KITP IRONIC14, Nov. 18, 2014

Local moment physics in doped $CaFe_2As_2$: A dual description

Young-June Kim

University of Toronto

Physics
UNIVERSITY OF TORONTO

Acknowledgements

H. Gretarsson

Theory

L. Ortenzi
L. Boeri
I. Mazin

Samples

W. Wu, S. R. Julian (Toronto)

Z. J. Xu, J. S. Wen, G. D. Gu (BNL)

R. H. Yuan Z. G. Chen, N.-L. Wang (IOP Beijing)

S. Khim, K. H. Kim (Seoul Natl. U)

M. Ishikado, I. Jarrige, S. Shamoto (JAEA)

J.-H. Chu, I. R. Fisher (Stanford)

S. R. Saha, T. Drye, J. Paglione (Maryland)

S. Kasahara, Y. Mastuda (Kyoto)

A. Sefat (Oak Ridge)

Chenglin Zhang, Pengcheng Dai (Tennessee/Rice)

Argonne + CHESS

Jungho Kim
Diego Casa
Mary Upton
Thomas Gog

K. Finkelstein

Advanced Photon Source

UNIVERSITY OF TORONTO

Ontario

NSERC CRSNG

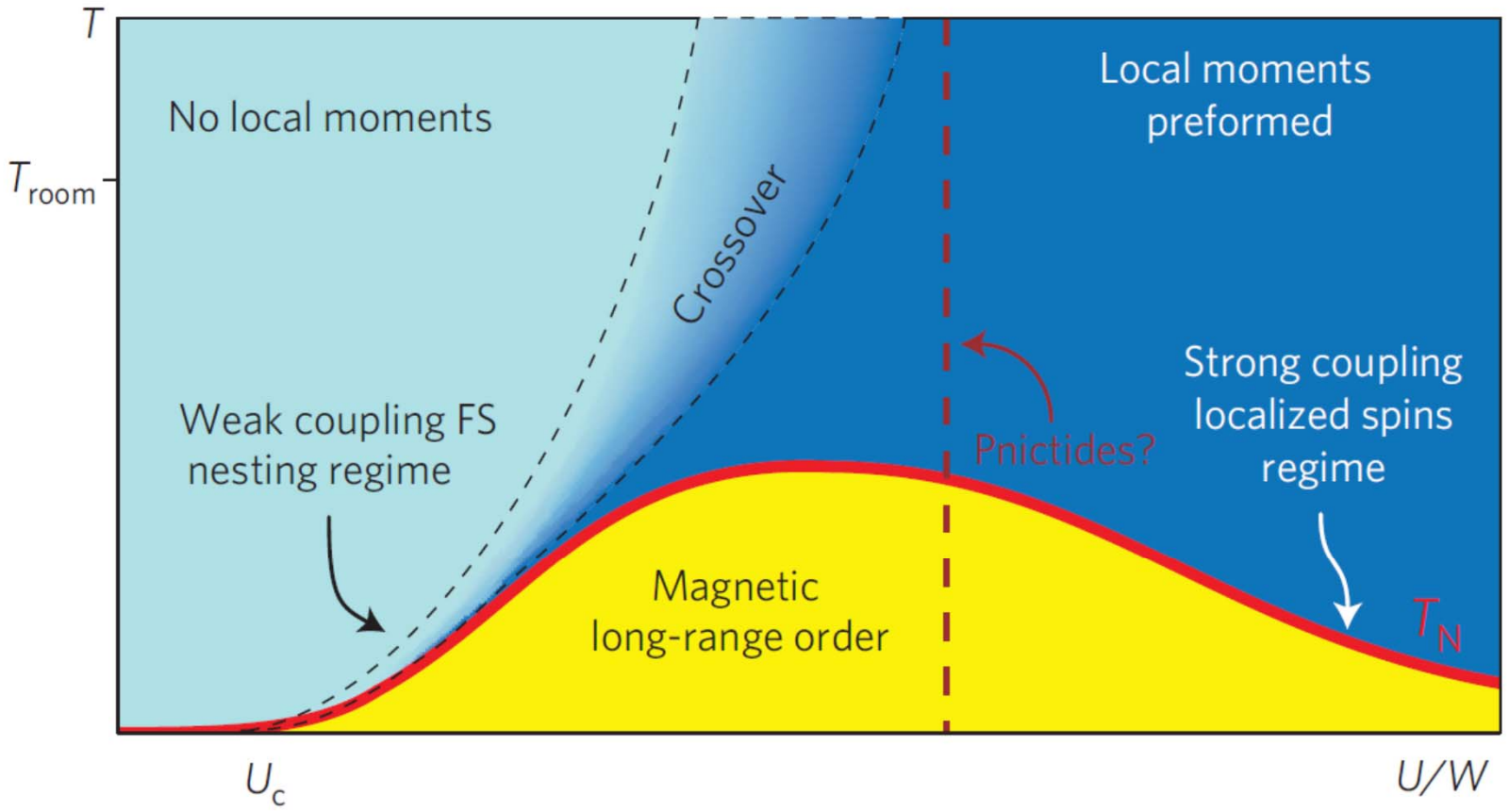
NSF

CHESS

Outline

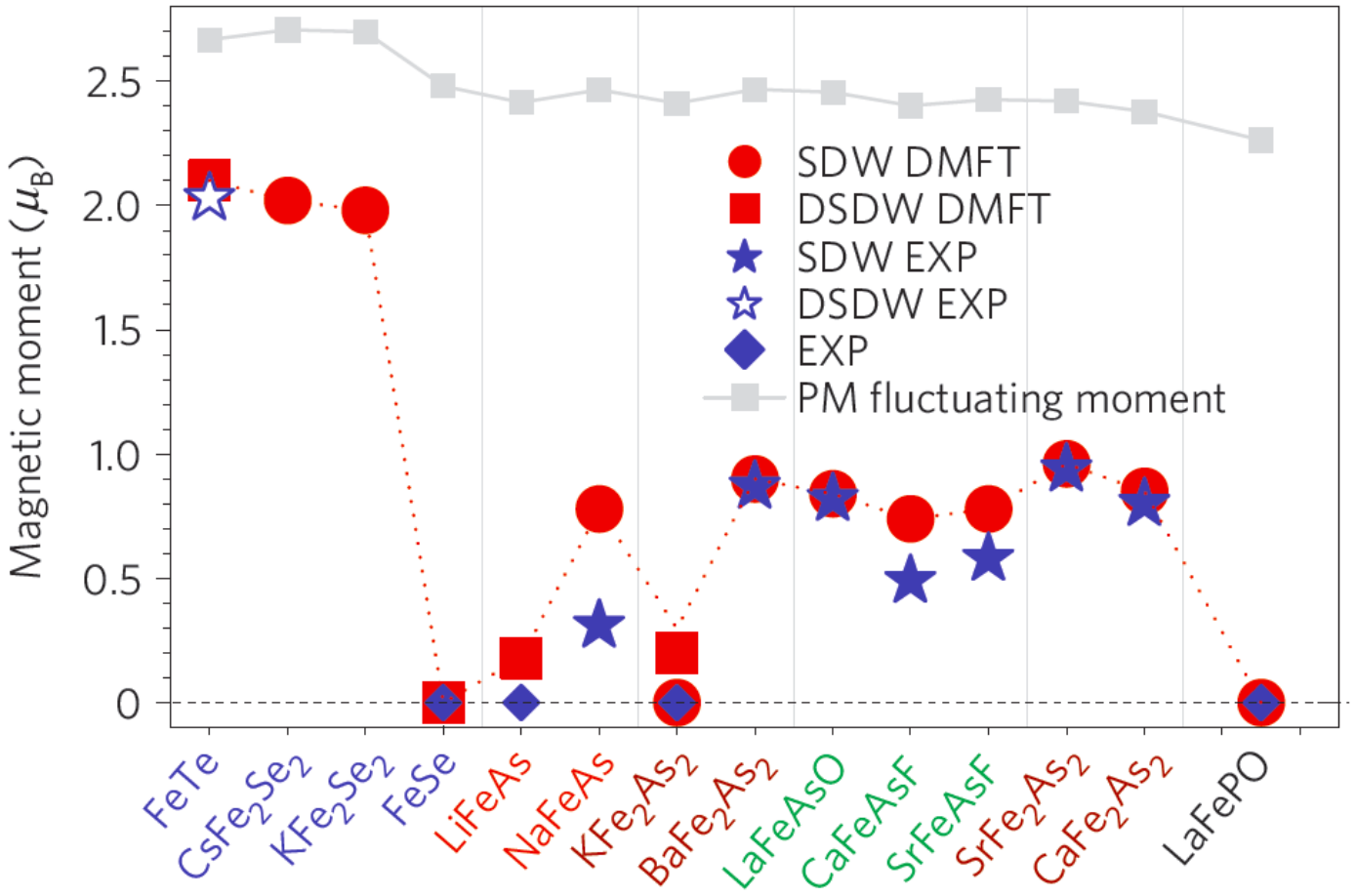
1. X-ray Emission Spectroscopy
   - What do we measure? Fluctuating local moments
2. Survey of Fe based materials
   - Material dependence
   - Temperature and doping dependence? Not much
3. What about $CaFe_2As_2$?
   - Large temperature dependence
     - Spin-state transition description
     - Reduced Stoner theory description

Local vs. itinerant



Dai, Hu, and Dagotto, Nat. Phys. 8, 709 (2012)

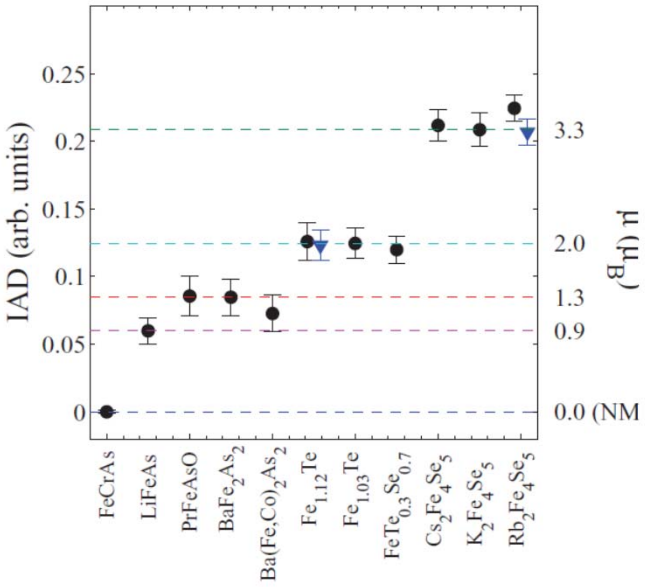
Magnetic Moment



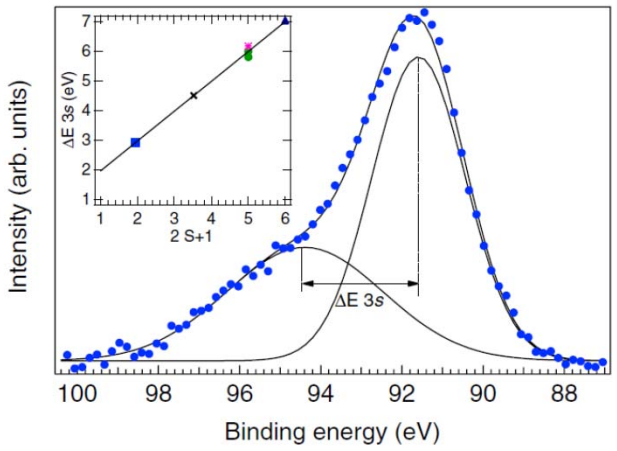
Z. P. Yin, K. Haule, and G. Kotliar, Nature Mater. 10, 932 (2011)

Local moments – experiments

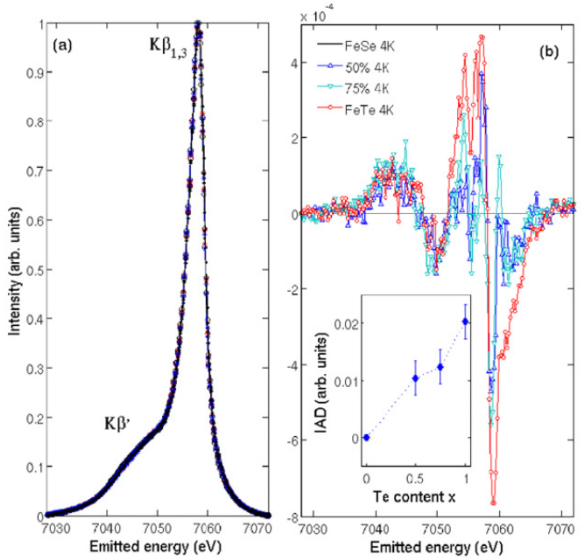
- Need experimental probes for measuring Local, Fluctuating moment:
  - Q and E integrated Inealstic Neutron Scattering
  - X-ray spectroscopy



Gretarsson et al. PRB 83, 100509 (2011)

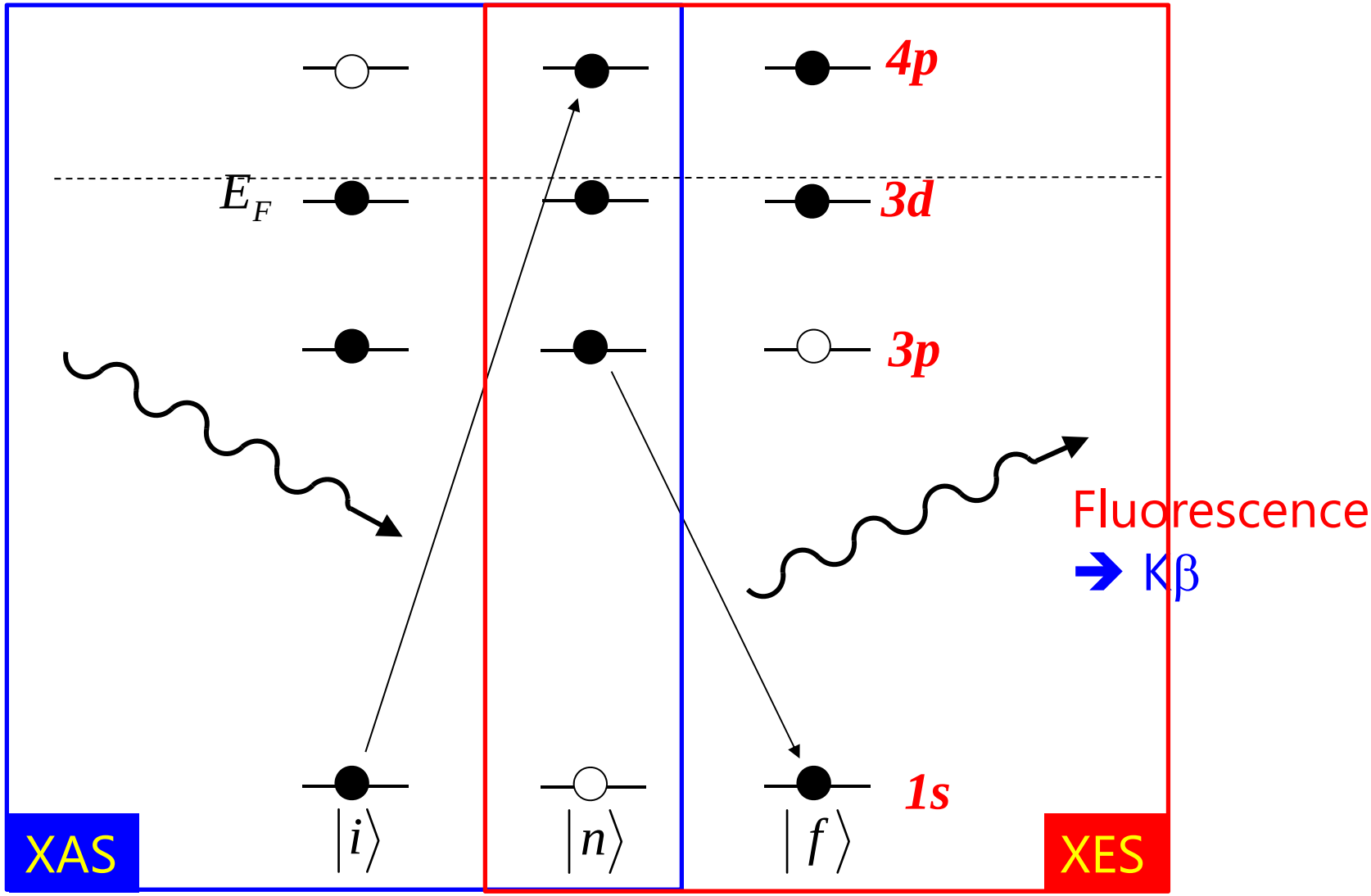


Bondino et al. PRL 102, 267001 (2008)



Simonelli et al. JPCM 24, 415501 (2012)

X-ray Absorption vs. Emission

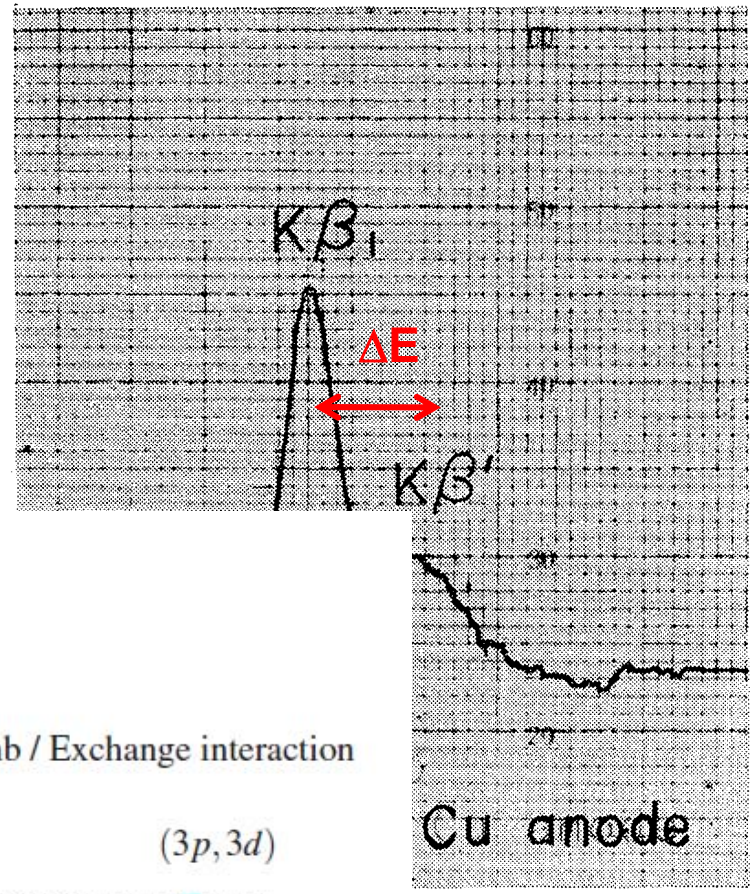


JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN, Vol. 14, No. 12, DECEMBER 1959

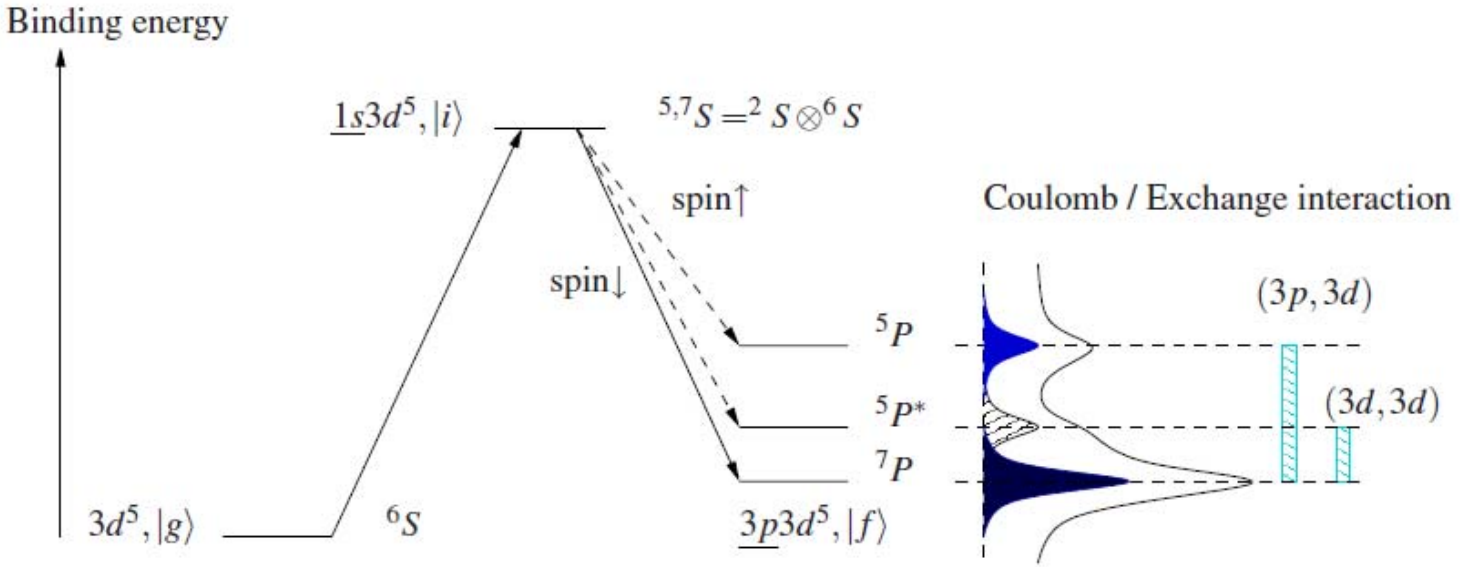
The X-ray Non-diagram Lines $K\beta'$ of Some Compounds of the Iron Group

By Kenjiro TSUTSUMI

Department of Physics, Faculty of Science, Osa



J-P Rueff and A. Shukla, RMP 2010



Multiplet structure

Vanko and de Groot, Phys. Rev. B 75, 177101 (2007)

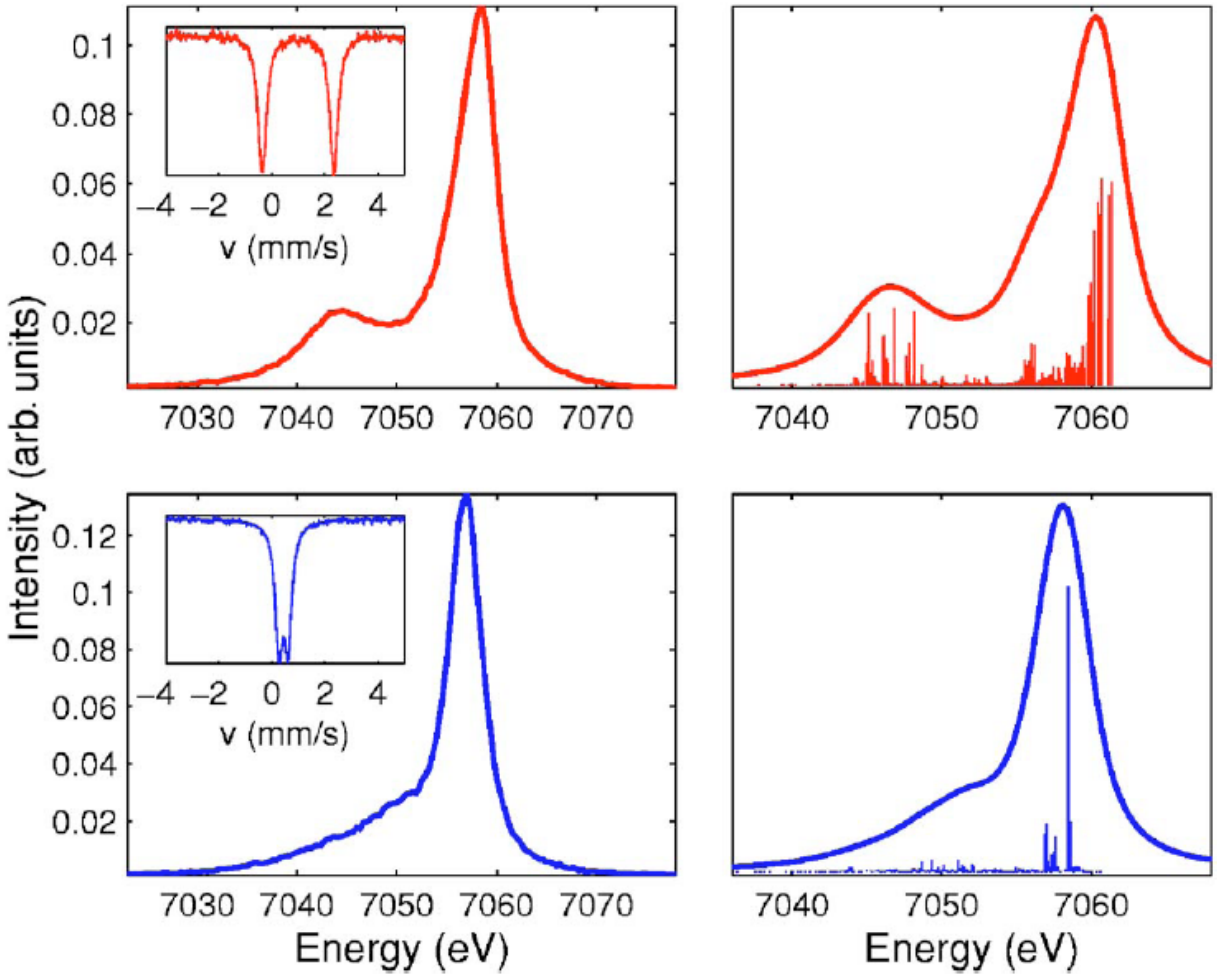
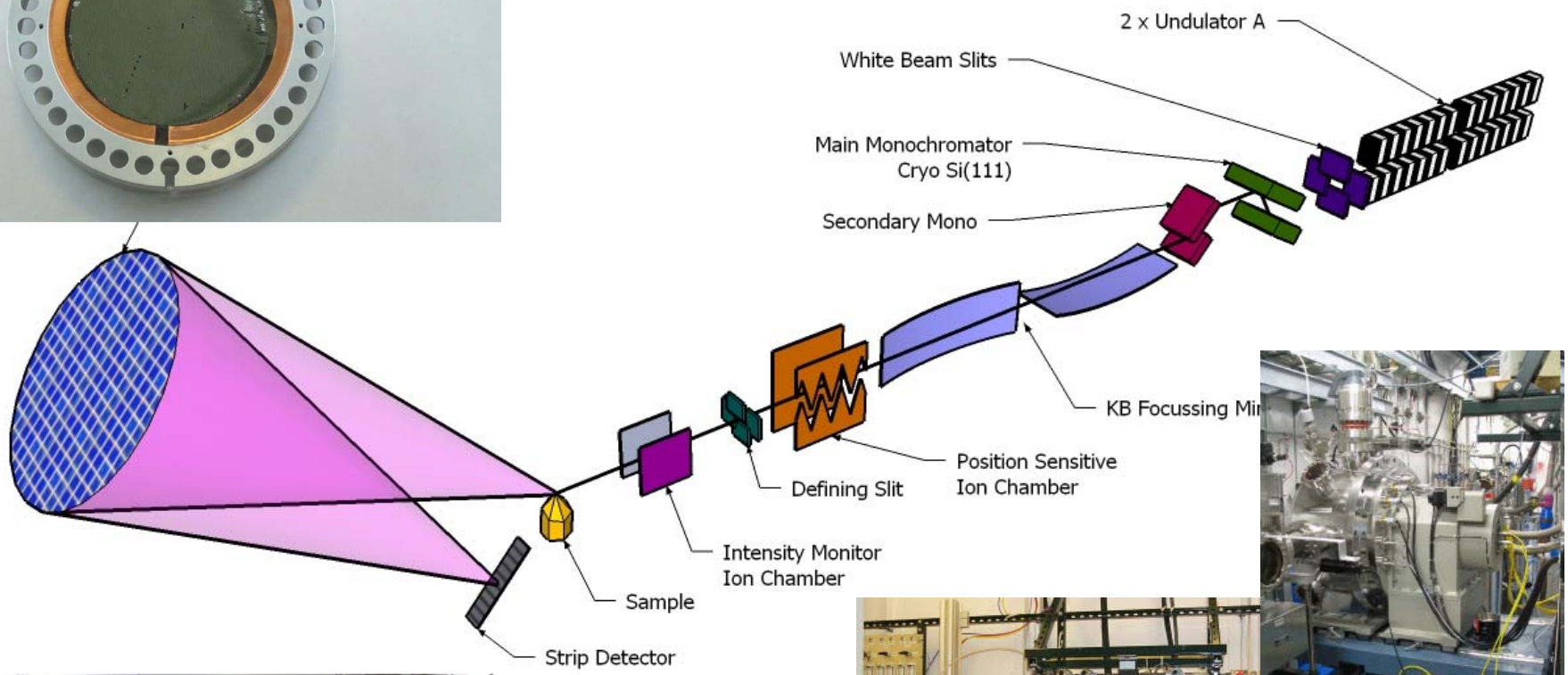
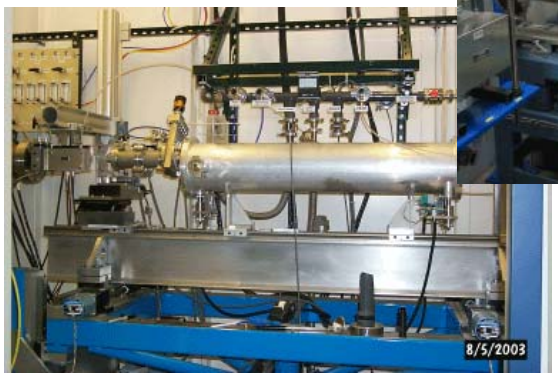
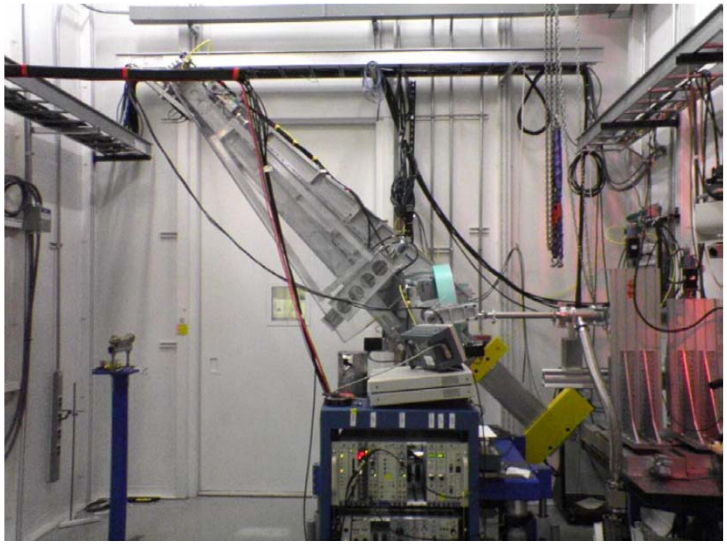


FIG. 1. (Color online) Experimental (left panel) and theoretical (right panel) $K\beta$ spectra of $[Fe(phen)_2(NCS)_2]$, in its HS (top) and LS (bottom) forms. Insets in the experimental part display the Mössbauer spectra.

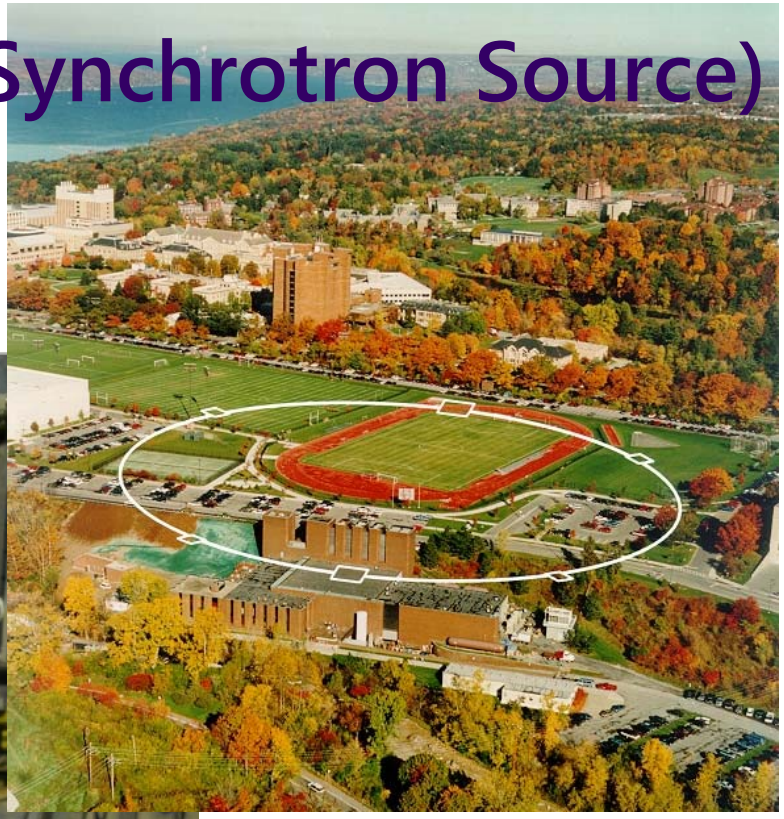

2 x Undulator A
White Beam Slits
Main Monochromator
Cryo Si(111)
Secondary Mono
KB Focussing Mi
Position Sensitive
Ion Chamber
Defining Slit
Intensity Monitor
Ion Chamber
Sample
Strip Detector

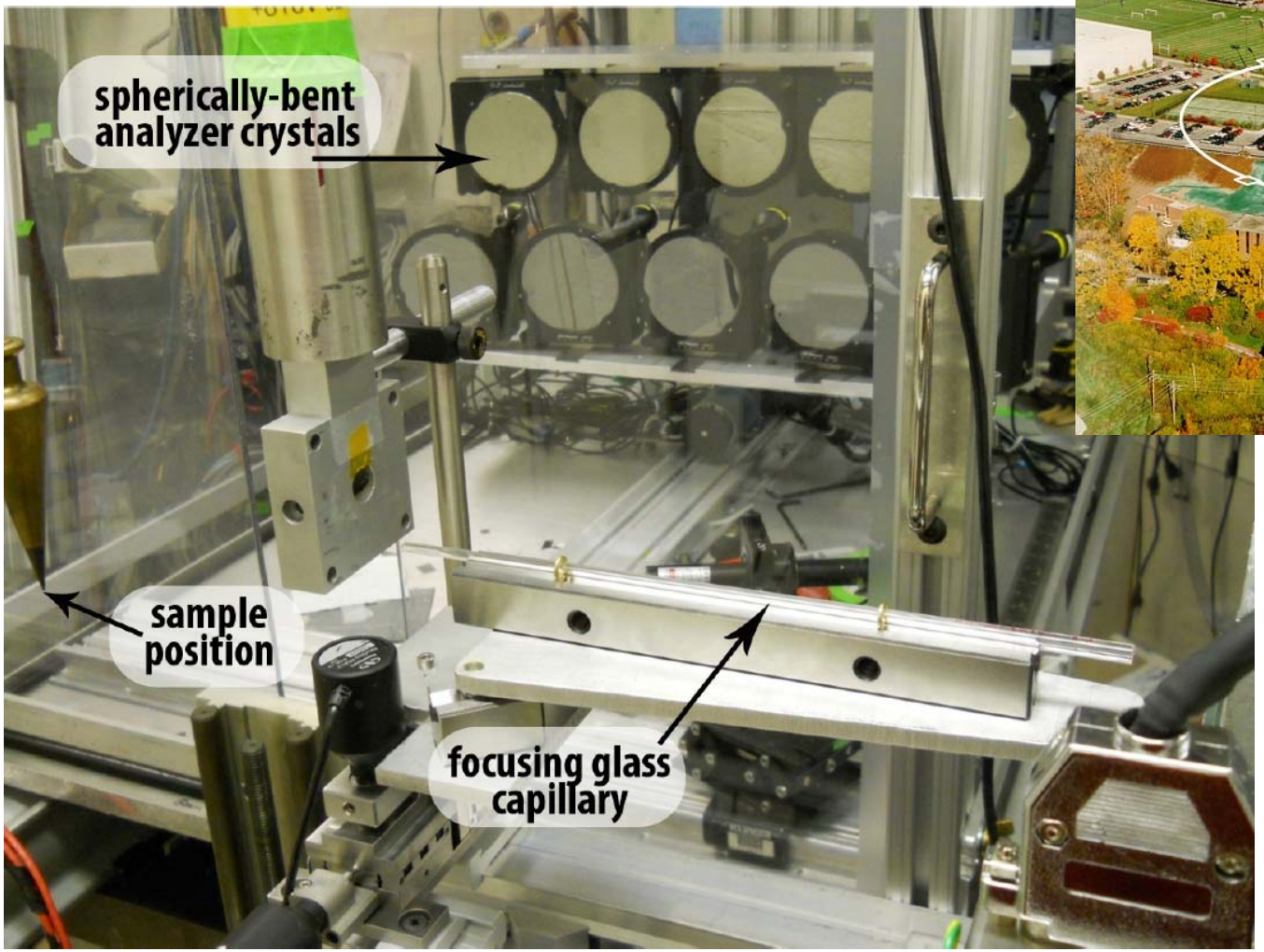

8/5/2003



APS 9ID

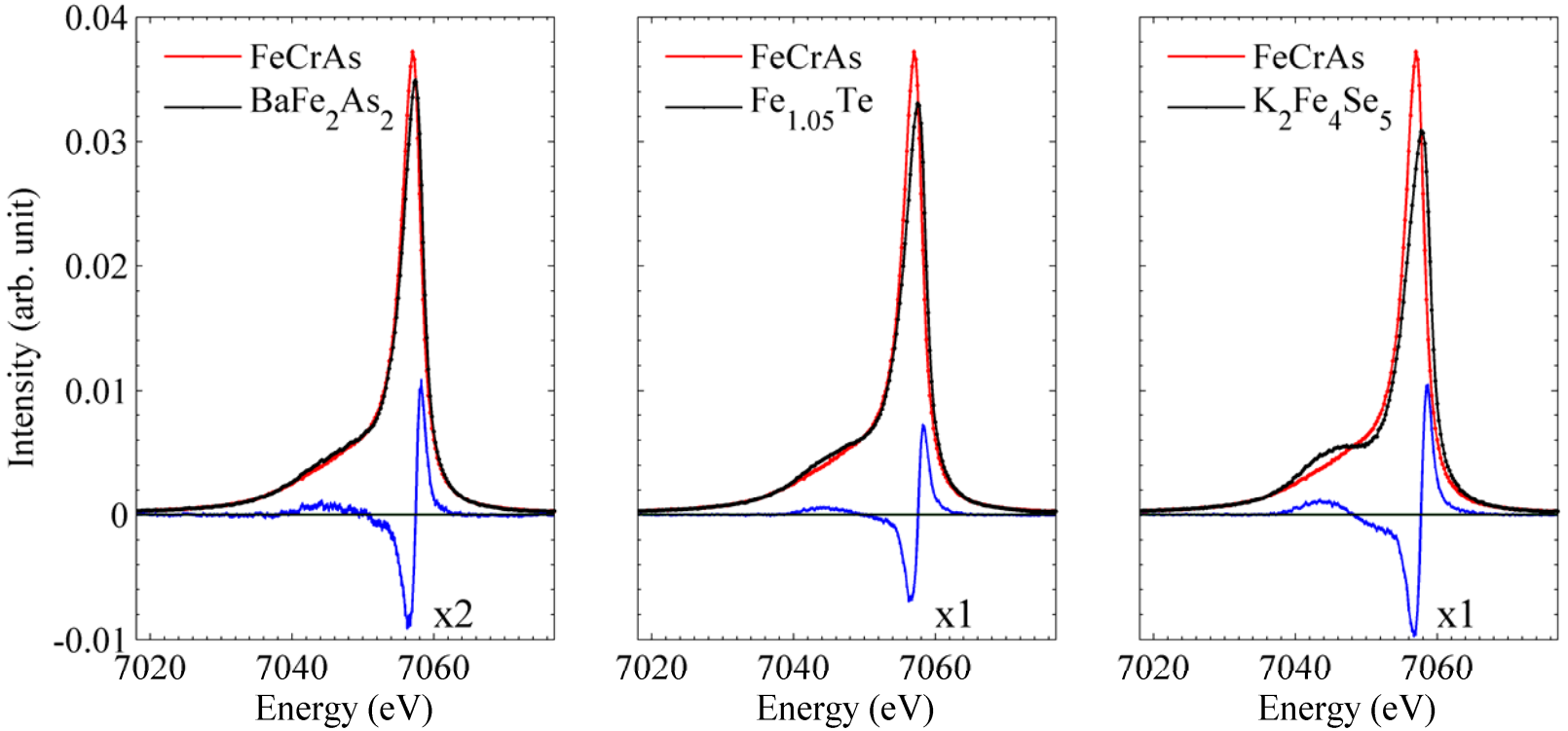
CHESS (Cornell High Energy Synchrotron Source)





C1 XES station
Ken Finkelstein

Spectra comparison

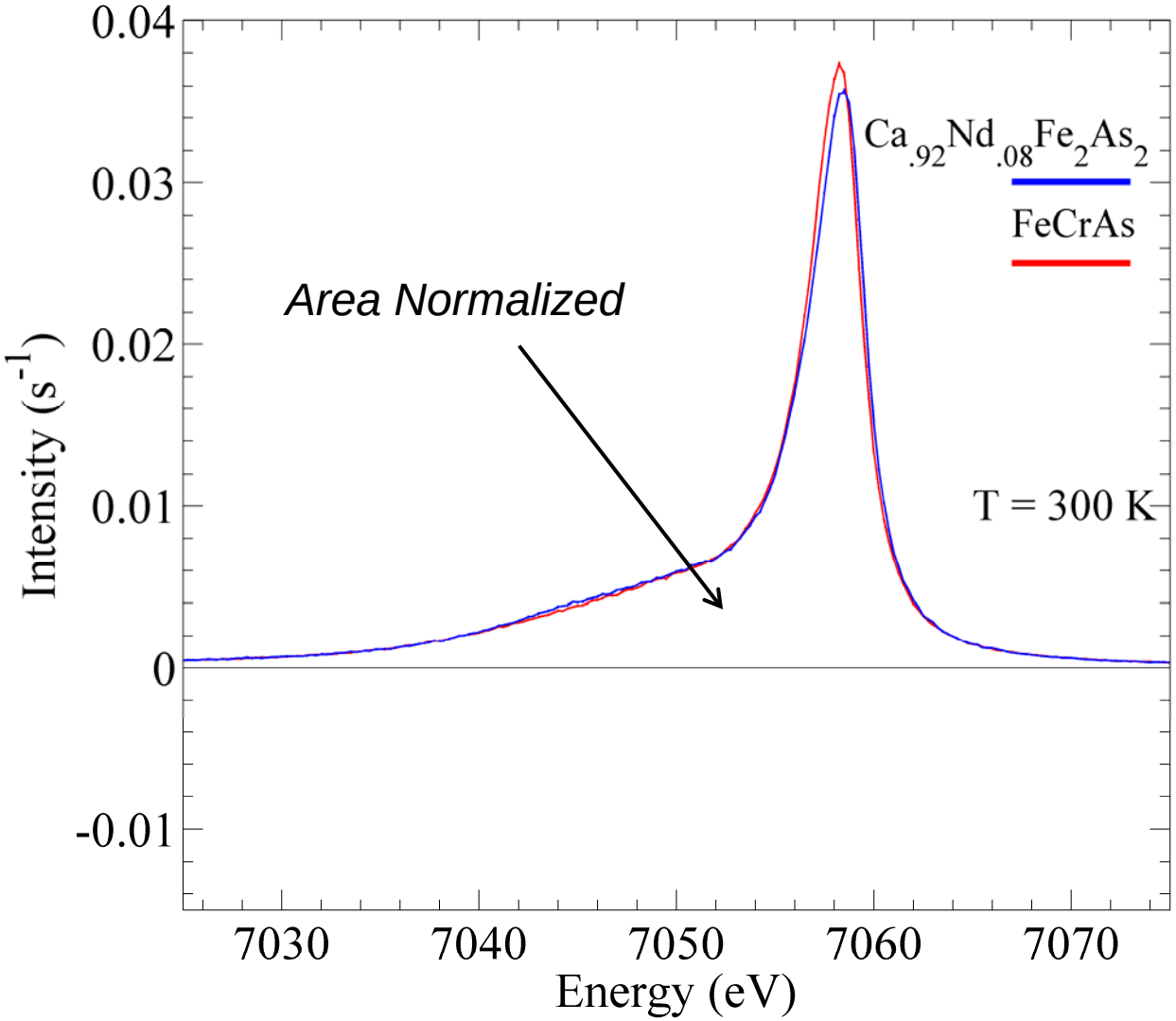


How to obtain Quantitative information?

$$IAD = \int \left| I(E) - I_{ref}(E) \right| dE$$

Vanko, de Groot et al. J. Phys. Chem. B 110, 11647 (2006)

Integrated Absolute Difference (IAD)



A reference sample required

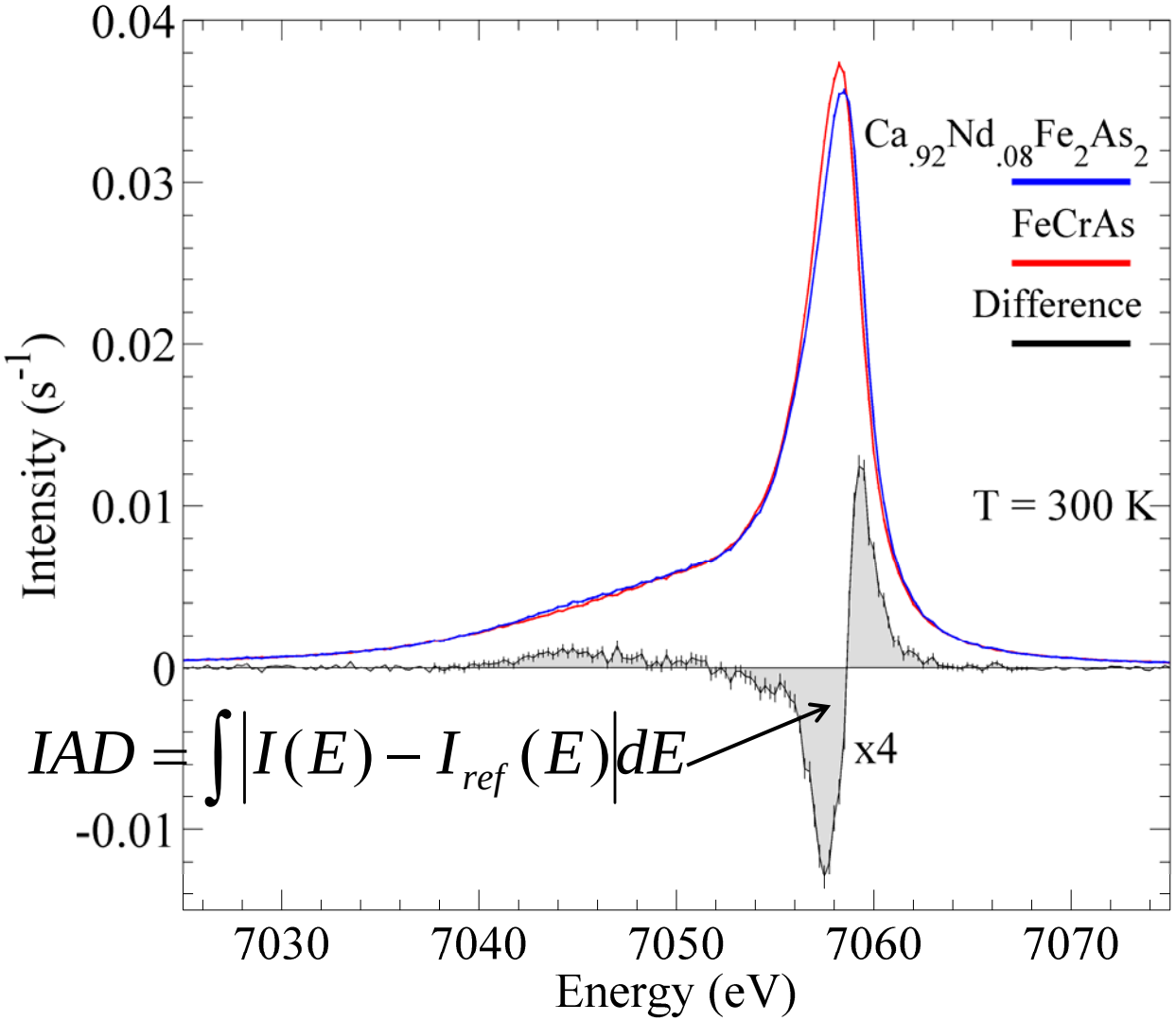
FeCrAs:

1. Same local environment as Fe-based SC (tetrahedral)
2. No magnetic moment (neutron scattering Mossbauer and band calculation)

W. Wu, S. Julian et al., EPL 2009

I. Swainson et al., Can. J. Phys. 2011

Integrated Absolute Difference



A reference sample required

FeCrAs:

1. Same local environment as Fe-based SC (tetrahedral)
2. No magnetic moment (neutron scattering Mossbauer and band calculation)

W. Wu, S. Julian et al., EPL 2009

I. Swainson et al., Can. J. Phys. 2011

IAD is a reliable measure of the Fe spin state

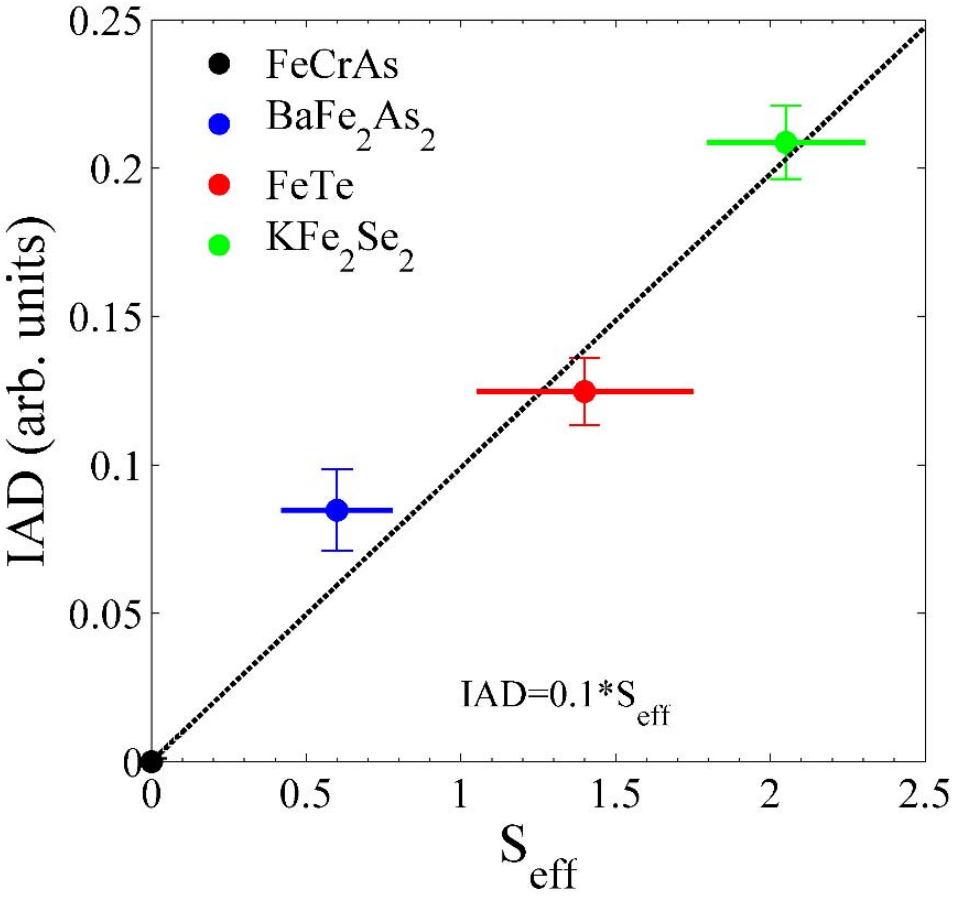
Outline

1. X-ray Emission Spectroscopy
   - What do we measure?
2. Surve
   - Ma
   - Ter
3. What
   - Larg
     - Spi
     - Reduced Stoner theory description

Instantaneous measurement of
Fluctuating local moment

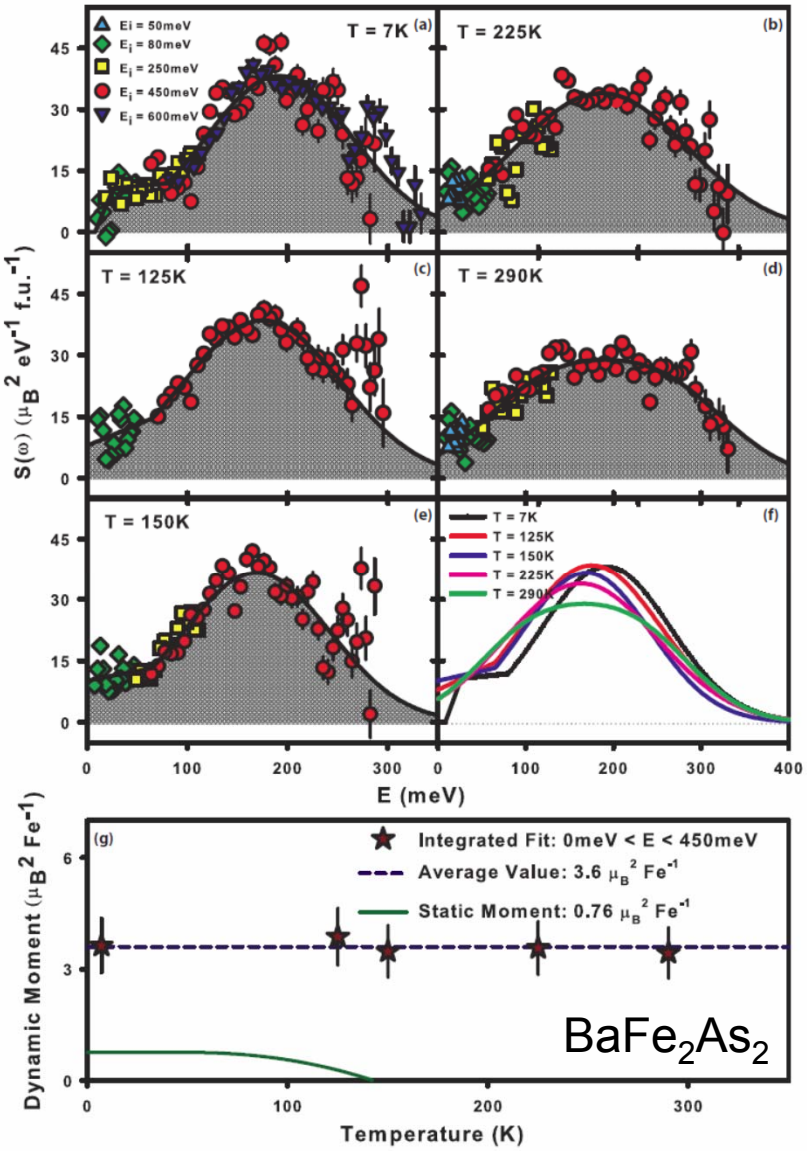
- Instantaneous: Femtosecond time scale (core hole lifetime)
- Local: Atomic length scale (exchange coupling between 3p and 3d)

Scaling vs. neutron sum rule



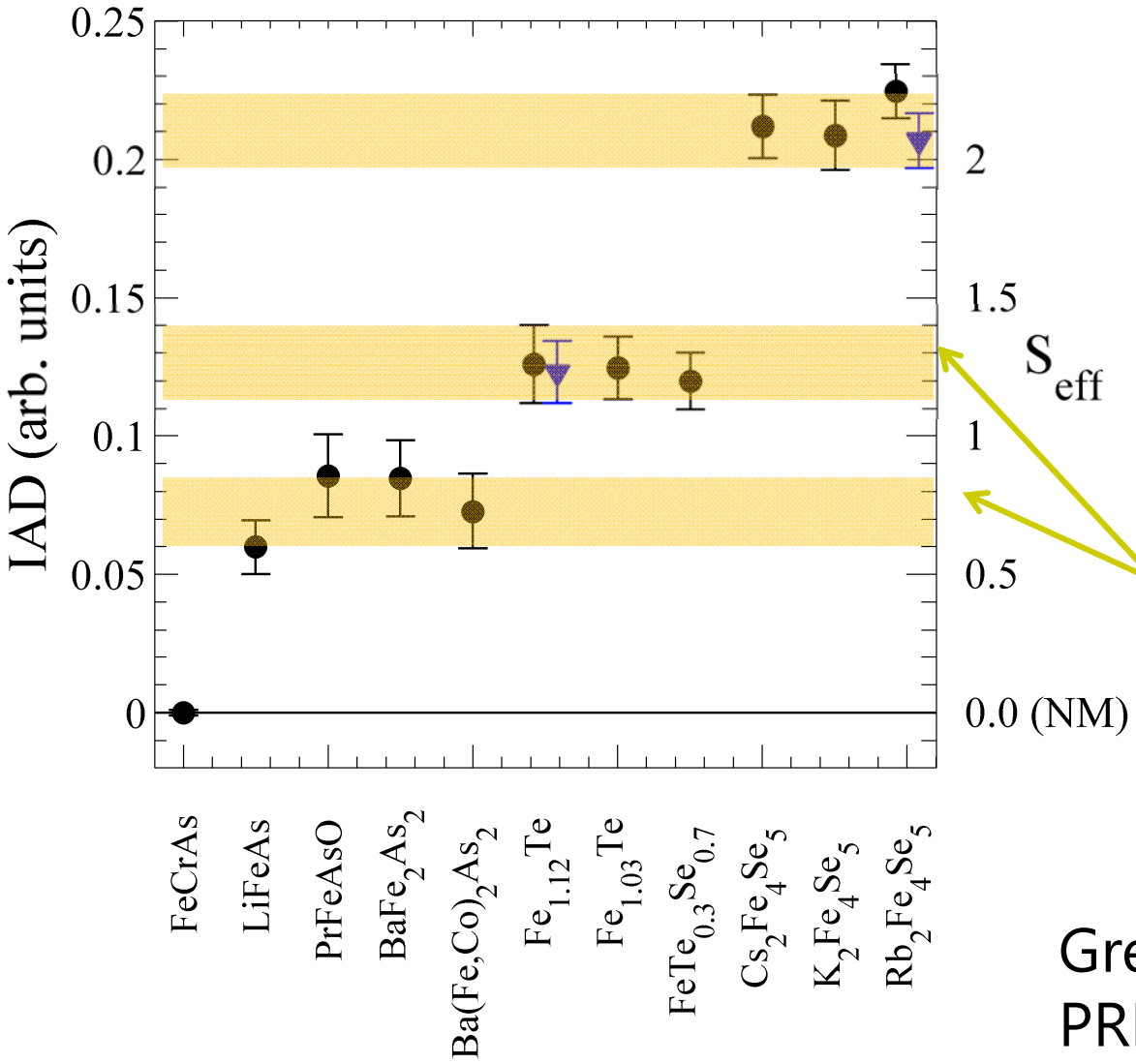
$$\int S(Q,E)dQdE = S_{eff}\left(S_{eff}+1\right)$$

Zaliznyak et al., PRL 107, 216403 (2011)
Wang et al., Nat. Comm. 2, 580 (2011)



Harriger et al., PRB 86, 140403(R) (2012)

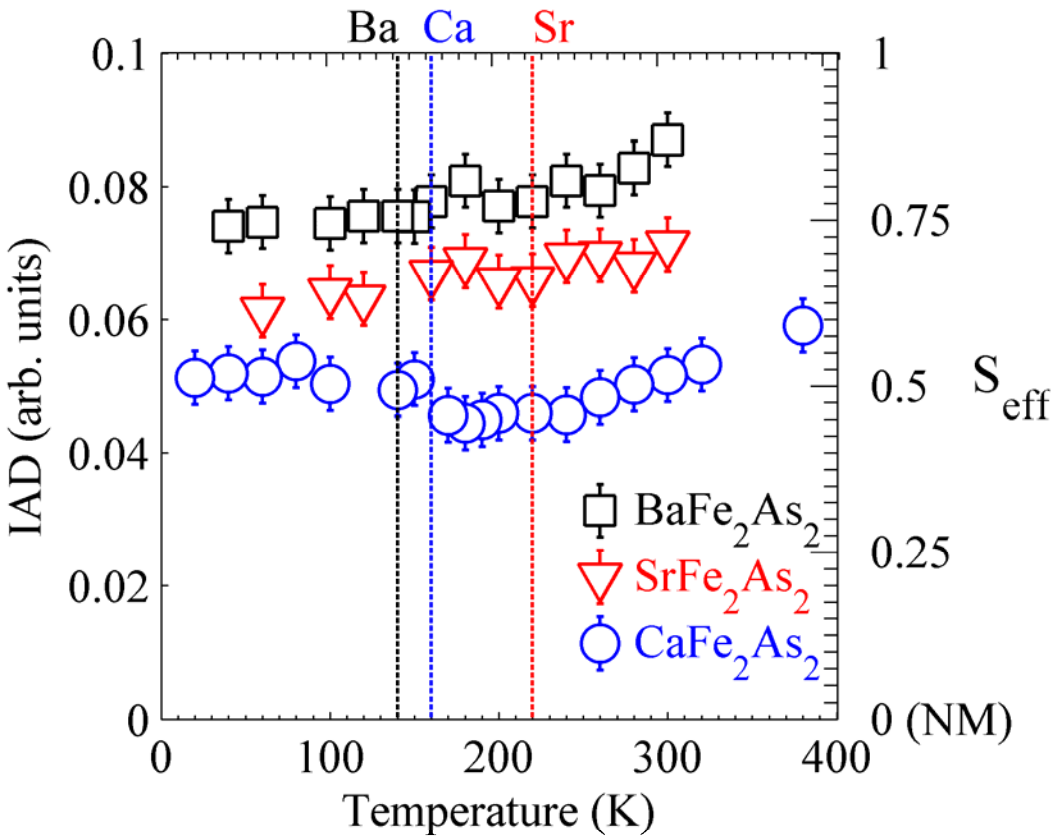
Materials Survey

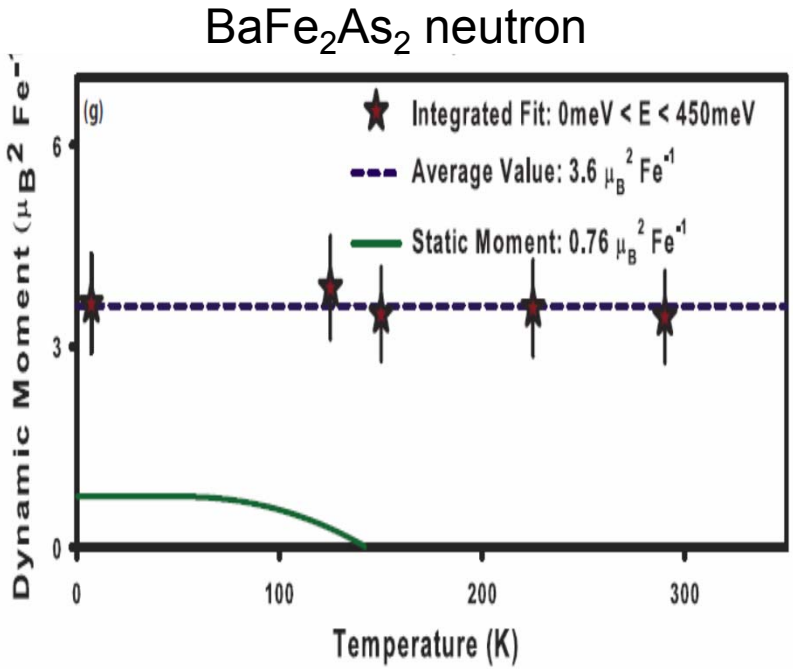


Not integer-multiples of 1/2

Gretarsson et al.
PRB 84, 100509 (R) (2011)

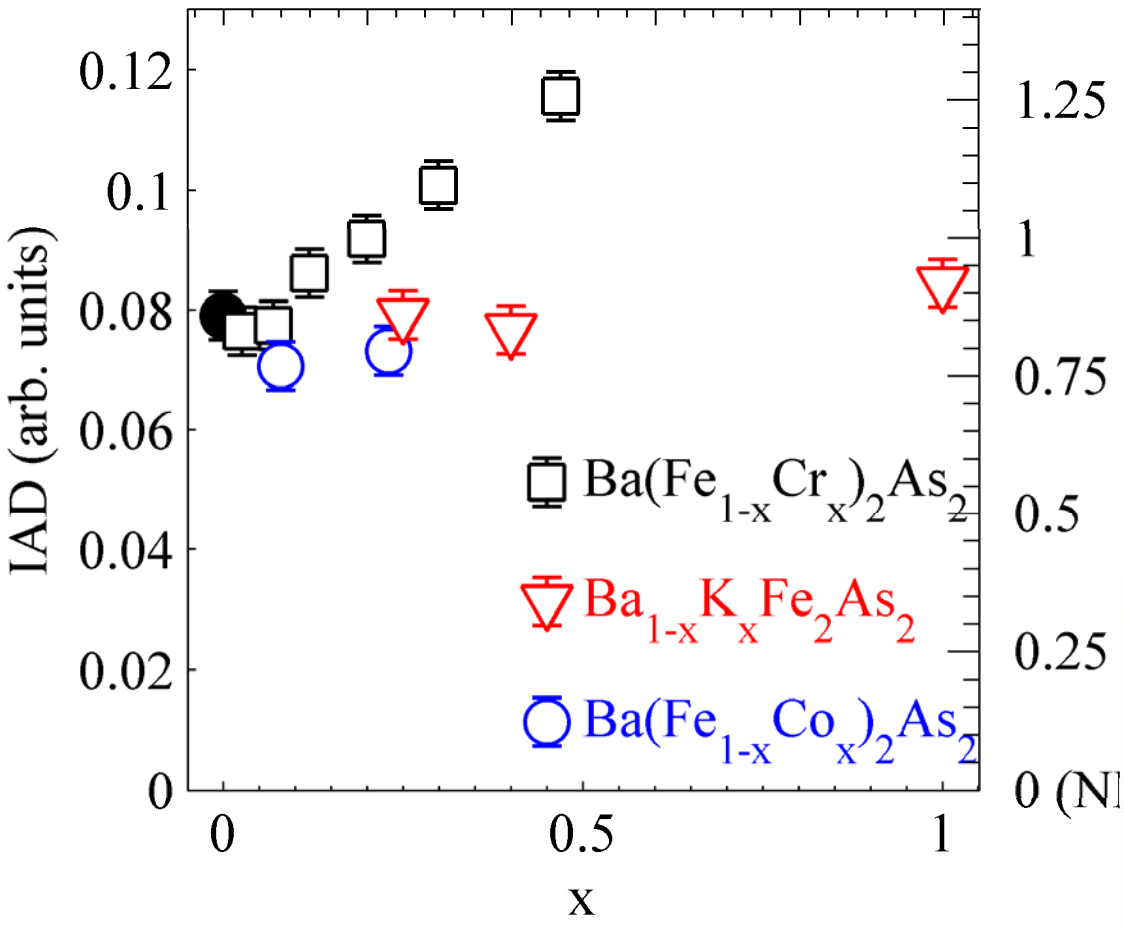
Temperature dependence

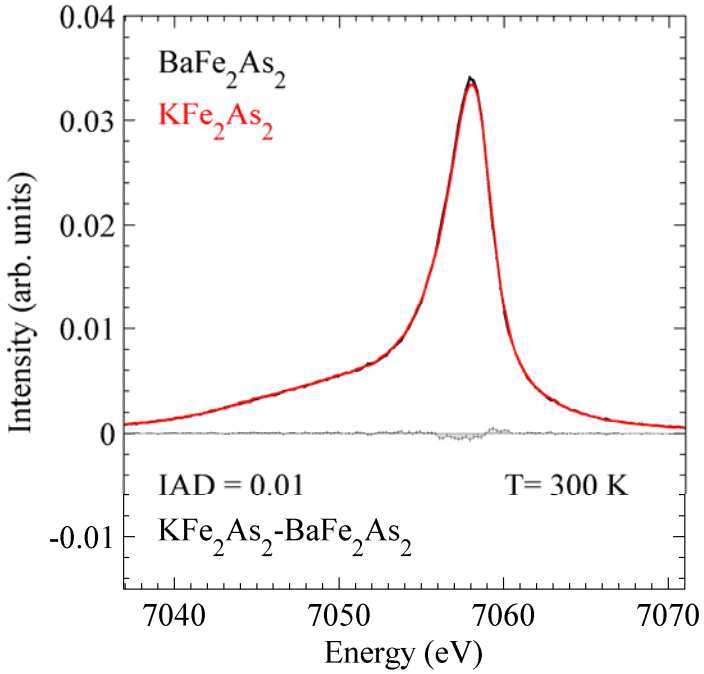


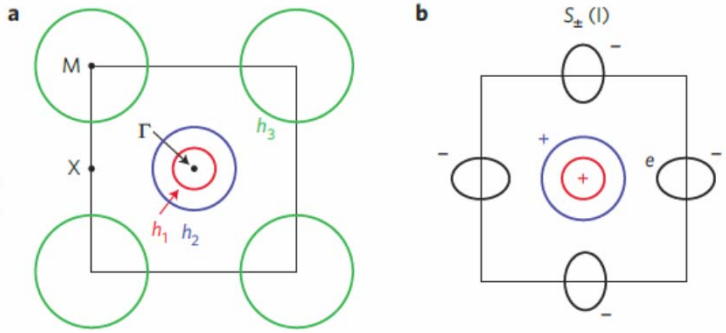


Harriger et al., PRB 86, 140403(R) (2012)

Doping dependence



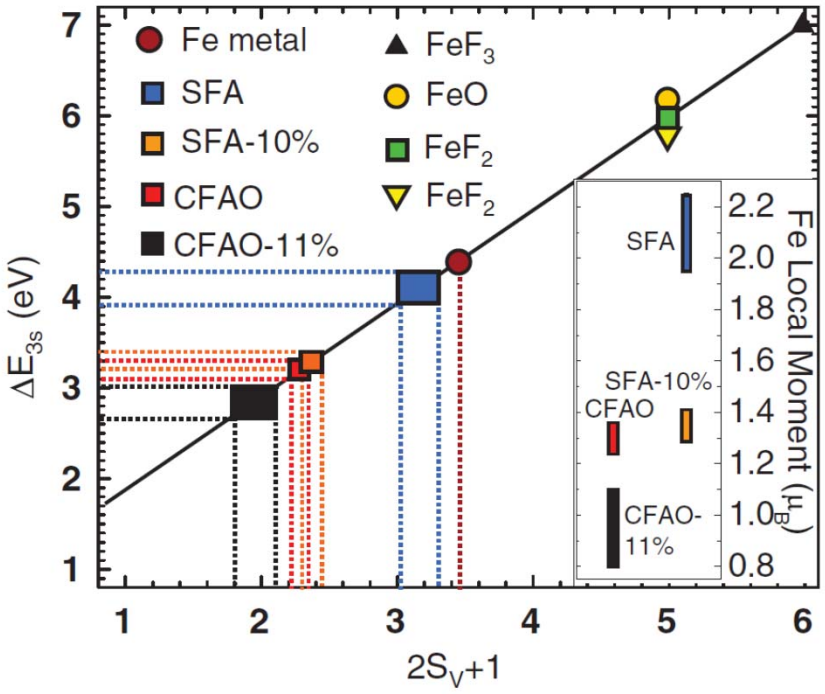




F. F. Tafti et al., Nat. Phys. 9, 349 (2013)

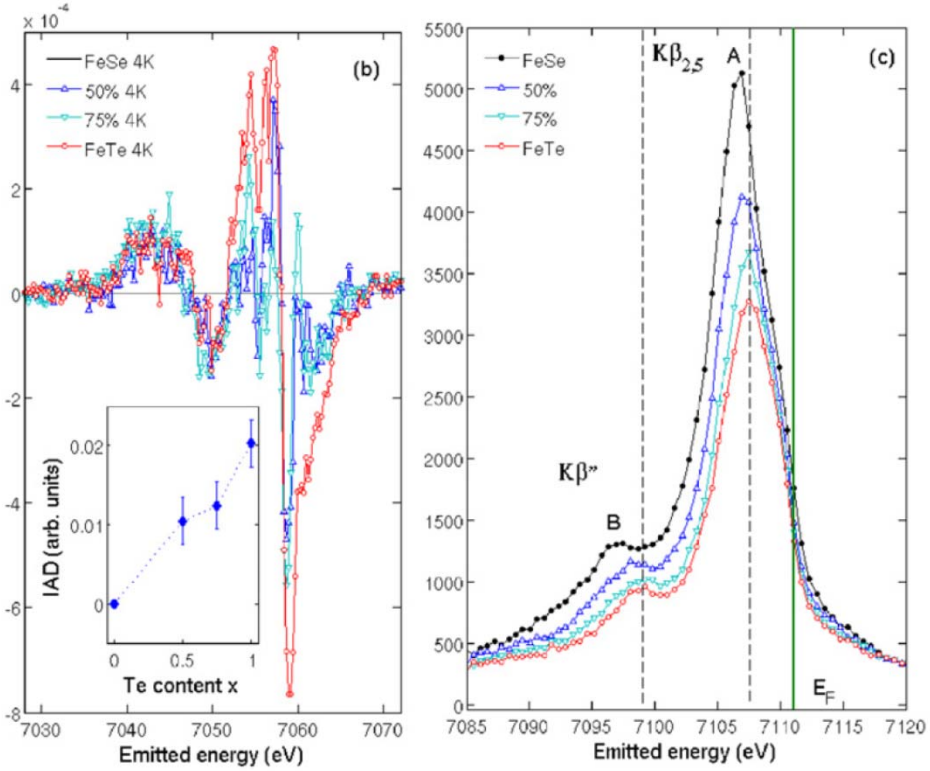
Other doping dependence studies

3s XPS
Sr(Fe,Co)2As2 and CeFeAsO



Vilmercarti et al. PRB 85, 220503 (2012)

Fe Kβ XES
Fe(SeTe)



Simonelli et al. JPCM, 24, 415501 (2012)

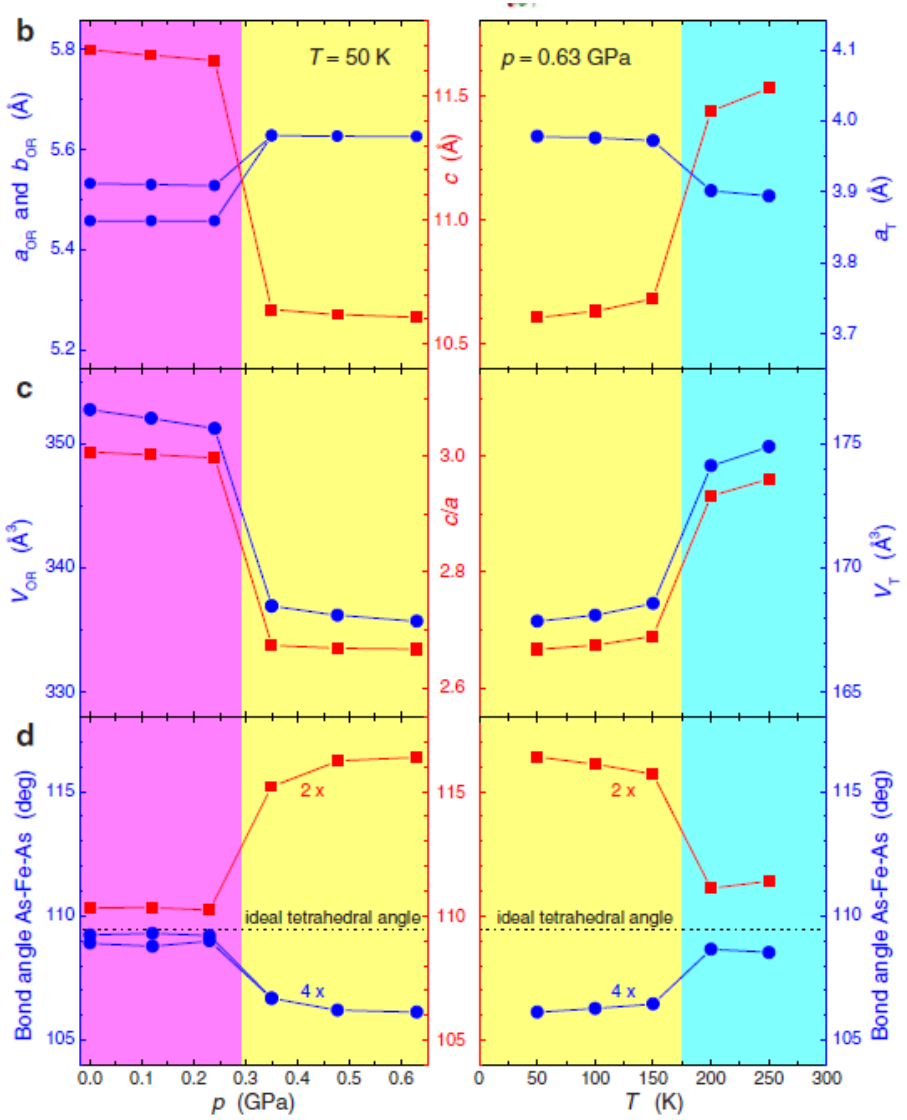
Outline

1. X-ray Emission Spectroscopy
   - What do we measure?
2. Survey of Fe based materials
   - Material dependence
   - Temperature and doping dependence?
3. What
   - Larg
     - Spi
     - Re

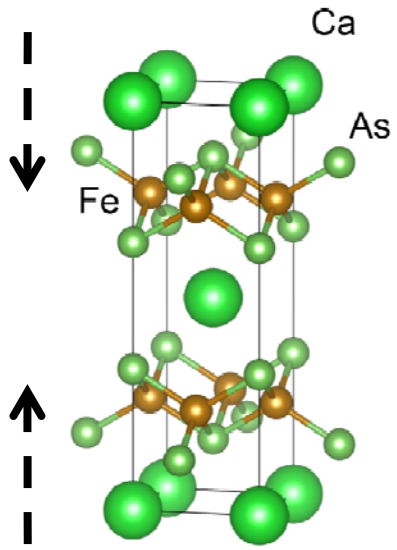
- Non-zero moments for all samples studied ($2S_{eff}$ is not an integer)
- Very weak temperature dependence*
- Very weak doping dependence*

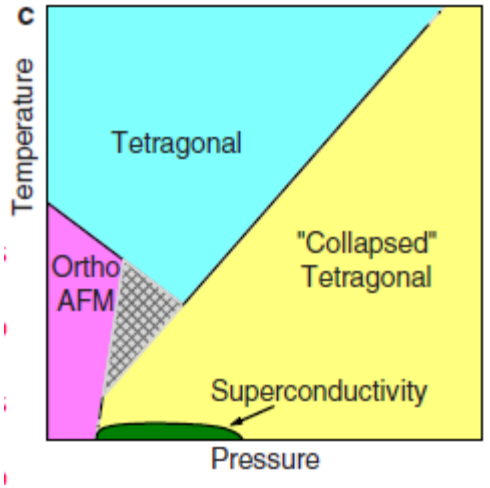
Collapsed Tetragonal (cT) phase

$CaFe_2As_2$



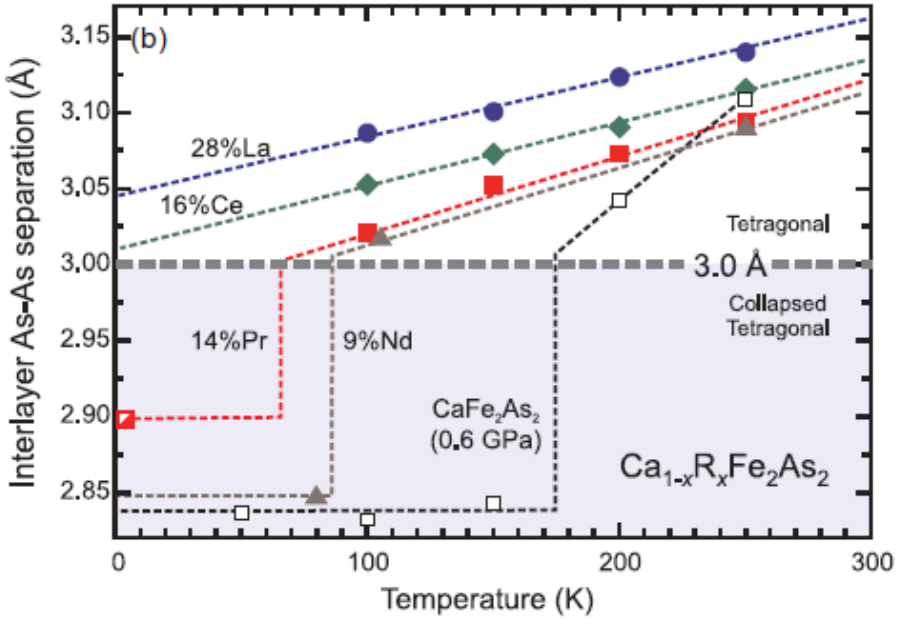
Kreyssig et al. Phys. Rev. B 78, 184517 (2008)





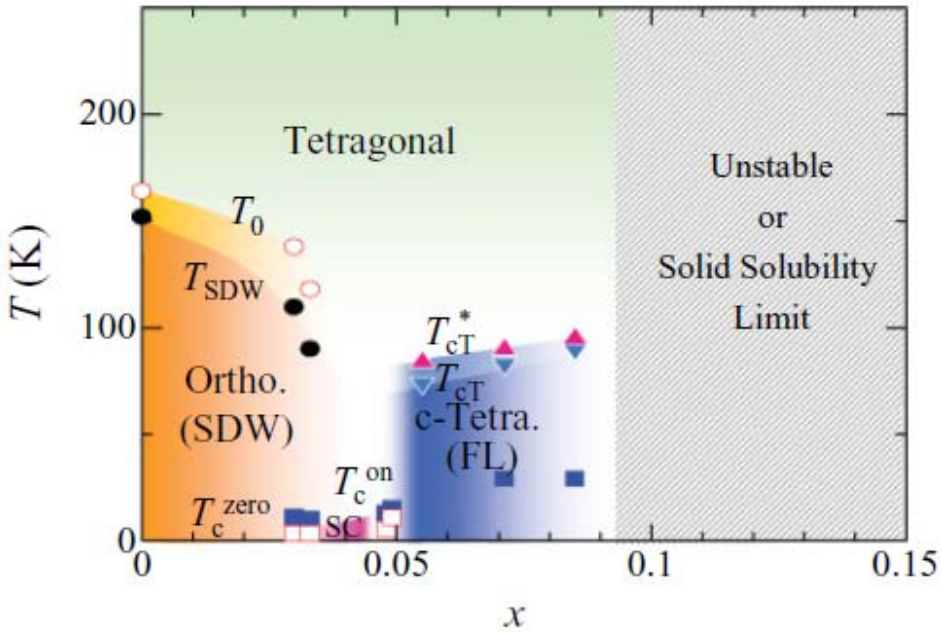
cT phase in ambient pressure

Rare-Earths doping



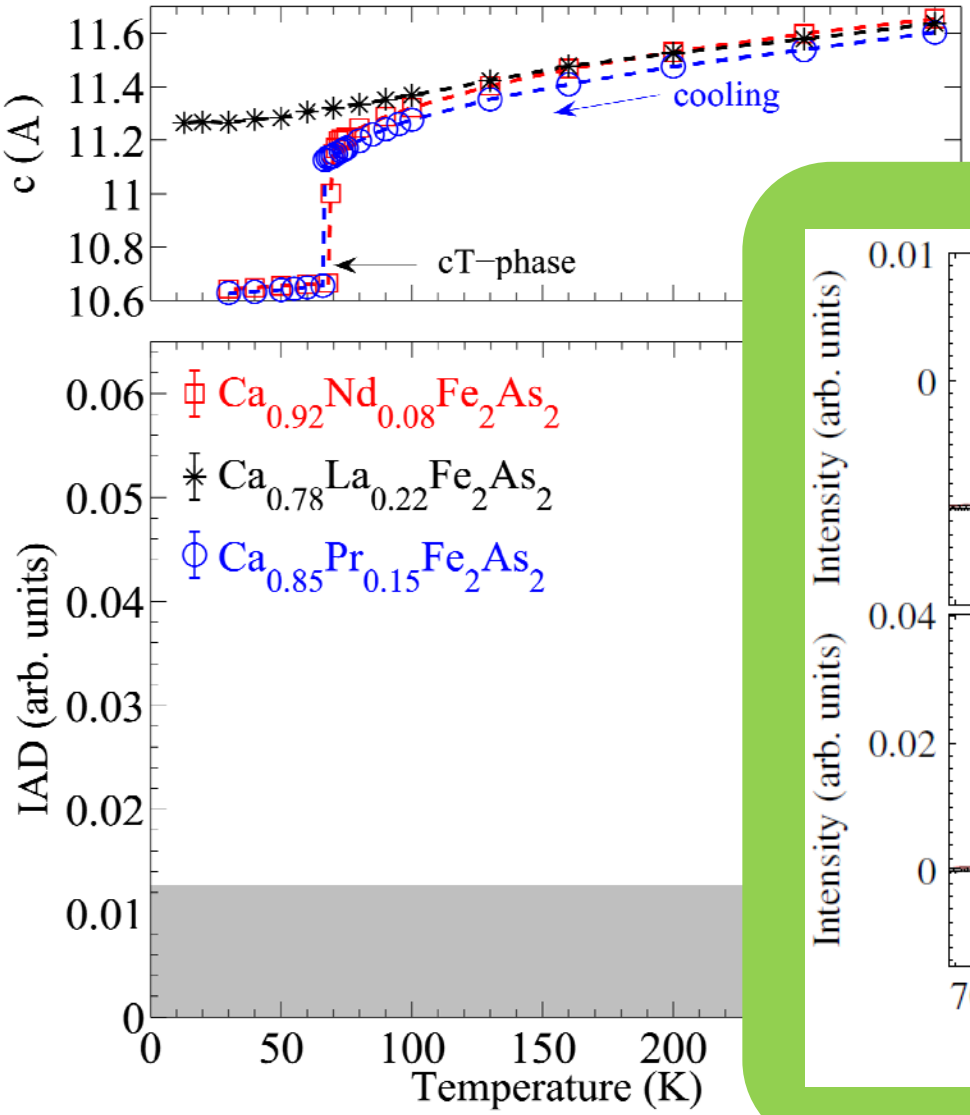
Saha, Paglione et al.
Phys. Rev. B
85, 024525 (2012)

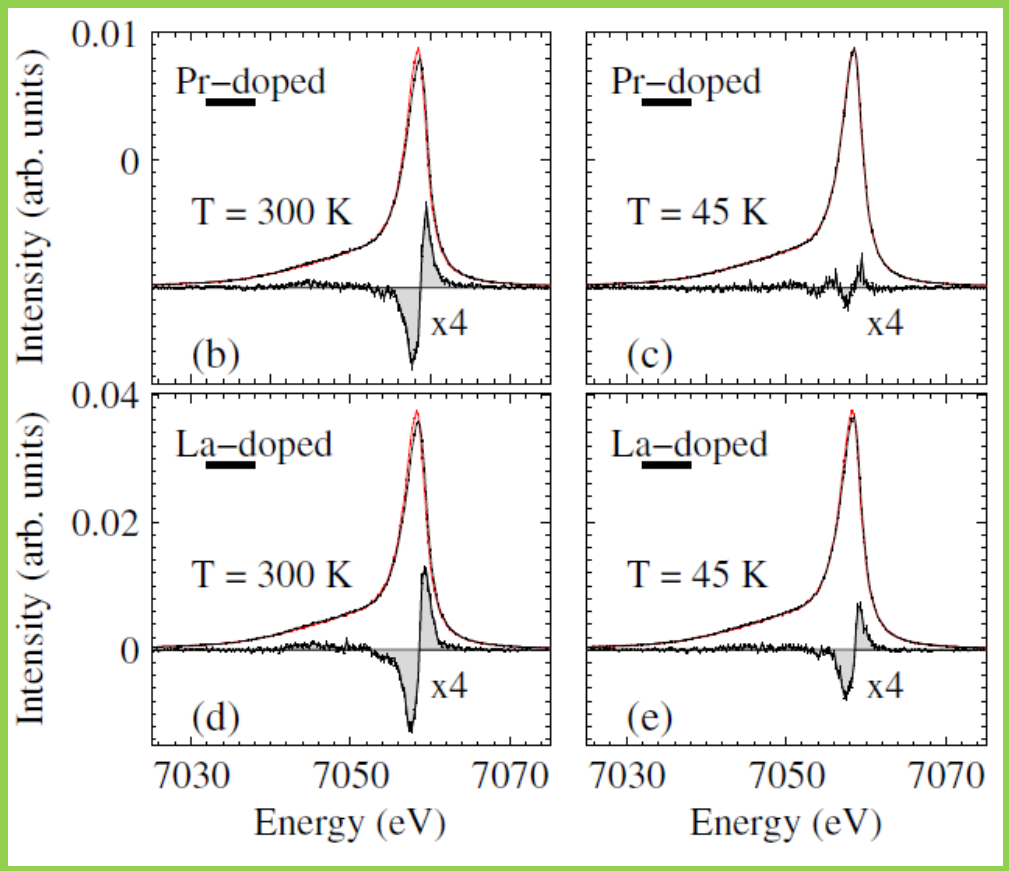
P doping (As site)



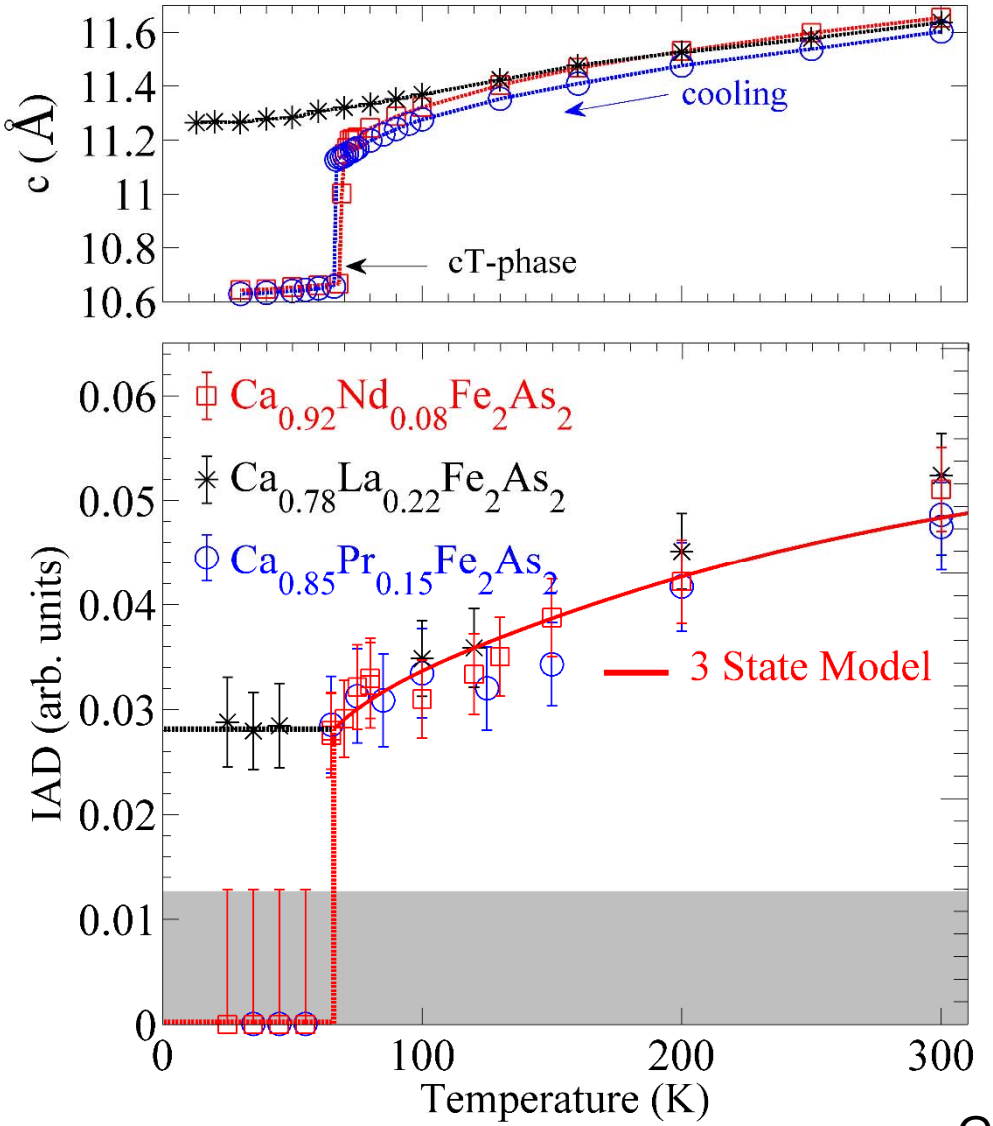
Kasahara et al.
Phys. Rev. B
83, 060505 (R) (2011)

Rare-Earths doped $CaFe_2As_2$

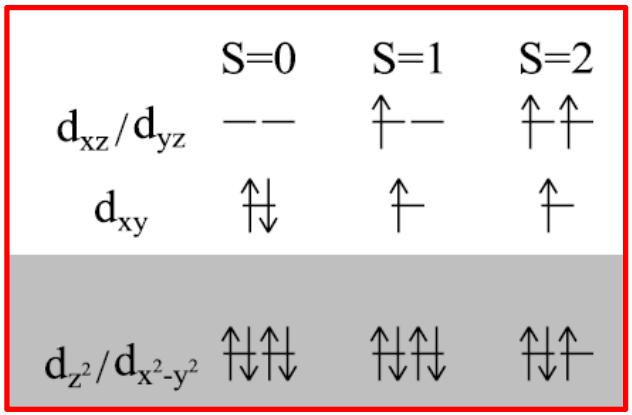




RE doped $CaFe_2As_2$



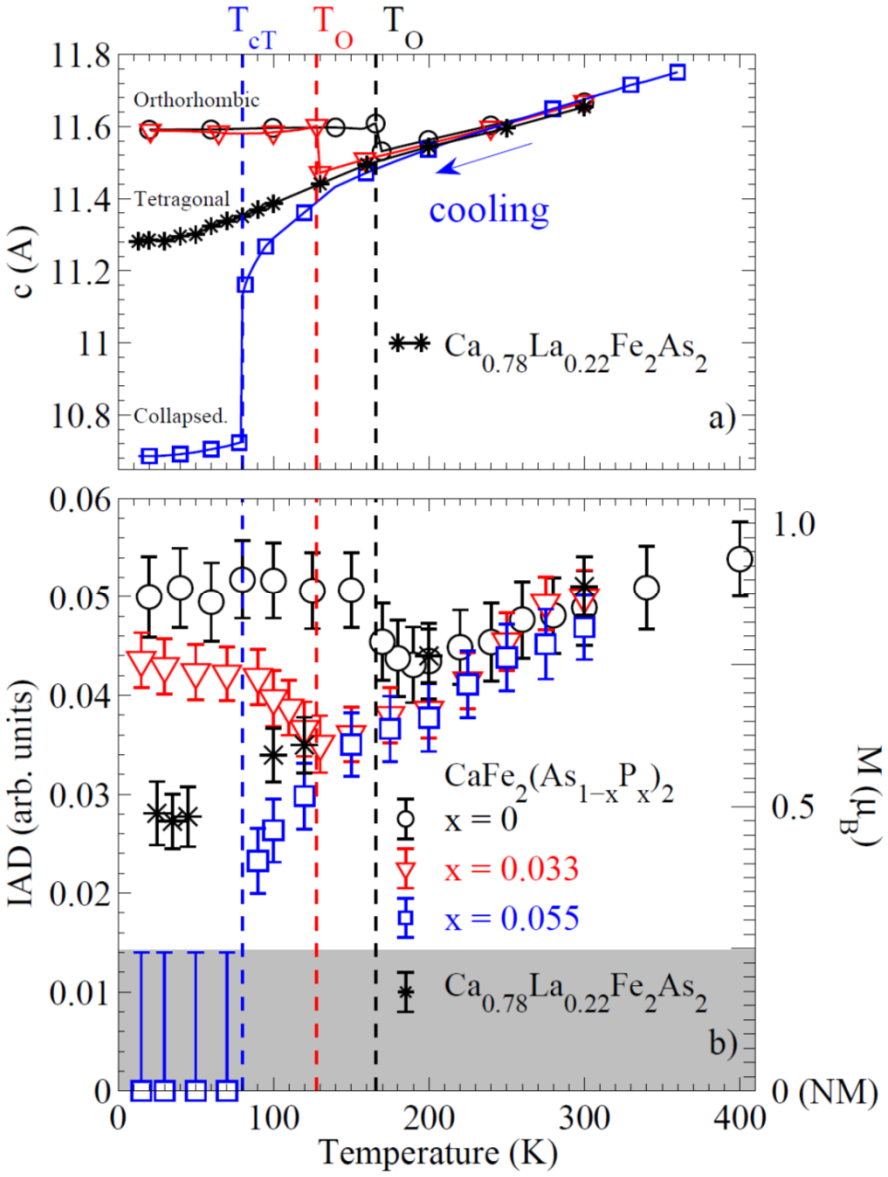
3 spin-state model



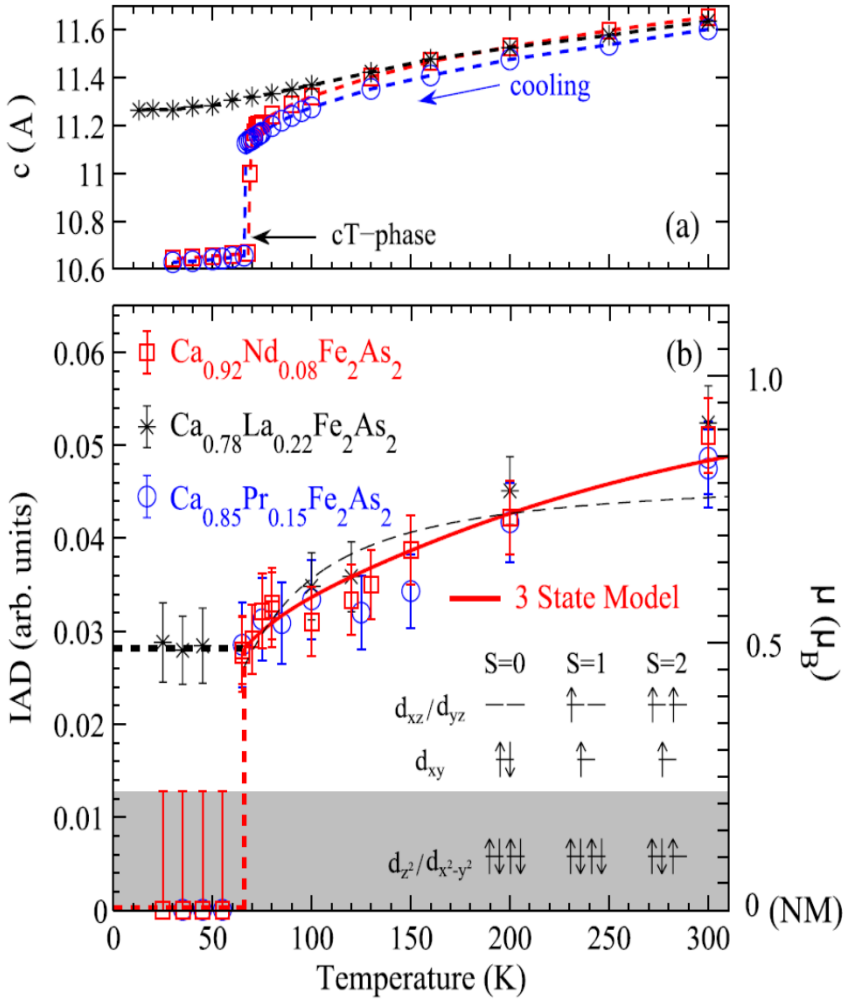
Hund's coupling J_H ~ crystal field splitting (?)

Gretarsson et al. PRL 110, 047003 (2013)

P doped $CaFe_2As_2$



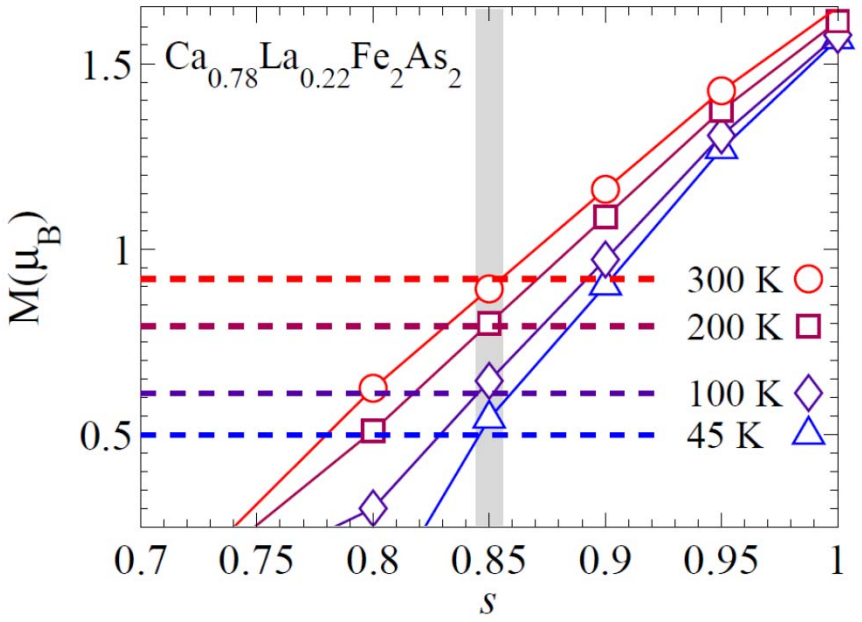
RE doped Ca122

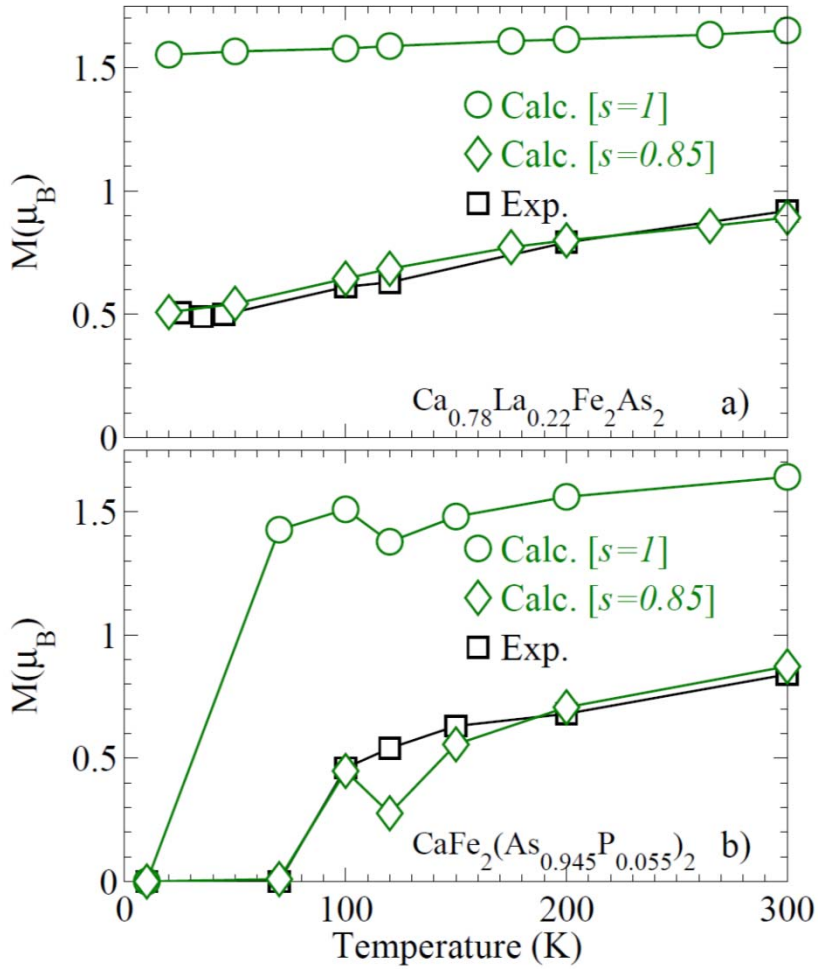


Reduced Stoner Theory

- Renormalization of LSDA Stoner parameter

$$I \rightarrow sI \ (0 < s < 1)$$





L. Ortenzi, L. Boeri, I. Mazin, Gretarsson, YJK et al., arXiv:1408.4058

Conclusions

- X-ray Emission Spectroscopy provides
  - Instantaneous measurement of
  - Fluctuating local moment
  - By comparing with inelastic neutron scattering, absolute scale can be found
- All pnictides have non-integer $2S_{eff}$ and large fluctuating local moment at all temperatures.
  - Not much of doping and temperature dependence
- $CaFe_2As_2$
  - Zero moment in the collapsed tetragonal phase
  - Large temperature dependence: explained by reduced Stoner theory LSDA calculation (structural origin)