Orbitals and Polarons in Fe – based Superconductors

- **Electron correlations in Fe based SC: "Lower Hubbard bands"**
- **Nematic order, orbitals, and spin fluctuations in Fe based SC**
- **Temperature dependent electronic structure: "red/blue shift"**

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TECHNISCHE UNIVERSITÄT DRESDEN

Thanks to

ARPES

S. Borisenko

S. Fedorov, Y. Kushnirenko, J. Maletz, S. Thirupathaiah, Z. Liu — IFW Dresden
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Timur Kim — Diamond Light Source
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NMR/NQR

H. Grafe

S.H. Baek

G. Lang, E. Brüning, P. Lepucki — IFW Dresden
E. Brüning F. Hammerath

Synthesis

S. Aswartham

S. Wurmehl, R. Kappenberger — IFW Dresden
I. Morozov et al. — Moscow (MSU)
T. Wolf — Karlsruhe (KIT)
J. M. Ok, J. S.Kim — U Pohang

Transport Magnetisation

C. Hess

C. Hess, F. Caglieris, X. Hong, C. Wuttke — IFW Dresden
A. Wolter-Giraud

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Theory

J. van den Brink, D. Efremov — IFW Dresden
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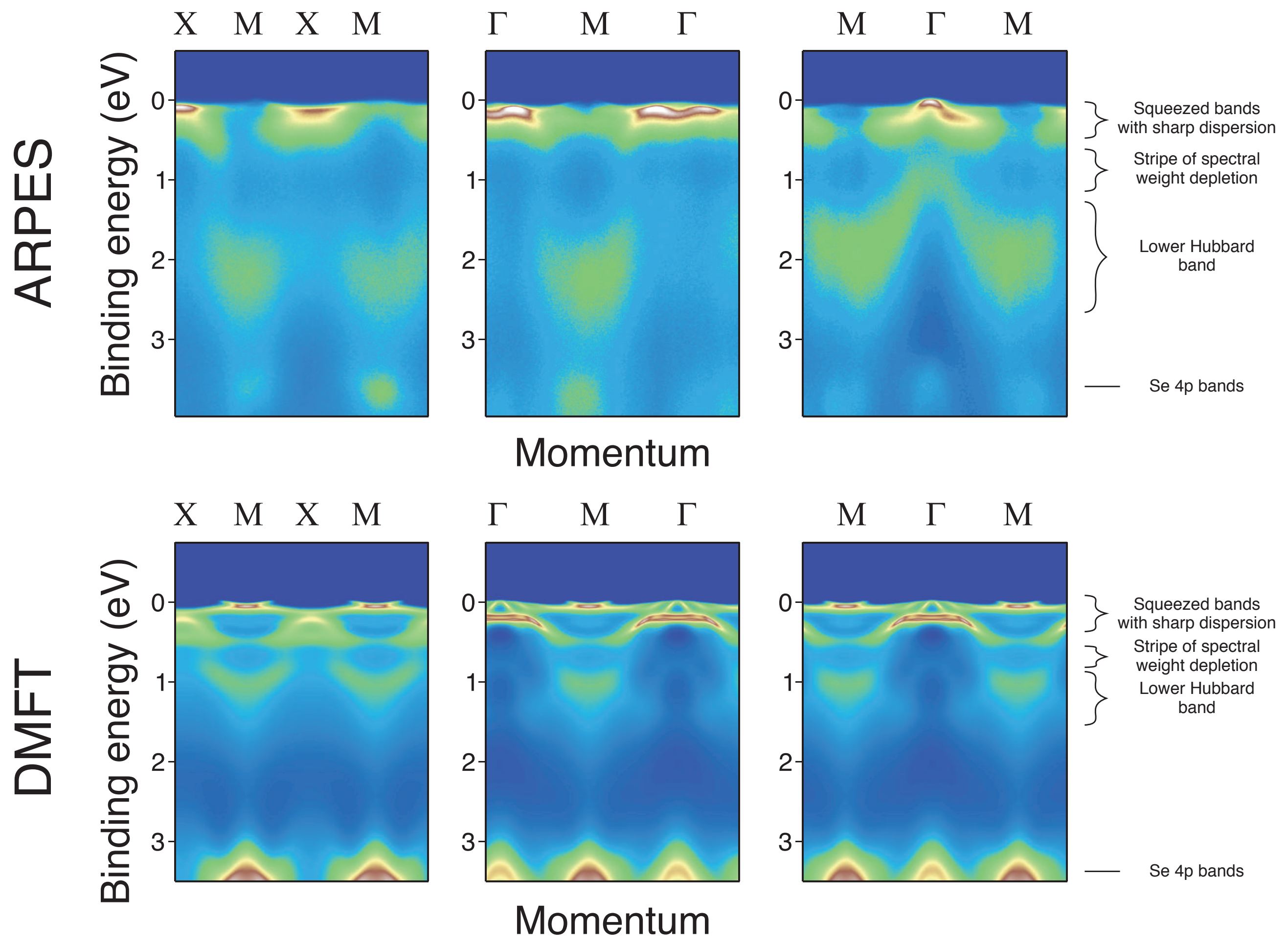
M. Aichhorn, Y.Sassa — U Graz, ETH Zürich

Priority Program SPP1458 (2010 – 2017): “Iron Pnictides Superconductors: Materials and Mechanisms“

Electronic correlations: "Lower Hubbard bands"



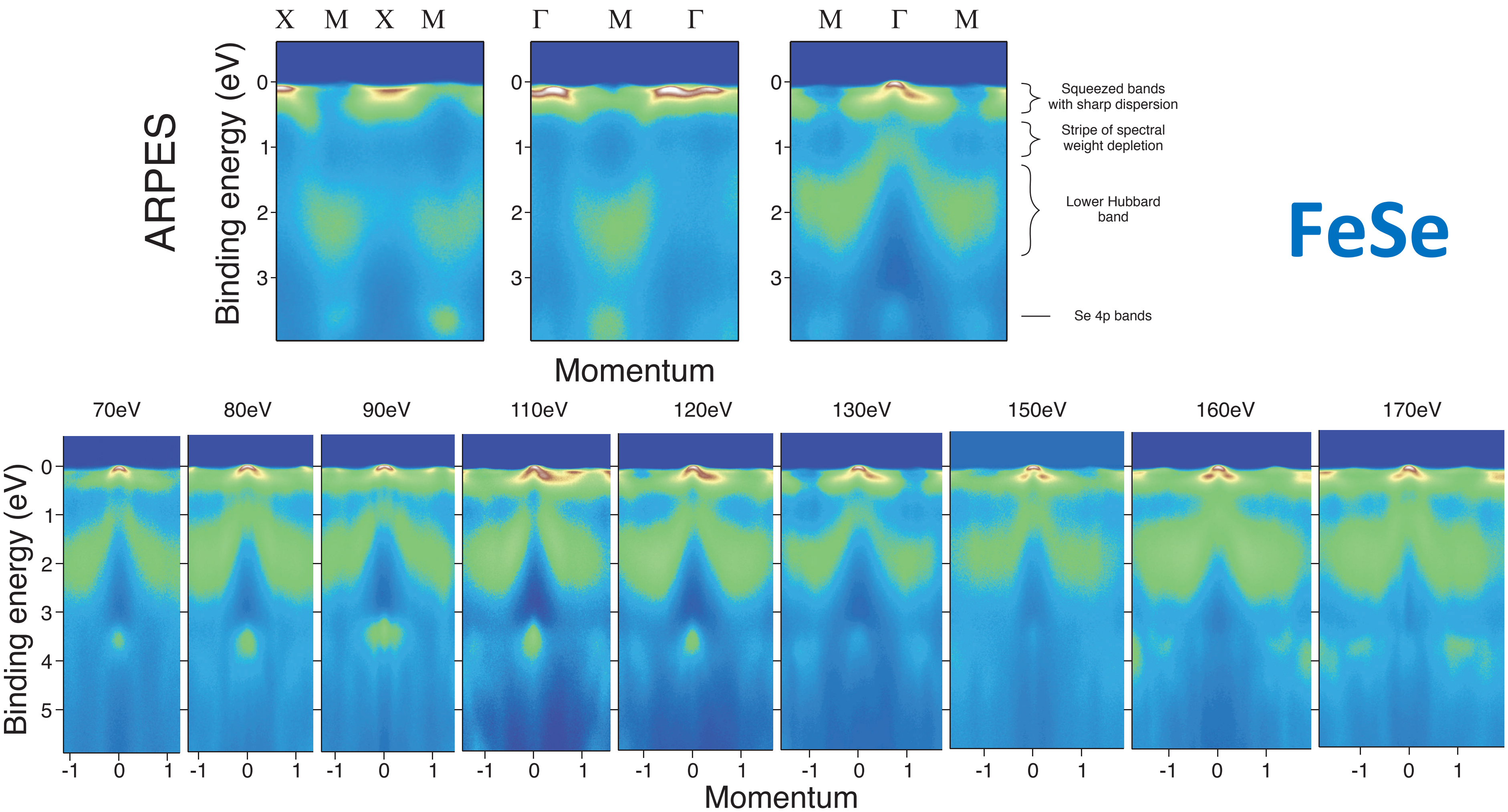
FeSe

Direct observation of dispersive lower Hubbard band in iron-based superconductor FeSe

D. V. Evtushinsky,[1,*] M. Aichhorn,[2] Y. Sassa,[3,4] Z.-H. Liu,[1] J. Maletz,[1] T. Wolf,[5] A. N. Yaresko,[6] S. Biermann,[7] S. V. Borisenko,[1] and B. Büchner[1,8]

See also M. Watson, R. Valenti et al.

Electronic correlations: “Lower Hubbard bands”



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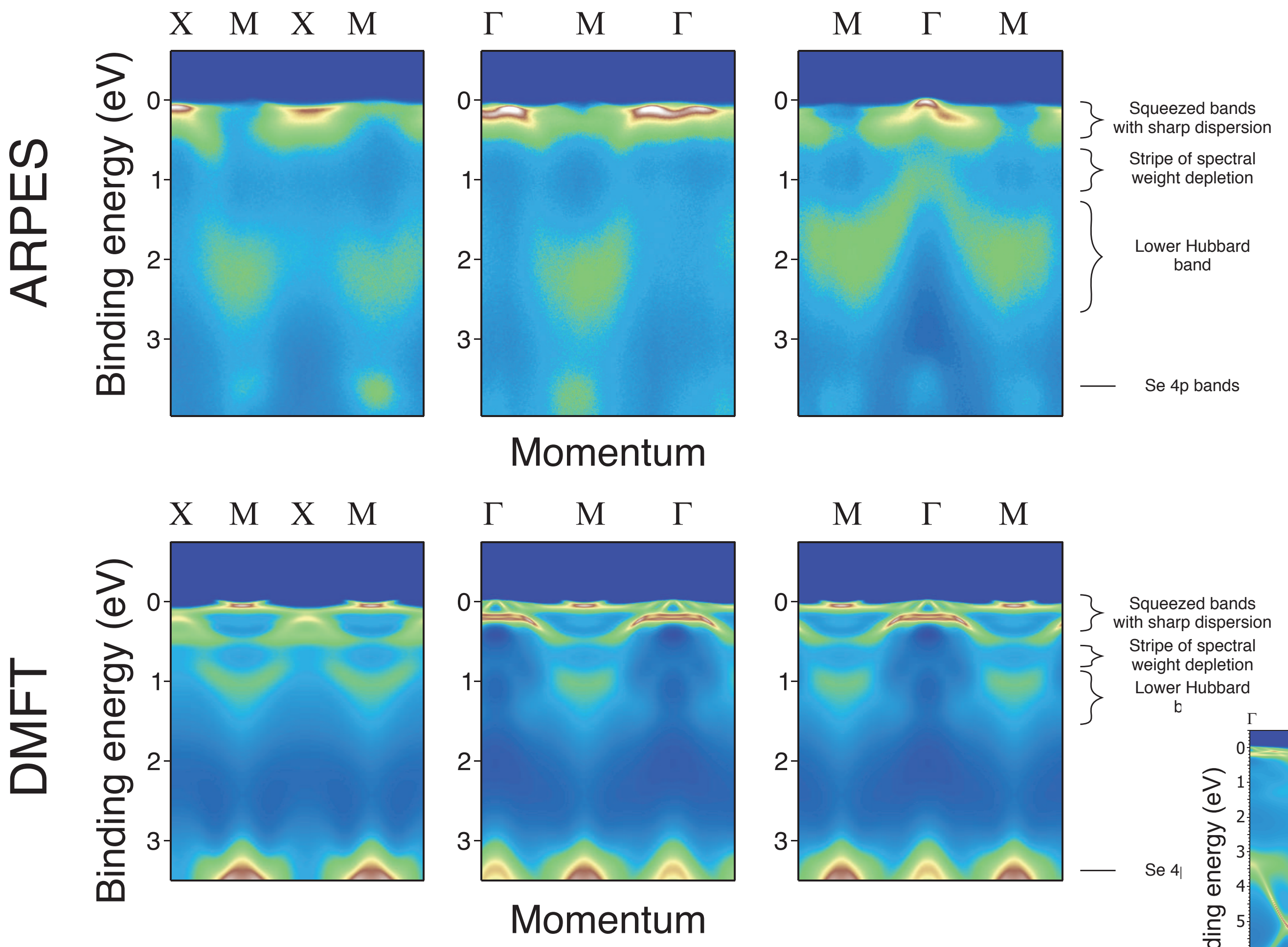

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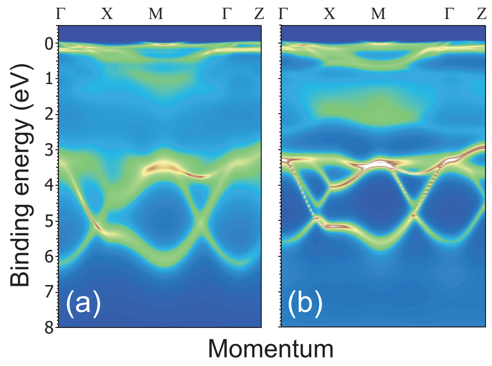
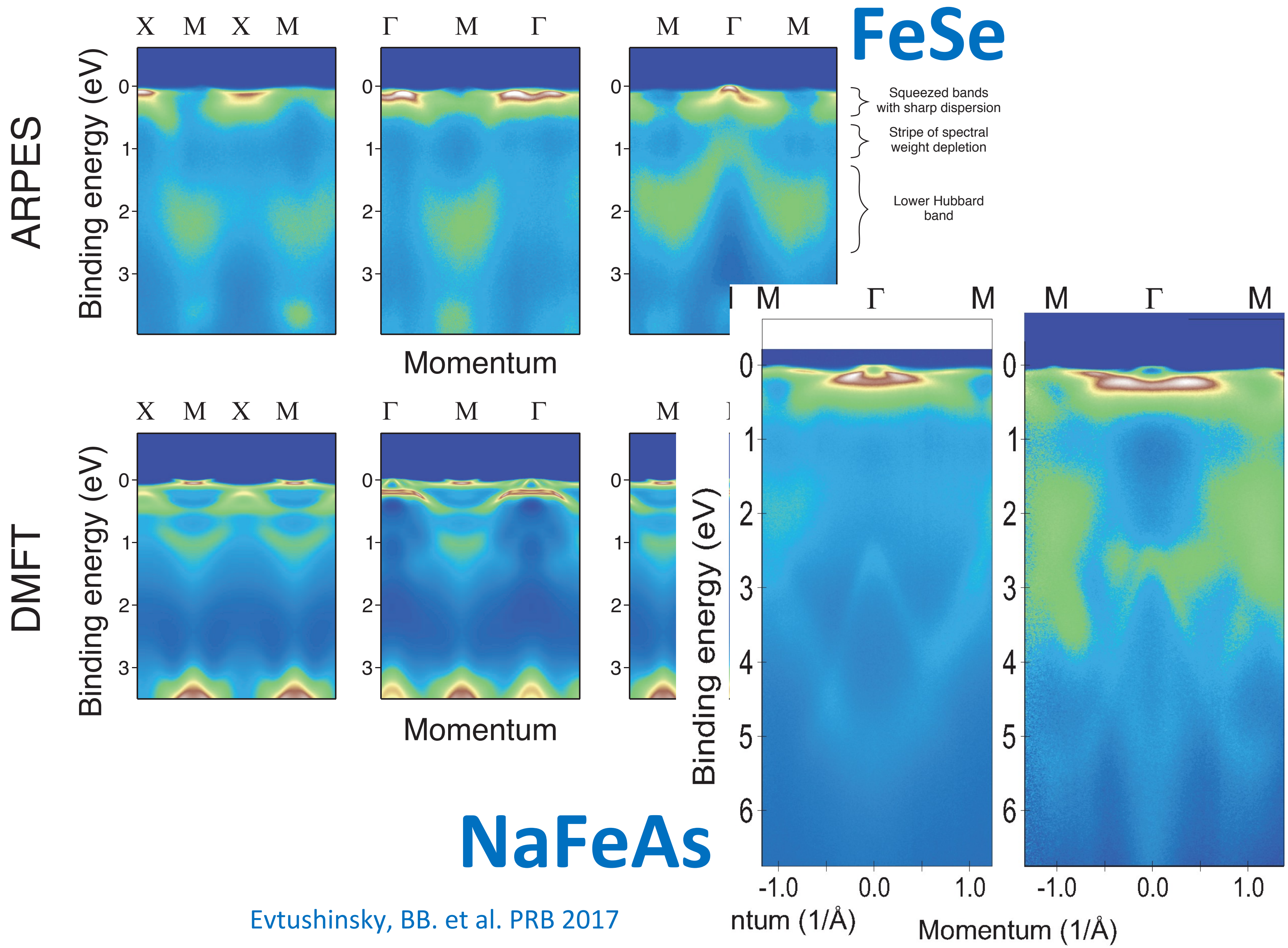


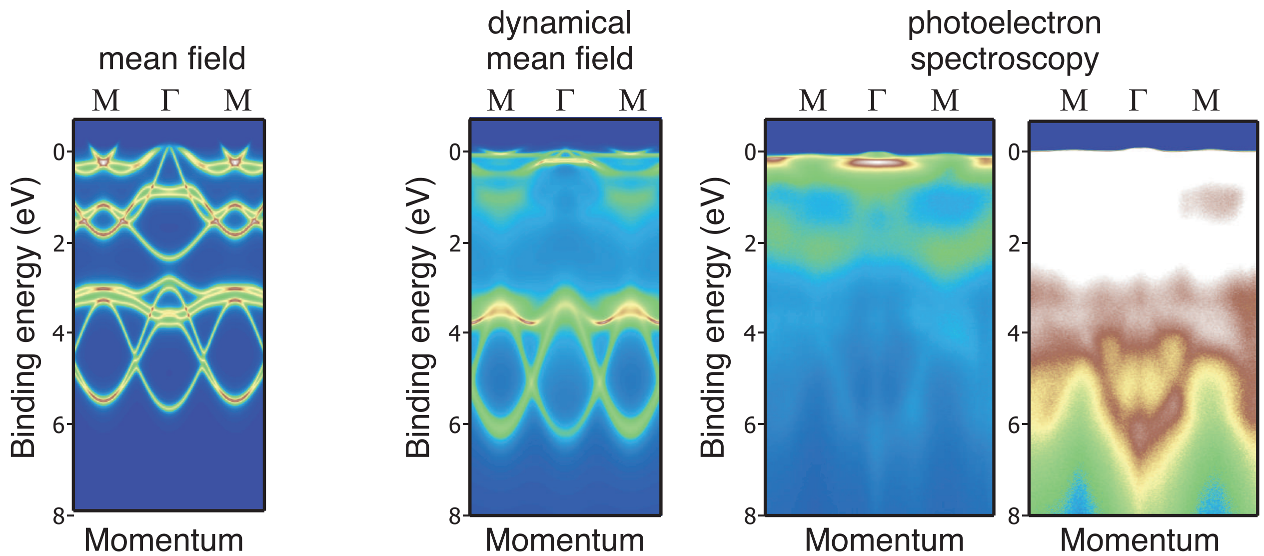
Fig. S 4: Calculated spectral function using two different variants of the analytic continuation method for the self energy. Left (a) using an artifical Greens function, right (b) using a rescaling of the self energy.

Electronic correlations: “Lower Hubbard bands”

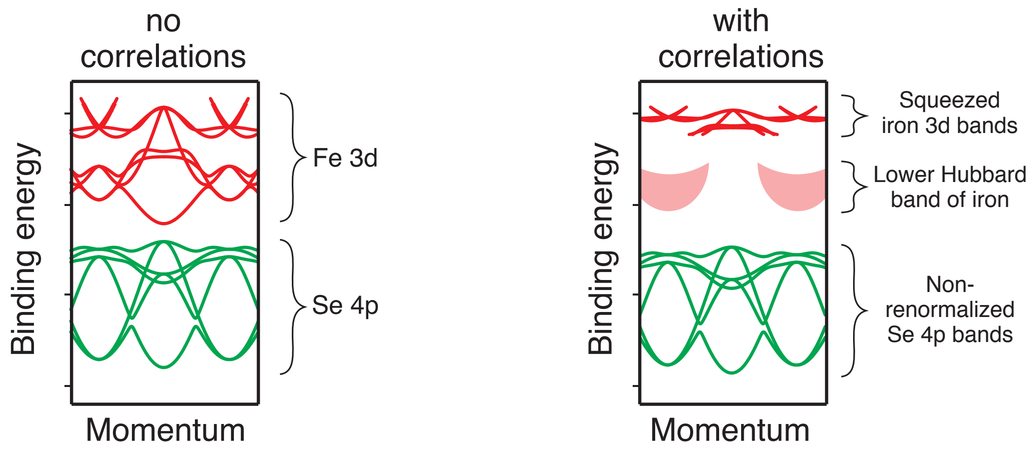


Evtushinsky, BB. et al. PRB 2017

Electronic correlations: “Lower Hubbard bands”



FeSe



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Conclusions

Sizeable electronic correlations in Fe-based SC

“dispersive“ lower Hubbard bands with contributions from all 5 orbitals

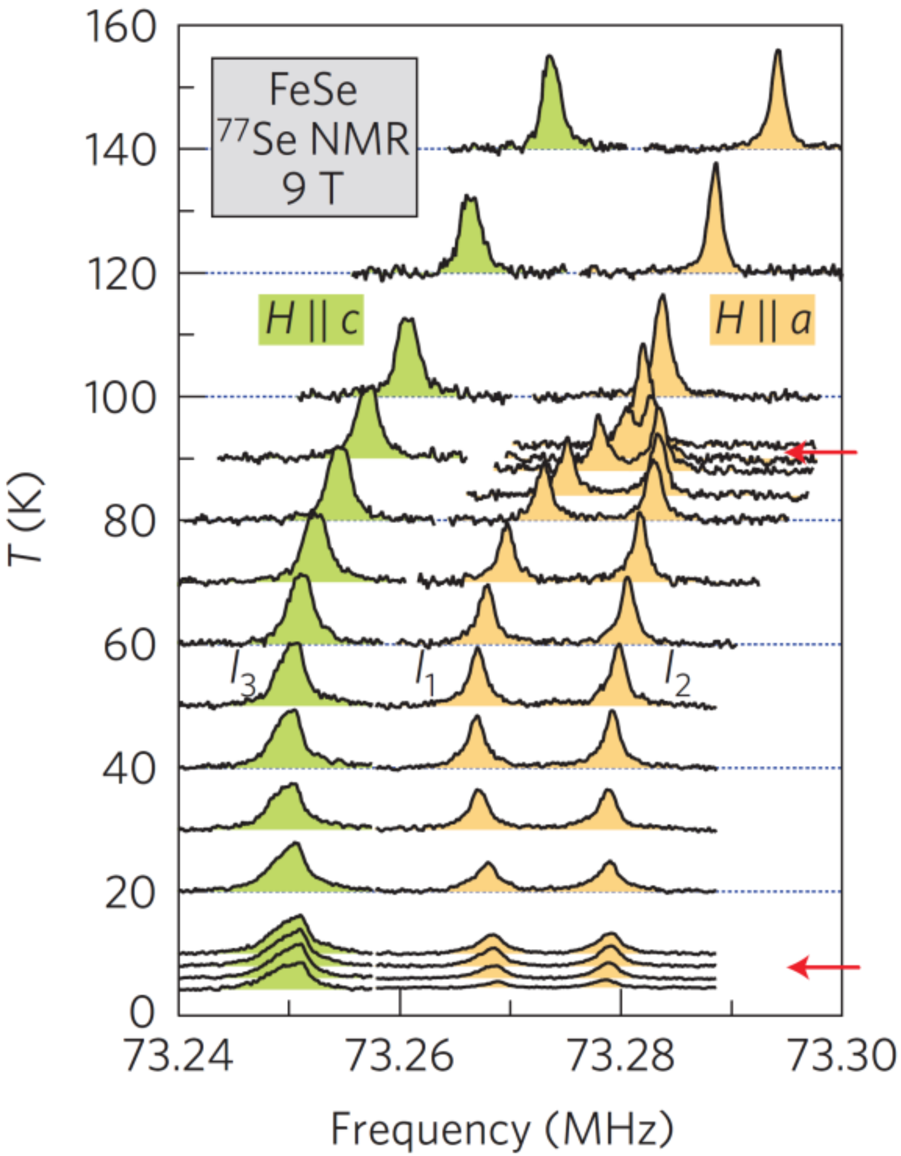
ARPES on Fe based SC shows both

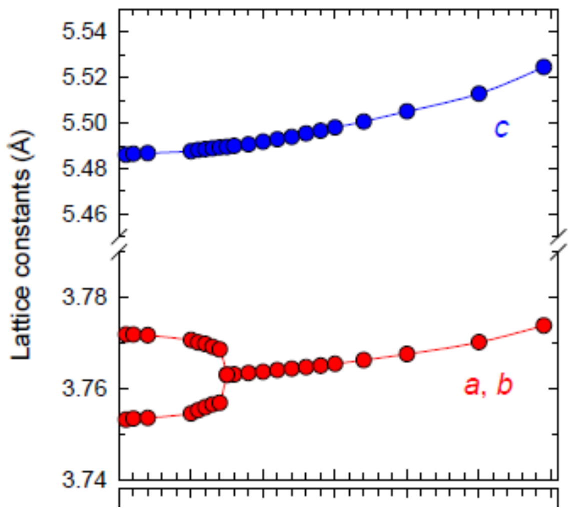
“itinerant e$^-$“ with orbital character

and

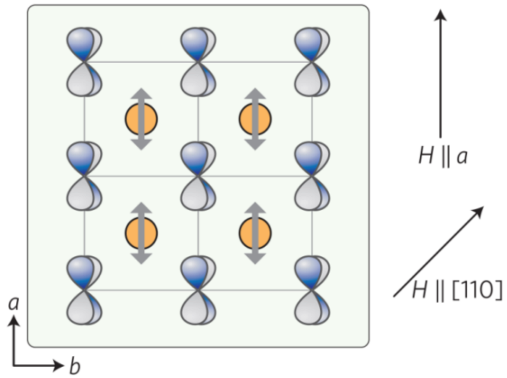
“local physics“ of Fe 3d orbitals

Nematic order, orbitals, and spin fluctuations





- Tiny structural distortion
- In-plane anisotropy of κ comparable of to $\kappa_c - \kappa_{a,b}$



S. Baek, BB et al., Nat. Mat. 2015

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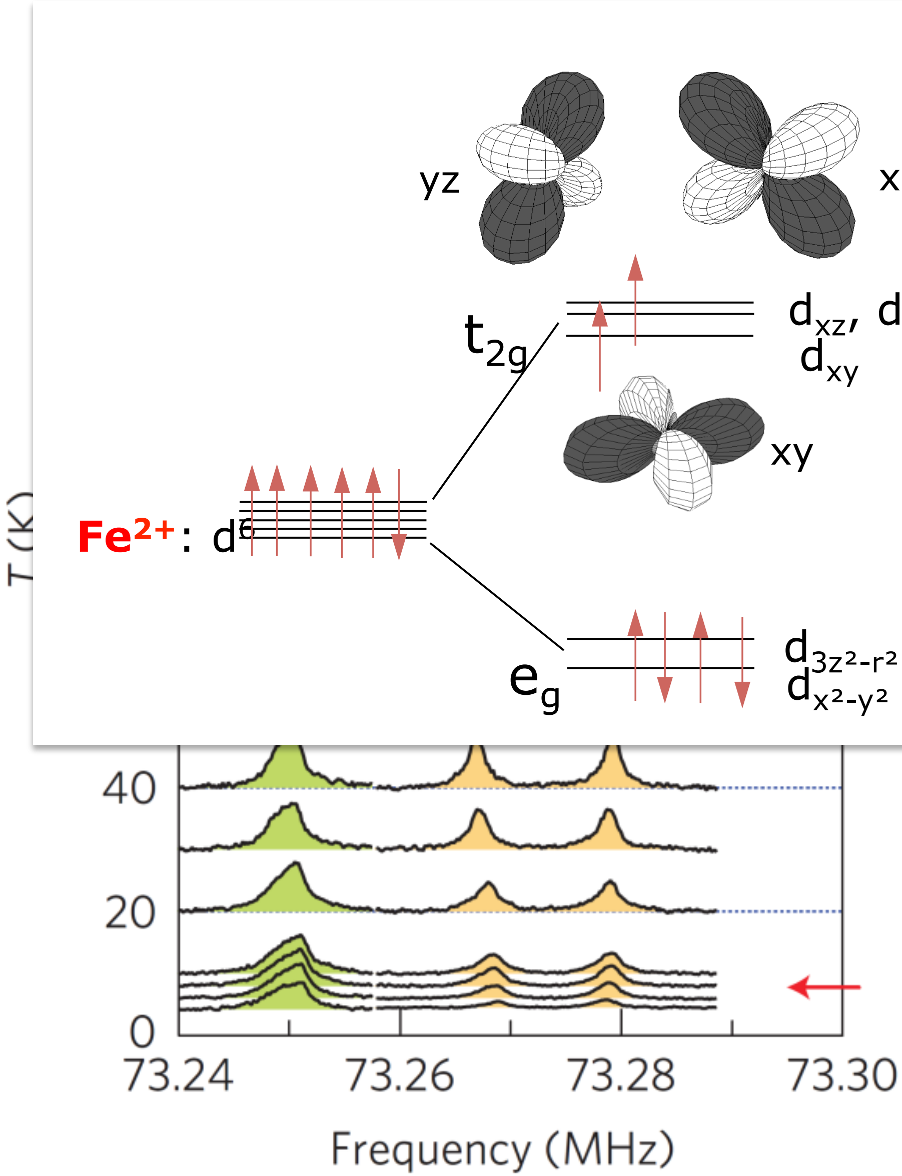

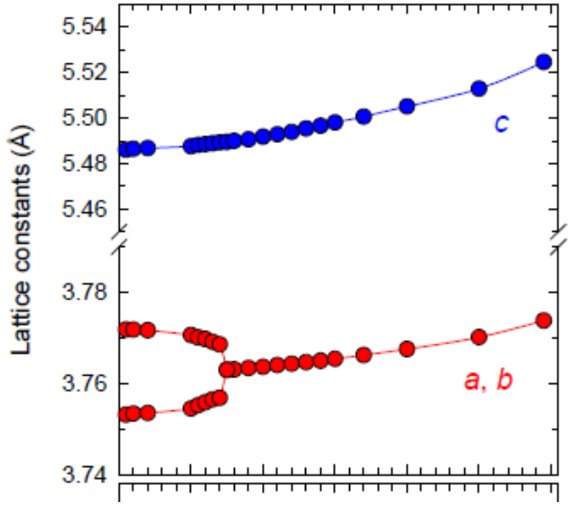

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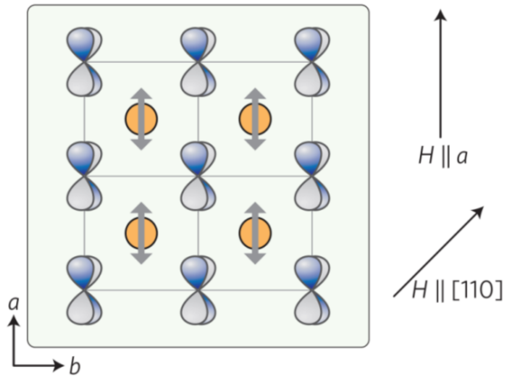
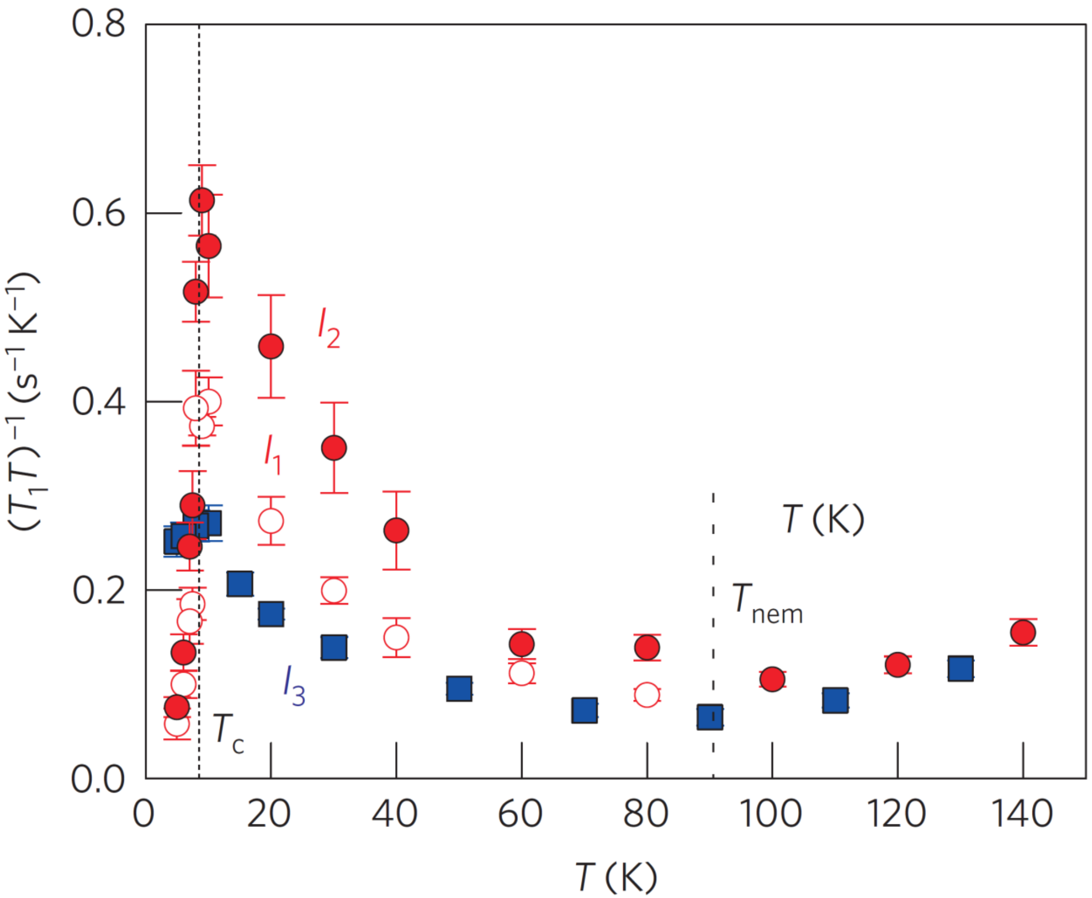
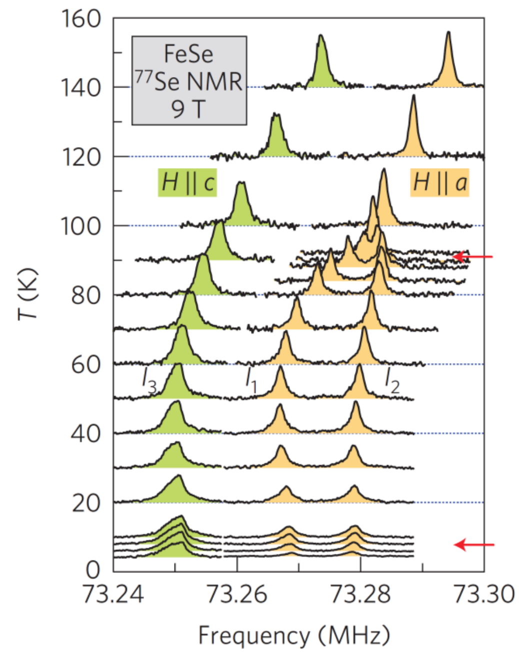


S. Baek, BB et al., Nat. Mat. 2015

FeSe: nematic order but no slow (NMR) spin fluctuations





Above T_{nem}: typical T_1 for Fe based sc far away form T_N, **$(T_1T)^{-1}$ a K^2_{spin}**

At T_{nem}: No drastic change of T_1

Well below T_{nem}: Increase of $1/(T_1T)$ signaling the proximity of a magnetic instability

S. Baek, BB et al., Nat. Mat. 2015

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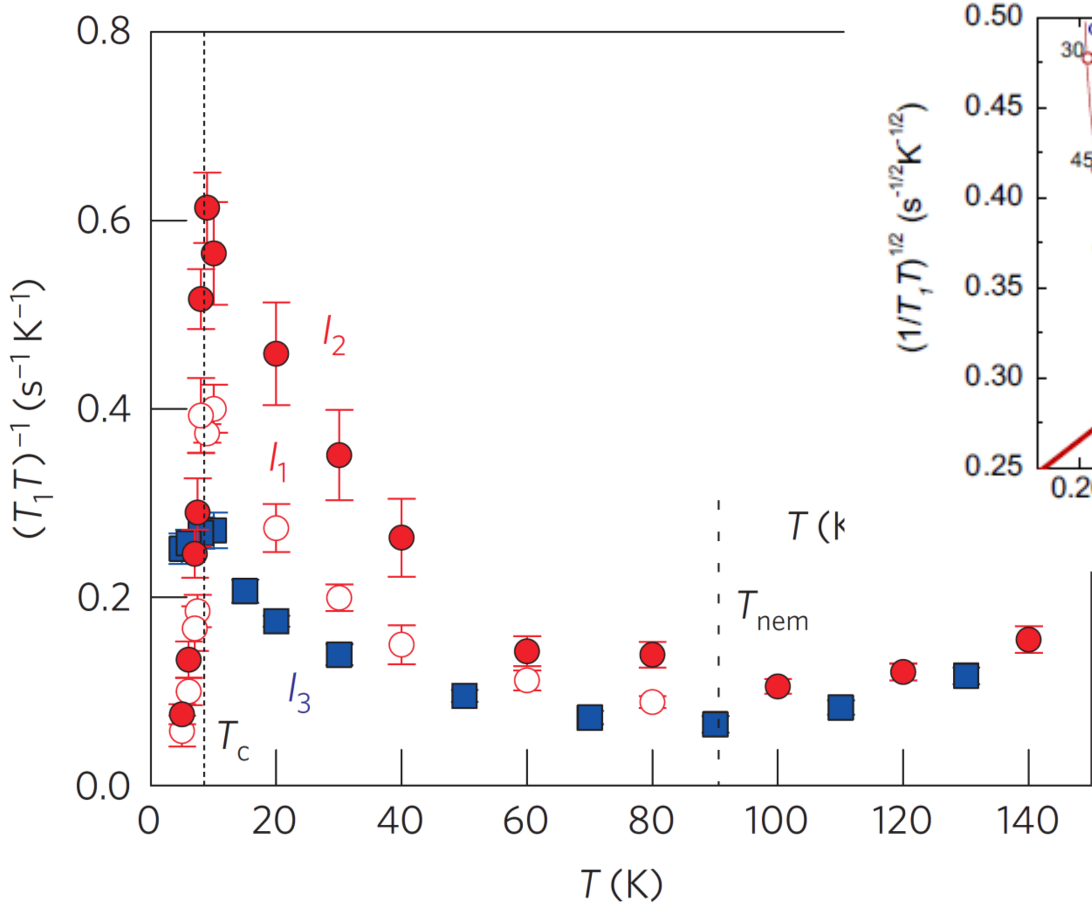
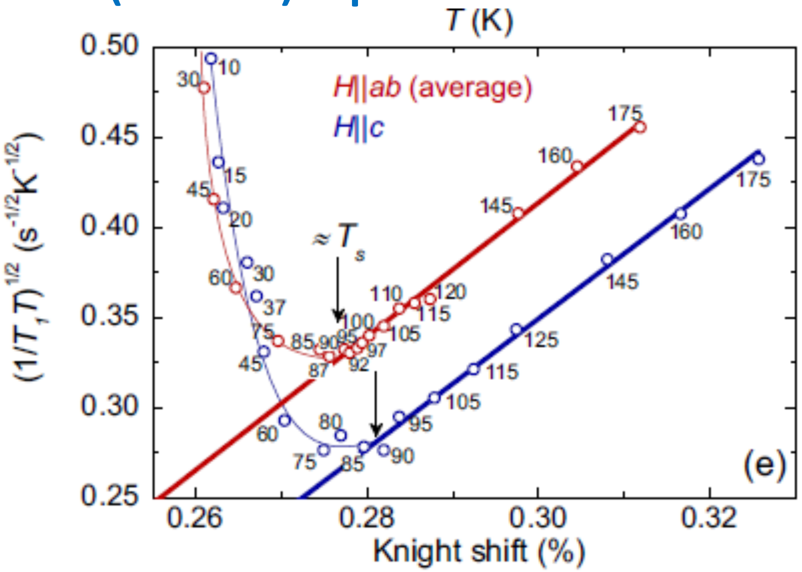
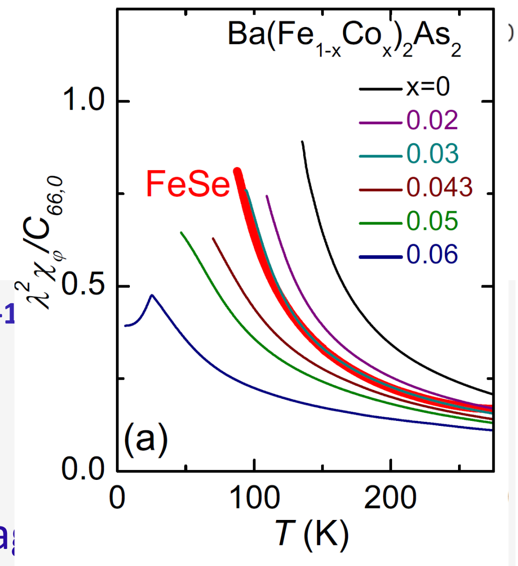




A.E. Böhmer et al., PRL 2015



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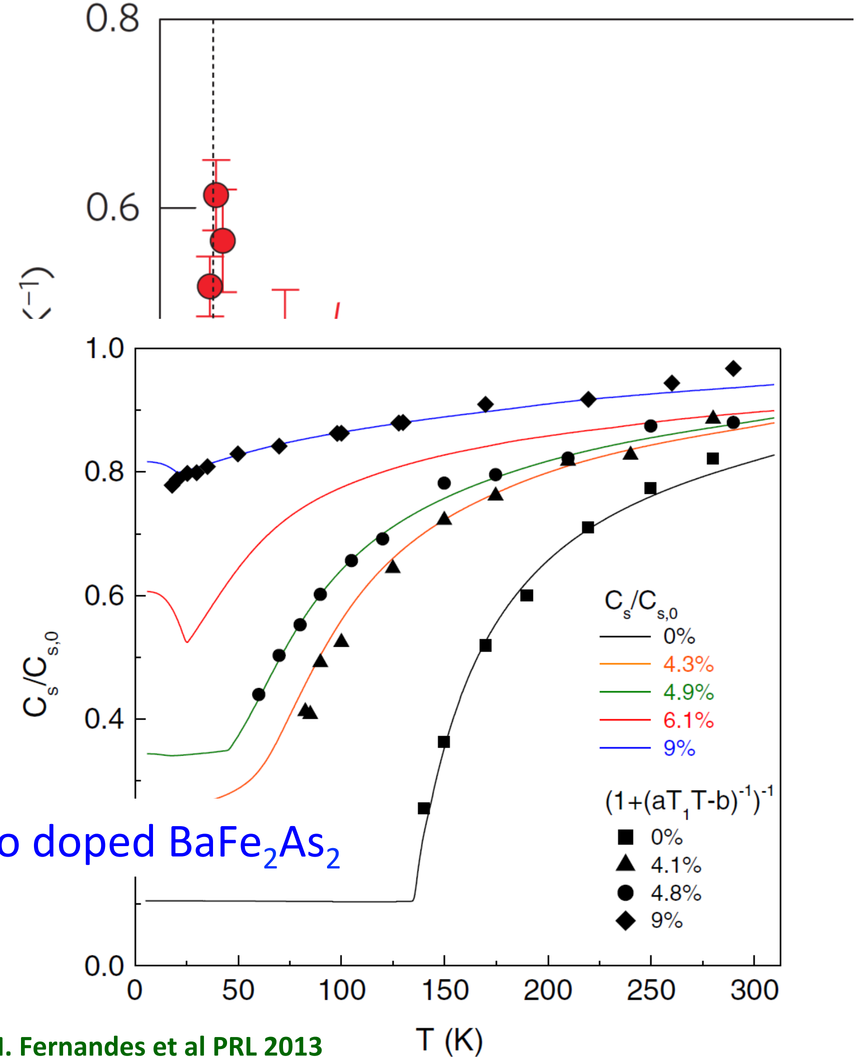
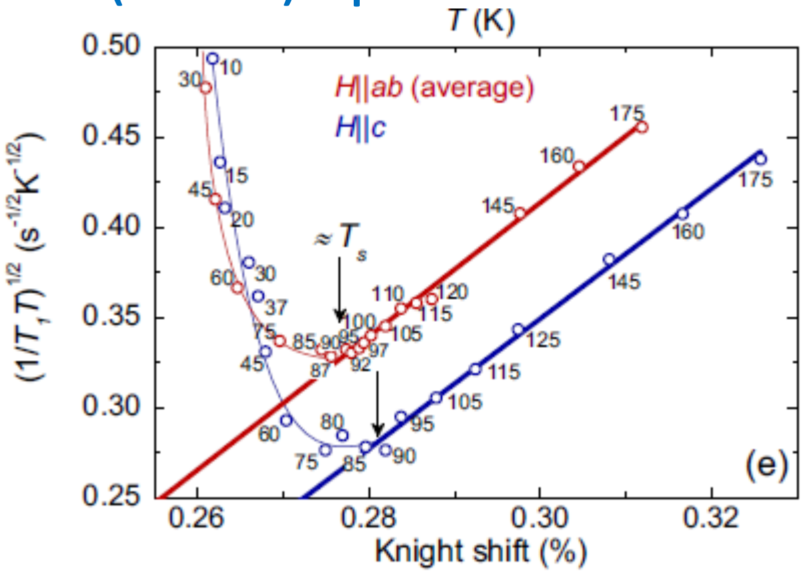


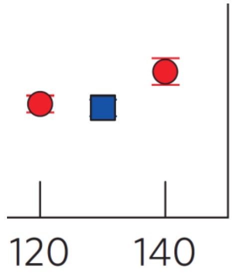
Co doped $BaFe_2As_2$

R.M. Fernandes et al PRL 2013

FIG. 2 (color online). Comparison between the relative shear modulus $C_s/C_{s,0}$ (continuous lines, from Ref. [8]) and the rescaled NMR $1/T_1T$ (closed symbols, from Ref. [3]) for different "effective" Co concentrations in $Ba(Fe_{1-x}Co_x)_2As_2$. The



A.E. Böhmer et al., PRL 2015



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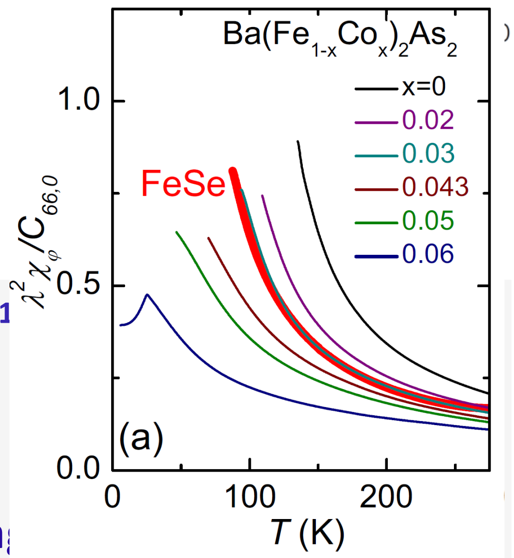

NMR on FeSe: Conclusions

Data: FeSe shows orbital order and pronounced nematic fluctuations!

experimental signatures for lattice/electrons similar to findings in 122 …

but long range magnetic order and slow spin fluctuations are missing…

→ data with striking difference to findings in Ba122

-> from NMR no evidence for "conventional spin-driven" nematicity!

S. Baek, BB et al., Nat. Mat. 2015

Many scenarios for a "magnetic origin" of nematic order in FeSe

which are consistent with the NMR data!

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nature physics

ARTICLES

PUBLISHED ONLINE: 24 AUGUST 2015 | DOI: 10.1038/NPHYS3434

Effect of magnetic frustration on nematicity and superconductivity in iron chalcogenides

J. K. Glasbrenner[1]*, I. I. Mazin[2], Harald O. Jeschke[3], P. J. Hirschfeld[4], R. M. Fernandes[5] and Roser Valentí[3]

understanding the more exotic derivatives of the FeSe system. The FeSe phase diagram is distinct from the pnictides: the orthorhombic distortion, which is likely to be of a 'spin-nematic' nature in numerous pnictides, is not accompanied by magnetic order in FeSe, and the superconducting transition temperature T_c rises significantly with pressure before decreasing. Here we show that the magnetic interactions in FeSe, as opposed to most pnictides, demonstrate an unusual and unanticipated frustration, which suppresses magnetic (but not nematic) order, triggers ferro-orbital order in the nematic phase and can

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nature physics

ARTICLES

PUBLISHED ONLINE: 7 SEPTEMBER 2015 | DOI: 10.1038/NPHYS3456

Nematicity and quantum paramagnetism in FeSe

Fa Wang[1,2], Steven A. Kivelson[3] and Dung-Hai Lee[4,5]*

In common with other iron-based high-temperature superconductors, FeSe exhibits a transition to a 'nematic' phase below 90 K in which the crystal rotation symmetry is spontaneously broken. However, the absence of strong low-frequency magnetic fluctuations near or above the transition has been interpreted as implying the primacy of orbital ordering. In contrast, we establish that quantum fluctuations of spin-1 local moments with strongly frustrated exchange interactions can lead to a nematic quantum paramagnetic phase consistent with the observations in FeSe. We show that this phase is a fundamental expression of the existence of a Berry's phase associated with the topological defects of a Néel antiferromagnet, in a manner analogous to that which gives rise to valence bond crystal order for spin-1/2 systems. We present an exactly solvable model realizing the nematic quantum paramagnetic phase, discuss its relation with the spin-1 J_1–J_2 model, and construct a field theory

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PRL 115, 116401 (2015) PHYSICAL REVIEW LETTERS week ending 11 SEPTEMBER 2015

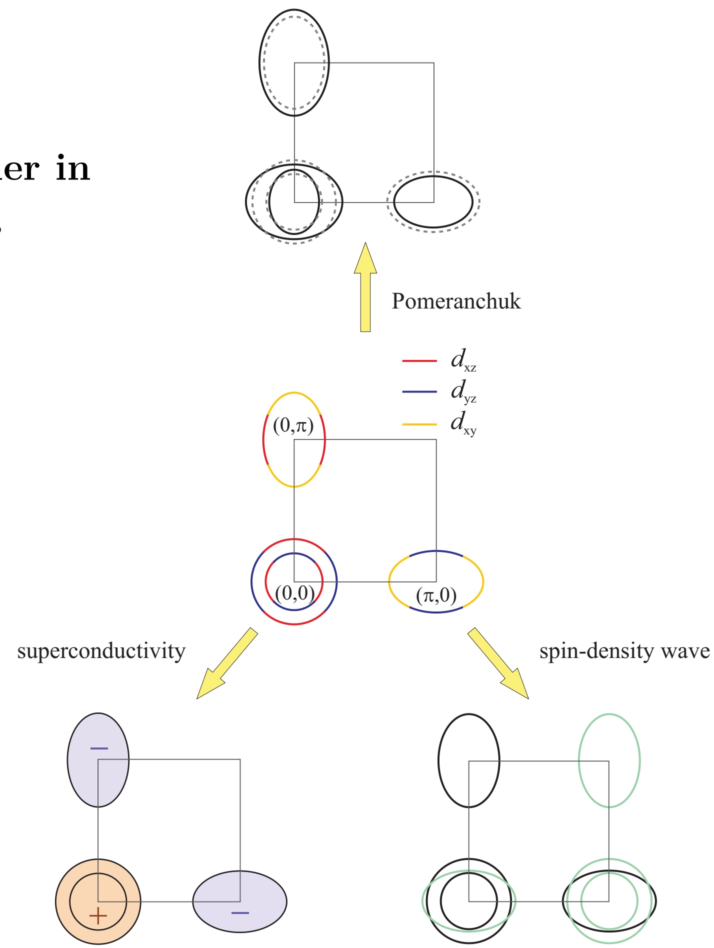
Antiferroquadrupolar and Ising-Nematic Orders of a Frustrated Bilinear-Biquadratic Heisenberg Model and Implications for the Magnetism of FeSe

Rong Yu[1,2] and Qimiao Si[3]

Another scenario: Pomeranchuk versus SDW instability

Magnetism, superconductivity, and spontaneous orbital order in iron-based superconductors: who comes first and why?

Andrey V. Chubukov[1], M. Khodas [2,3], and Rafael M. Fernandes[1]



in systems with large Fermi energies, such as $BaFe_2As_2$, LaFeAsO, and NaFeAs, orbital order is induced by stripe magnetism. However, in systems with small Fermi energies, such as FeSe, the system develops a spontaneous orbital order, while magnetic order does not develop. Our results provide a unifying description of different iron-based materials.

ARPES on FeSe: Band splitting due to nematic order

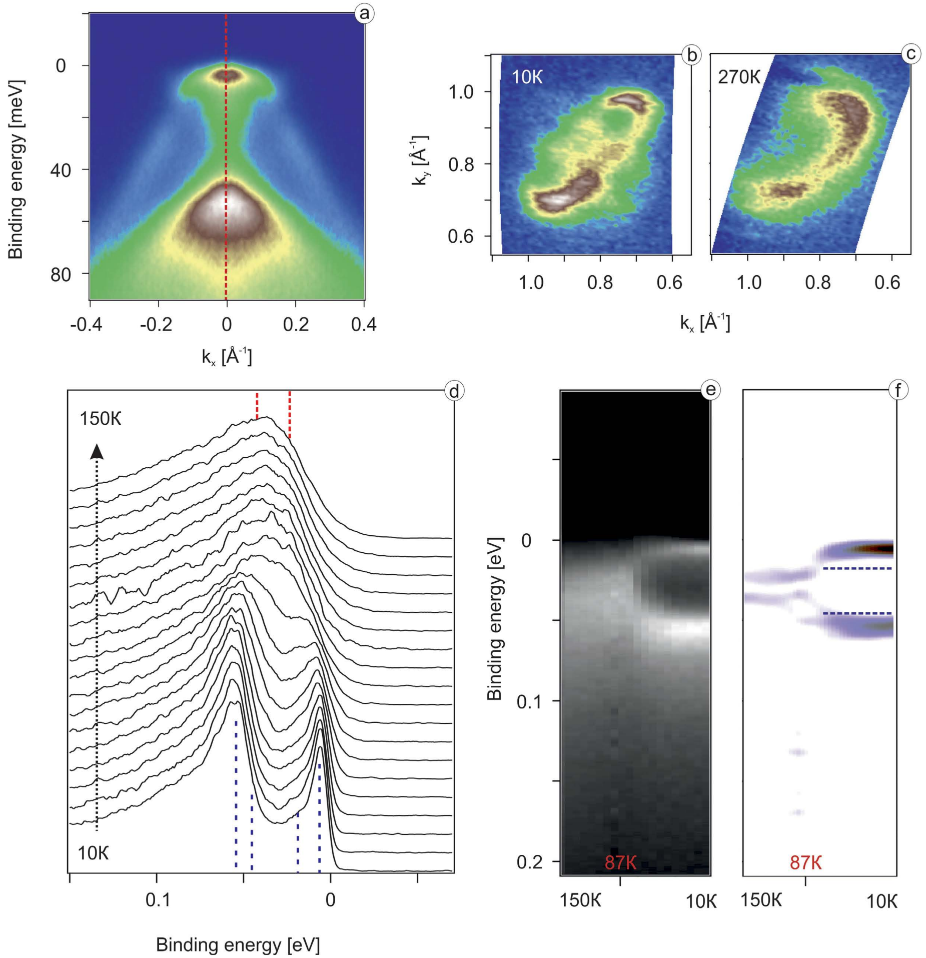


Figure 3. (**a**) High resolution ARPES data along the shortest *A*–*A* direction in vicinity of the *A* point; (**b**) high resolution ARPES derived Fermi surface in vicinity of *A* point measured with $h\nu = 28$ eV and T = 10 K; (**c**) ARPES derived Fermi surface in vicinity of *A* point measured with $h\nu = 28$ eV and T = 270 K; (**d**) EDC curves taken at the *A* point measured at temperatures from 10 K to 150 K; (**e**,**f**) color plot representation of data from panel (**d**) and its second derivative, respectively.

Effect of nematic ordering on electronic structure of FeSe

A. Fedorov[1,2,3], A. Yaresko[4], T. K. Kim[5], Y. Kushnirenko[1], E. Haubold[1], T. Wolf[6], M. Hoesch[5], A. Grüneis[2], B. Büchner[1] & S. V. Borisenko[1]

SCIENTIFIC REPORTS Published: 10 November 2016

Similar data
M. Watson, A. Coldea et al.
PRB 2016

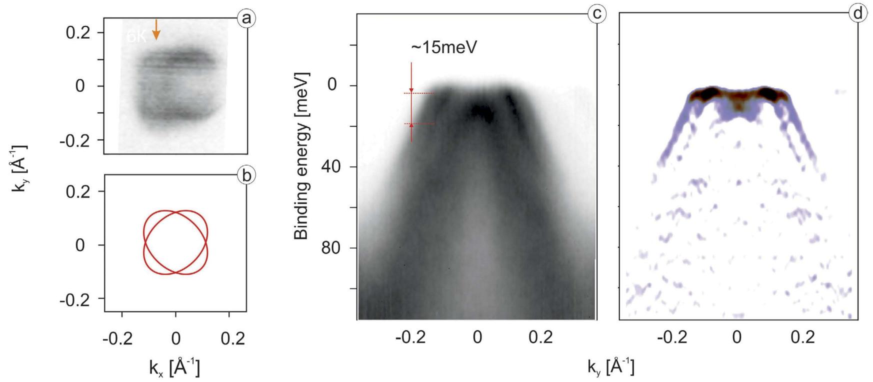


Figure 4. (**a**) High resolution ARPES derived Fermi surface in vicinity of *Z* point measured with $h\nu = 23$ eV; (**b**) cartoon of the two domain Fermi surface in vicinity of *Z* point; (**c**,**d**) high resolution energy cut along the shortest *Z*–*Z* direction at $k_x = 0.05$ Å^{-1} and its second derivative respectively.

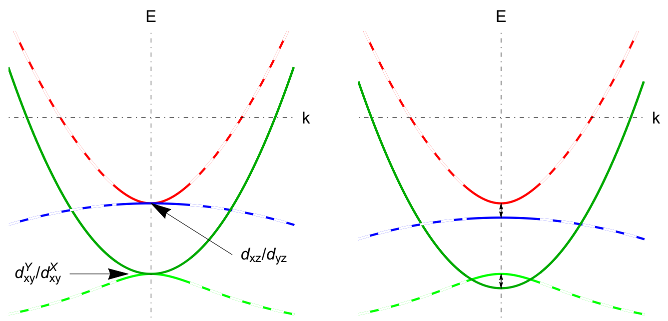
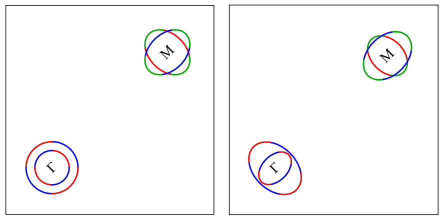


FIG. 16: The splittings in
point in the 2Fe BZ for in
fixed trajectory. The M p
coordinates and the cut is
panel – above the nematic
nematic phase. Solid and
with near-pure and mixed



Competing instabilities, orbital ordering and splitting of band degeneracies from a parquet renormalization group analysis of a 4-pocket model for iron-based superconductors: application to FeSe

Rui-Qi Xing[1], Laura Classen[2], Maxim Khodas[3], and Andrey V. Chubukov[1]

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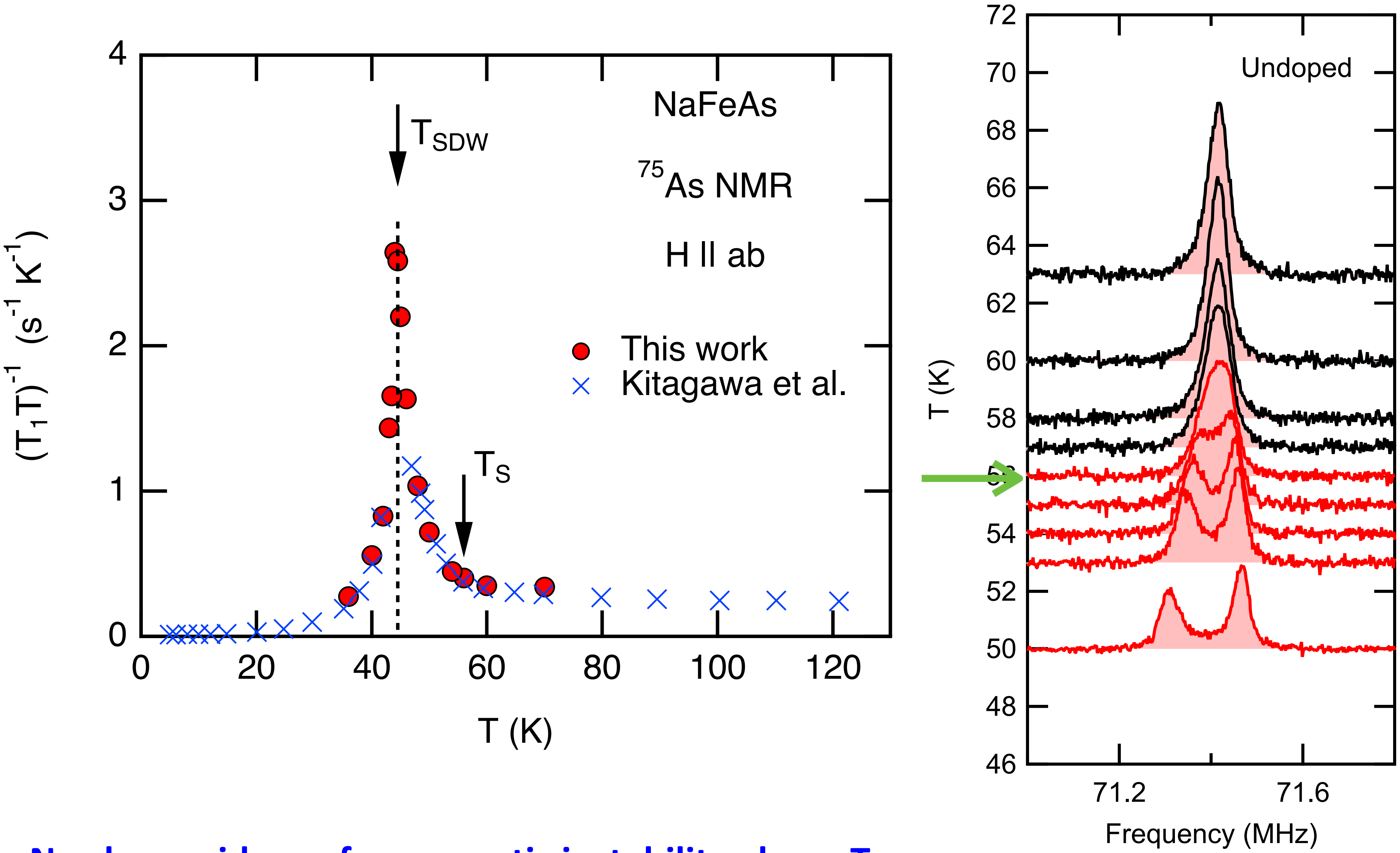
S. Baek, BB et al., Nat. Mat. 2015

Many scenarios for a "magnetic origin" of nematic order in FeSe as well as spontaneous orbital order are consistent with the NMR data!

Spin fluctuations and nematic order as seen by NMR: Striking differences between FeSe and $BaFe_2As_2$!

What about other systems?

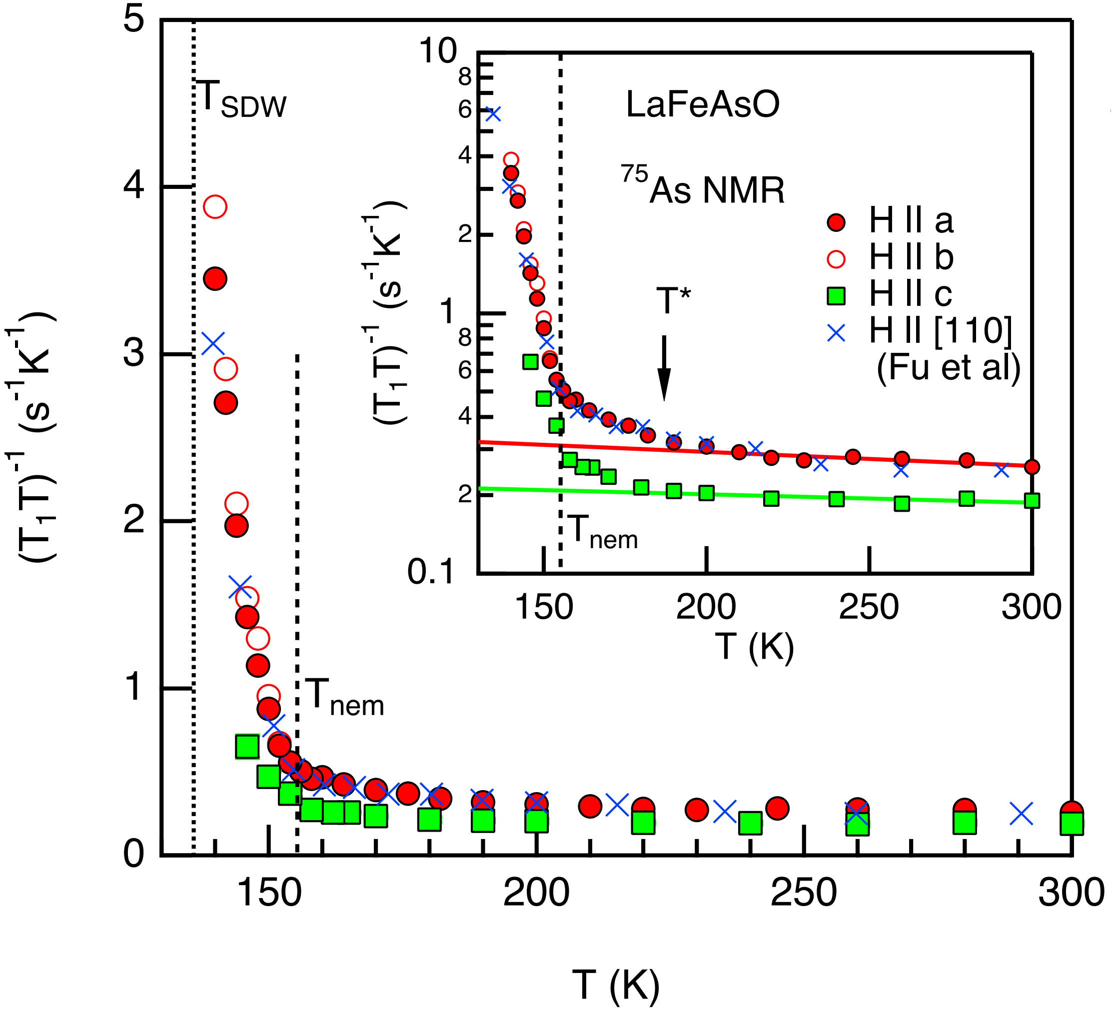
NMR on NaFeAs

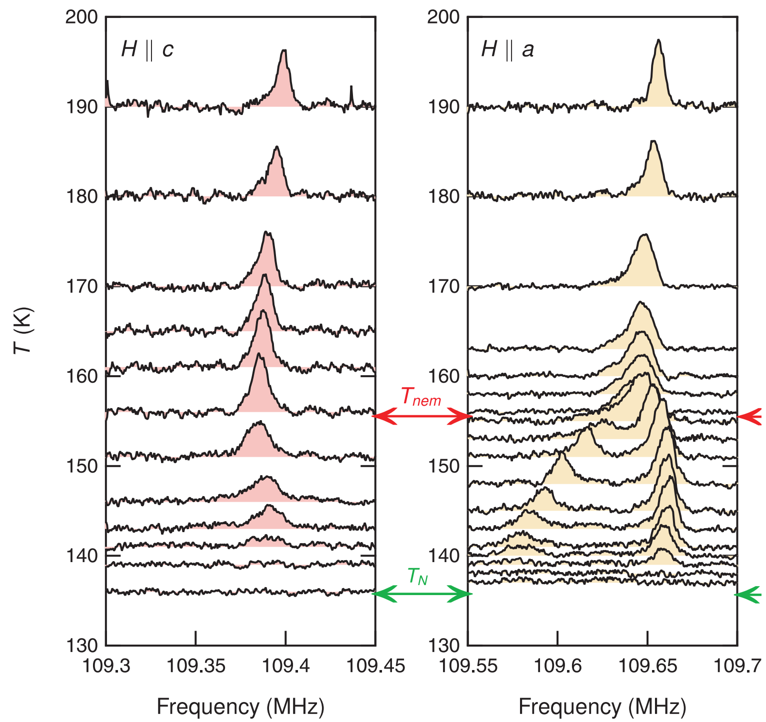


No clear evidence for magnetic instability above T_{nem}

Strong (>> FeSe) enhancement of slow spin fluctuations at T_{nem}

NMR on LaOFeAs (1111)





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Spin fluctuations and nematic order as seen by NMR: FeSe vs $BaFe_2As_2$

Scaling between lattice softening and spin fluctuations ($BaFe_2As_2$) not generic!

Weak influence of nematic order on (slow) spin fluctuations (FeSe) is an exception!

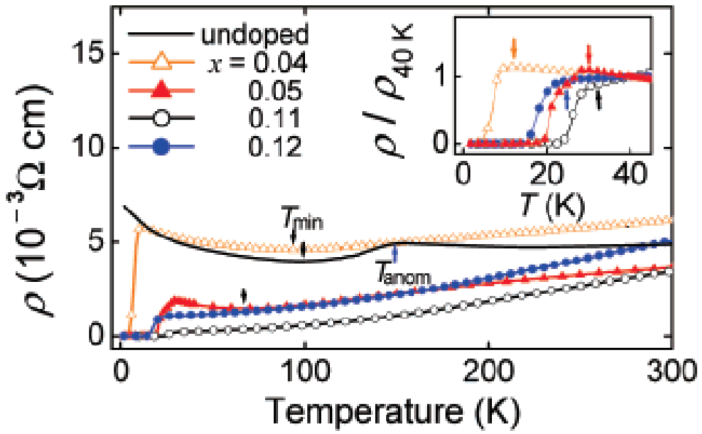
coupling between orbitals/lattice and (slow) spin fluctuations from NMR

FeSe $T_N=0$ ← $T>T_{nem}$ — **NaFeAs, LaOFeAs** $T_N < T_{nem}$ — $T<T_{nem}$ → **$BaFe_2As_2$** ($T_{nem}= T_N$) $T_N = T_{nem}$

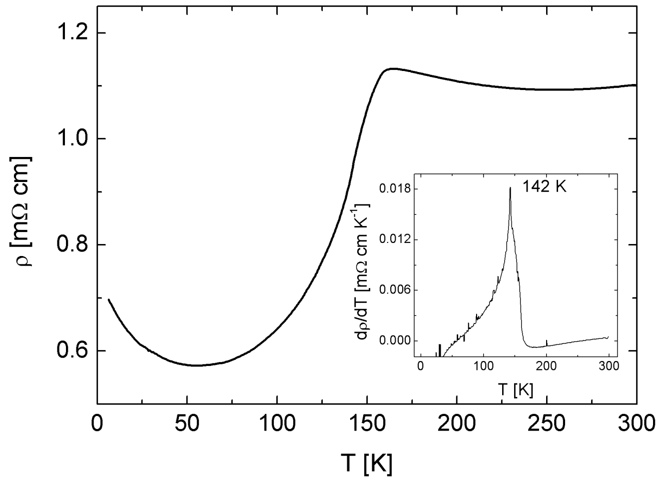
Doping "orbital-ordered systems": orbital polarons?

Most Fe based superconductors are "good metals"

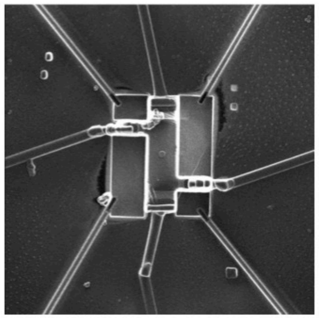
Exception: 1111 (in particular doped LaOFeAs)

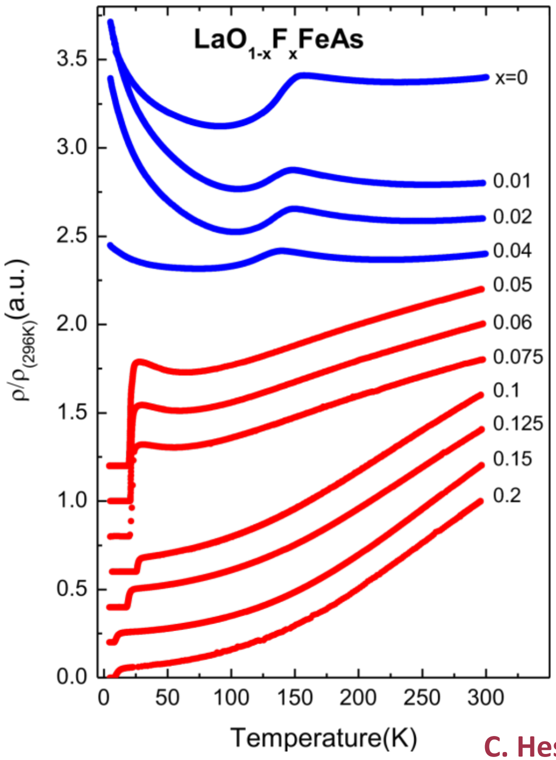


Y. Kamihara et al., J. Am. Chem. Soc. 2008



F. Caglieris, M. Fujioka et al.





C. Hess, BB et al., EPL 2009

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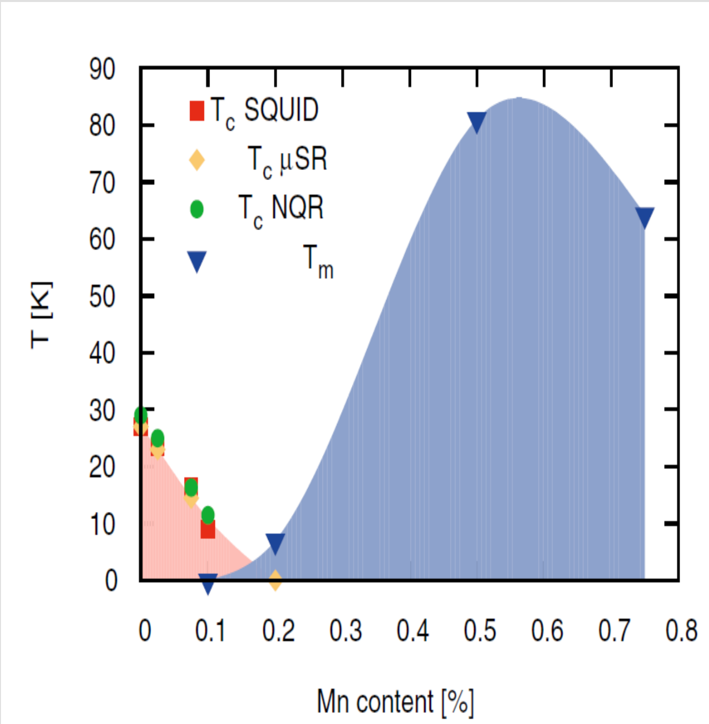
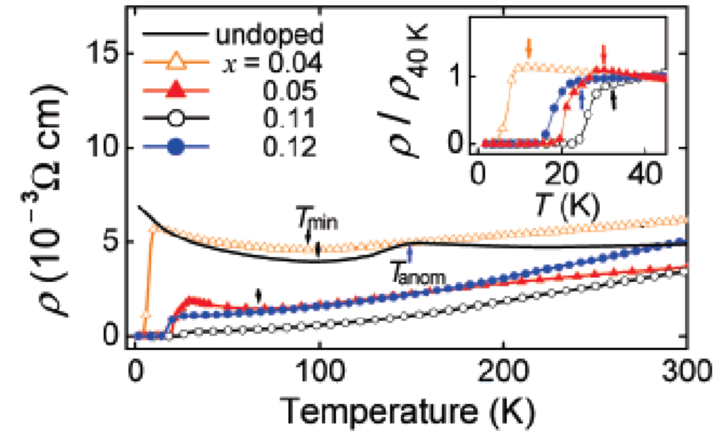
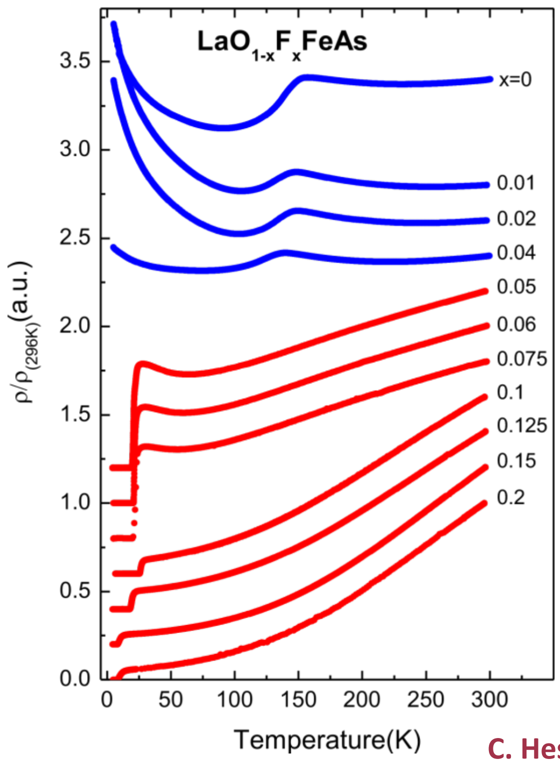


Substitution of Fe by tiny amounts of Mn
→ Drastic suppression of superconductivity

M. Sato et al. , J. Phys. Soc. Jpn. 2010
F. Hammerath, et al. Phys. Rev. B 2014
F. Hammerath et al. Phys. Rev. B 2015

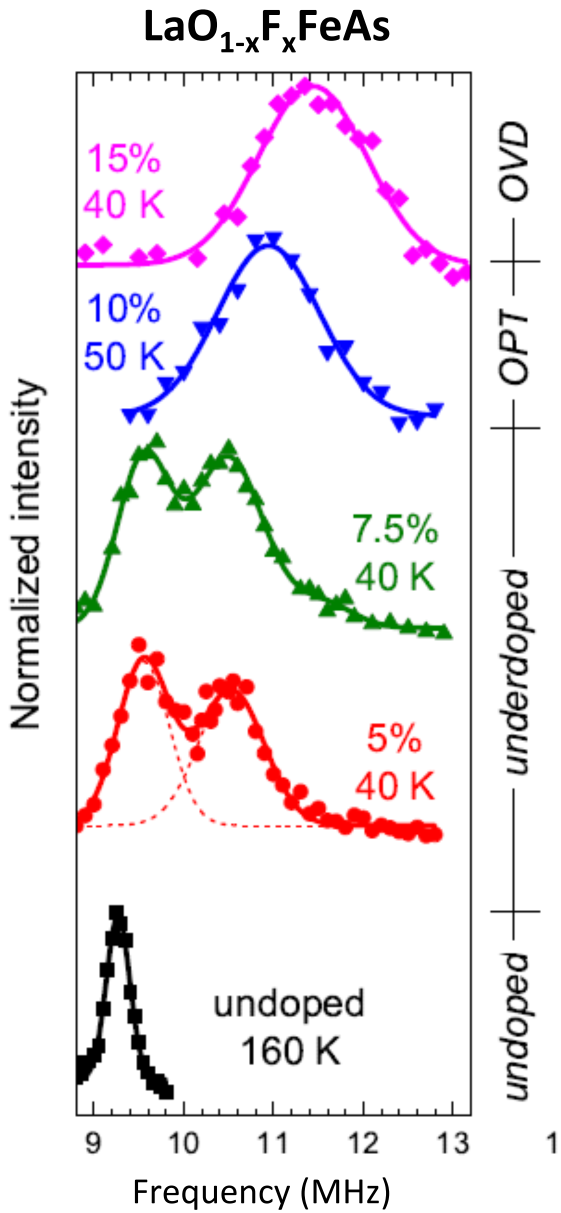


Y. Kamihara et al., J. Am. Chem. Soc. 2008

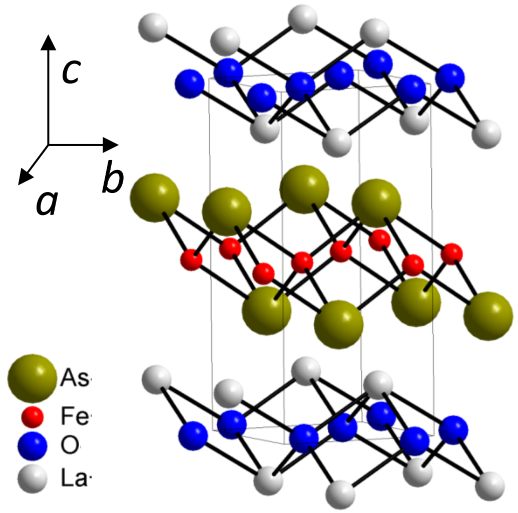


C. Hess, BB et al., EPL 2009

Doping “orbital-ordered systems”: orbital polarons?



NQR spectrum =
histogram of the electric
field gradient (at the As sites)

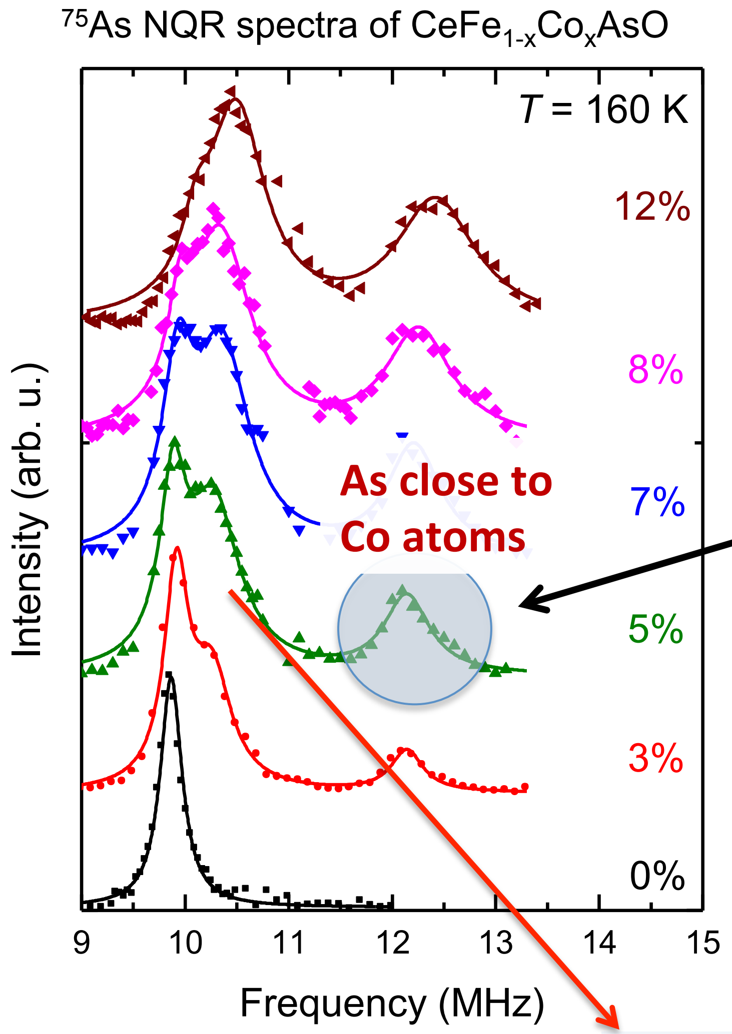


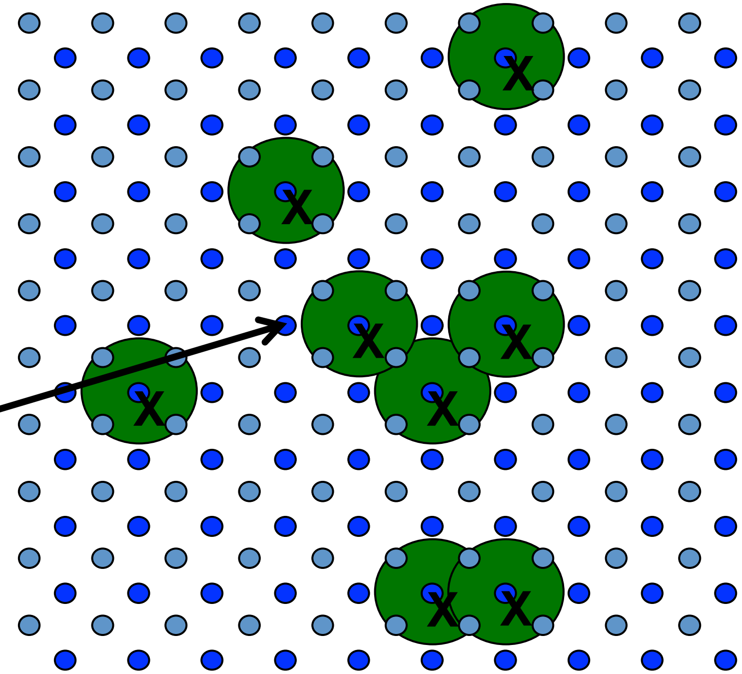
MESSAGE:
One doped electron creates „cluster“ of about
9 As sites with differnt charge/structure

Distortion due to F atoms?

G. Lang, BB et al., PRL2010

Doping “orbital-ordered systems”: orbital polarons?





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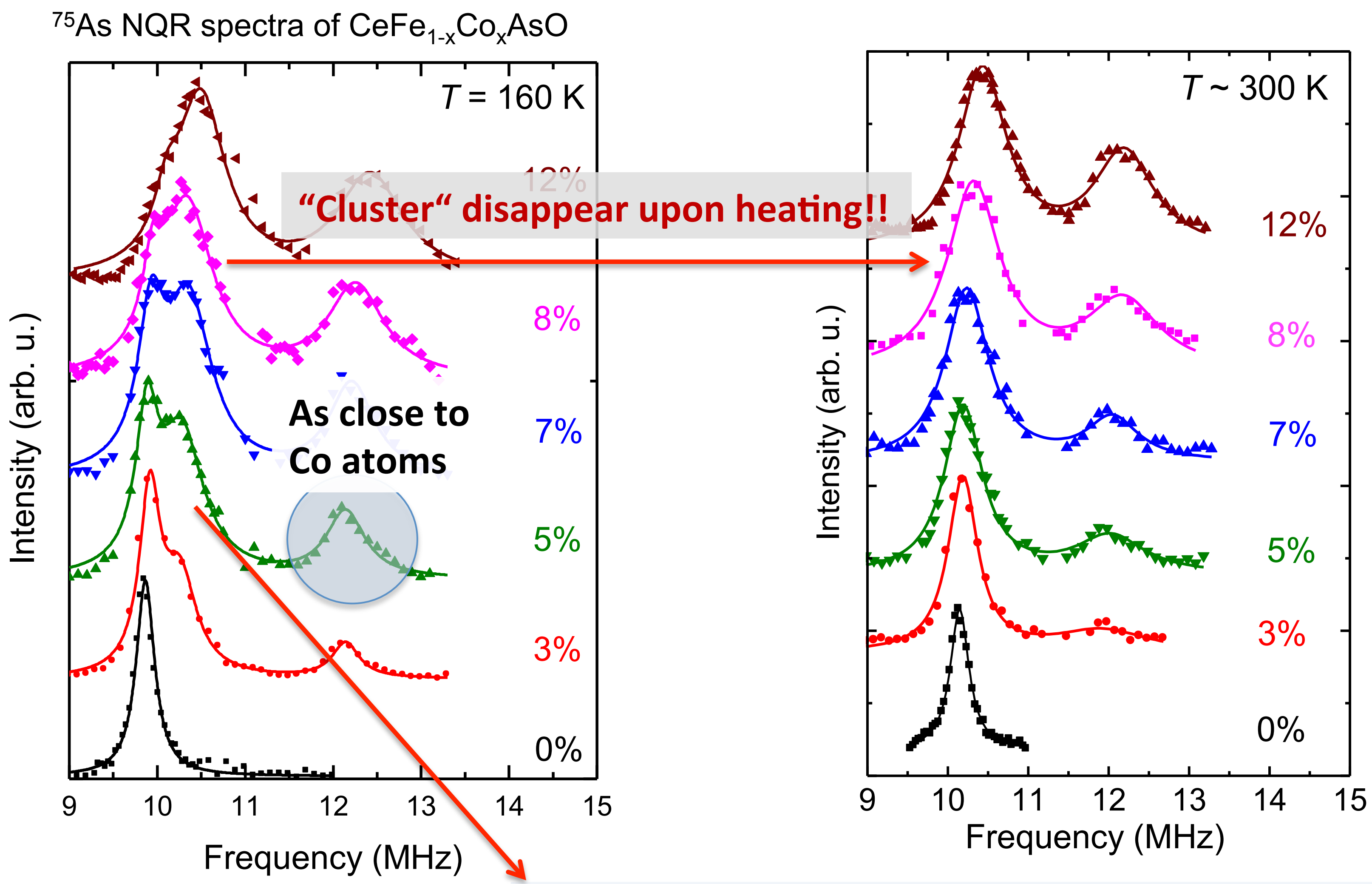
Doping “orbital-ordered systems”: orbital polarons?



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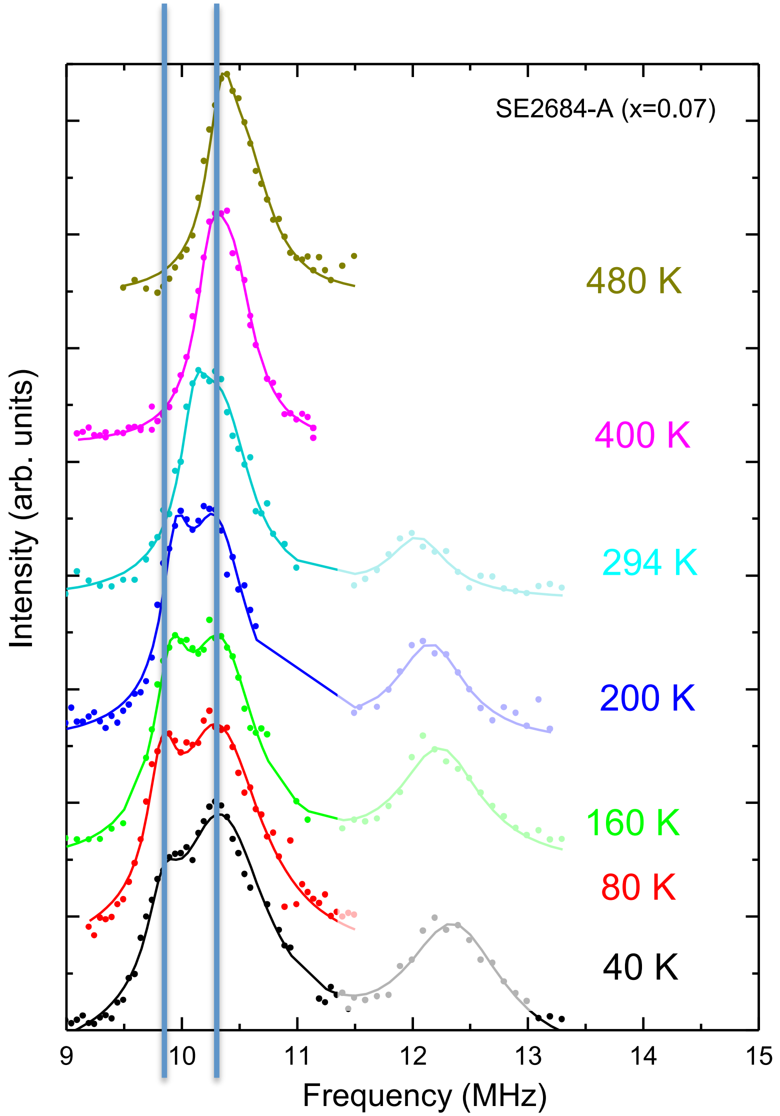
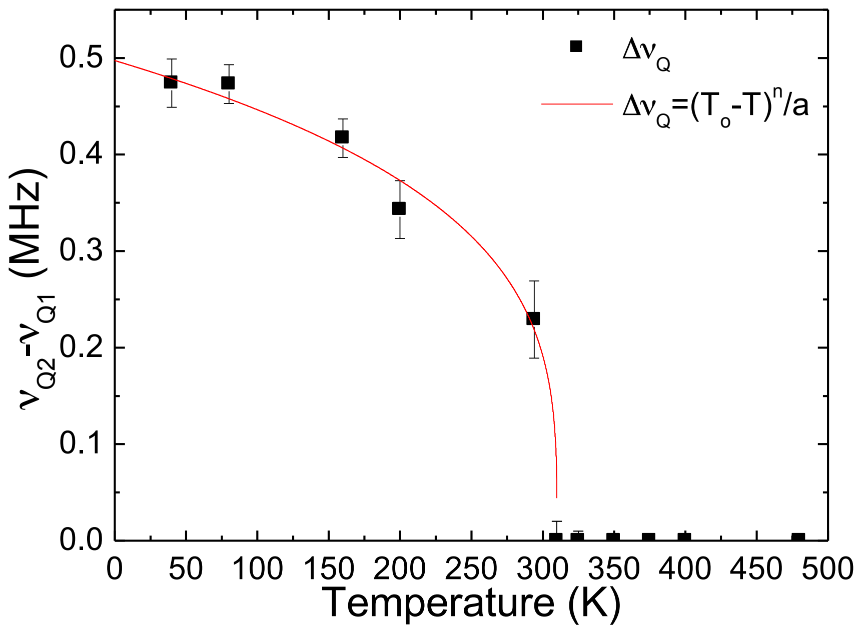
Doping "orbital-ordered systems": orbital polarons?

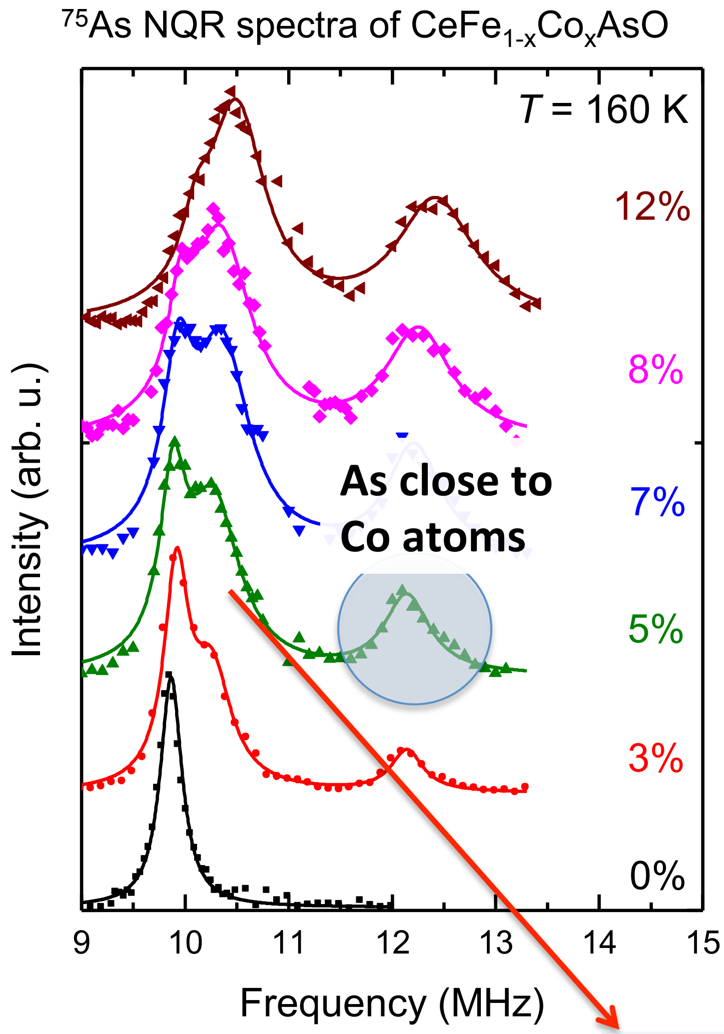


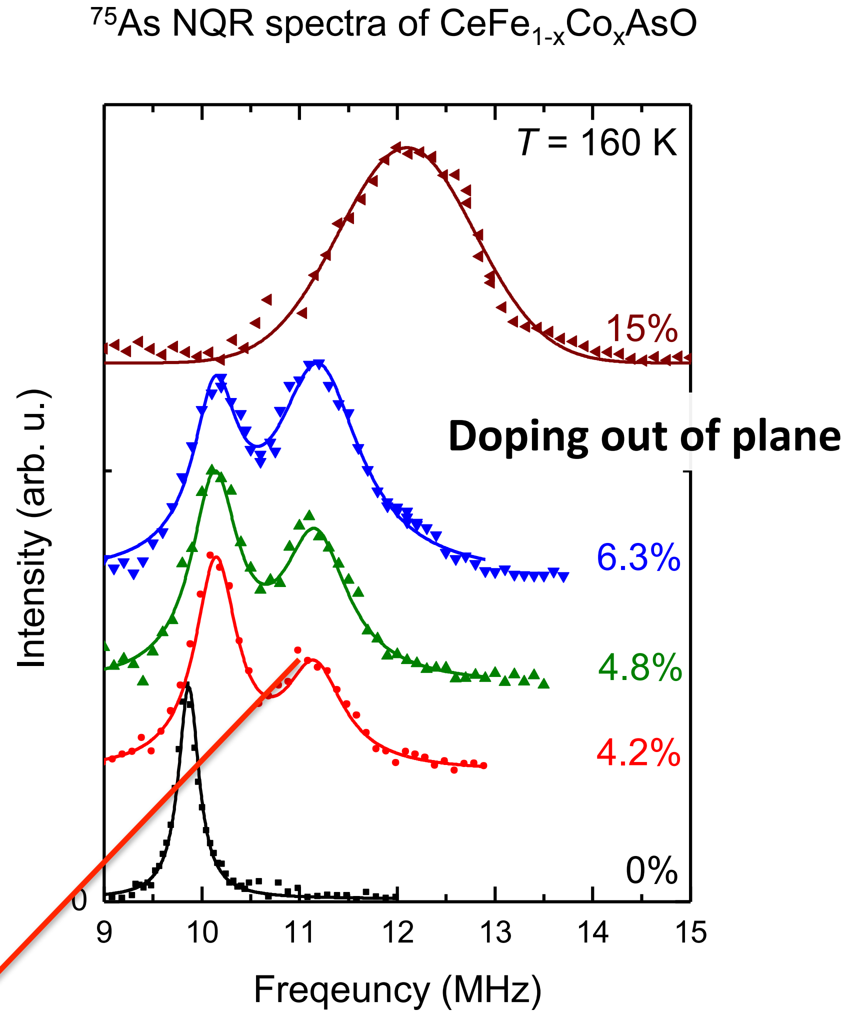
T dependence of the NQR frequency for 7% Co doped Ce1111



Splitting of the NQR lines appears below T ~ 310 K!
T dependence of the splitting: ~ order parameter of a "phase transition"!

Doping “orbital-ordered systems”: orbital polarons?

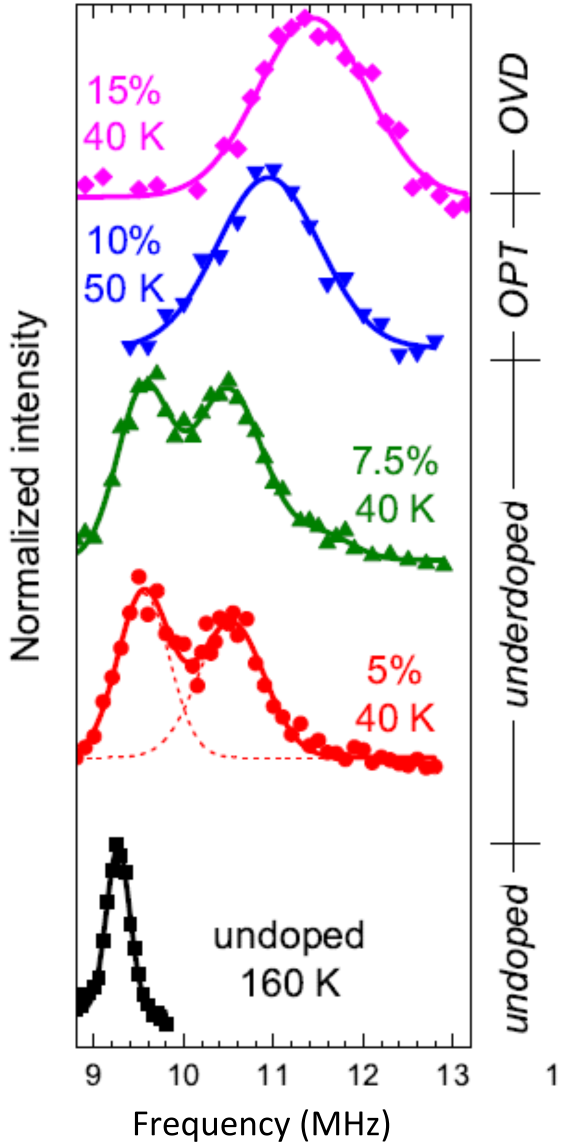




“Cluster“ disappear upon heating!!

MESSAGE:
One doped electron creates “cluster“ of about 9 As sites with differnt charge/structure

Doping “orbital-ordered systems”: orbital polarons?



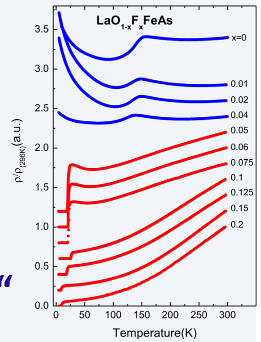
MESSAGE:

One doped electron creates „cluster“ of about 9 As sites with differnt charge/structure

Distortion NOT due to F or Co atoms!!

“Cluster“ merge at about 10 % doping

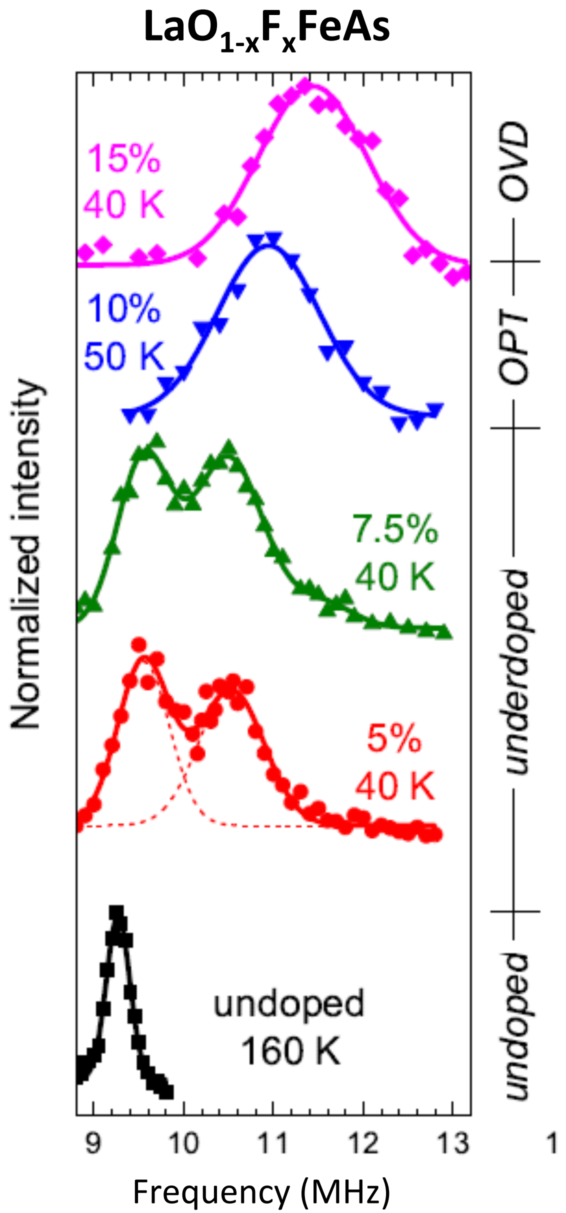
single broad line, i.e. single As site
transition “from very bad metal to metal“



Overdoped: shift of broad line with increasing x

G. Lang, BB et al., PRL2010

Doping "orbital-ordered systems": orbital polarons?



G. Lang, BB et al., PRL2010

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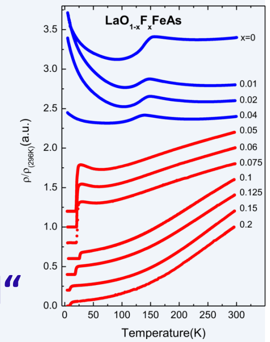
Distortion NOT due to F or Co atoms!!



"Cluster" merge at about 10 % doping

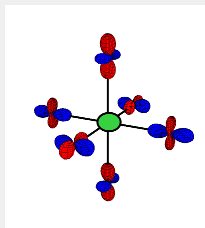
single broad line, i.e. single As site
transition "from very bad metal to metal"

Overdoped: shift of broad line with increasing x

Similar behavior in manganites, cobaltates etc.

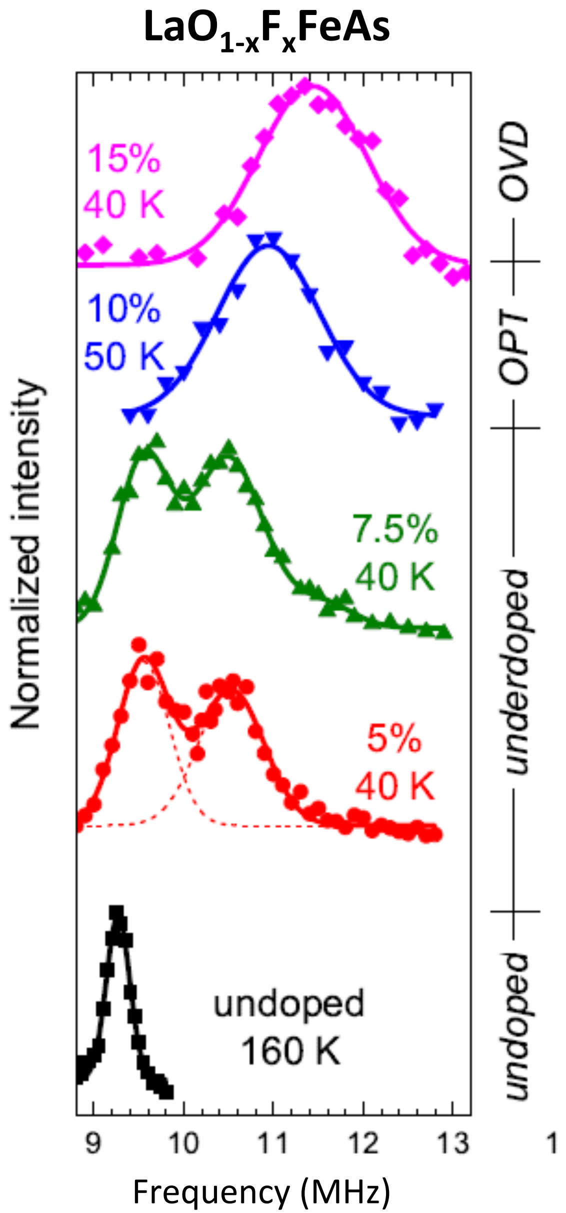
Attributed to "Orbital Polarons"
Charge polarizes local orbital structure

- **inhomogenous charge, structure**
- **inhomogenous magnetism**
- **metal insulator transition when polarons merge**
- **...**



orbital polaron

Doping “orbital-ordered systems”: orbital polarons?



G. Lang, BB et al., PRL2010

MESSAGE:
One doped electron creates “cluster“ of about 9 As sites with differnt charge/structure

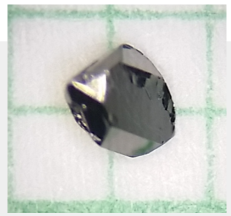
QUESTIONS:

Are 1111-type Fe-based SC (more or less) itinerant systems with “orbital physics“ (charge <-> spin <-> lattice) ?

Are the interactions/dynamics leading to “clusters“ in 1111 also important for properties of other Fe-based SC?

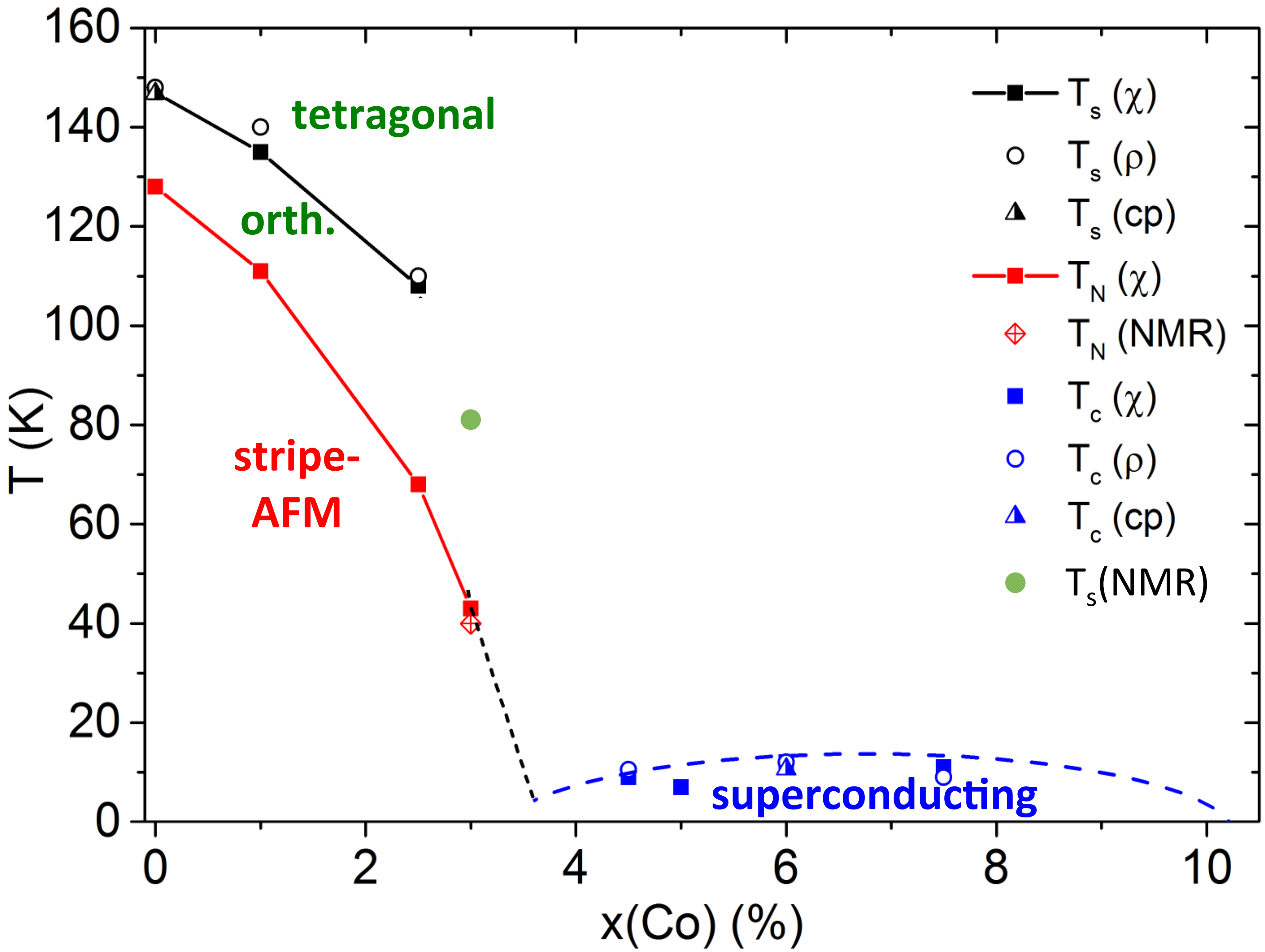
Is there any connection to SC?
(T_c up to 58K in inhomogeneous 1111-type systems)

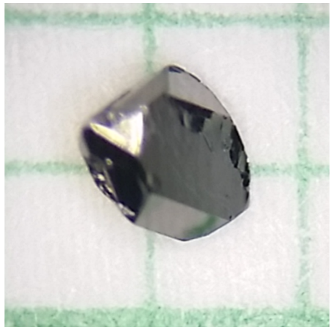
CHALLENGES & work in progress:



Improving size and quality of crystals !!
→ sophisticated experiments to study “clusters“ (STM etc.)
→ better knowlege & understanding of local structure

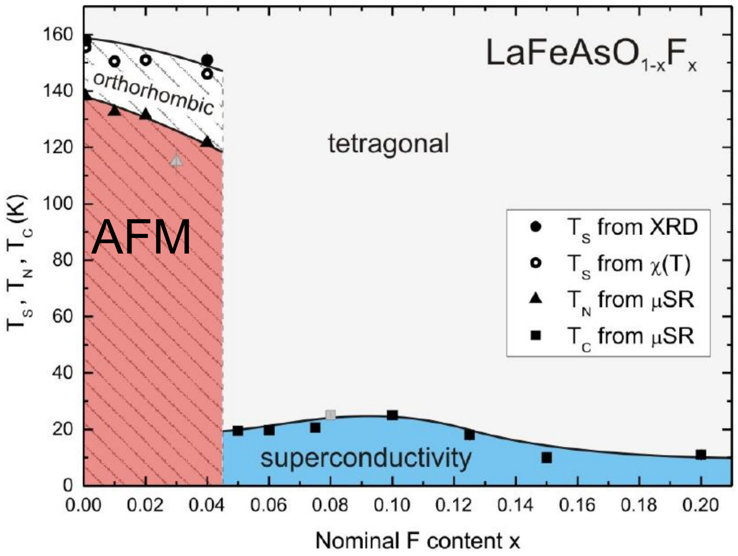
Phase diagram of Co-doped La 1111 revisited …



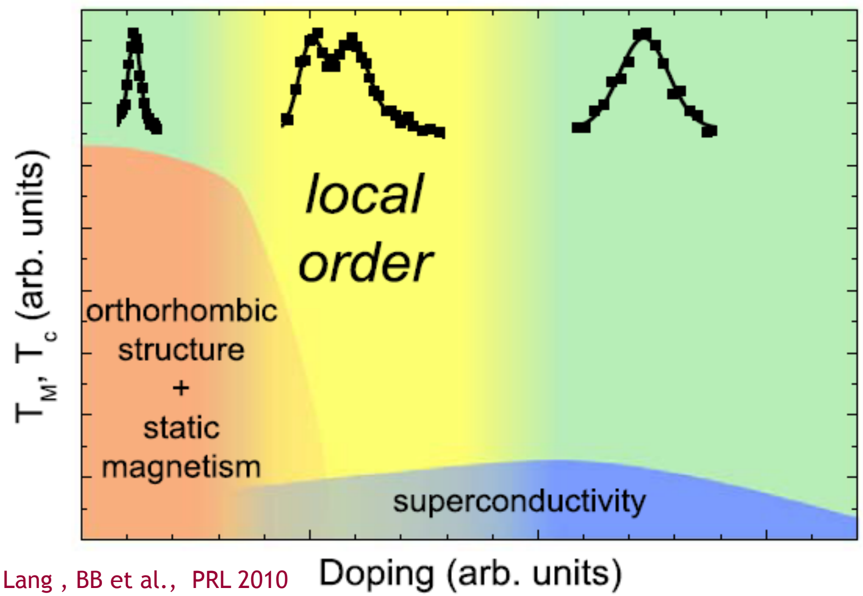


Different phase diagrams: Consequences of charge/orbital polarons

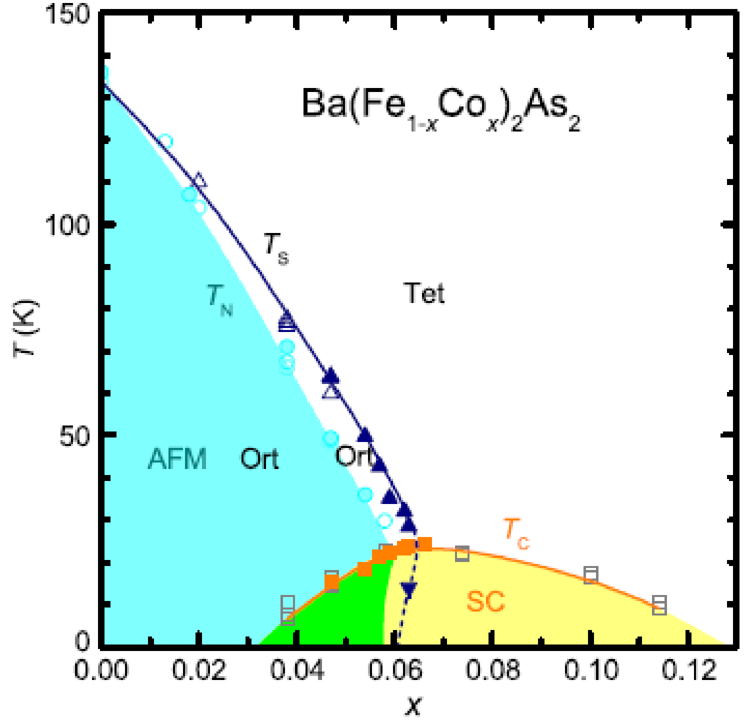
Apparent difference of phase diagrams of 1111 and 122 system



Luetkens , BB et al., Nature Materials **8**, 305 (2009)

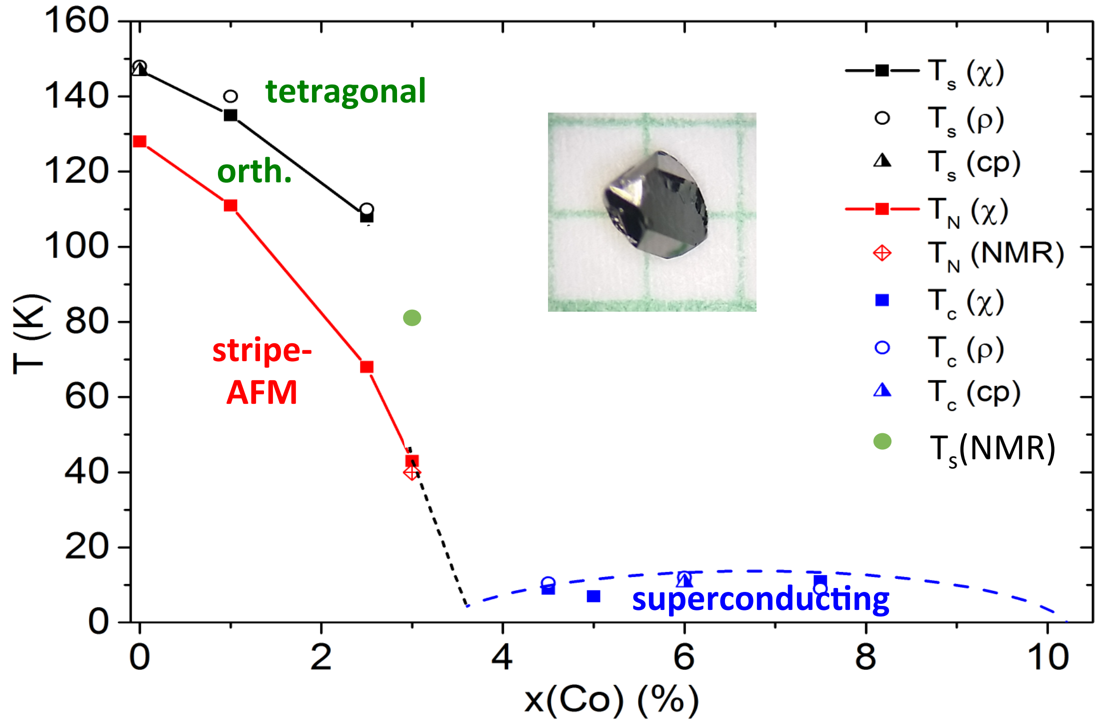


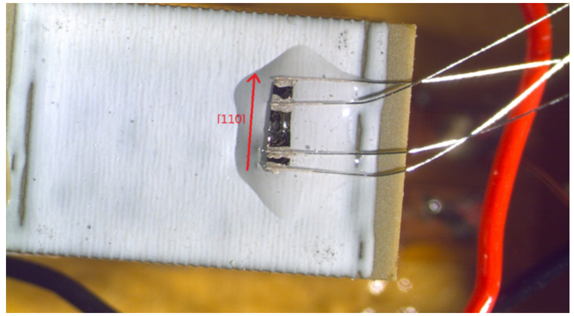
G. Lang , BB et al., PRL 2010

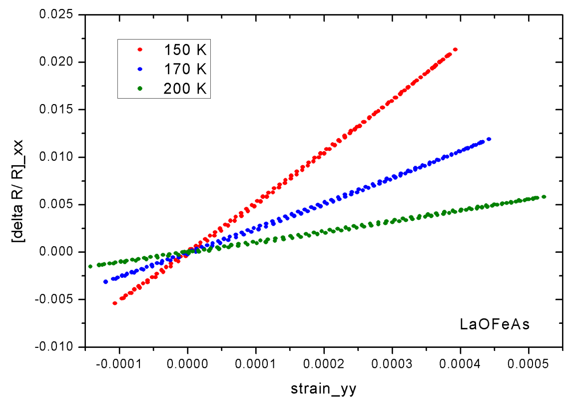


e.g. Nandi et al., Phys. Rev. Lett. (2010)

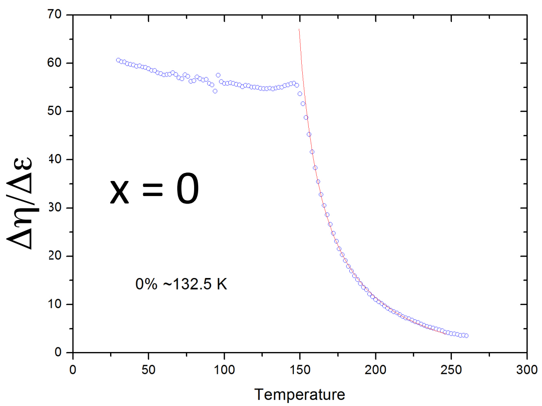
“Electronic nematicity in Co-doped La 1111 …“

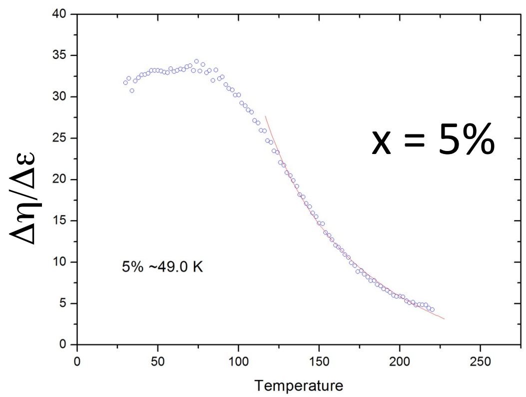


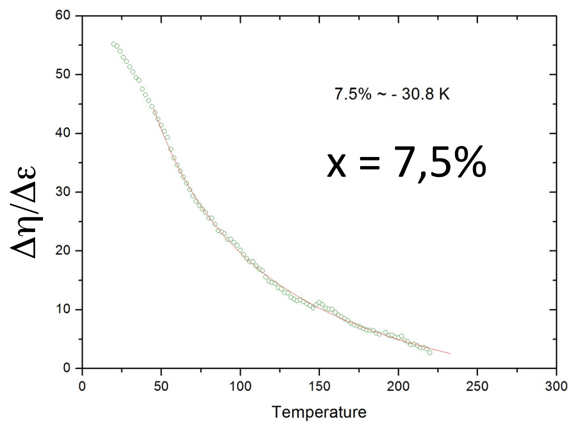




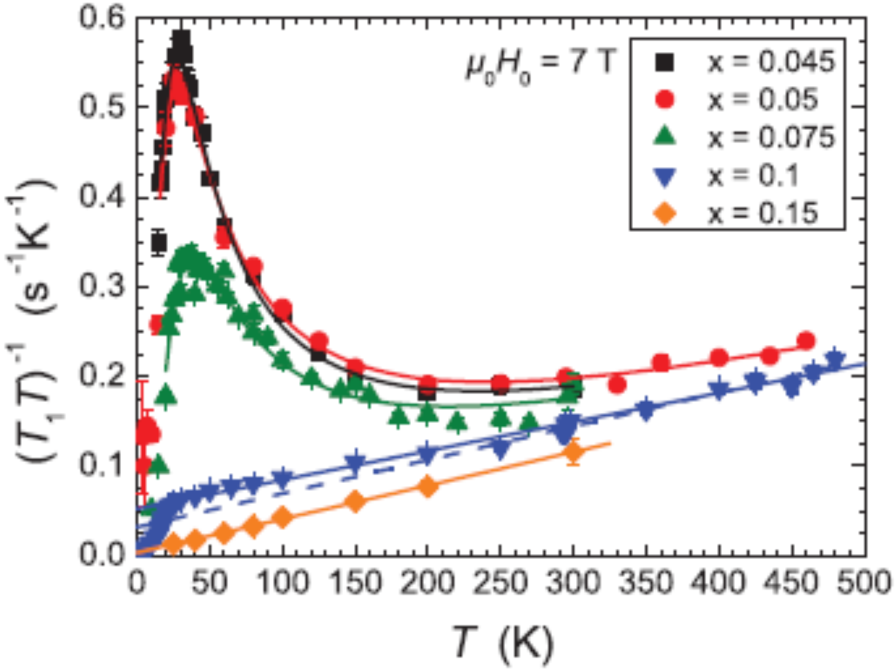
Strain dependence of the resistance of Co doped La-1111: nematic susceptibility

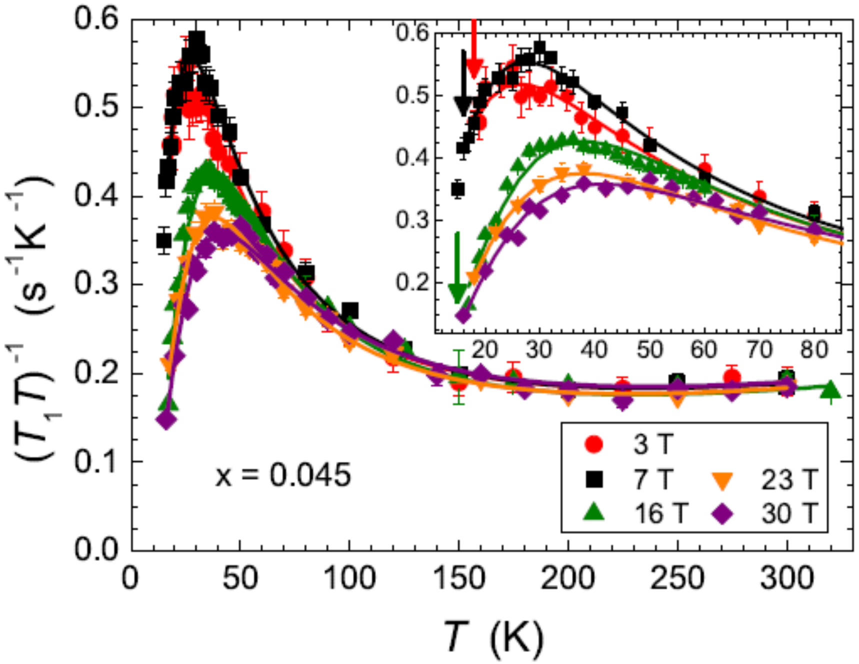




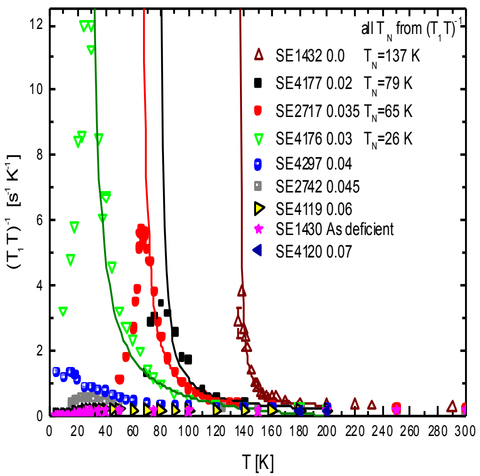


Slowing down of spin fluctuations in F doped La 1111

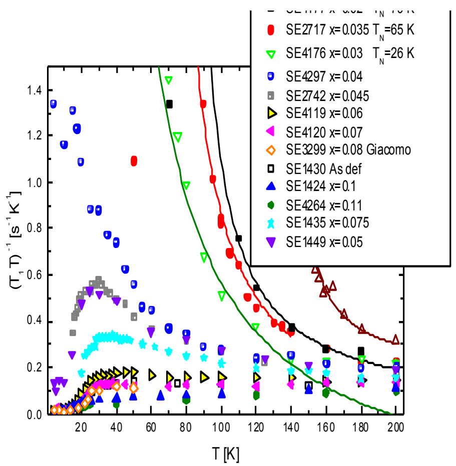




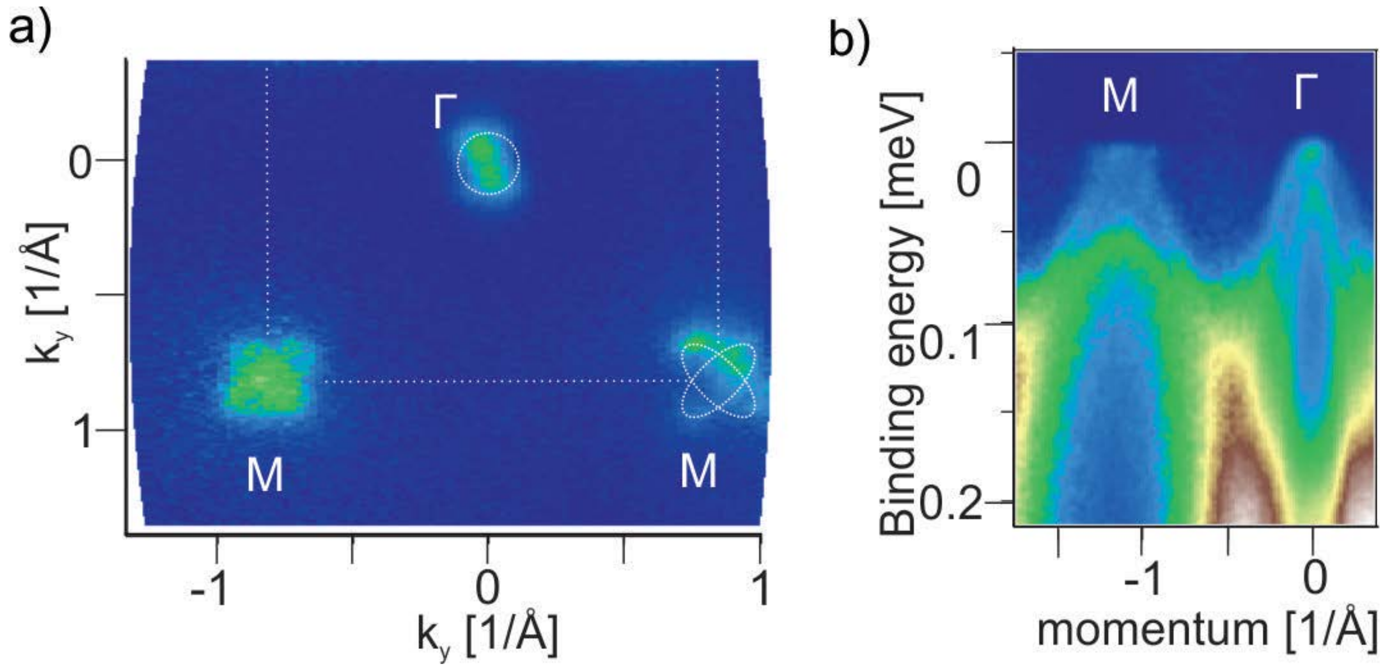
F. Hammerath, P. Caretta, BB et al., PRB 2013



work in progress



T dependent electronic structure: “red/blue shift“



FeSe

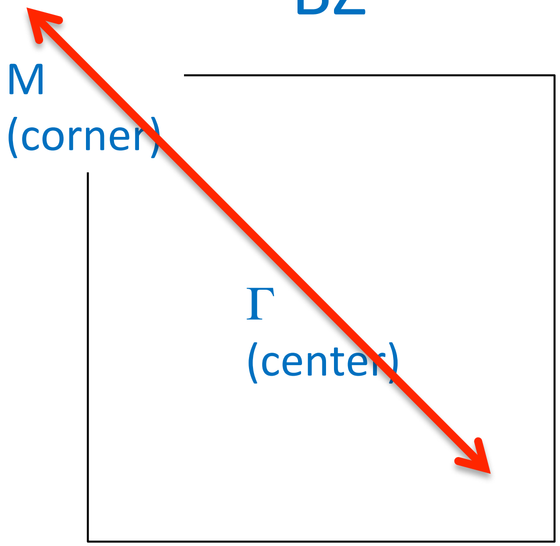
Well established: **very small hole and electron pockets in FeSe**
strong deviation from DFT

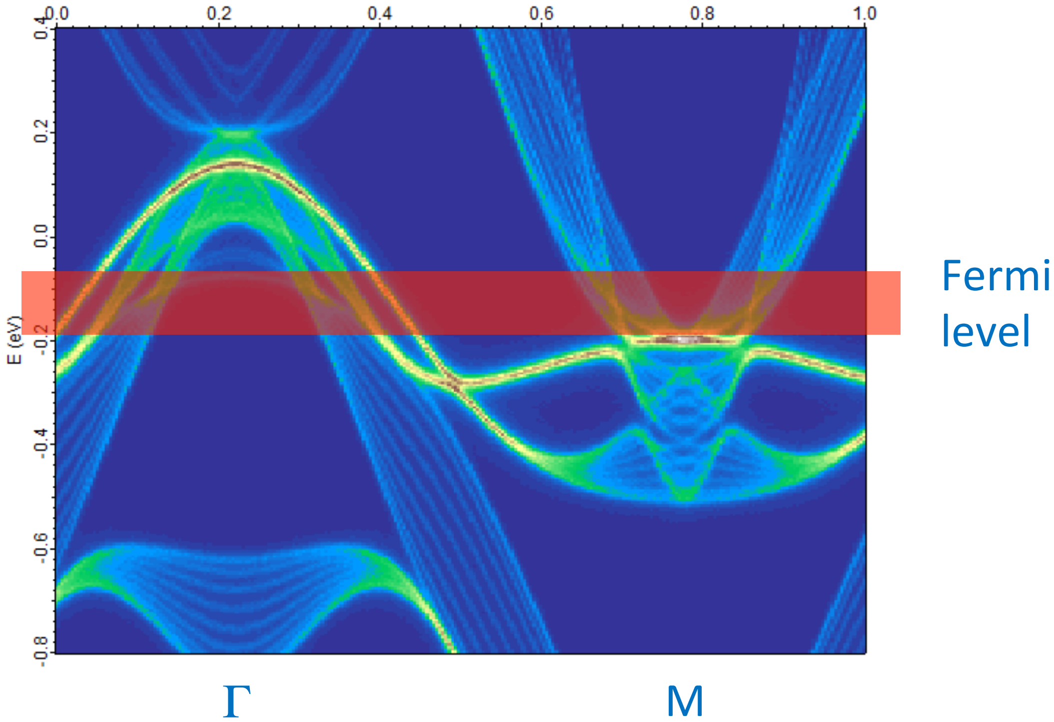
Anomalous temperature evolution of the electronic structure of FeSe

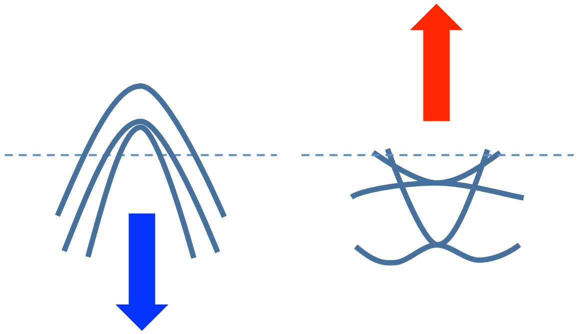
Y. Kushnirenko [1], A. A. Kordyuk [2,3], A. Fedorov [1,4], E. Haubold [1], T. Wolf [5], B. Büchner[1] and S. V. Borisenko [1]

From DFT to ARPES

BZ





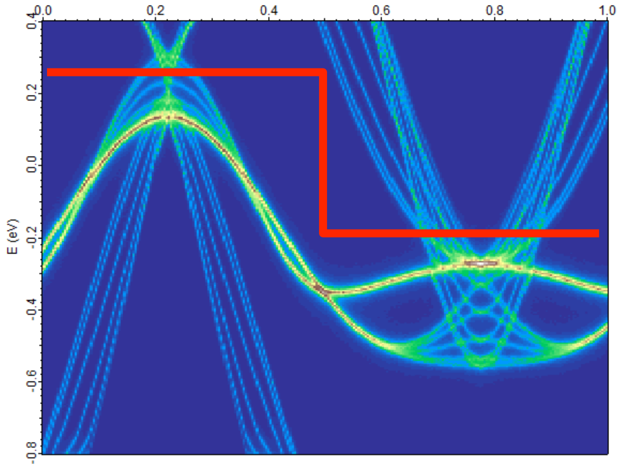


red/blue shift in Fe based SC

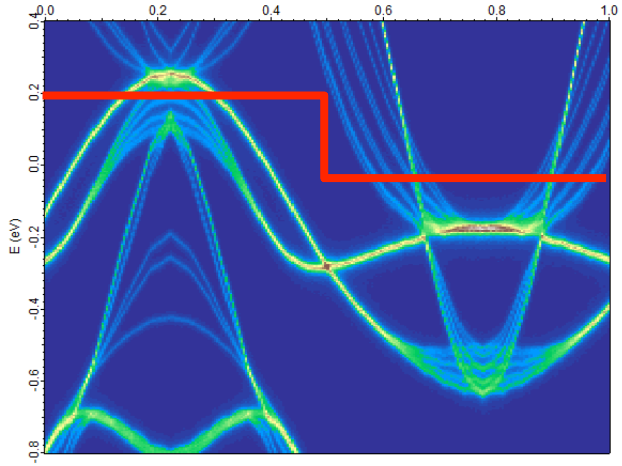
Courtesy of S. Borisenko

red/blue shift in Fe based SC

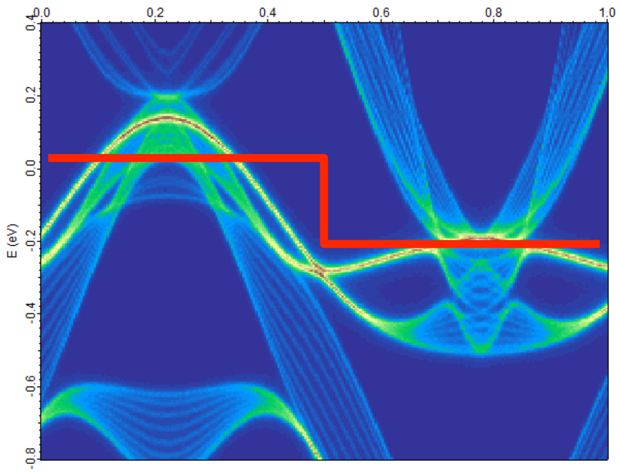
11



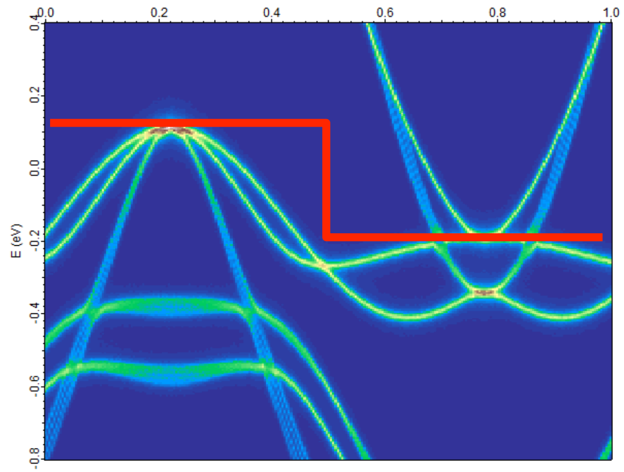
111



122

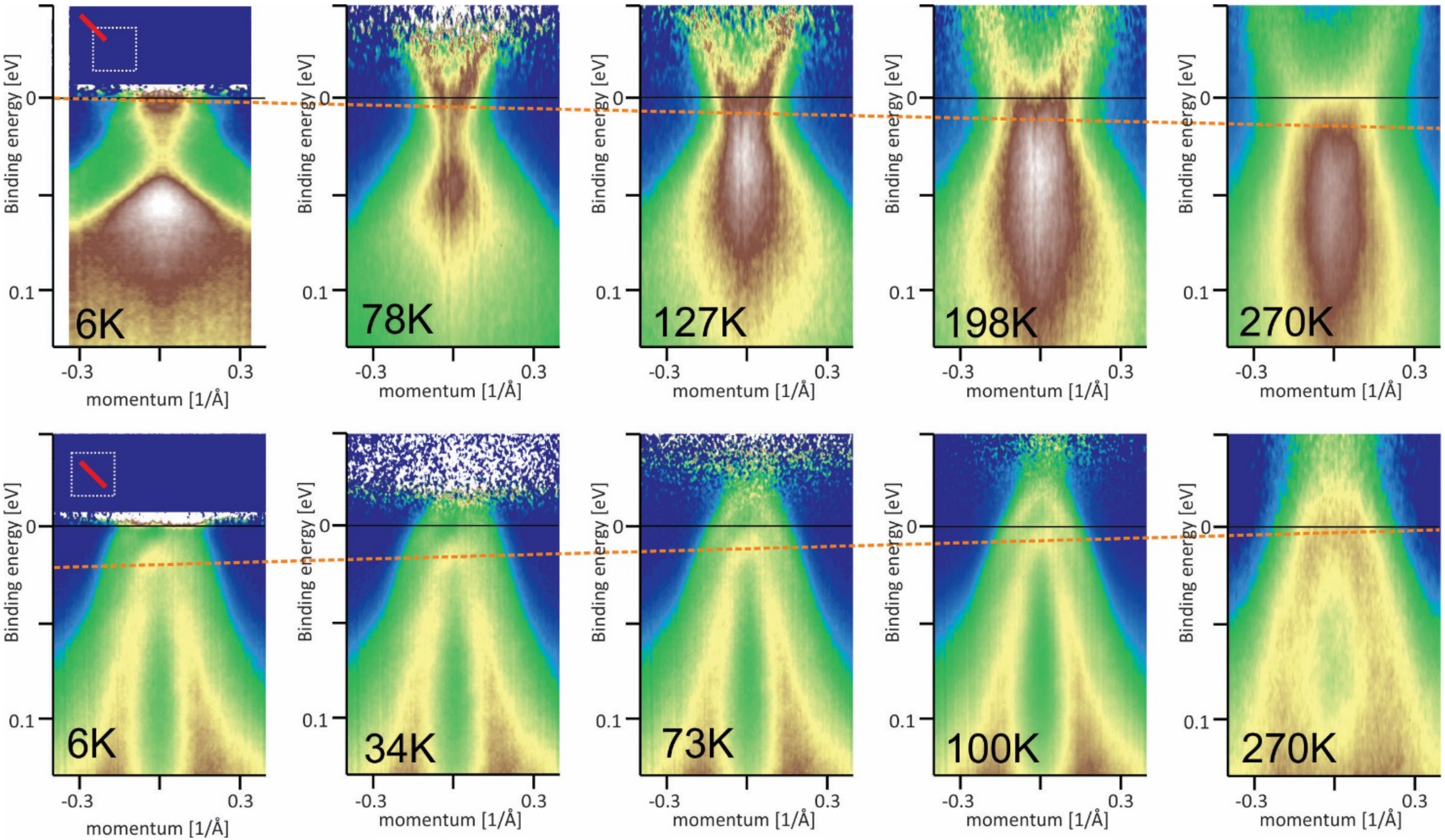


1111



Courtesy of S. Borisenko

T dependent electronic structure: Back to DFT



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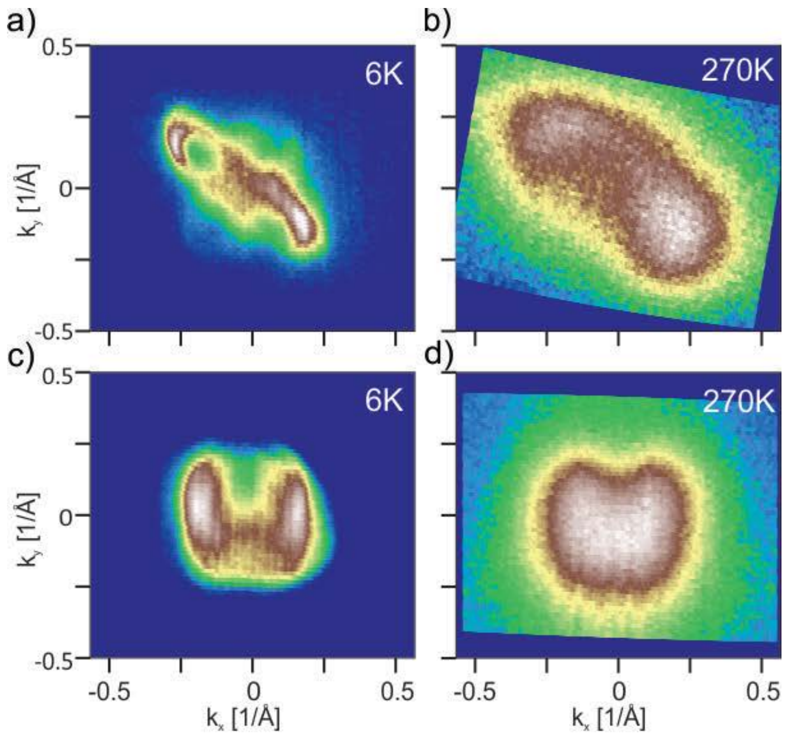

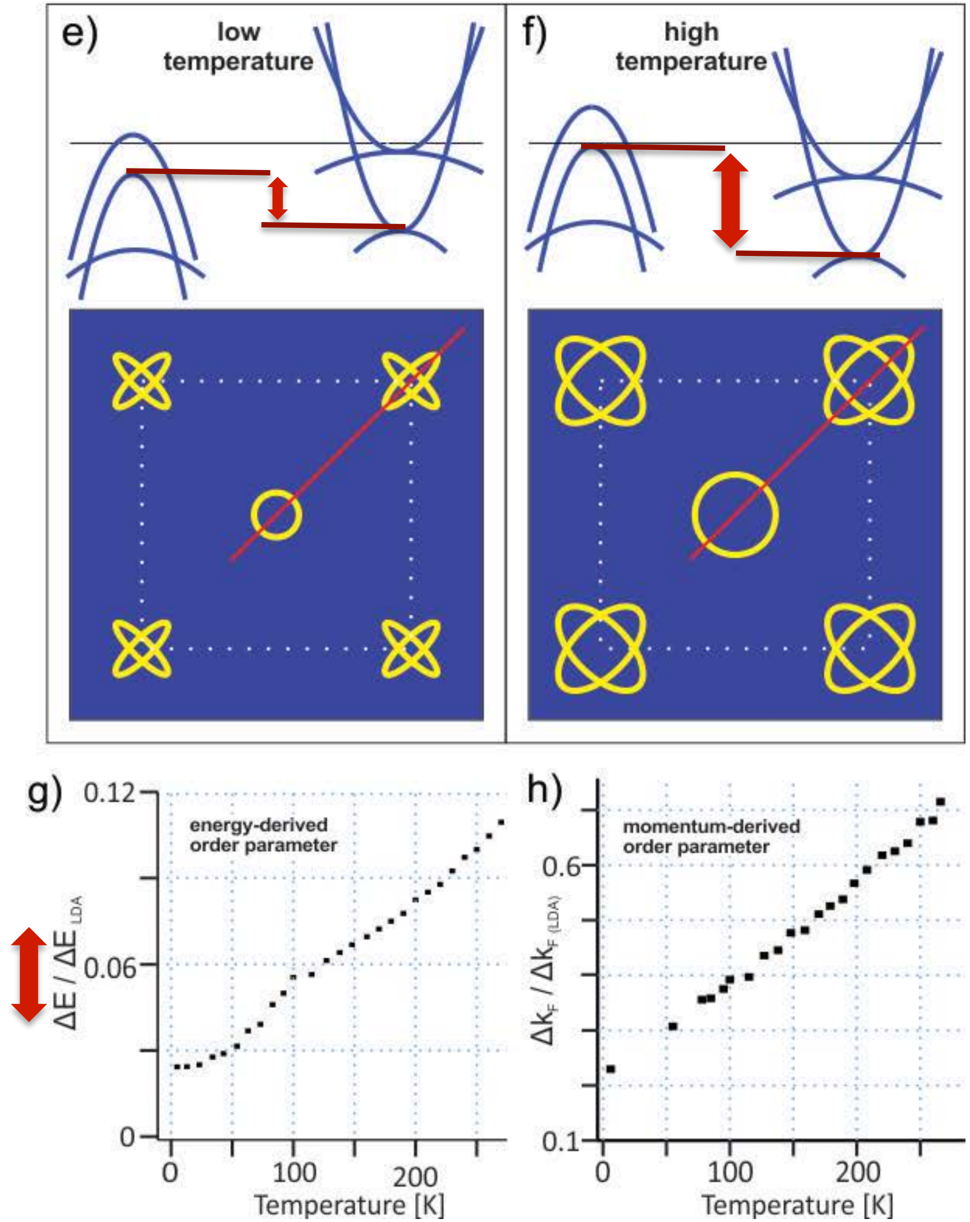

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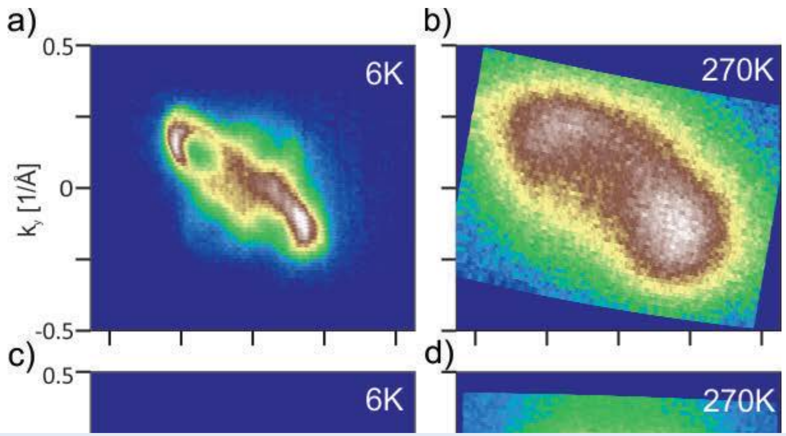
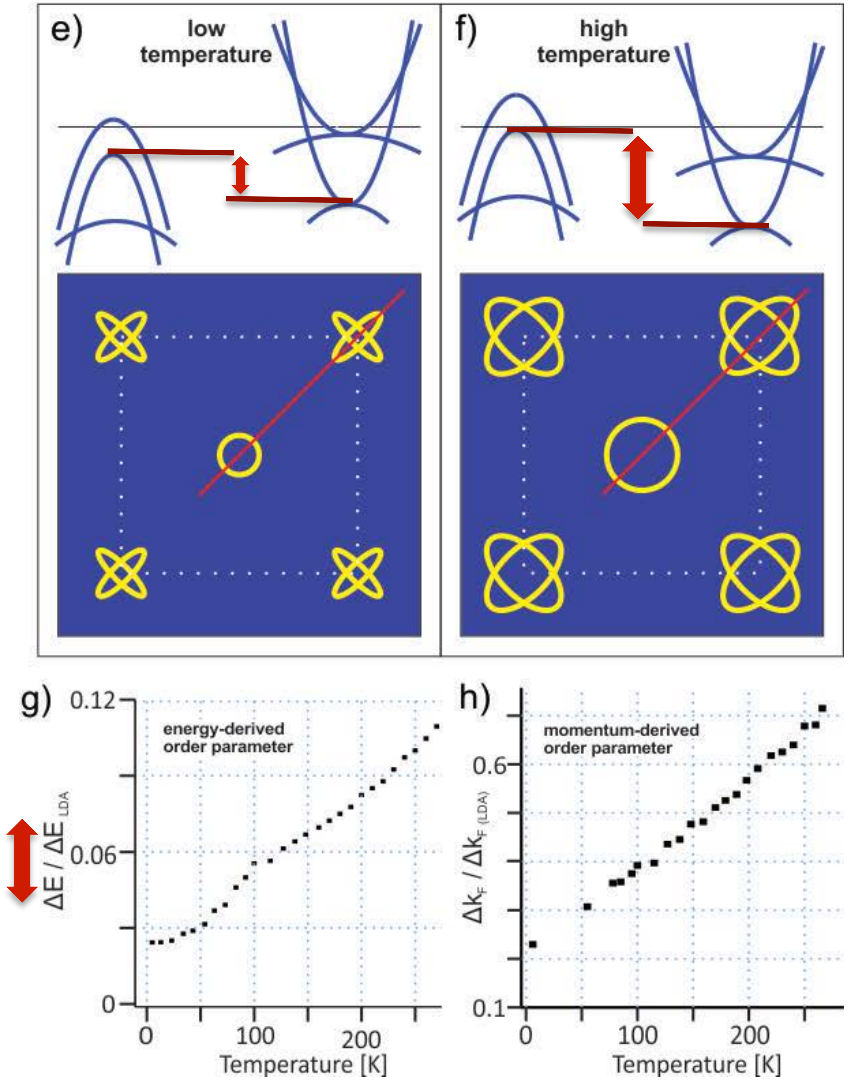




Questions & Challenges

Theory, discriminate between scenario(s)?

s+- Pomeranchuk (Lee et al, Chubukov et al.)
interpocket spin fluctuations (Benfatto et al.)
nematic fluctuations (Mazin et al.)
etc.

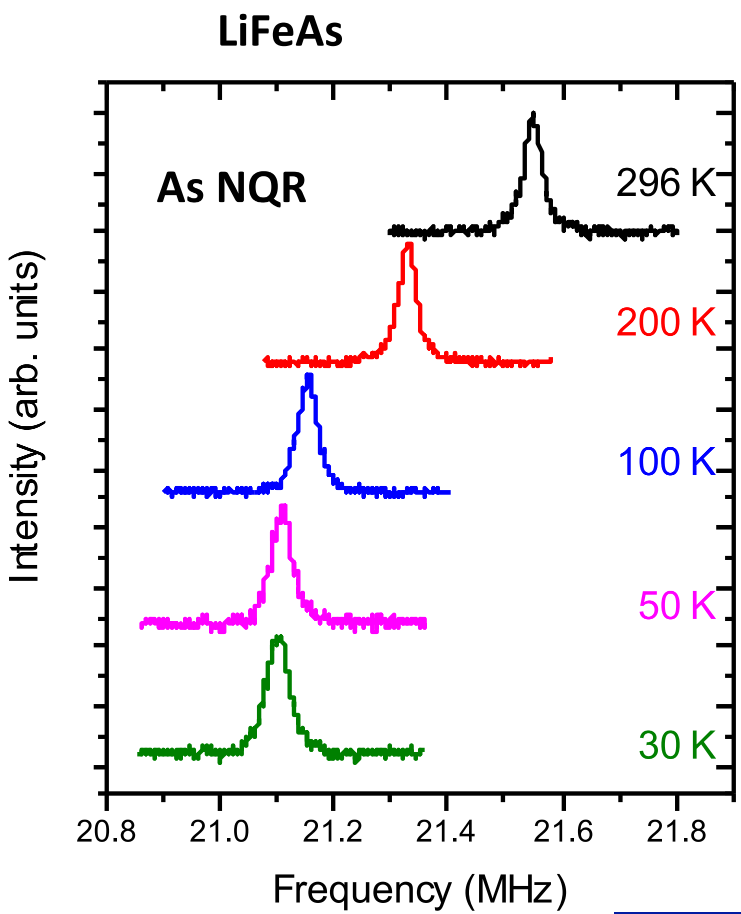
FeSe or generic for Fe- based SC?

work in progress …

Relationship to other physical properties?

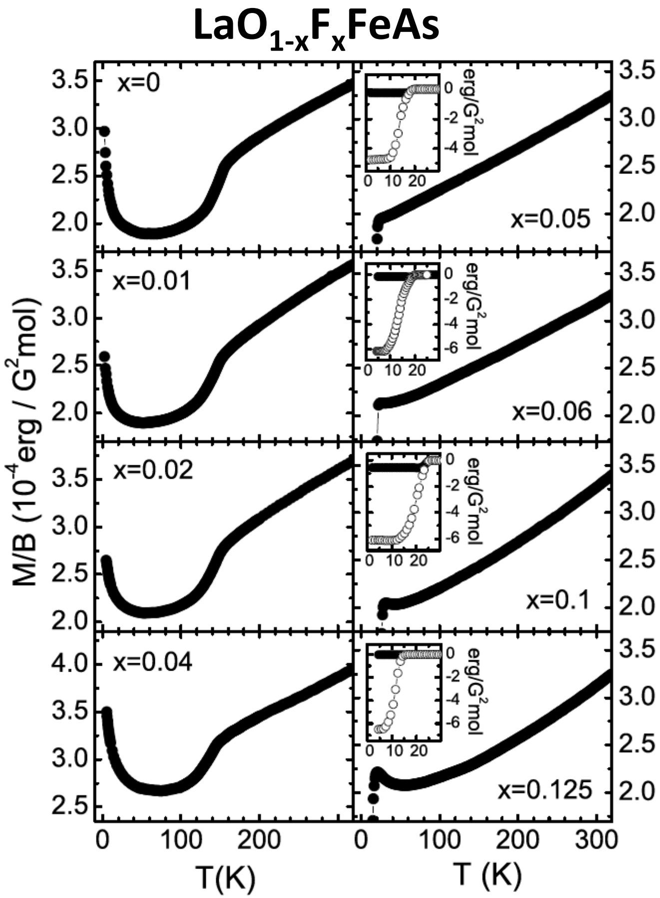
er[1] and S. V. Borisenko [1]

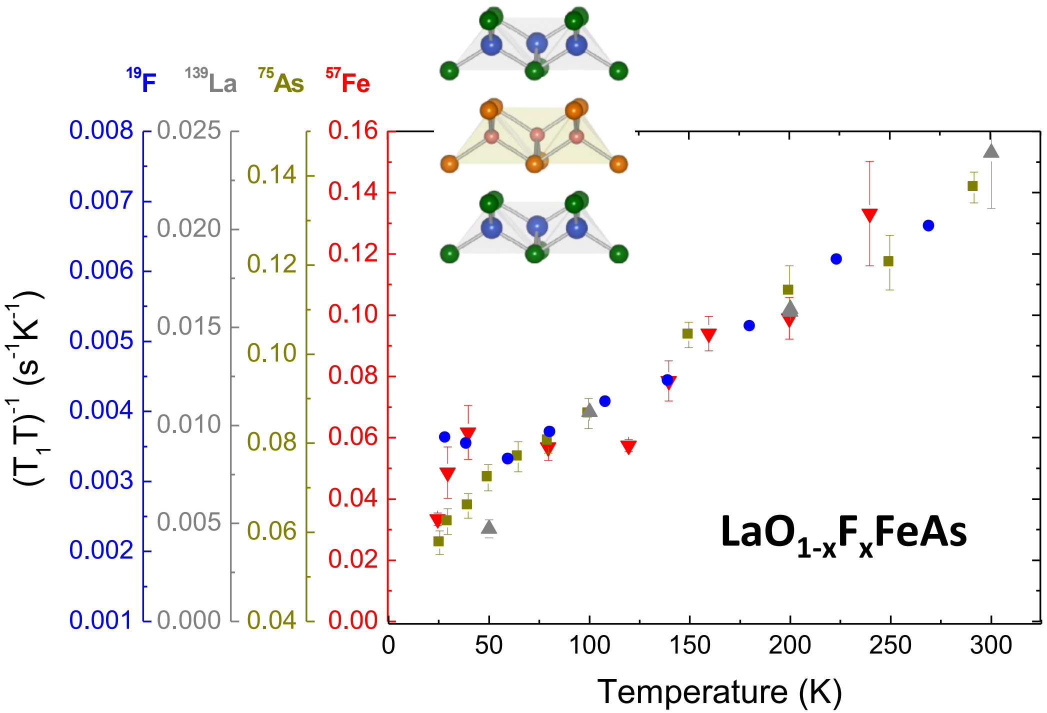
T dependent electronic structure: Back to DFT
Relationship to anomalous change of local structure?



Large T dependent changes of As NQR frequency seen in many Fe-based SC (1111, 122, 111…)
NQR frequency: electrical field gradient at the As nucleus
Signature of changes in mean Fe orbitals?

T dependent electronic structure: Back to DFT
Relationship to increase of magn. susceptibility χ?





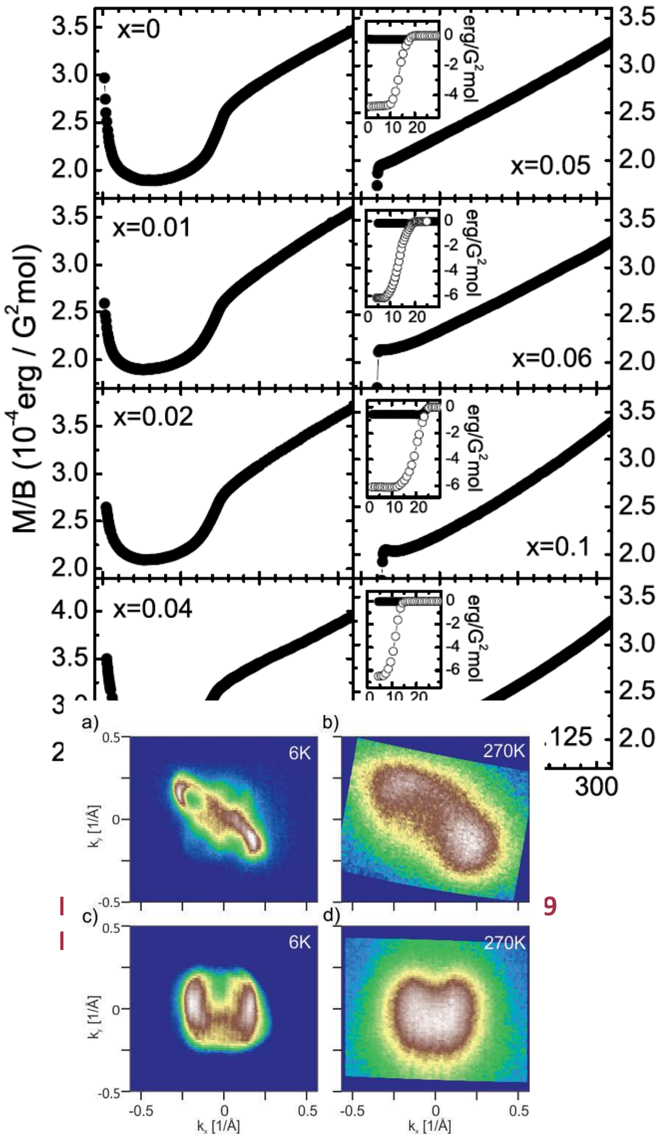
H.-J. Grafe, BB. et al., PRL 2008, NJP 2009
R. Klingeler, BB et al., PRB 2010

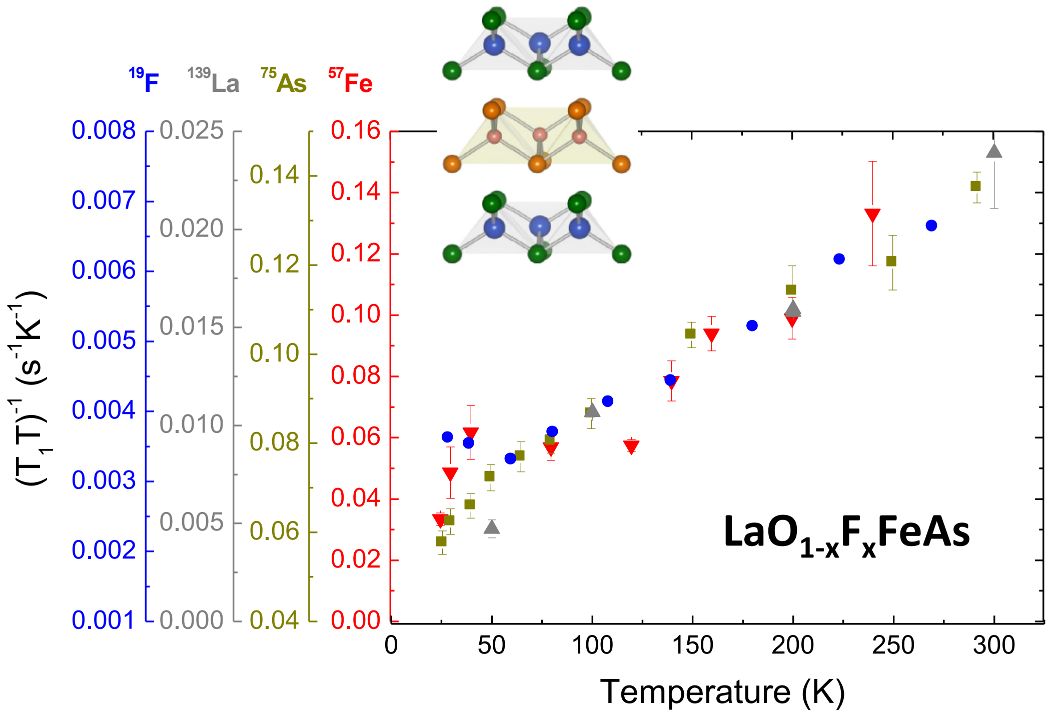
Anomalous increase of magnetic susceptibility with T

visible in χ, Knight shift, relaxation rate
“local effect”, i.e. not q dependent spin interaction
present for all doping contents, parent, overdoped …
seen in all Fe based SC, 1111, FeSe, LiFeAs, 122, …

T dependent electronic structure: Back to DFT
Relationship to increase of magn. susceptibility χ?

$LaO_{1-x}F_xFeAs$





Anomalous increase of magnetic susceptibility with T

- visible in χ, Knight shift, relaxation rate
- "local effect", i.e. not q dependent spin interaction
- present for all doping contents, parent, overdoped …
- seen in all Fe based SC, 1111, FeSe, LiFeAs, 122, …

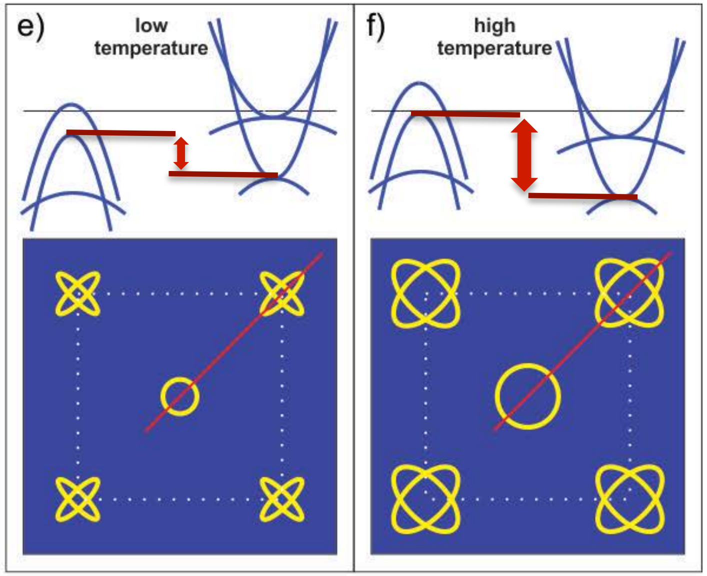
T dependent electronic structure: Back to DFT

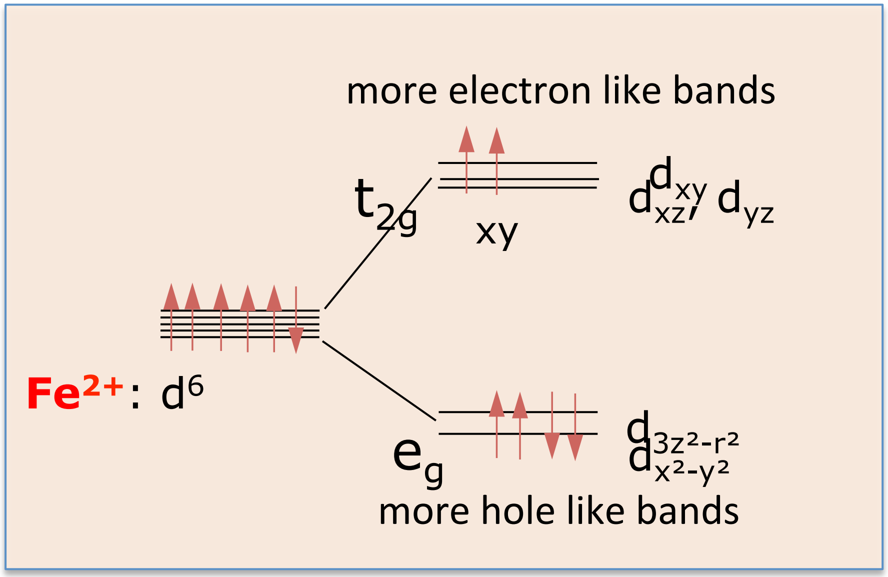
Qualitative picture

Both parts of FS expand, total charge constant

Number of electrons increases with T
Number of holes increases with T

“Orbital character” of electrons at the FS changes!!

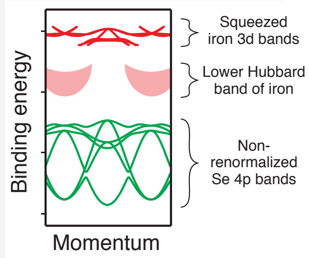




Conclusions and Questions

- **Electron correlations in Fe based SC: "Lower Hubbard bands"**

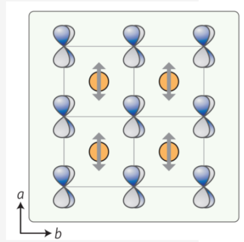
  ARPES + DMFT: "dispersive" lower Hubbard bands
  Sizeable electron correlations in Fe-based SC
  Relevance of local physics? Role of correlations for SC?



- **Nematic order, orbitals, and spin fluctuations in Fe based SC**

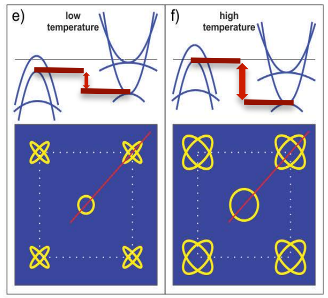
  Spin fluctuations and nematic order as seen by NMR: FeSe vs $BaFe_2As_2$
  Scaling between lattice softening and spin fluctuations ($BaFe_2As_2$) not generic!
  Weak influence of nematic order on spin fluctuations (FeSe) is an exception!
  Discrimination between different theoretical scenarios?

  As NQR on 1111 type systems: "evidence for (orbital) polarons"
  Are 1111-type Fe-based SC (nearly) itinerant systems with„orbital physics"?



- **Temperature dependent electronic structure: "red/blue shift"**

  ARPES on FeSe: Back to DFT with increasing T
  Discrimation between different theoretical models?
  Generic for all Fe-based SC?
  Relationship to other properties?



Thank you very much!!

GRK 1621

Deutsche Forschungsgemeinschaft DFG
Priority Program SPP1458 (2010 – 2017):
"Iron Pnictides Superconductors: Materials and Mechanisms"