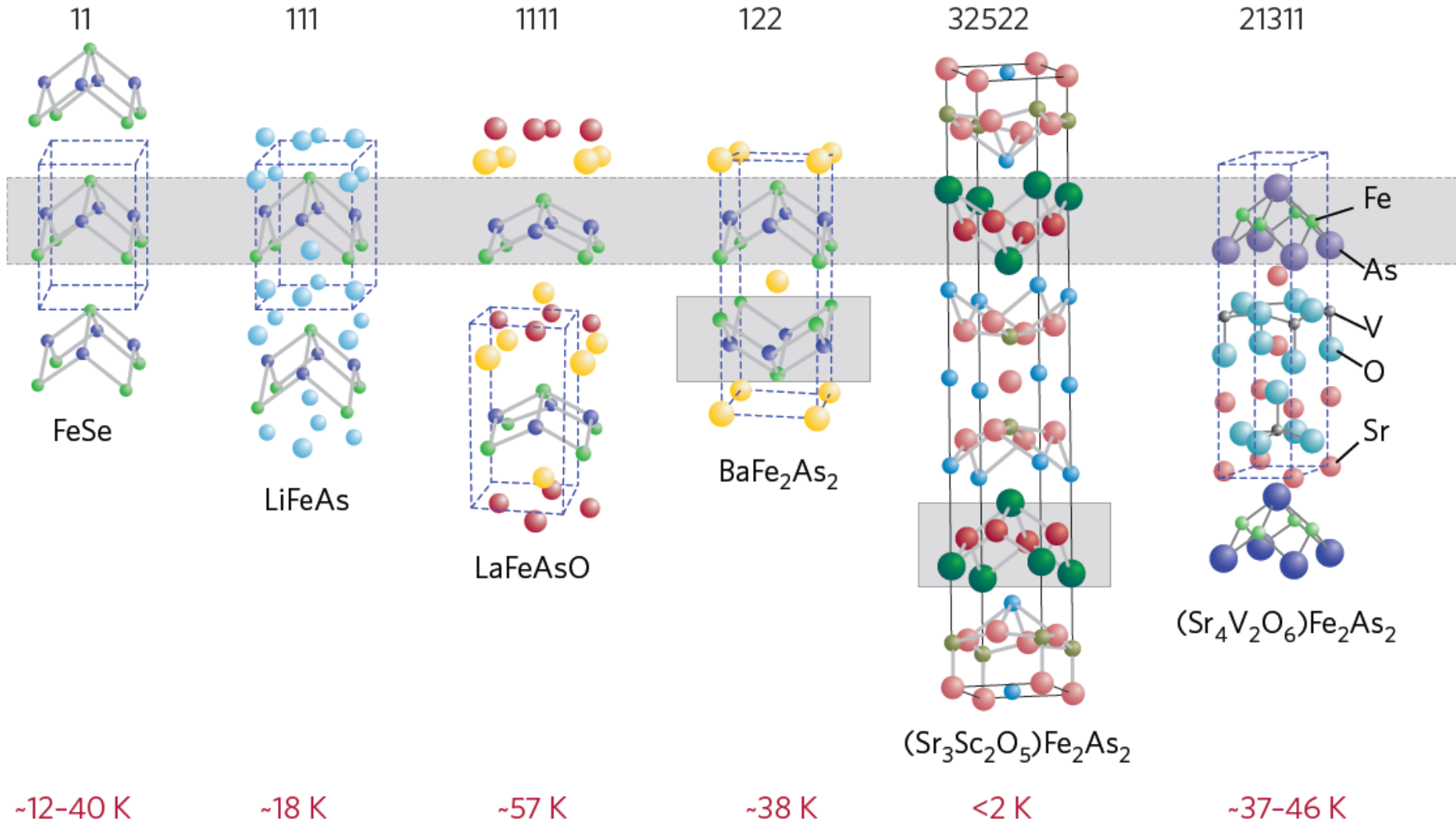
Theory:



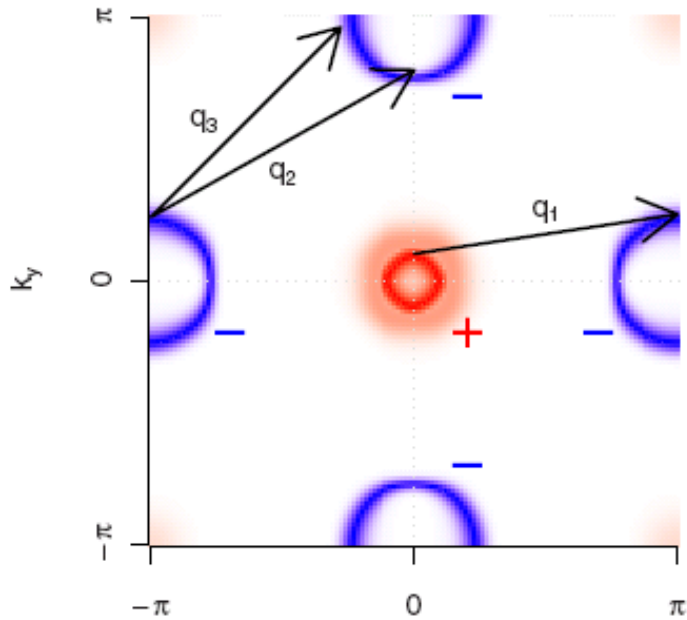
A. Akbari *et al.*,
Phys. Rev. B **80**, 100504R (2009)

Iron-arsenide superconductors

Fe-based superconductors



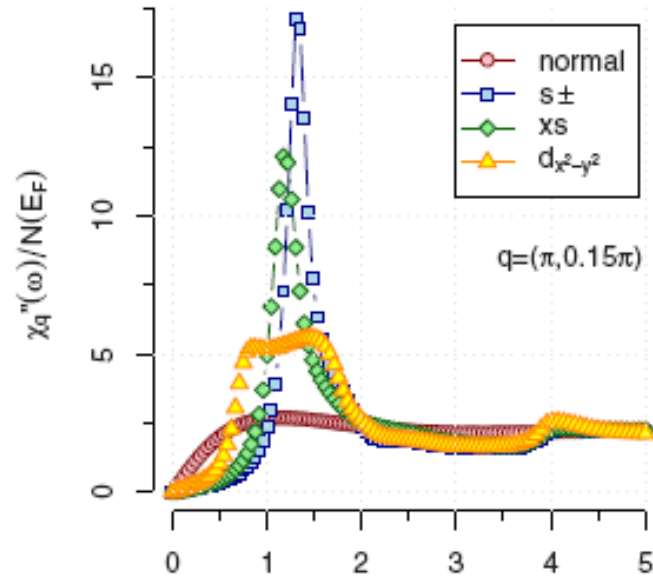
Resonant mode in Fe-based superconductors



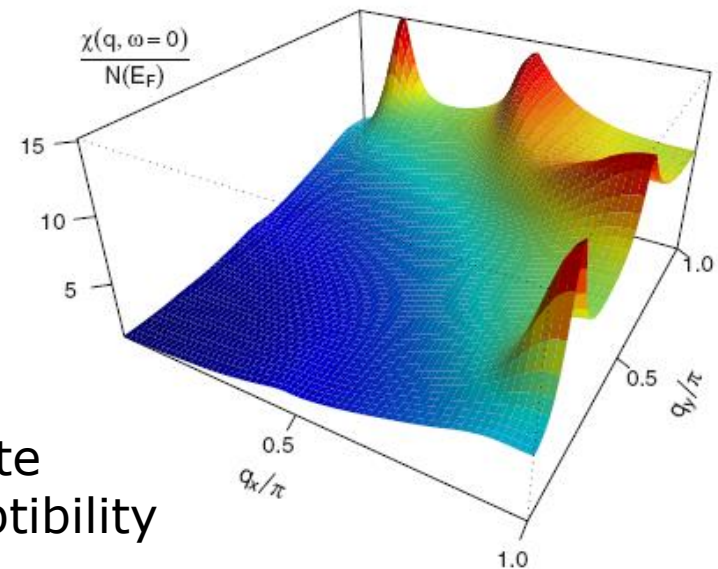
Isotropic, sign reversed
s-wave

T. A. Maier et al.,
PRB **79**, 134520 (2009);

see also Eremin et al.,
PRB **78** 140509 (2008).

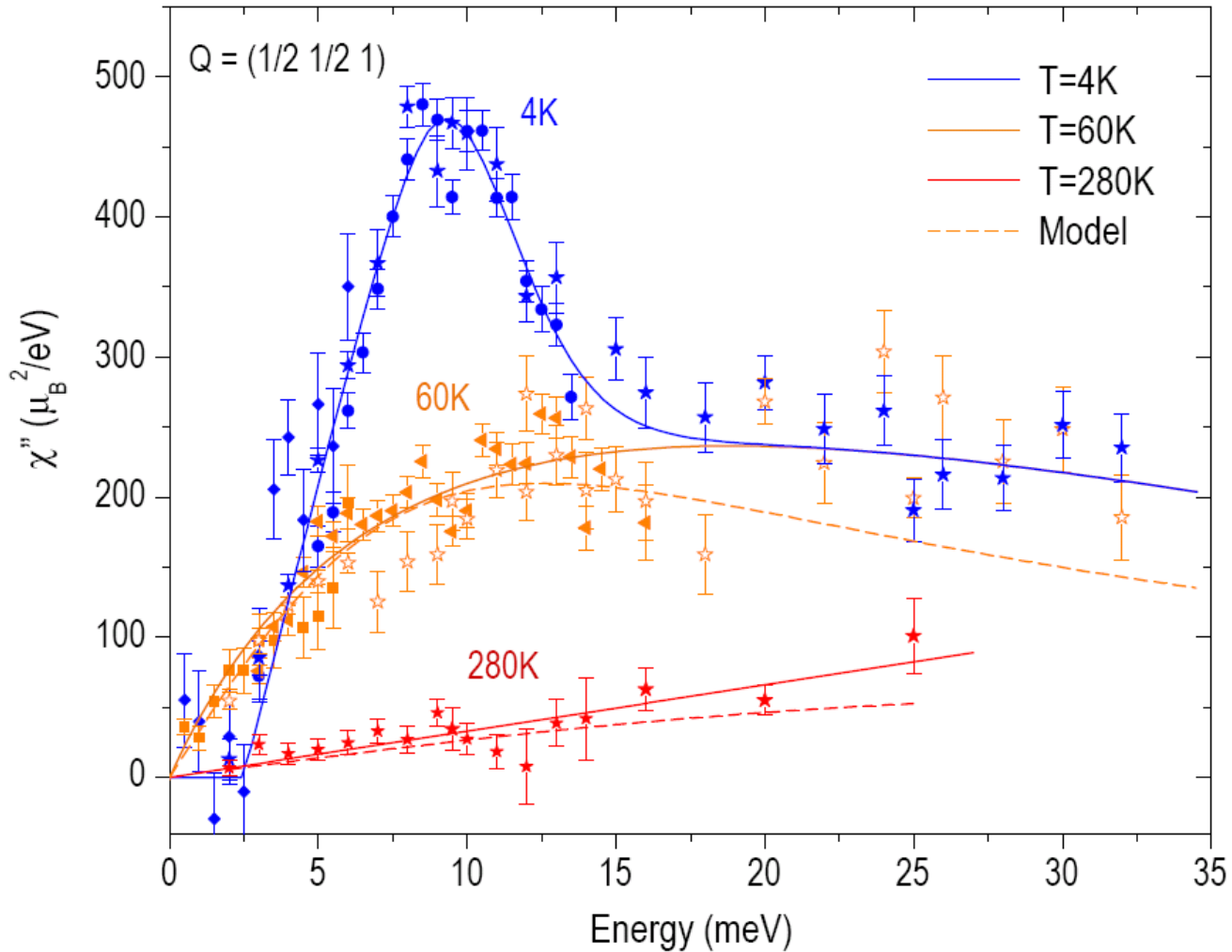


(a)



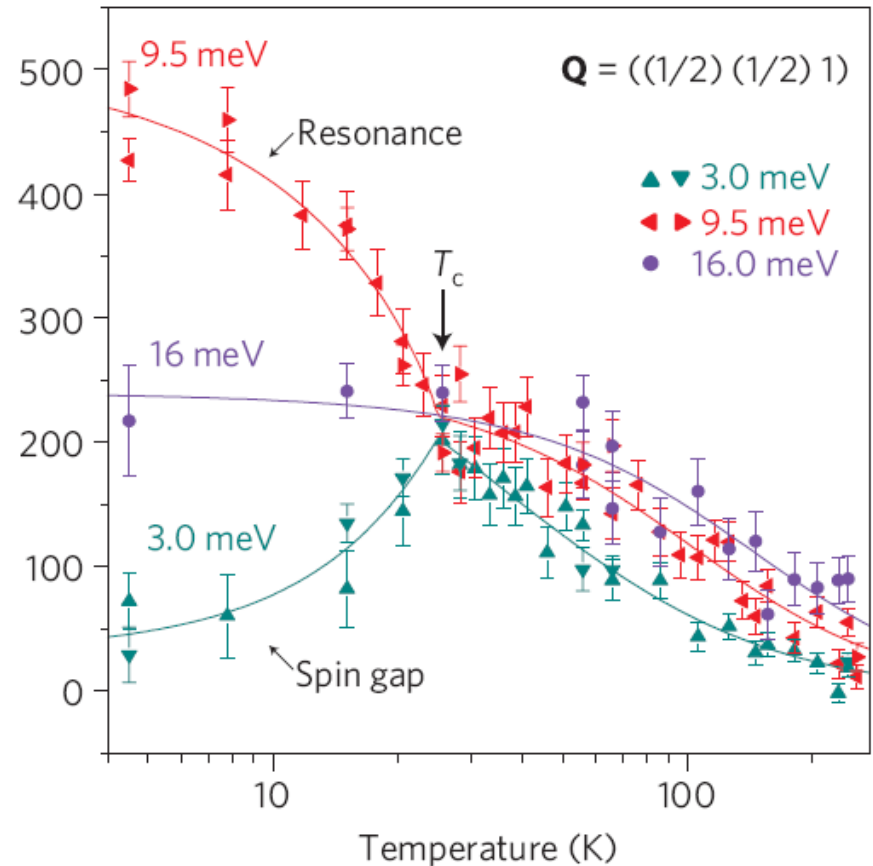
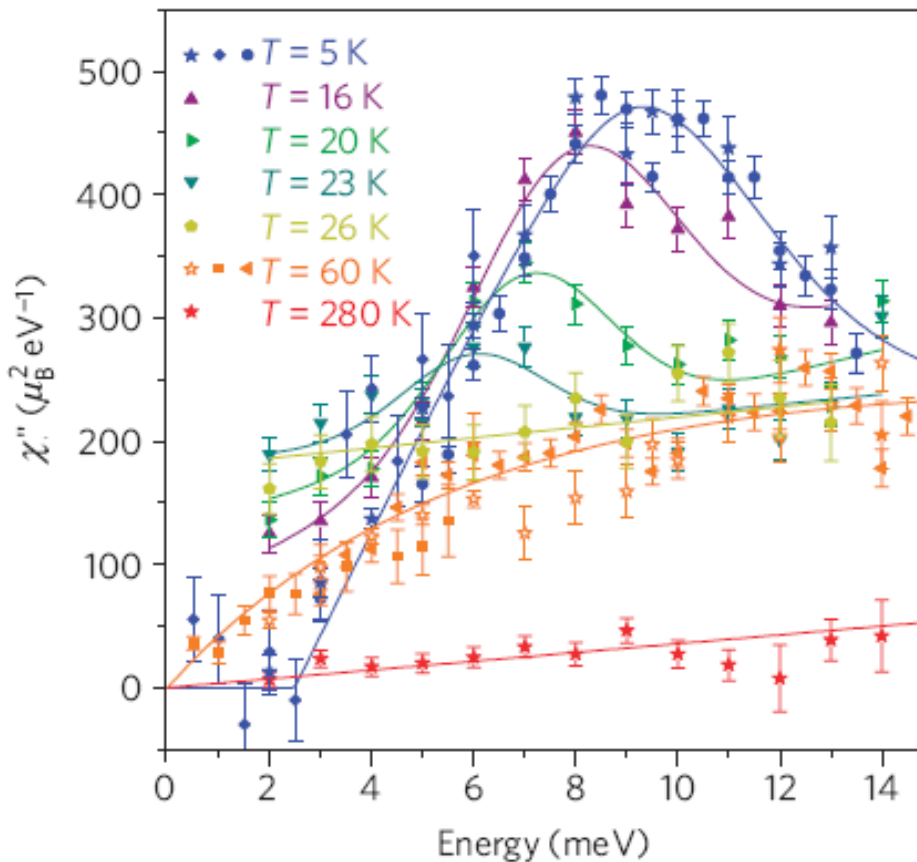
Normal state
spin susceptibility

Magnetic resonant mode in $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$



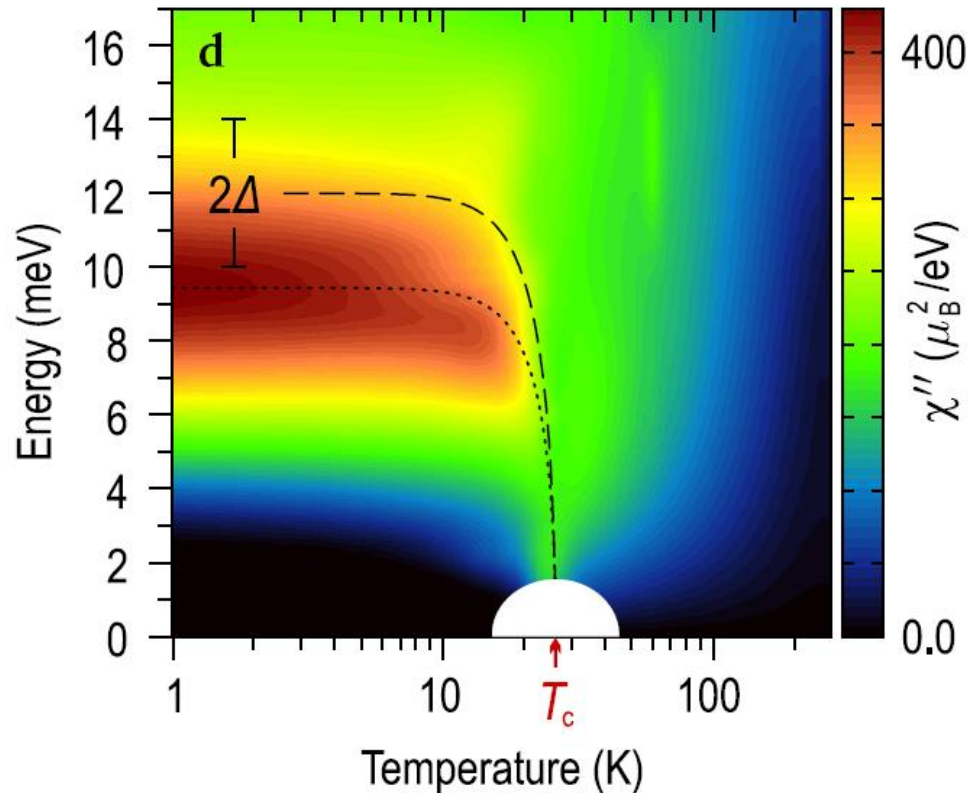
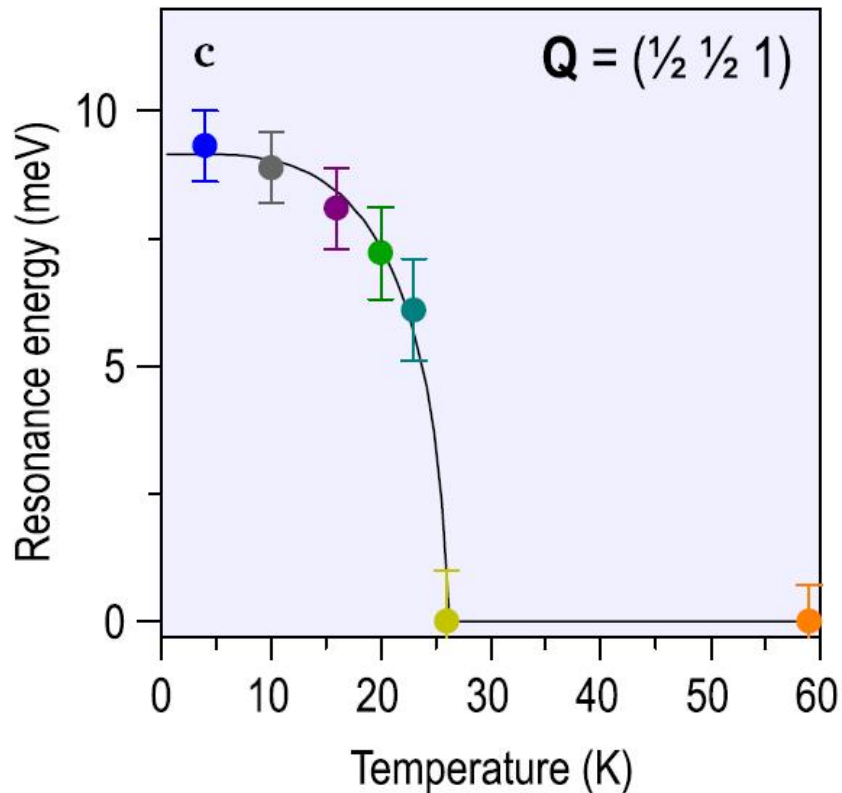
Magnetic resonant mode in $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$

$\text{BaFe}_{1.85}\text{Co}_{0.15}\text{As}_2$

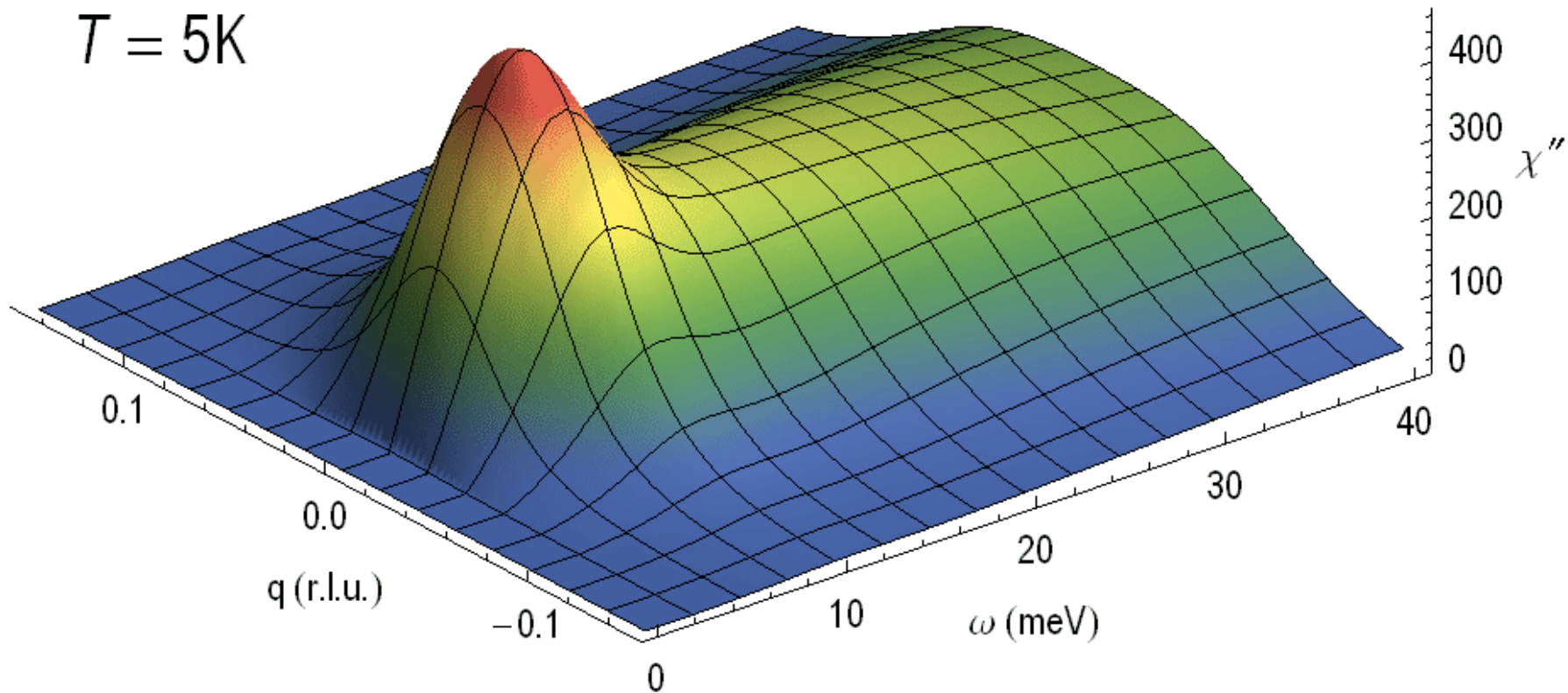


D. Inosov *et al.*, Nature Phys. **6**, 178 (2010)

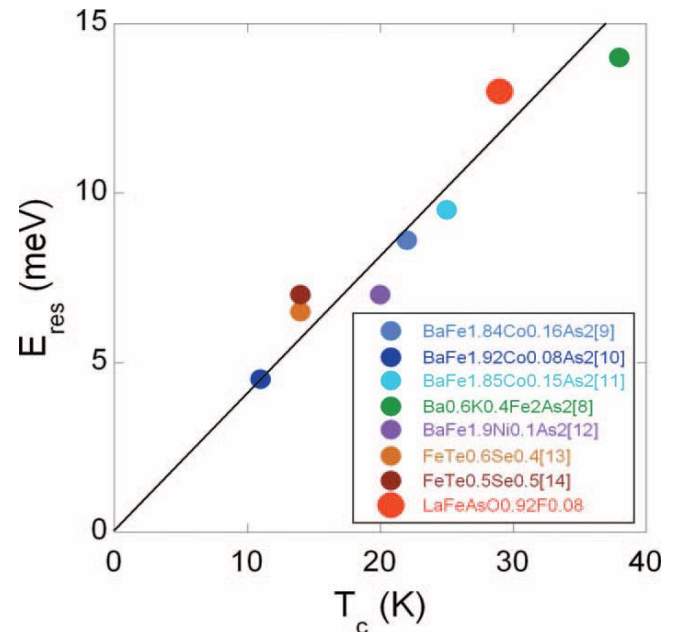
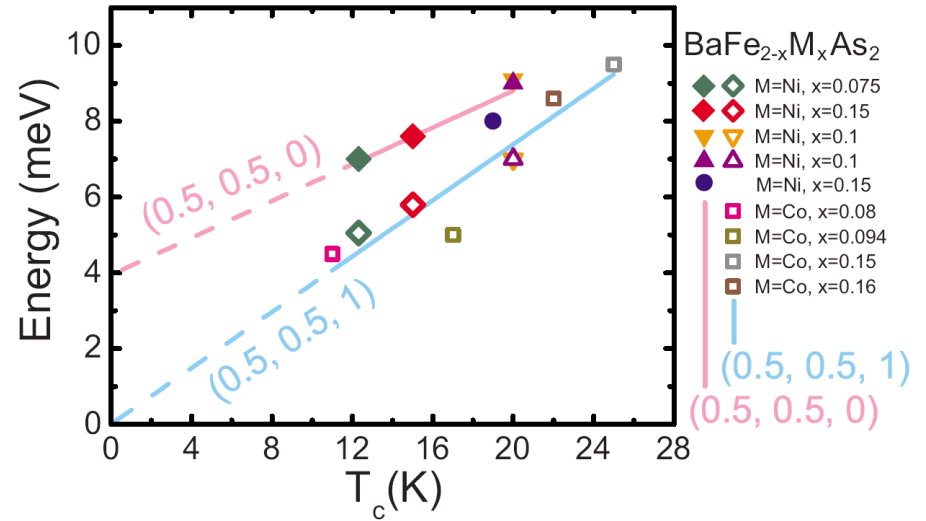
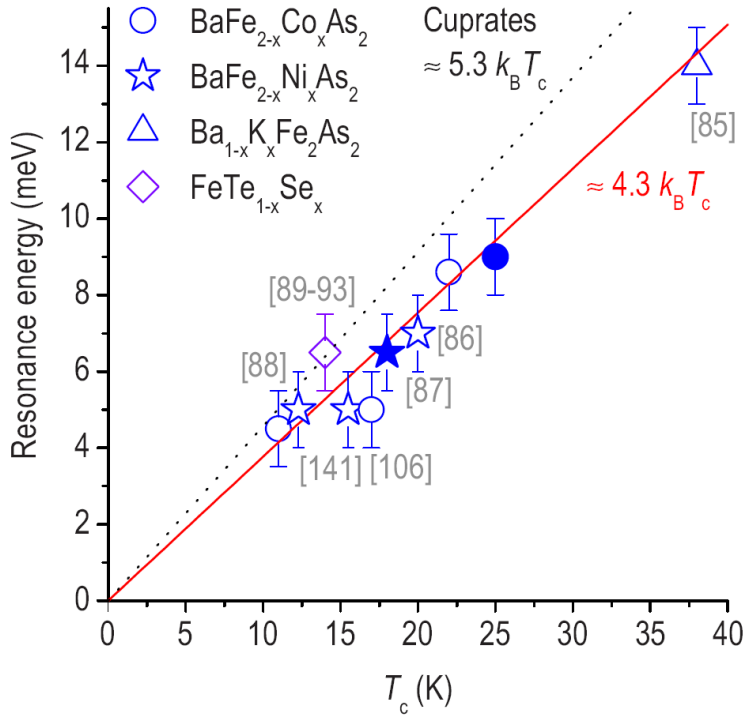
Temperature dependence of the resonance



Q -, ω -, and T -dependence of the spin excitations



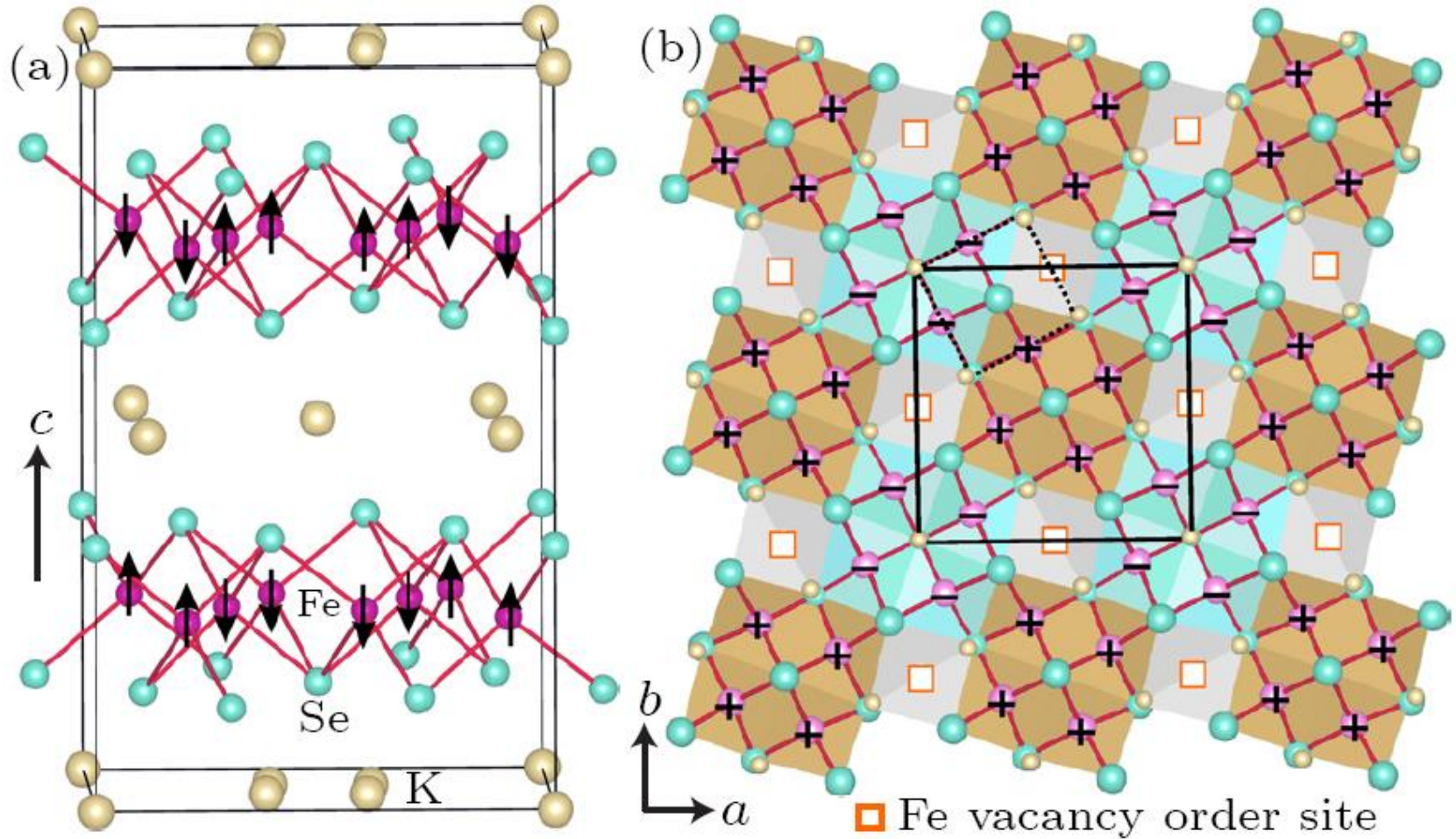
Linear relationship between E_{res} and T_c



J. T. Park, D. S. Inosov *et al.*, PRB (2010);
M. Wang *et al.*, PRB **81**, 174524 (2010);
S. Shamoto *et al.*, PRB **82**, 172508 (2010).

Magnetic resonant mode in
 $A_{1-x}Fe_{2-y}Se_2$

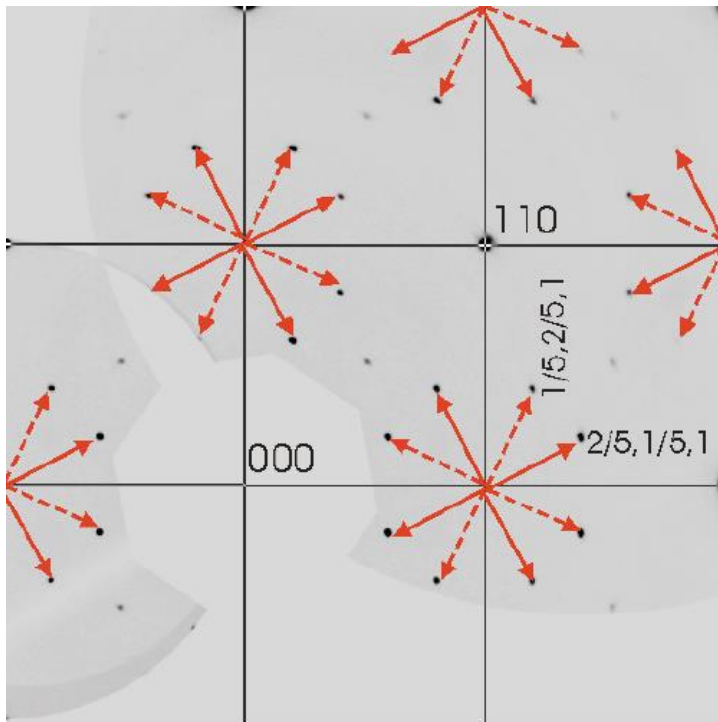
Iron selenides of the "245" family



F. Ye *et al.*, PRL **107**, 137003 (2011),
see also V. Yu. Pomjashin *et al.*, PRB (2011).

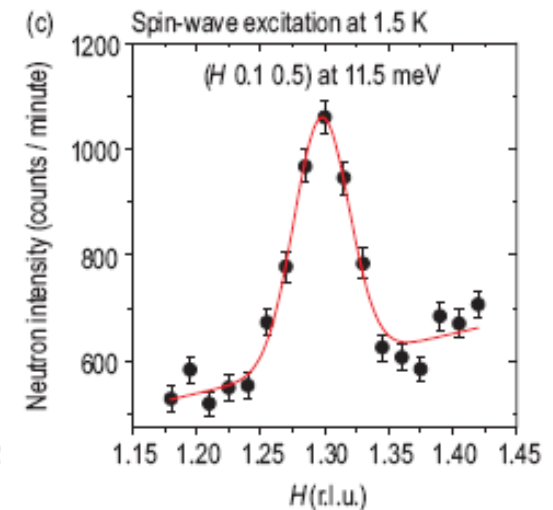
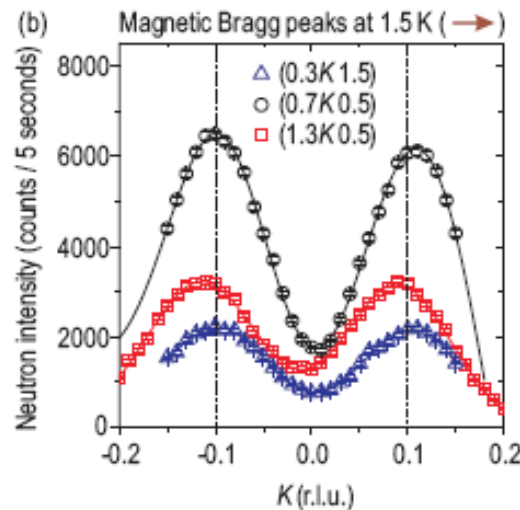
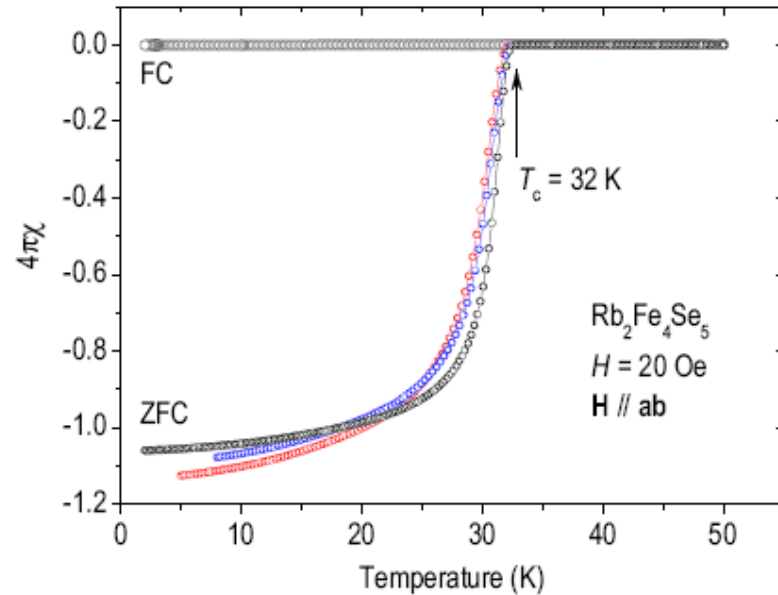
Magnetic order and iron-vacancy superstructure

Fe-vacancy ordering

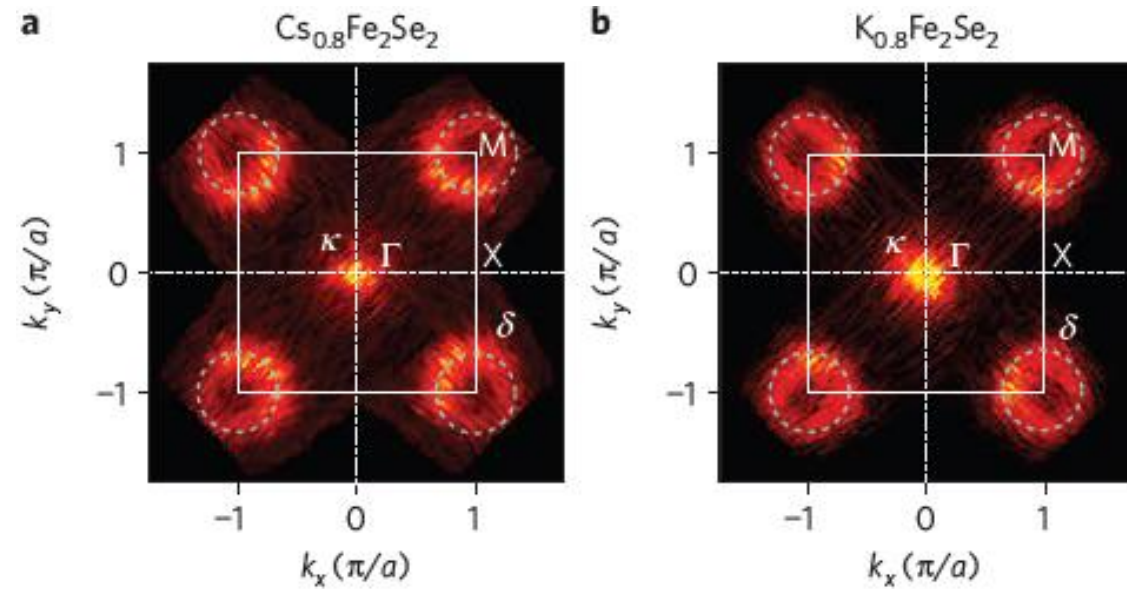


from V. Yu. Pomjakushin *et al.*,
Phys. Rev. B **83**, 144410 (2011);
JPCM **23**, 156003 (2011).

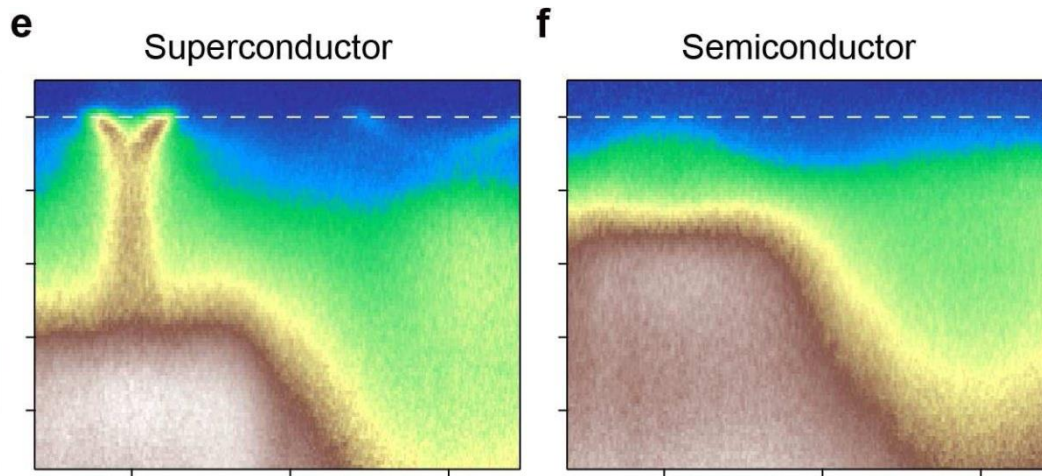
J. T. Park *et al.*,
PRL **107**, 177005 (2011)



Metal or insulator?

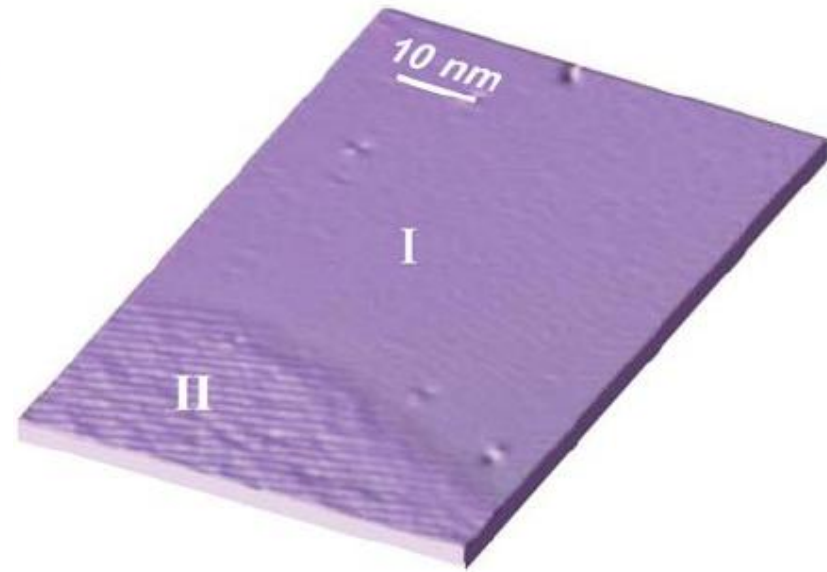
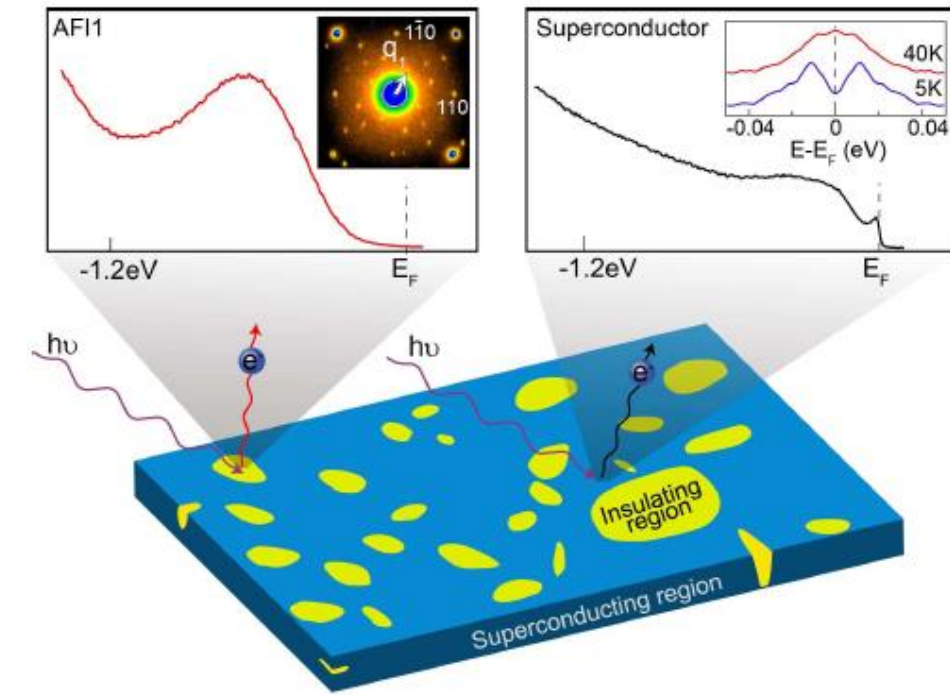


Y. Zhang *et al.*, *Nature Mater.* (2011),
see also T. Qian *et al.*, *PRL* (2011),
D. Mou *et al.*, *PRL* (2011),
X.-P. Wang *et al.*, *EPL* (2011), etc.

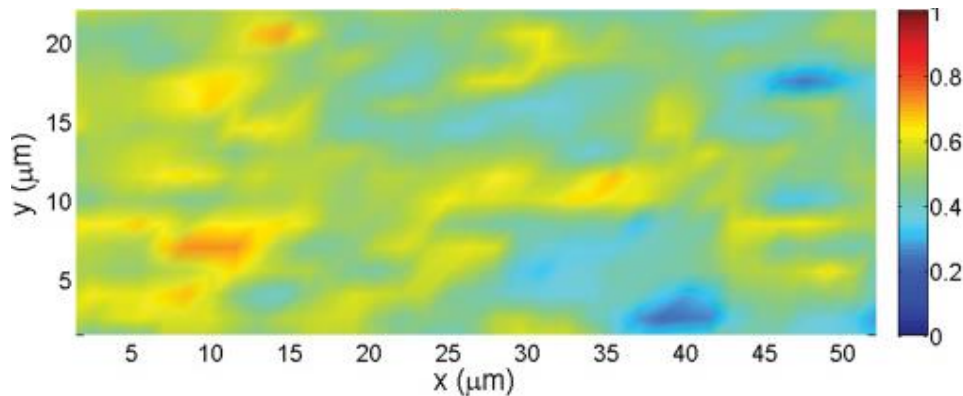


F. Chen *et al.*, *PRX* **1**, 021020 (2011)

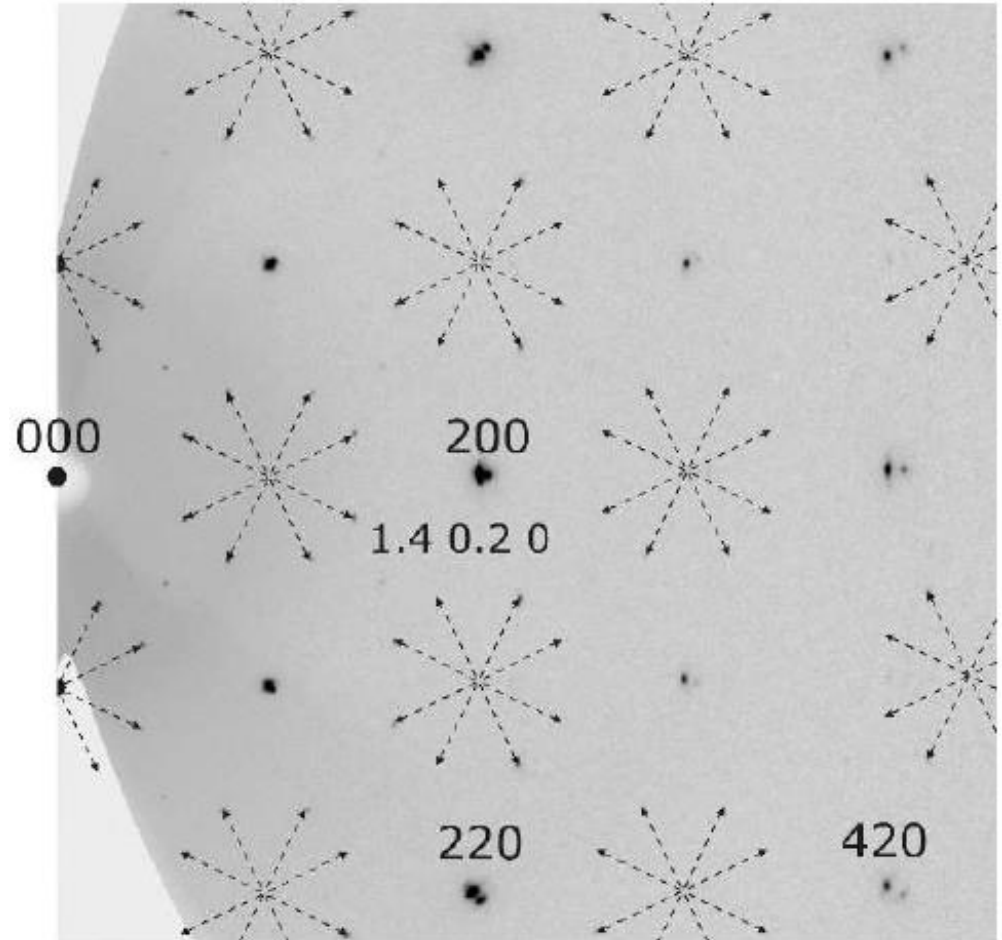
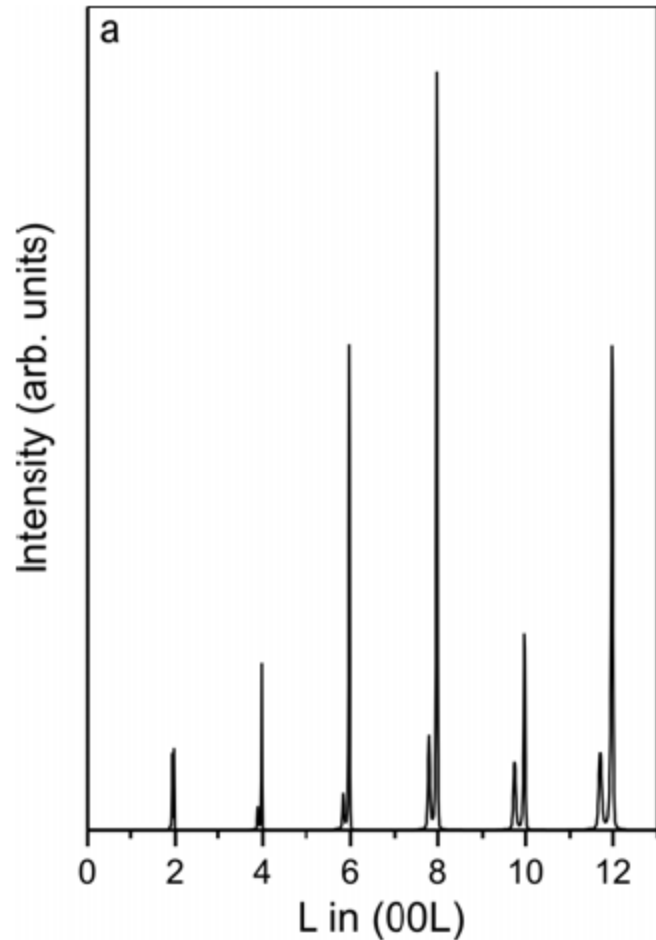
Nanoscale phase separation



W. Li *et al.*, Nat. Phys. **8**, 126 (2012)
A. Ricci *et al.*, PRB **84**, 060511(R)
F. Chen *et al.*, PRX **1**, 021020 (2011)



Nanoscale phase separation

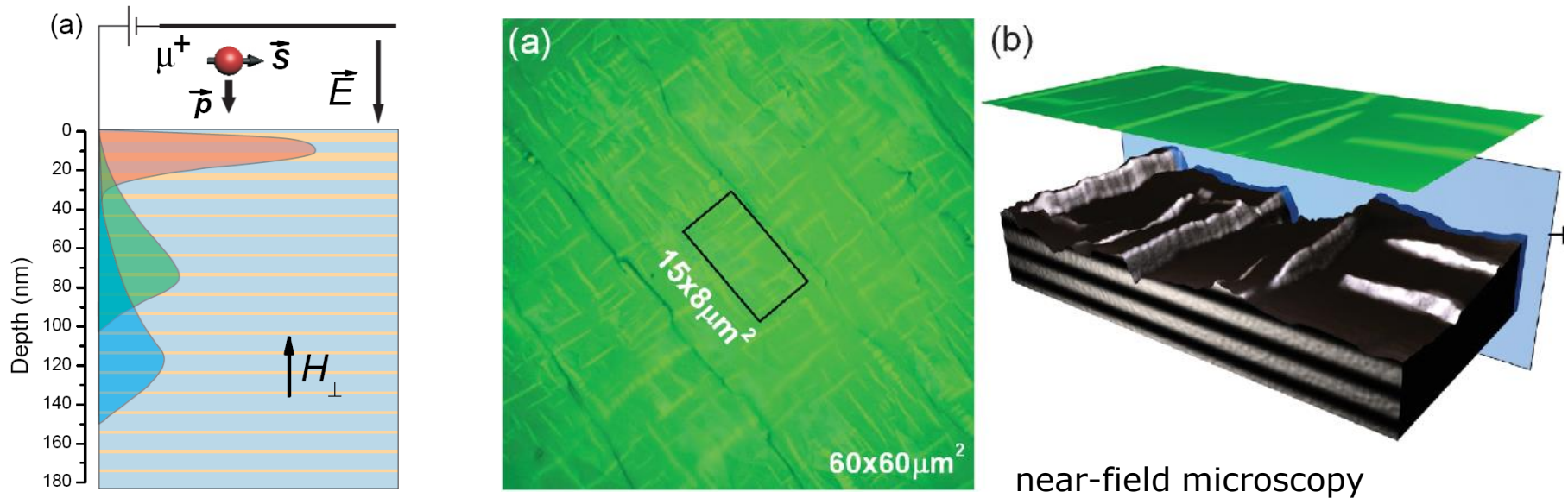


A. Bosak *et al.*, arXiv:1112.2569; V. Yu. Pomjakushin *et al.*, arXiv:1204.5449

See also:

X. G. Luo *et al.*, NJP **13**, 053011 (2011); Y. Liu *et al.*, SUST **25**, 075001 (2012); etc.

Nanoscale layering of the two phases



A. Charnukha *et al.*, PRL **109**, 017003 (2012)

See also:

S. C. Speller *et al.*, arXiv:1204.5472

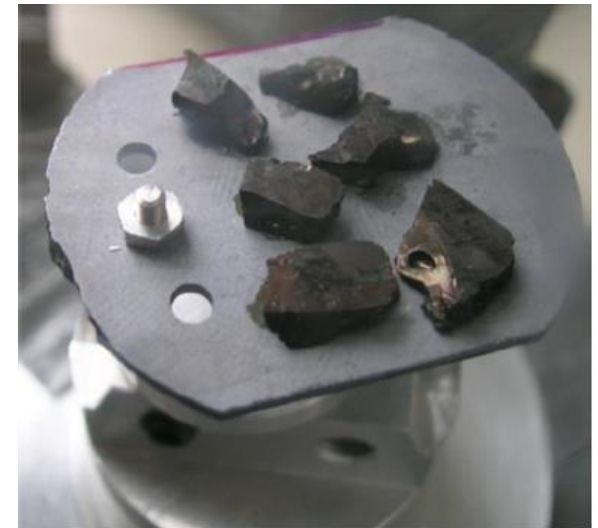
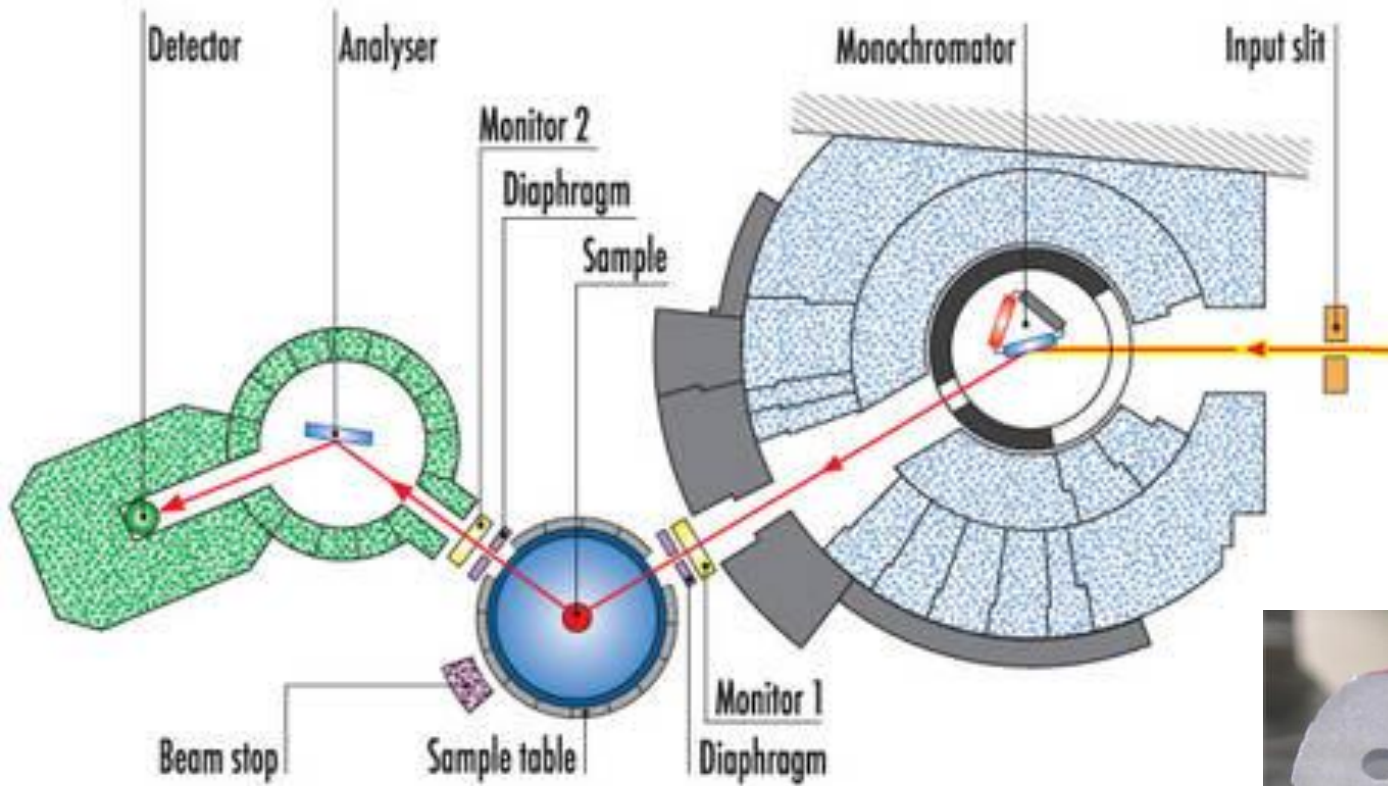
R. H. Yuan *et al.*, Sci. Rep. **2**, 221 (2012)

What is the composition and structure of the superconducting phase?

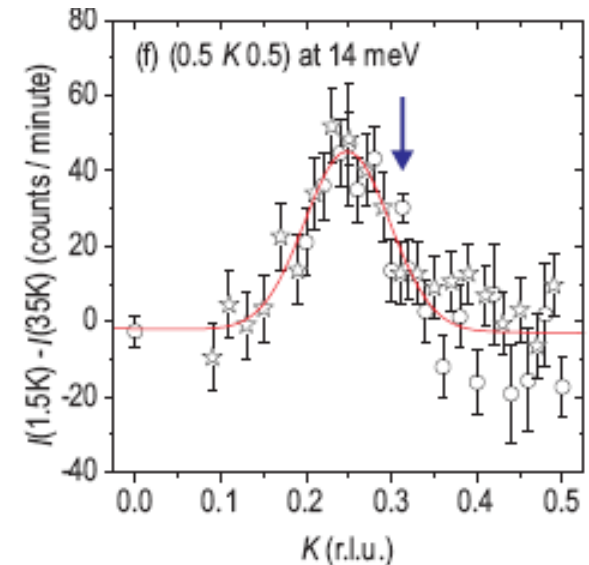
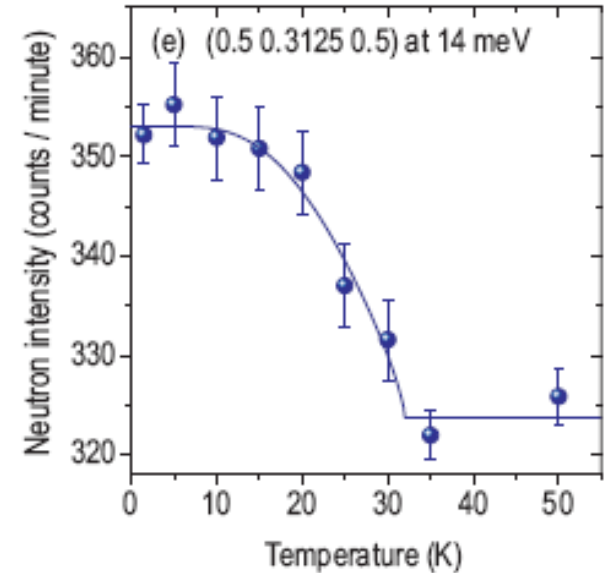
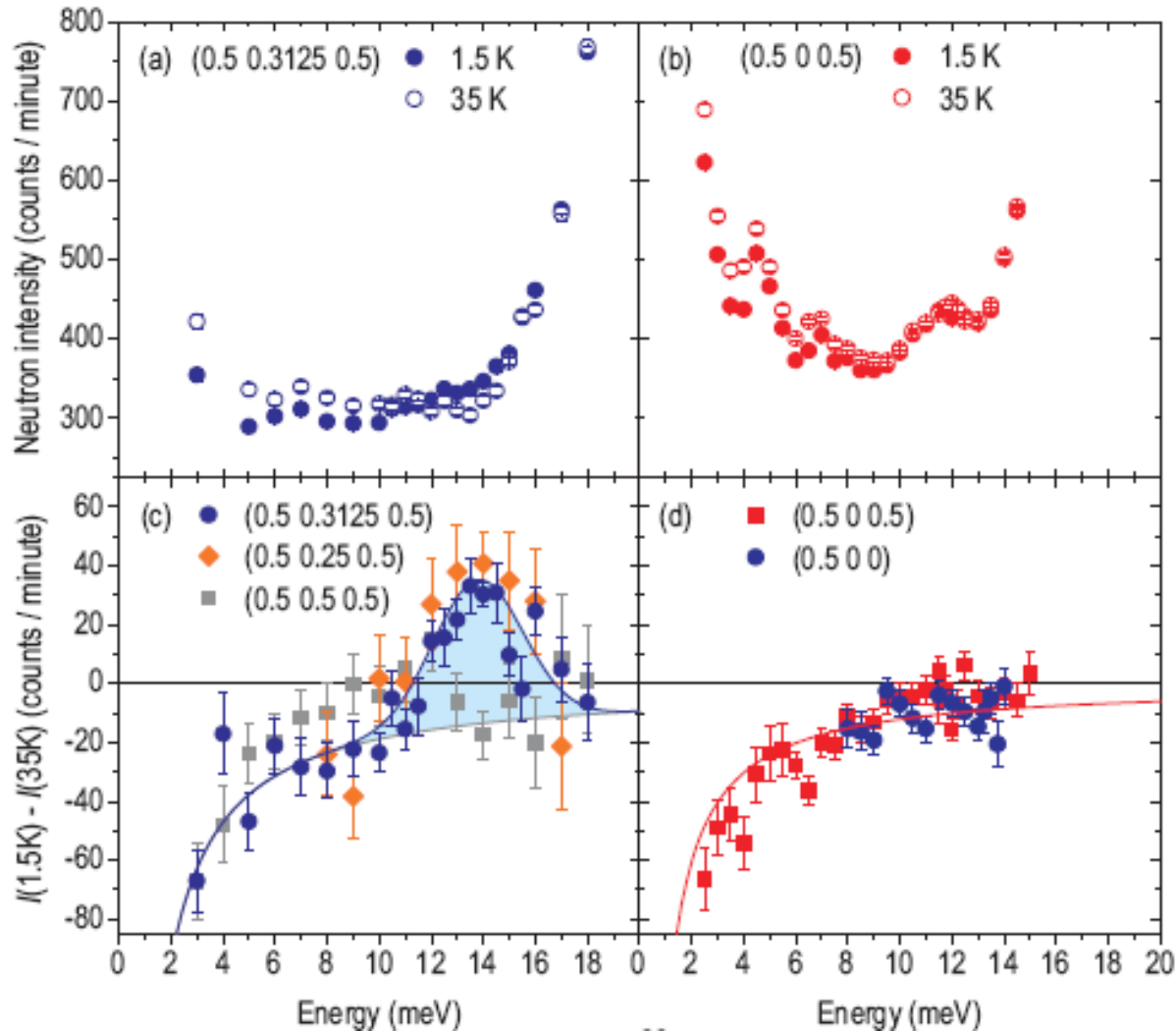
- doping level/concentration of the alkali metal (K, Rb, or Cs)
- presence of vacancies
- vacancy order or disorder

**Inelastic neutron scattering
on $A_{1-x}Fe_{2-y}Se_2$**

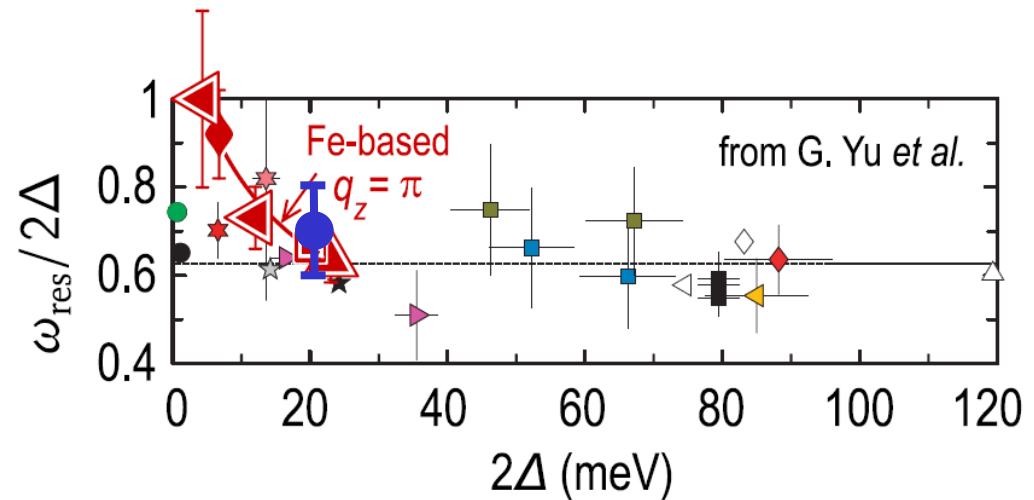
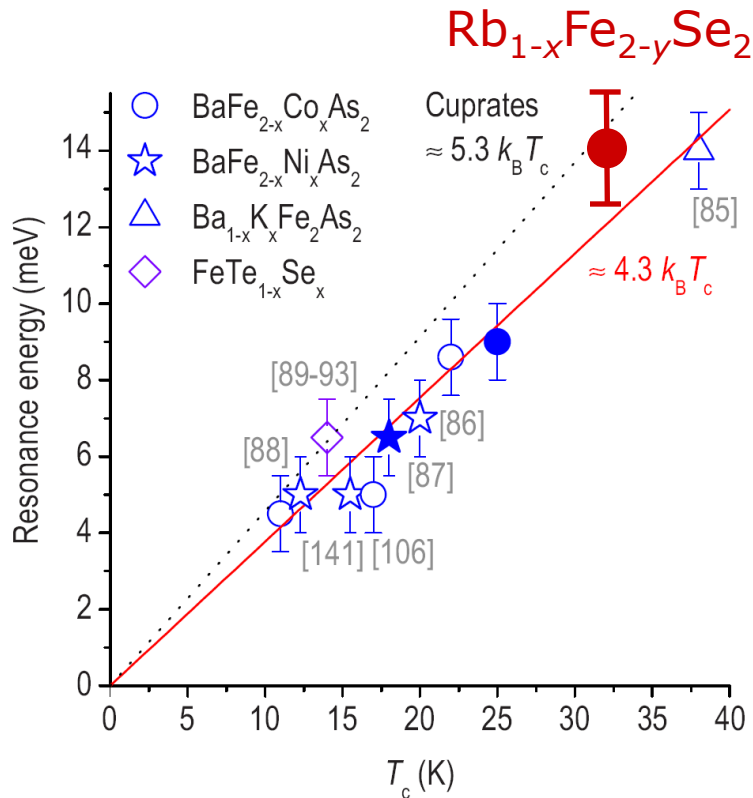
IN8 triple-axis spectrometer (ILL)



Resonant mode in $\text{Rb}_{1-x}\text{Fe}_{2-y}\text{Se}_2$



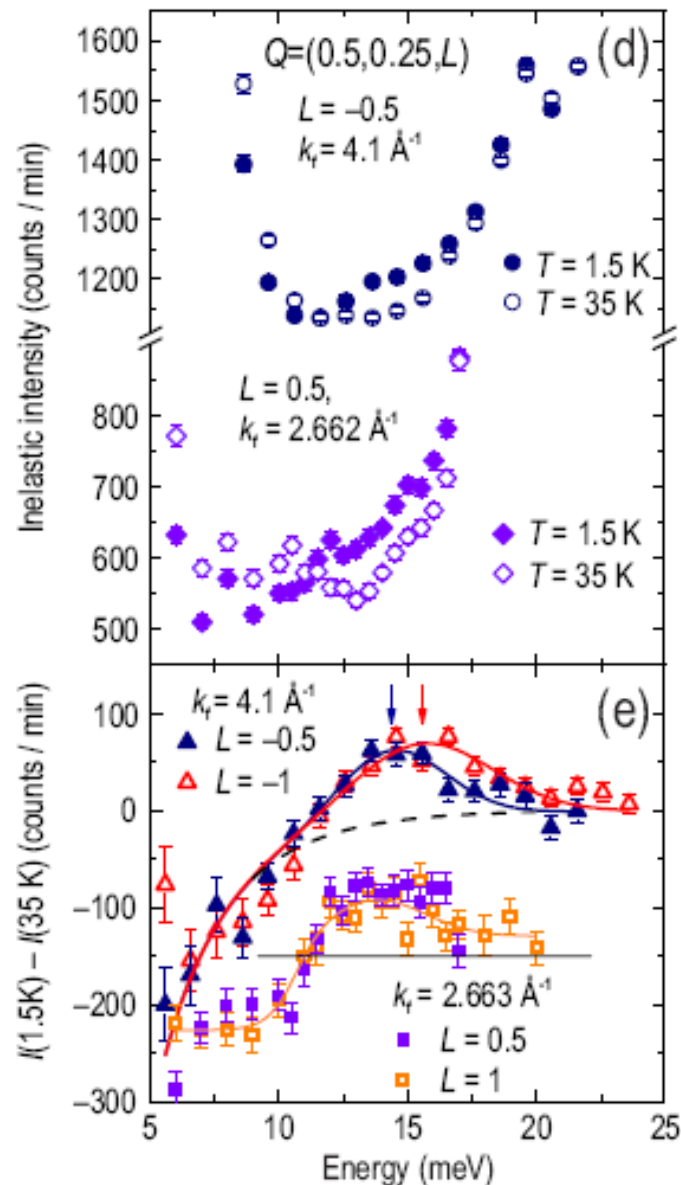
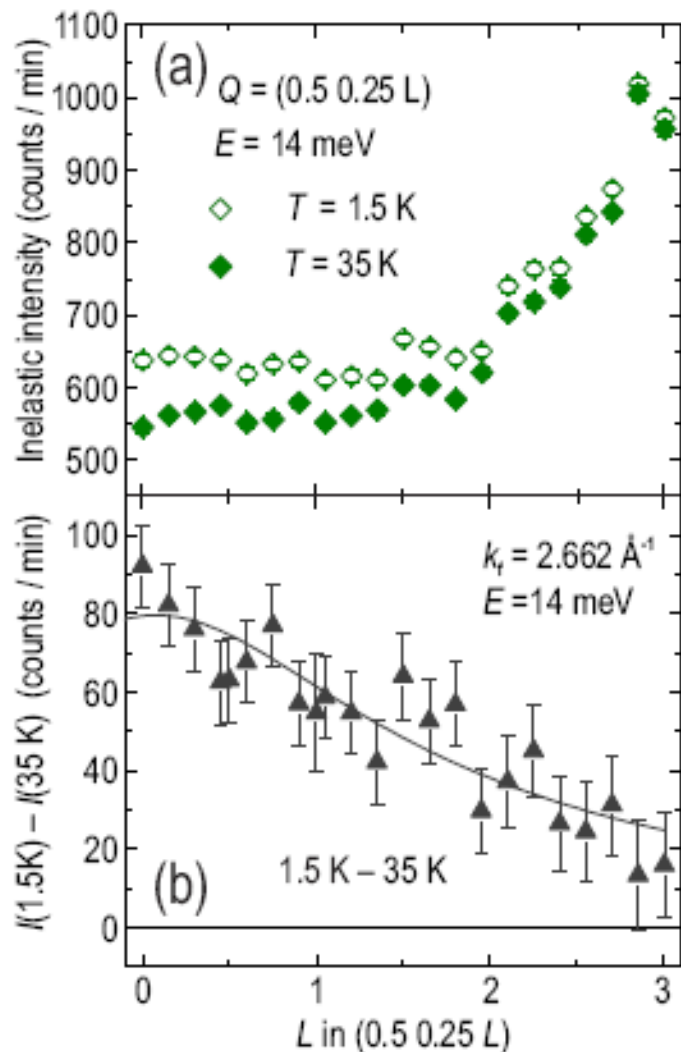
Linear relationship between E_{res} and T_c



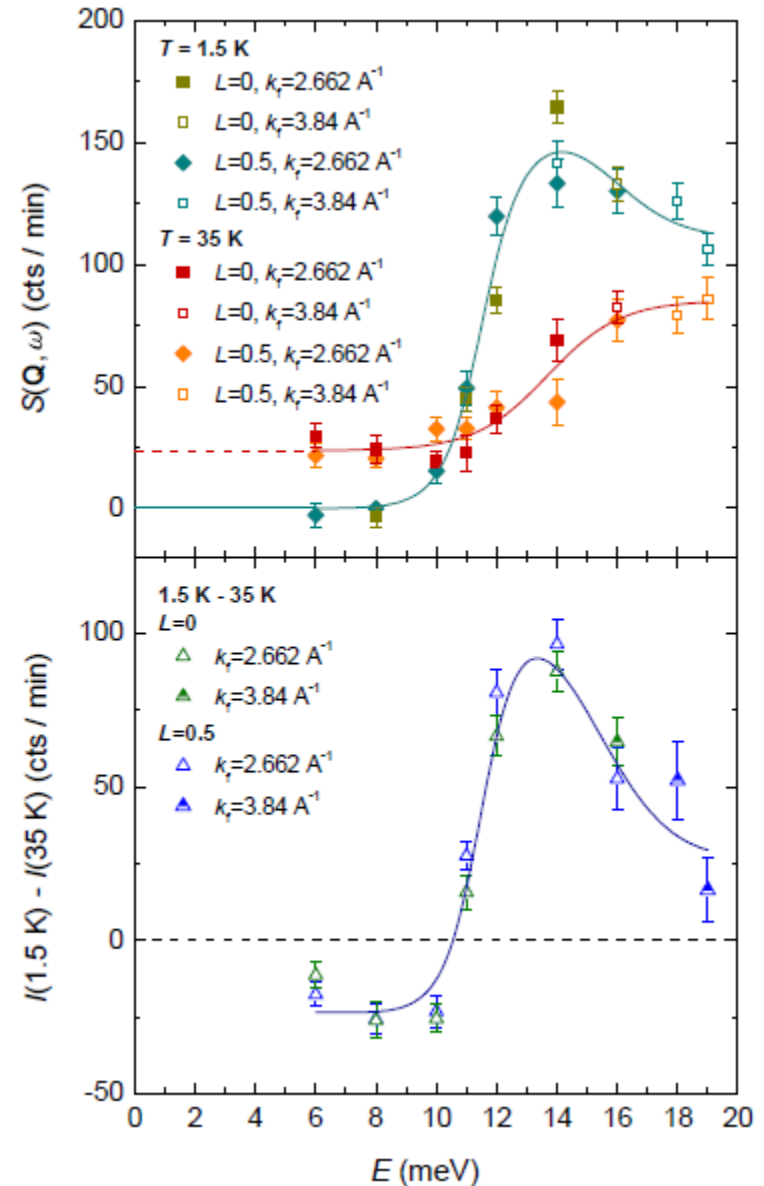
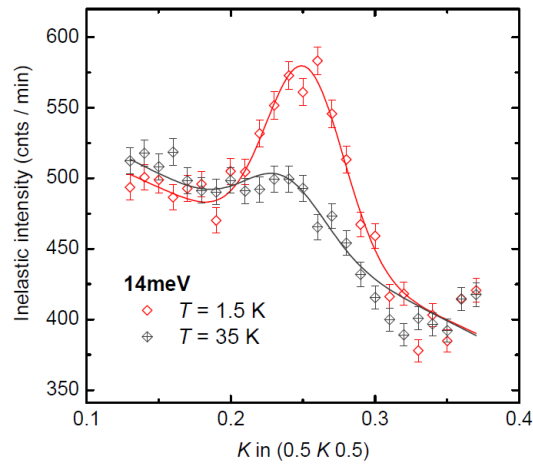
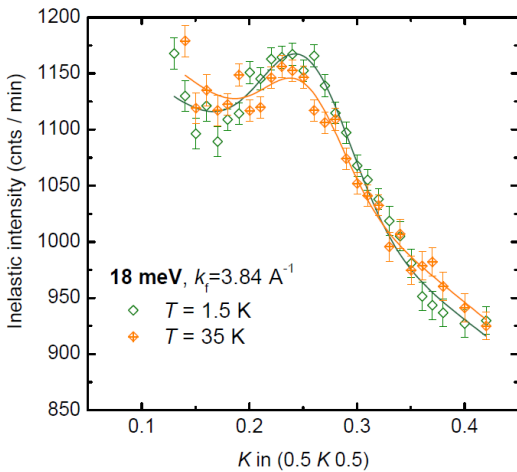
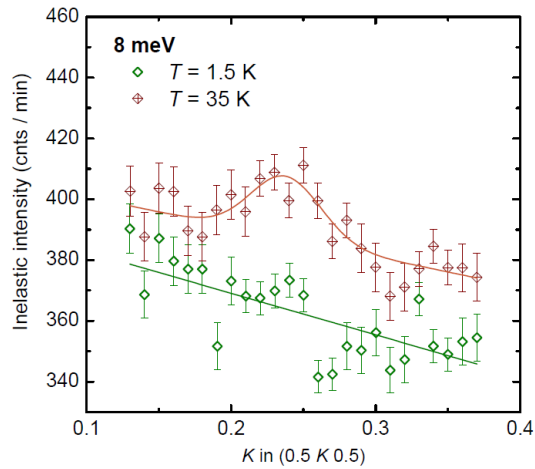
D. Inosov *et al.*, PRB **83**, 214520 (2011)

J. T. Park, D. S. Inosov *et al.*, PRB (2010);
 M. Wang *et al.*, PRB **81**, 174524 (2010);
 S. Shamoto *et al.*, PRB **82**, 172508 (2010).

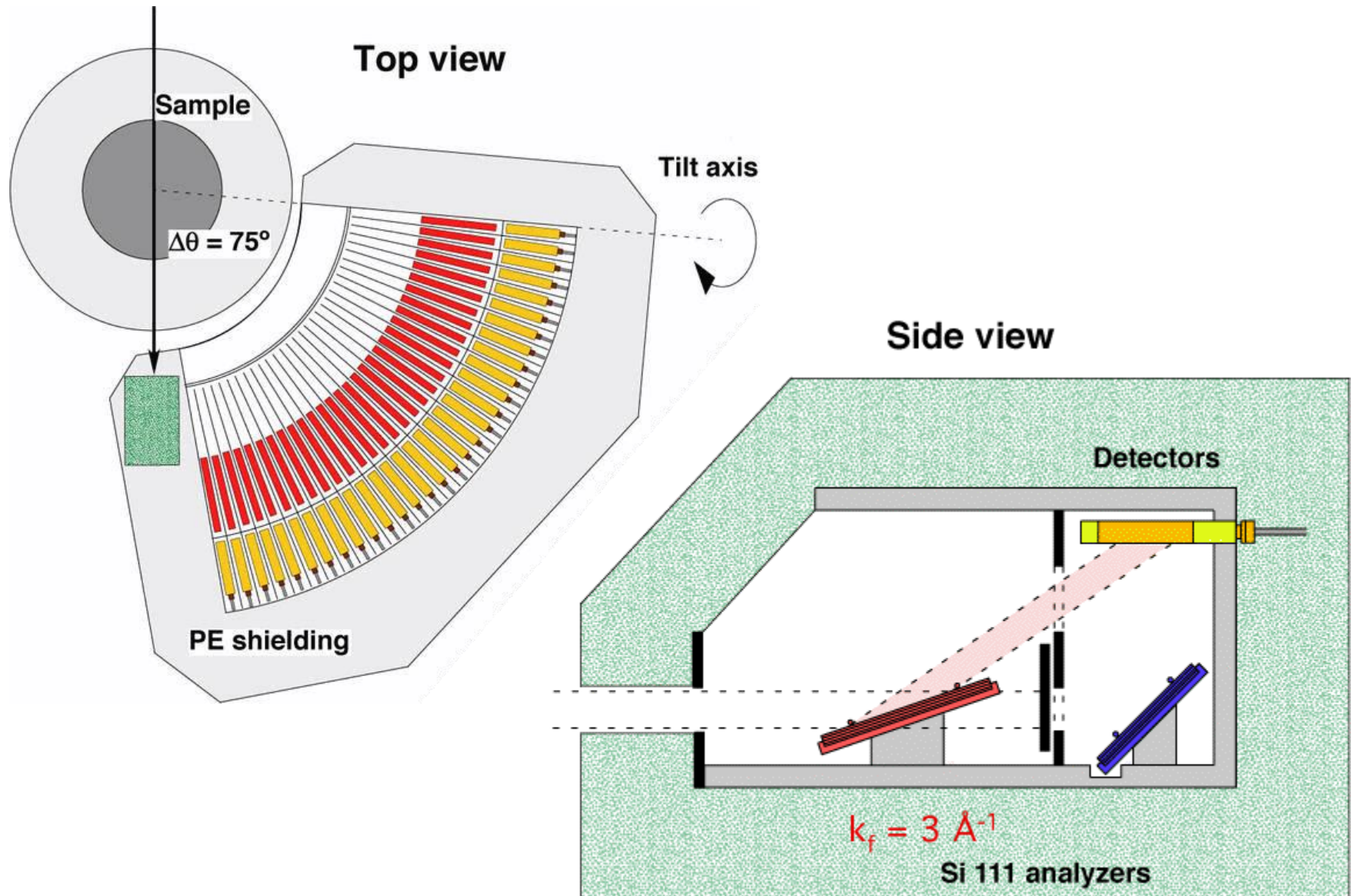
Quasi-two-dimensionality of the resonant mode



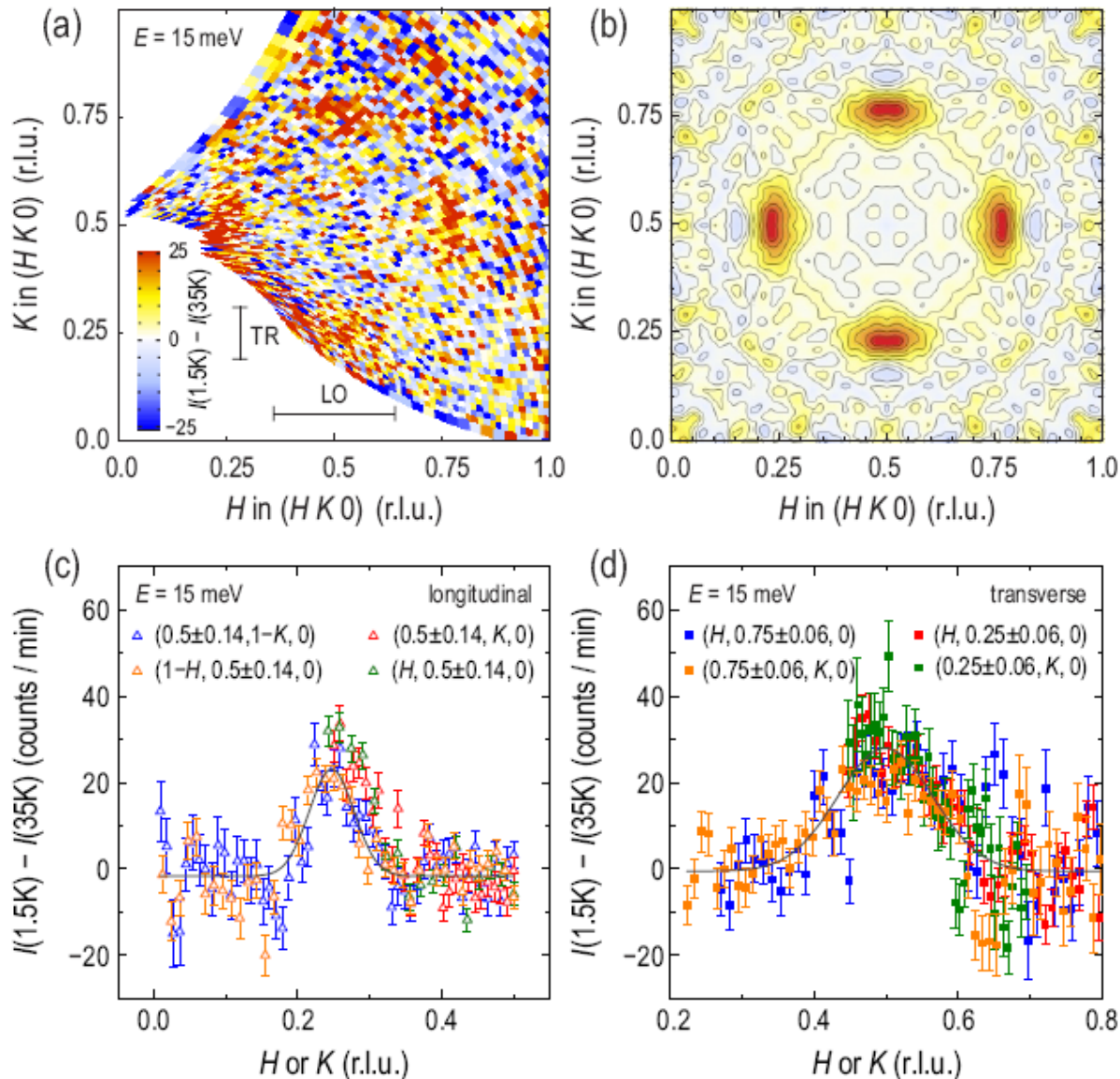
Normal-state response



FlatCone multi-analyzer at IN8

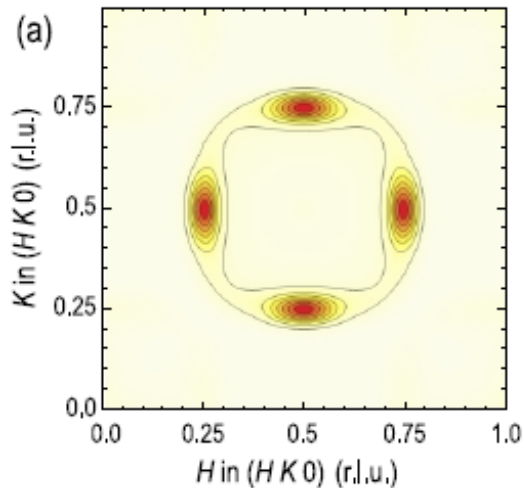


Reciprocal-space structure of the resonance



$(HK0)$ scattering plane

Bulk-sensitive estimates of the electron count



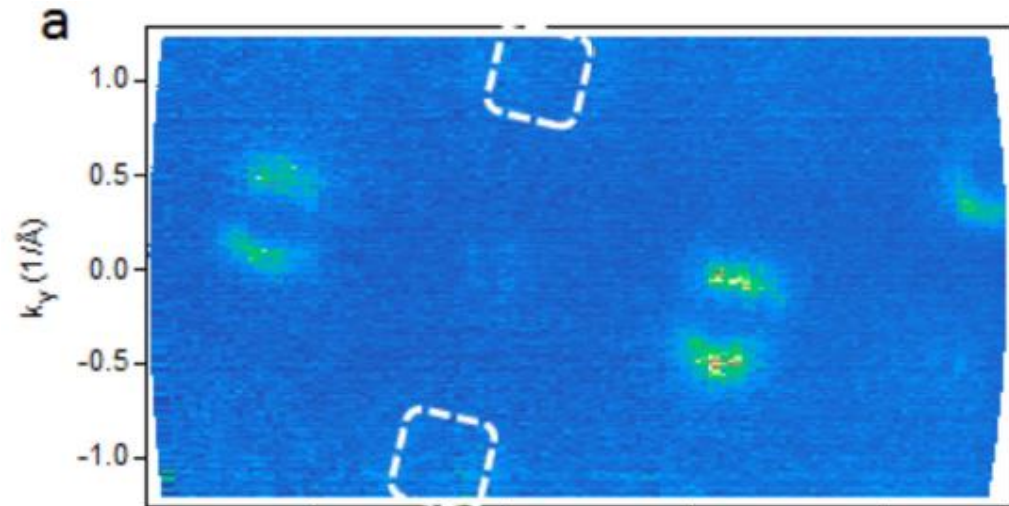
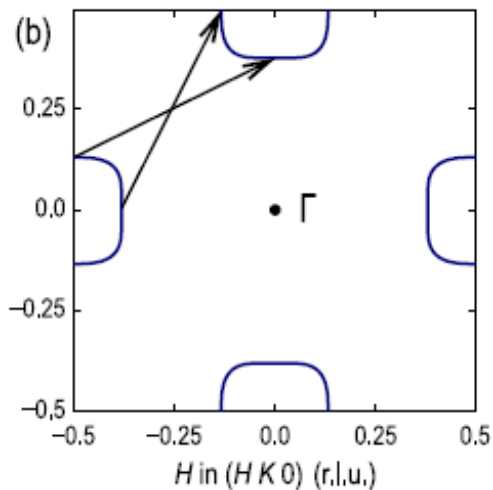
\Rightarrow **0.18 electrons/Fe (INS + theory)**

NMR: 0.15 electrons/Fe

Y. Texier *et al.*, PRL **108**, 237002 (2012)

ARPES: 0.15 electrons/Fe

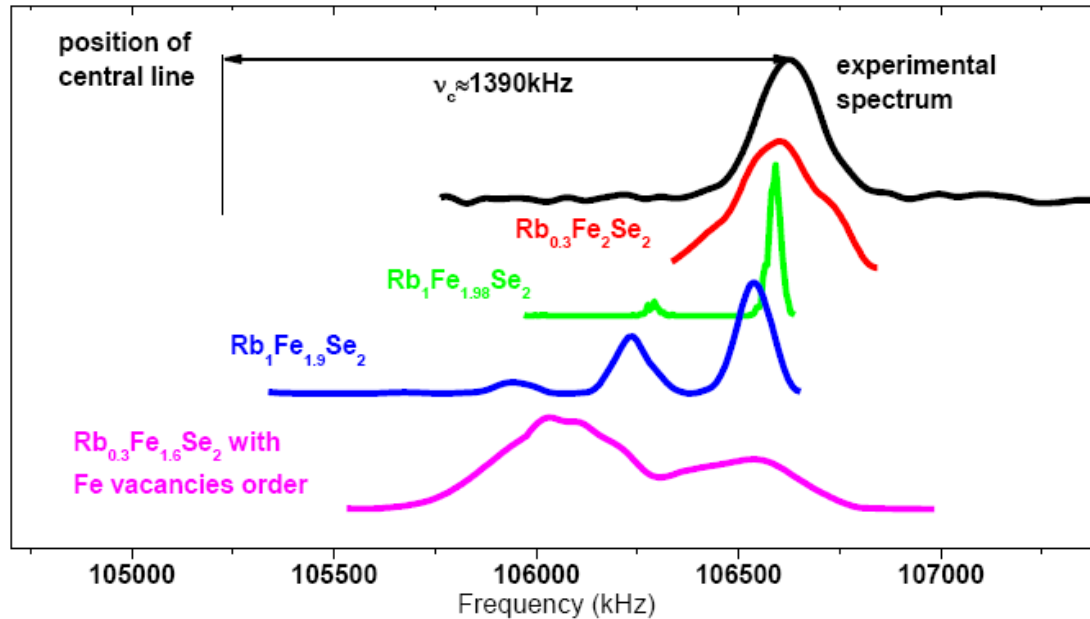
S. V. Borisenko *et al.*, arXiv:1204.1316



calculations by T. A. Maier
Phys. Rev. B **85** (2012), 140511(R)

No superstructure in the Fe layer!

NMR evidence for a vacancy-free SC phase

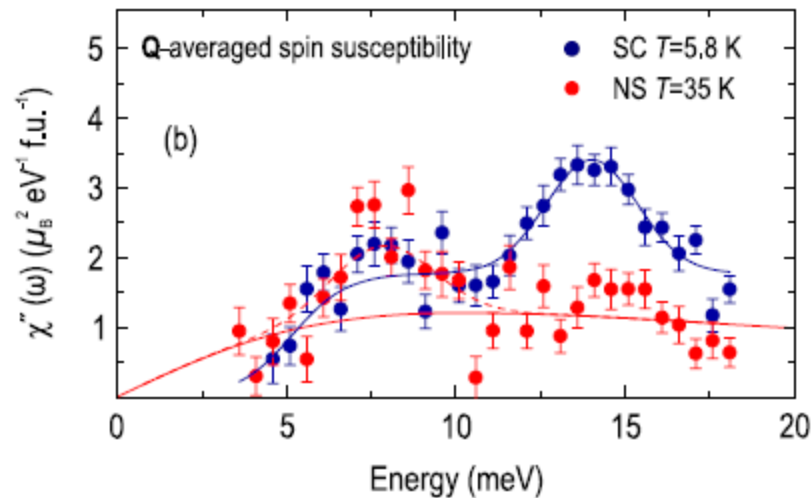
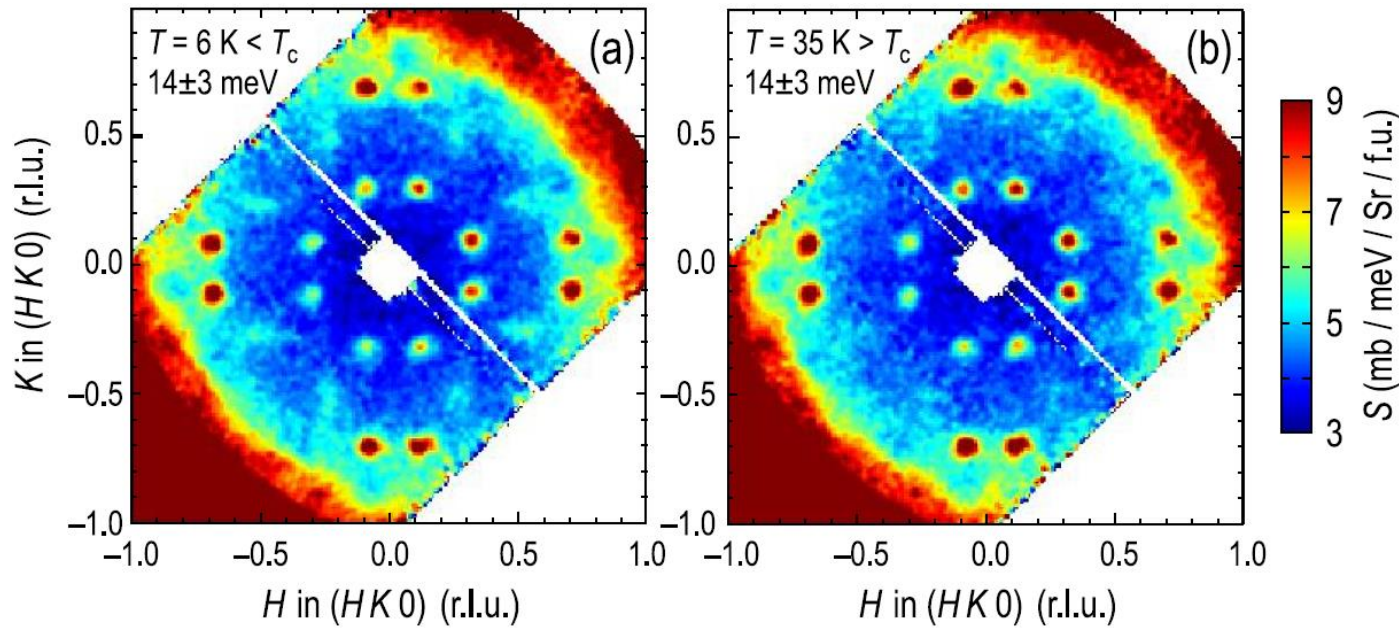


Y. Texier, J. Bobroff *et al.*, Phys. Rev. Lett. **108**, 237002 (2012)

Superconducting phase has no Fe vacancies!

It must be associated with the “compressed” minority phase with the $\text{A}_{0.3}\text{Fe}_2\text{Se}_2$ composition.

Spin excitations and resonant mode in $K_{1-x}Fe_{2-y}Se_2$



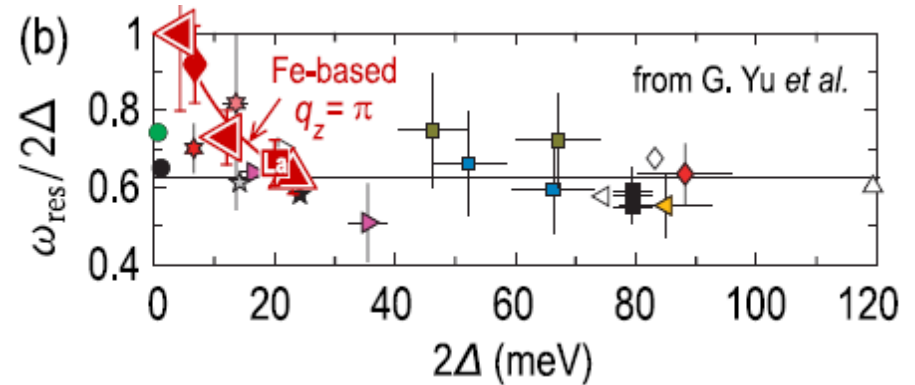
Total resonant spectral weight: $0.011 \pm 0.003 \mu_B^2/\text{f.u.}$

G. Friemel *et al.*, EPL **99**, 67004 (2012)

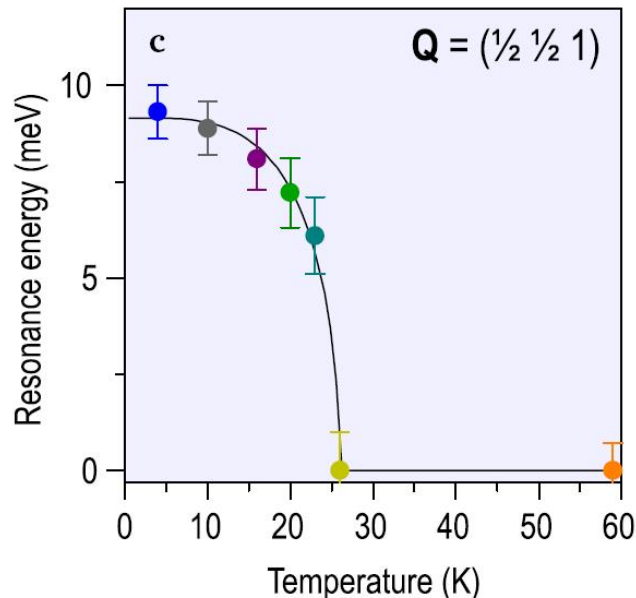
See also: A. Taylor *et al.*, PRB **86**, 094528

Summary, or what do we call a resonant mode?

1. Magnetic spectral weight.
2. Exciton of an "itinerant" character below the particle-hole continuum.
3. Temperature dependence, with an onset at T_c .



D. Inosov *et al.*, PRB **83**, 214520 (2011)



Thank you for your attention



PhD positions available in the neutron scattering group
at the Technical University of Dresden