FeSe: a model system for Fe based superconductors

IFW
Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

TECHNISCHE UNIVERSITÄT DRESDEN

Bernd Büchner

Institute for Solid State Research, IFW Dresden

Institute for Condensed Matter Physics, TU Dresden

Deutsche Forschungsgemeinschaft
DFG

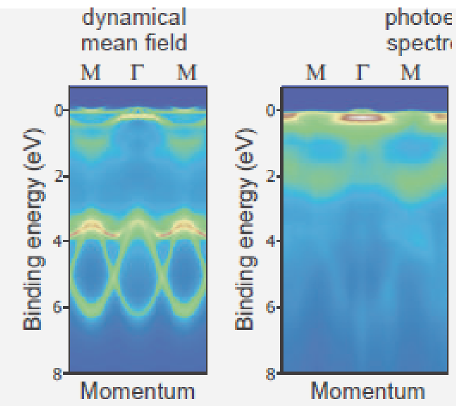
DFG Priority Program SPP1458 (2010 – 2016):

„Iron Pnictides Superconductors: Materials and Mechanisms“

OUTLINE

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

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



Orbital-driven nematicity in FeSe

nature materials

S-H. Baek[1*], D. V. Efremov[1], J. M. Ok[2], J. S. Kim[2], Jeroen van den Brink[1,3] and B. Büchner[1,3]

NMR	S.-H. Baek, H. Grafe	IFW Dresden
Theory	D. Efremov, J. v.d. Brink	IFW Dresden
Synthesis	J. M. Ok, J. S.Kim	U Pohang

Phase diagram of 1111 pnictides: Evidence for Orbital Polarons?

NMR/NQR	G. Lang, H. Grafe, F. Hammerath, E. Brüning	IFW Dresden
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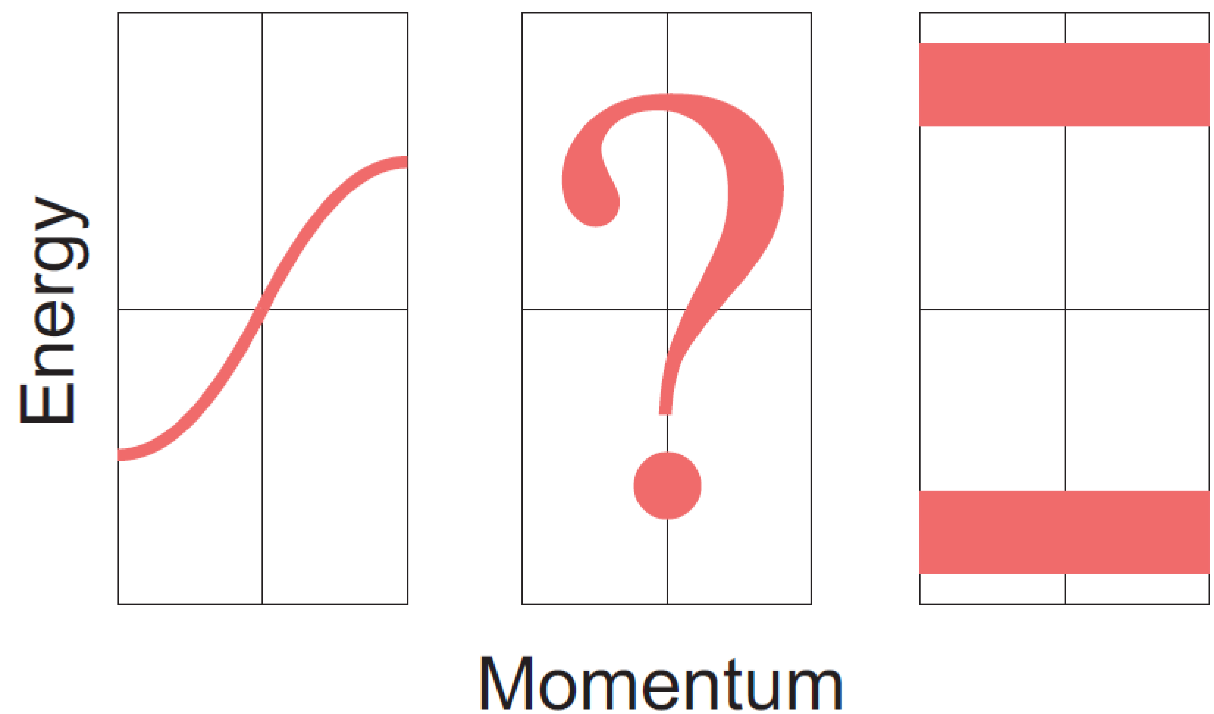
[1] *Institute for Solid State Research, IFW Dresden, P. O. Box 270116, D-01171 Dresden, Germany*
[2] *Institute of Theoretical and Computational Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria*
[3] *Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland*
[4] *Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany*
[5] *Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*
[6] *Centre de Physique Theorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France*

ARPES

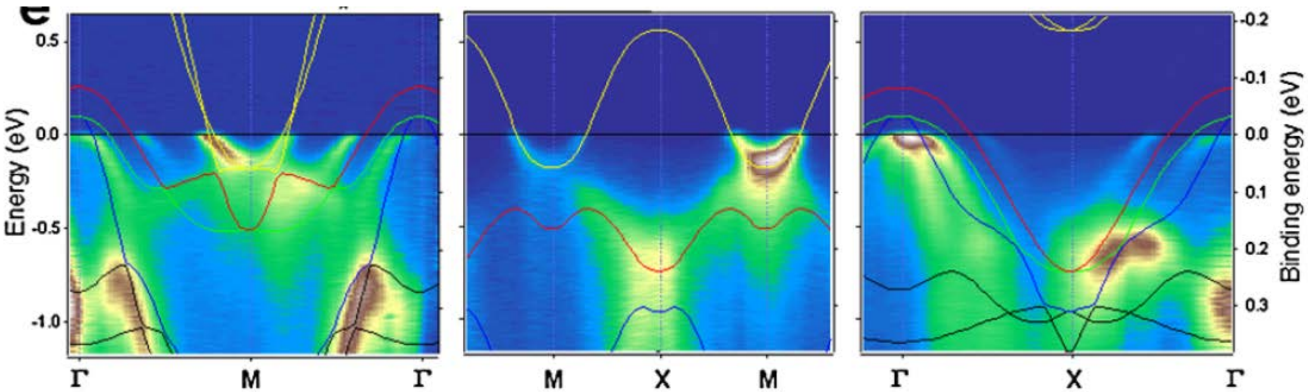
THEORY

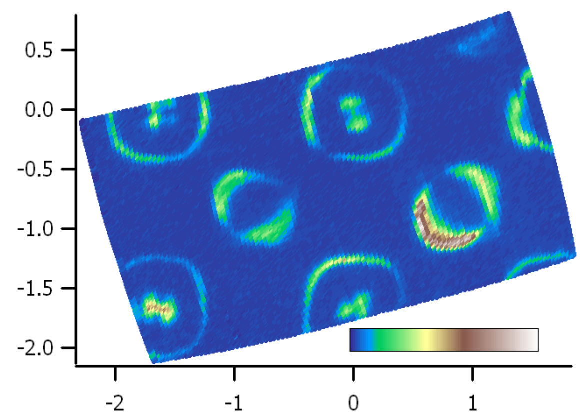
CRYSTAL



Renormalized bands close to E_F

Superconducting material: LiFeAs

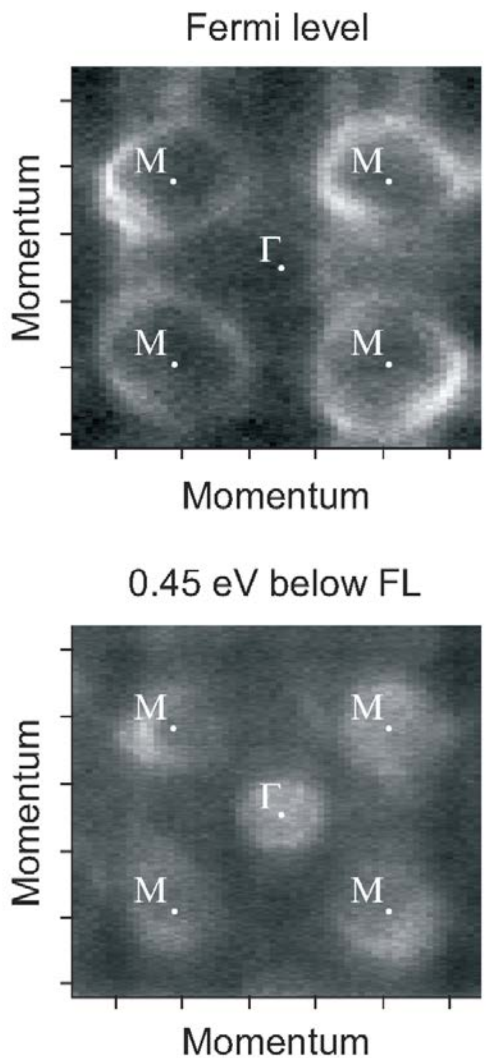


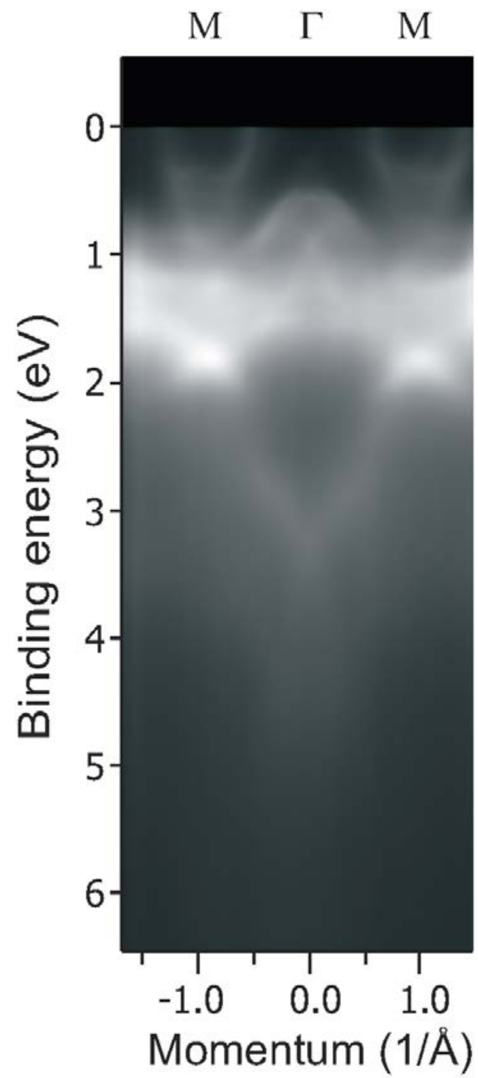


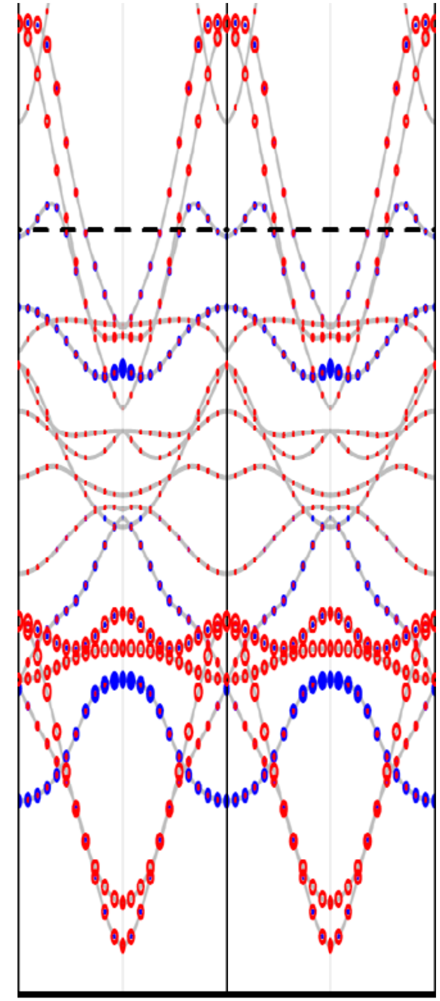
Renormalization ~ 3

Borysenko *et al., PRL* (2010)

122-structure, no iron atoms: $BaNi_2As_2$

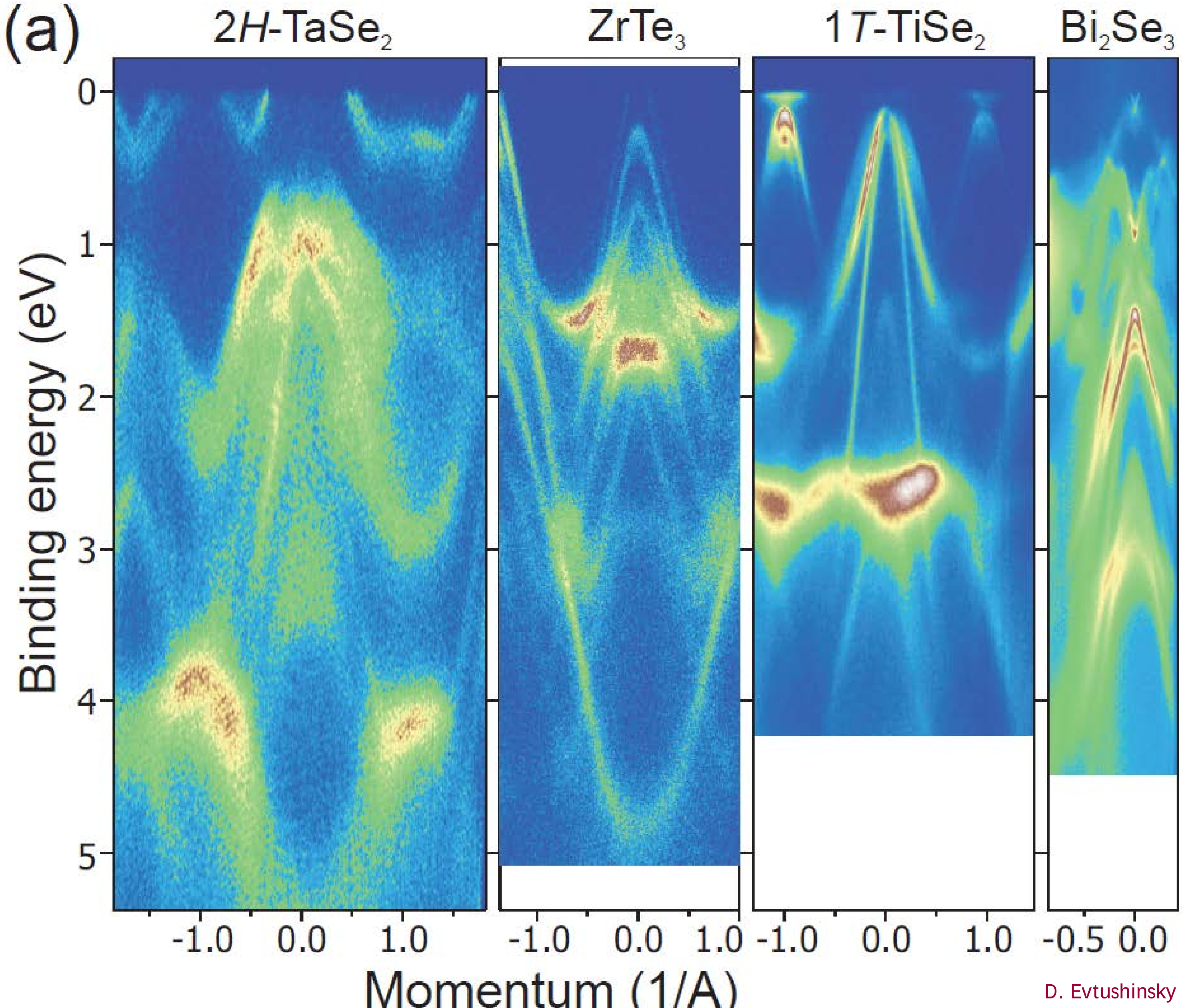






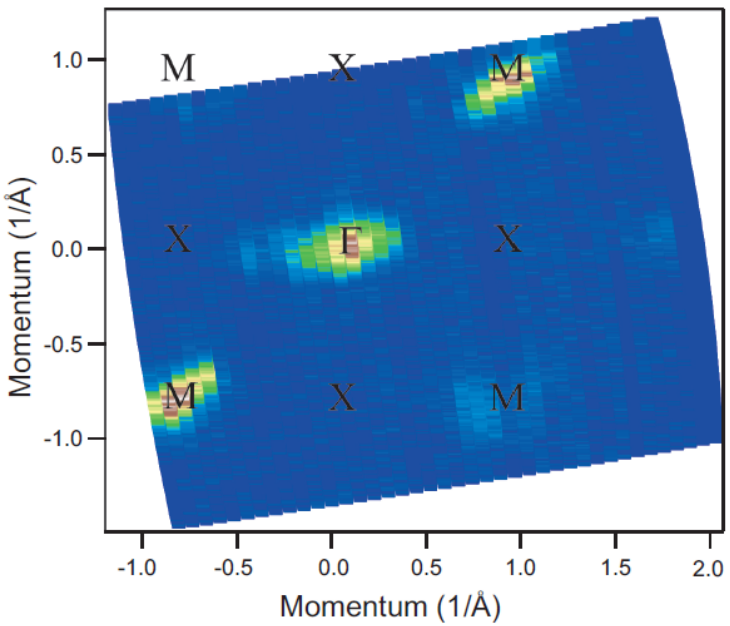
Renormalization ~ 1

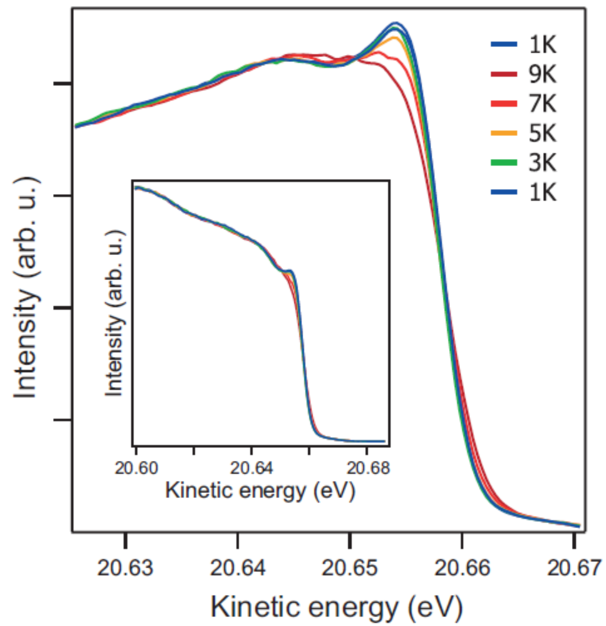
Kim, Evtushinskiy, Yaresko *et. al.*



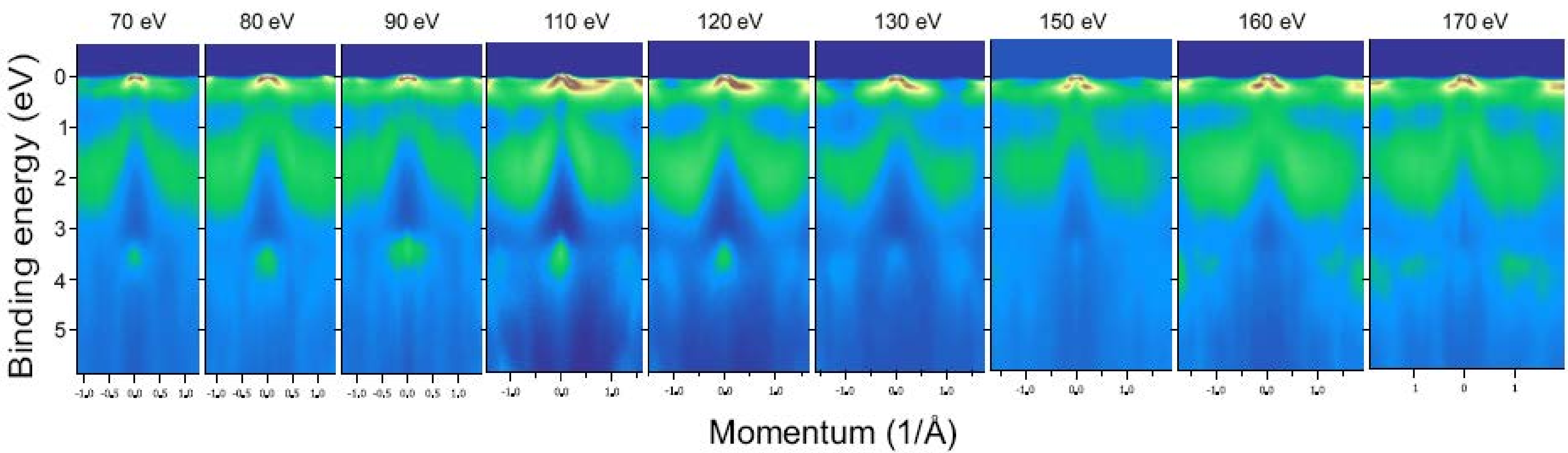
D. Evtushinsky et al, Arxiv

ARPES on FeSe

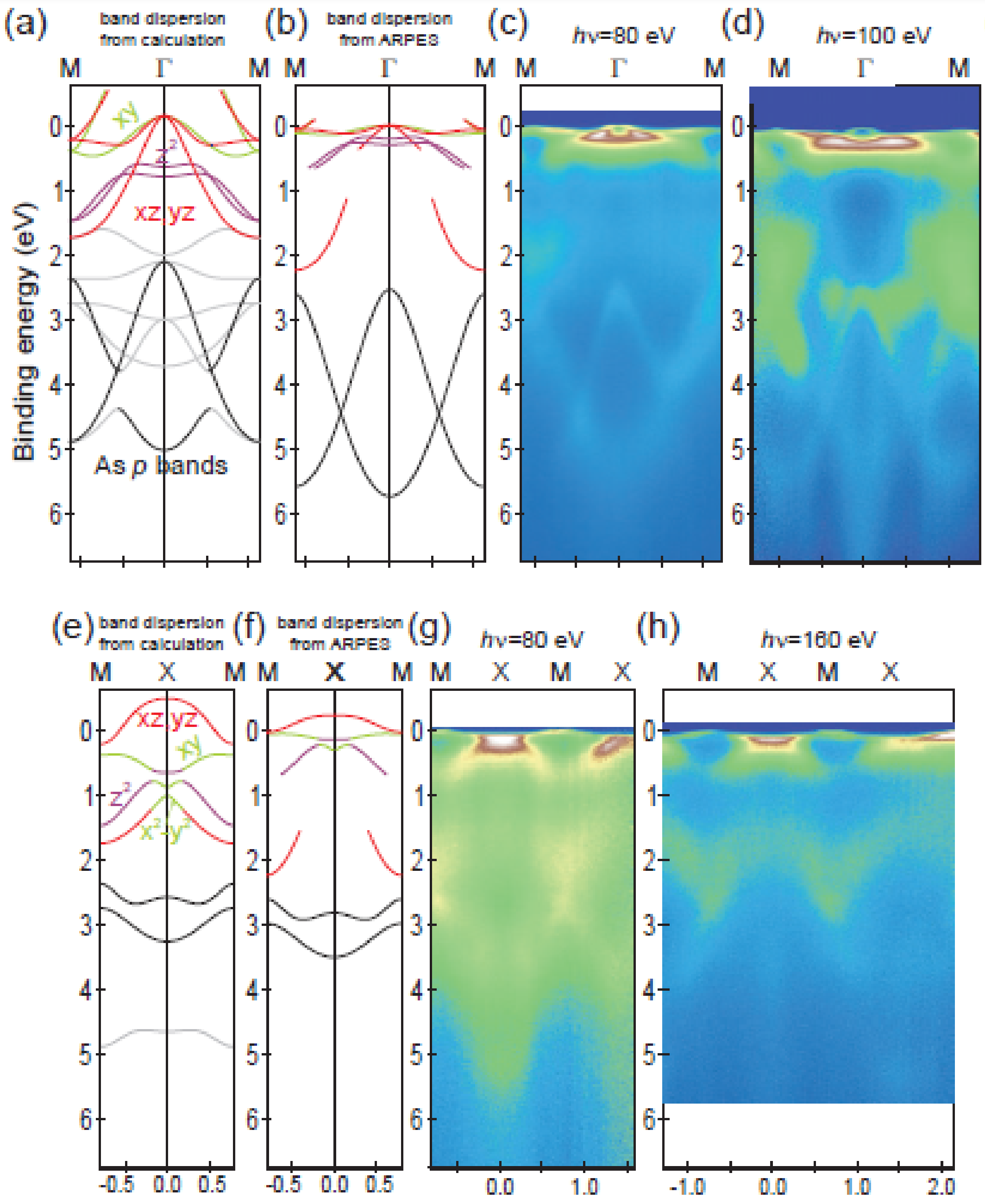




see also
Maletz et al., PRB 2014



ARPES on NaFeAs



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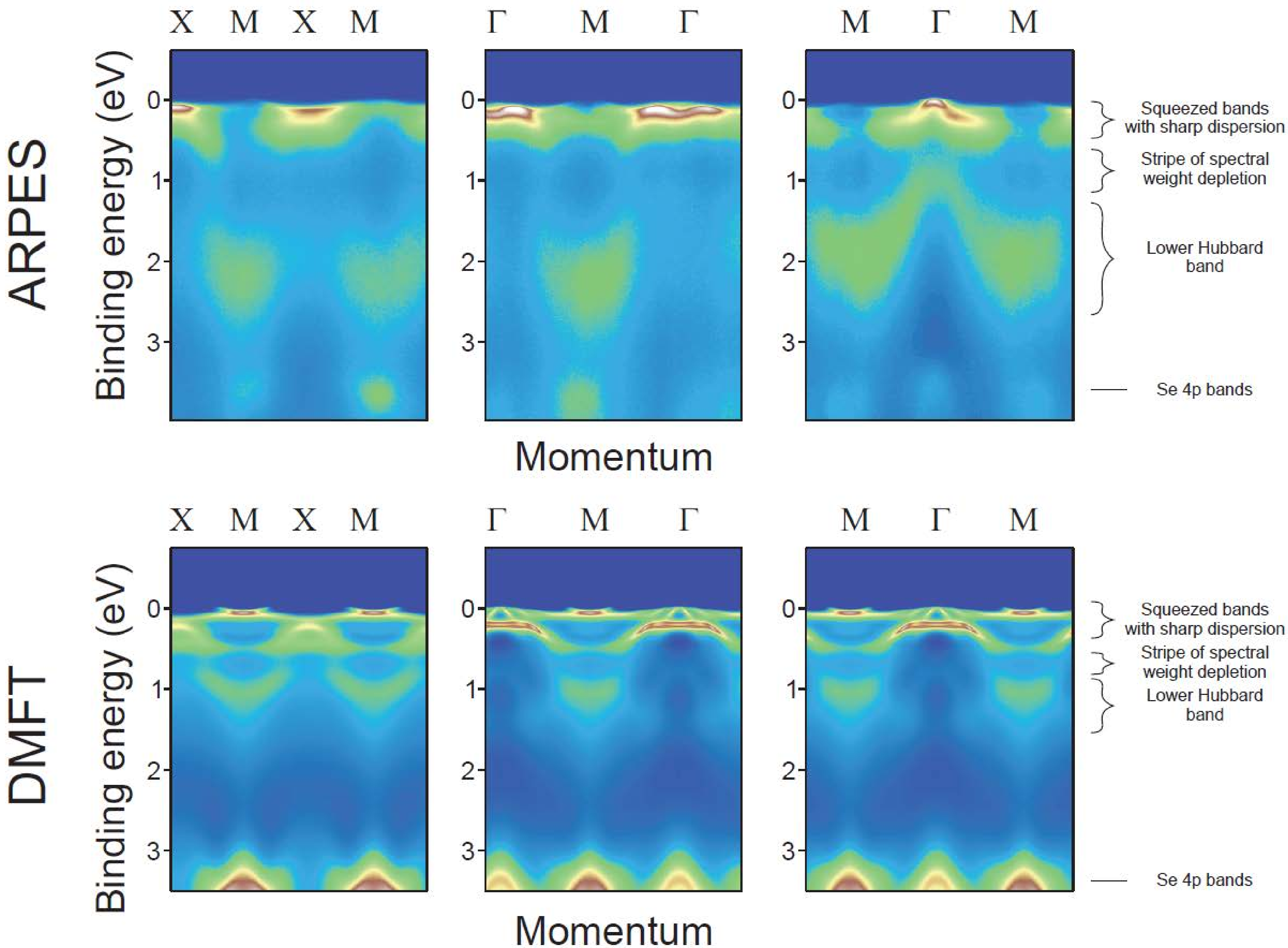
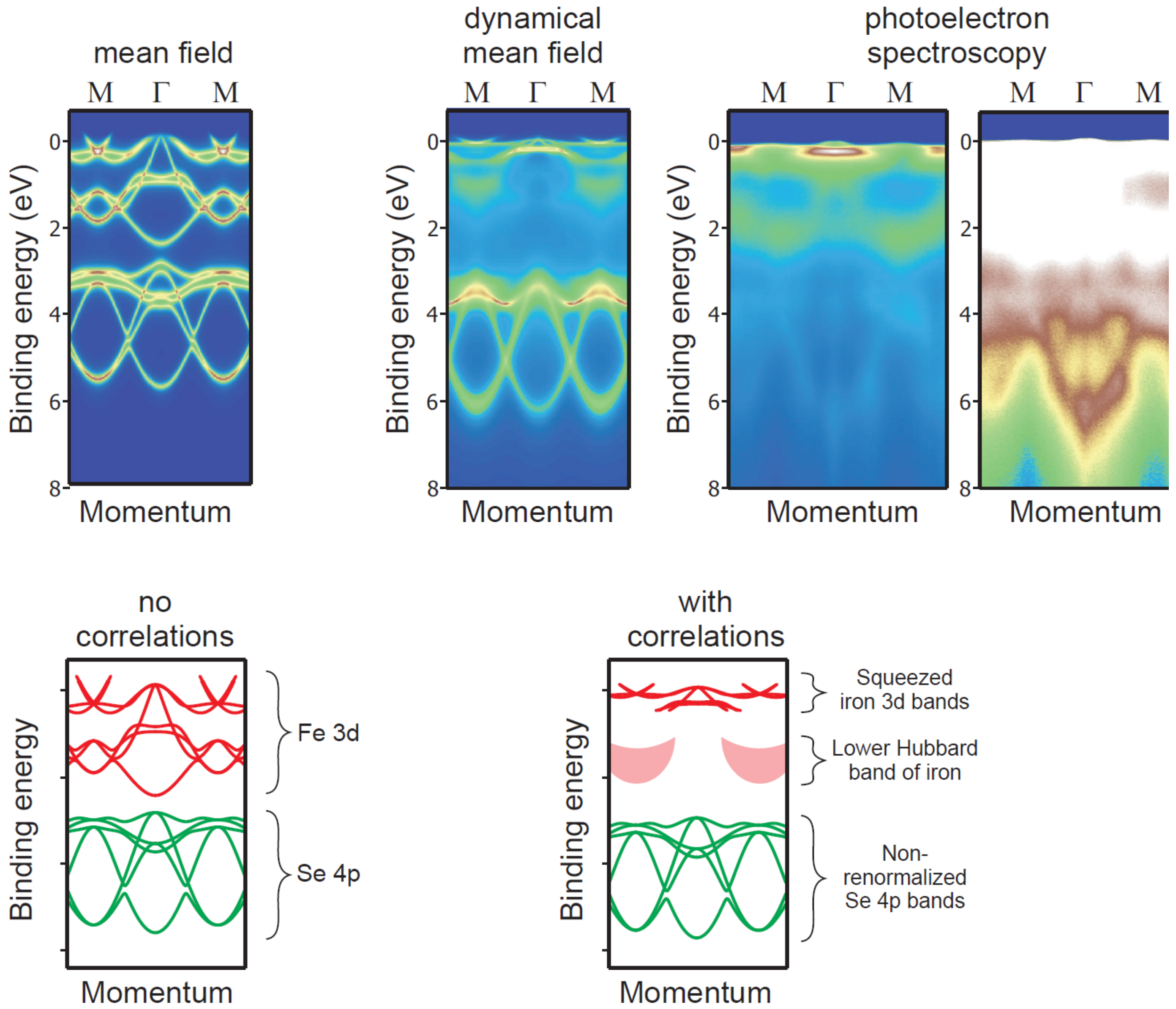


ARPES on FeSe: Theory and Experiment



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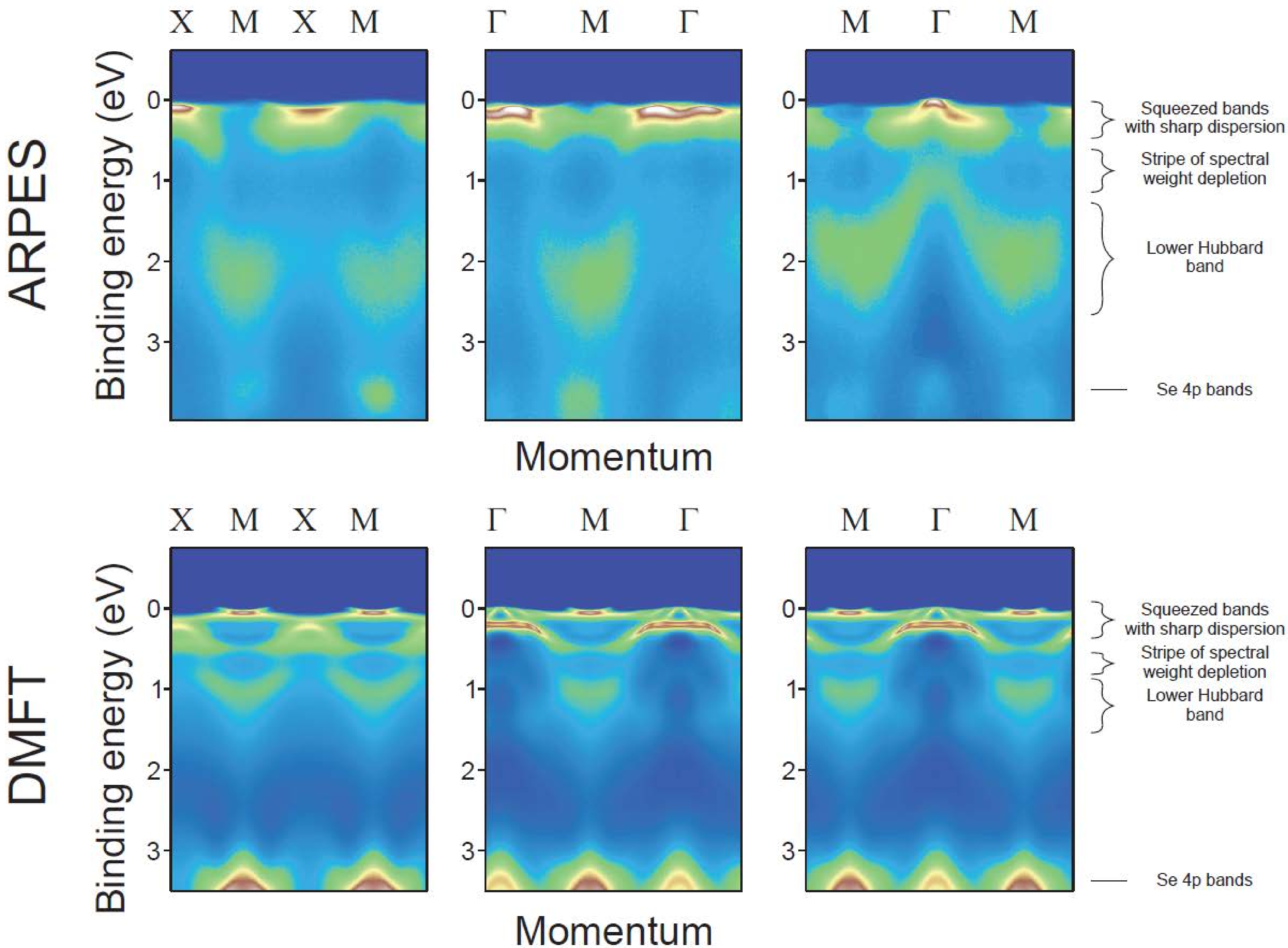

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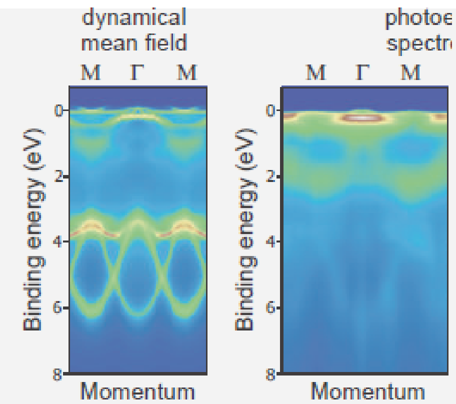

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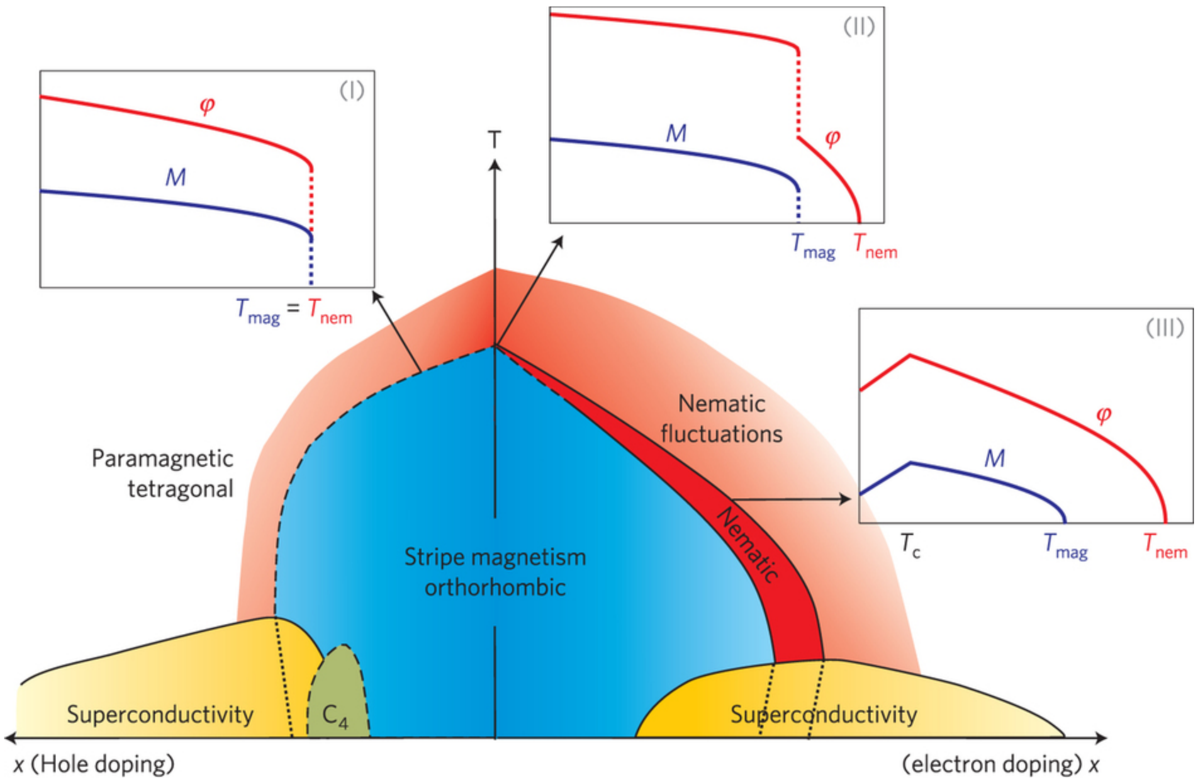
Nematic Order in Fe based SC (Ba122 type)

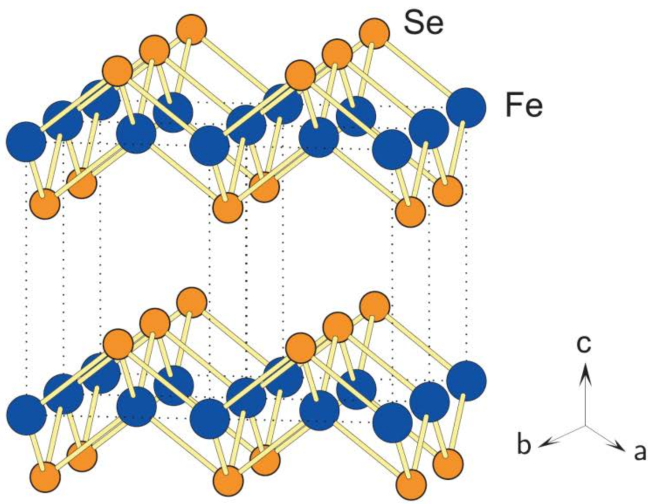


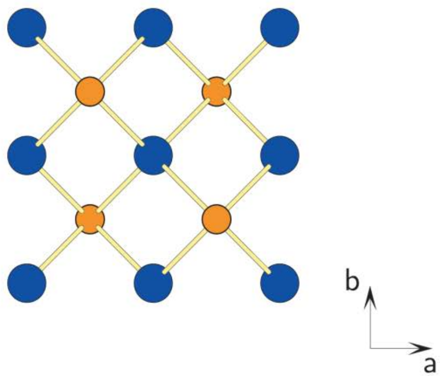
R. Fernandes, A. Chubukov, J. Schmalian
Nat. Phys. 2014

- Nematic order in iron-based superconductors is a well-established experimental fact.
- Origin remains controversial: orbital order or spin-driven Ising-nematic order.

“Nematic order is in the class of correlation-driven electronic instabilities, like superconductivity and density-wave transitions.”

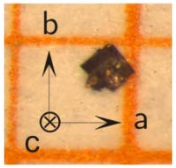
FeSe the most simple Fe based superconductor

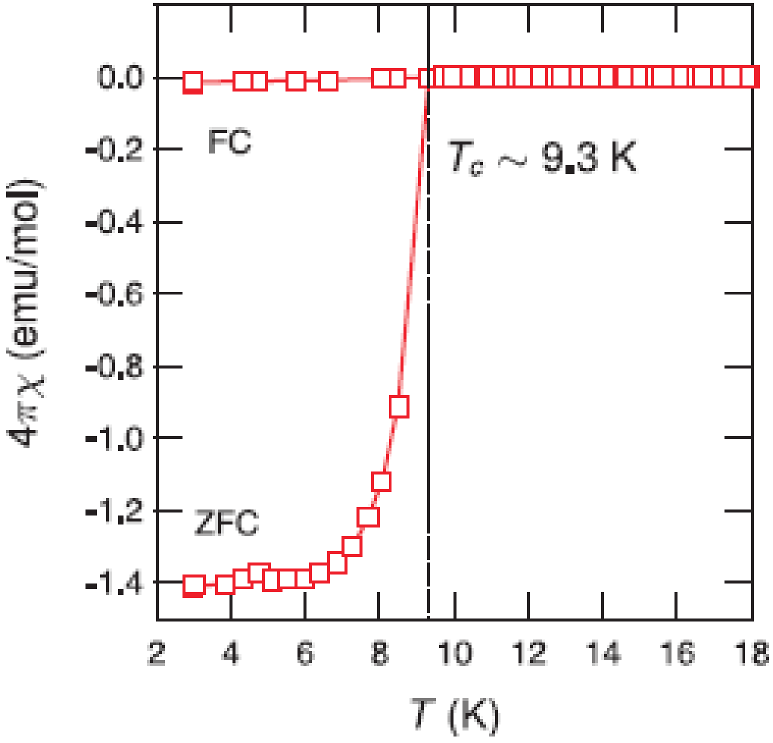




- Superconductivity Tc ~9.3 K
- No magnetic oder

FeSe
„11“





Sample:
J.M. Ok & J.S. Kim,
Pohang University, Korea

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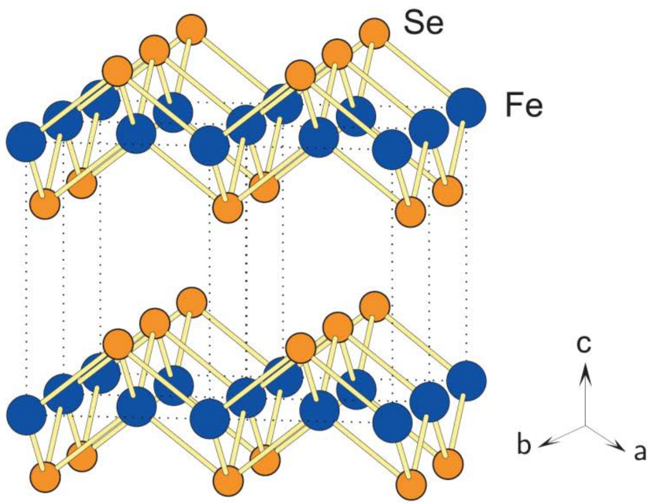

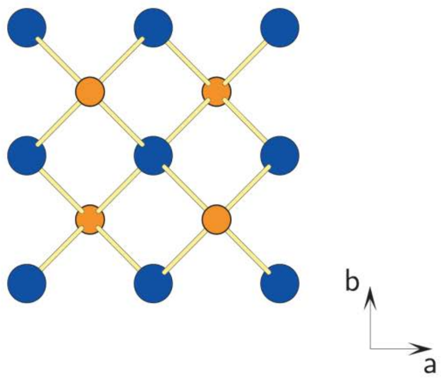

- Superconductivity Tc ~9.3 K
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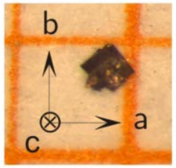
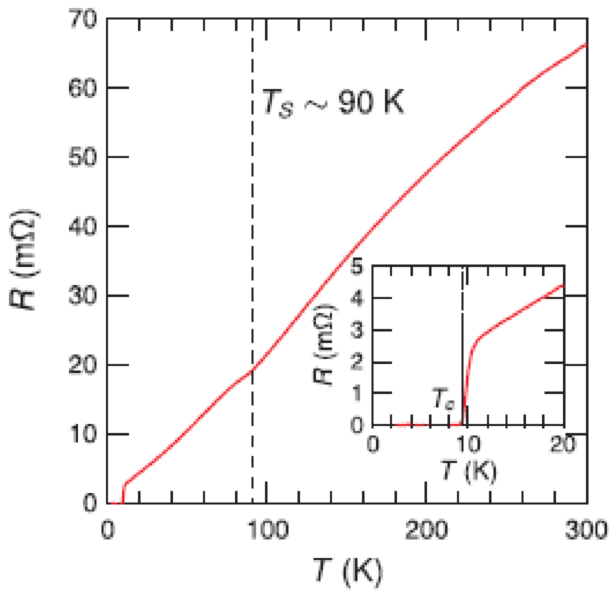
- Structural phase transition at ~ 90K

FeSe „11“





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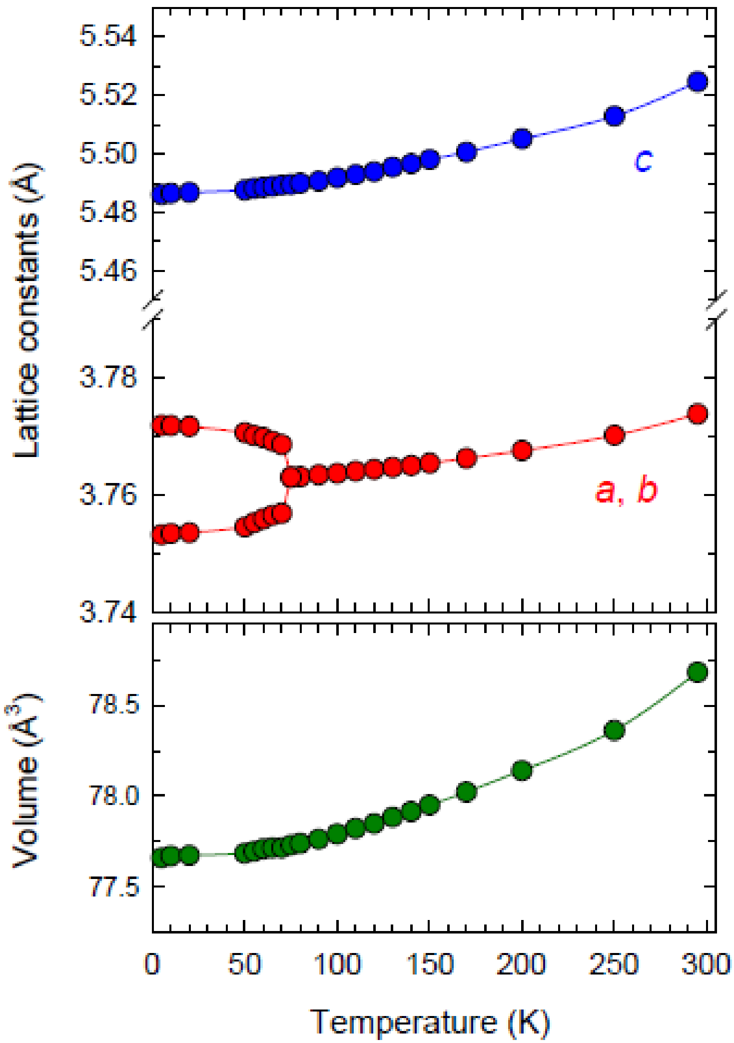

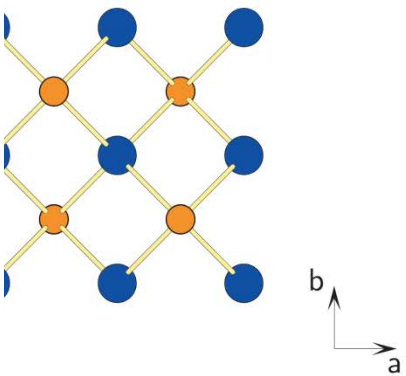

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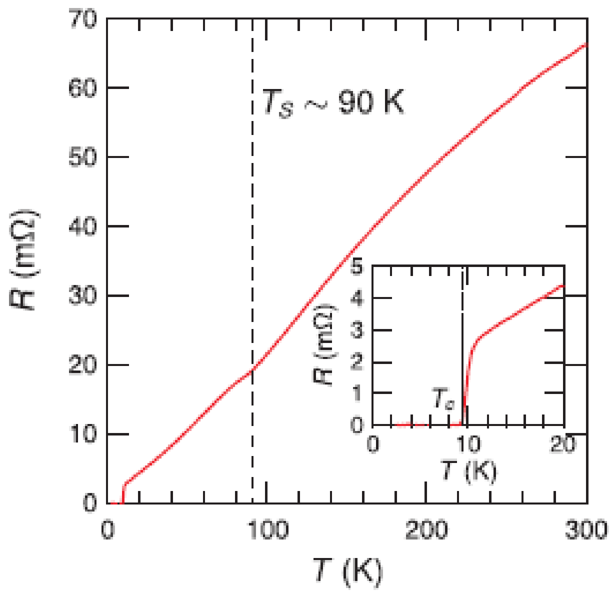
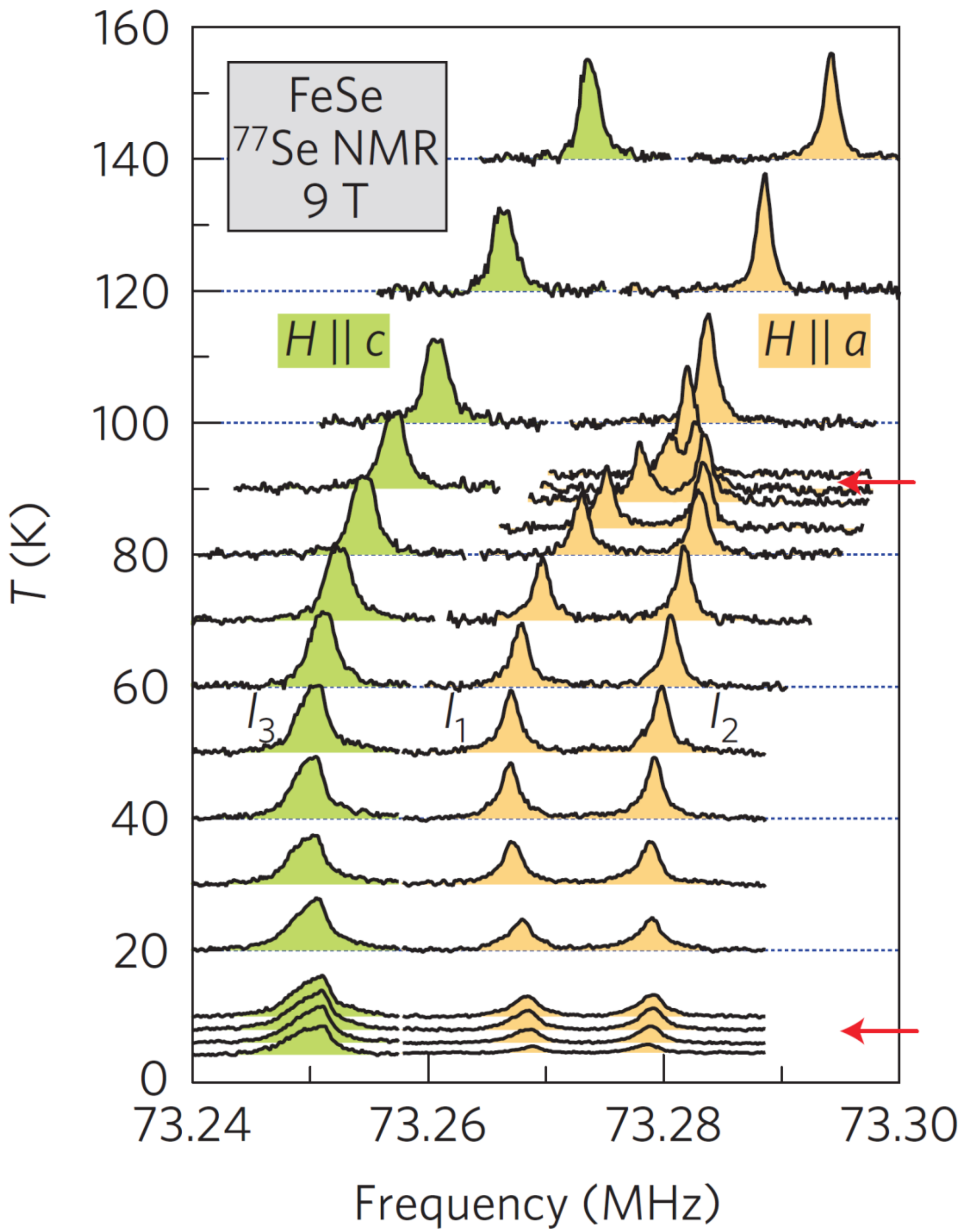


S. Margadonna et al., Chem. Comm. (2008)

NMR on FeSe

Splitting of NMR lines below the structural tetragonal to orthorhombic transition!

- ^{77}Se: nuclear spin ½,
  no quadrupol splitting
- 2 Se sites with different local magnetic field
- Not due to magnetic oder



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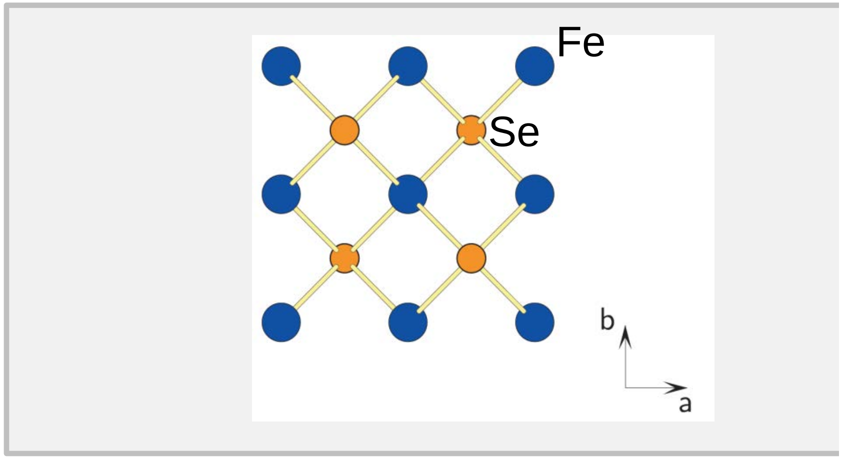

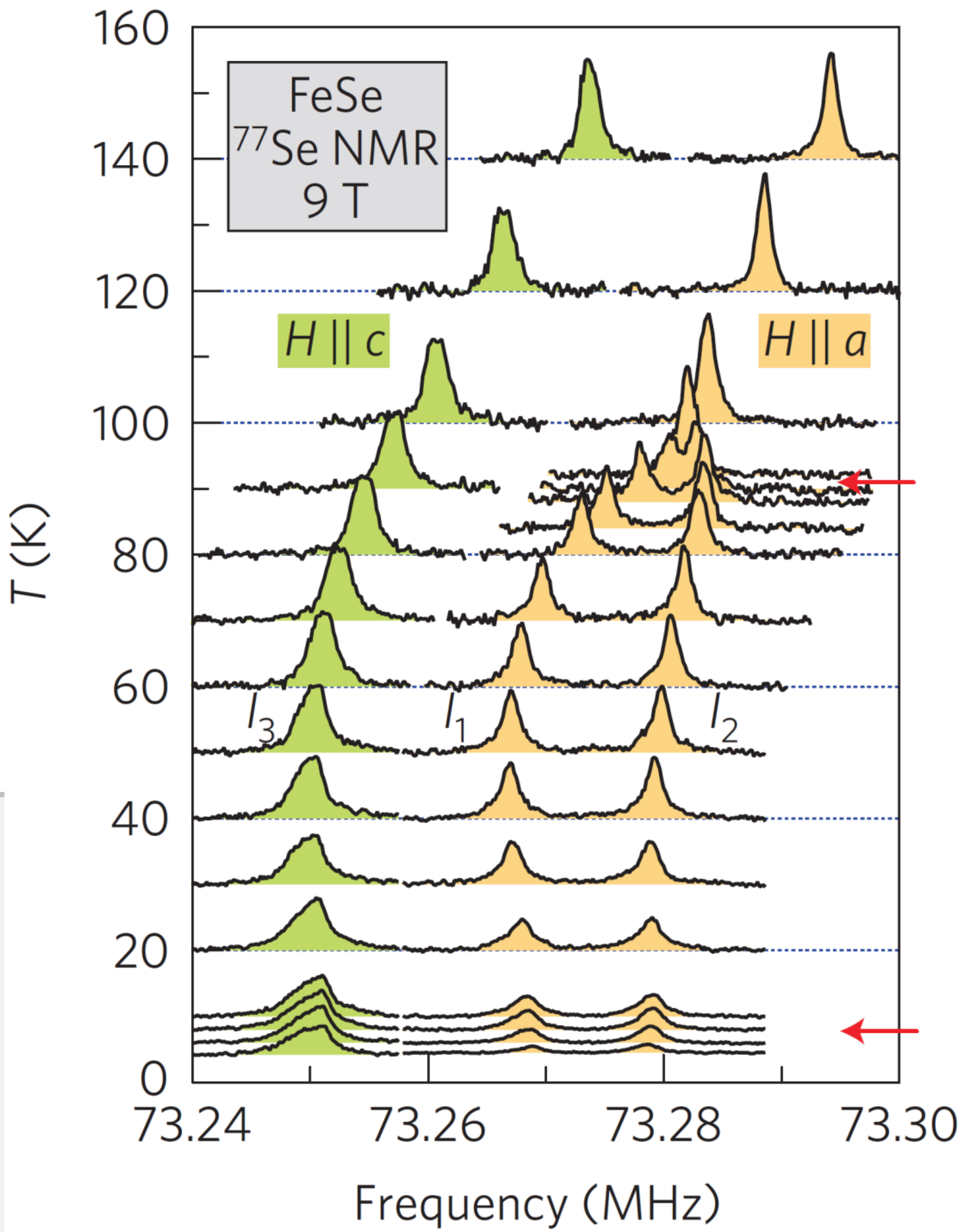

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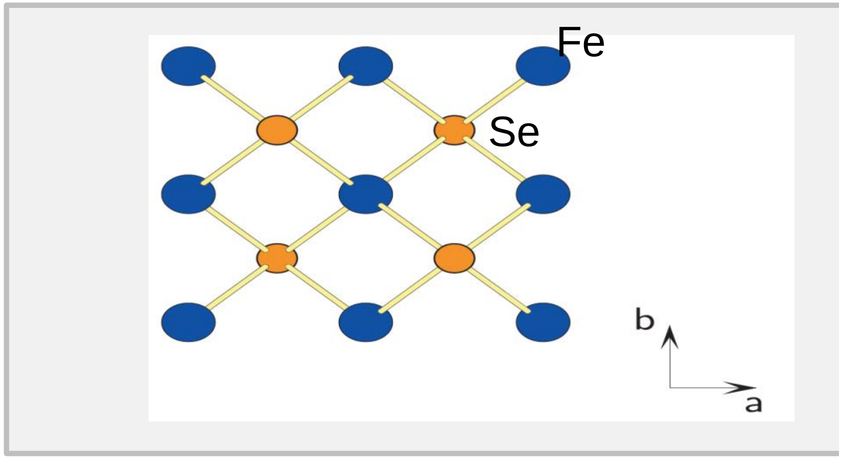

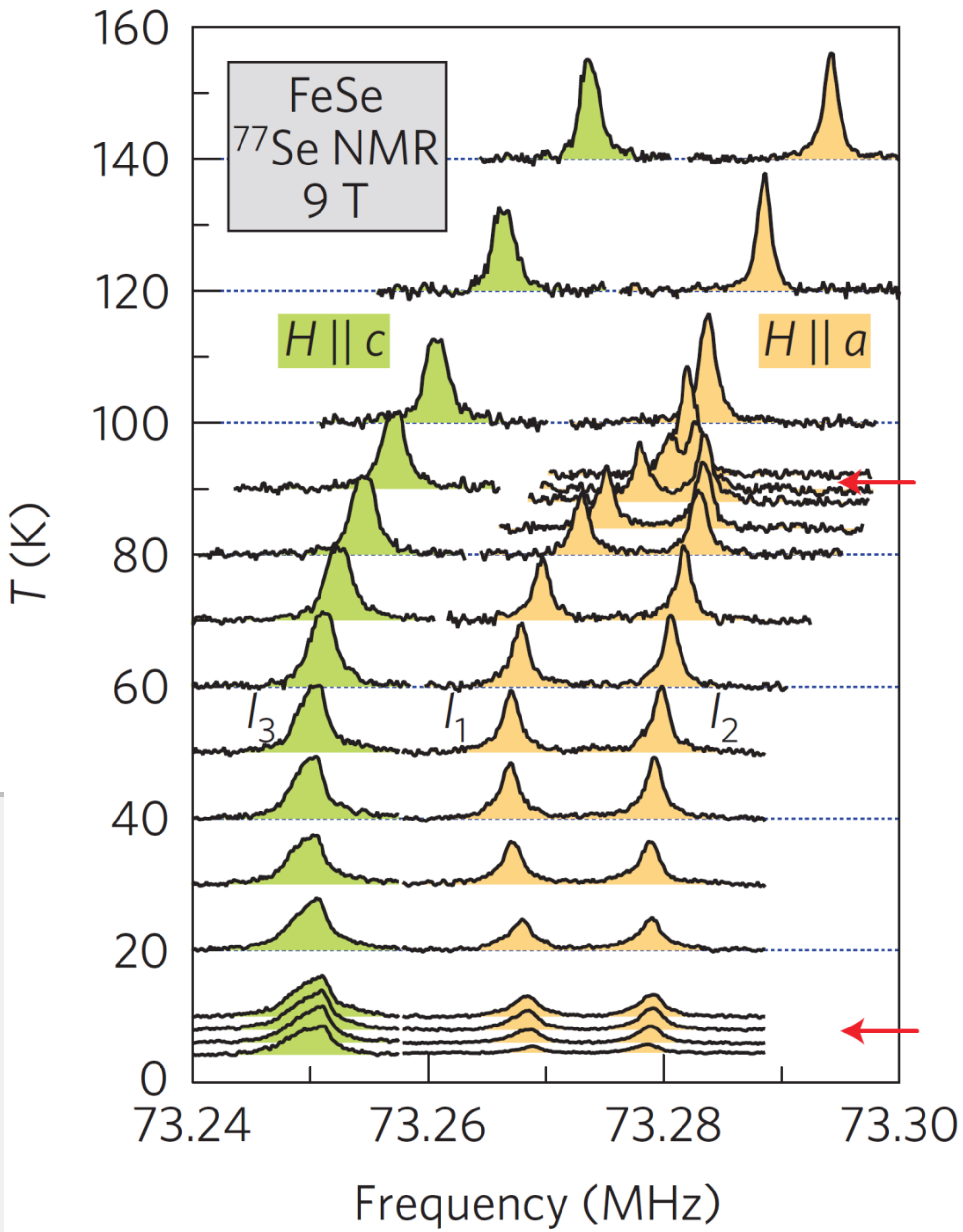

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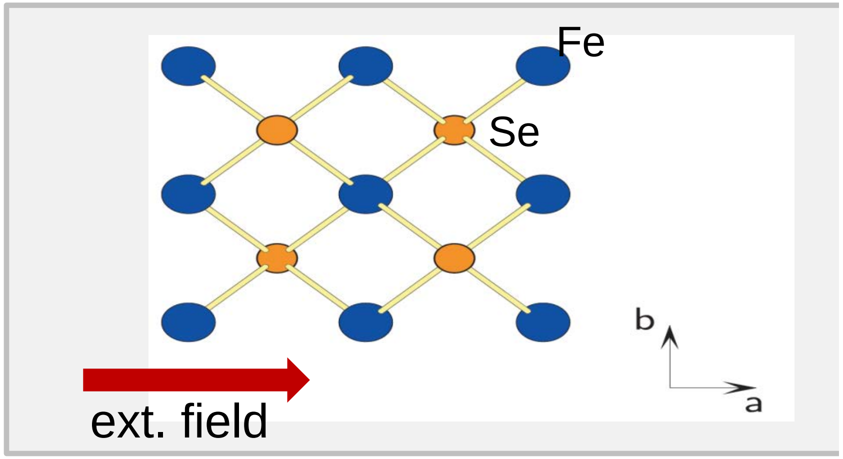

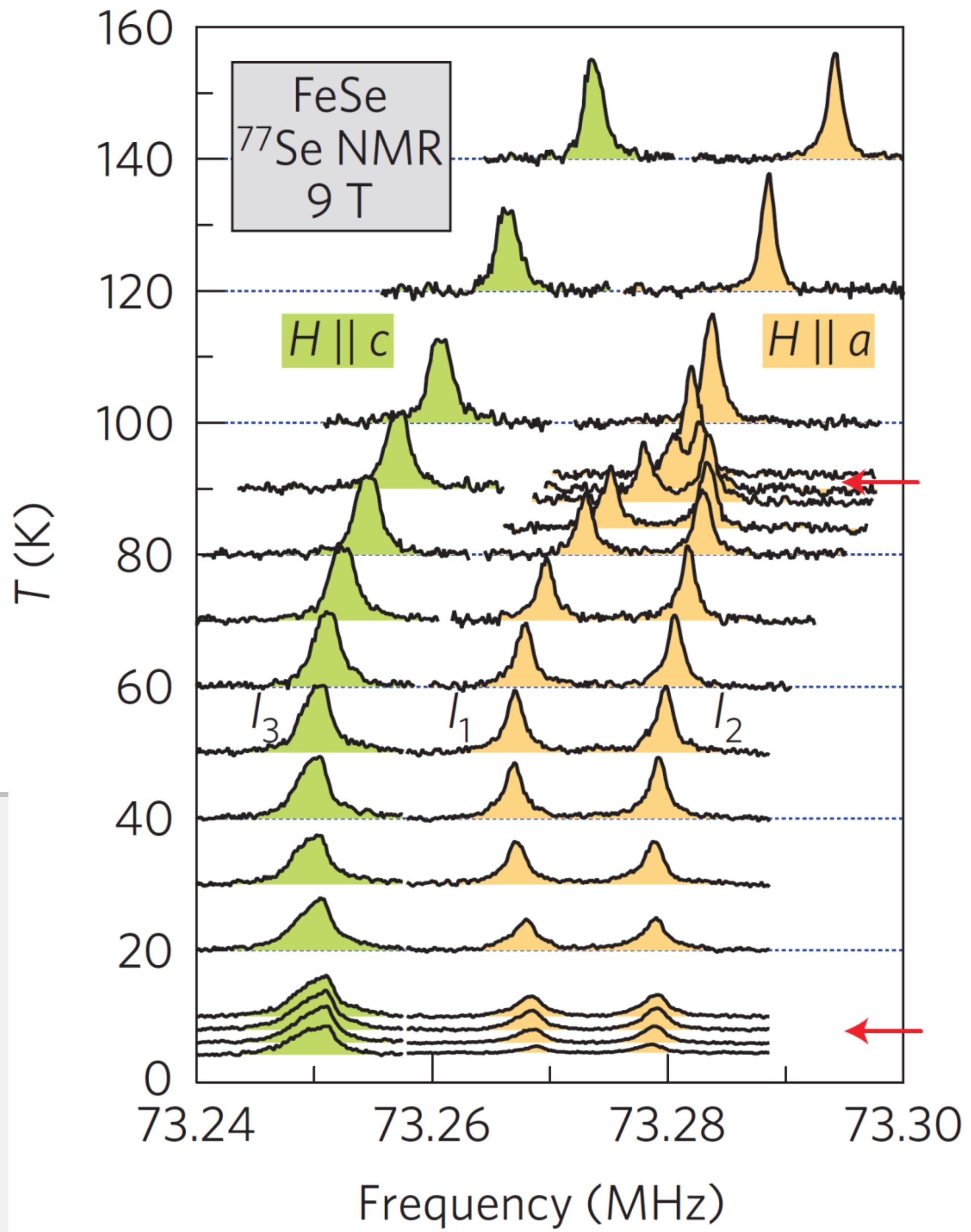

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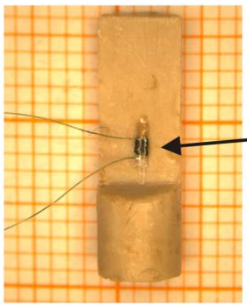
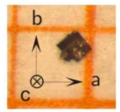
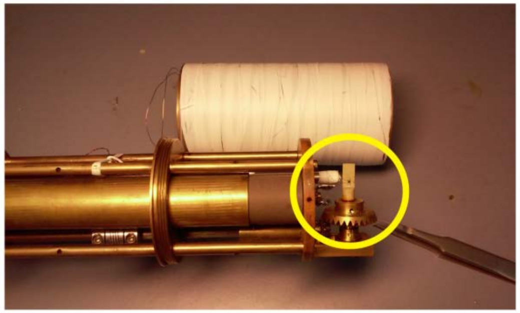
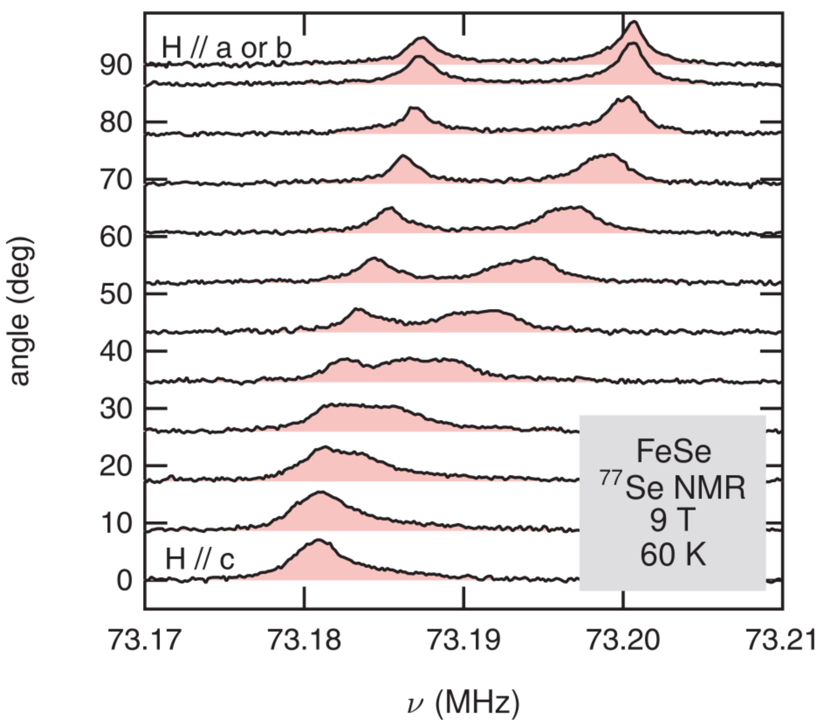


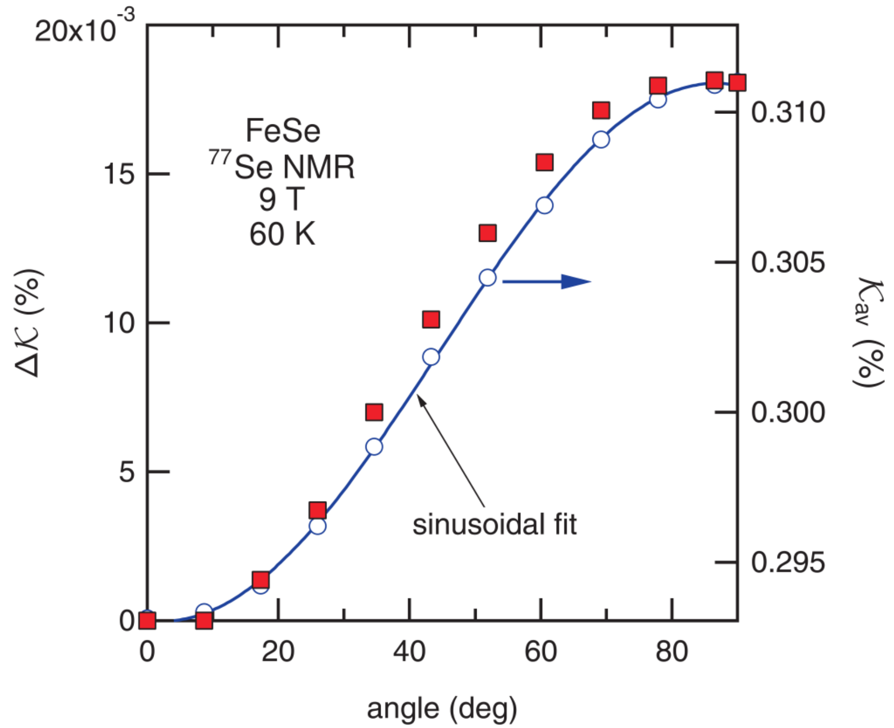
Flat NMR coil with a plate-like FeSe single crystal inside





Mounted to a goniometer





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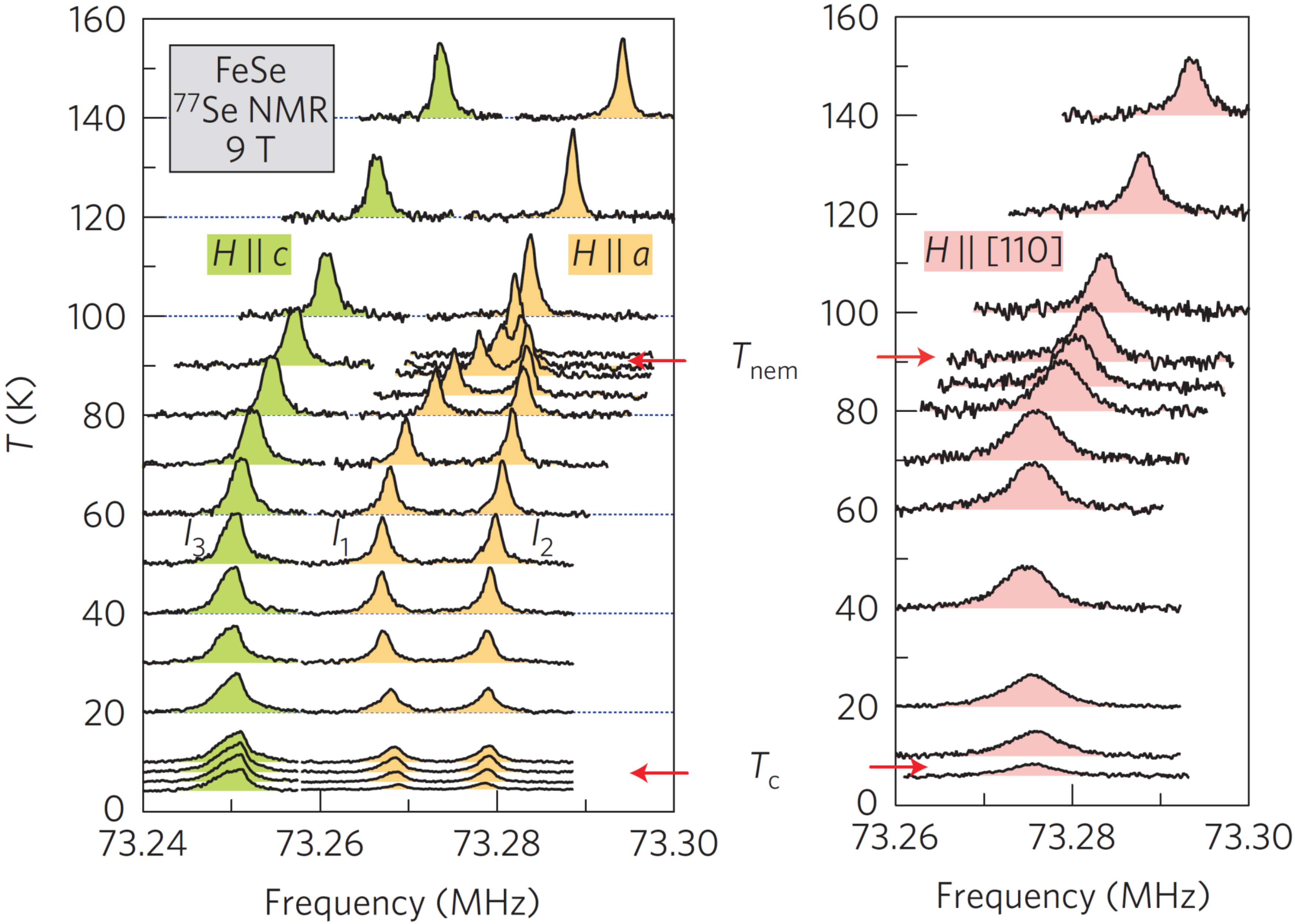

FeSe
77Se NMR
9 T
H || c
H || a
H || [110]
T (K)
Frequency (MHz)
T nem
T c
l3
l1
l2
160
140
120
100
80
60
40
20
0
73.24
73.26
73.28
73.30

NMR on FeSe

Splitting of NMR lines below the structural tetragonal to orthorhombic transition!

- ^{77}Se: nuclear spin ½,
  no quadrupol splitting

- 2 Se sites with different
  Knight shift κ

Paramagnetic state

$$\kappa = A_{hf}\,\chi_{spin} + \kappa_{chem}$$

Splitting of lines is caused by the anisotropy of the hyperfine coupling and the spin susceptibility

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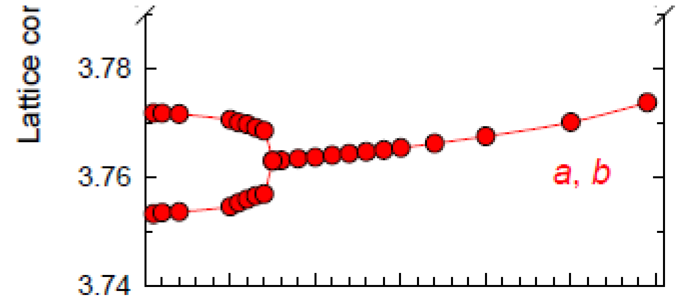

- ^{77}Se: nuclear spin ½,
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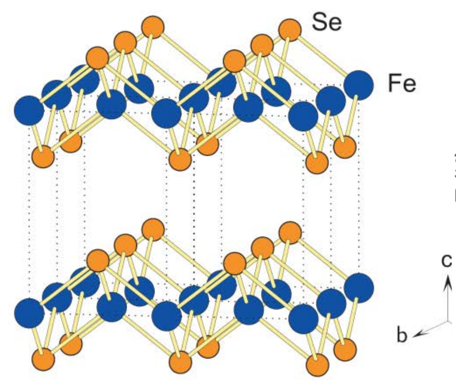
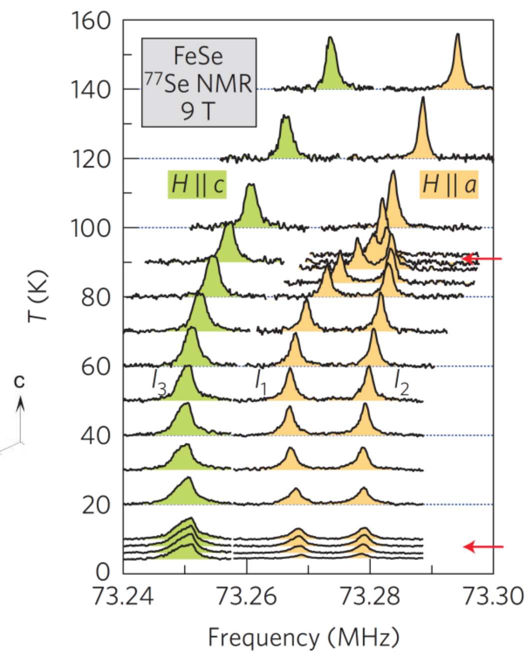
- 2 Se sites with different Knight shift κ

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

Paramagnetic state

$\kappa = A_{hf}\,\chi_{spin} + \kappa_{chem}$





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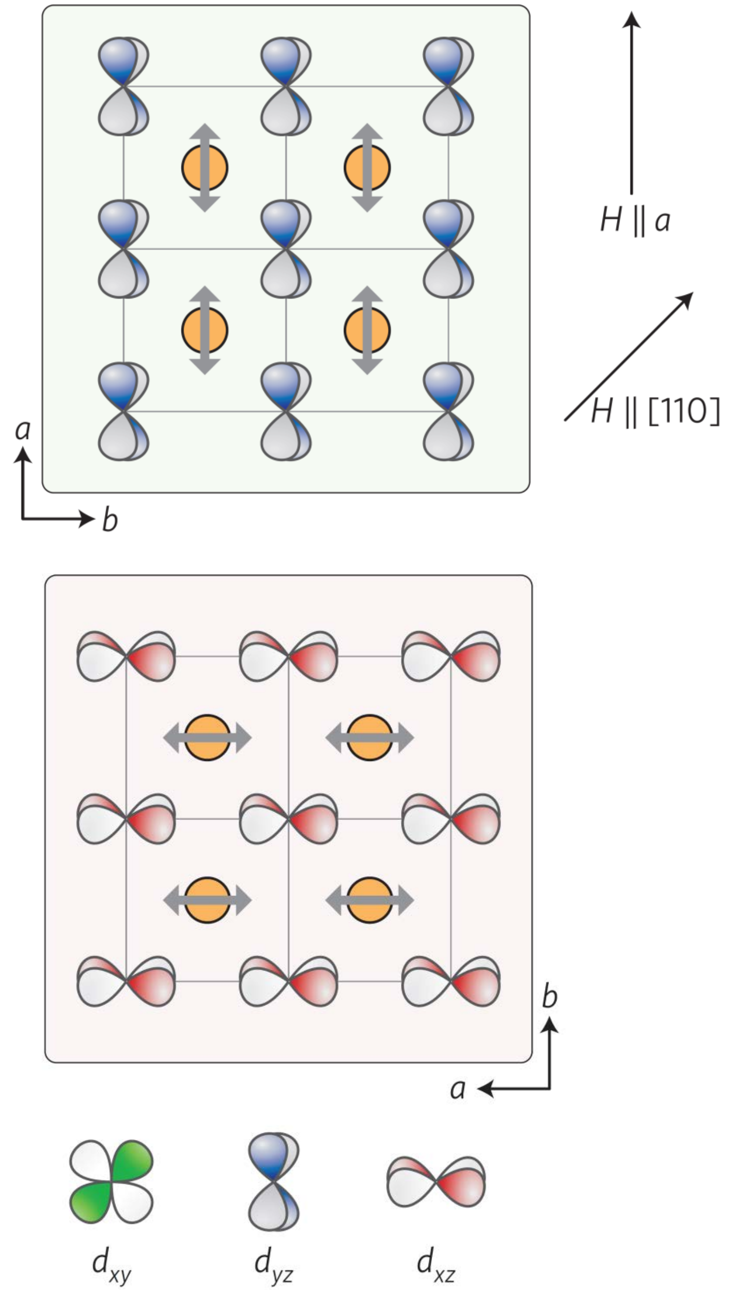


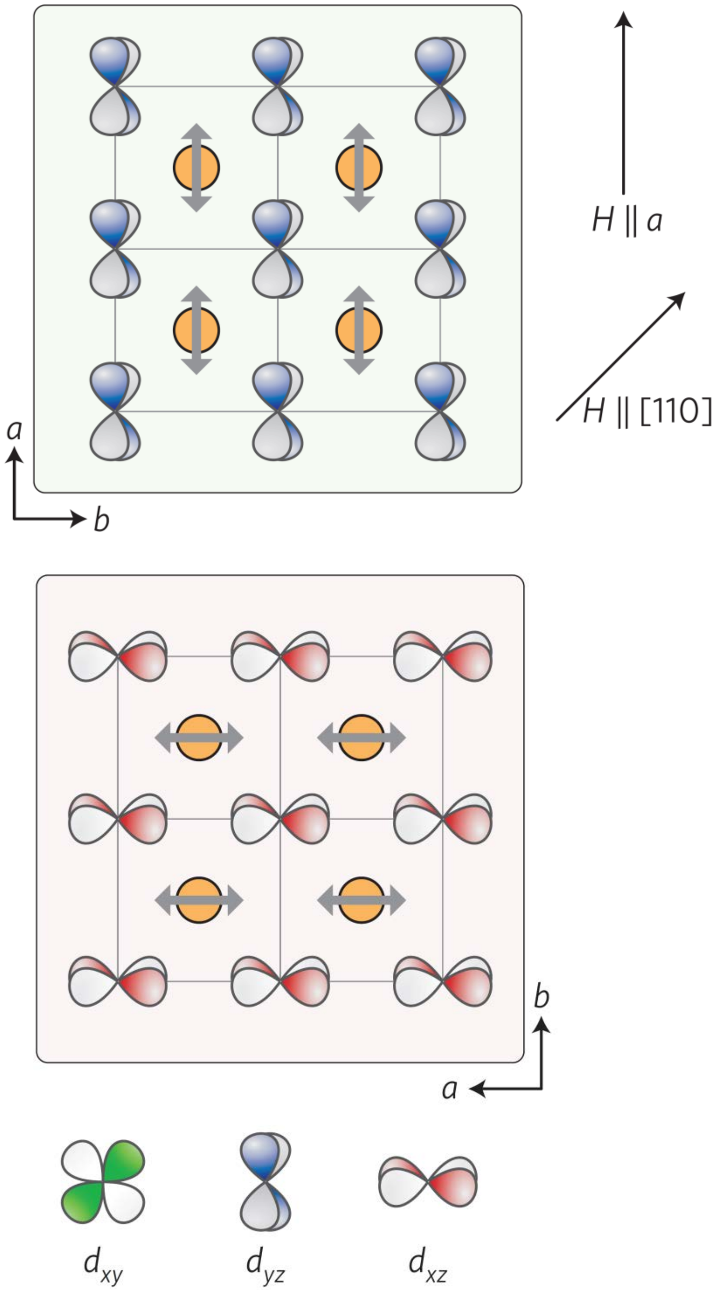
NMR on FeSe

Order parameter Ψ for ferro-orbital-order
(difference of occupation for d_{xz}, d_{yz} orb.)

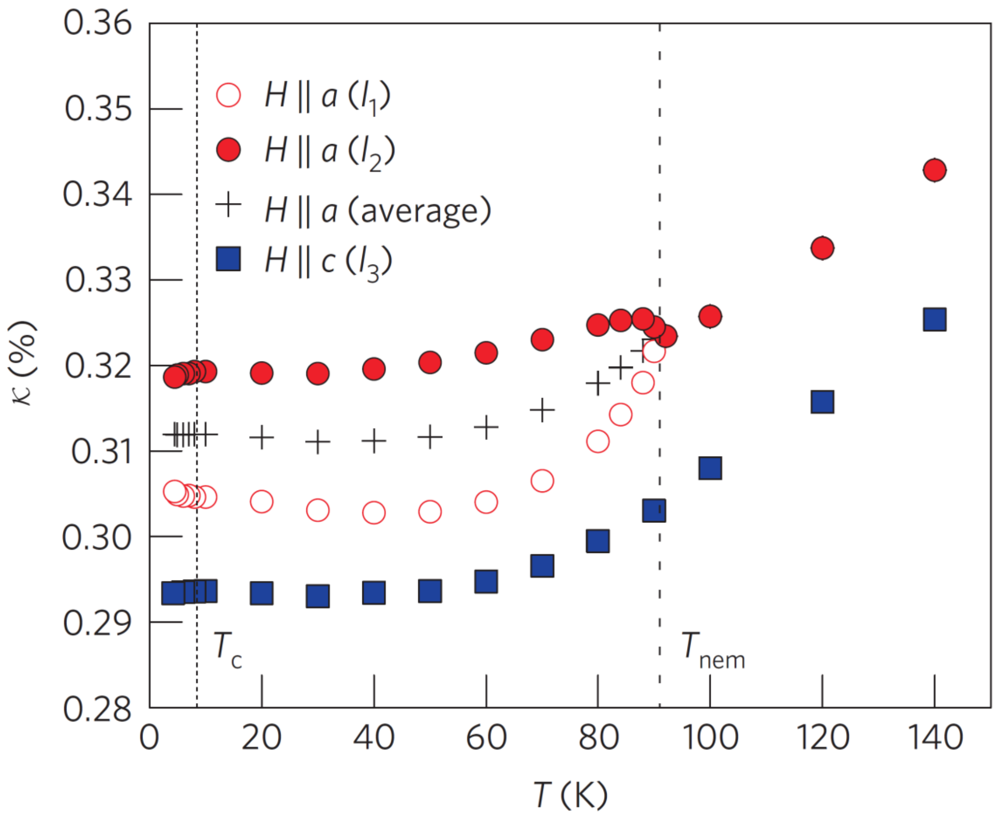
$$(A_{hf}^{xx} - A_{hf}^{yy}) \propto \Psi$$

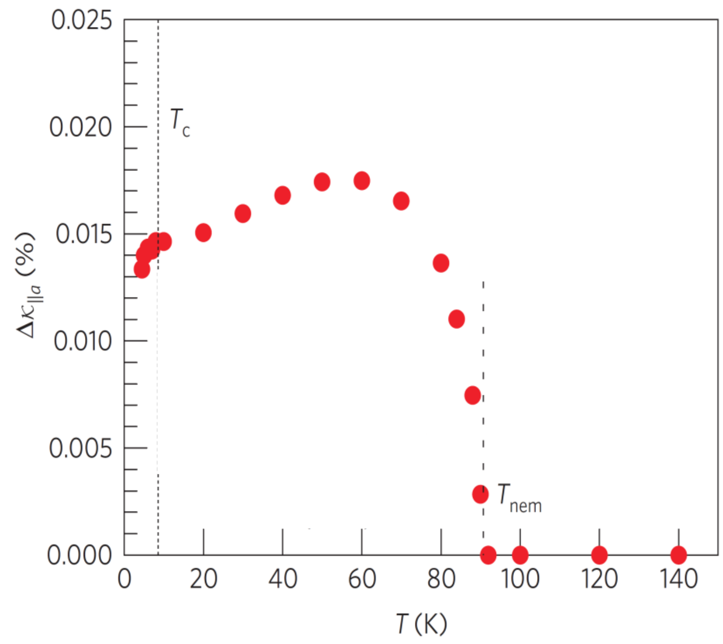
$$\Delta K \propto \Psi$$

Splitting of NMR lines is a signature of
A ferro- orbital order in FeSe



NMR on FeSe: T dependence of the line splitting





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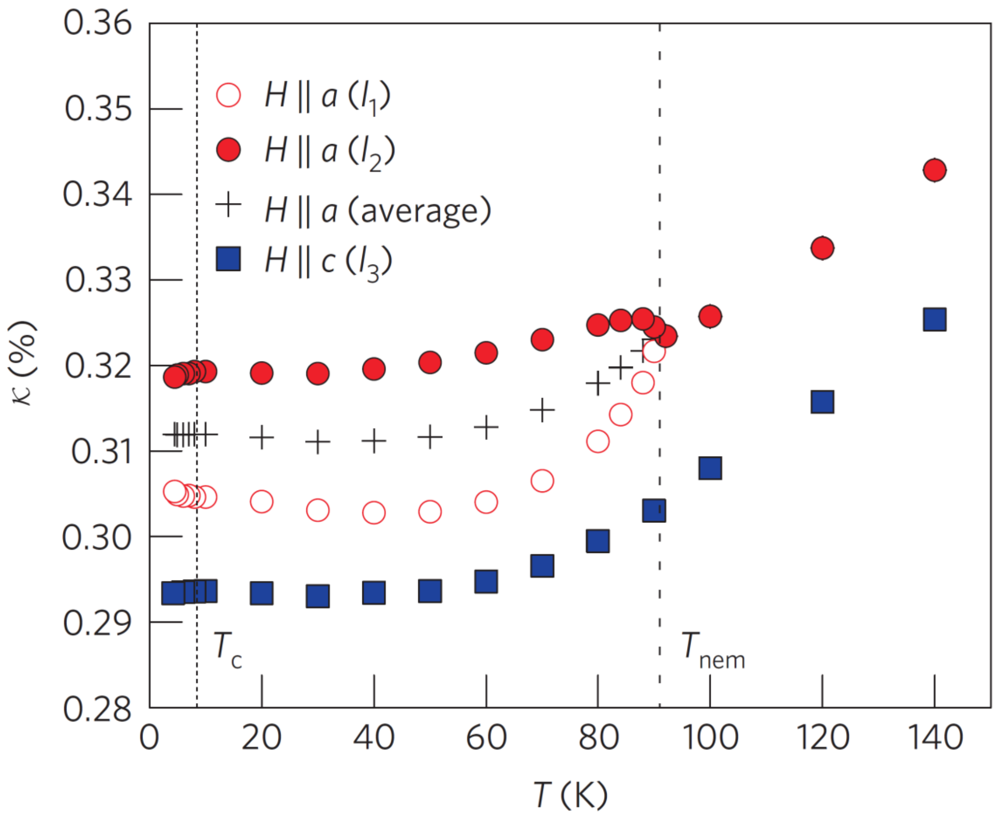
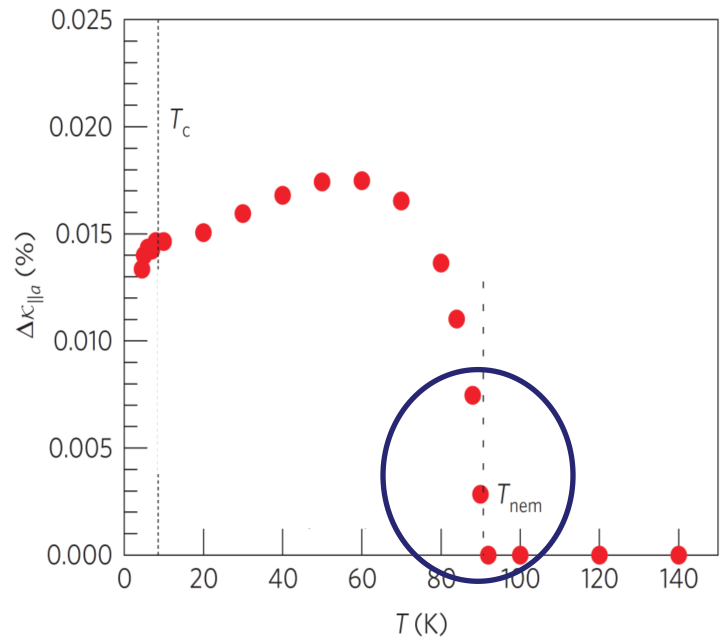
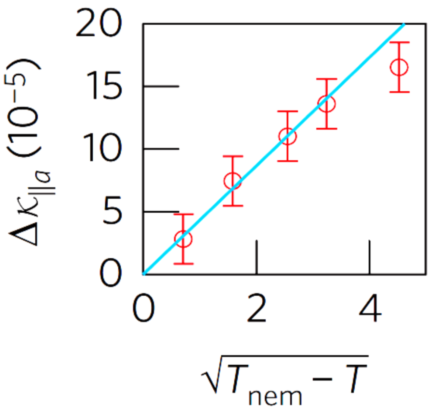
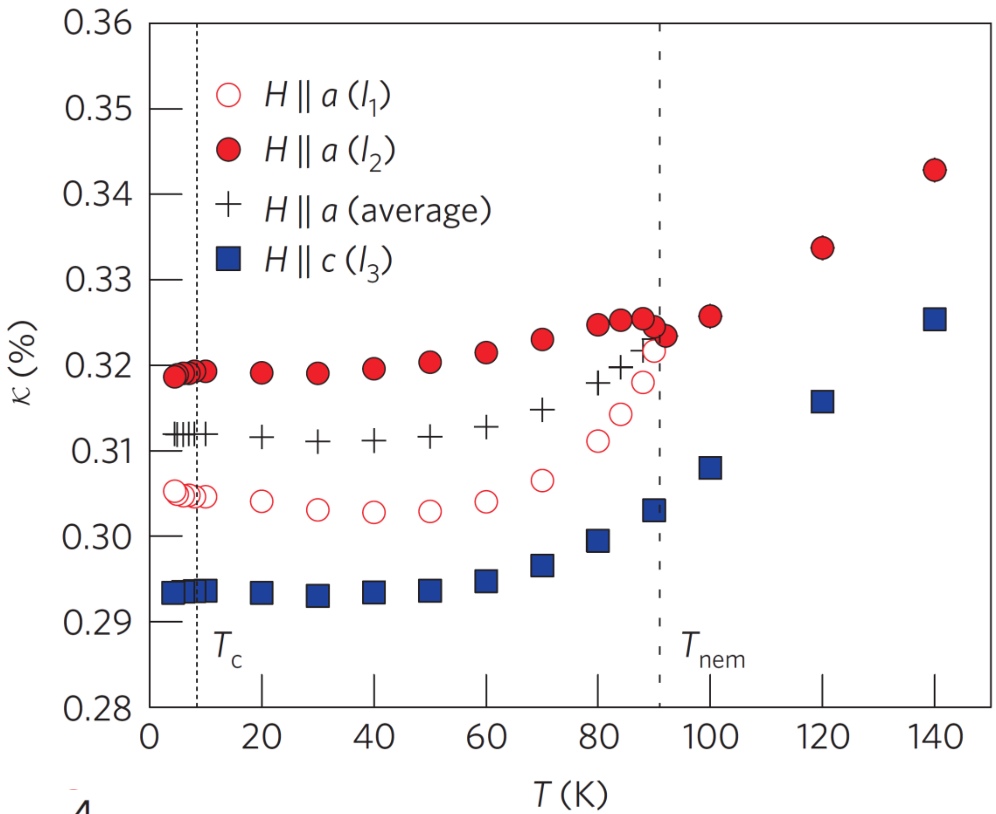


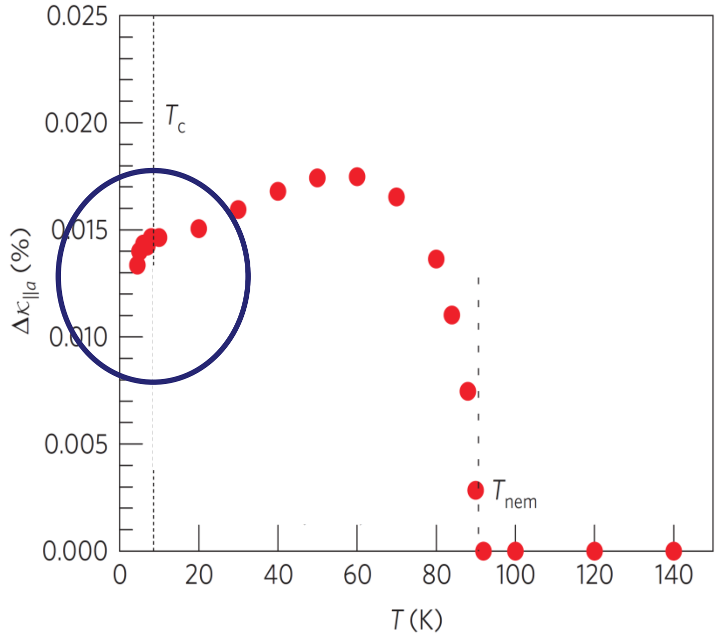


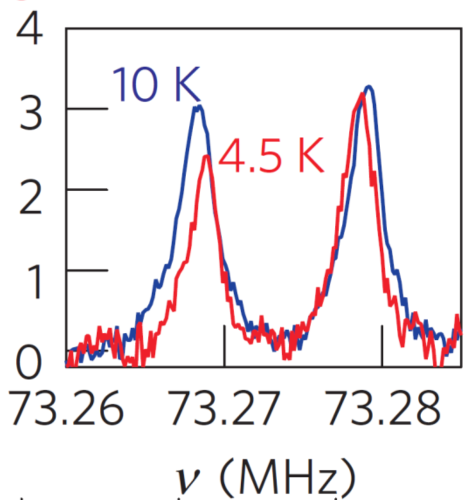


At T_{nem}: typical behavior of an order parameter

NMR on FeSe: T dependence of the line splitting





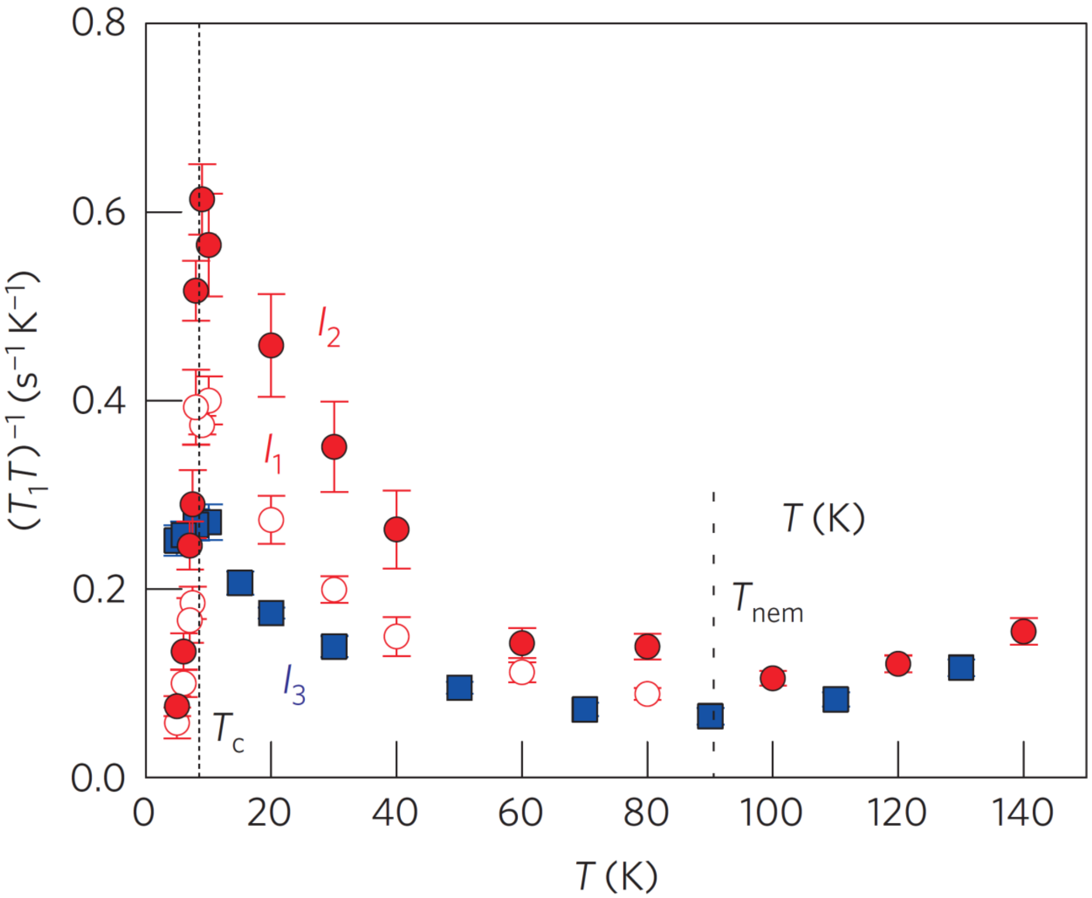


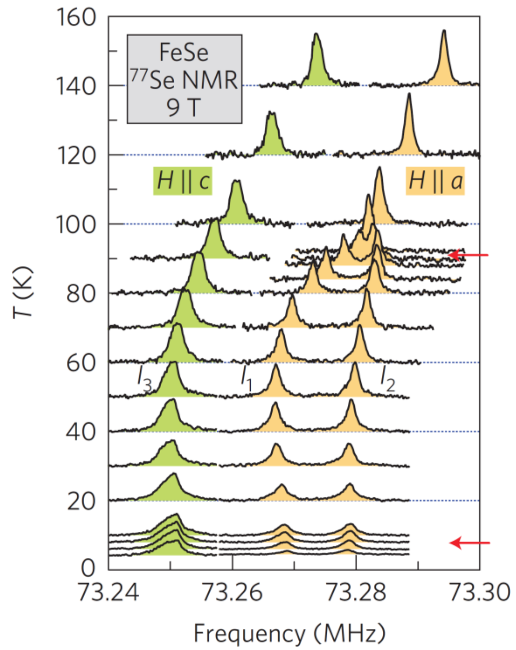
At T_c: (slight) reduction of line splitting

- typical for competing order parameters (FOO ←→ SC)

- supporting interpretation with electronic origin of the transition at T_{nem}

NMR on FeSe: Relaxation rate T_1



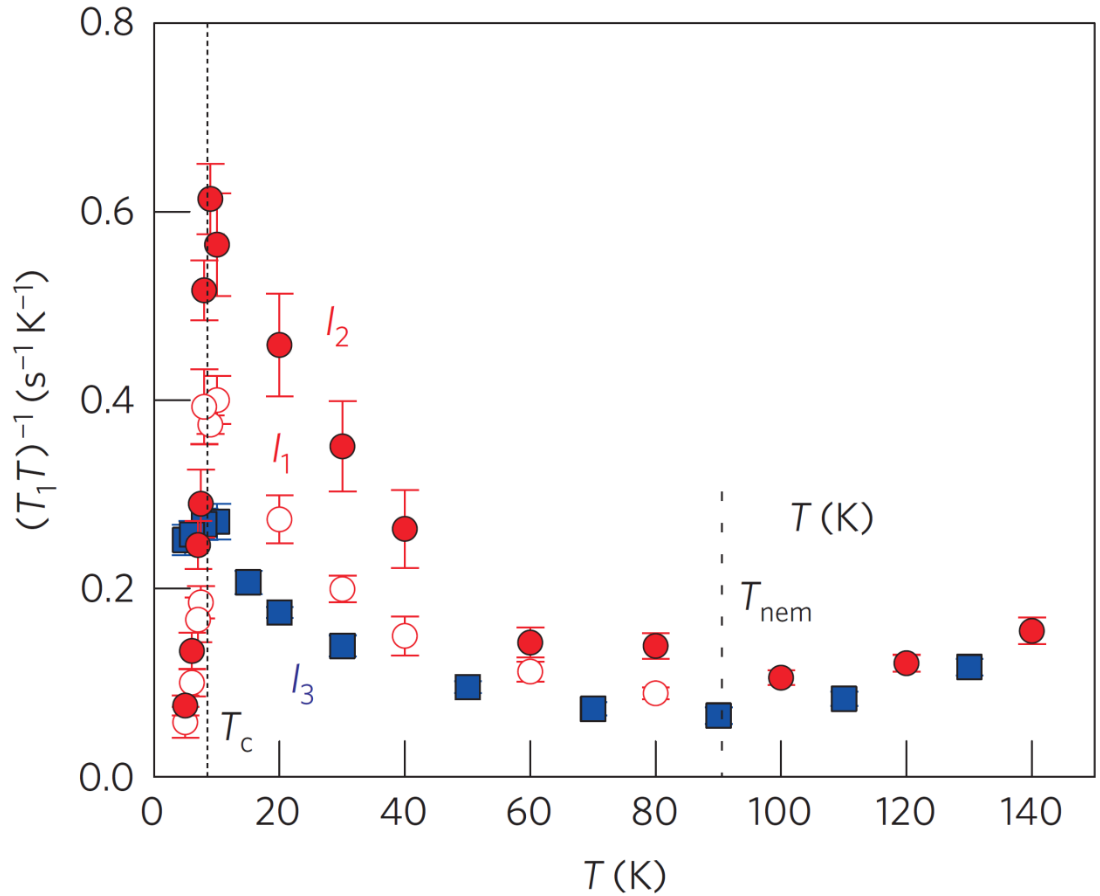


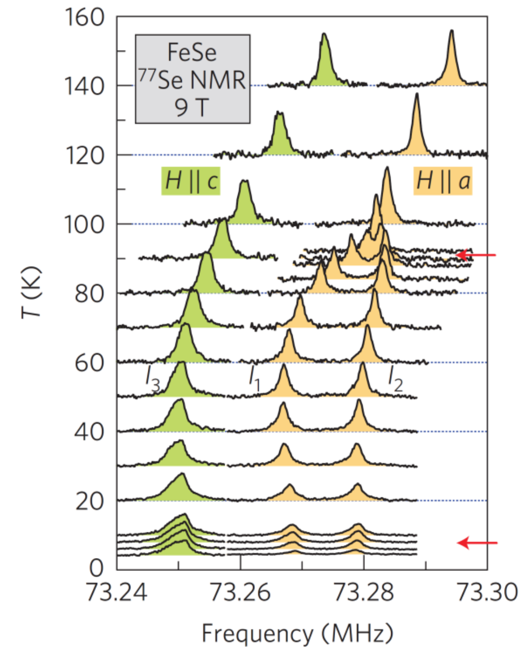
Clear differences of T_1 for the three NMR lines

anisotropic hyperfine coupling: $(T_1T)^{-1} \propto \sum_q (A_{hf}(q))^2 \chi''(q,\omega)/\omega$

Caution: T dependence of T_1 influenced by T dependend A_{hf}

NMR on FeSe: Relaxation rate T_1



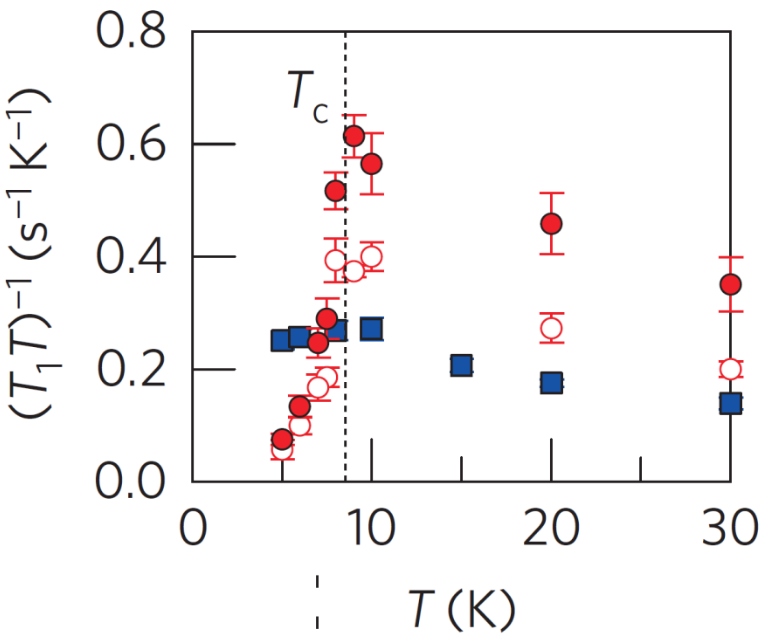


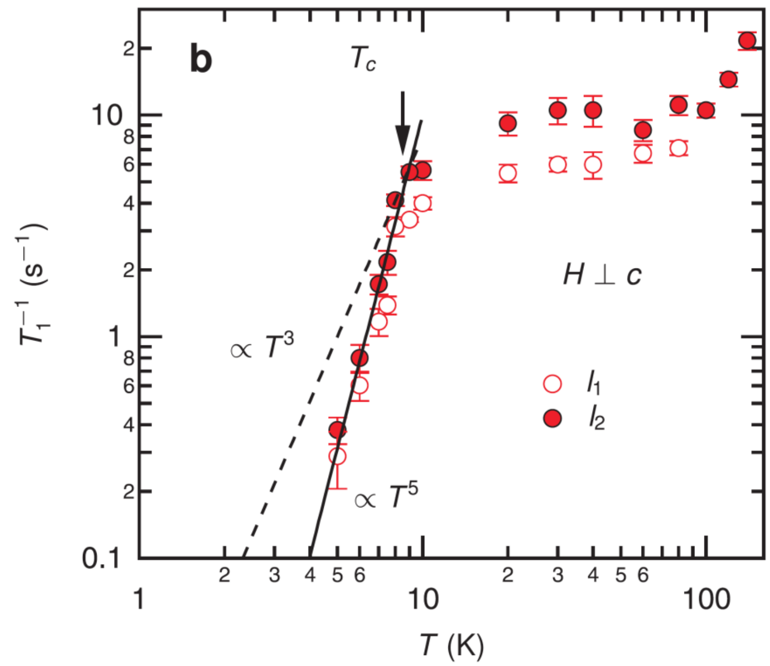
Above T_{nem}: typical T_1 for Fe based sc far away form T_N, $\mathbf{(T_1T)^{-1} \alpha\ \kappa^2_{spin}}$

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

NMR on FeSe: Relaxation rate T_1





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Elastic constant vs T_1 in Co doped Ba122

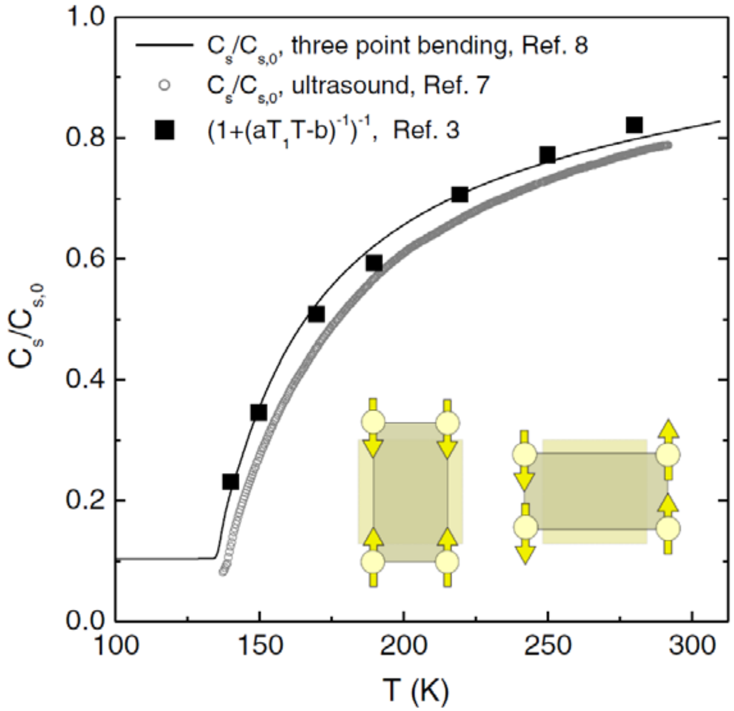


FIG. 1 (color online). Scaling between the shear modulus C_s (open symbols, from Ref. [7], continuous line from Ref. [8]) and the NMR spin-lattice relaxation rate $1/T_1$ (closed symbols, from Ref. [3]) in the tetragonal phase of the parent compound $BaFe_2As_2$. $C_{s,0}$ denotes the noncritical, high-temperature shear modulus. The fitting parameters are $a = 0.65\,(\mathrm{sK})^{-1}$ and $b = 1.3$ in Eq. (2). The inset schematically represents the magnetoelastic coupling, which makes bonds connecting antiparallel (parallel) spins expand (shrink).

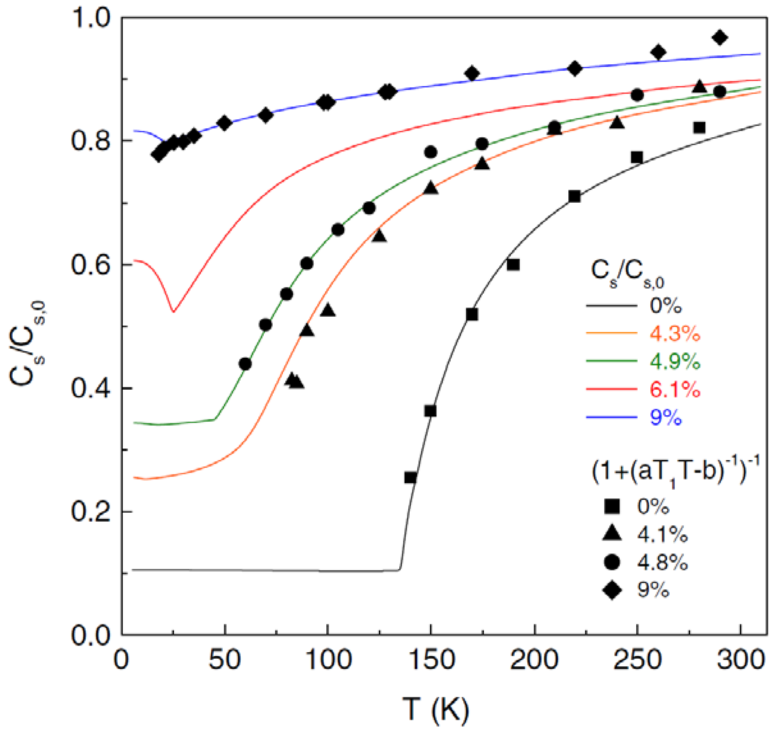
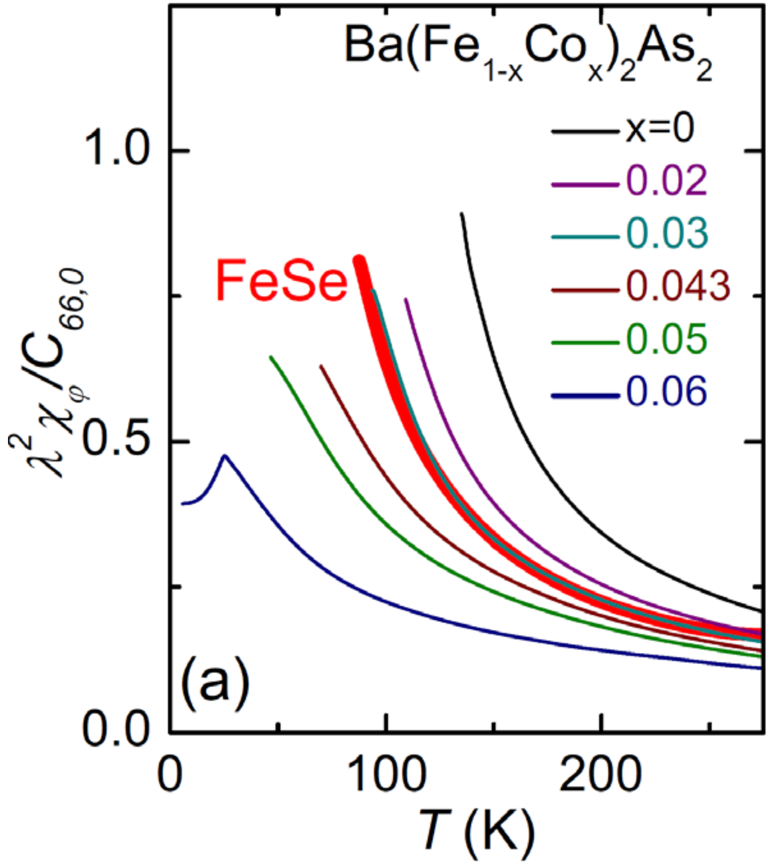


FIG. 2 (color online). Comparison between the relative shear modulus $C_s/C_{s,0}$ (continuous lines, from Ref. [8]) and the rescaled NMR $1/T_1T$ (closed symbols, from Ref. [3]) for different "effective" Co concentrations in $Ba(Fe_{1-x}Co_x)_2As_2$. The

R.M. Fernandes, A.E. Böhmer, C. Meingast, and J. Schmalian, PRL 2013

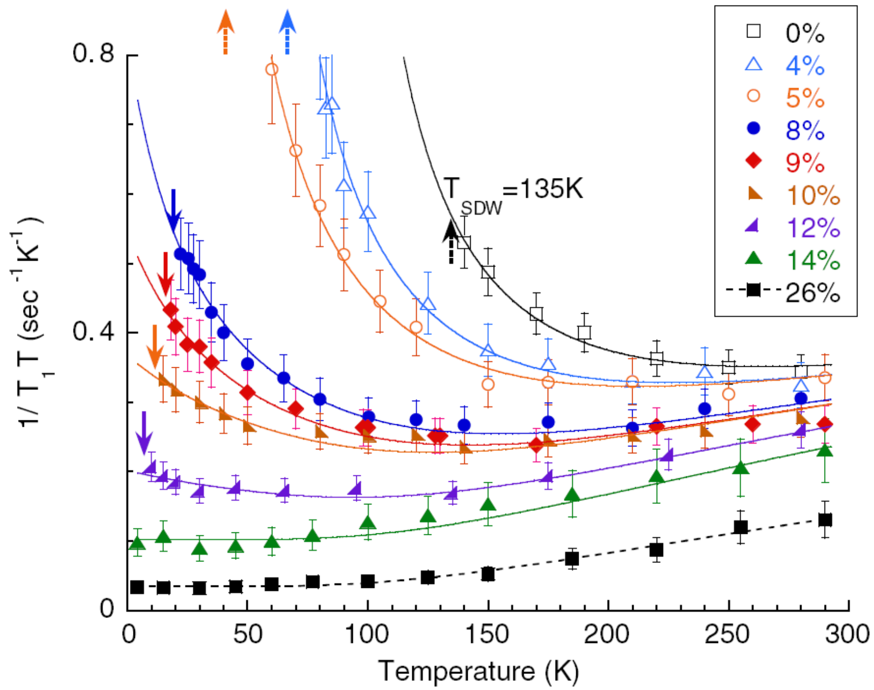
Strong evidence for a magnetically driven structural phase transition in (doped) Ba-122!

Elastic constant vs T1 in FeSe



A.E. Böhmer et al., ArXiv: 1407.5497

NMR on $Ba(Fe_{1-x}Co_x)_2As_2$:

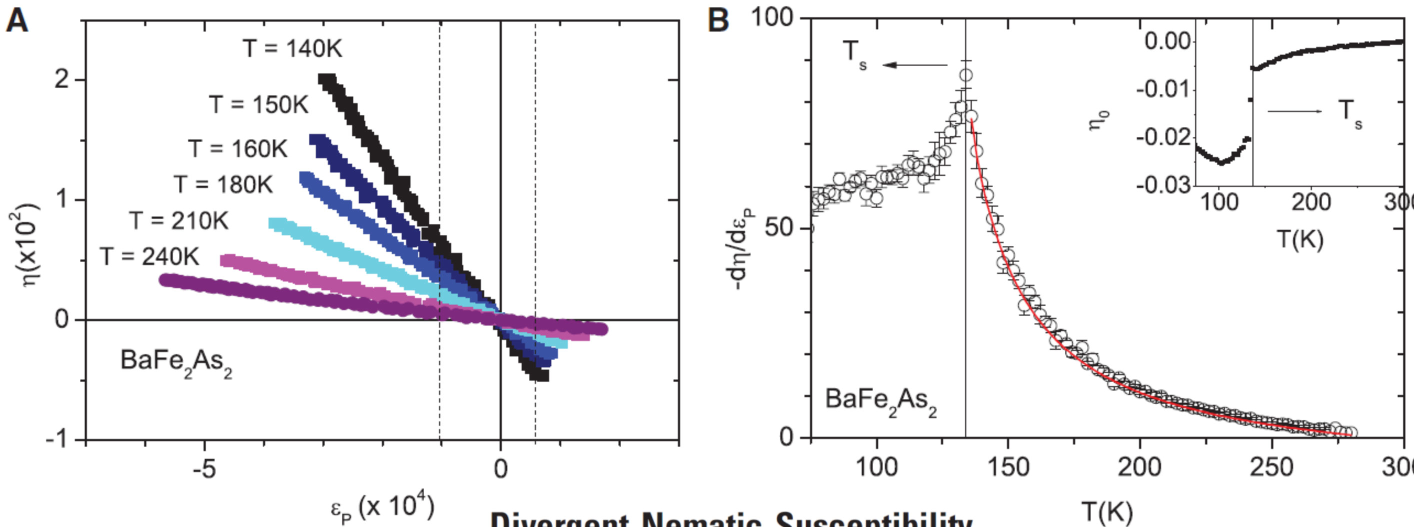


Ning *et al.* PRL 104, 037001 (2010)

No evidence for a magnetically driven structural phase transition in FeSe!

Divergent nematic susceptibility in (doped) Ba122

Fig. 2. (**A**) Representative data for $BaFe_2As_2$ showing the relative change of resistivity ($\eta = \Delta\rho/\rho_0$) as a function of strain ($\varepsilon_P = \Delta L/L$) at several temperatures above T_S. The nematic response was obtained by a linear fit of the data near zero applied voltage [$-5 \times 10^{-5} < \varepsilon_P(V) - \varepsilon_P(0) < 1 \times 10^{-4}$, indicated by the vertical dashed lines]. (**B**) Temperature dependence of the nematic response $d\eta/d\varepsilon_P$. Vertical line indicates the struc-



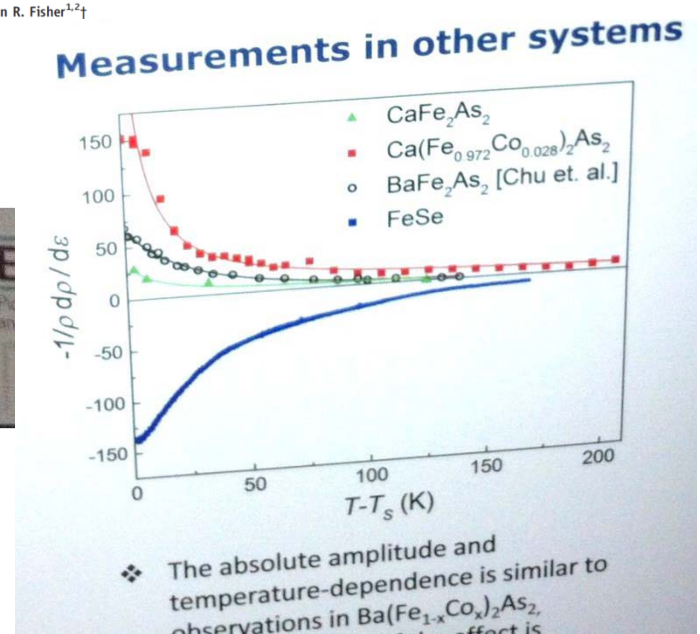
Divergent Nematic Susceptibility in an Iron Arsenide Superconductor

Jiun-Haw Chu,[1,2]*† Hsueh-Hui Kuo,[1,2] James G. Analytis,[1,2] Ian R. Fisher[1,2]†

Very similar behaviour found in FeSe

The effect of strain on the electronic properties of superconducting FeSe

A. Narayanan[1], **M. D. Watson**[1], N.R. Davies, T. Kim[2], A. A. Haghirirad[1], S. Blake[1], C. Meingast[3], T. Wolf[3], A. I. Coldea[1]
[1]Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX1 3PU, UK
[2]Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, UK
[3]Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany



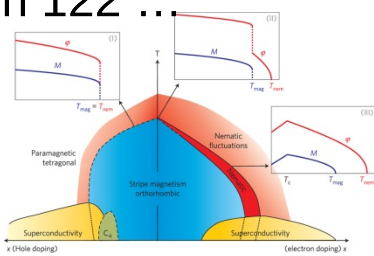
NMR on FeSe: Consequences, Speculations…

Data: FeSe shows orbital order and pronounced nematic fluctuations!

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

but magnetic order and slow spin fluctuations are missing…

→ **(conv.) „Spin-driven“ nematicity can be excluded!**



Interpretation: Orbital fluctuations are responsible for nematic fluctuations in FeSe!

other possibilities???

Consequence: **There are orbital fluctuations in Fe based superconductors with a pronounced influence on the electronic properties!**

Speculations: Orbital fluctuations responsible for nematicity in all Fe based sc?

slowing down of spin-fluctuations (& lattice) as secondary effect

Orbital fluctuations crucial for superconductivity?

- Orbital <> lattice: large T_c in FeSe (pressure, monolayers)
- Orbital fluctuations mediate pairing in FeSe (and …)

→ theories by Kontani et al., etc. … s+/+ instead of s+/-

NMR on FeSe -- CONCLUSIONS

→ clear signatures of the structural transition in the NMR (splitting of lines)

→ pronounced anisotropy of the hyperfine coupling suggesting orbital order

→ angular dependence of the NMR signal consistent with ferro-orbital order similar to that in other Fe based superconductors

→ signatures of a competition between orbital order and superconductivity

→ structural phase transition (orbital order) decoupled from magnetic instability

→ **Clear evidence for nematic electronic order in FeSe but no evidence of a magnetic origin of this order**

Orbital-driven nematicity in FeSe

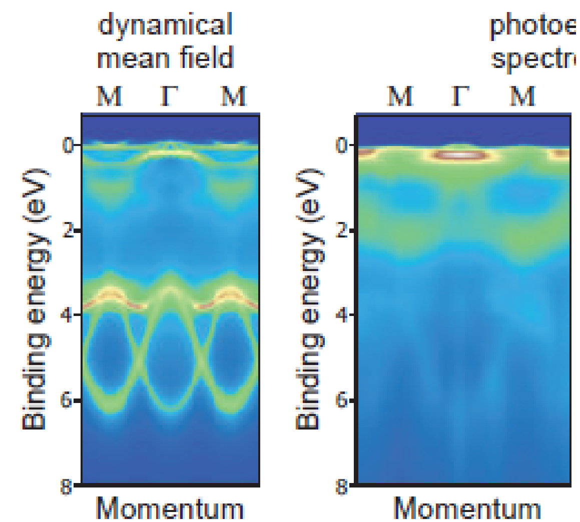
S-H. Baek[1]*, D. V. Efremov[1], J. M. Ok[2], J. S. Kim[2], Jeroen van den Brink[1,3] and B. Büchner[1,3]

nature materials

NMR	S.-H. Baek, H. Grafe	IFW Dresden
Theory	D. Efremov, J. v.d. Brink et al.	IFW Dresden
Synthesis	J. M. Ok, J. S.Kim	U Pohang

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

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



Deutsche Forschungsgemeinschaft DFG

DFG Priority Program SPP1458 (2010 – 2016):

„Iron Pnictides Superconductors: Materials and Mechanisms“