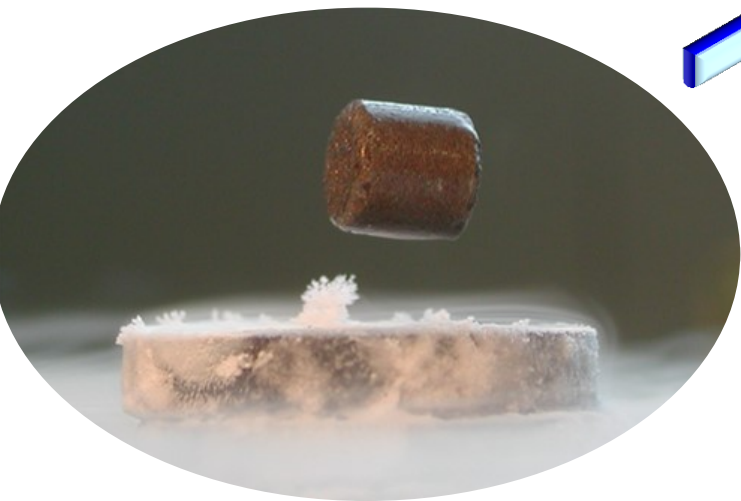


Effect of the electron-phonon coupling on phonons in iron based superconductors

Ilya Sergeev, PETRA III, Hamburg, Germany



- Fe superconductors: overview
- Study of lattice dynamics in $LnFeAsO$
- Study of lattice dynamics in $EuFe_2As_2$

Fe-superconductors. Overview

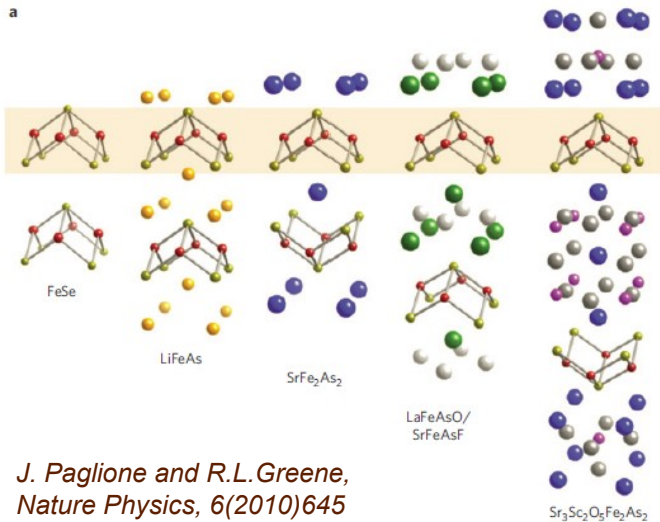
J|A|C|S
COMMUNICATIONS

Published on Web 02/23/2008

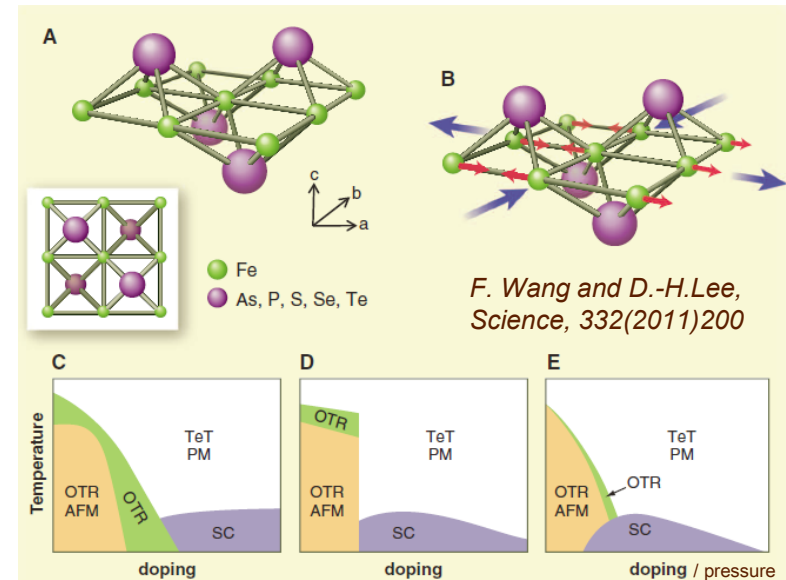
Iron-Based Layered Superconductor $\text{La}[\text{O}_{1-x}\text{F}_x]\text{FeAs}$ ($x = 0.05-0.12$)
with $T_c = 26$ K

Yoichi Kamihara,^{*,†} Takumi Watanabe,[‡] Masahiro Hirano,^{†,§} and Hideo Hosono^{†,§}

Crystallographic structures of Fe-superconductors



Phase diagrams of Fe-superconductors

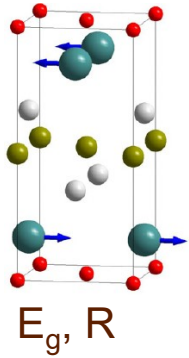
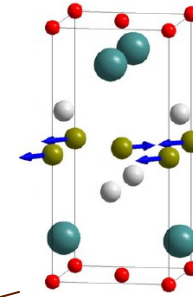
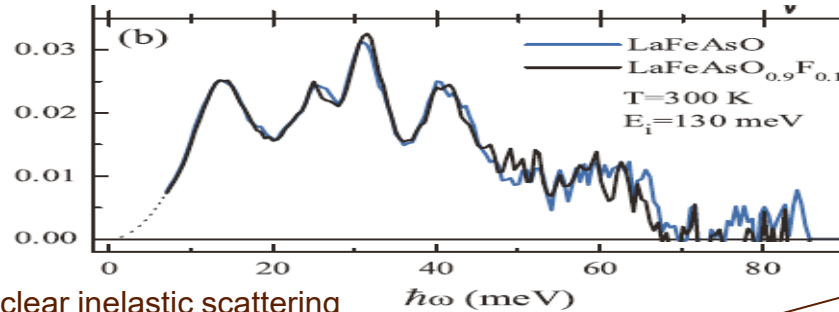


- superconductivity originates within Fe layer
- suppression of magnetism by doping or by pressure leads to SC
- unconventional superconductors: magnetic(?) excitations are the “glue” of the Cooper pair

Measurements of phonons in FeSCs

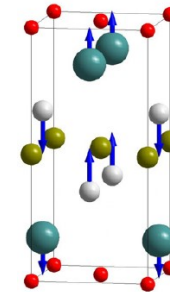
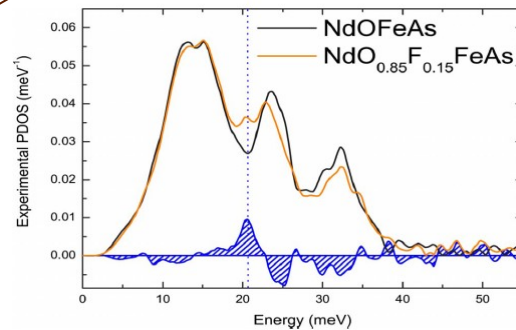
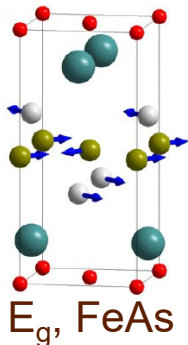
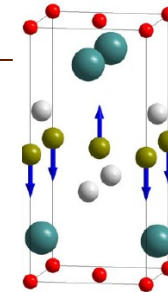
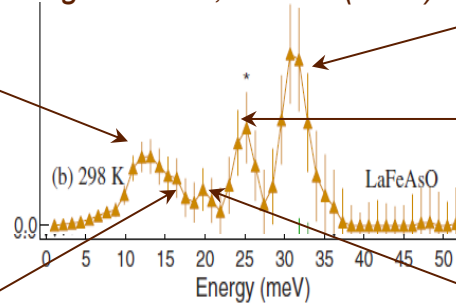
inelastic neutron scattering

Christianson et al., PRL 101 (2008) 157004



nuclear inelastic scattering

Higashitaniguchi et al., PRB 78(2008)174507



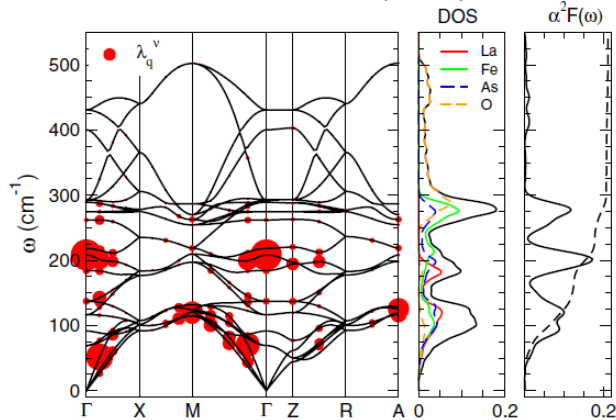
inelastic X-ray scattering

Le Tacon et al., PRB 78 (2008) 140505(R)

Theoretical phonon calculations

Electron-phonon properties of LaFeAsO

Boeri et al., PRL, 101(2008)026403

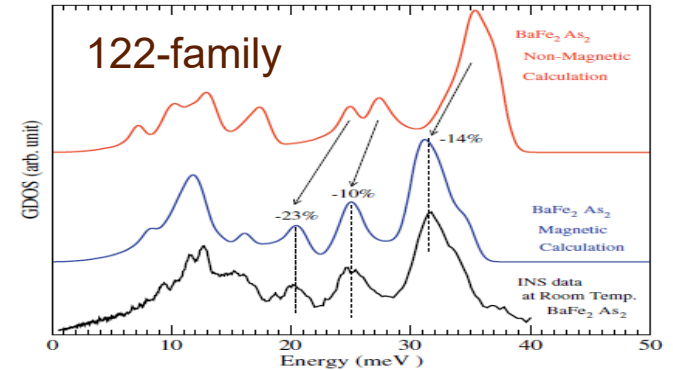


The theory predicts $T_c=0.8\text{K}$ due to the phonon mediated Cooper pairing. Much smaller than exp. $T_c = 25\text{K}$

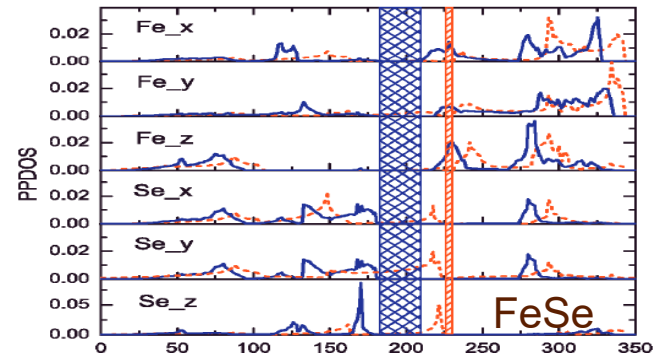
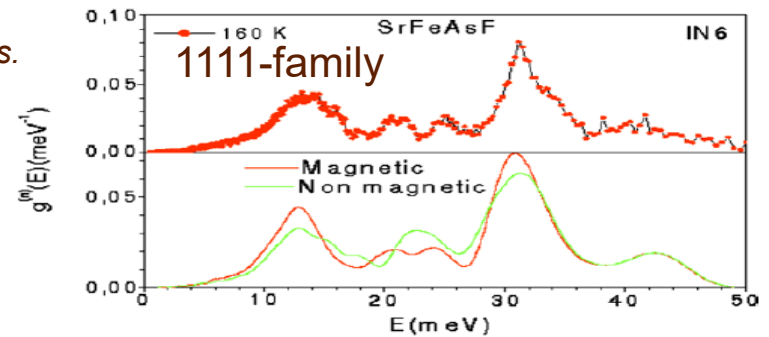
Theory predicts significant effect of the local magnetic moment on the phonon structure. It suggest to use phonons to reveal presence of the Fe magnetic moment.

Dependence of phonons on magnetism

T. Yildirim, Physica C 469(2009) 425



Zbiri et al., J.Phys. Cond.Matt 22(2010)315701



11-family

Wang et al., Physica C 472(2012)29

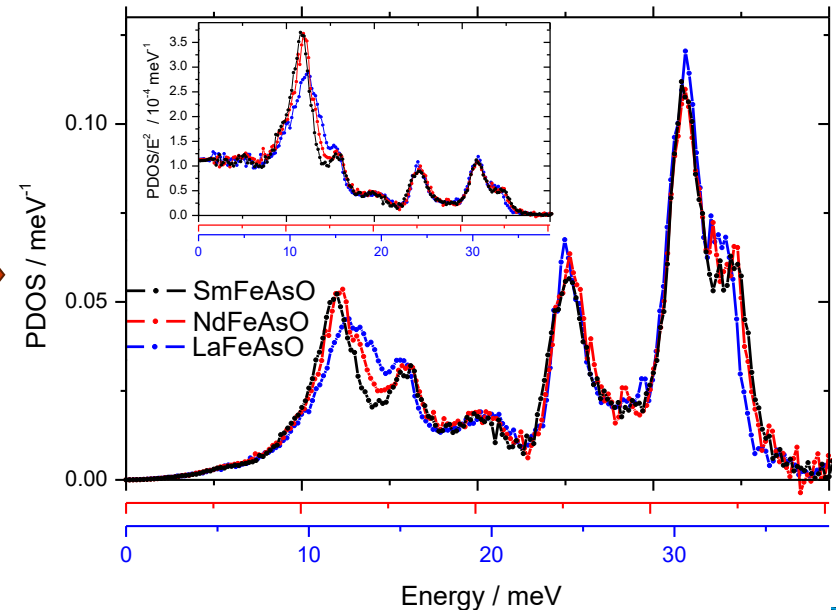
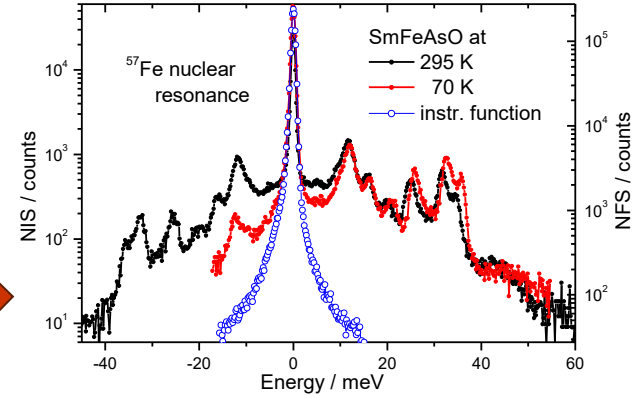
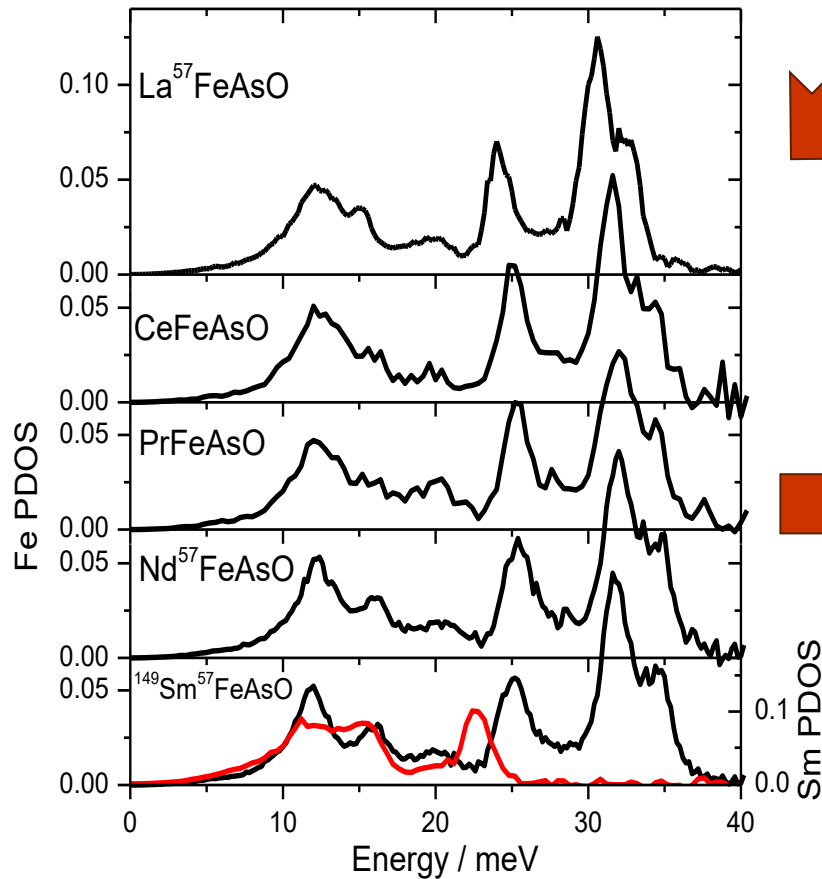


Fe PDOS for parent 1111 compounds

Sergueev et al., PRB 87 (2013) 064302

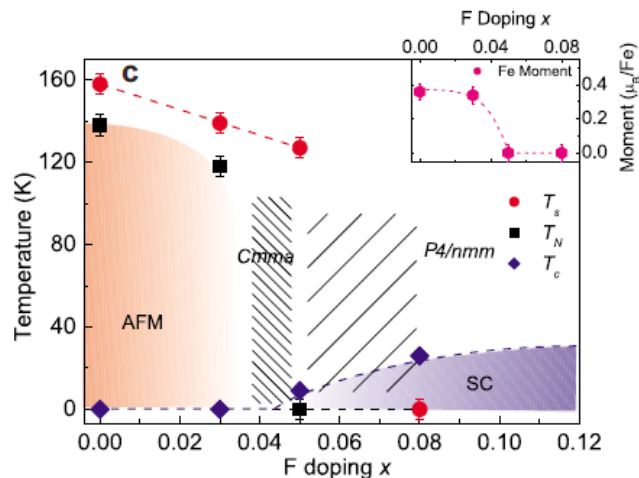
Measurements at ID18. $\Delta E = 0.7$ meV

Fe PDOS for different compounds at room temperature



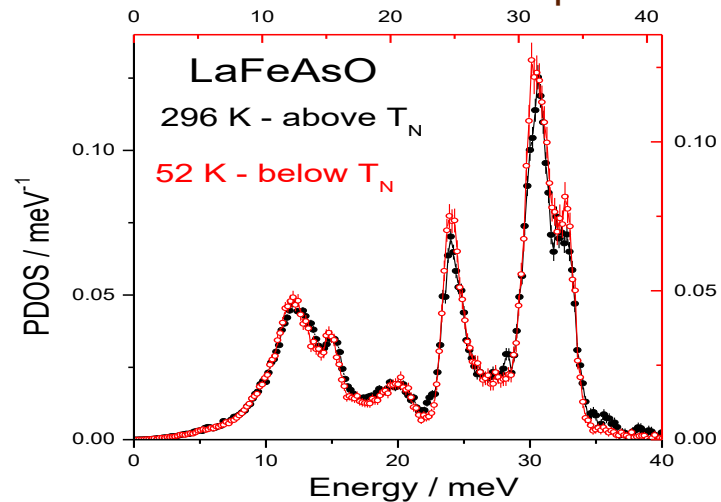
Fe PDOS for $\text{LaFeAsO}_{1-x}\text{F}_x$ at 0 and 296 K

Phase-diagram for $\text{LaFeAsO}_{1-x}\text{F}_x$

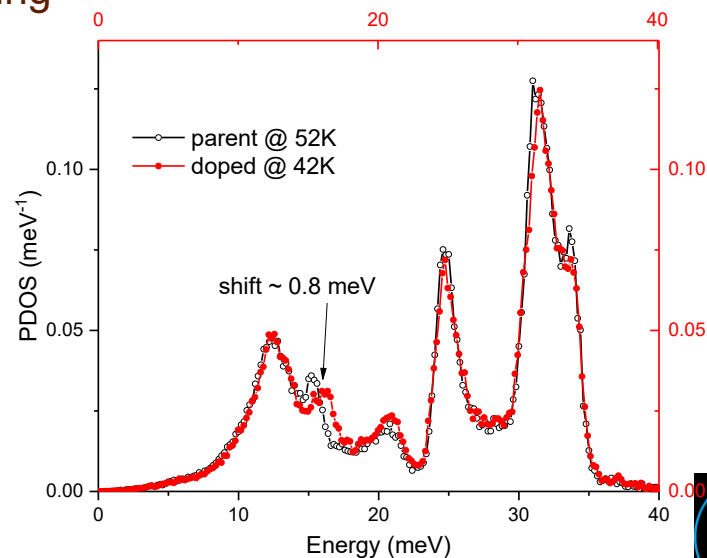
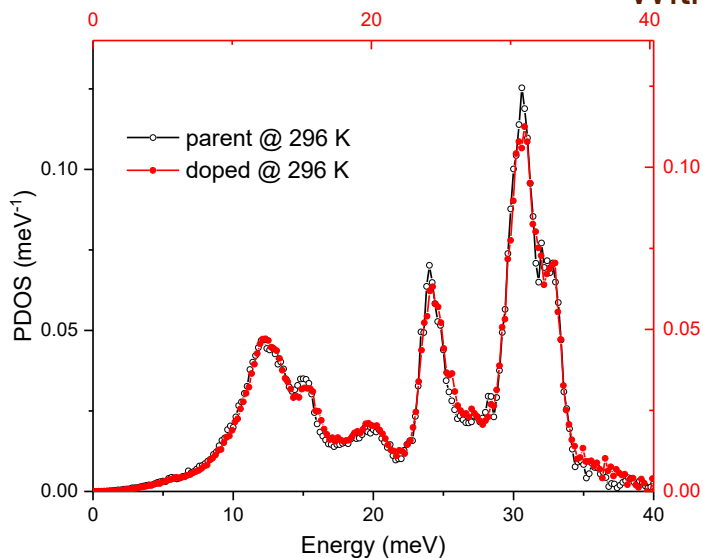


Q. Huang et al. PRB 78 (2008) 054529

Above and below Neel temperature



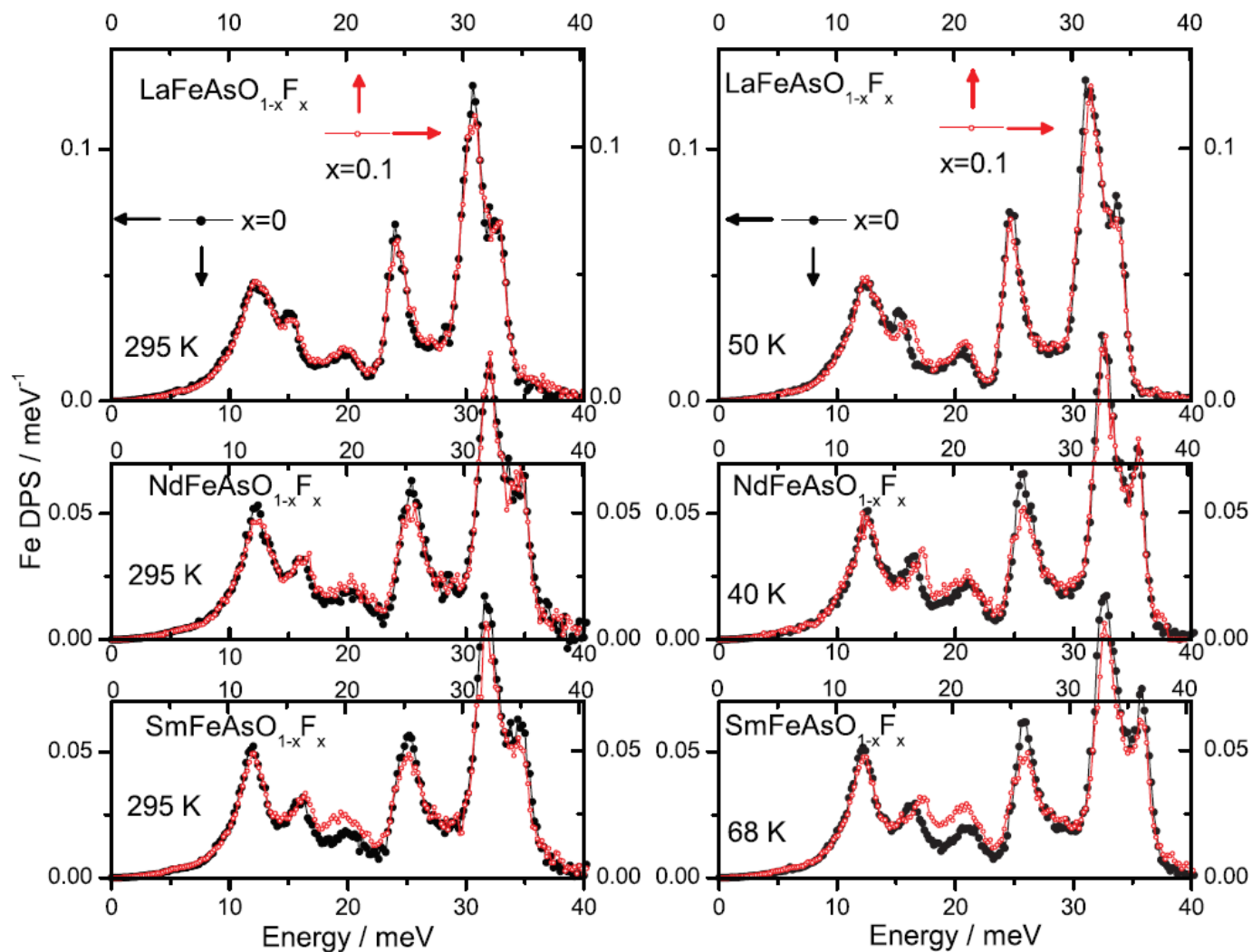
With doping



Fe PDOS for parent / doped 1111 compounds

Room temperature

Low temperature



LaFeAsO_{1-x}F_x

NdFeAsO_{1-x}F_x

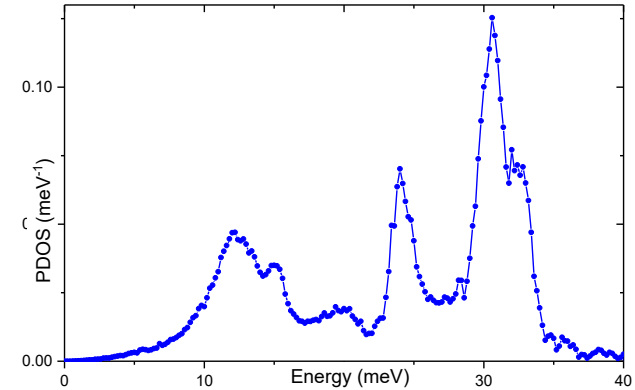
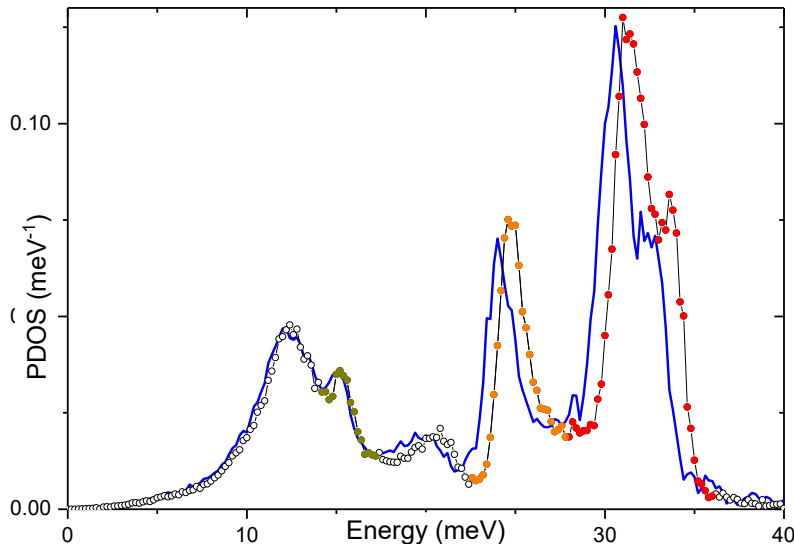
SmFeAsO_{1-x}F_x



How to find “peak” energy

Options to find peaks:

- Fit by peak function $\leftarrow ? \rightarrow$ peak shape unknown
- Use COM position $\leftarrow ? \rightarrow$ depends on chosen E-range
- Our solution: search for relative shift compared to reference spectrum by least square fit. Obtain value with statistical error.



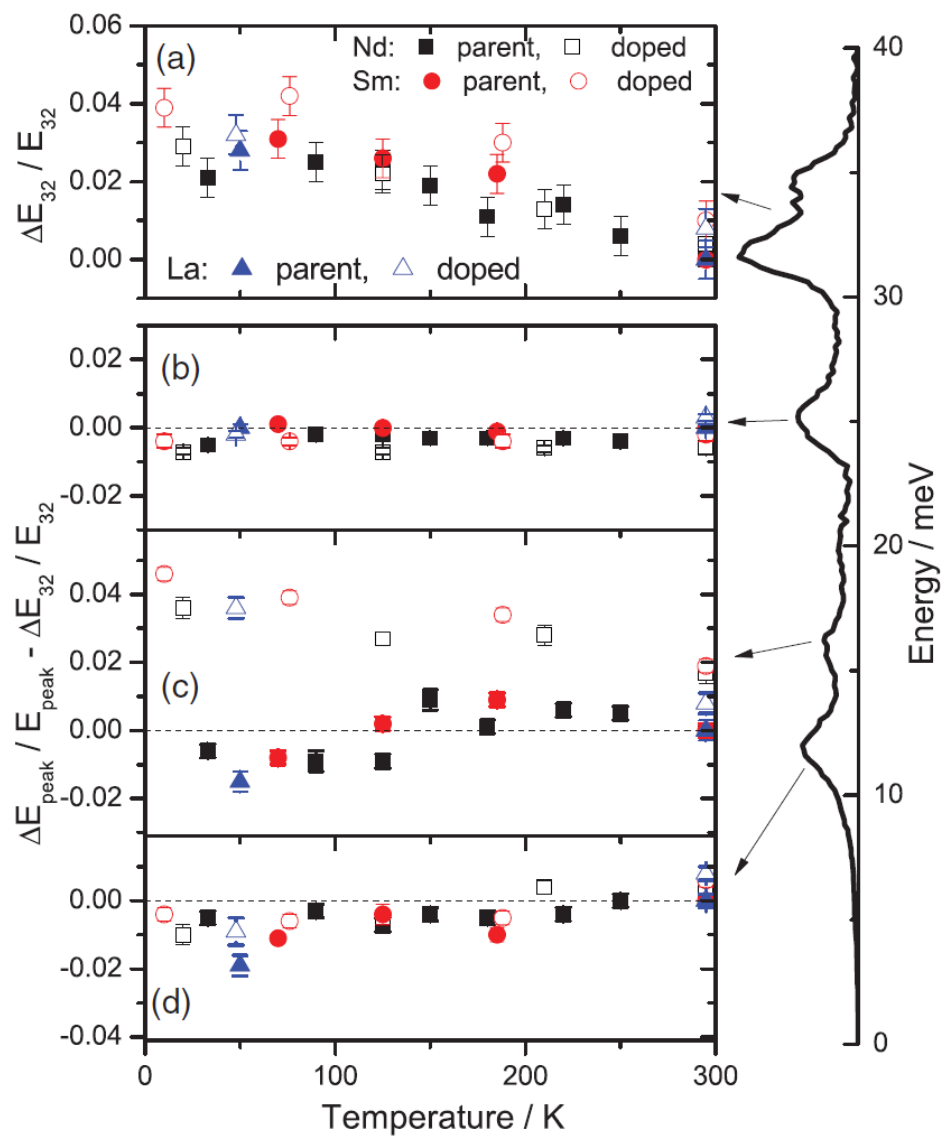
Interpolation: $D(E)$



Theoretical function for LSF:
 $F(E) = \beta \cdot D(E \cdot (1+\alpha))$

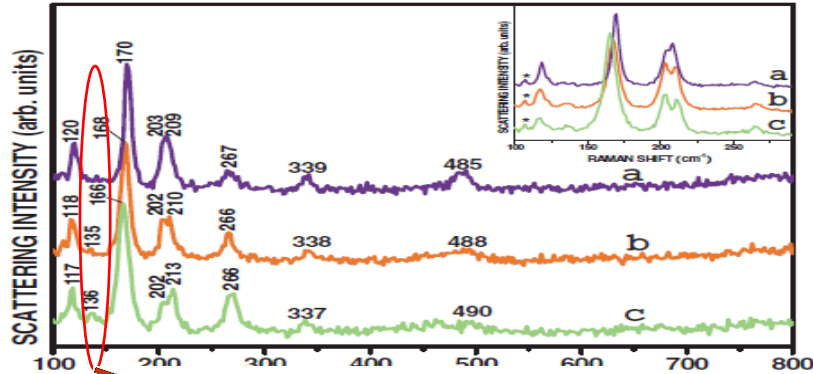
$\alpha = \Delta E / E$ – relative “peak” shift
 $\beta (1/ \alpha)$ – scaling factor

Peaks positions vs T for parent and doped compounds



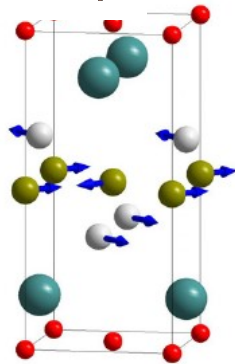
Raman scattering data with 1111 compounds

Raman scattering of $\text{NdFeAsO}_{1-x}\text{F}_x$
 Zhang et al., PRB 79 (2009) 052507

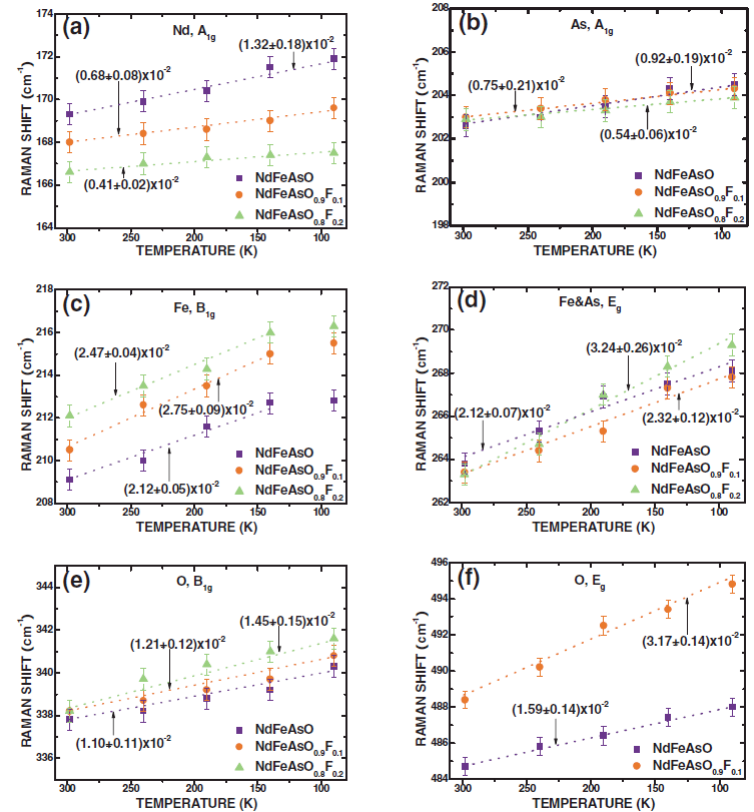


E_g of As and Fe
 at ~ 16 meV (130 cm^{-1})

weak or invisible for
 1111 family



T-dependence of other modes

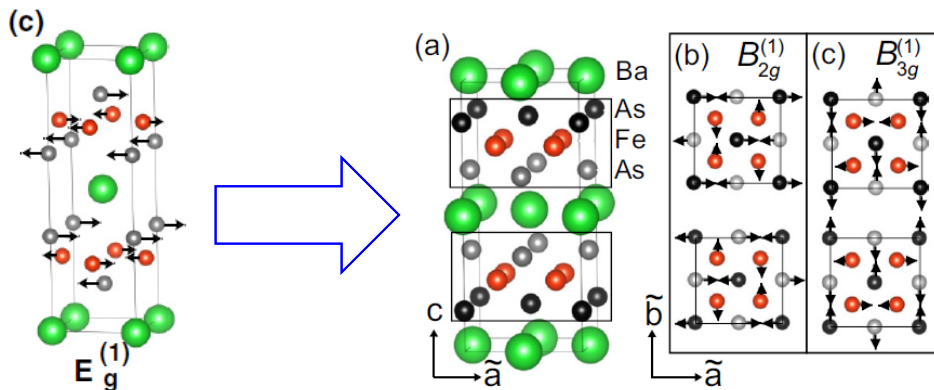


Raman scattering data with 122 compounds

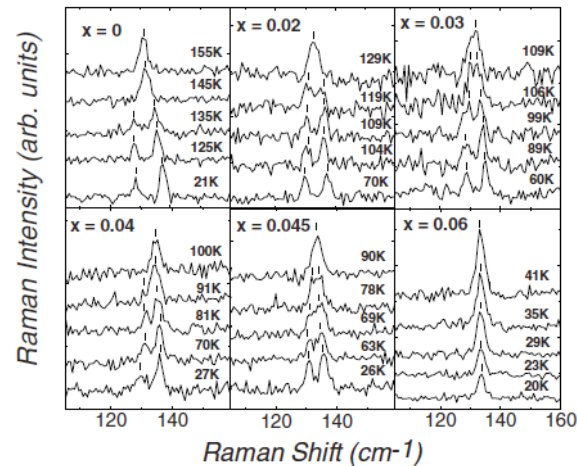
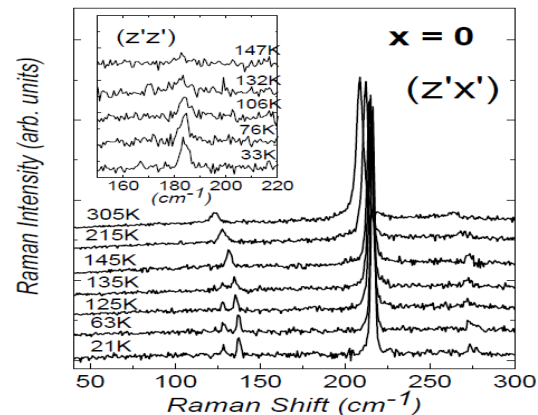
Raman scattering on BaFe_2As_2

Chauviere et al. PRB 80 (2009) 094504

Baum et al., PRB 98(2018) 075113

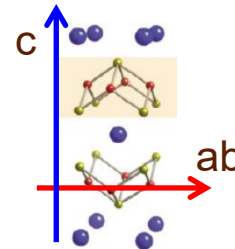
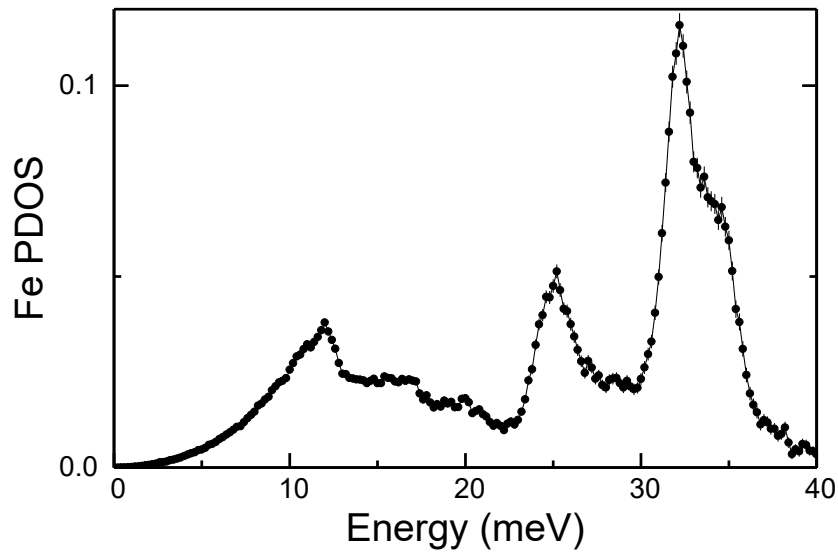


Gap between $B_{2g}^{(1)}$ and $B_{3g}^{(1)}$:
 theory : 2.8 meV
 exp : 1.2 meV

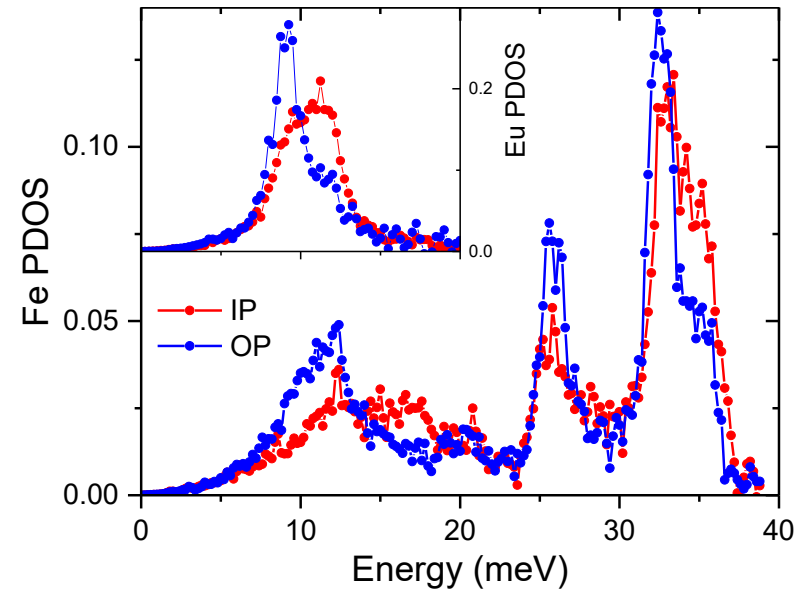


EuFe_2As_2 . NIS measurements at room T

EuFe_2As_2
NIS on powder

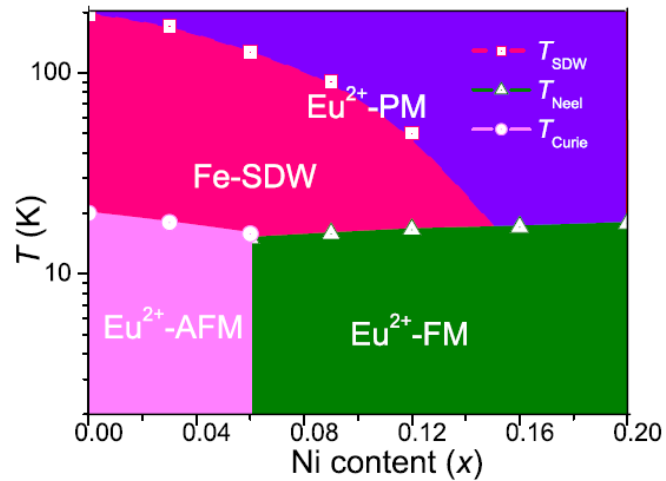


EuFe_2As_2
NIS on single crystal



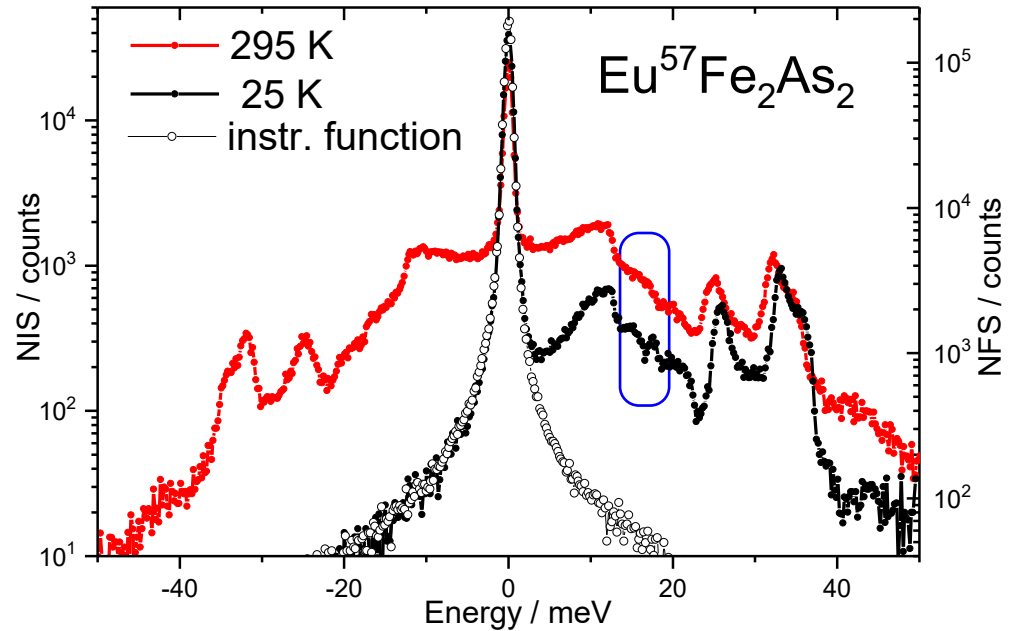
Phase diagram of EuFe_2As_2

Phase diagram of $\text{EuFe}_{2-x}\text{Ni}_x\text{As}_2$

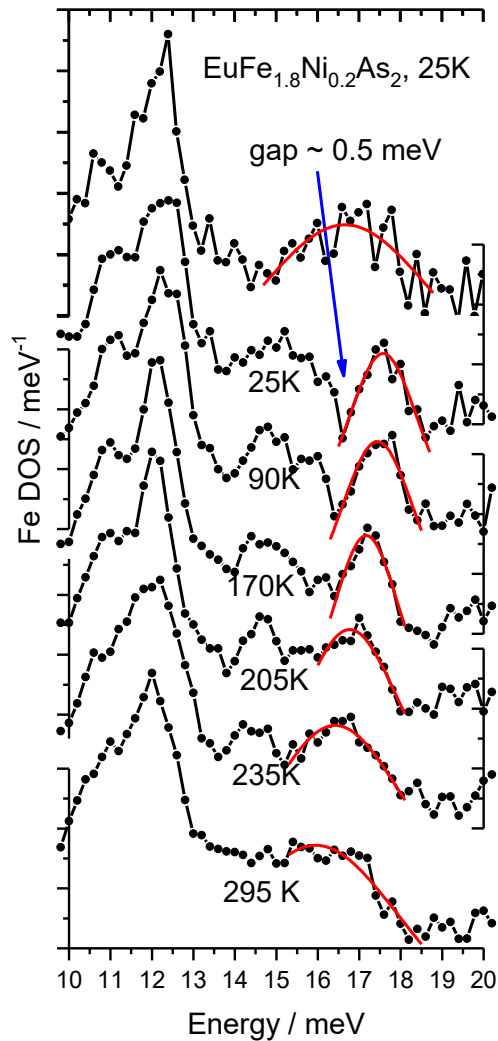


Ren et al., PRB 79 (2009) 094426

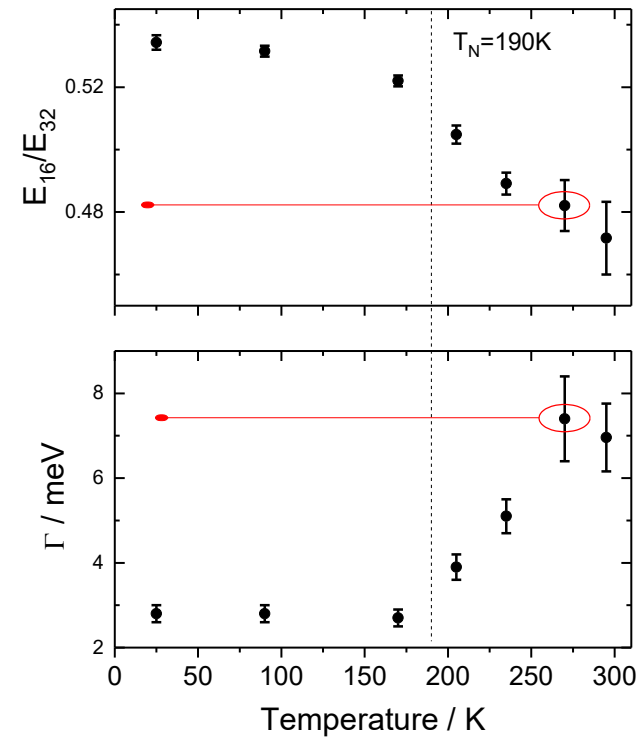
NIS on EuFe_2As_2 at low and room T



T – dependence of phonons in EuFe_2As_2



T – dependence of the phonon line position and width obtained by Lorentz fit

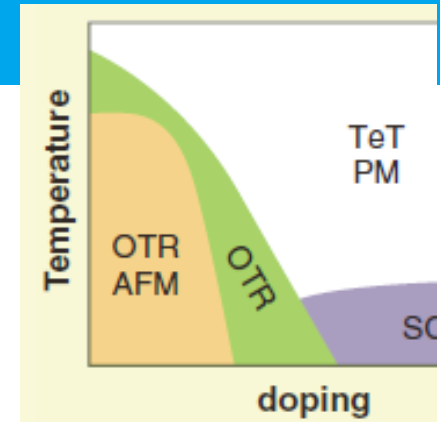


Theory proposition for spin-dynamics

A key role for unusual spin dynamics in ferropnictides

I. I. Mazin and M. D. Johannes*

Nature Physics 5 (2009) 141

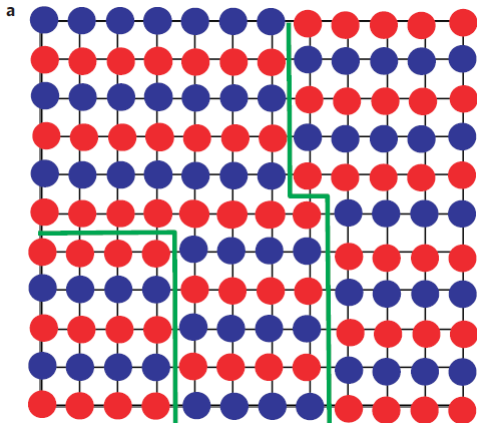


- AF magnetic
- orthorhombic

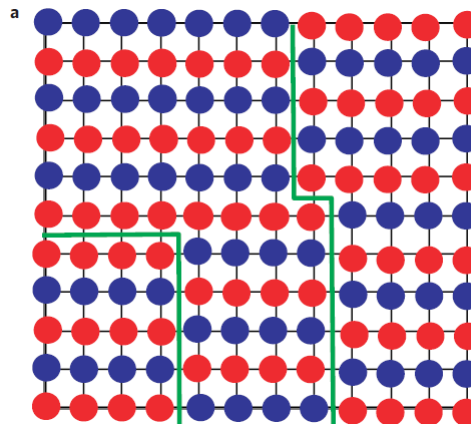
- paramagnetic
- orthorhombic

- paramagnetic
- tetragonal

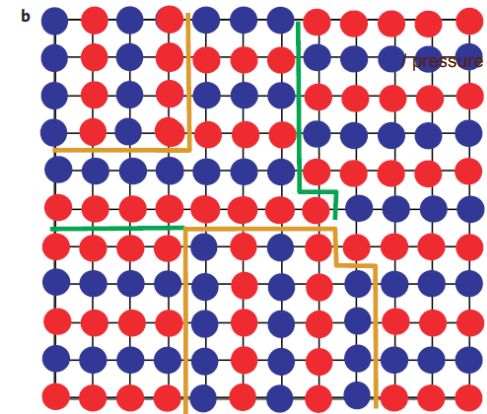
- * domain walls fixed
- * all domains with same direction (x/y symmetry broken)



- * dynamic domain walls
- * all domains with same direction (x/y symmetry broken)

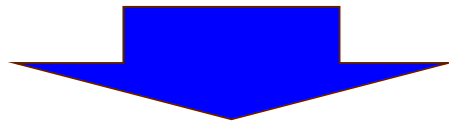


- * dynamic domain and twin walls
- * twins at different directions (x/y symmetry conserve)



Conclusion

- There are anomalies in the T – dependence of the phonon structure for FeSc of 1111 and 122 families.
- They can be related to the structural transition, spin-lattice coupling, e-ph coupling, ...???
- Characteristic E scale of anomalies is $0.1 - 1$ meV. E –resolution of current HRM is $0.7 - 1$ meV



Investigation of the T evolution of the phonon anomalies requires monochromator with 0.1 meV E resolution (spectrograph).

Other useful capability of the spectrograph is simultaneous measurements of different samples (doped / parent FeSc)

Acknowledgment



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**Thank you for your
attention**

