



RUB



RUHR-UNIVERSITÄT BOCHUM

# NEMATIC FLUCTUATIONS IN IRON-BASED SUPERCONDUCTORS WITHOUT STRIPE-TYPE MAGNETISM

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Fei Chen

Morten Christensen

Rafael Fernandes



UNIVERSITY OF MINNESOTA

Roser Valentí

Vladislav Borisov (Uppsala University)



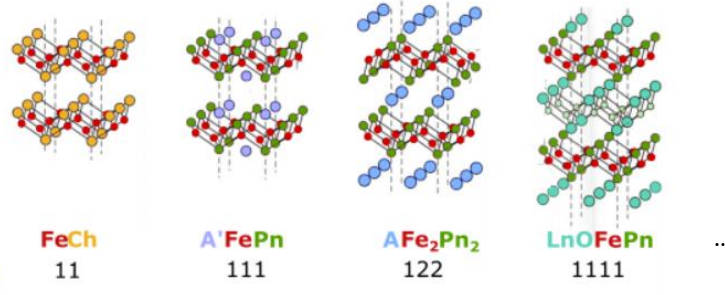
**Funding:**

*DFG SFB/TRR288 ELASTO-Q-MAT*

*Helmholtz Impuls- und Vernetzungsfond*

*Ames Laboratory, US DOE, under contract No. DE-AC02-07CH11358*

# A large variety of iron-based materials



substitutions



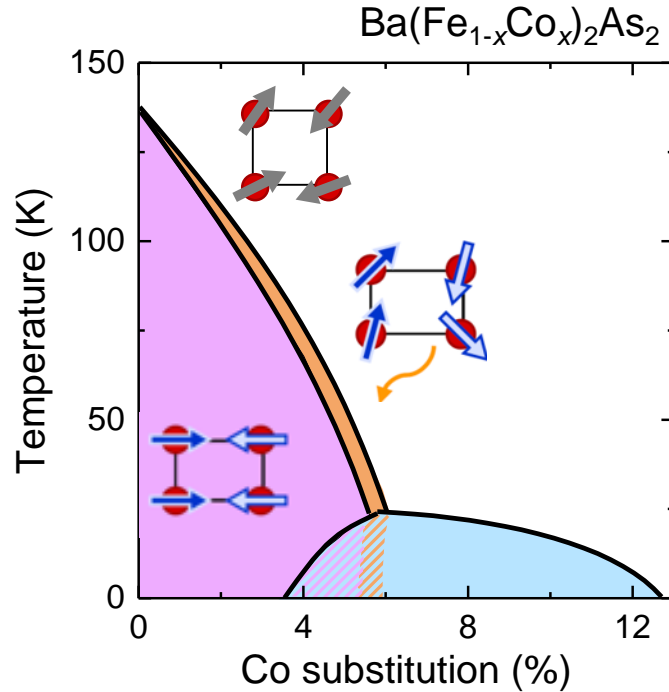
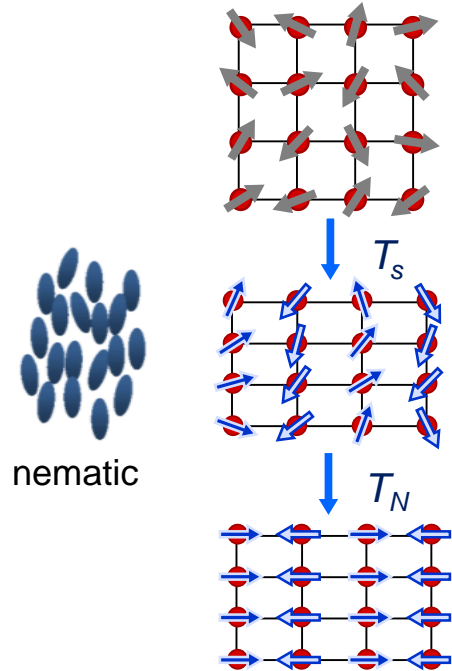
substitutions

H	A																Pn Ch										He
Li	Be																	B	C	N	O	F	Ne				
Na	Mg	Ln																	Al	Si	P	S	Cl	Ar			
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr										
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe										
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn										
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt																			

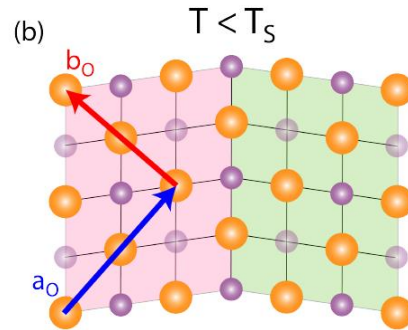
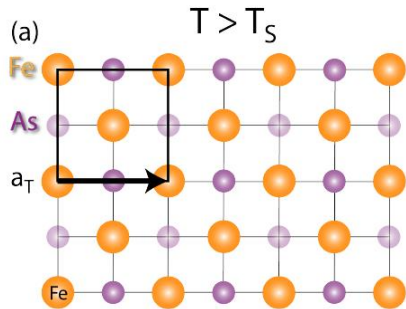
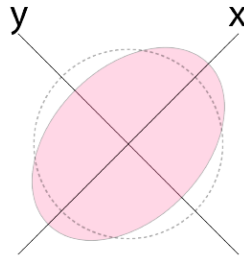
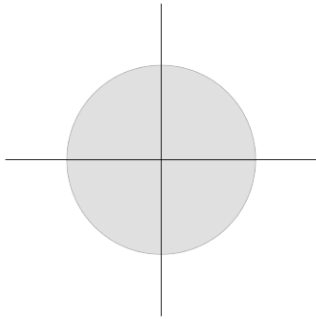
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

A. Böhmer, A. Kreyssig,  
Phys. Unserer Zeit **48**, 70 (2017)

# Typical phase diagram of 122 iron-based compounds

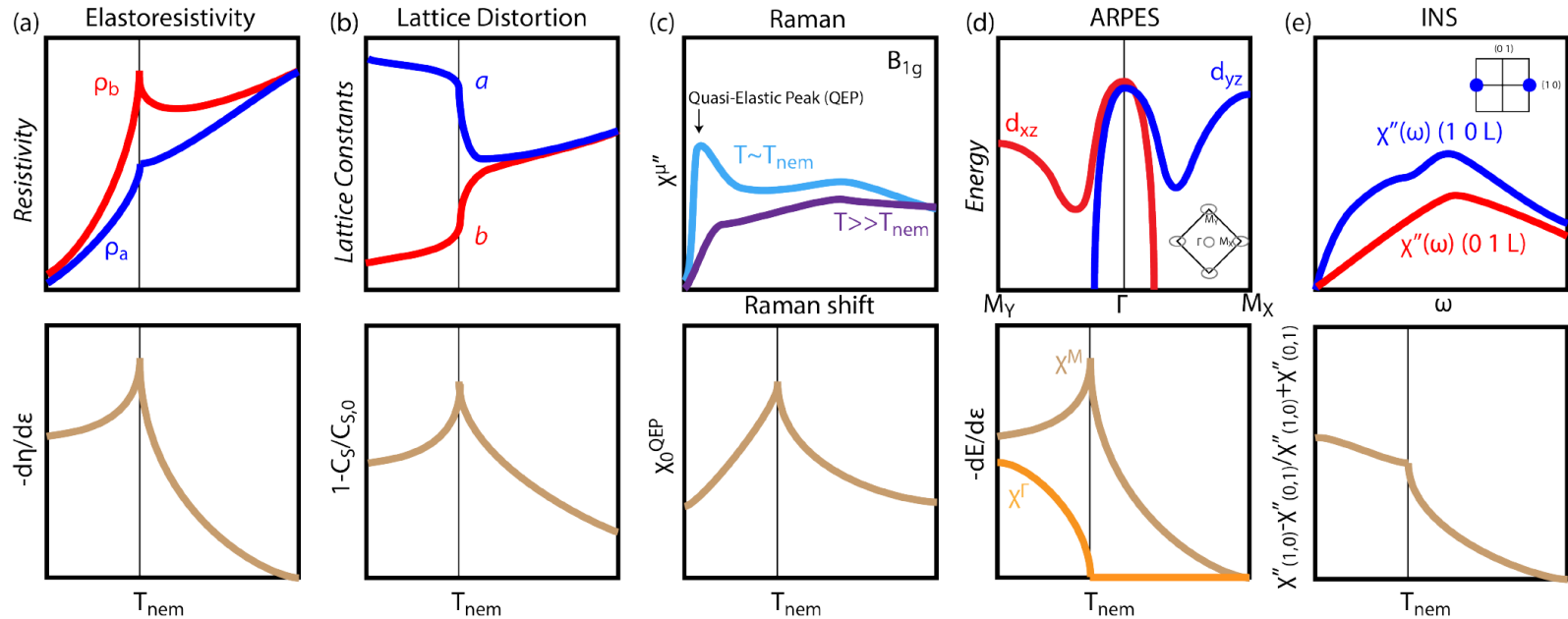


# Nematicity in iron-based superconductors



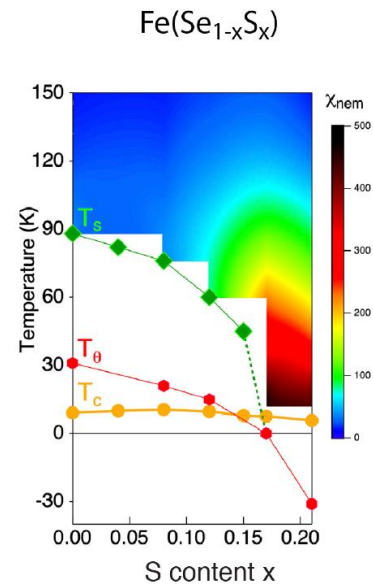
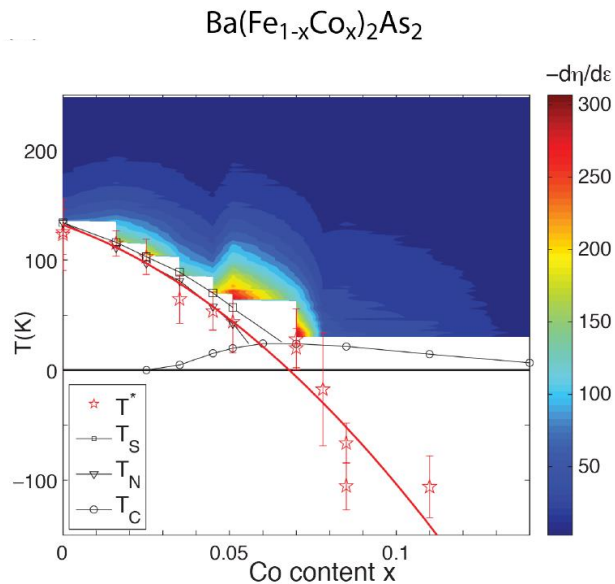
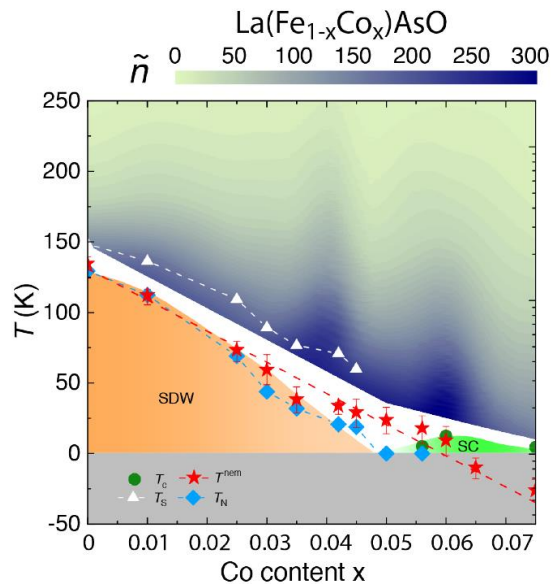
A. Böhmer, J.-H. Chu, S. Lederer and  
M. Yi, (in preparation)

# Model character of the iron-based systems (since 2008)



A. Böhmer, J.-H. Chu, S. Lederer and M. Yi, (in preparation)

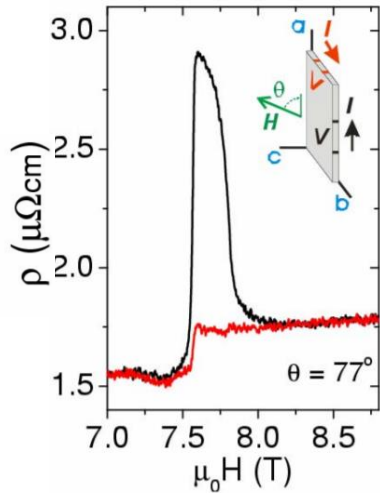
# Role of nematic fluctuations in superconducting pairing?



Hong et al., Phys. Rev. Lett. **125**, 067001 (2020)  
 Chu et al., Science **337**, 710 (2012)  
 Hosoi et al., PNAS **113**, 8139 (2016)

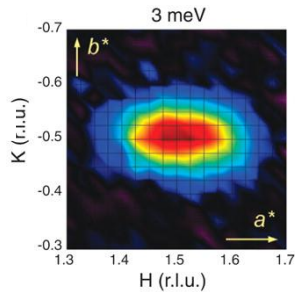
# Multiple observations of electronic anisotropy

$\text{Sr}_3\text{Ru}_2\text{O}_7$



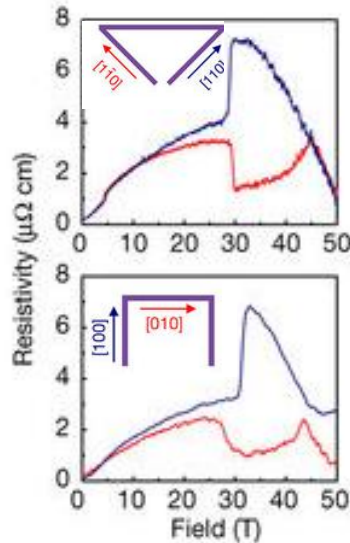
Borzi et al., Science  
**315**, 214 (2007)

$\text{YBa}_2\text{Cu}_3\text{O}_{6.45}$



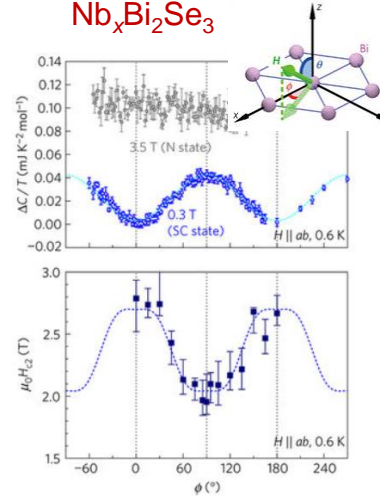
Hinkov et al., Science  
**319**, 597 (2008)

$\text{CeRhIn}_5$



Ronning et al., Nature  
**548**, 313 (2017)

$\text{Cu}_x\text{Bi}_2\text{Se}_3$   
 $\text{Sr}_x\text{Bi}_2\text{Se}_3$   
 $\text{Nb}_x\text{Bi}_2\text{Se}_3$



Yonezawa et al., Nature  
Physics **13**, 123 (2017)

$\text{Sr, BaNi}_2\text{As}_2$

$\text{CeAuSb}_2$

Magic-angle twisted  
bilayer graphene

$\text{CsV}_3\text{Sb}_5$

...

Eckberg et al., Nature  
Physics **16**, 346 (2020)

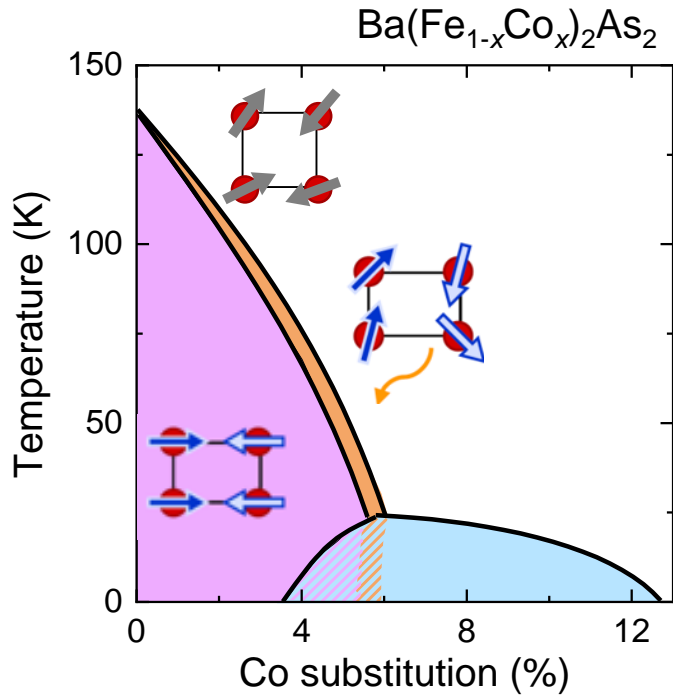
Seo et al, Phys. Rev. X  
**10**, 011035 (2020)

Cao et al., Science **372**,  
264 (2021)

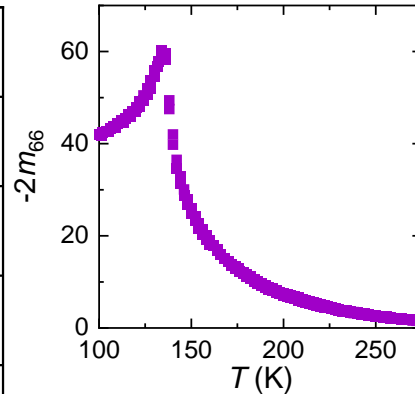
Xiang et al., arxiv  
2104.06909 (2021)



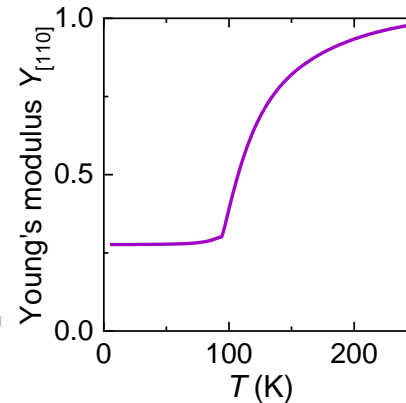
# „Nematicity standard“: $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$



Elastoresistance

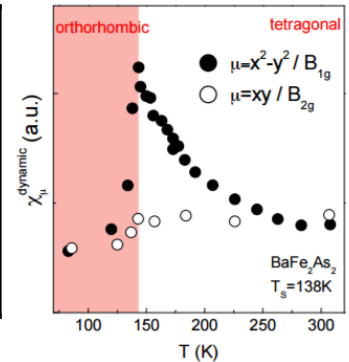


Shear modulus



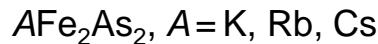
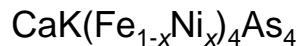
Böhmer et al., PRL 112,  
047001 (2014)

Electronic Raman



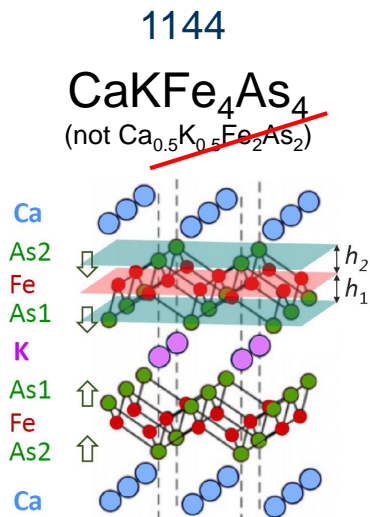
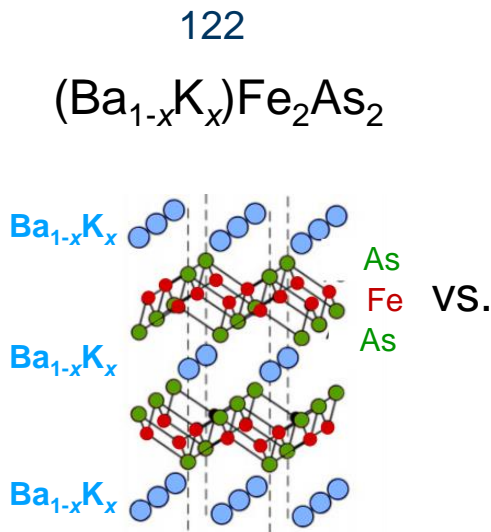
Gallais et al., Comptes  
Rendus Physique (2016)

## Iron-based materials with no stripe-type magnetic order?



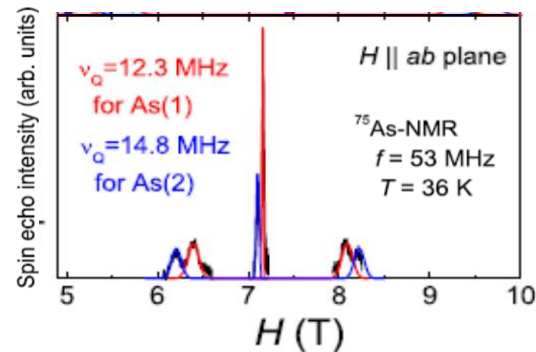
# A special derivative structure type of iron-based superconductors

K	Ca
Rb	Sr
Cs	Ba



Iyo et al., JACS 2016

Two inequivalent As sites



Cui et al, PRB **96**, 104512 (2017)

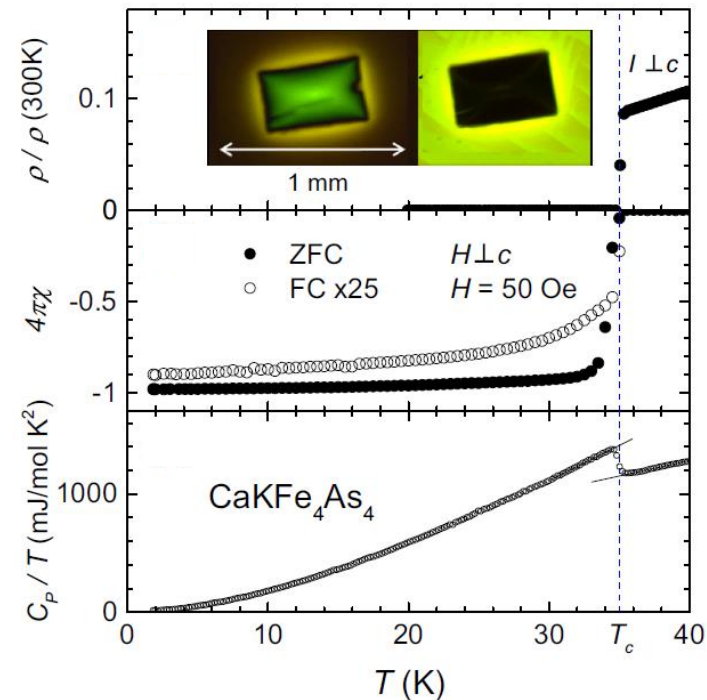
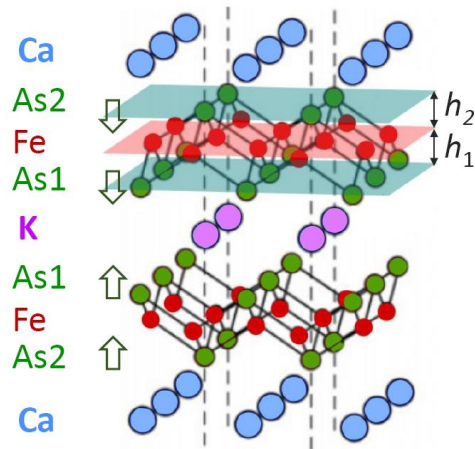
$$h_1 = 1.4124(4) \text{ \AA}$$

$$h_2 = 1.3951(4) \text{ \AA}$$

$$h_1 - h_2 = 0.0173(8) \text{ \AA}$$

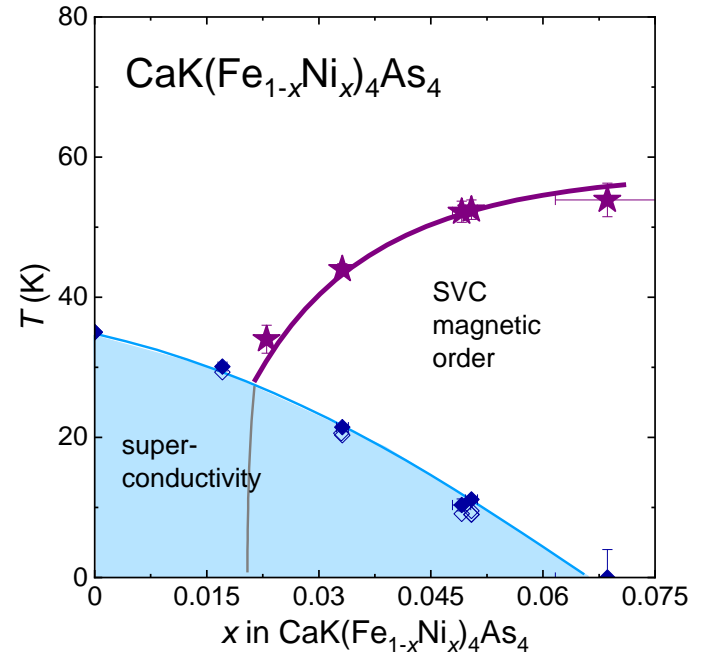
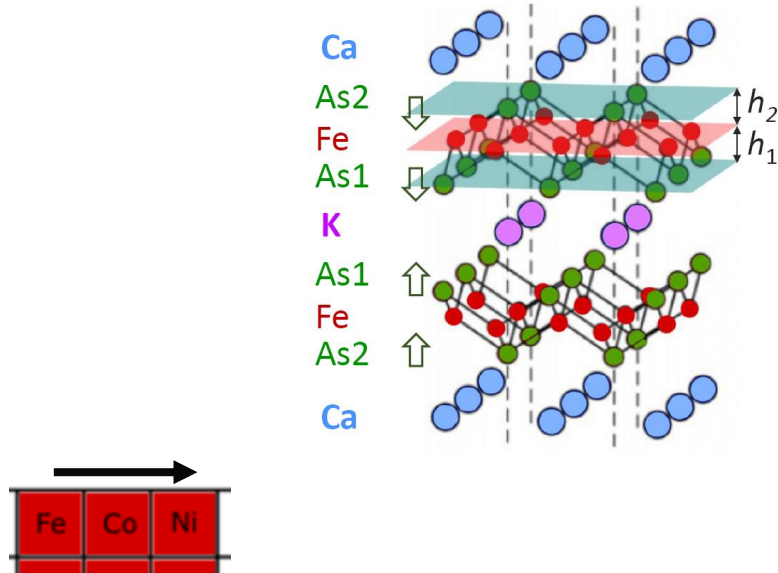
Böhmer et al., arXiv:2011.13207

# Superconductivity in $\text{CaKFe}_4\text{As}_4$



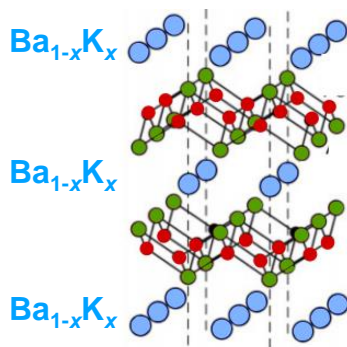
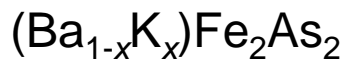
Meier et al., Phys. Rev. B, 94, 064501 (2016)

# Magnetic order achieved by electron-doping



Meier et al., npj Quantum Materials **3**, 5 (2018)

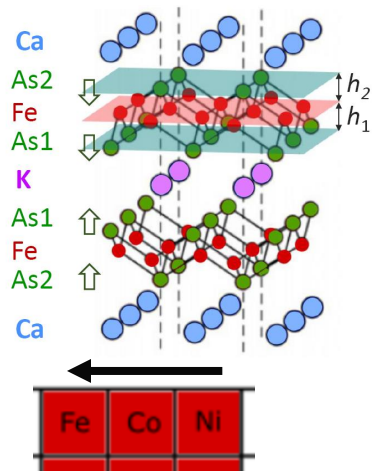
# Comparison: hole-doped 122 and electron-doped 1144



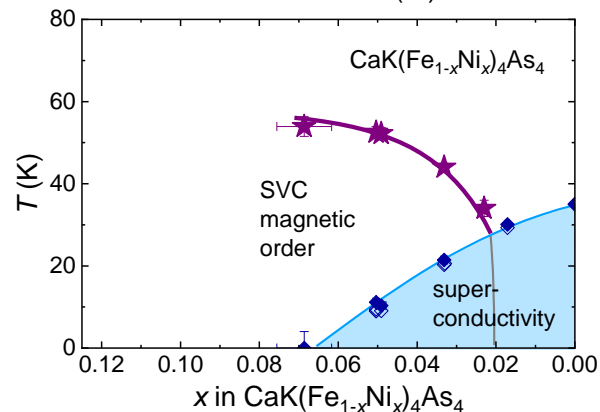
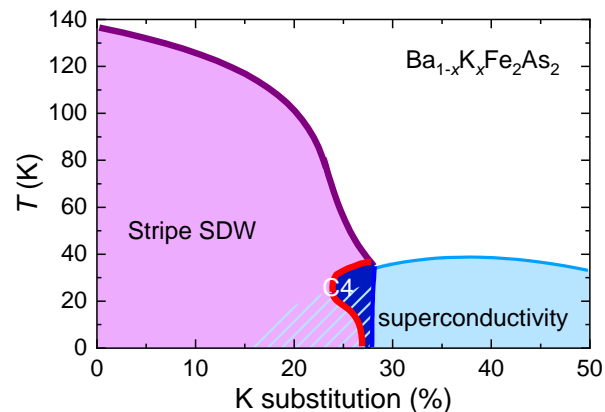
K	Ca
Rb	Sr
Cs	Ba

Meier et al., Phys. Rev. B, 94, 064501 (2016)

Meier et al., npj Quantum Materials 3, 5 (2018)



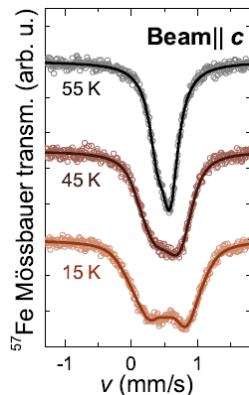
Fe	Co	Ni
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# Different magnetic order types

## Experimental evidence

### Mössbauer

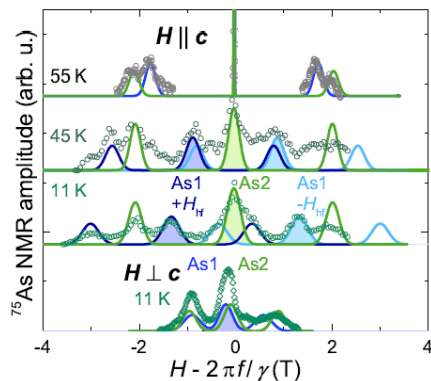


W. Meier et al., npj Quantum Materials **3**, 5 (2018)

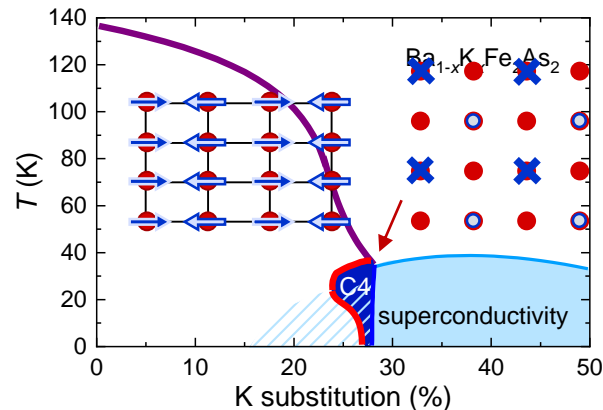
### Neutron diffraction

Kreyssig et al, Phys. Rev. B **97**, 224521 (2018)

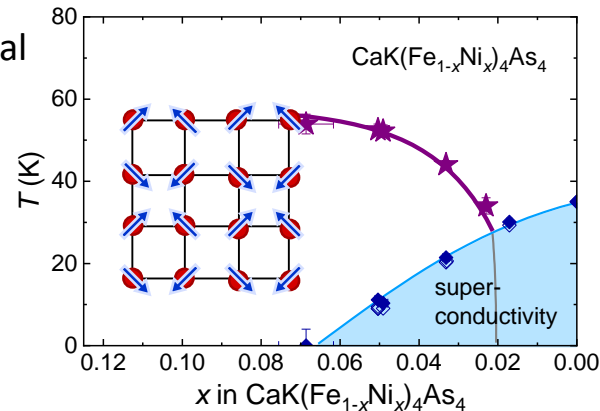
### NMR



## Stripe-type magnetic order



## Spin-vortex crystal magnetic order, hedgehog type



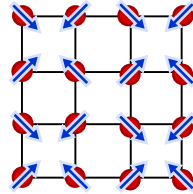
# Magnetic phases in Ginzburg-Landau parameter space

$$\mathbf{M}(\mathbf{r}) = \mathbf{M}_1 \cos(\mathbf{Q}_X \mathbf{r}) + \mathbf{M}_2 \cos(\mathbf{Q}_Y \mathbf{r})$$

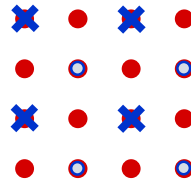
$$\mathbf{Q}_X = (\pi, 0), \mathbf{Q}_Y = (0, \pi)$$

$$\mathcal{F} = r_0 (M_1^2 + M_2^2) + \frac{u}{2} (M_1^2 + M_2^2)^2 - \frac{g}{2} (M_1^2 - M_2^2)^2 + 2w (M_1 \cdot M_2)^2$$

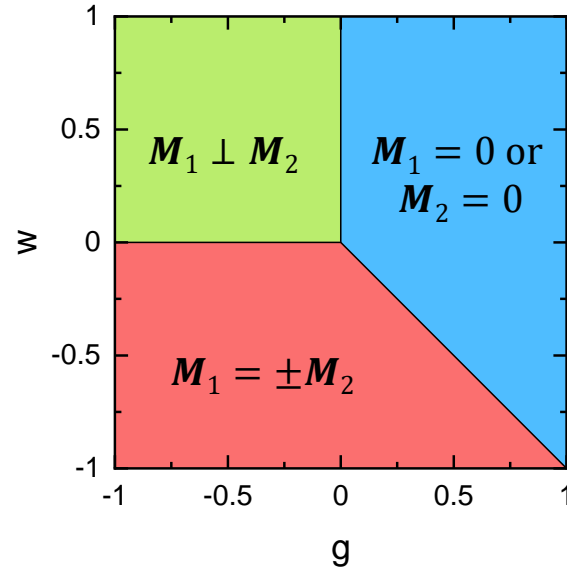
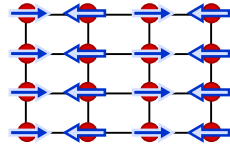
Spin-vortex crystal



Spin-charge density wave

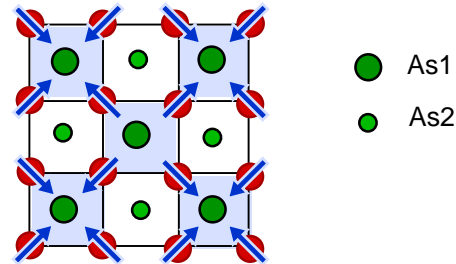
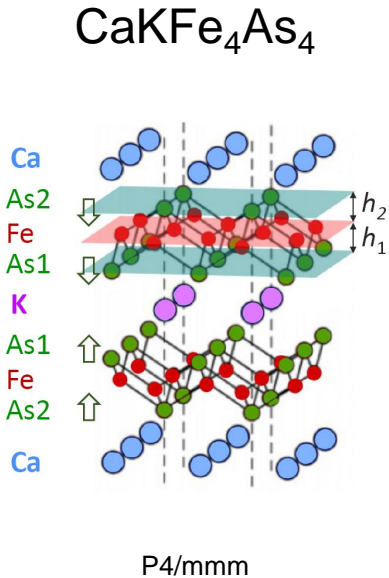


Stripe-spin density wave



Fernandes, Kivelson, and Berg, PRB **93**, 014511 (2016)

# Consequence of inequivalent As-sites in the 1144 crystal structure



## Symmetry-breaking field

- characterized by  $\boldsymbol{\eta} = \eta \hat{z}$
- couples to SVC phase:

$$F \sim -\boldsymbol{\eta} \cdot (\mathbf{M}_1 \times \mathbf{M}_2)$$



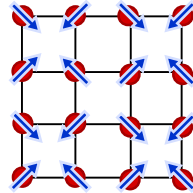
# Magnetic phases in Ginzburg-Landau parameter space

$$\mathbf{M}(\mathbf{r}) = \mathbf{M}_1 \cos(\mathbf{Q}_X \mathbf{r}) + \mathbf{M}_2 \cos(\mathbf{Q}_Y \mathbf{r})$$

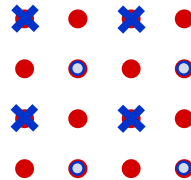
$$\mathbf{Q}_X = (\pi, 0), \mathbf{Q}_Y = (0, \pi)$$

$$\mathcal{F} = r_0 (\mathbf{M}_1^2 + \mathbf{M}_2^2) + \frac{u}{2} (\mathbf{M}_1^2 + \mathbf{M}_2^2)^2 - \frac{g}{2} (\mathbf{M}_1^2 - \mathbf{M}_2^2)^2 + 2w (\mathbf{M}_1 \cdot \mathbf{M}_2)^2$$

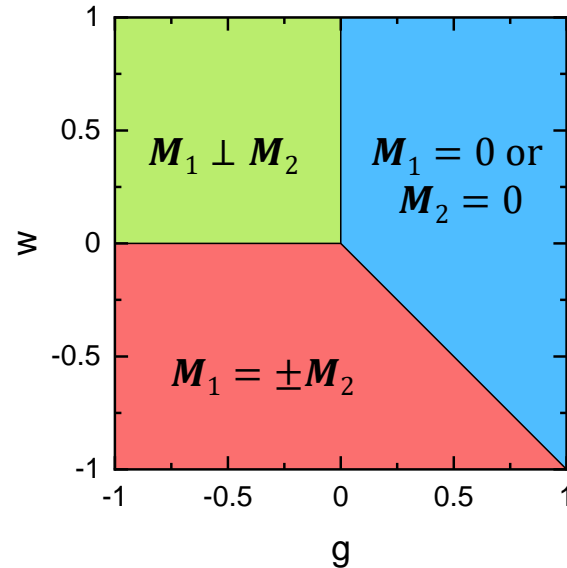
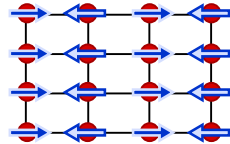
Spin-vortex crystal



Spin-charge density wave



Stripe-spin density wave



Fernandes, Kivelson, and Berg, PRB **93**, 014511 (2016)

# Magnetic phases in Ginzburg-Landau parameter space

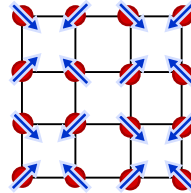
$$\mathbf{M}(\mathbf{r}) = \mathbf{M}_1 \cos(\mathbf{Q}_X \mathbf{r}) + \mathbf{M}_2 \cos(\mathbf{Q}_Y \mathbf{r})$$

$$\mathbf{Q}_X = (\pi, 0), \mathbf{Q}_Y = (0, \pi)$$

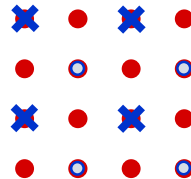
$$\mathcal{F} = r_0 (\mathbf{M}_1^2 + \mathbf{M}_2^2) + \frac{u}{2} (\mathbf{M}_1^2 + \mathbf{M}_2^2)^2 - \frac{g}{2} (\mathbf{M}_1^2 - \mathbf{M}_2^2)^2 + 2w (\mathbf{M}_1 \cdot \mathbf{M}_2)^2 - \eta (\mathbf{M}_1 \times \mathbf{M}_2) \cdot \hat{z},$$

Effect on nematic fluctuations?

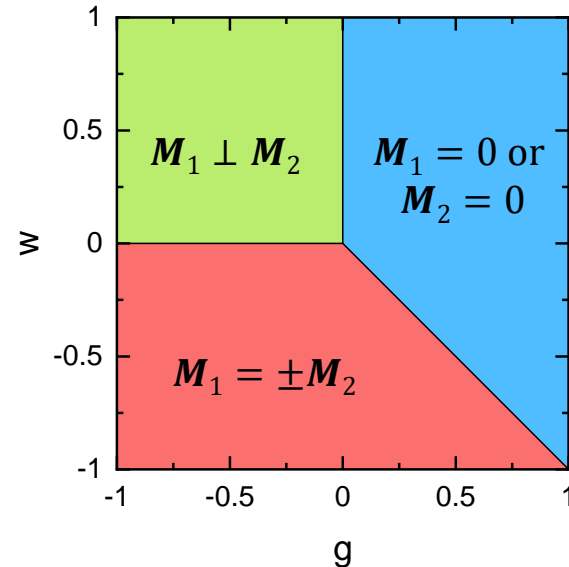
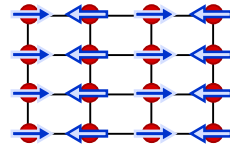
Spin-vortex crystal



Spin-charge density wave

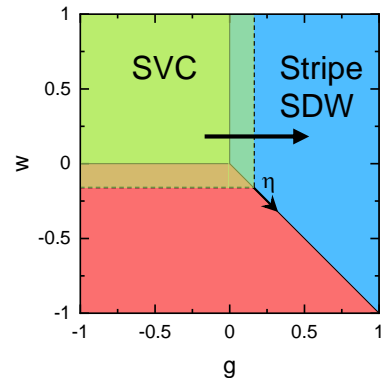


Stripe-spin density wave



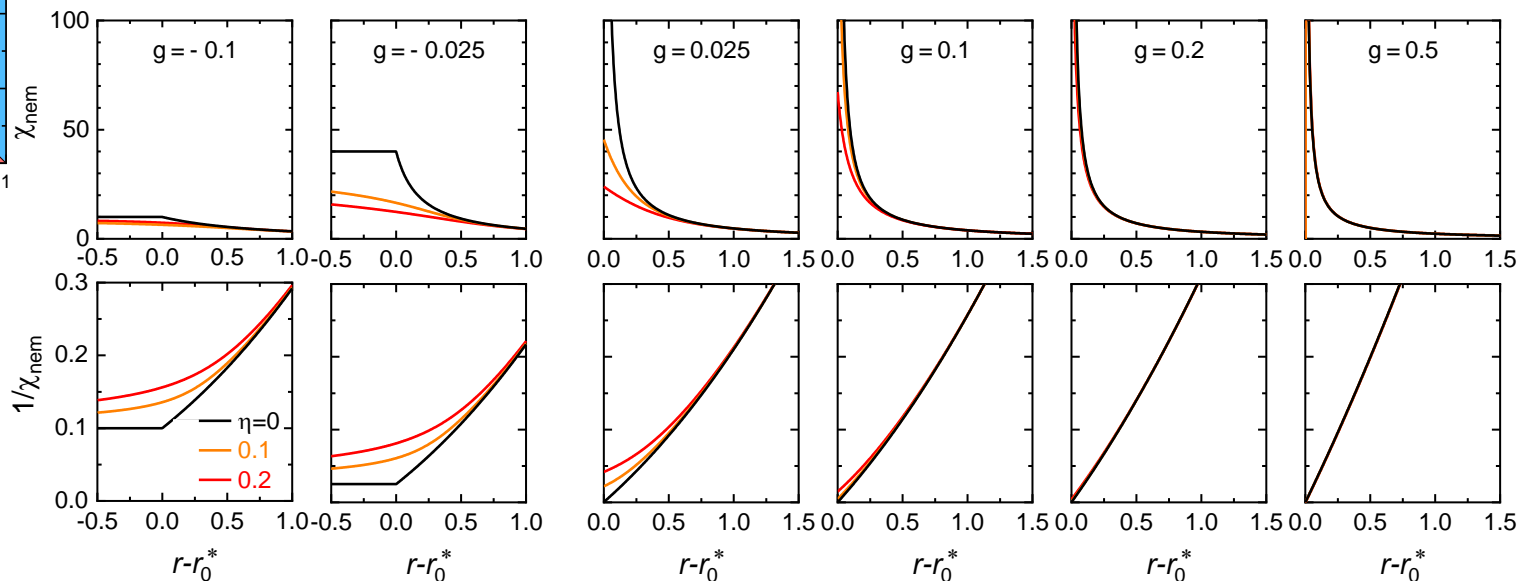
Fernandes, Kivelson, and Berg, PRB **93**, 014511 (2016)

# Expectation for nematic susceptibility



Ginzburg-Landau, 2 dimensions

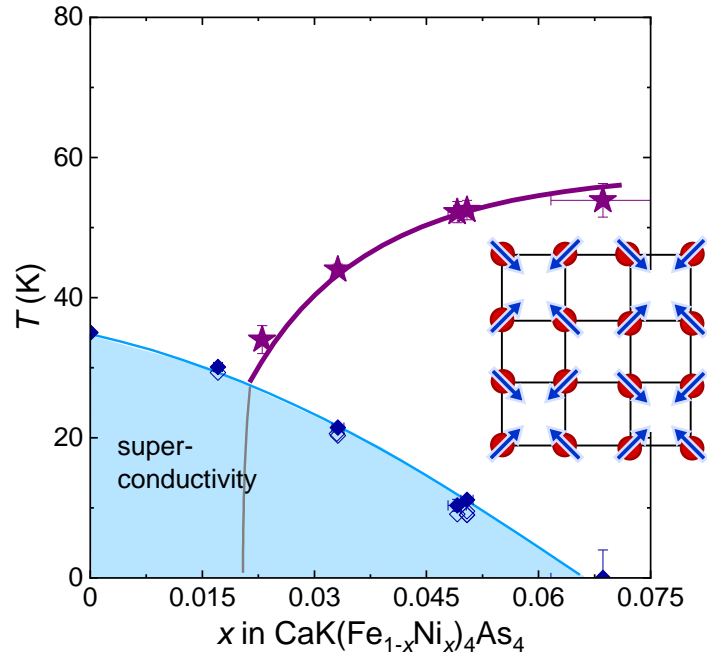
M. Christensen, Fei Chen



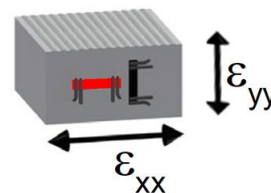
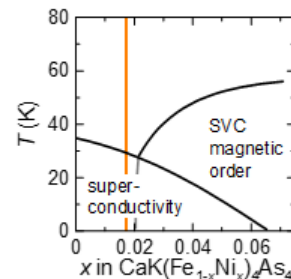
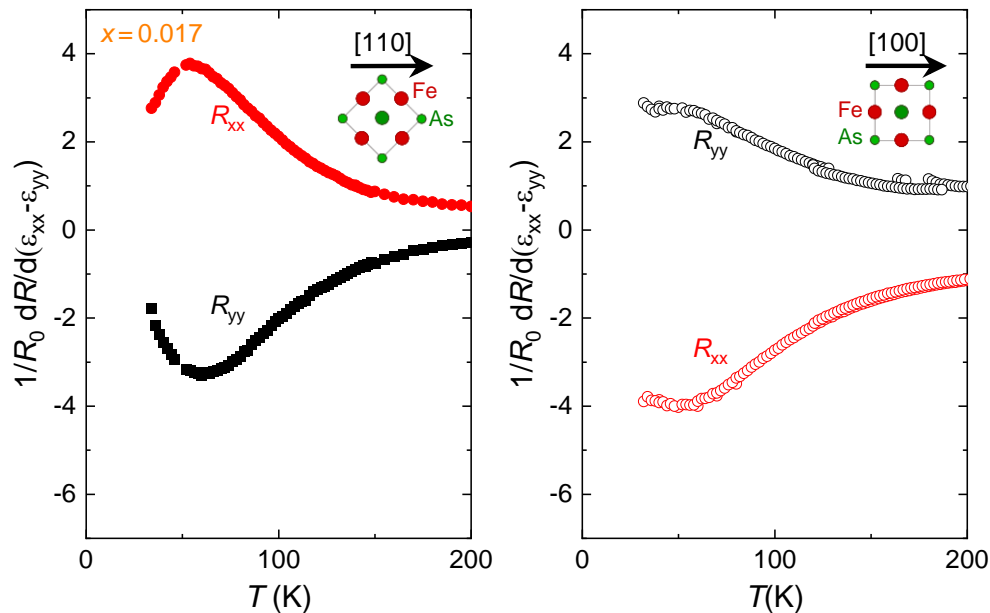
Böhmer et al.,  
arXiv:2011.13207

# Experimental study of the nematic susceptibility

- Elastoresistance
- Elastic modulus



# Elastoresistance of $\text{CaK}(\text{Fe}_{1-x}\text{Ni}_x)_4\text{As}_4$



$$m_{B_{2g}} = k \cdot \chi_{\text{nem}}^{B_{2g}}$$

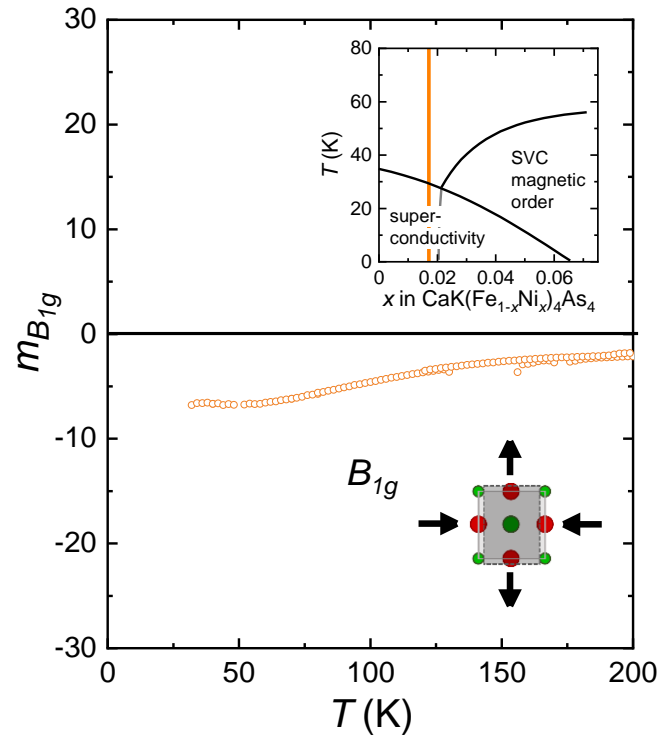
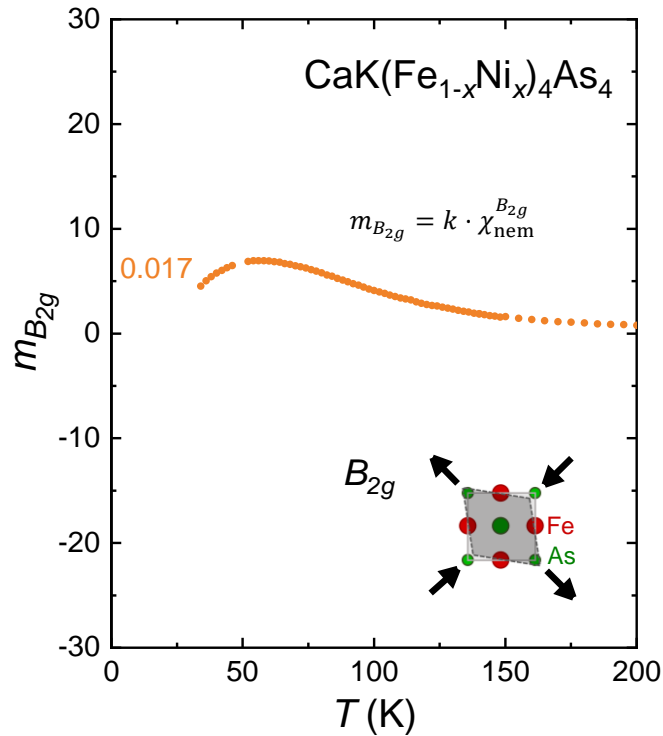
$$m_{A_{1g}} = \frac{1}{1 - \nu_{[100]}} \left[ \frac{d(\Delta R/R_0)_{[100]}}{d\epsilon_{[100]}} + \frac{d(\Delta R/R_0)_{[010]}}{d\epsilon_{[010]}} \right]$$

$$= \frac{1}{1 - \nu_{[110]}} \left[ \frac{d(\Delta R/R_0)_{[110]}}{d\epsilon_{[110]}} + \frac{d(\Delta R/R_0)_{[\bar{1}10]}}{d\epsilon_{[\bar{1}10]}} \right]$$

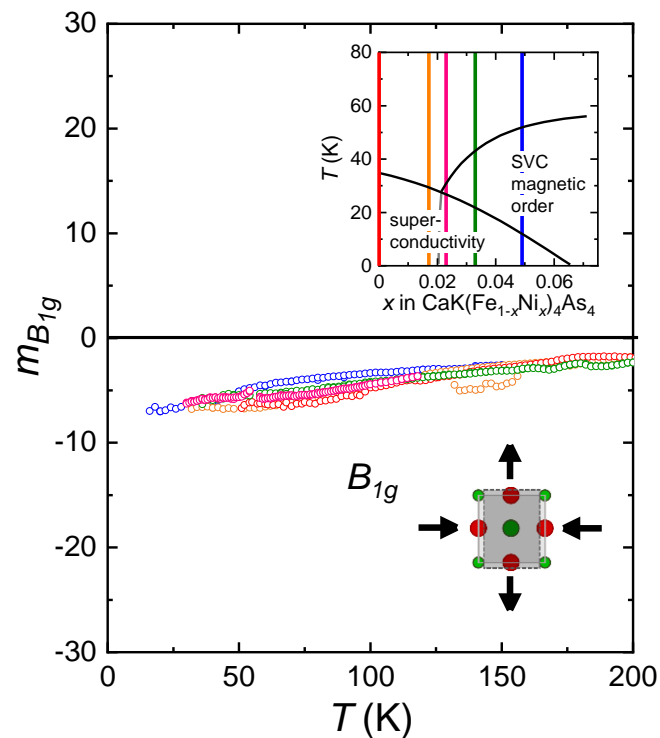
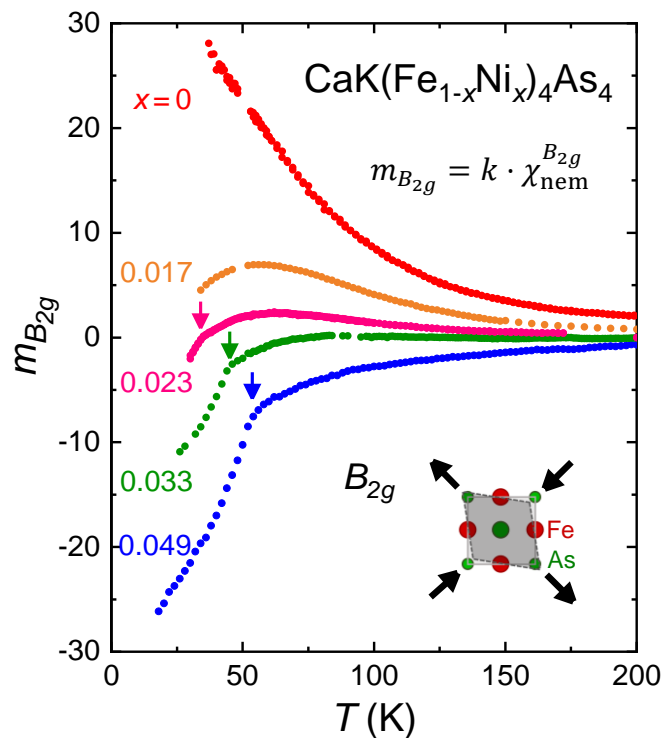
$$m_{B_{1g}} = \frac{1}{1 + \nu_{[100]}} \left[ \frac{d(\Delta R/R_0)_{[100]}}{d\epsilon_{[100]}} - \frac{d(\Delta R/R_0)_{[010]}}{d\epsilon_{[010]}} \right]$$

$$m_{B_{2g}} = \frac{1}{1 + \nu_{[110]}} \left[ \frac{d(\Delta R/R_0)_{[110]}}{d\epsilon_{[110]}} - \frac{d(\Delta R/R_0)_{[\bar{1}10]}}{d\epsilon_{[\bar{1}10]}} \right]$$

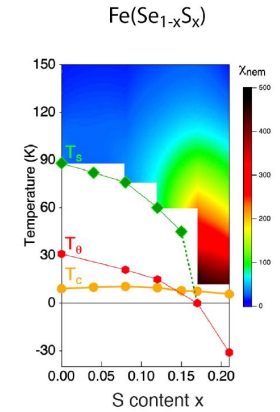
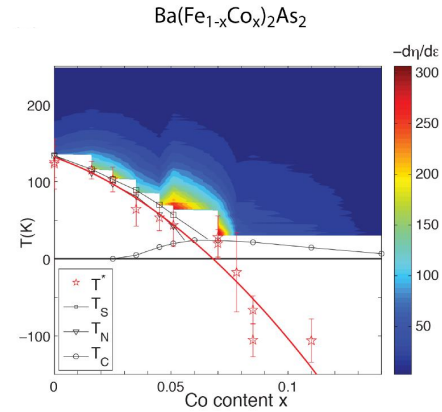
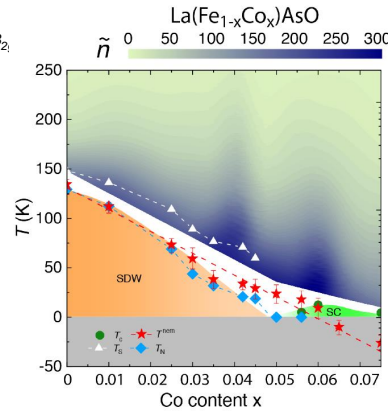
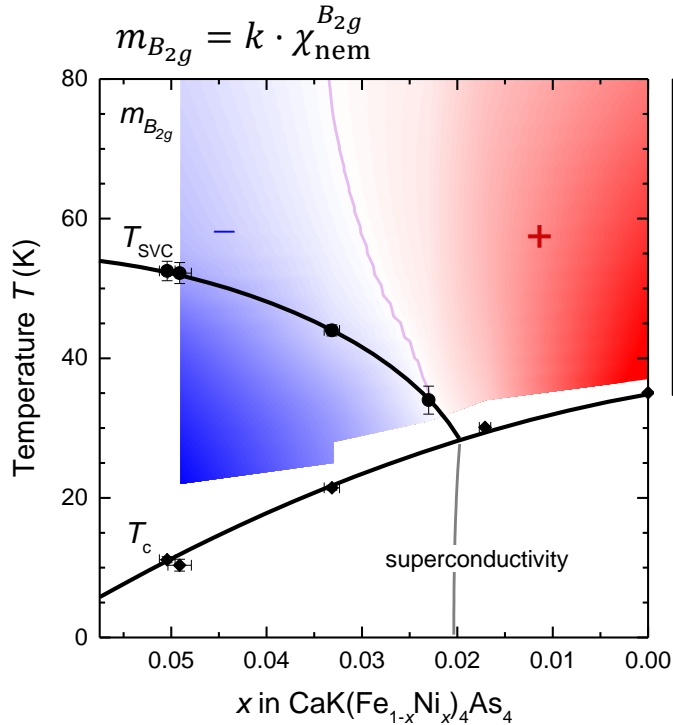
# Elastoresistance of $\text{CaK}(\text{Fe}_{1-x}\text{Ni}_x)_4\text{As}_4$



# Elastoresistance of $\text{CaK}(\text{Fe}_{1-x}\text{Ni}_x)_4\text{As}_4$

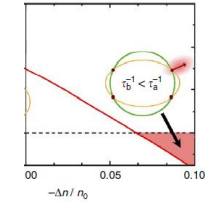


# Unexpected(?) sign change of the elastoresistance



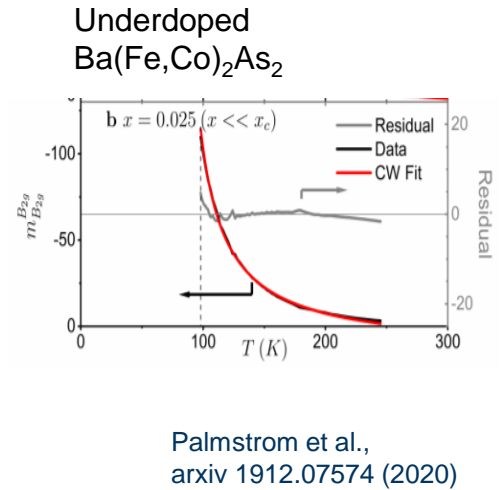
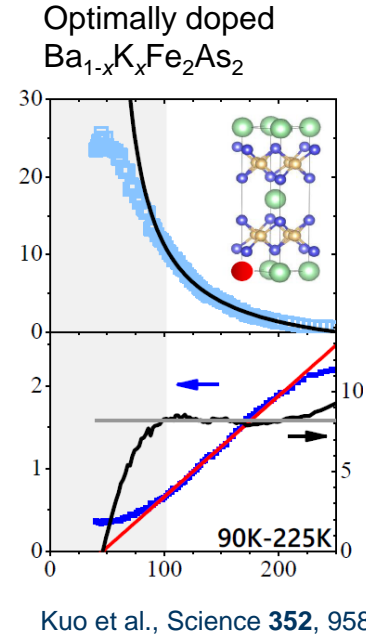
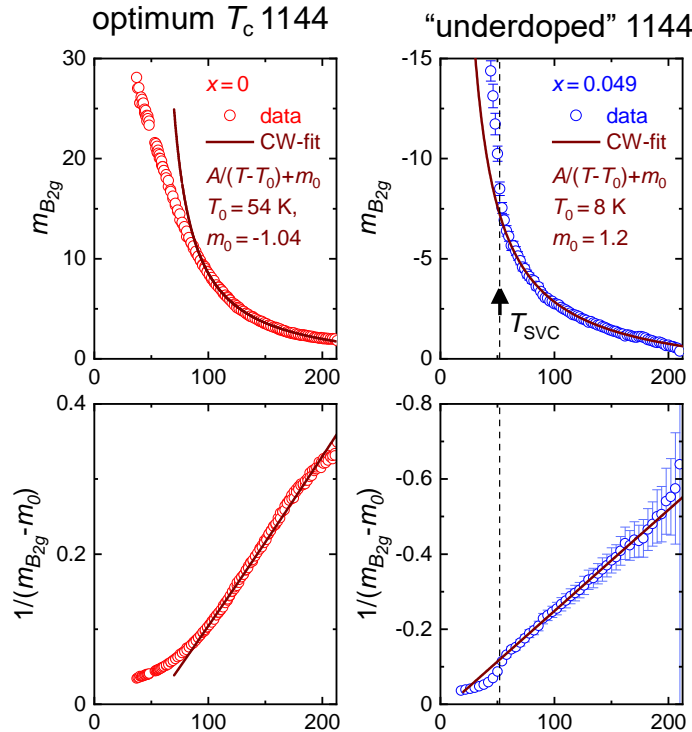
Hong et al., Phys. Rev. Lett. **125**, 067001 (2020)  
 Chu et al., Science **337**, 710 (2012)  
 Hosoi et al., PNAS **113**, 8139 (2016)

See:  
 Blomberg et al., Nat. Commun. **4**, 1914 (2013)  
 Sanchez et al., arXiv:2006.09444

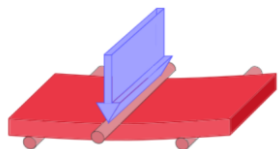




# Temperature dependence of the elastoresistance



# Bending modulus of $\text{CaK}(\text{Fe},\text{Ni})_4\text{As}_4$

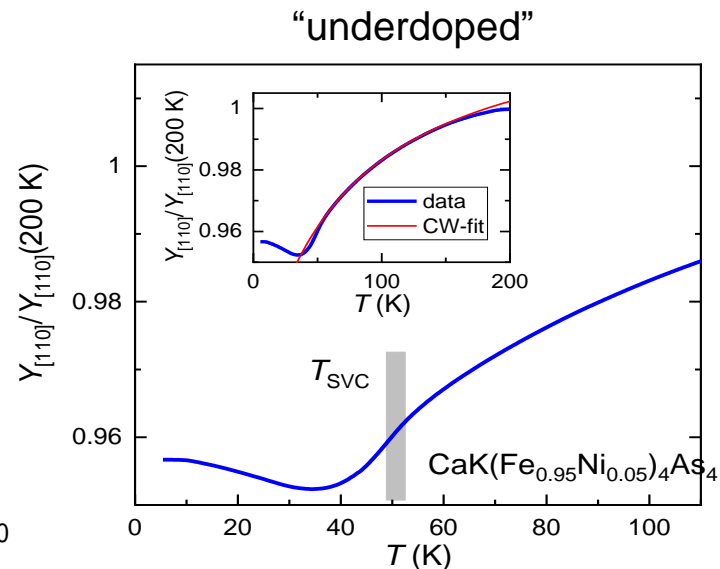
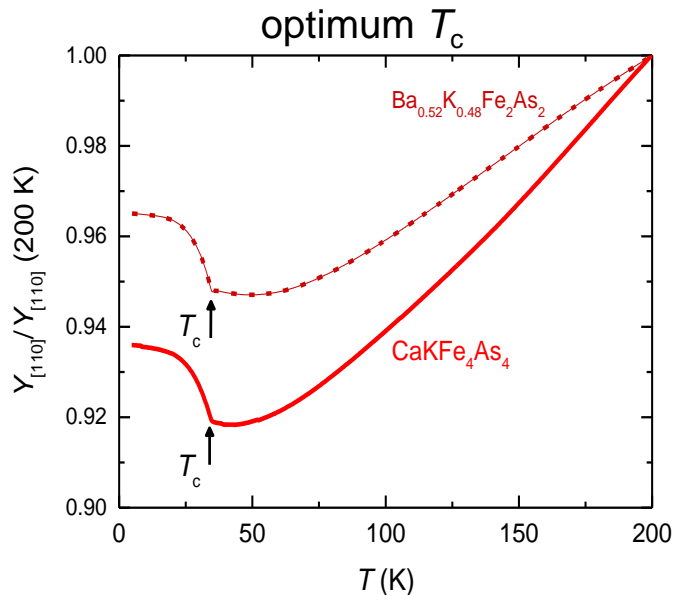


$$Y_{[110]} = 4 \left( \frac{1}{C_{66}} + \frac{1}{\gamma} \right)^{-1}$$

$$\gamma = \frac{C_{11} + C_{12}}{2} - \frac{C_{13}^2}{C_{33}}$$

$$\frac{C_{66}}{C_{66,0}} = 1 - \frac{\lambda^2}{C_{66,0}} \chi_{\text{nem}}$$

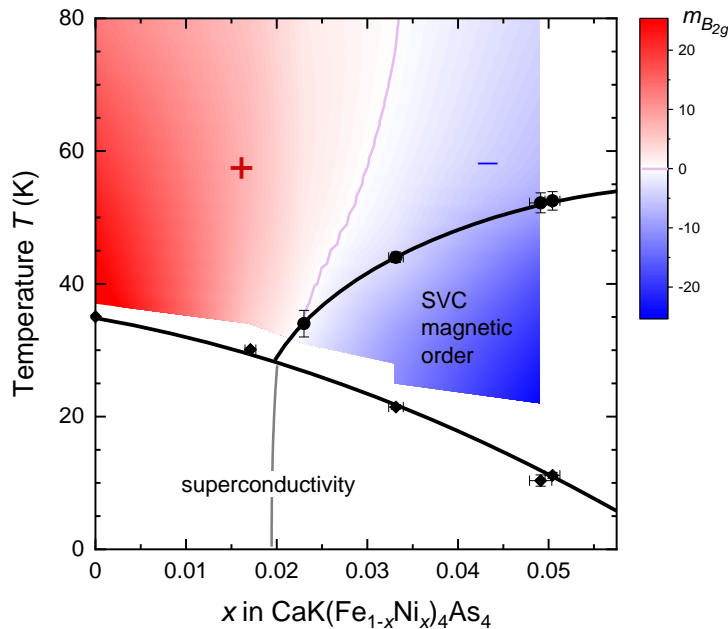
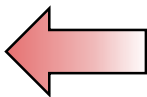
Three-point bending in a capacitance dilatometer  
See: Böhmer et al., PRL **112**, 047001 (2014)



# Summary: Evolution of nematic fluctuations in $\text{CaK}(\text{Fe}_{1-x}\text{Ni}_x)_4\text{As}_4$

- “Sub-Curie-Weiss”  $T$ -dependence
- Very similar to  $\text{Ba}_{0.5}\text{K}_{0.5}\text{Fe}_2\text{As}_2$
- Consequence of almost degenerate magnetic orders?

More hole-doped?



- Nematic fluctuations finite but far from critical
- Curie-Weiss-like temperature dependence

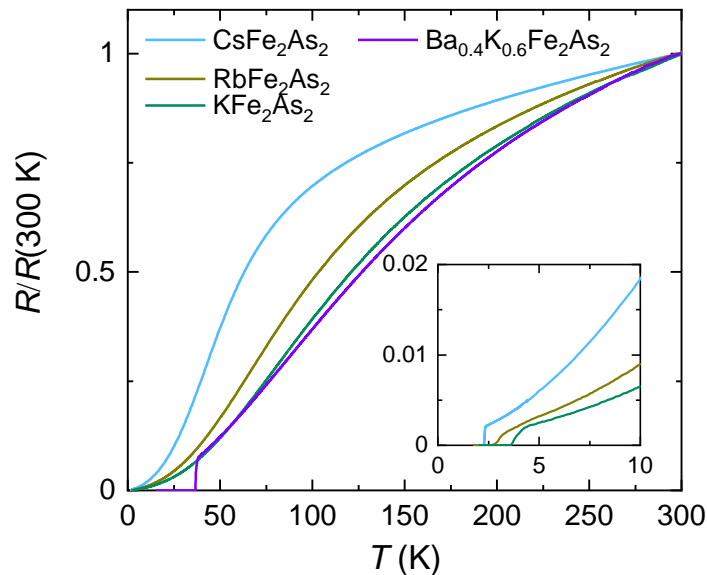
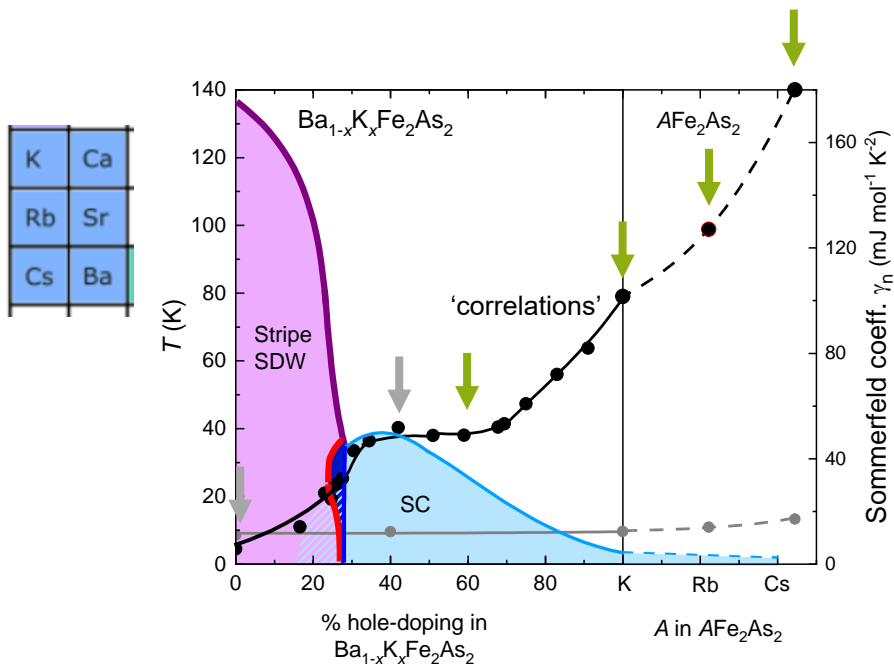
$$m_{B_{2g}} = k \cdot \chi_{nem}^{B_{2g}}$$



Prefactor of elastoresistance:

- Clear doping dependence
- Likely temperature dependent

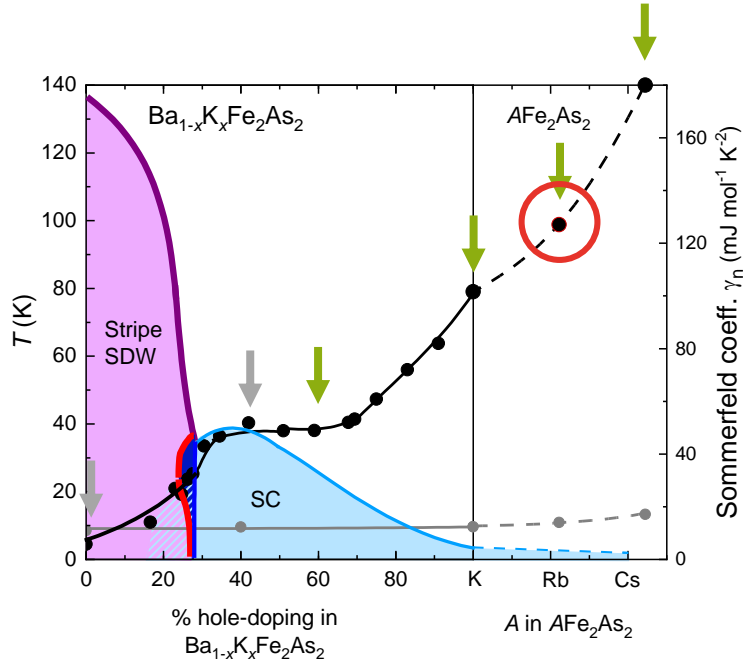
# The “extremely hole-doped” $A\text{Fe}_2\text{As}_2$ ( $A=\text{K}, \text{Rb}, \text{Cs}$ )



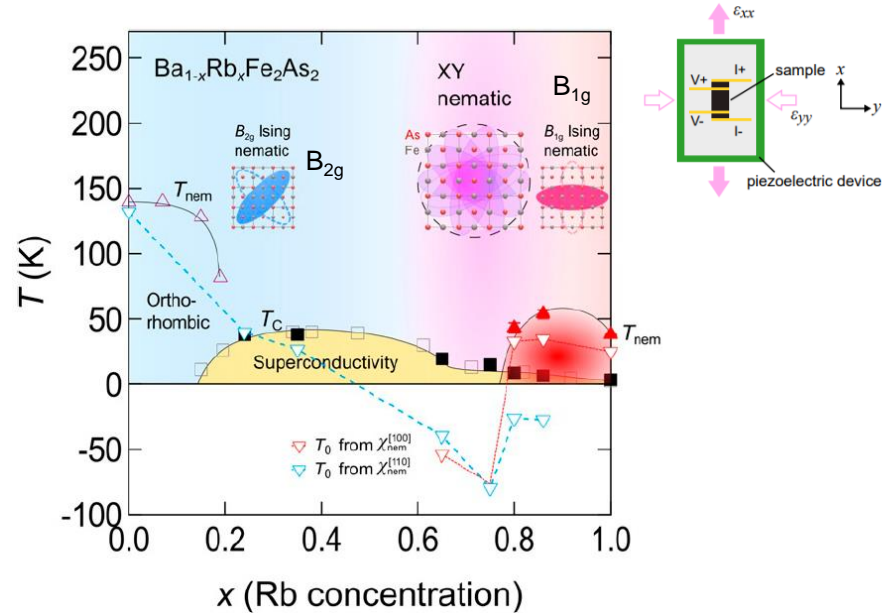
Hardy et al., PRB **94**, 025113 (2016)

# Change of nematic direction?

K	Ca
Rb	Sr
Cs	Ba

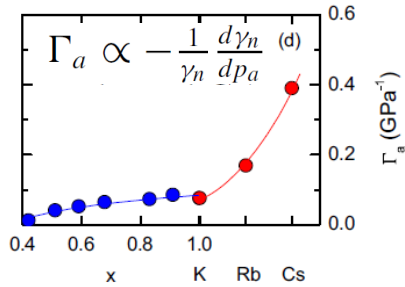


Hardy et al., PRB **94**, 025113 (2016)

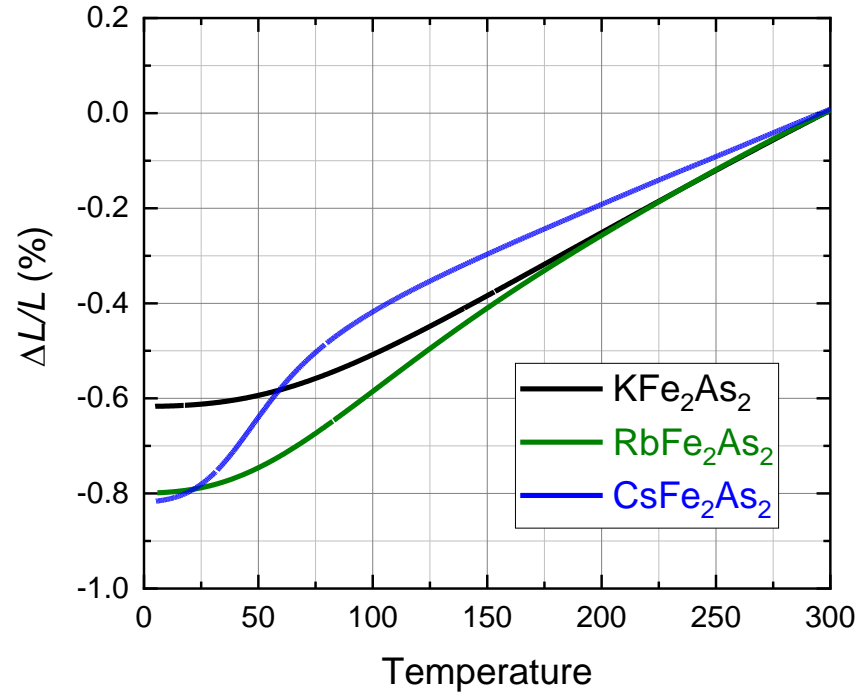
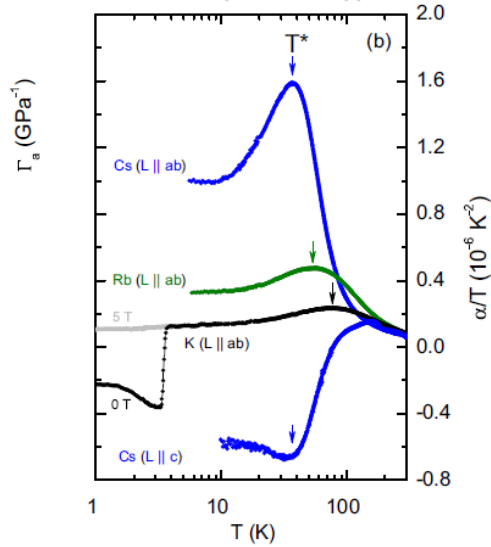


Ishida et al., PNAS, 117, 6424–6429, (2020)

# Strain dependence and thermal expansion

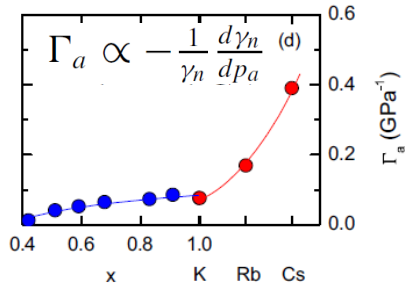


$$\alpha = \frac{1}{V} \frac{dV}{dT} = - \frac{dS}{dp}$$

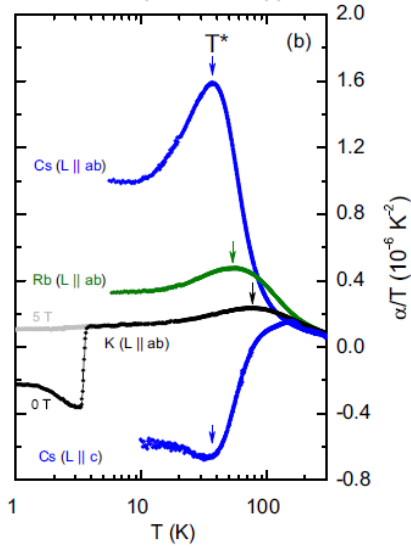


Hardy et al., PRB **94**, 025113 (2016)

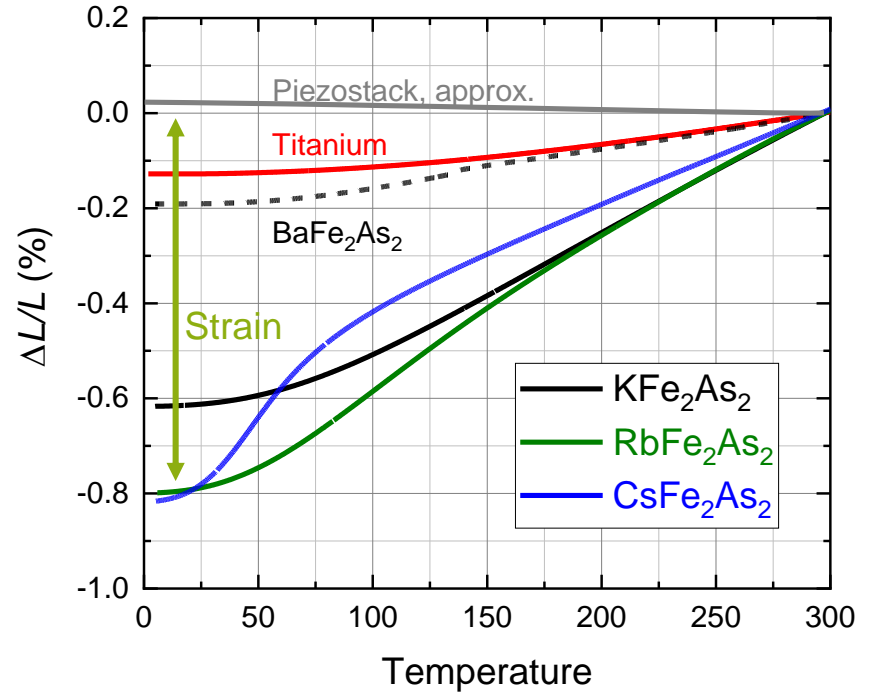
# Strain dependence and thermal expansion



$$\alpha = \frac{1}{V} \frac{dV}{dT} = -\frac{dS}{dp}$$



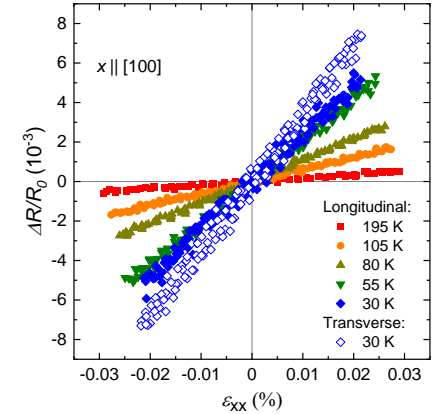
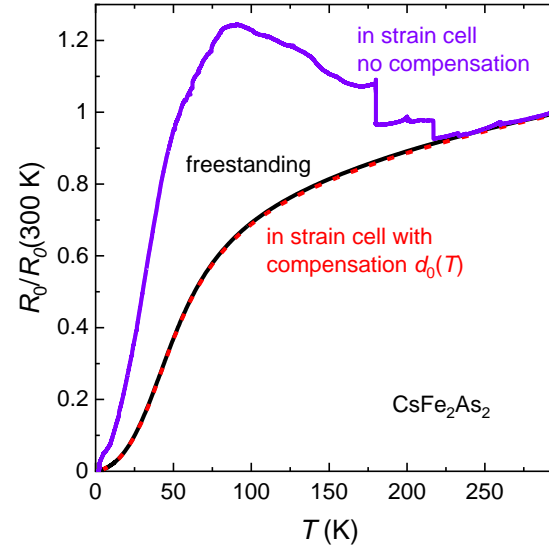
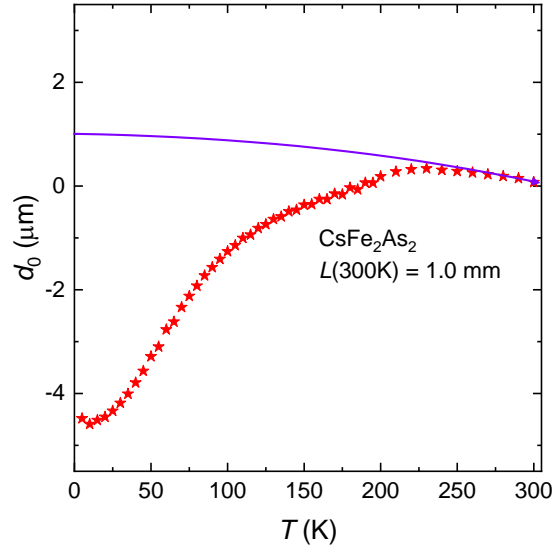
Hardy et al., PRB **94**, 025113 (2016)



# Successful active strain compensation



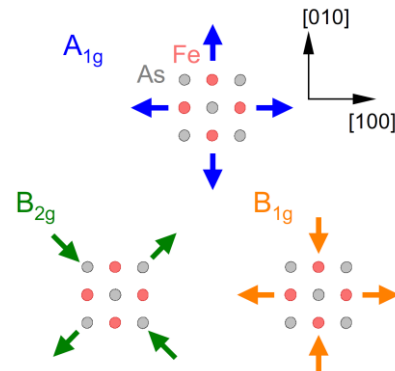
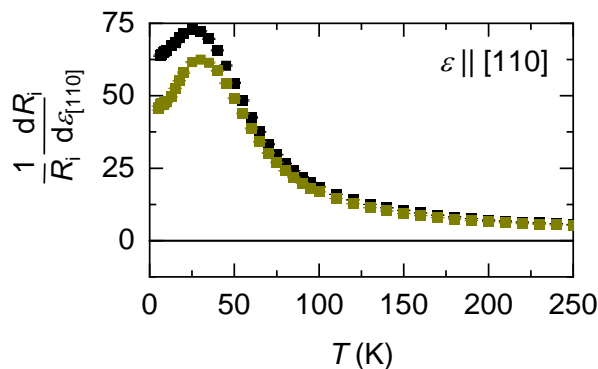
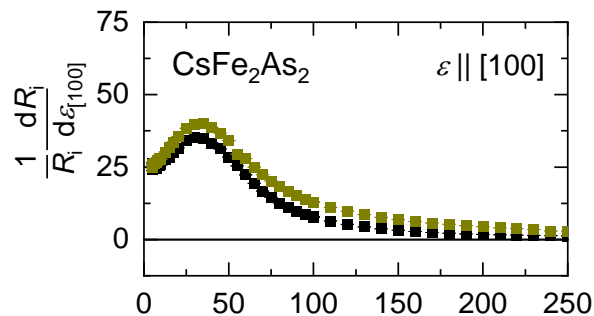
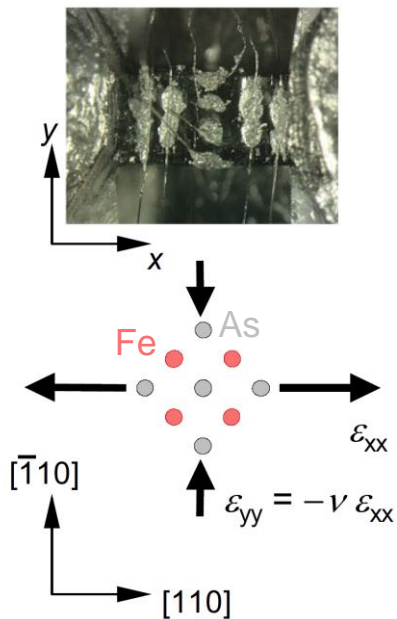
Razorbill  
CS100, CS120



Wiecki et al., Phys. Rev. Lett. **125**, 187001 (2020)

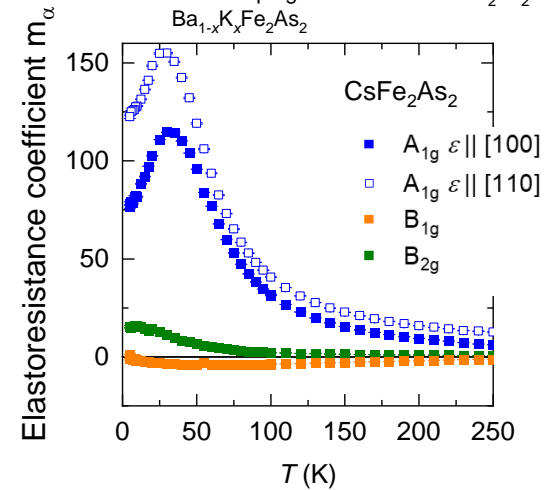
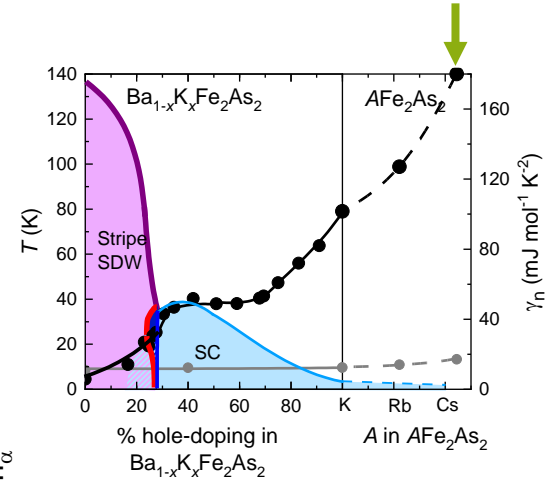
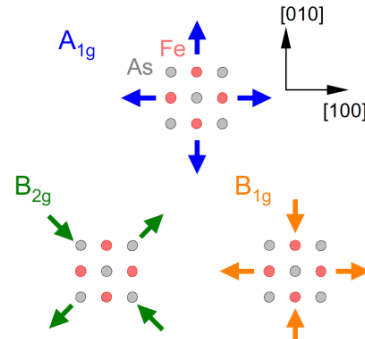


# Symmetry-resolved elastoresistance

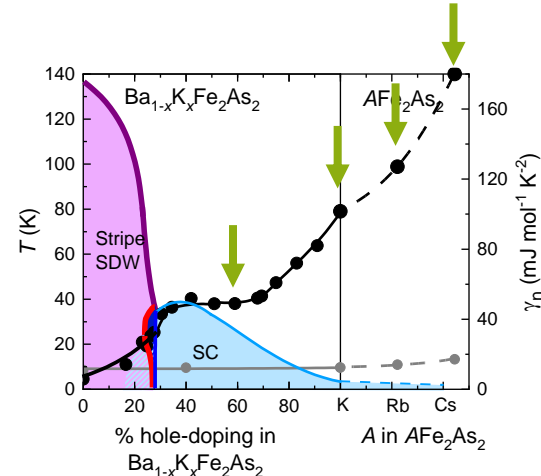
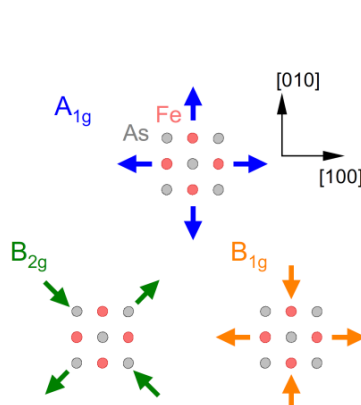


$$\begin{aligned}
 m_{A_{1g}} &= \frac{1}{1 - \nu_{[100]}} \left[ \frac{d(\Delta R/R_0)_{[100]}}{d\epsilon_{[100]}} + \frac{d(\Delta R/R)_{[010]}}{d\epsilon_{[100]}} \right] \\
 &= \frac{1}{1 - \nu_{[110]}} \left[ \frac{d(\Delta R/R_0)_{[110]}}{d\epsilon_{[110]}} + \frac{d(\Delta R/R)_{[\bar{1}10]}}{d\epsilon_{[110]}} \right] \\
 m_{B_{1g}} &= \frac{1}{1 + \nu_{[100]}} \left[ \frac{d(\Delta R/R_0)_{[100]}}{d\epsilon_{[100]}} - \frac{d(\Delta R/R)_{[010]}}{d\epsilon_{[100]}} \right] \\
 m_{B_{2g}} &= \frac{1}{1 + \nu_{[110]}} \left[ \frac{d(\Delta R/R_0)_{[110]}}{d\epsilon_{[110]}} - \frac{d(\Delta R/R)_{[\bar{1}10]}}{d\epsilon_{[110]}} \right]
 \end{aligned}$$

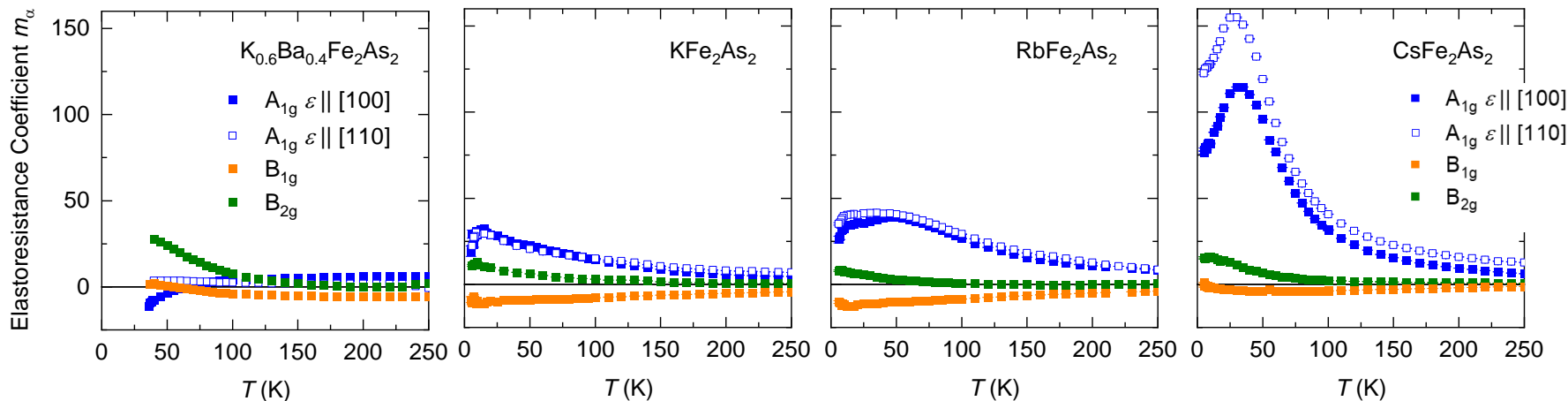
# Elastoresistance evolution



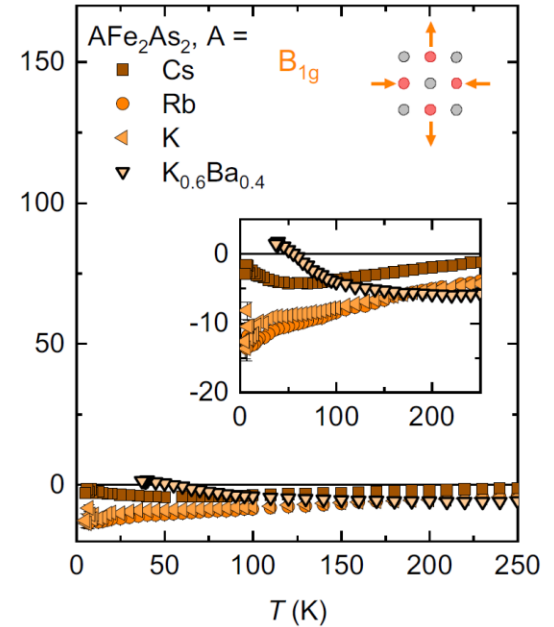
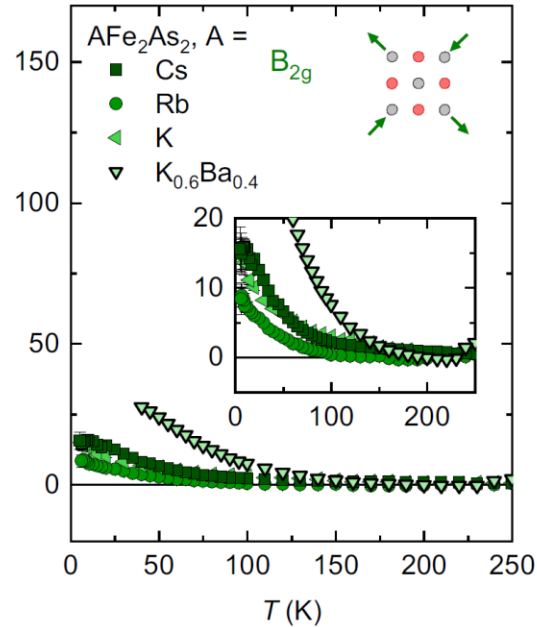
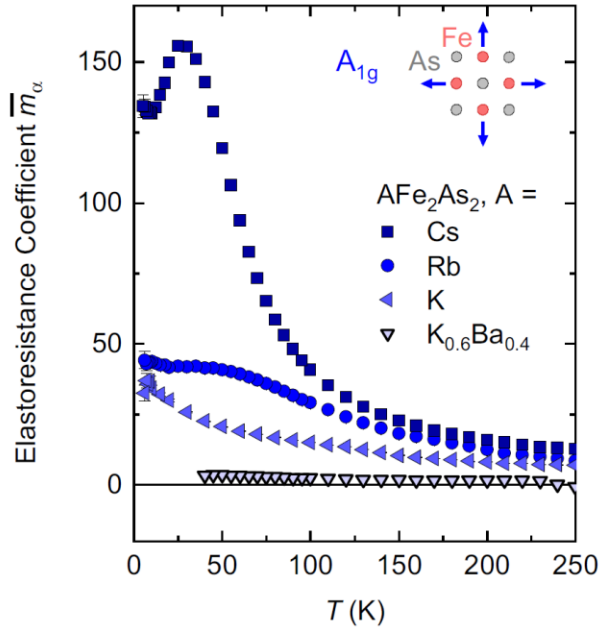
# Elastoresistance evolution



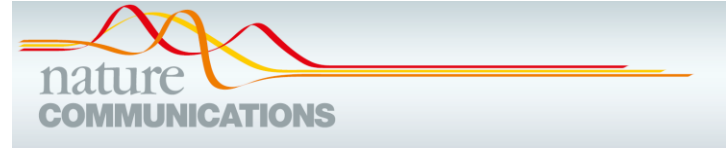
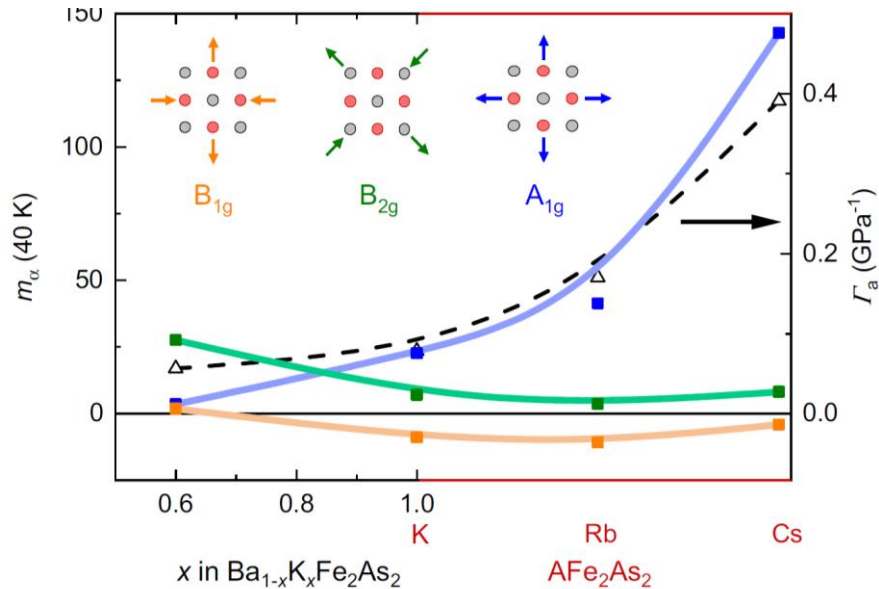
Wiecki et al., Nature Communications **12**, 4824 (2021)



# Elastoresistance evolution



Wiecki et al., Nature Communications **12**, 4824 (2021)



## Emerging symmetric strain response and weakening nematic fluctuations in strongly hole-doped iron-based superconductors,

P. Wiecki, M. Frachet, A.-A. Haghighirad, T. Wolf, C. Meingast, R. Heid and A. E. Böhmer, Nature Communications **12**, 4824 (2021)

# (Weak) nematic behavior in iron-based materials also in less obvious cases

