Nematic fluctuations and lattice coupling in FeSe and $Ba(Fe_{0.97}Co_{0.03})_2As_2$

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Acknowledgements

- Collaborators
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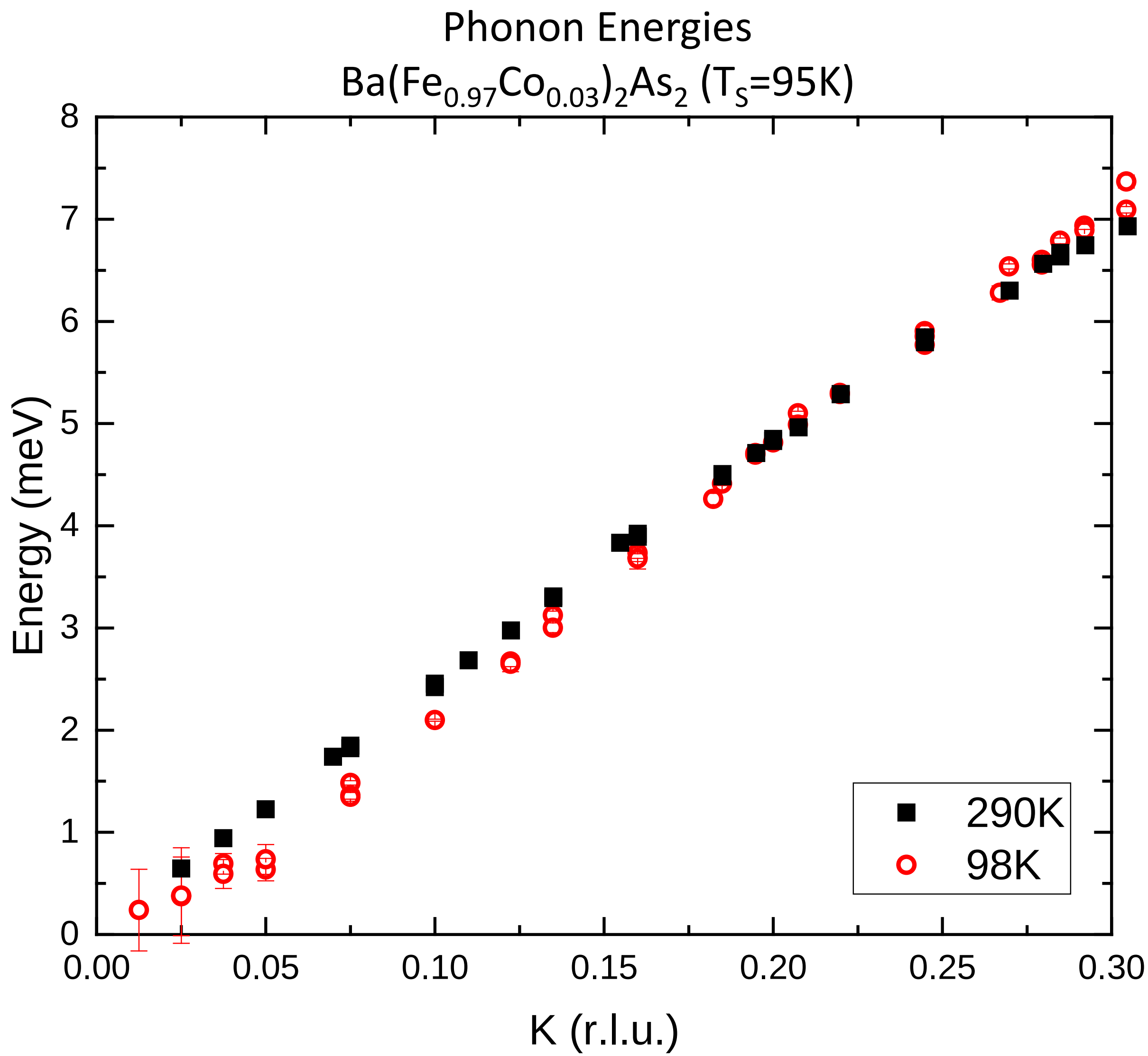
Overview

- Measure TA phonon energy near (2k0) for small k
- Observe k-dependent phonon softening
- This softening is due to nematic fluctuations



Previous Studies: 122 Pnictides & FeSe

- $SrFe_2As_2$, $BaFe_2As_2$
  - D. Parshall *et al*., Phys. Rev. B **91**, 13446 (2015)
- Co-doped Ba-122 (OP)
  - F. Weber *et al*., Phys. Rev. B **98**, 014516 (2018)
- FeSe
  - **Structural transition at 90K**
  - Superconducting below 9K (bulk crystal)
  - No antiferromagnetic ordered state
- $Ba(Fe_{1-x}Co_x)_2As_2$
  - **UD: x=0.03 → T_S=95K, no superconducting state**
  - OP: x=0.06 → T_c=25K, no structural transition

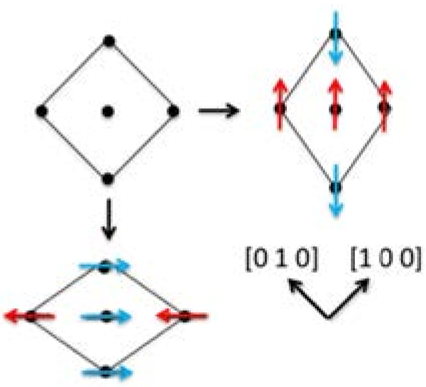
FeSe and $Ba(Fe_{0.97}Co_{0.03})_2As_2$

	FeSe	**$Ba(Fe_{0.97}Co_{0.03})_2As_2$**
Structure Above T_S	Tetragonal	Tetragonal
T_S	90K	95K
Structure Below T_S	Orthorhombic	Orthorhombic
Magnetic Order	NA	AFM
T_c	9K	NA

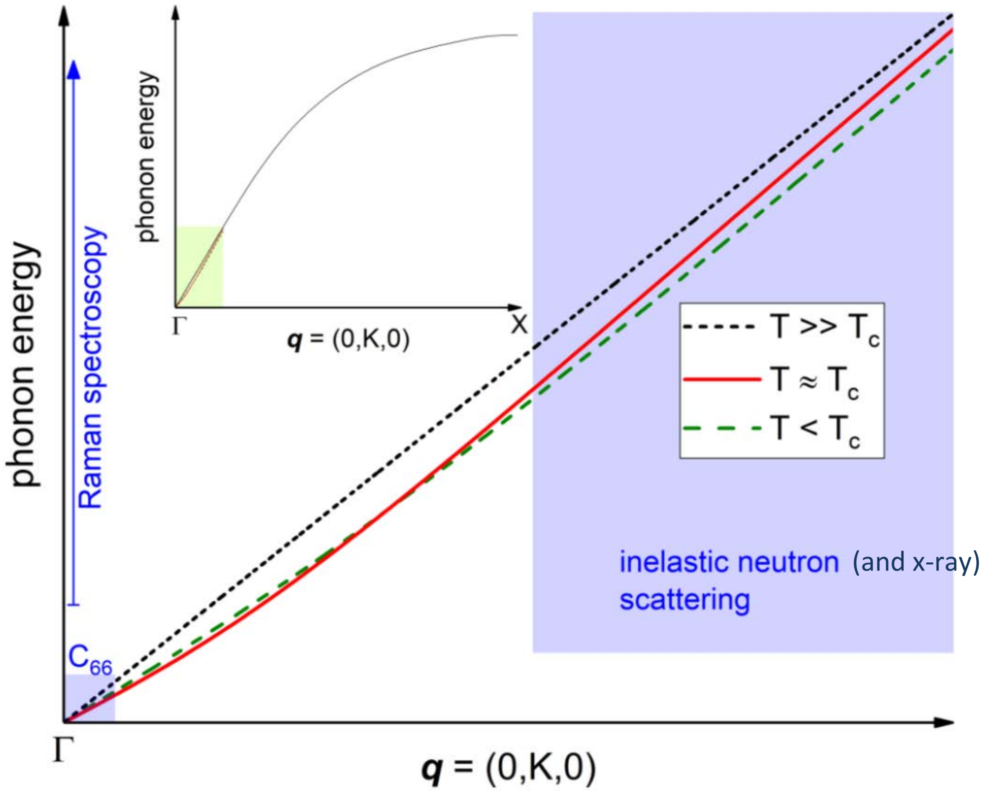
- Our goal is to compare the two materials near the structural transition
  - Different behavior between FeSe and Ba-122 of NMR spin-relaxation measurements at T_S
  - Similar shear modulus measurements between them
  - Different nematic susceptibility between OP and UD Ba-122

Inelastic Scattering Measurements: $E_{ph}(\mathbf{q})$

- Phonon softening is measureable at finite q with inelastic scattering measurements
- This TA phonon connects to the shear modulus near q=0



D. Parshall *et al*., Phys. Rev. B **91**, 13446 (2015)



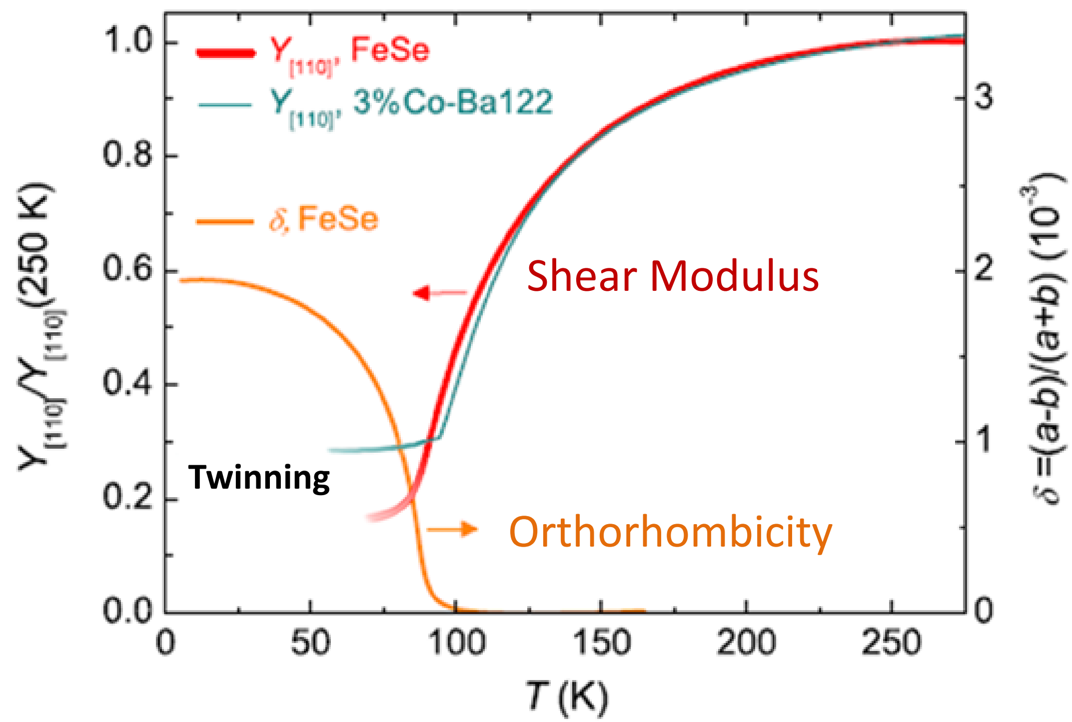
F. Weber *et al*., Phys. Rev. B **98**, 014516 (2018)

Shear Modulus Measurements: C_{66}

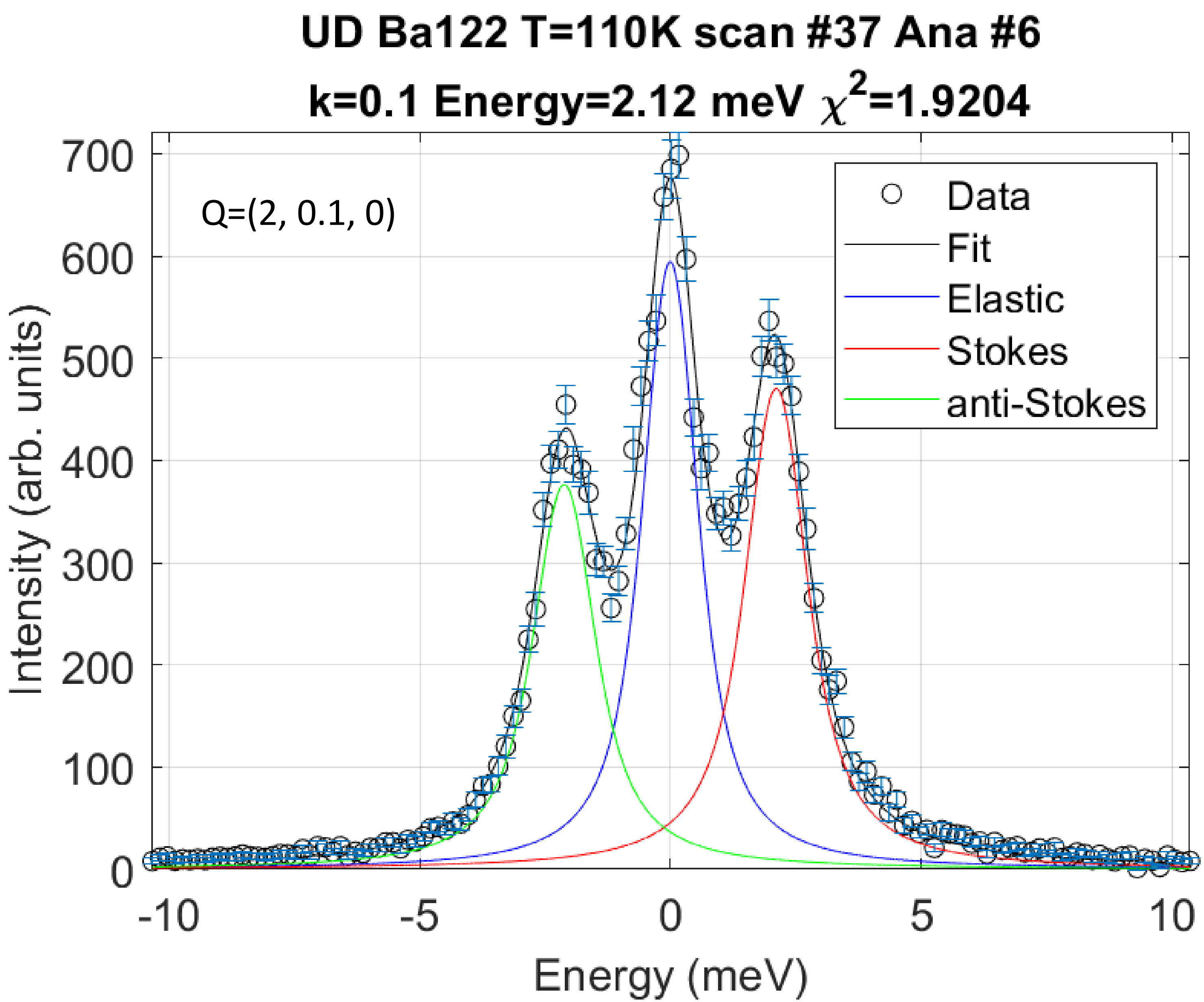
- C_{66} is measureable directly through resonant ultrasound or indirectly through 3-point bending
- Low-q phonon dispersion

$$\sqrt{C_{66}} \propto \frac{dE}{dq}(q \to 0)$$

- Contradicts finite-q measurements



A. E. Böhmer *et al.,* Phys Rev Lett **114,** 027001 (2015)

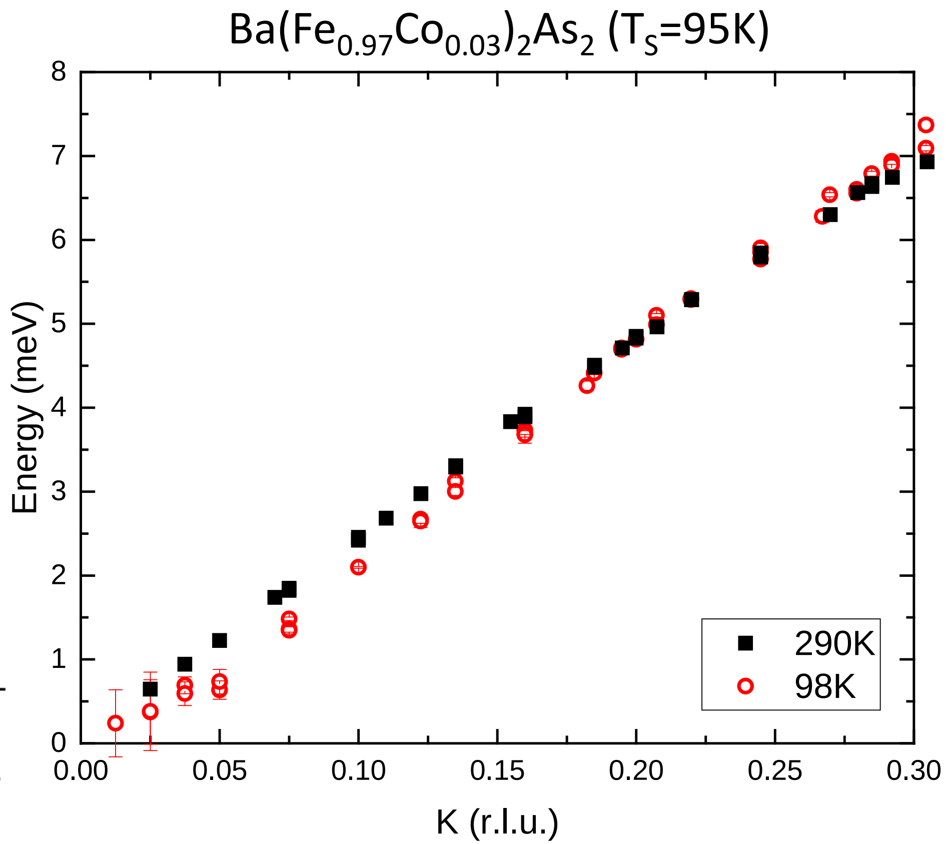


- Fit with resolution function, peaks are resolution limited

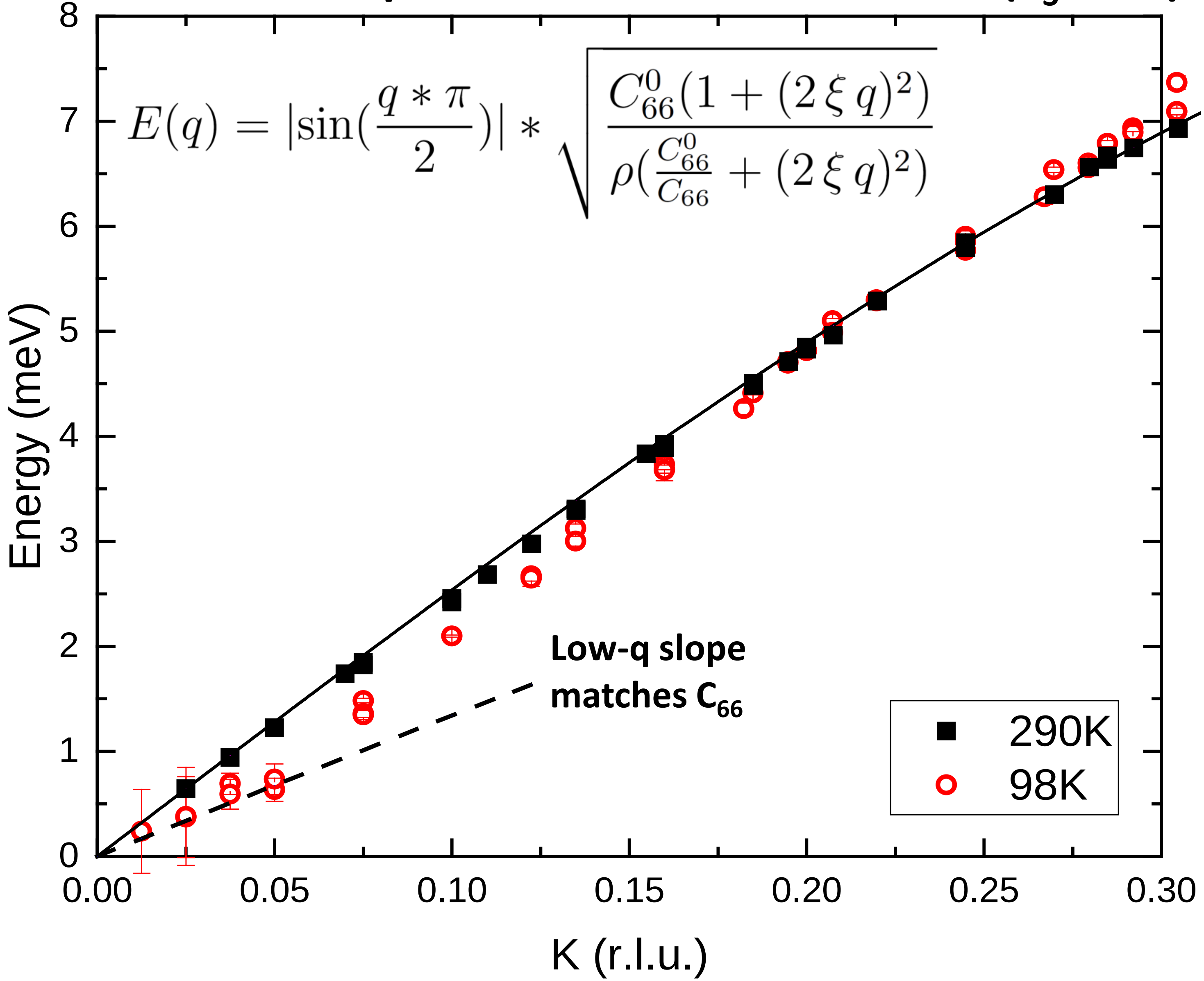
Phonon Dispersion Fitting

- Fit energy using measureable parameters C^0_{66} & C_{66}
- C^0_{66}: Unmodified shear modulus
- C_{66}: Modified shear modulus
- ξ: Nematic correlation length

$$E(q) = |\sin(\frac{q * \pi}{2})| * \sqrt{\frac{C^0_{66}(1 + (2\,\xi\,q)^2)}{\rho(\frac{C^0_{66}}{C_{66}} + (2\,\xi\,q)^2)}}$$



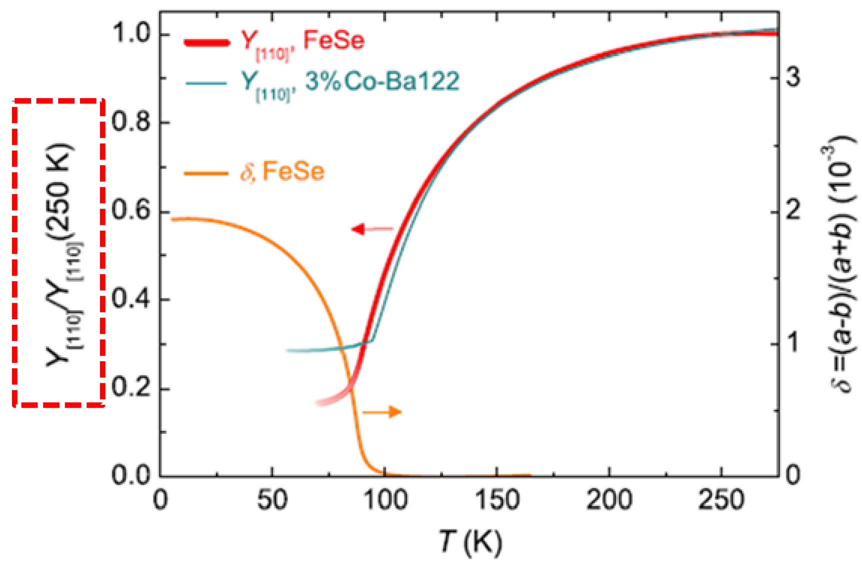
Phonon Dispersion at 98K in UD Ba-122 (T_S=95K)



- Nematic correlation length ξ fits the curve connecting high-q and low-q portions
- Need to find right values for C_{66}^0 & C_{66} at lower temperatures

3-Point Bending Measurements

- C_{66} data taken from $Y_{[110]}(T)/Y_{[110]}(T{=}250K)$, scaled to 1 at high temperature
- If $C^0_{66} / C_{66} = 1$, ξ-terms cancel: we can say nothing about the nematic correlation length

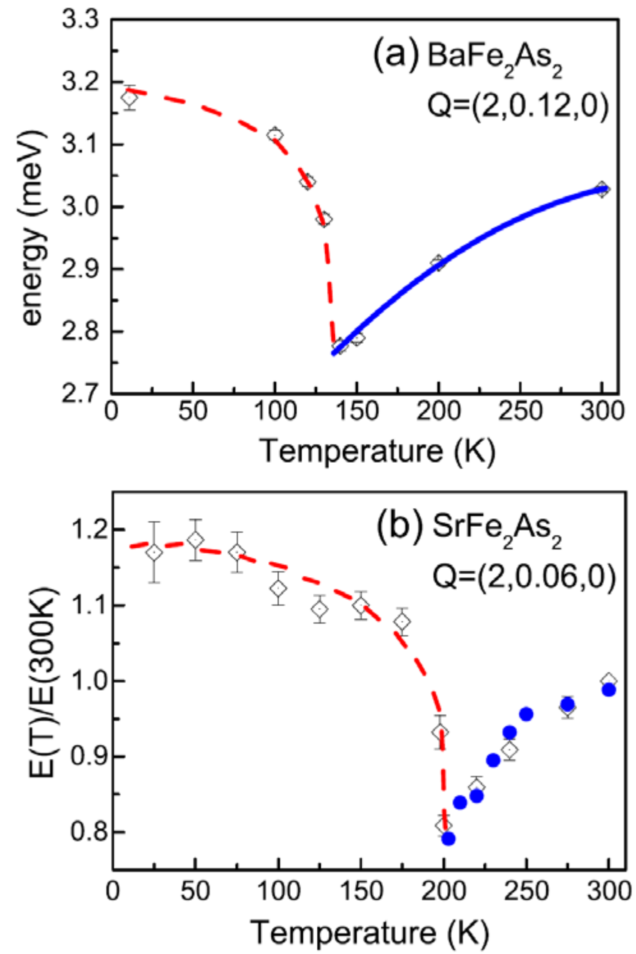


$$E(q) = |\sin(\frac{q * \pi}{2})| * \sqrt{\frac{C^0_{66}(1 + (2\,\xi\,q)^2)}{\rho(\frac{C^0_{66}}{C_{66}} + (2\,\xi\,q)^2)}}$$

We have to make assumptions about the shear modulus and the interaction with the nematic fluctuations to fit the data

$SrFe_2As_2$ & $BaFe_2As_2$

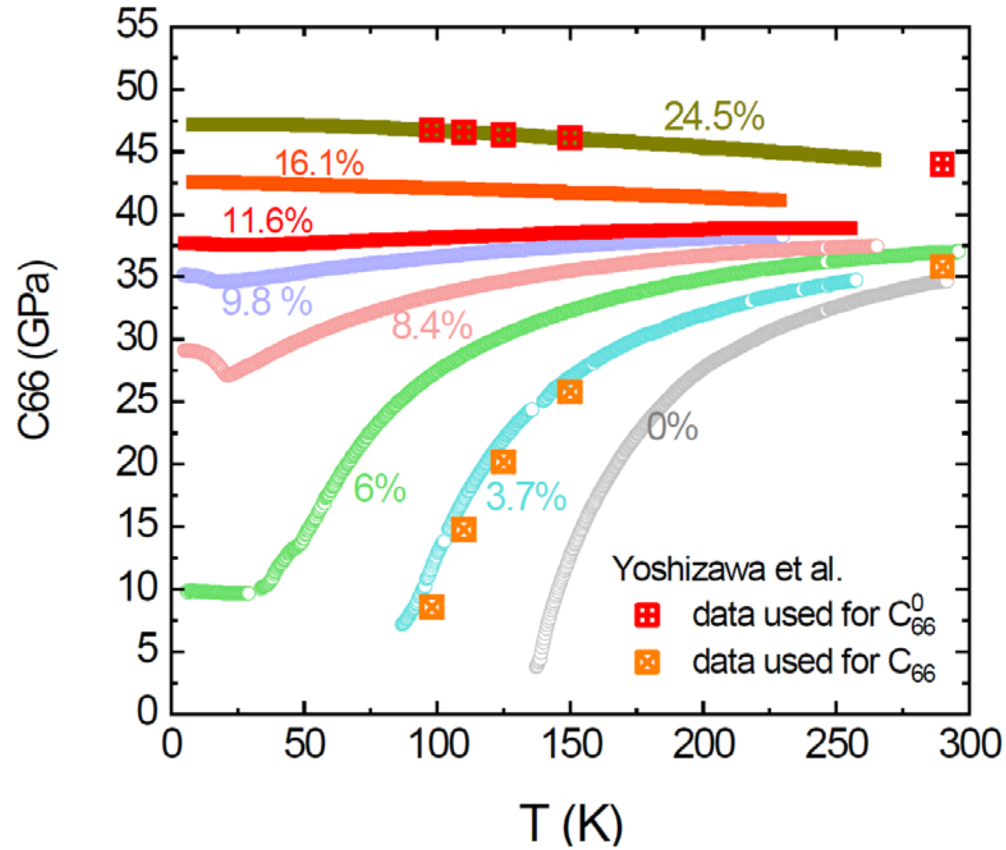
- $SrFe_2As_2$ and $BaFe_2As_2$ phonon softening tracks magnetic order
  - Magnetic fluctuations appear above T_S and persist at high temperature in $SrFe_2As_2$
- Implies nematic fluctuations contribute even at room temperature



D. Parshall *et al.*, Phys. Rev. B **91**, 13446 (2015)

Resonant Ultrasound Measurements

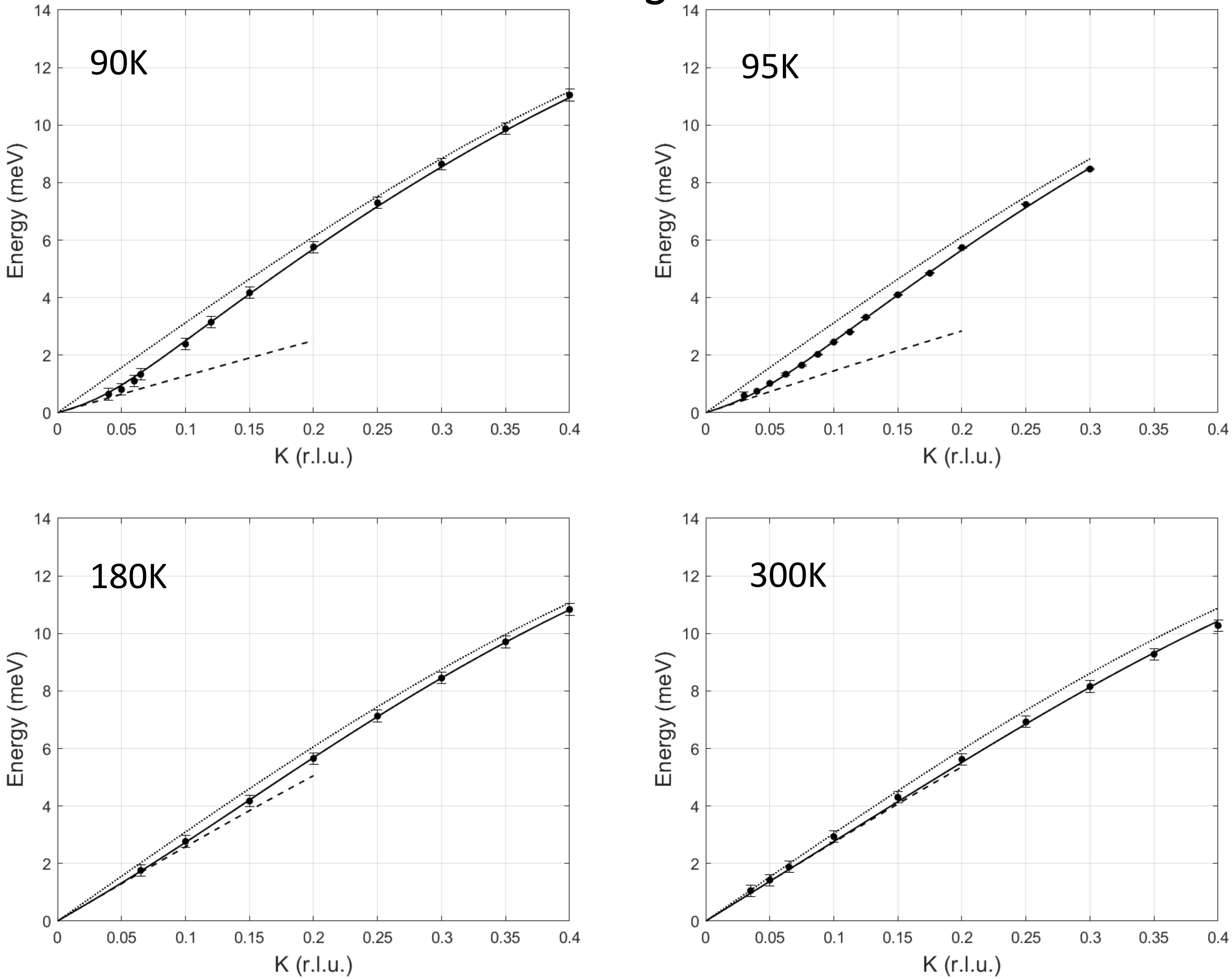
- Clear effect in C_{66} at high temperatures as doping changes in $Ba(Fe_{1-x}Co_x)_2As_2$
- Use C_{66} data for highly overdoped sample to C^0_{66} in the underdoped sample
  - We lack C_{66} data for "overdoped" FeSe! We will apply C_{66} data for OD Ba-122 to C^0_{66} in FeSe



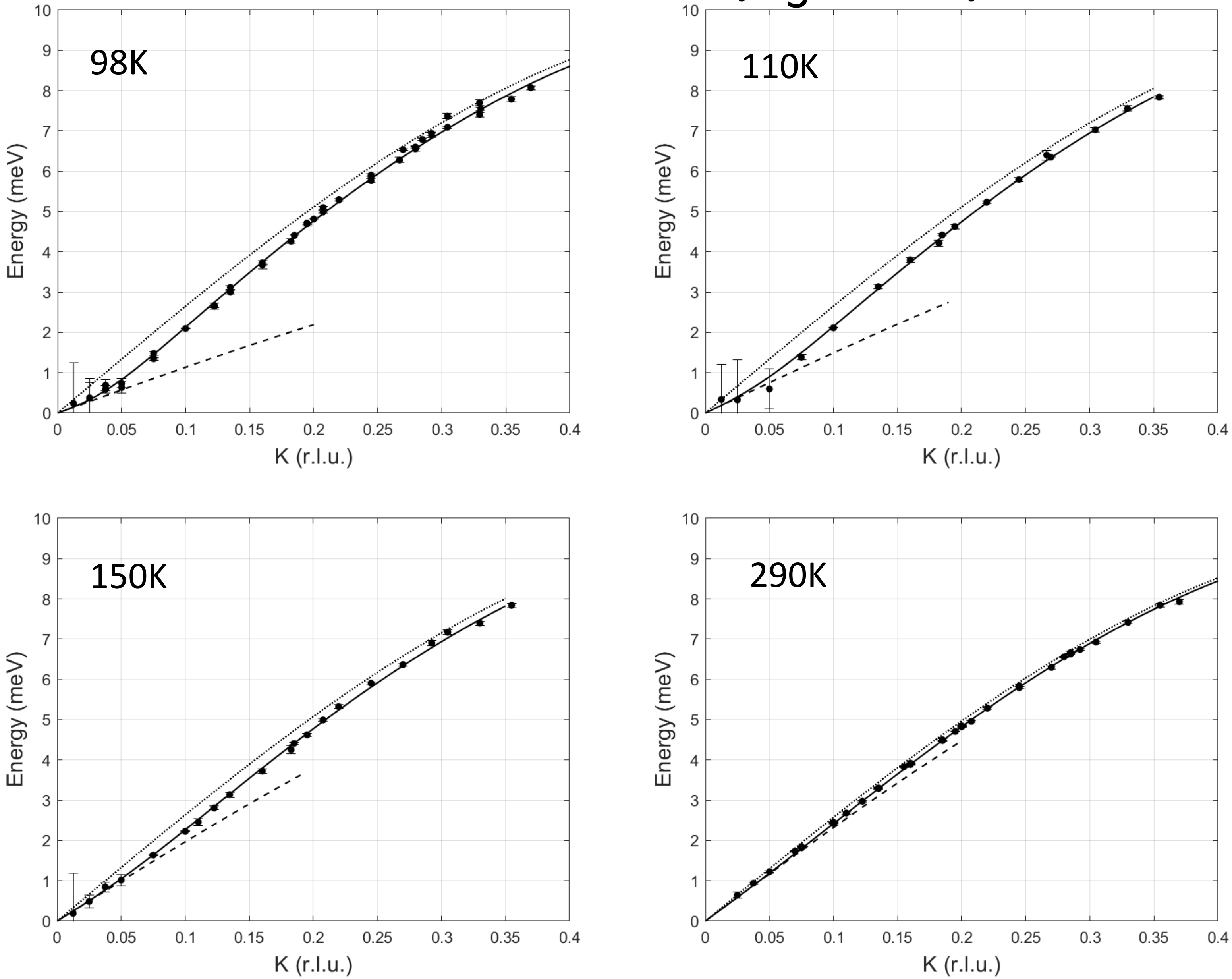
M. Yoshizawa and S. Simayi, Mod Phys Lett B **26,** 1230011 (2012)

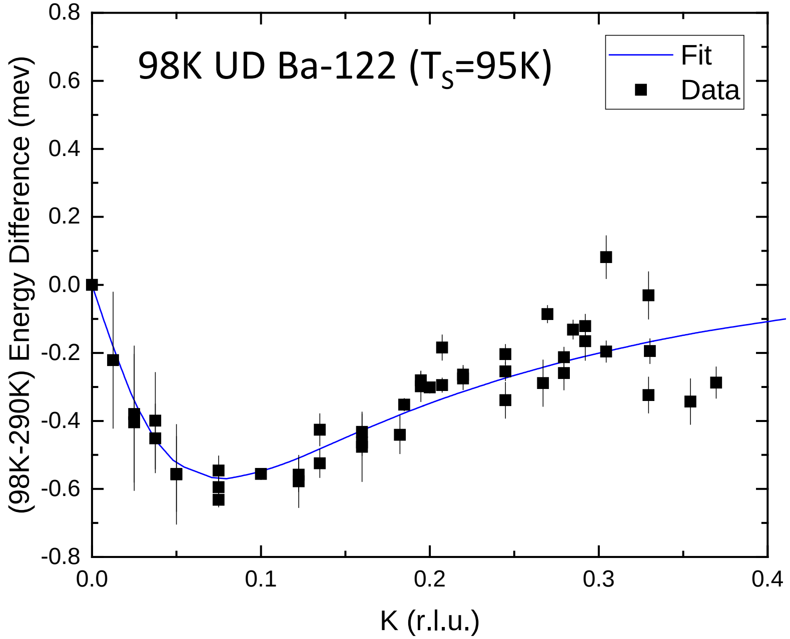
$$E(q) = |\sin(\frac{q*\pi}{2})| * \sqrt{\frac{C^0_{66}(1+(2\,\xi\,q)^2)}{\rho(\frac{C^0_{66}}{C_{66}}+(2\,\xi\,q)^2)}}$$

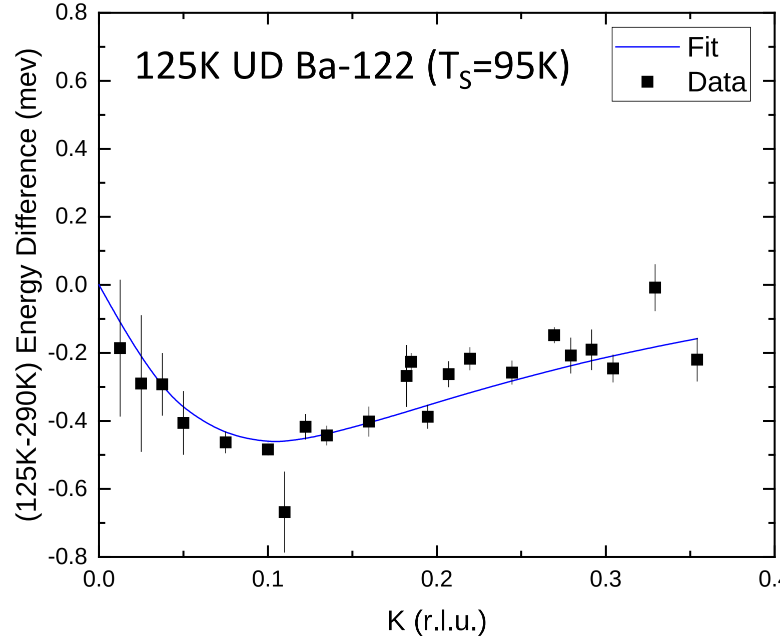
FeSe (T_S=90K)

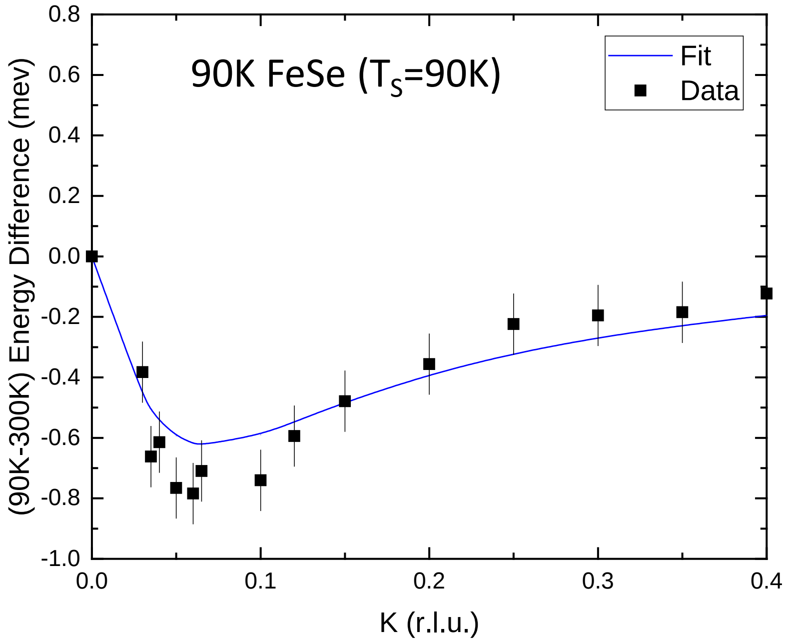

90K
95K
180K
300K
Energy (meV)
K (r.l.u.)
0
2
4
6
8
10
12
14
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4

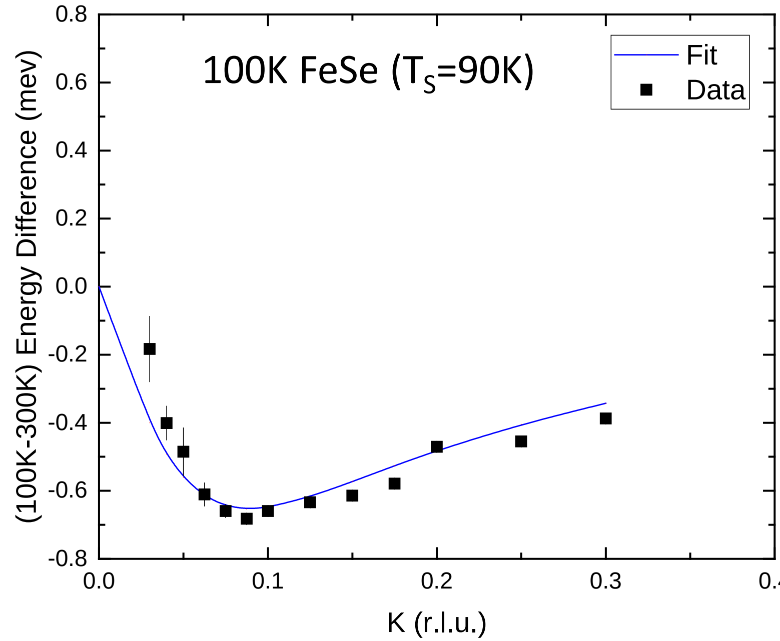
3%Co-Ba122 (T_S=95K)



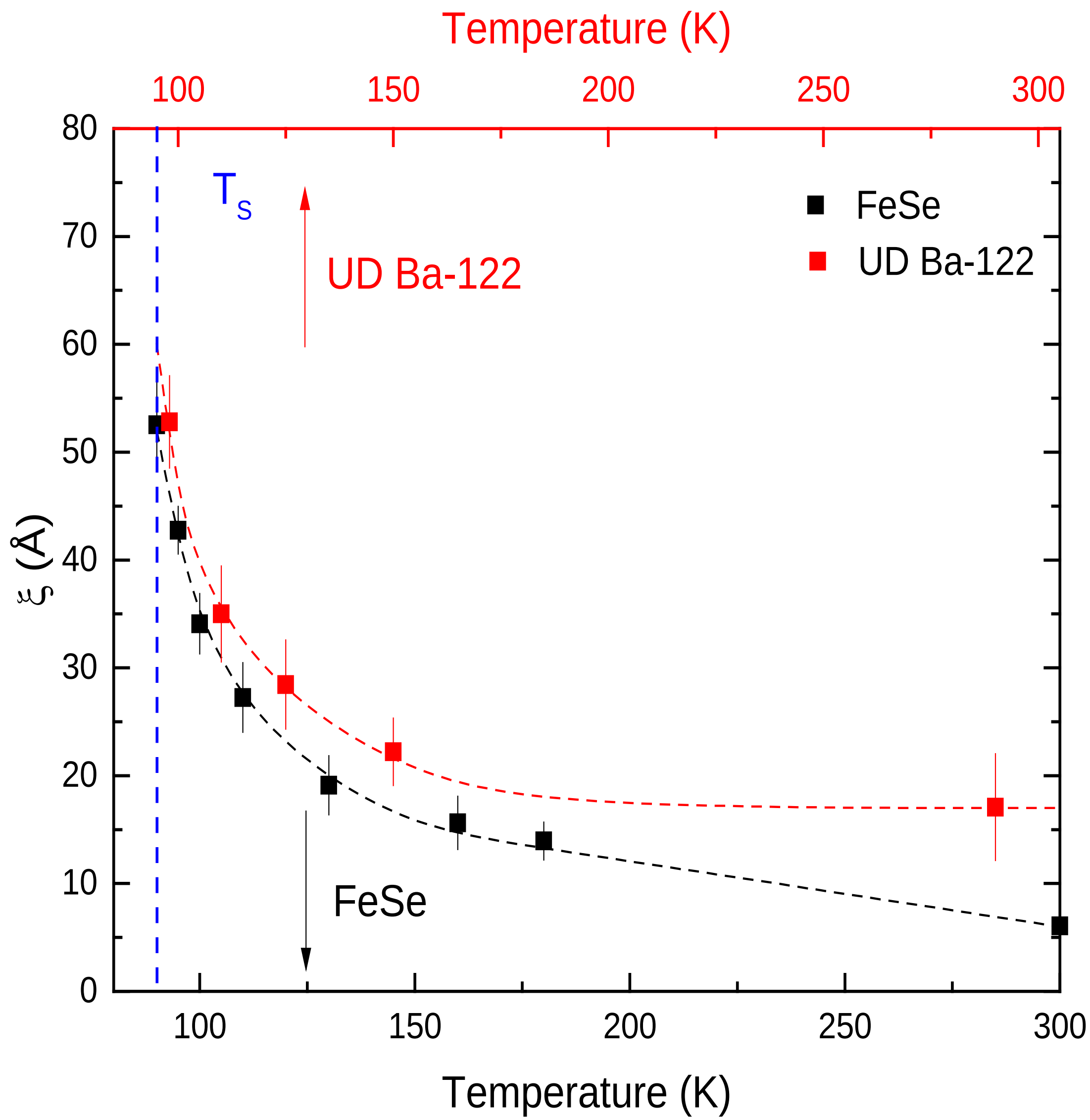

98K UD Ba-122 (T$_S$=95K)
Fit
Data
(98K-290K) Energy Difference (mev)
K (r.l.u.)
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
0.0
0.1
0.2
0.3
0.4


125K UD Ba-122 (T$_S$=95K)
Fit
Data
(125K-290K) Energy Difference (mev)
K (r.l.u.)
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
0.0
0.1
0.2
0.3
0.4

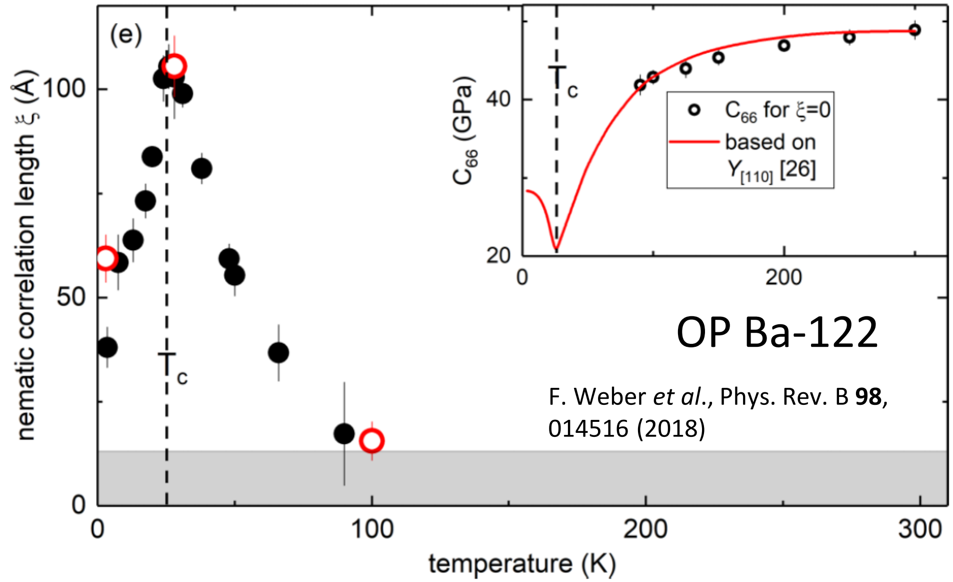

90K FeSe (T$_S$=90K)
Fit
Data
(90K-300K) Energy Difference (mev)
K (r.l.u.)
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
0.0
0.1
0.2
0.3
0.4

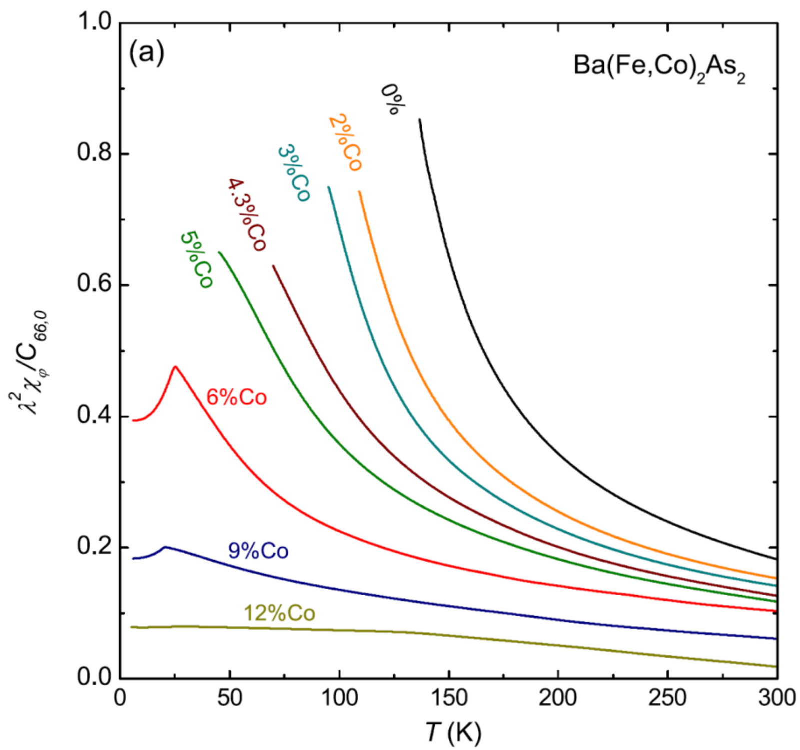

100K FeSe (T$_S$=90K)
Fit
Data
(100K-300K) Energy Difference (mev)
K (r.l.u.)
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
0.0
0.1
0.2
0.3
0.4

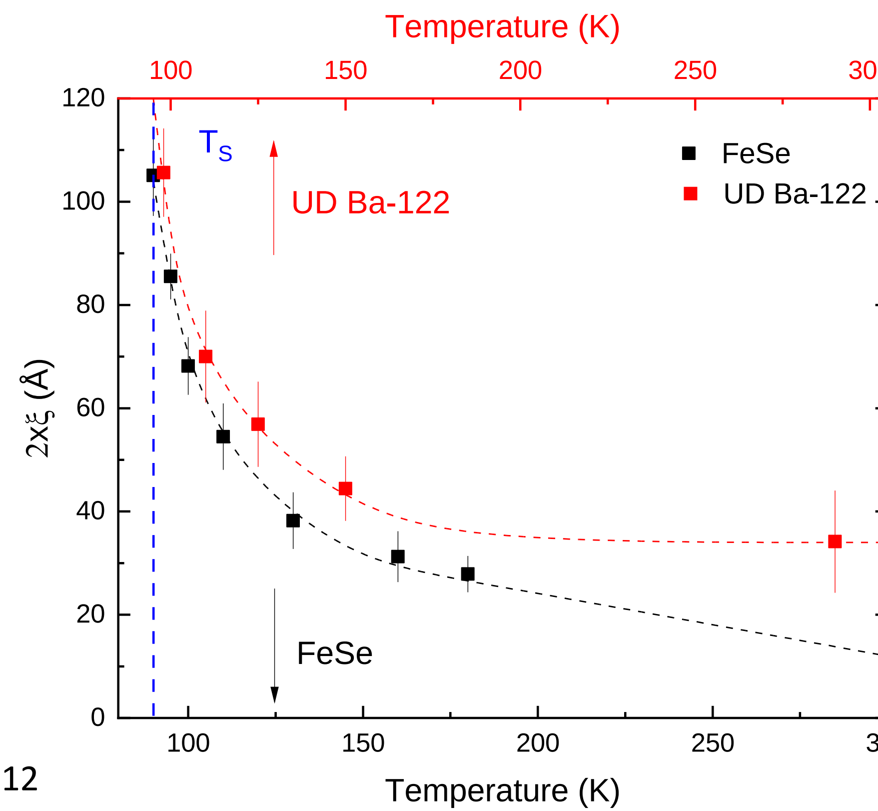
- Nematic correlation length ξ vs. T in FeSe and UD Ba-122
- ξ increases towards T_S but does not diverge
- ξ maximum is on the order of ~55 Å or 14-15 unit cells



- Similar behavior for ξ upon approaching T_S in non-superconducting samples vs. T_c in OP Ba-122
- Contrast with nematic susceptibility below



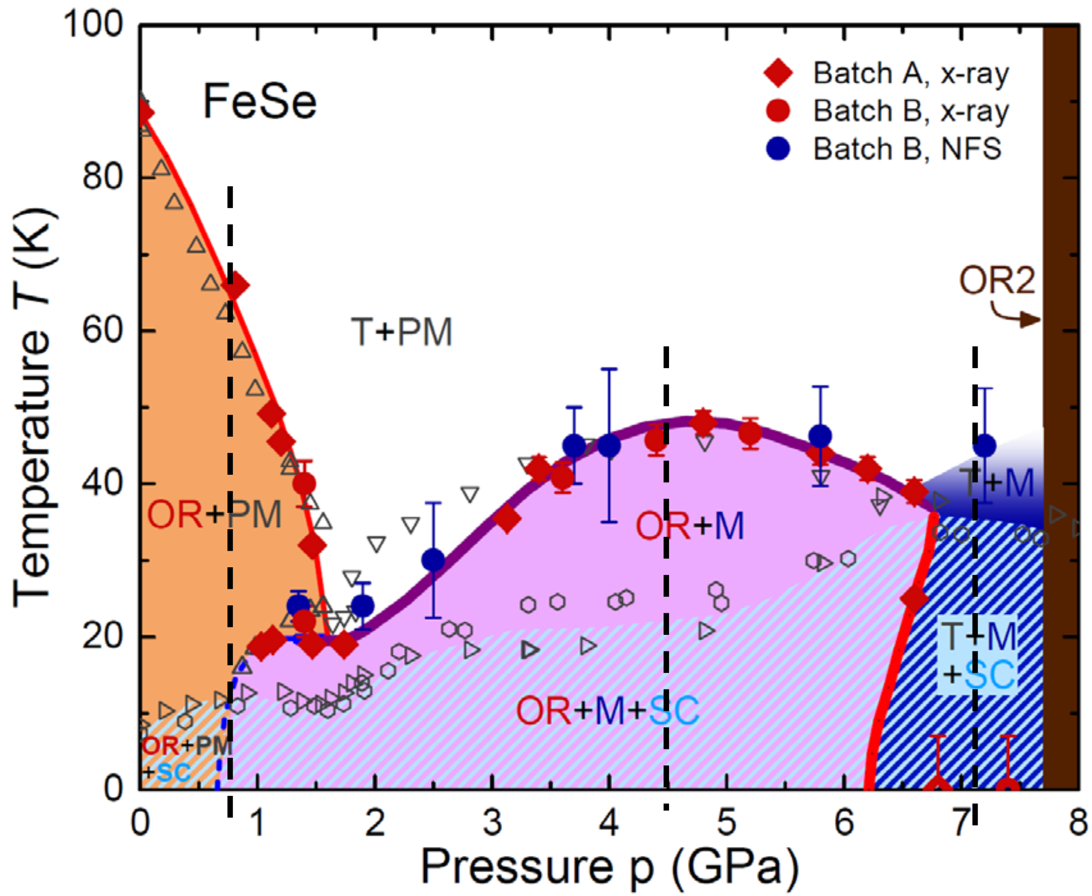




A. E. Böhmer and C. Meingast, C. R. Physique, 17 (2016), 90-112

Ongoing Work: High-Pressure Experiments in FeSe

- Hydrostatic pressure allows access to different phases in FeSe
- Of primary interest are the magnetic phases (~4.5 GPa) and tetragonal superconducting (~7.5 GPa)



A. E. Böhmer *et al.*, arXiv:1803.09449 [cond-mat.supr-con] (2018)

Summary

- Published Young's modulus data explains low-q dispersion for both FeSe and 3% Co-doped Ba-122, but nematic susceptiblity differs
- Nematic correlation length ξ does not diverge when approaching the structural phase transition
- Similarities between OP/UD Ba-122 and FeSe of ξ in contrast with shear modulus and NMR studies
- Ongoing Work: OP Ba-122, FeSe under pressure