RIXS and XMCD for the study of high Tc superconductors

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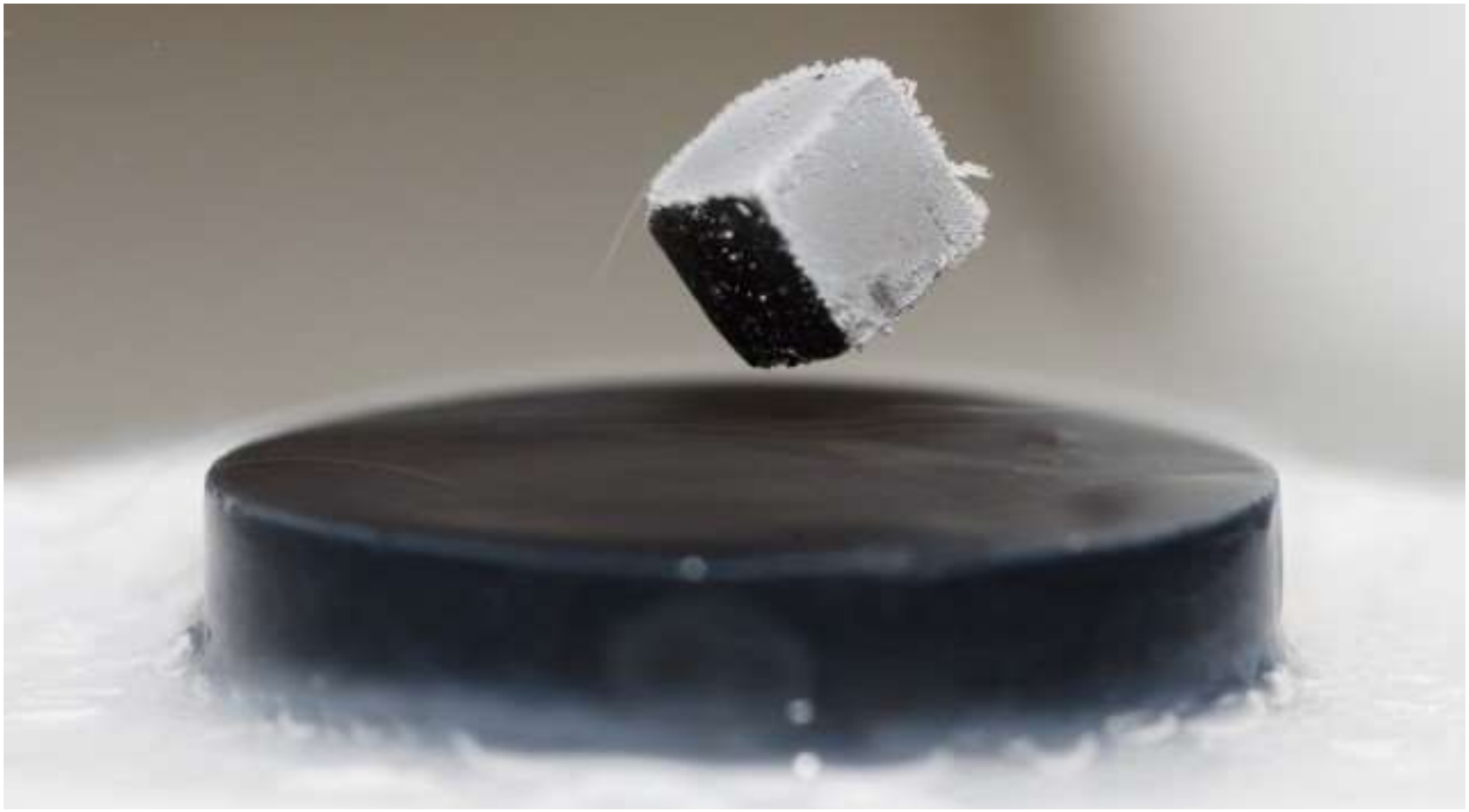
Summary

- The case of cuprate high Tc superconductors
- XMCD of cuprates
- Cu L_3 RIXS and spin excitations in cuprates

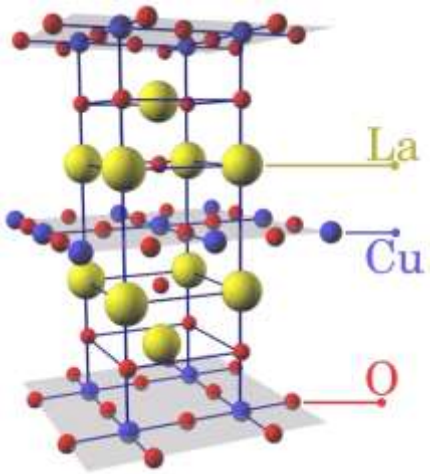
POLITECNICO MILANO 1863

PAUL SCHERRER INSTITUT PSI SWISS LIGHT SOURCE SLS

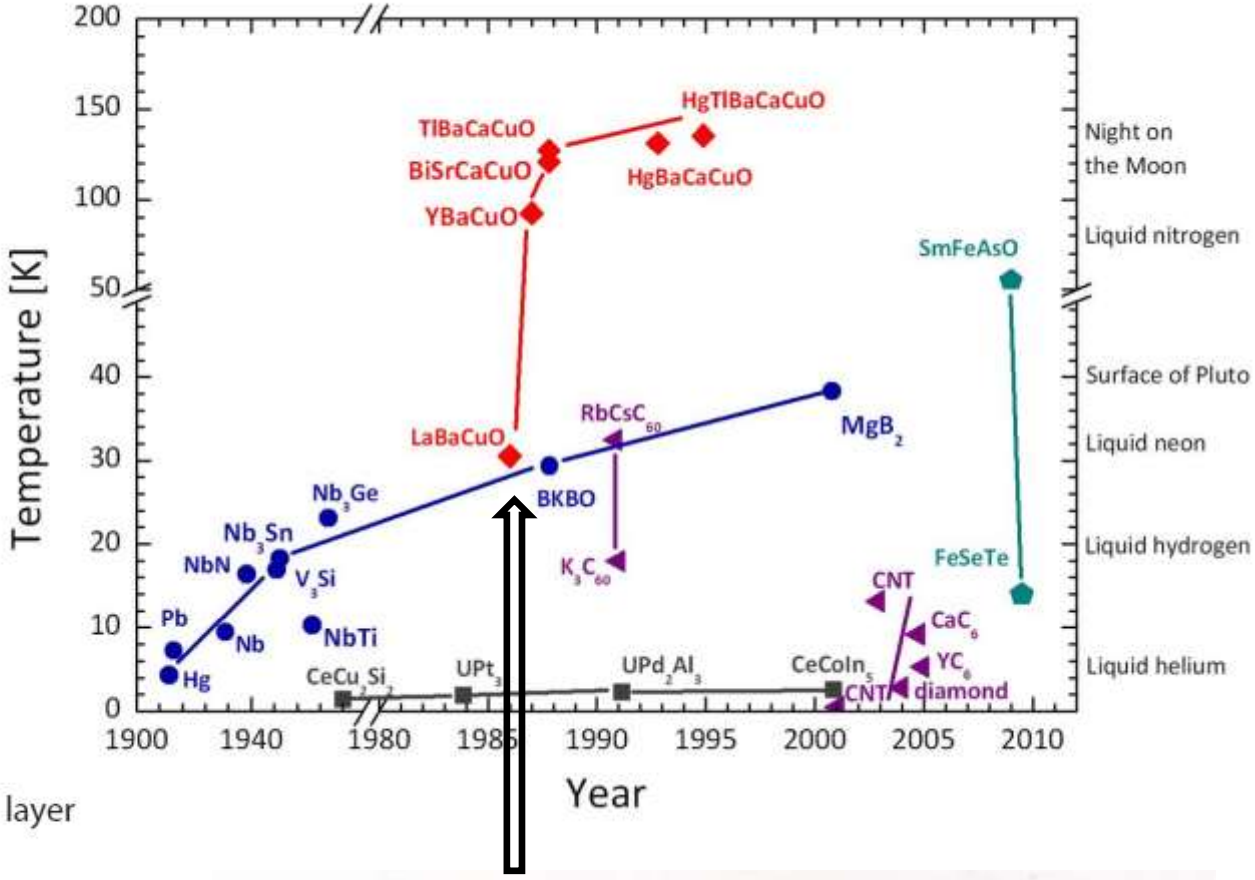
High Tc superconductors

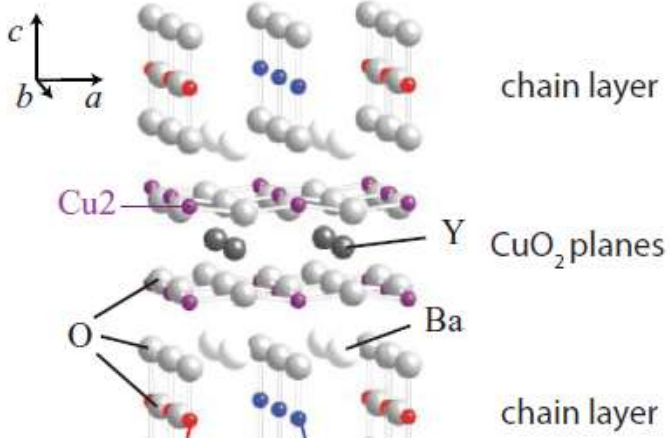


High Tc superconducting cuprates



$La_{2-x}Sr_xCuO_4$ (LSCO)





$YBa_2Cu_3O_{6+\delta}$ (YBCO)

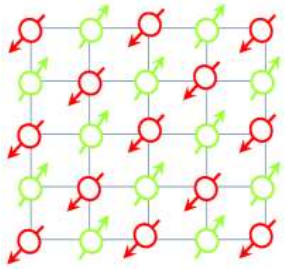
Possible High T_c Superconductivity in the Ba–La–Cu–O System

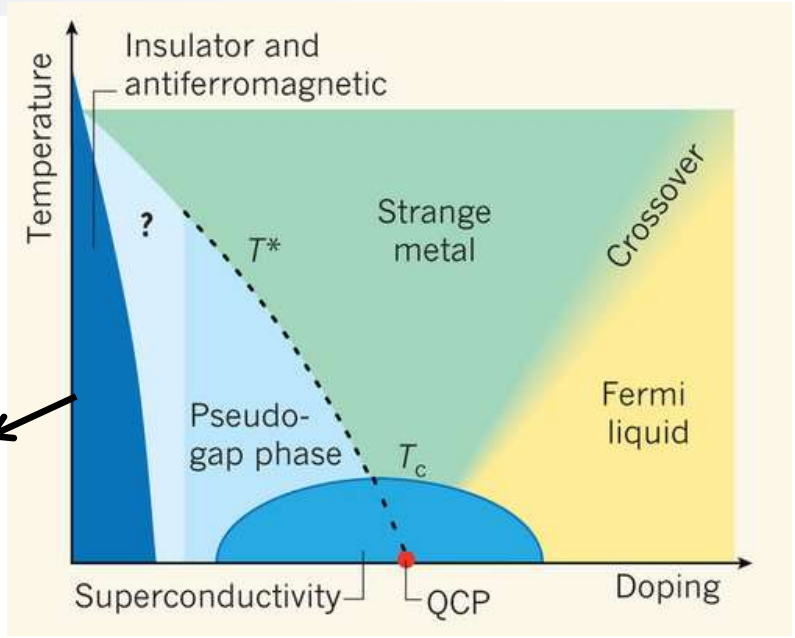
J.G. Bednorz and K.A. Müller
IBM Zürich Research Laboratory, Rüschlikon, Switzerland

Received April 17, 1986

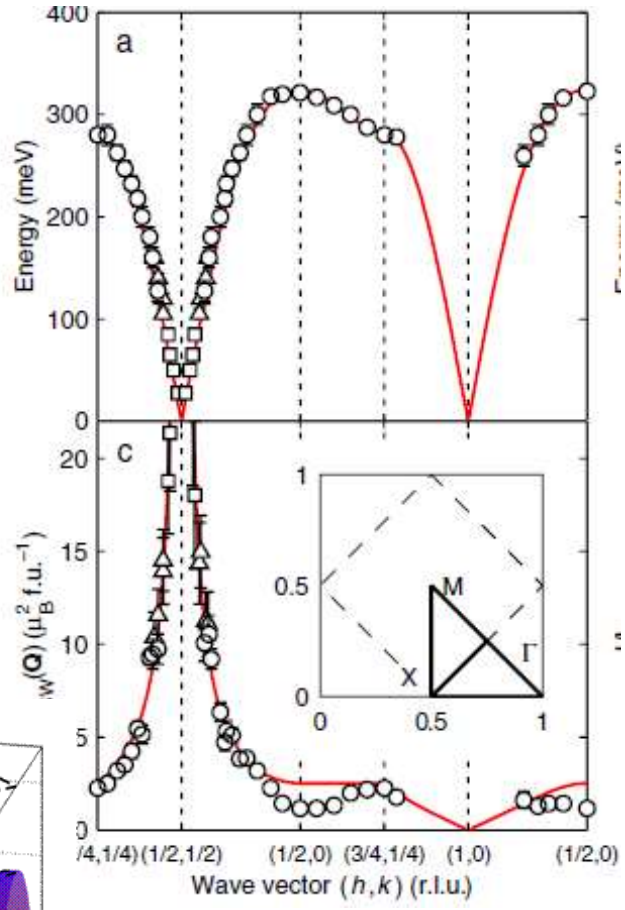
Spin excitations in HTcS: undoped AF

2D AF

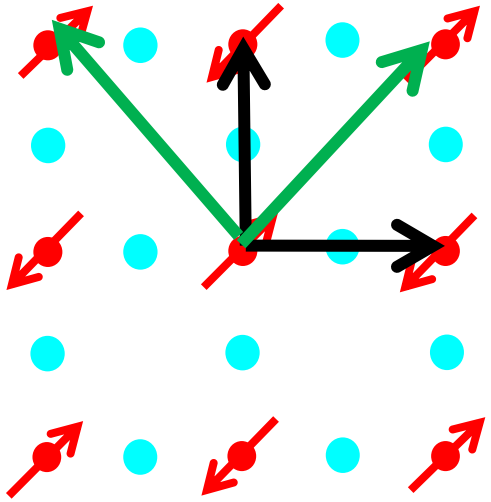




INS: La_2CuO_4

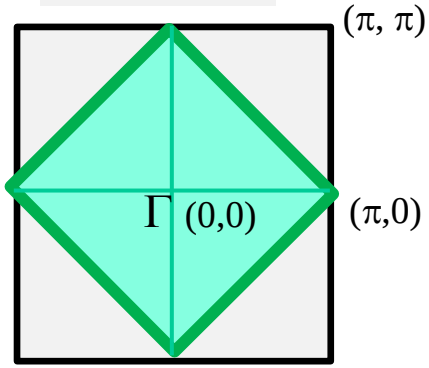


DIRECT SPACE

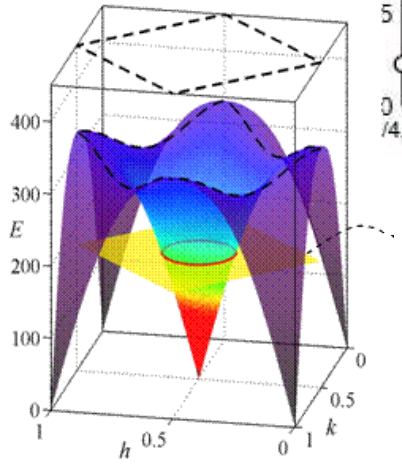


RECIPROCAL SPACE

nuclear BZ

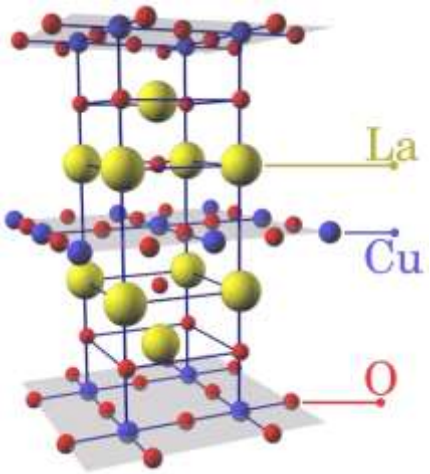


magnetic BZ

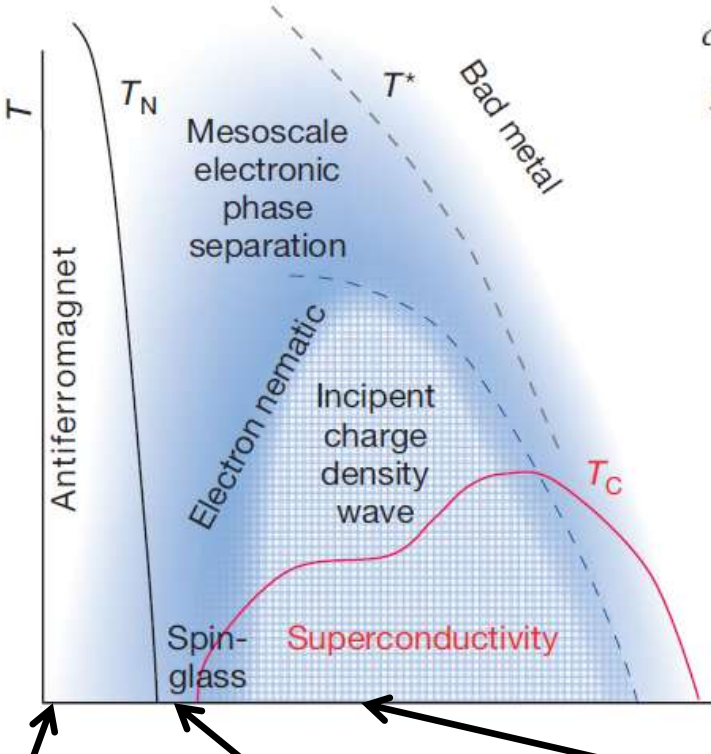


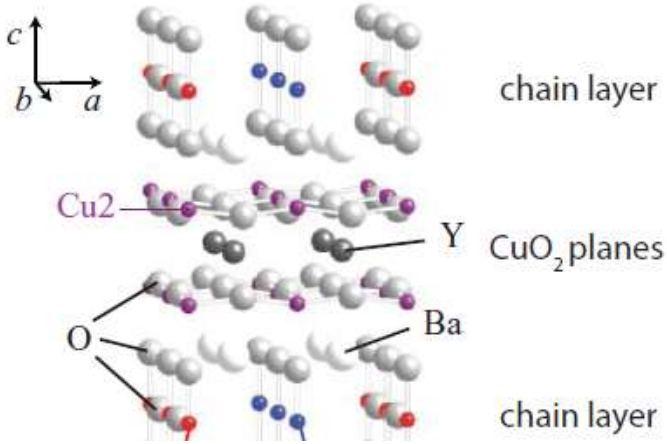
N. S. Headings, S. M. Hayden, R. Coldea, and T. G. Perring, Phys Rev Lett. **105** 247001 (2011)

The mysteries of HT_cS



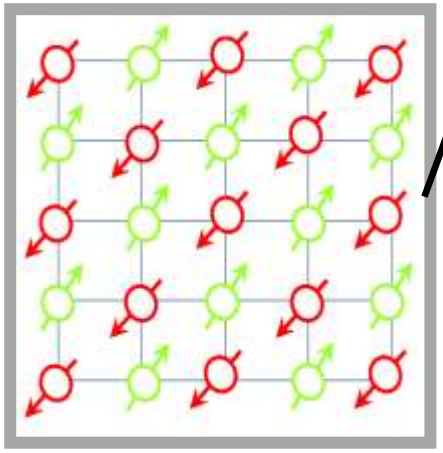
$La_{2-x}Sr_xCuO_4$ (LSCO)

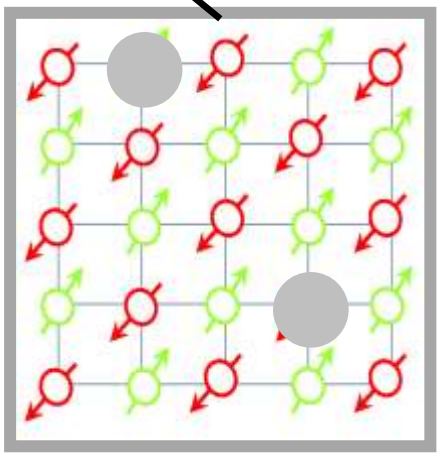


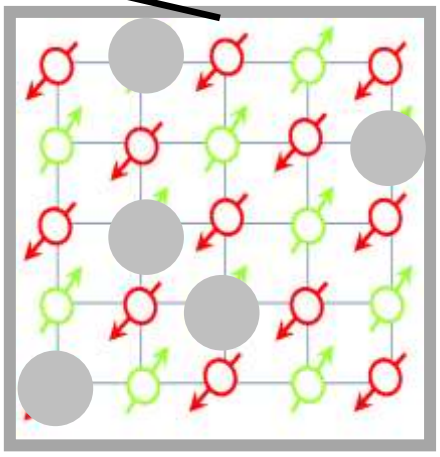


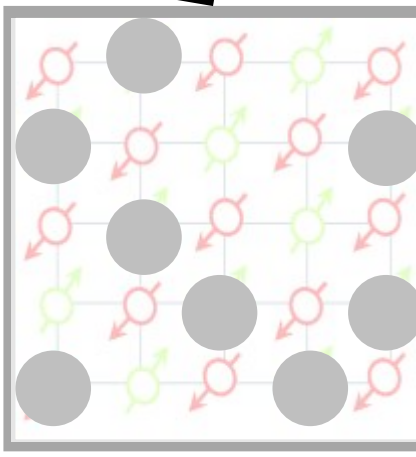
$YBa_2Cu_3O_{6+\delta}$ (YBCO)

Eduardo Fradkin and Steven A. Kivelson, Nature Physics, 8, 864 (2012)

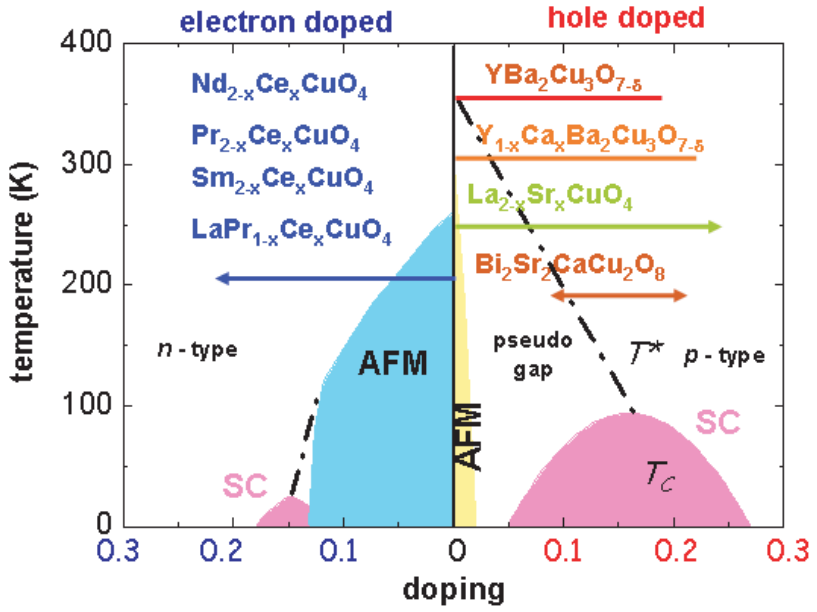




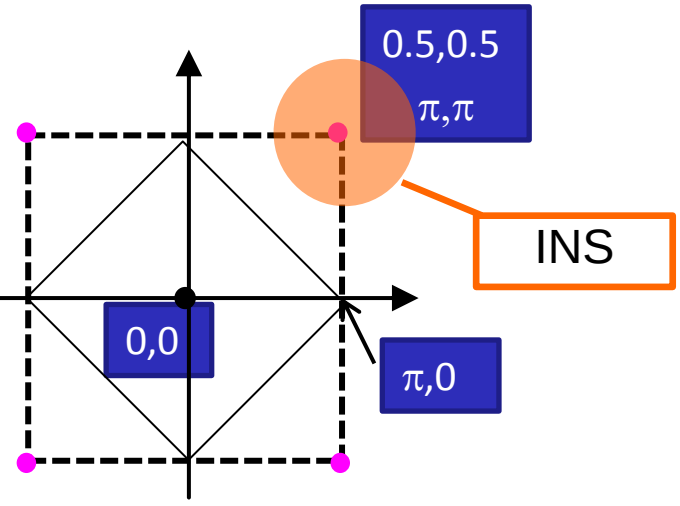


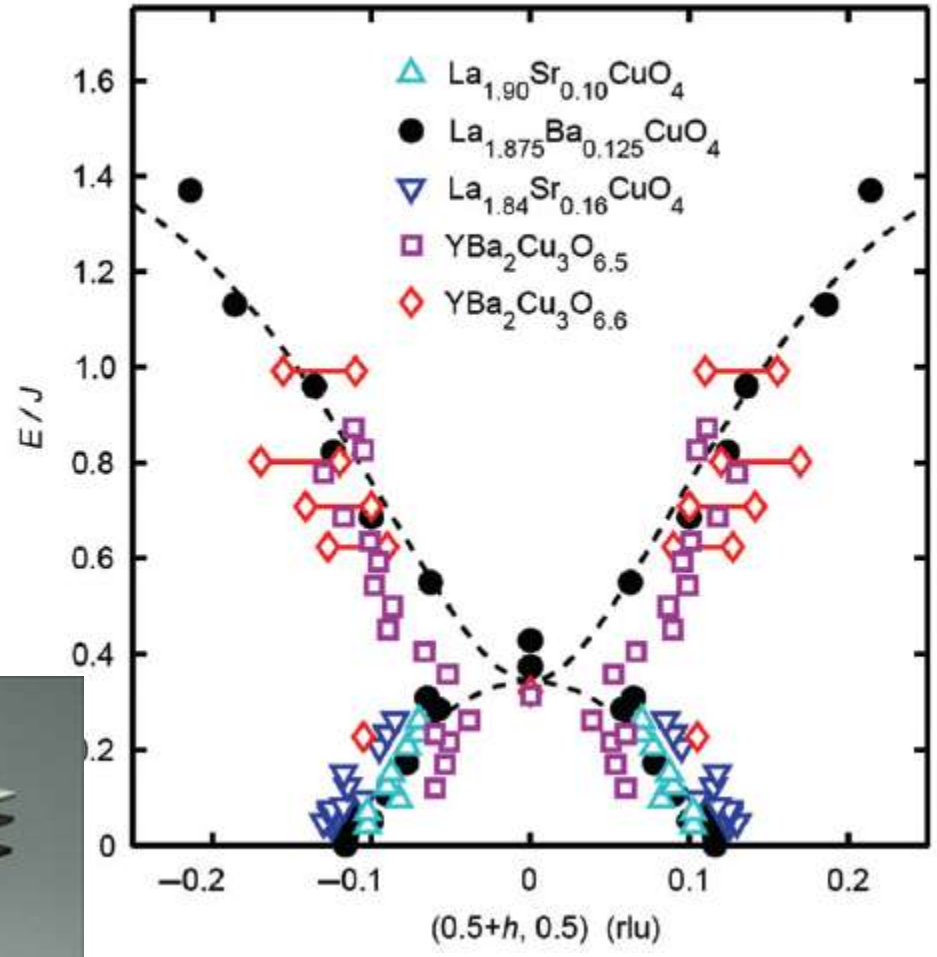


Spin excitations in HTcS: doped SC



http://for538.wmi.badw.de/projects/P4_crystal_growth/index.htm

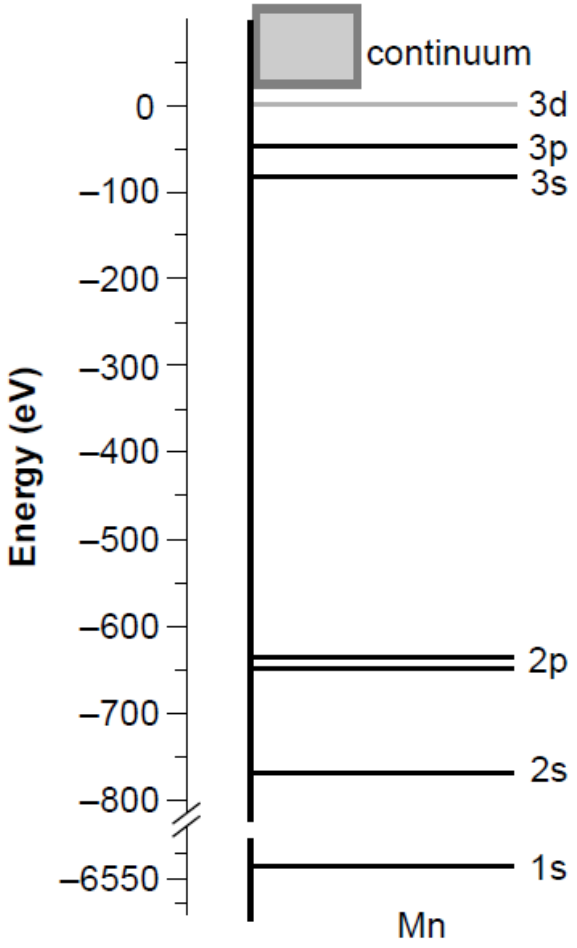


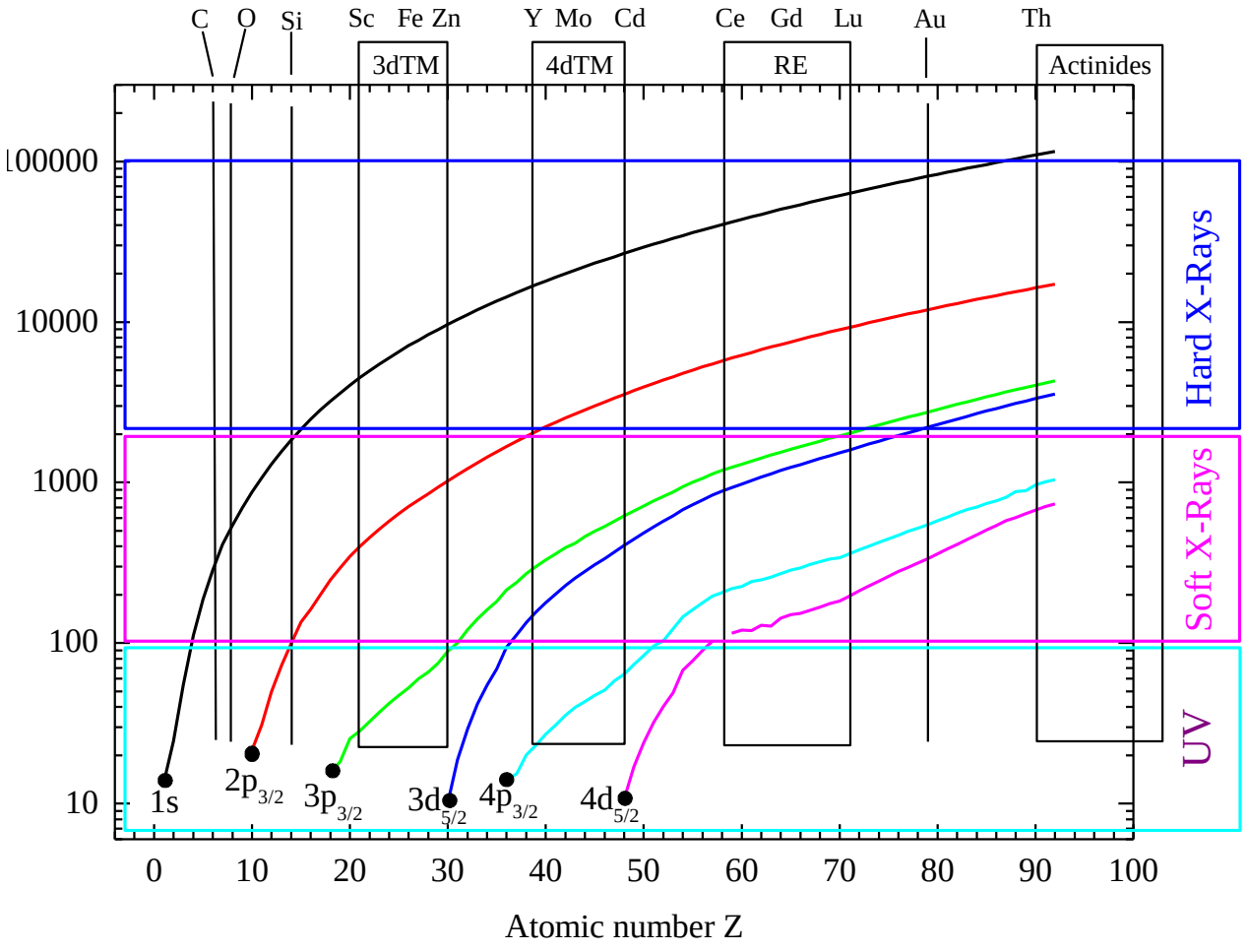


J.M. Tranquada, in *Handbook of High-Temperature Superconductivity: Theory and Experiment*, J.R. Schrieffer and J.S. Brooks, eds., Springer, 2007,

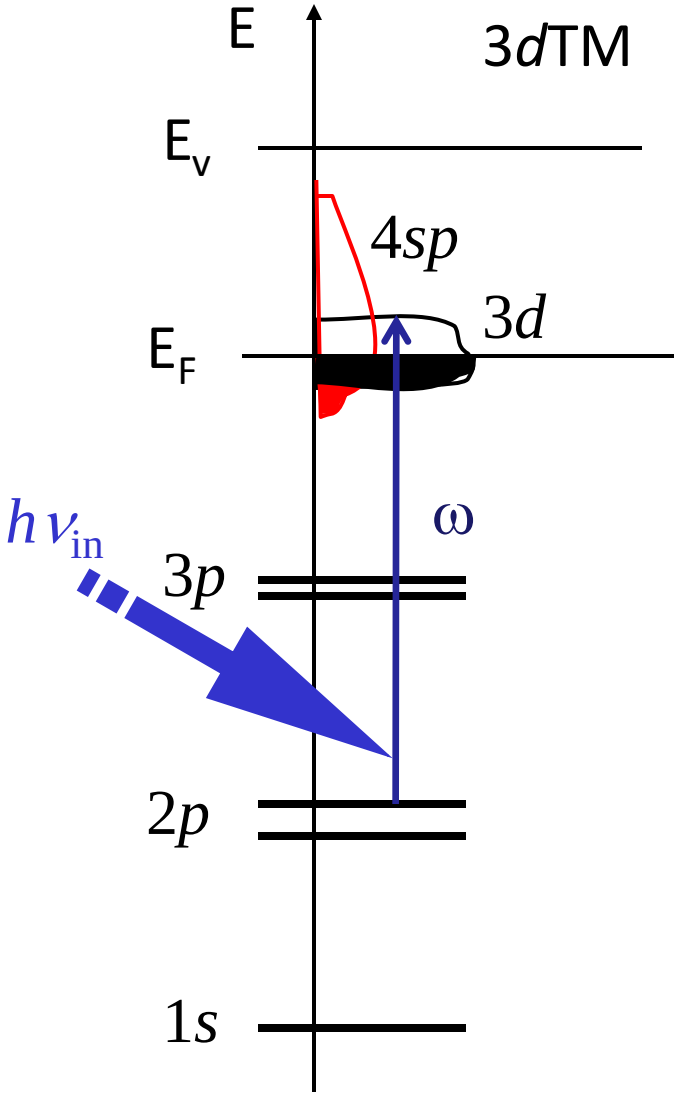
V. Hinkov et al, Eur. Phys. J. Special Topics 188, 113–129 (2010)

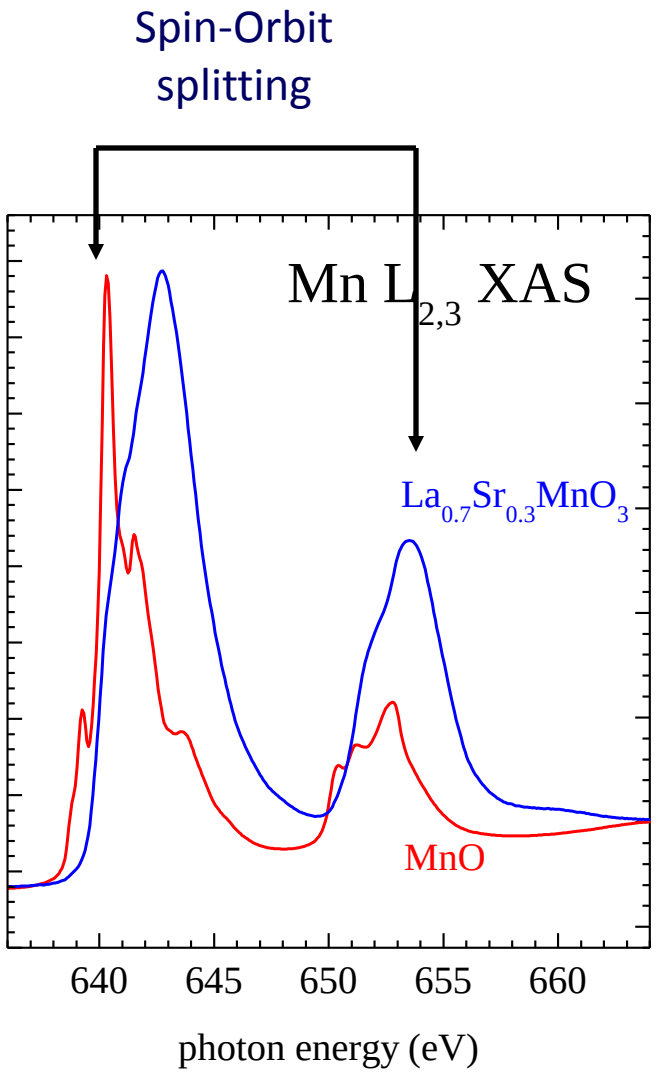
Core level binding energies and edges



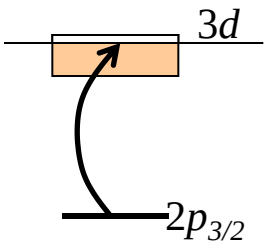


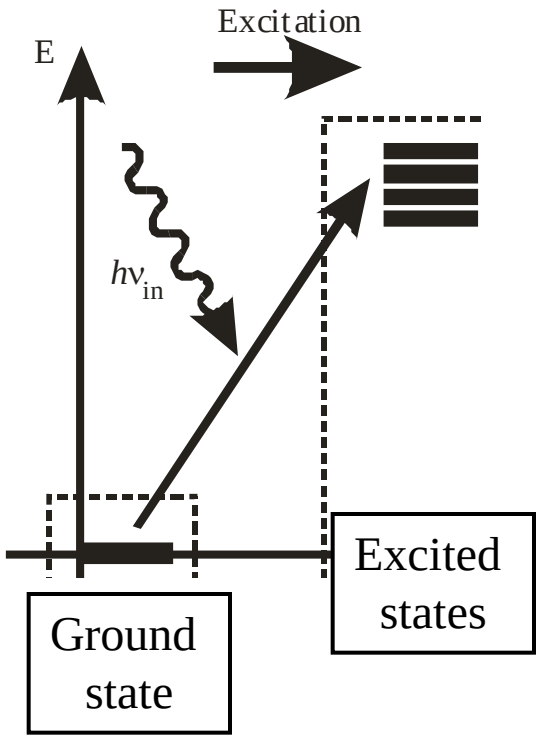
XAS of 3d transition metals

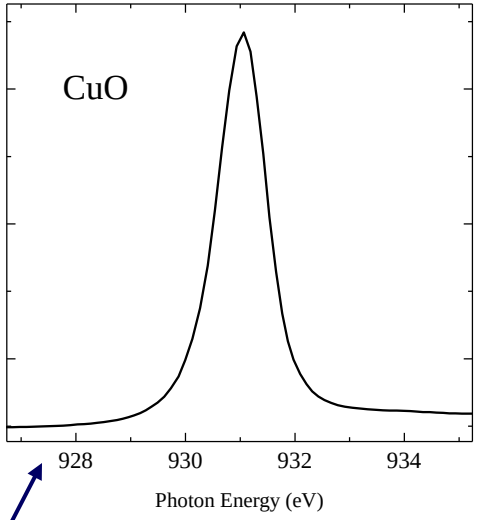


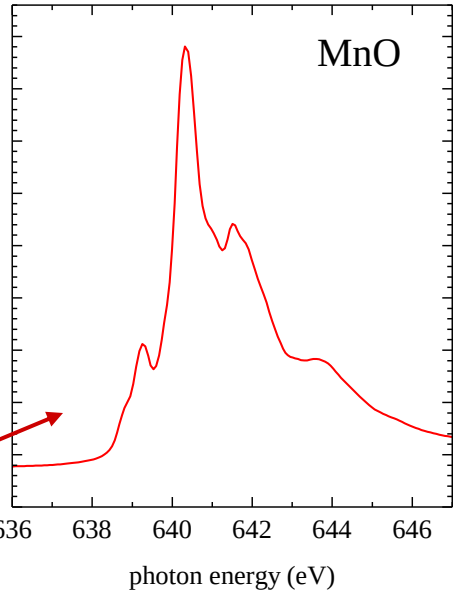


L_3 XAS and multiplets









$$3d^{\,n} \longrightarrow 2p^5 3d^{\,n+1}$$

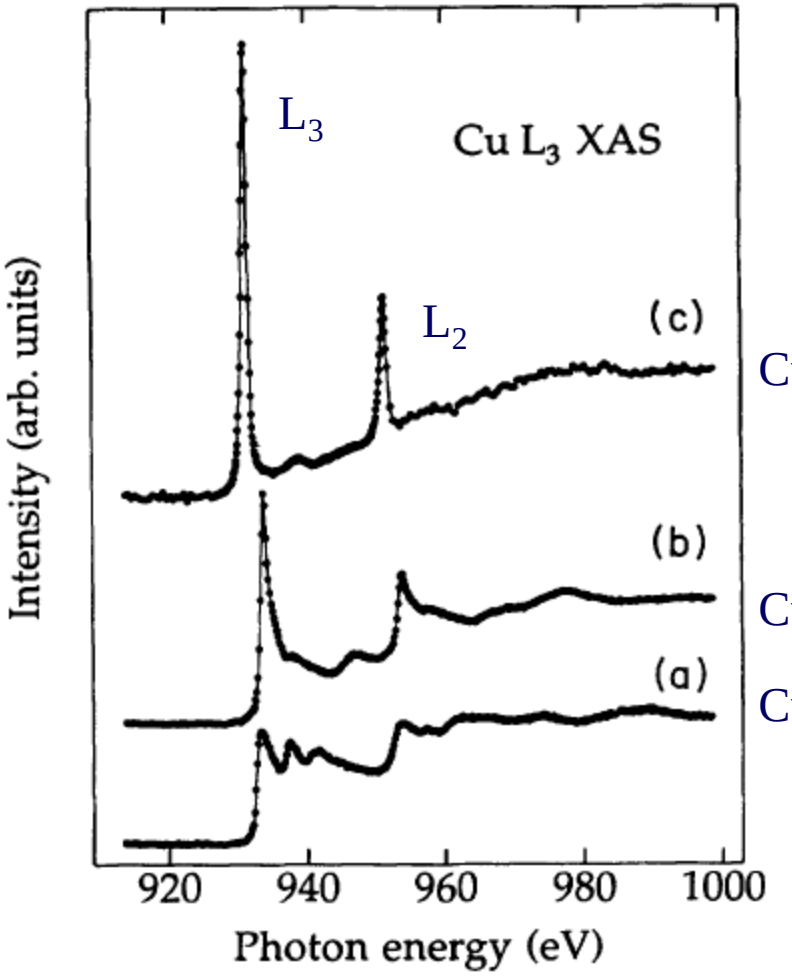
CuO: $3d^9 \rightarrow 3d^{10}$

One single peak

NiO: $3d^8 \rightarrow 3d^9$
MnO: $3d^5 \rightarrow 3d^6$

Many peaks

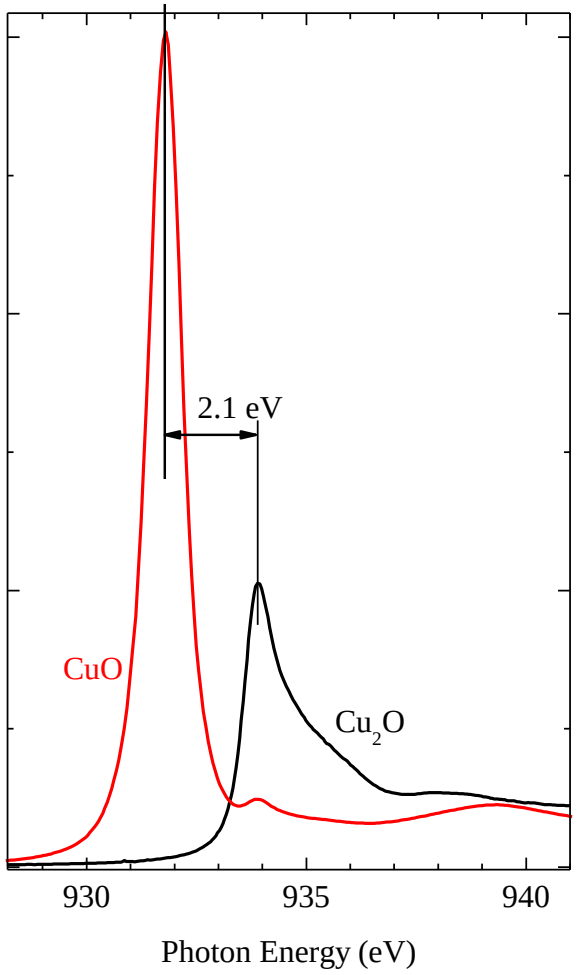
L_3 XAS and valence



CuO: Cu^{2+} is $3d^9$

Cu_2O: Cu^{1+} is $3d^{10}$

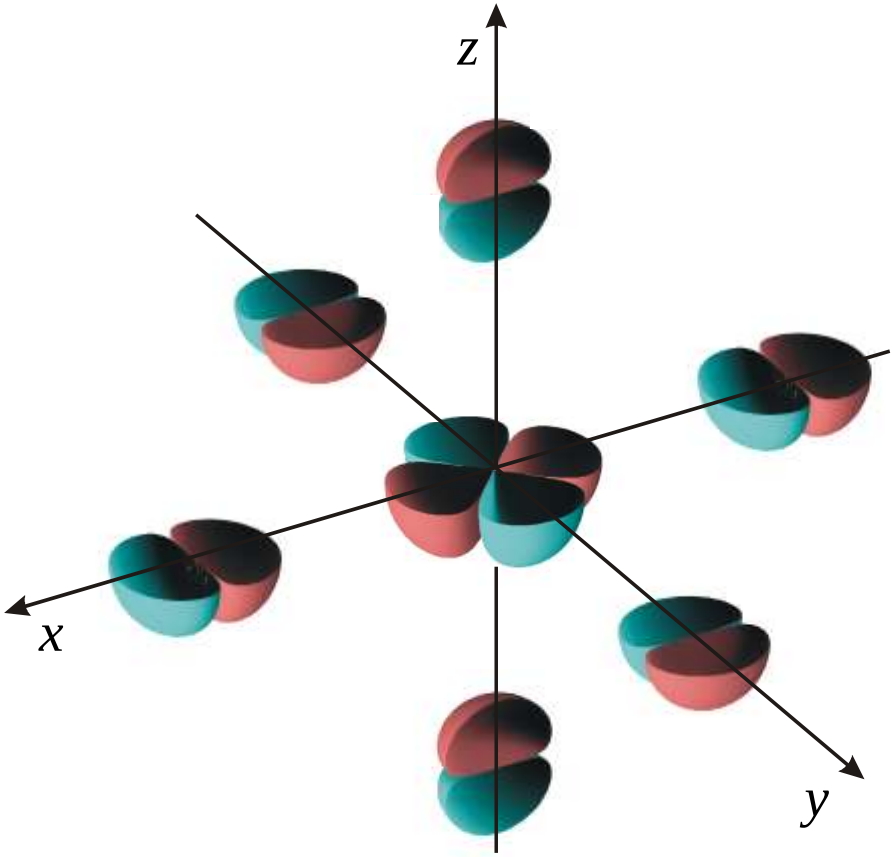
Cu metal: $3d^{10}4s^1$

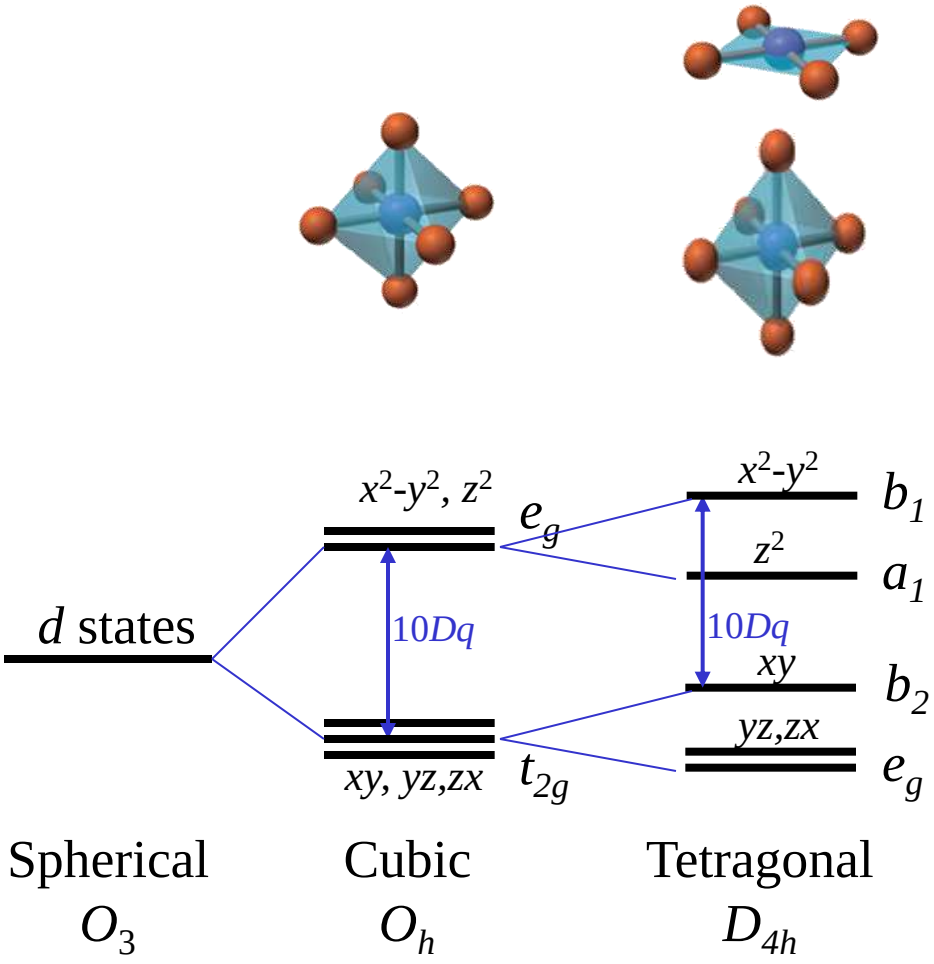


Source: M. Grioni *et al* PRB **45**, 3309 (1992)

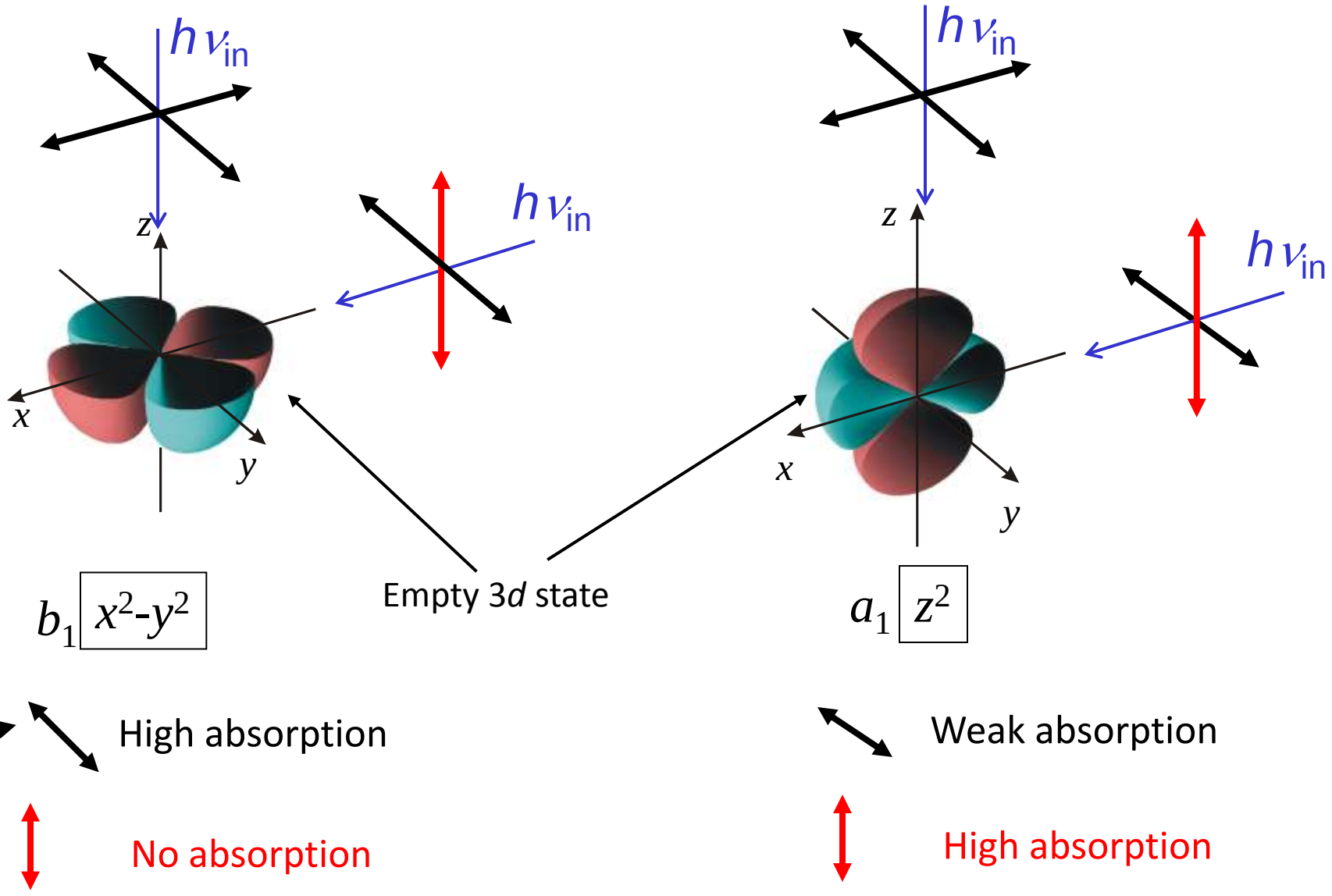
Source: M. Finazzi *et al* PRB **61**, 4629 (2000)

Crystal field



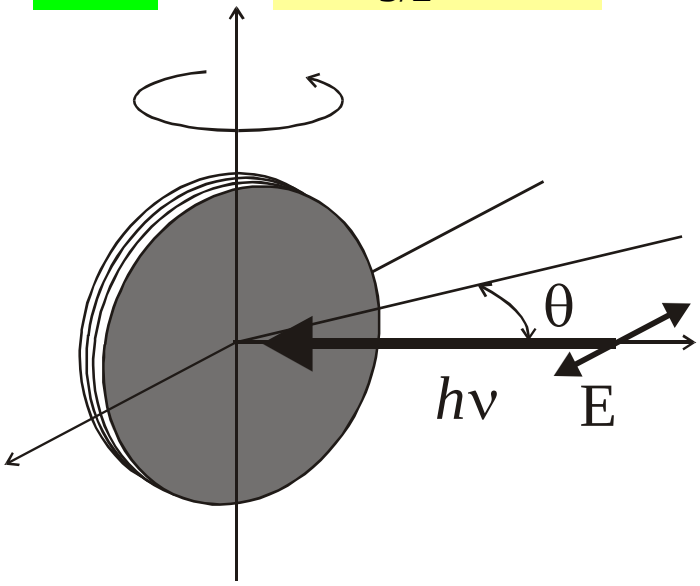


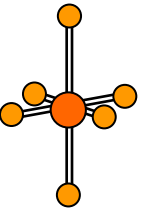
Linear polarization of x-rays and orbital orientation



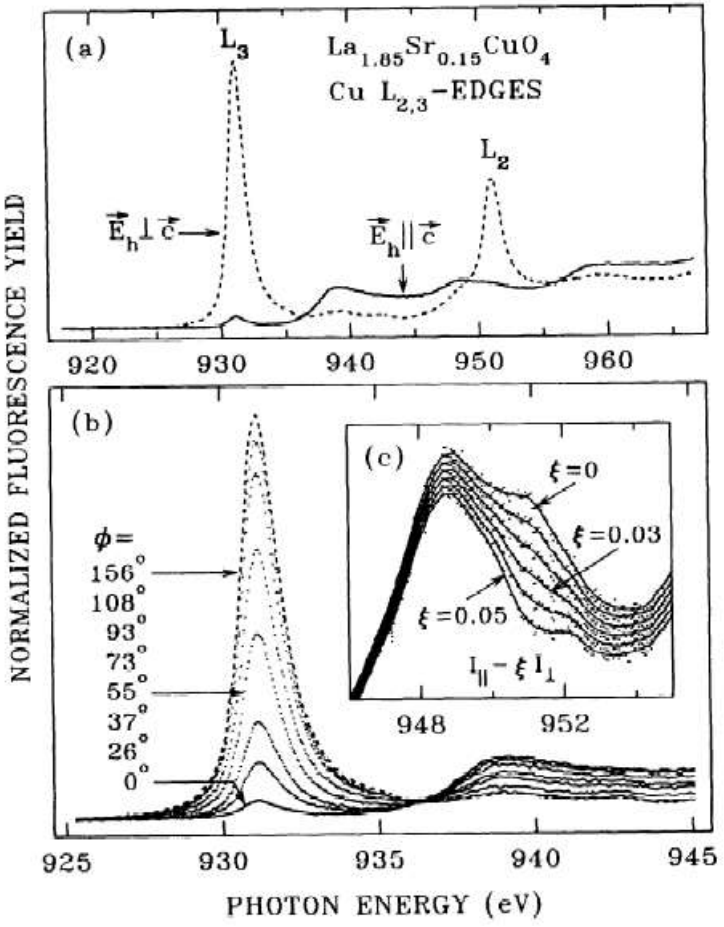
3*d* hole symmetry in cuprates

$3d^9 \rightarrow (2p_{3/2})^3 3d^{10}$





Result: the hole in Cu^{2+} has 100% x^2-y^2 symmetry



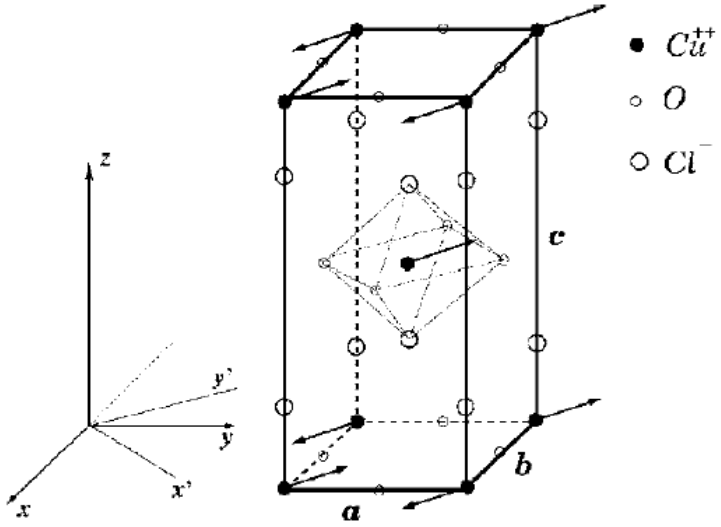
VOLUME 68, NUMBER 16 PHYSICAL REVIEW LETTERS 20 APRIL 1992

Out-of-Plane Orbital Characters of Intrinsic and Doped Holes in $La_{2-x}Sr_xCuO_4$

C. T. Chen, L. H. Tjeng, J. Kwo, H. L. Kao, P. Rudolf, F. Sette, and R. M. Fleming

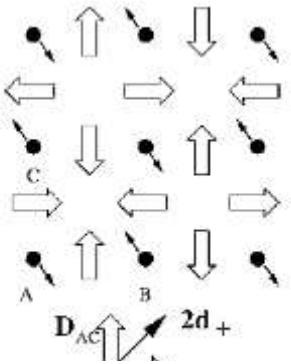
Weak ferromagnetism of cuprates

$Sr_2CuO_2Cl_2$



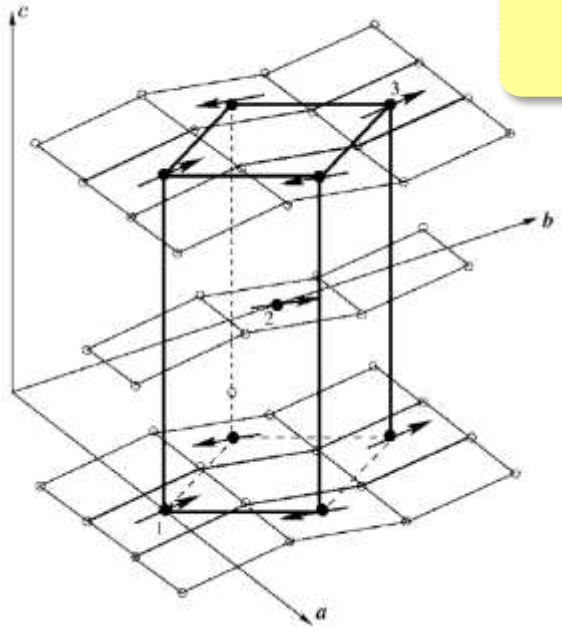
Perfectly flat CuO_2 planes

Spins are along (110), no out-of-plane component



Dzyaloshinskii-Moriya interaction

La_2CuO_4

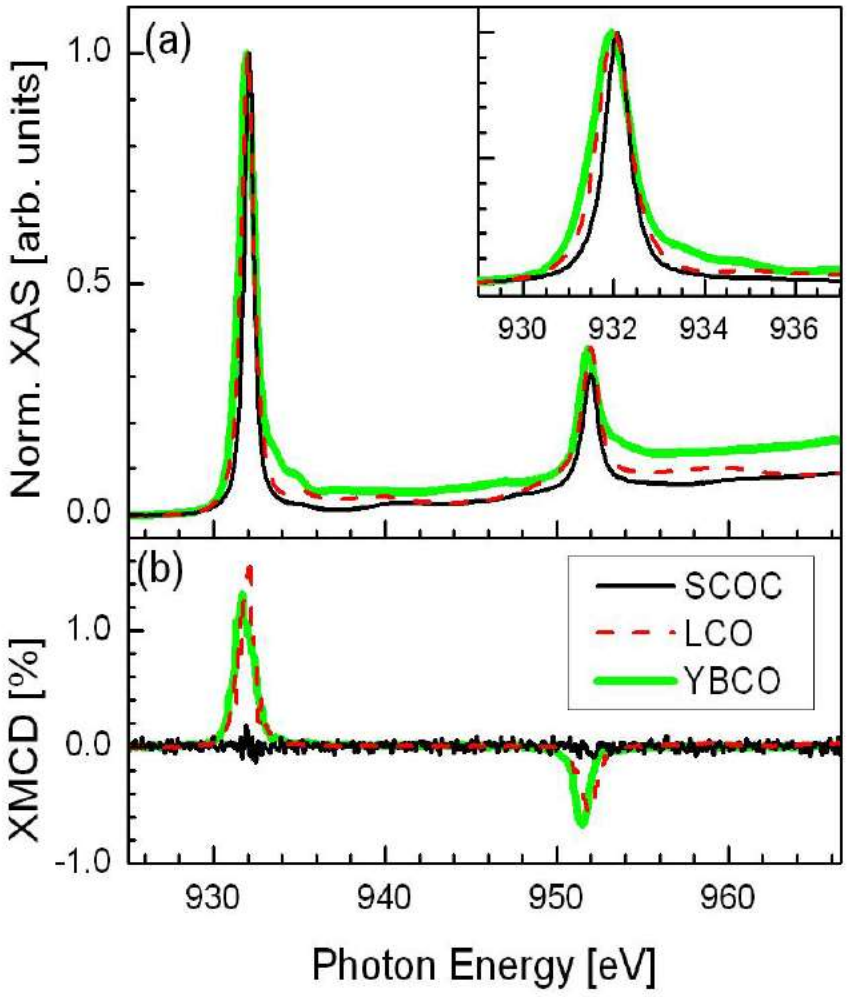


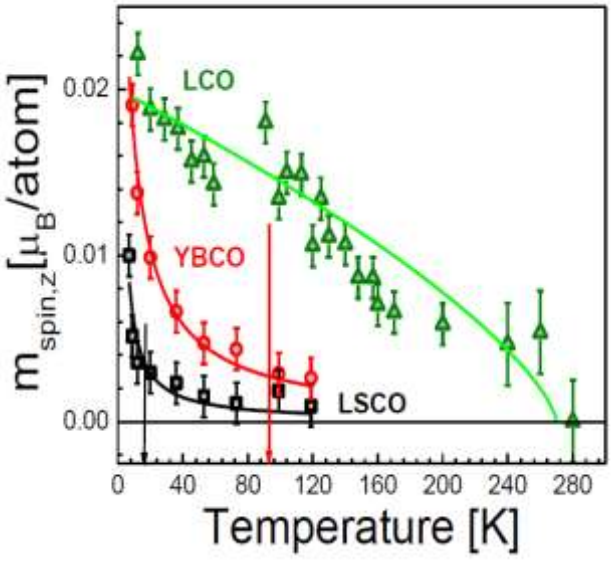
Buckled CuO_2 planes

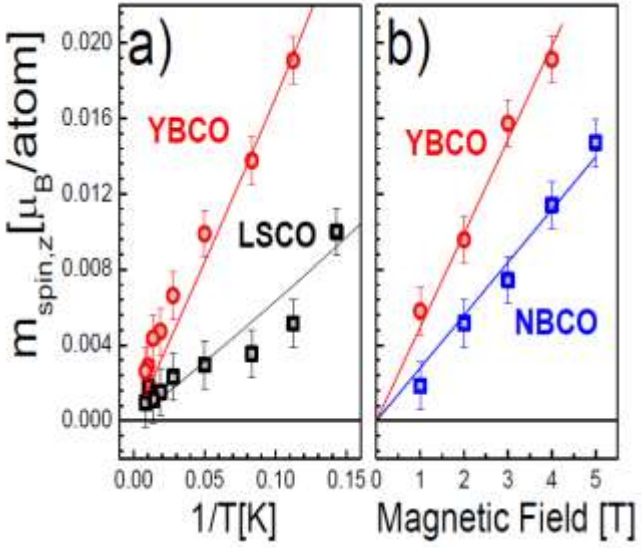
DM intercation induces out-of-plane spin component

L. Benfatto at al Phys. Rev. B **74**, 024416 (2006)

XMCD of cuprates

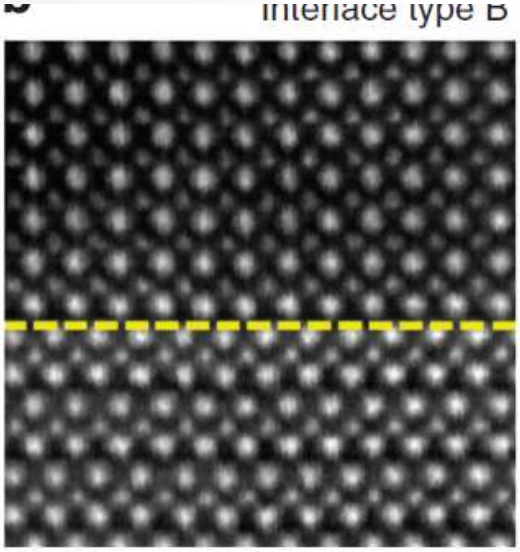


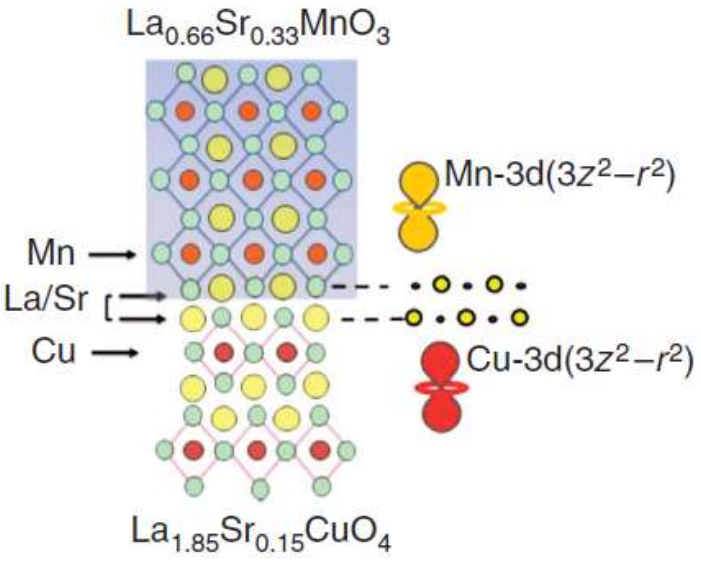


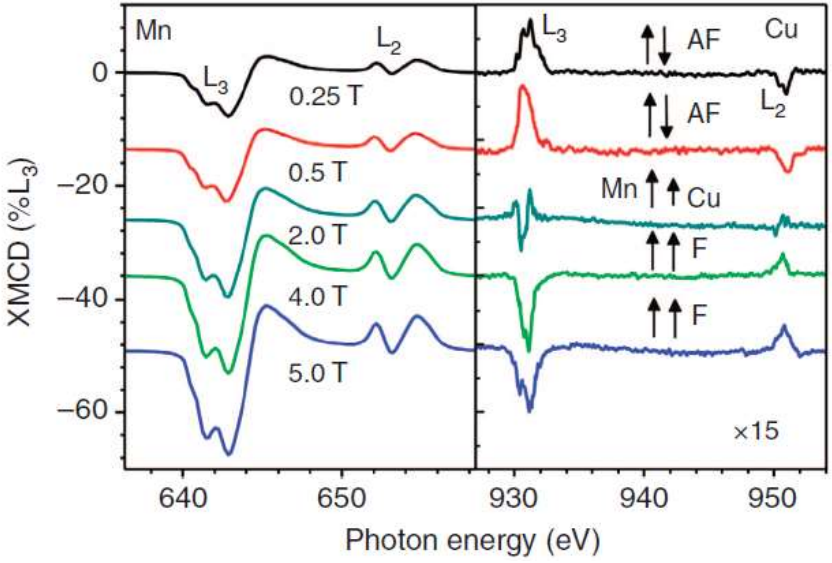


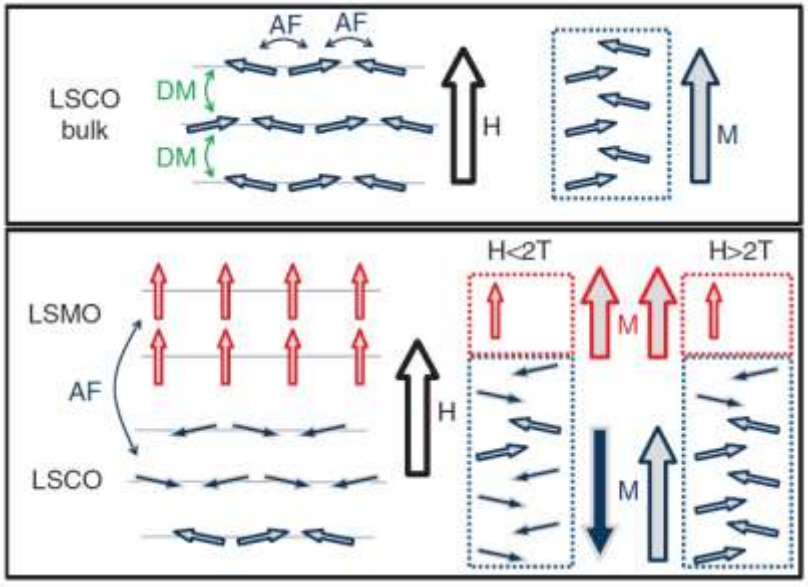
G. M. De Luca, G. Ghiringhelli, M. Moretti Sala, S. Di Matteo, M.W. Haverkort, H. Berger, V. Bisogni, J. C. Cezar, N. B. Brookes, and M. Salluzzo, Phys. Rev. B **82**, 214504 (2010)

Proximity effect: FM disturbs SC



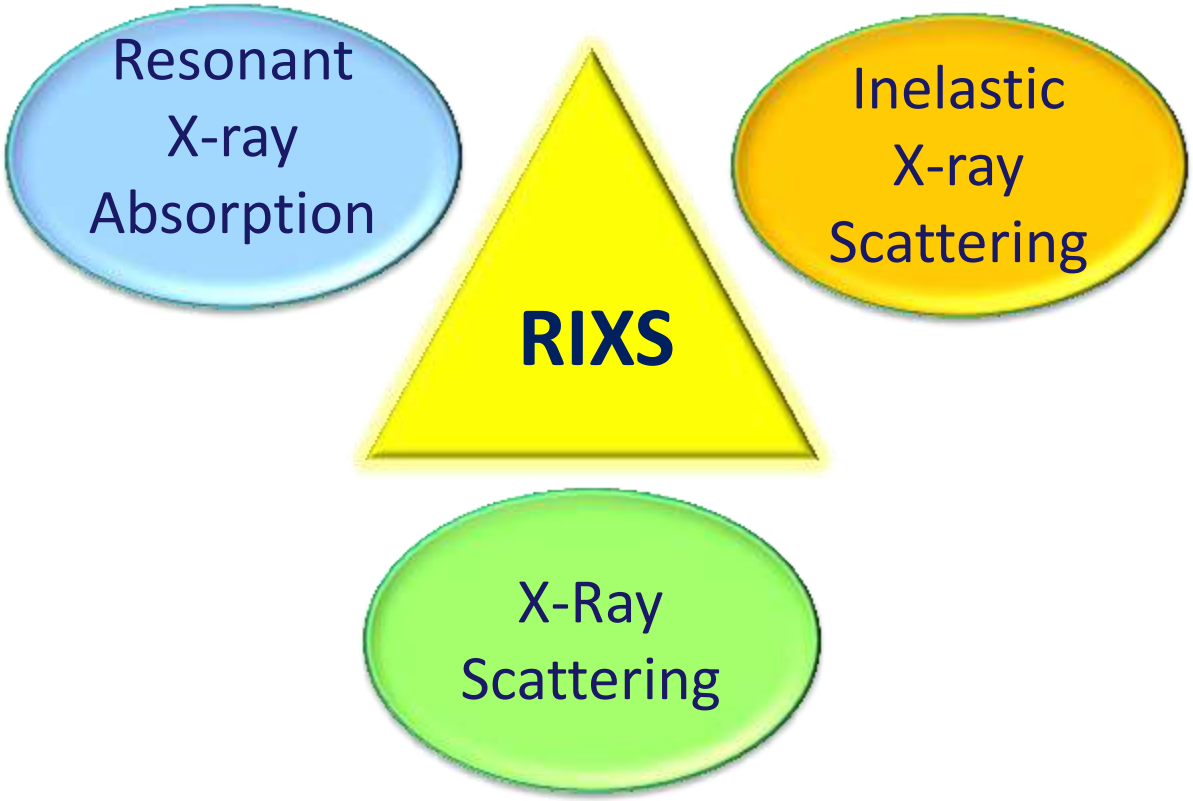


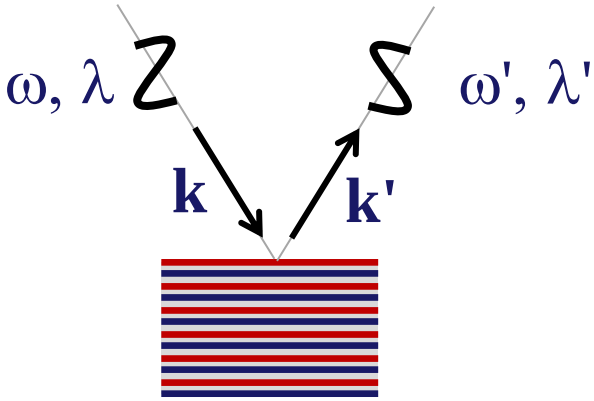




G.M. De Luca, G. Ghiringhelli, C.A. Perroni, V. Cataudella, F. Chiarella, C. Cantoni, A.R. Lupini, N.B. Brookes, M. Huijben, G. Koster, G. Rijnders & M. Salluzzo, Nat. Comm. 5, 5626 (2014)

Resonant Inelastic X-ray Scattering

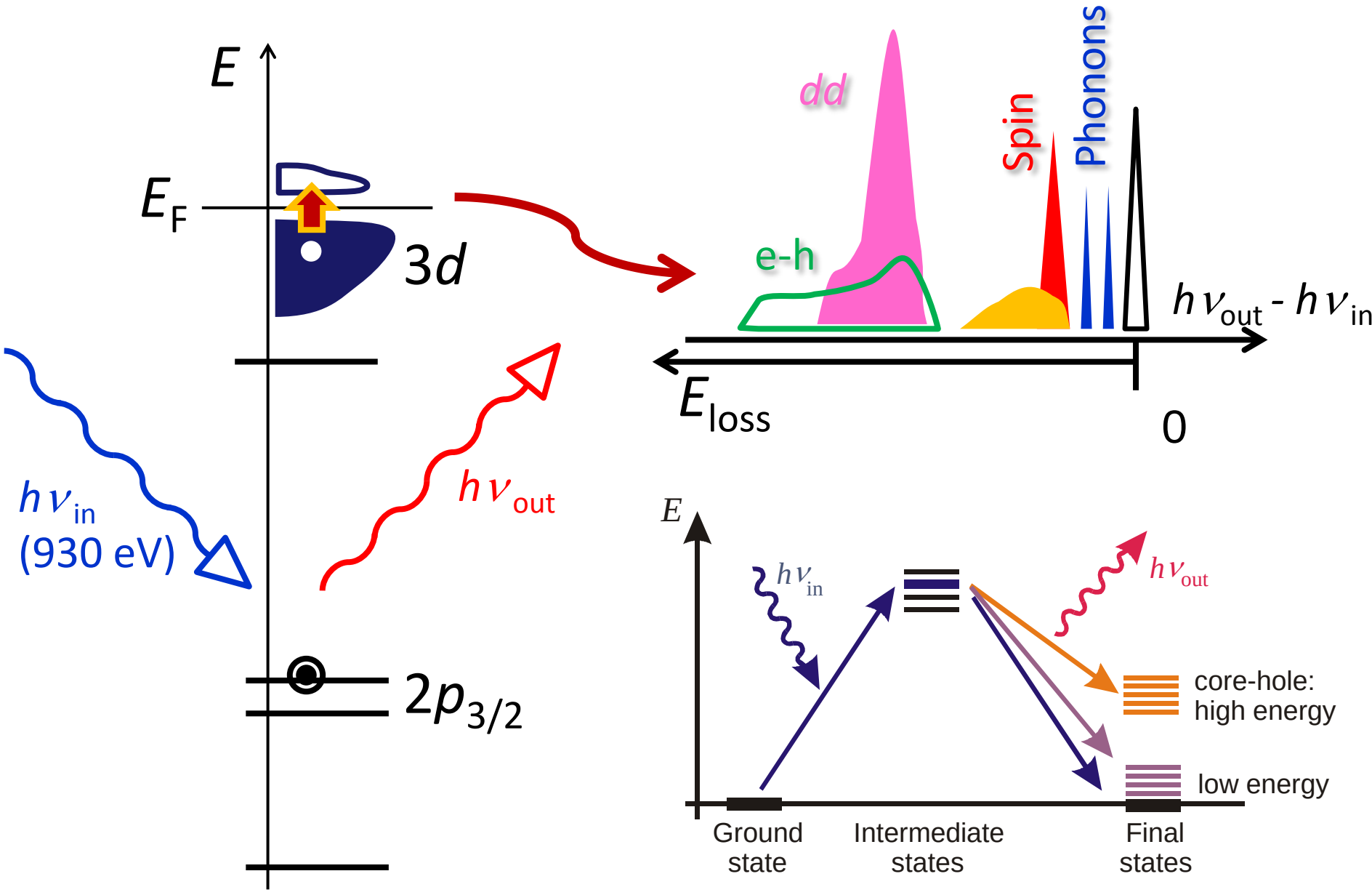




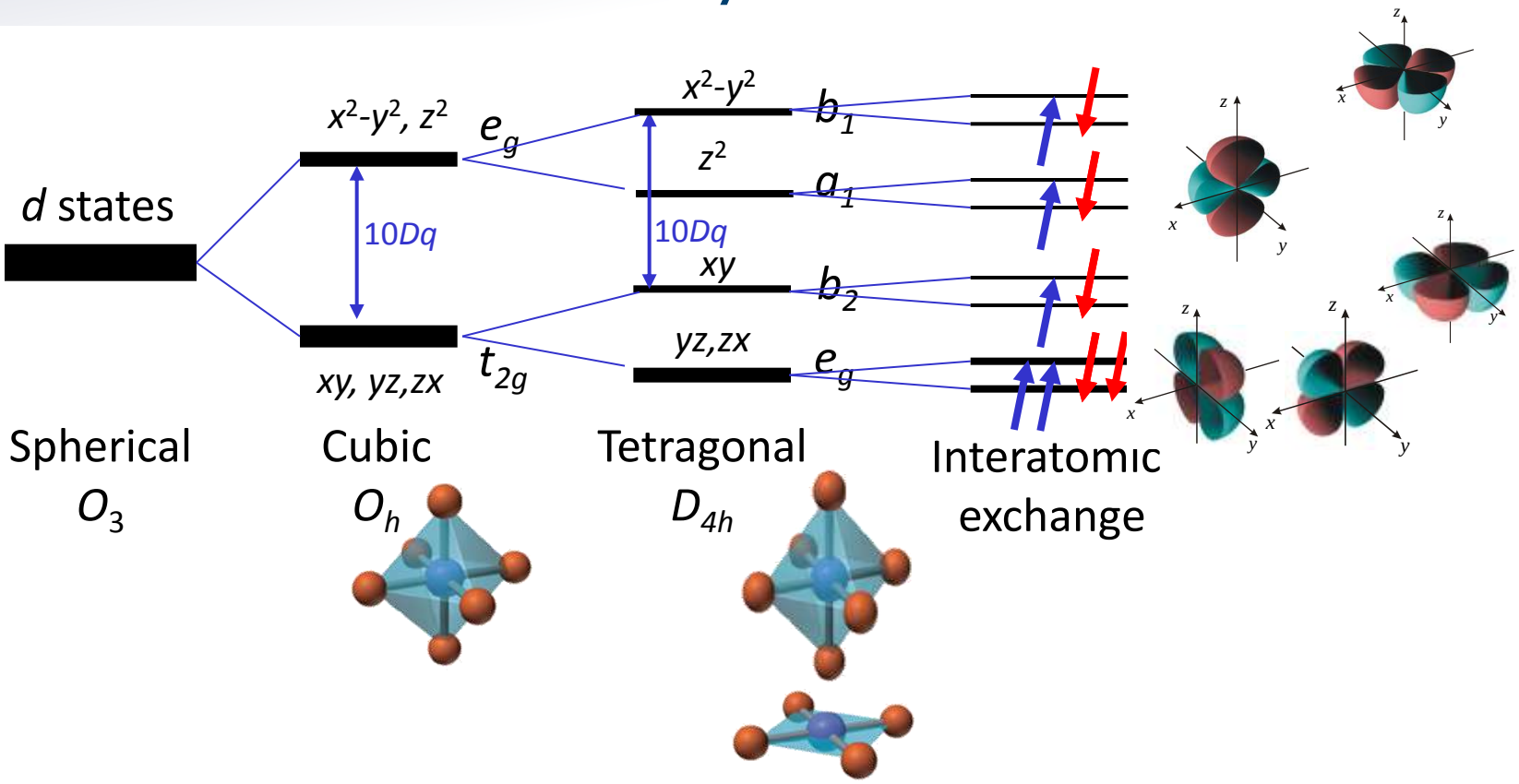
$\Omega = \omega - \omega'$

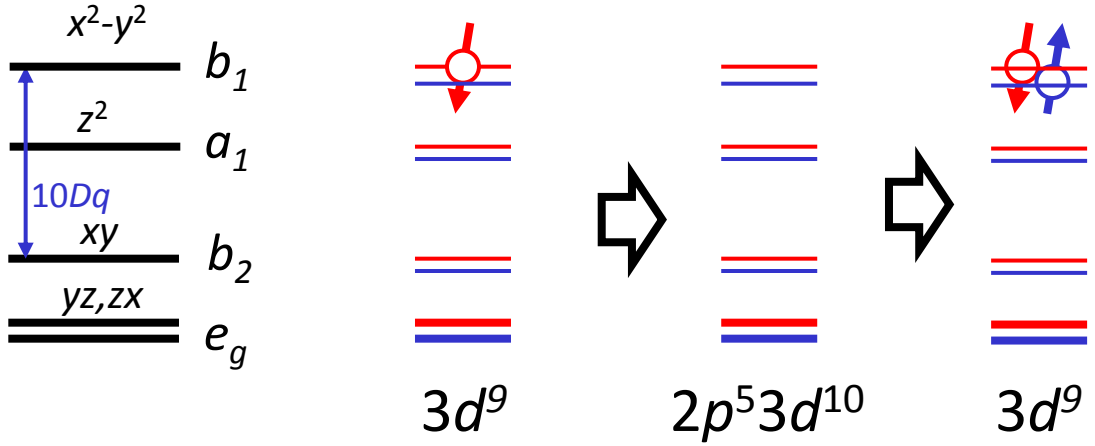
$\mathbf{q} = \mathbf{k}' - \mathbf{k}$

L_3 RIXS


E
E_F
3d
$2p_{3/2}$
$h\nu_{in}$
(930 eV)
$h\nu_{out}$
dd
Spin
Phonons
e-h
$h\nu_{out}$ - $h\nu_{in}$
E_{loss}
0
E
$h\nu_{in}$
$h\nu_{out}$
core-hole:
high energy
low energy
Ground
state
Intermediate
states
Final
states

dd excitations in Cu^{2+} systems

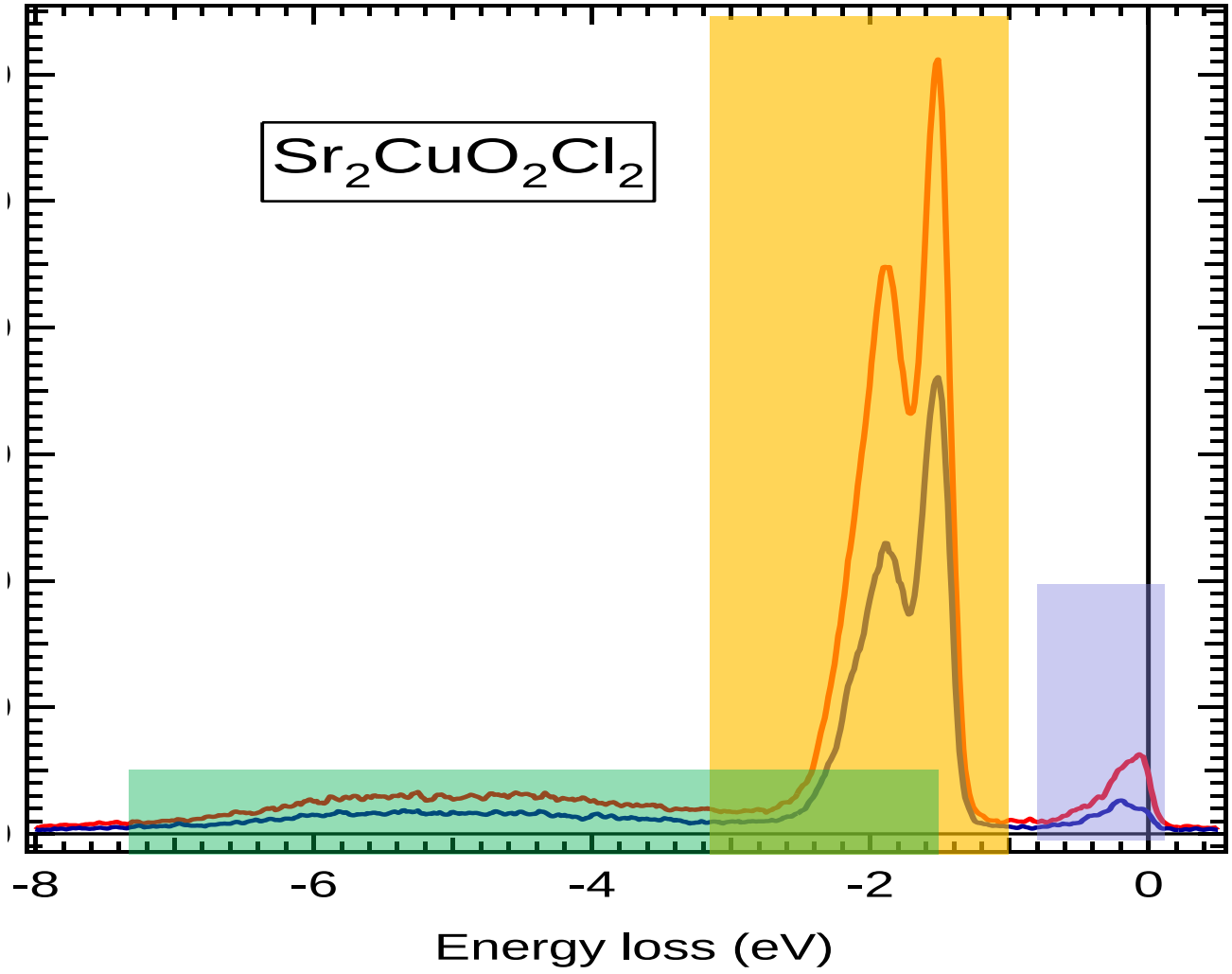




Cu L_3 RIXS of cuprates: mainly *dd* excitations

$3d^9 \longrightarrow 2p^5 3d^{10} \longrightarrow$

- $3d^9$: elastic, magnetic and phonons
- $3d^{9*}$: *dd* excitations
- $3d^{10}\underline{L}$: *Charge Transfer excitations*

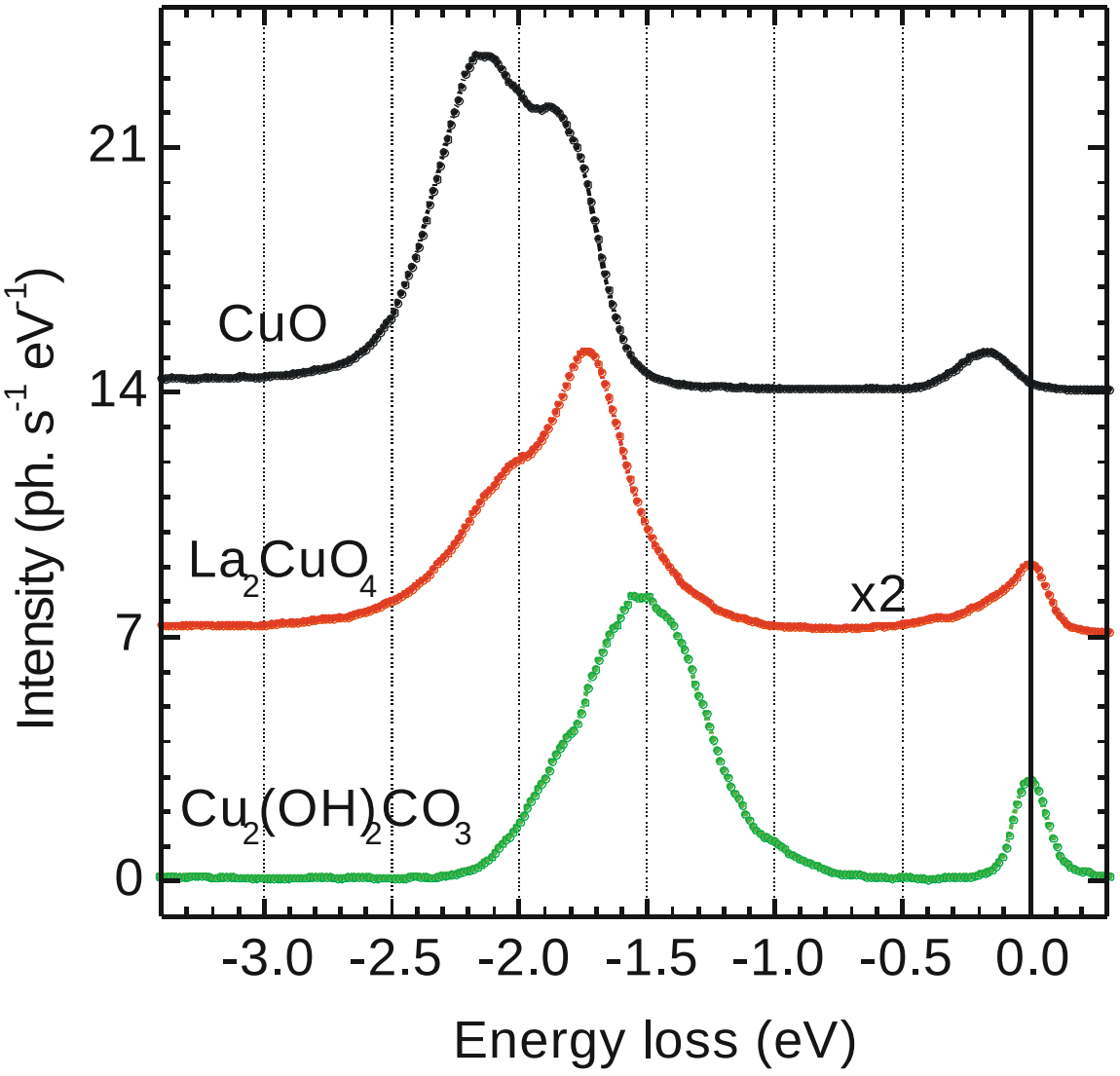


All final states are reached via 2 electric dipole allowed transitions!

Photons get coupled to electrons spin thanks to *2p* spin-orbit interaction

At L_3 edge elastic peak is very small (not the case at K)

Cu L_3 edge: CuO, La_2CuO_4, Malachite



Cu^{2+} in square approximately planar coordination

Cu-O distances:
CuO 1.7 – 2-2 Ang
LCO 1.9 – 2.4 Ang
Malachite 1.9 – 2.6 Ang

Different Cu^{2+} coordination, symmetry, hybridization

Different *dd* excitations

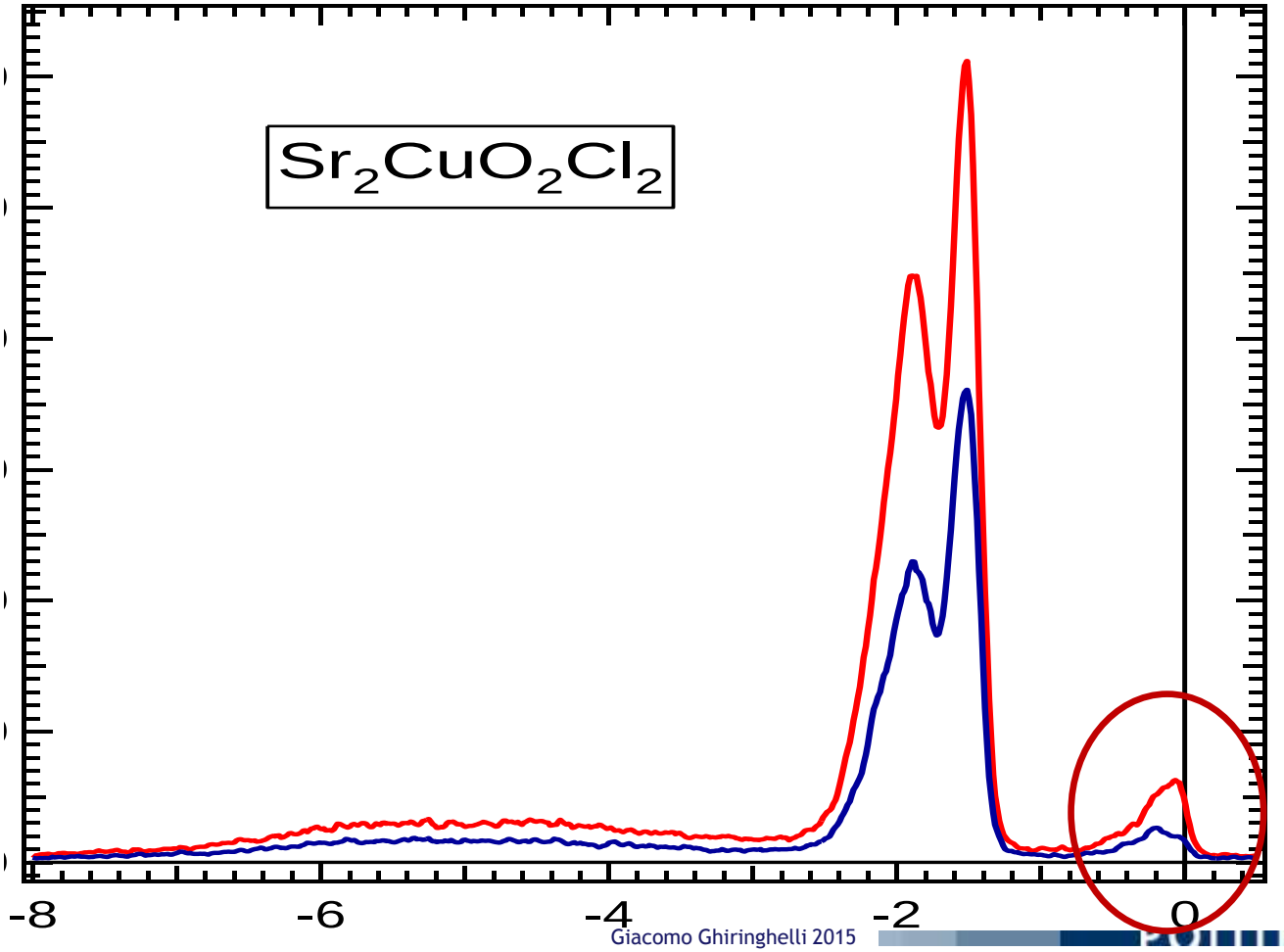
G. Ghiringhelli, A. Piazzalunga, X. Wang, A. Bendounan, H. Berger, F. Bottegoni, N. Christensen, C. Dallera, M. Grioni, J.-C. Grivel, M. Moretti Sala, L. Patthey, J. Schlappa, T. Schmitt, V. Strocov , and L. Braicovich, Eur.Phys. J. Special topics **169**, 199 (2009)

What about the "quasi-elastic" spectral features?

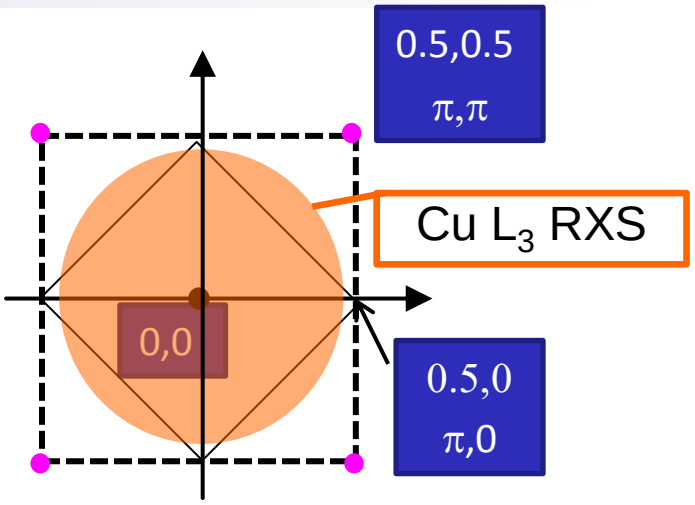
Phonons: up to 90meV

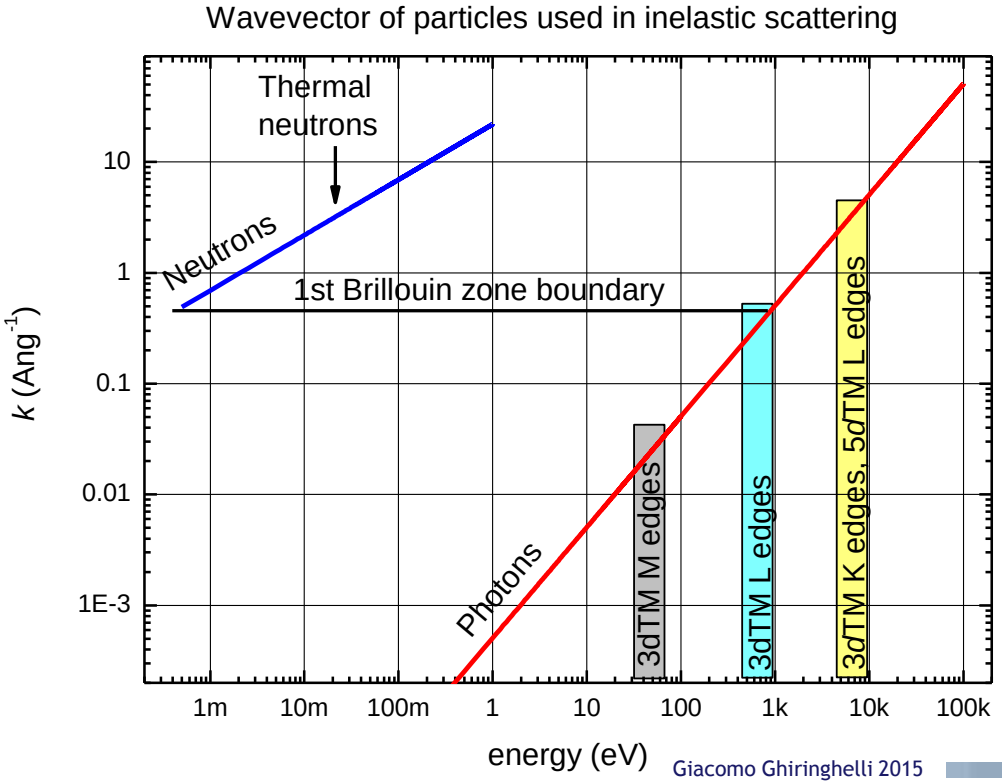
Magnons (2*J* at BZB): up to 300 meV (J_{eff} ≈ 140 meV)

Multi mangons...



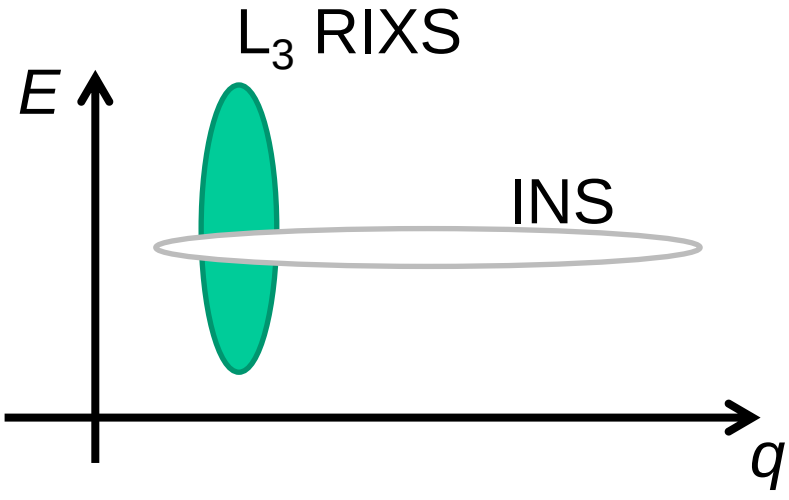
RIXS: Experimental conditions



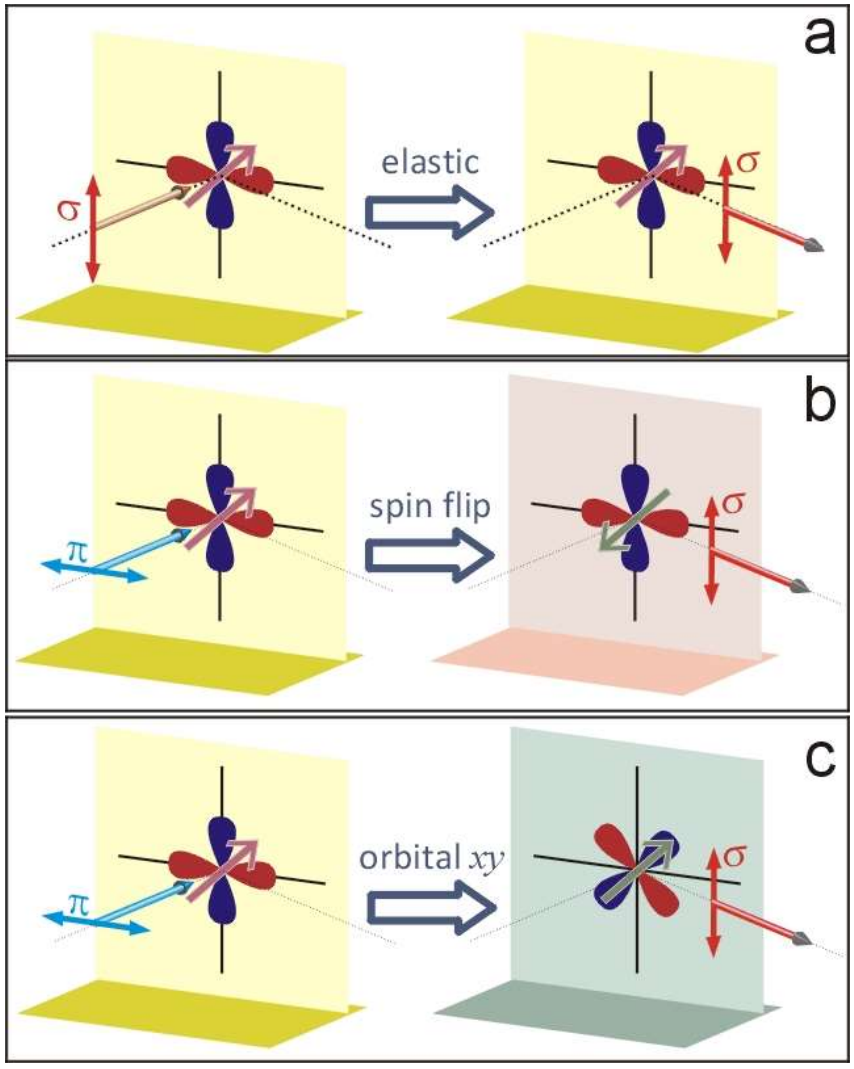


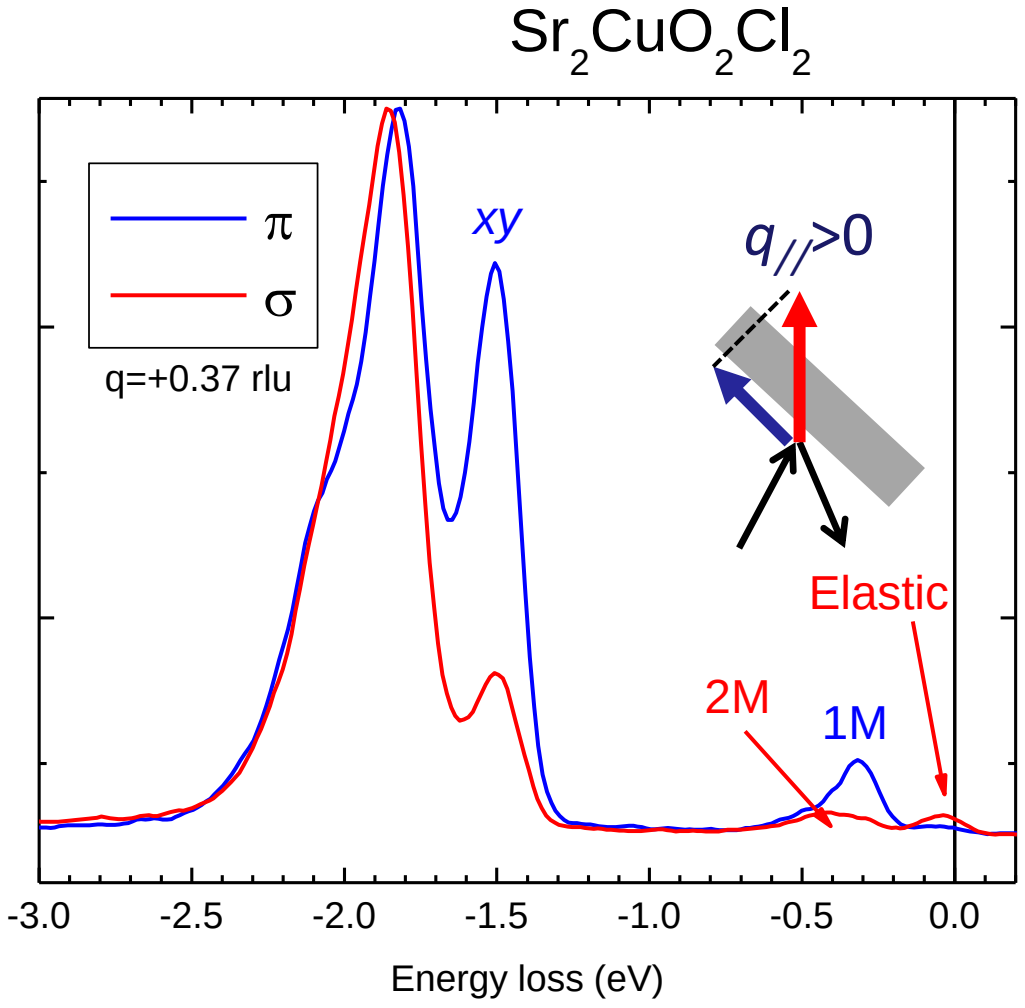
Cu L_3 resonance:

- E_0 = 930 eV
- q_{max} = 0.86 Ang^{-1}
- confined inside a region around Γ
- 2p core hole: spin-orbit interaction
- E resolution: 120-240 meV
- *q* resolution: 0.005 rlu
- ½ - 1 hour per spectrum



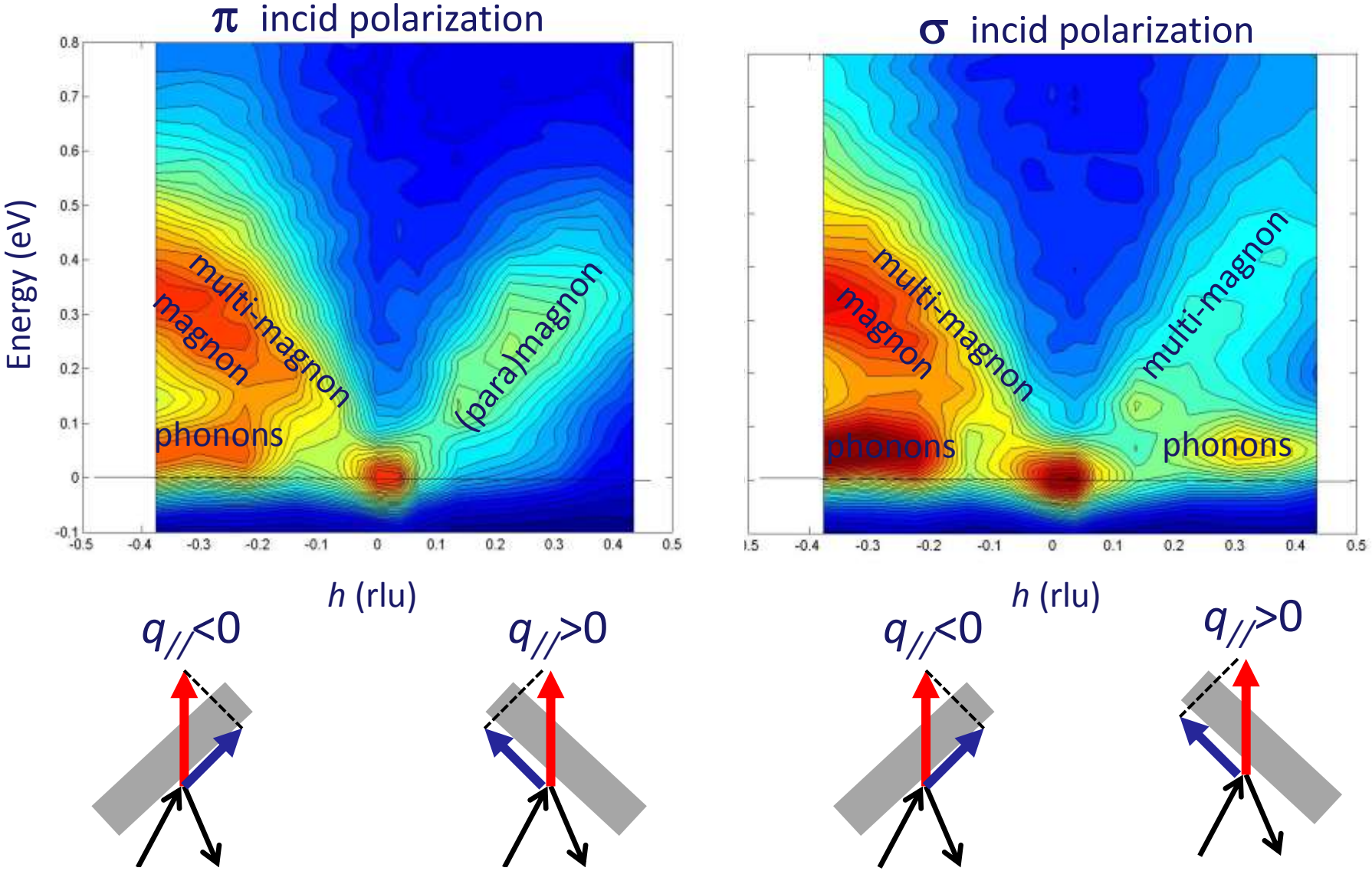
Polarization dep. of Cu L_3 RIXS intensity





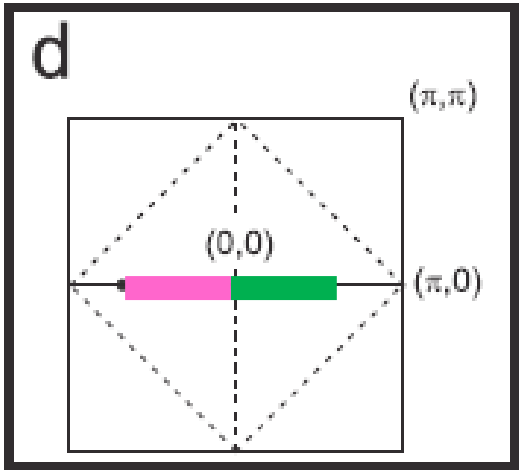
Polarization dependent cross-sections

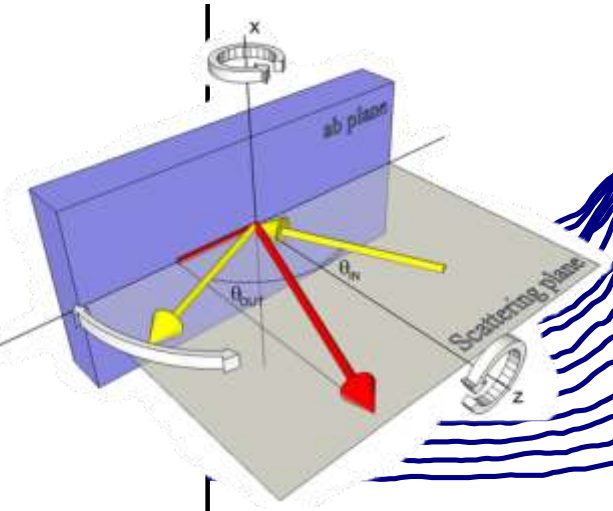
LSCO, opt. doping

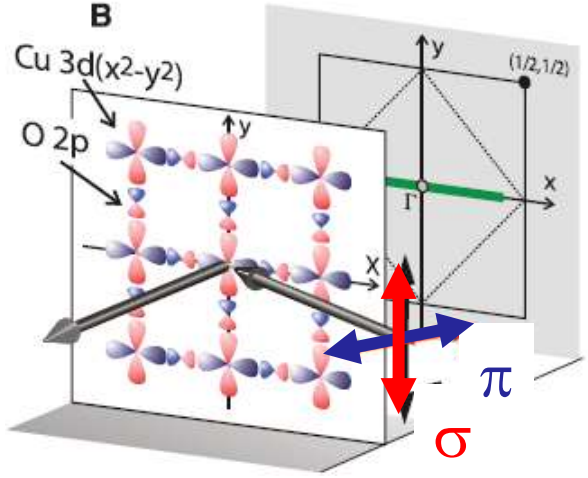


M. Hashimoto, L.Braicovich, M. Minola, GG et al. unpublished

First demonstration: La_2CuO_4







La_2CuO_4

$q_{//}>0$

$q_{//}<0$

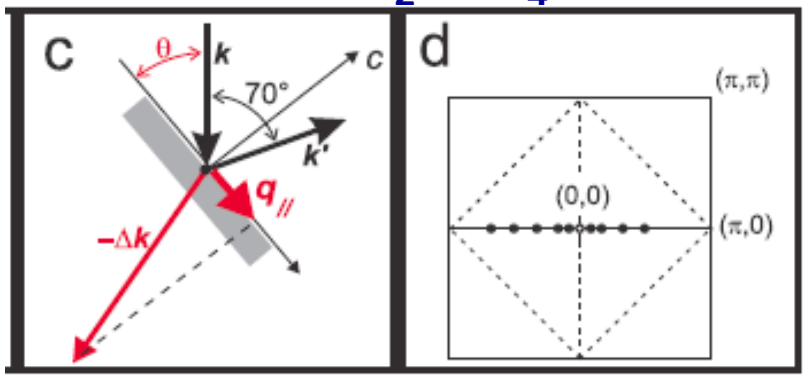
-3.5 -3.0 -2.5 -2.0 -1.5 -1.0 -0.5 0.0 0.5

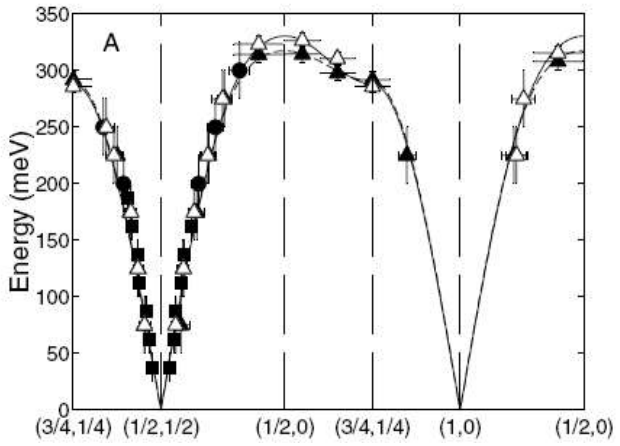
Energy loss (eV)

L. Braicovich, J. van den Brink, V. Bisogni, M. Moretti Sala, L. Ament, N.B. Brookes, G.M. de Luca, M. Salluzzo, T. Schmitt, and G. Ghiringhelli PRL **104** 077002 (2010)

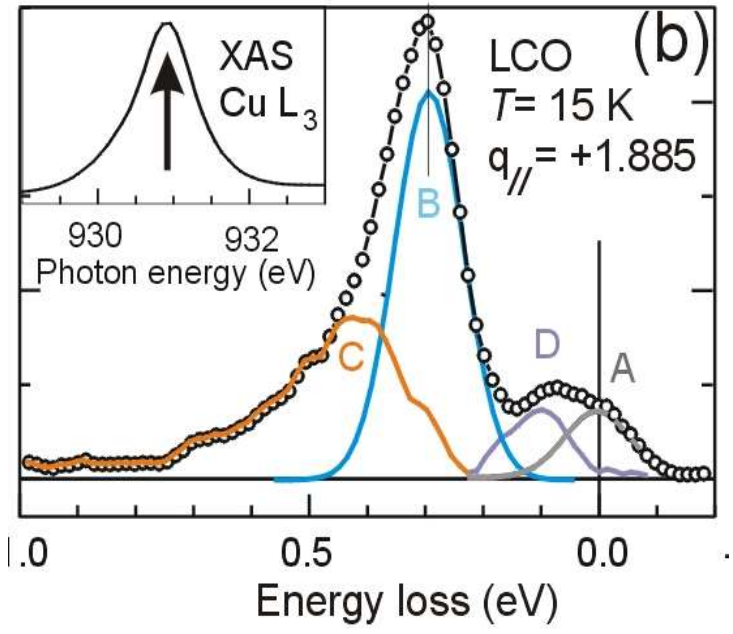
La_2CuO_4, RIXS vs INS

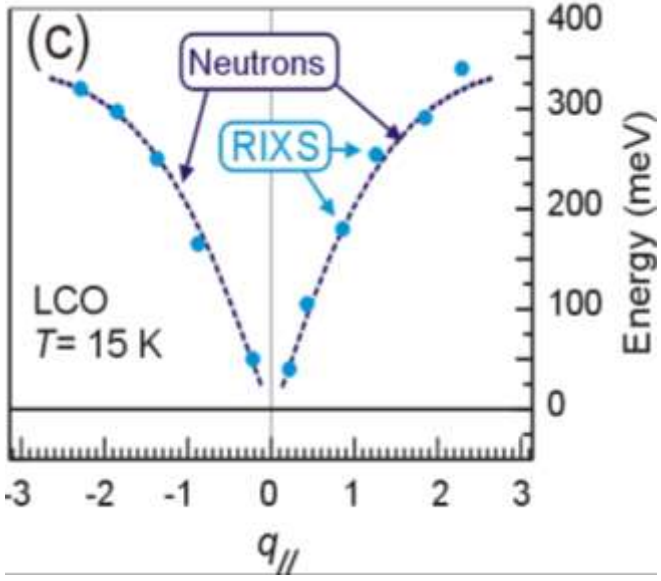
La_2CuO_4





R. Coldea et al, Phys. Rev. Lett. **86**, 5377 (2001).





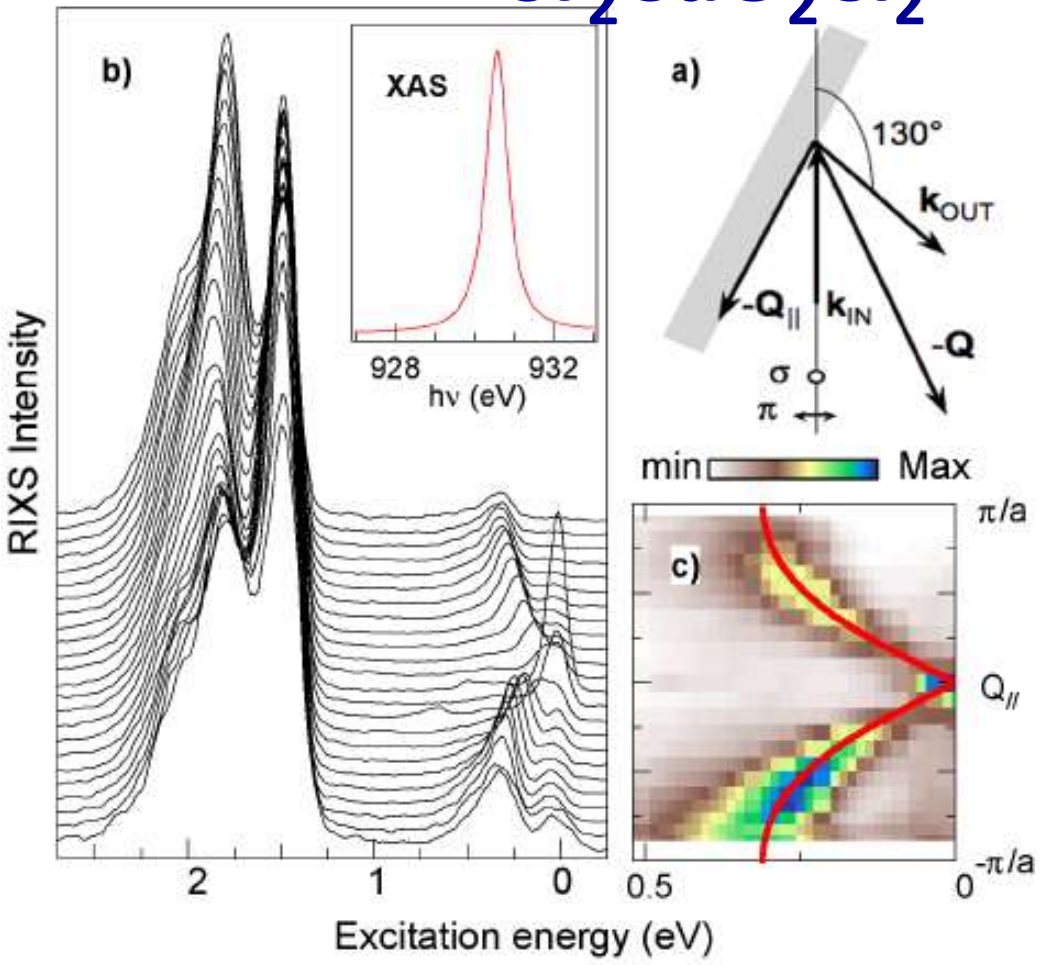
L. Braicovich, J. van den Brink, V. Bisogni, M. Moretti Sala, L. Ament, N.B. Brookes, G.M. de Luca, M. Salluzzo, T. Schmitt, and G. Ghiringhelli PRL **104** 077002 (2010)

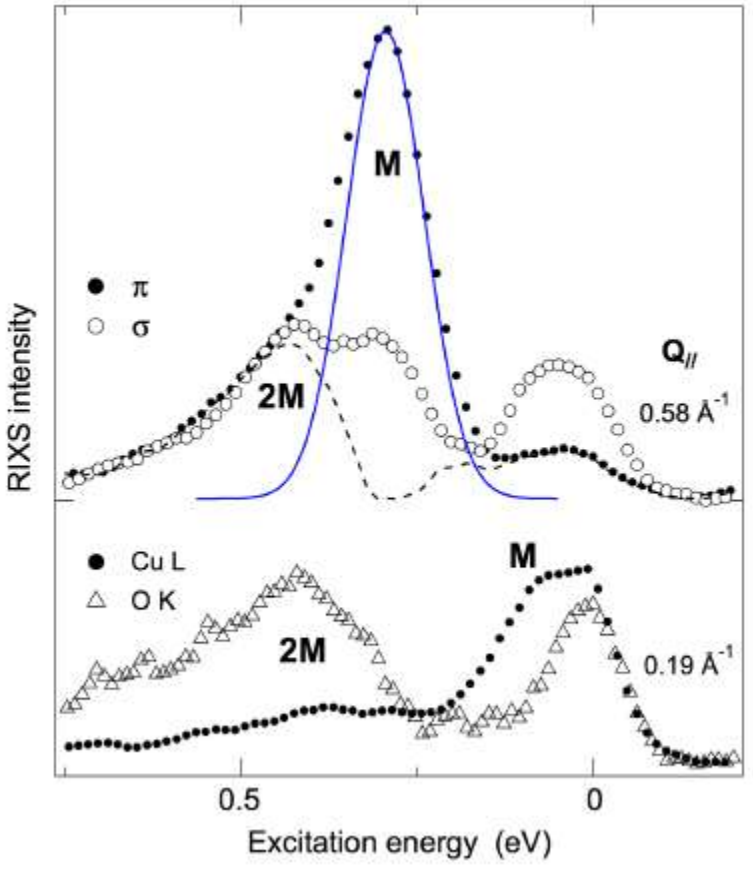
Magnetic excitations in AF cuprates

2008

$Sr_2CuO_2Cl_2$

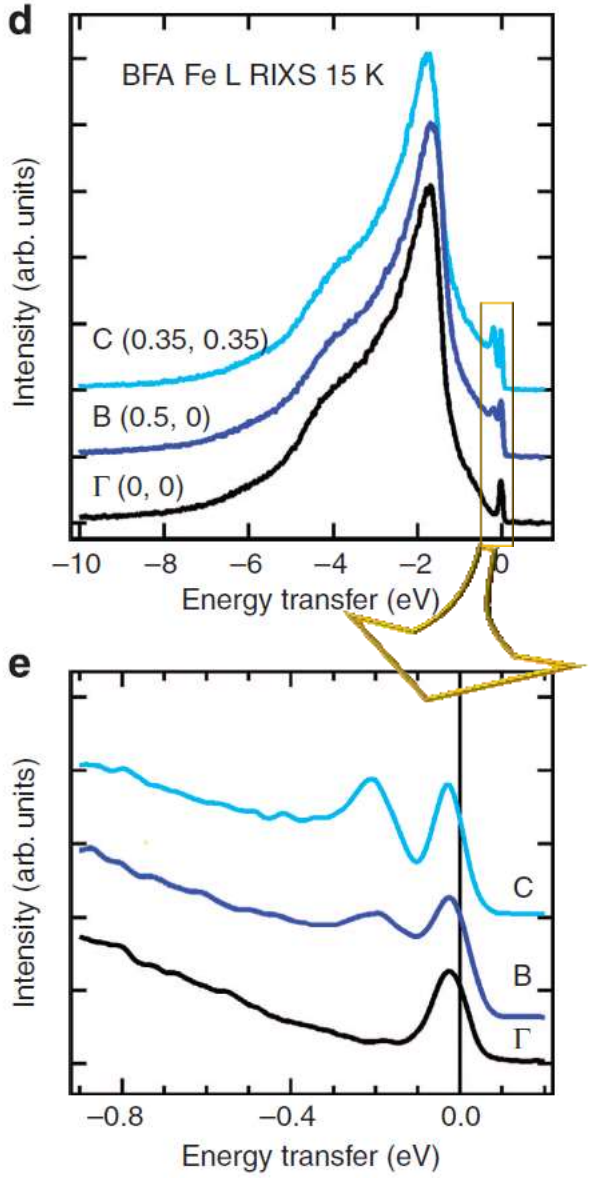
ΔE 0.12 eV

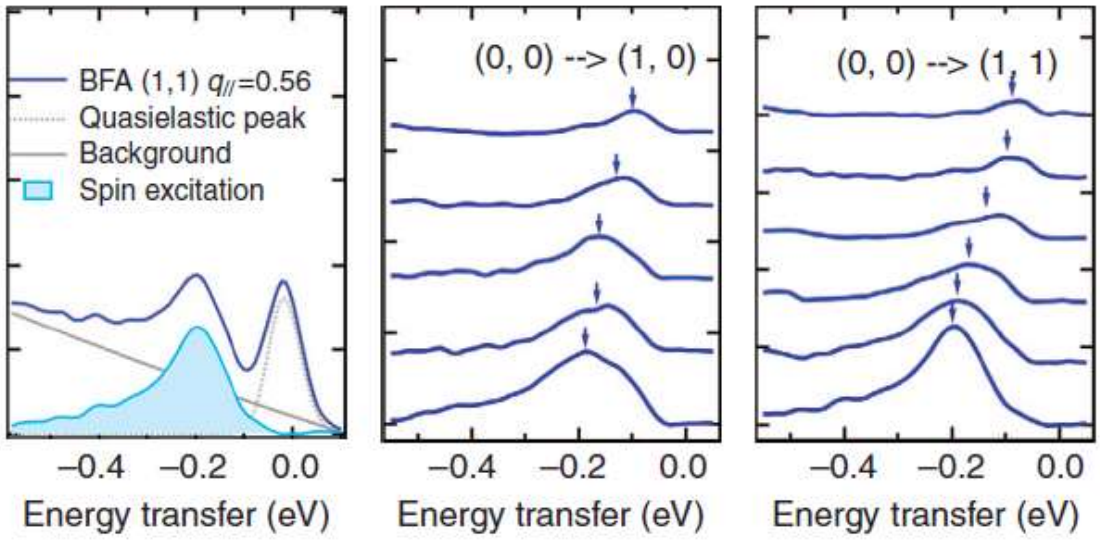


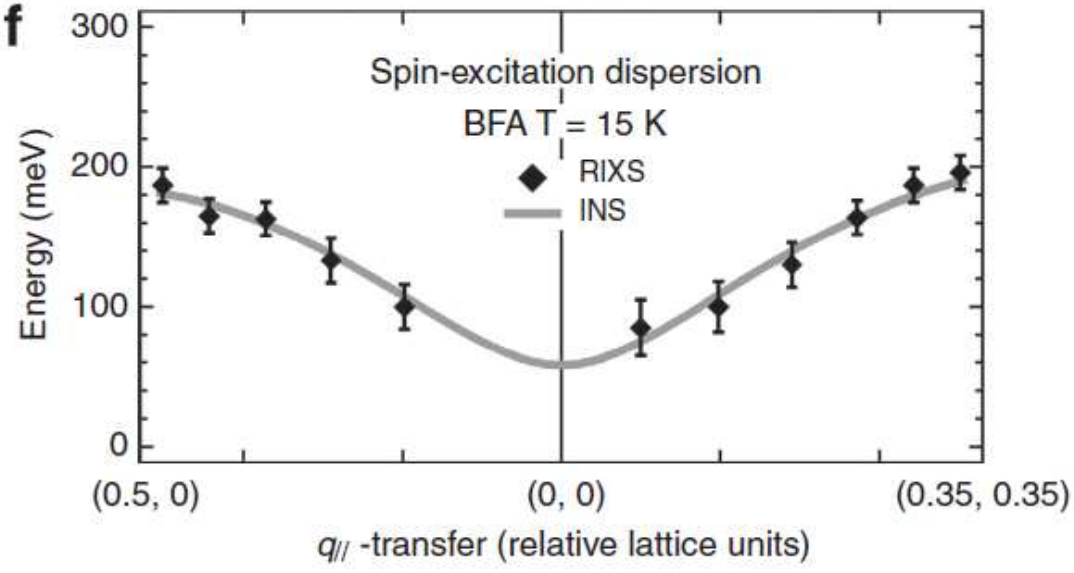


M. Guarise, B. Dalla Piazza, M. Moretti Sala, G. Ghiringhelli, L. Braicovich, H. Berger, J.N. Hancock, D. van der Marel, T. Schmitt, V.N. Strocov, L.J.P. Ament, J. van den Brink, P.-H. Lin, P. Xu, H. M. Rønnow, and M. Grioni. Phys. Rev. Lett. **105**, 157006 (2010)

Magnons at Fe L_3 edge in $BaFe_2As_2$

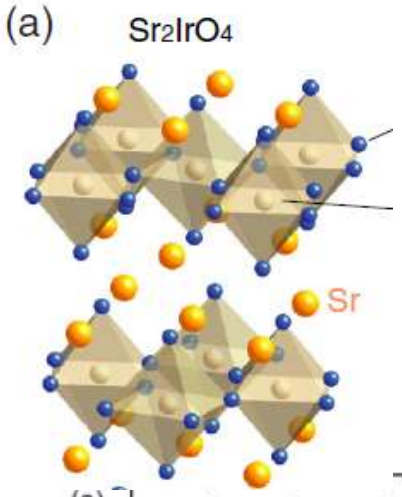






Ke-Jin Zhou, Yao-Bo Huang, Claude Monney, Xi Dai, Vladimir N. Strocov, Nan-Lin Wang, Zhi-Guo Chen, Chenglin Zhang, Pengcheng Dai, Luc Patthey, Jeroen van den Brink, Hong Ding & Thorsten Schmitt, Nature Comm. **4**, 1470 (2013)

Magnetic and orbital excitations in Sr_2IrO_4



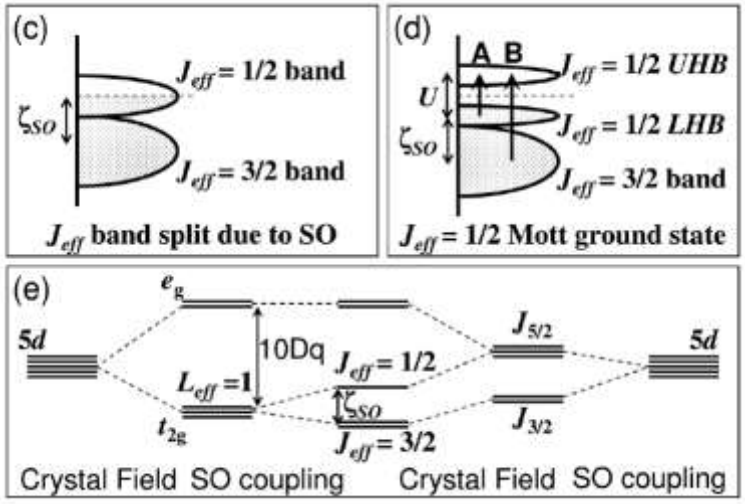
Ir^{4+}

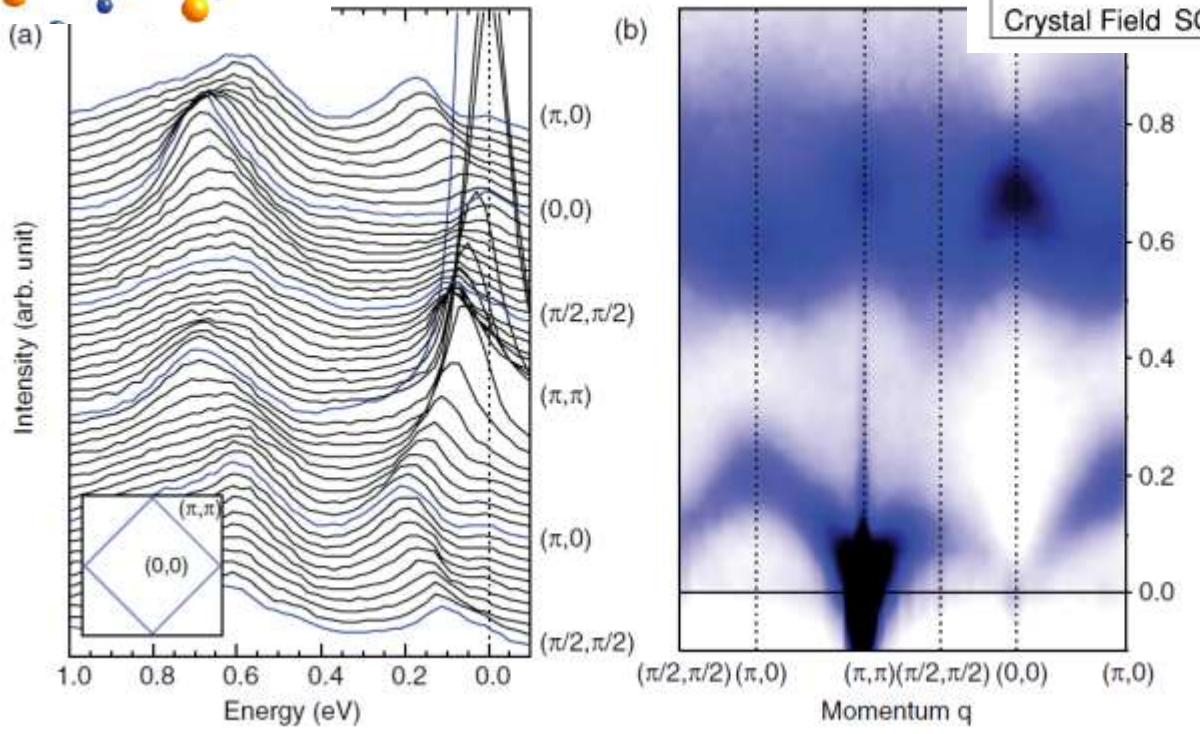
$5d^5$ ⇨

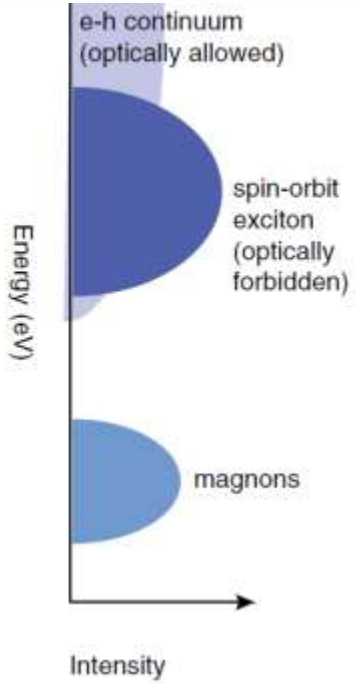
Strong spin-orbit in the 5*d*

$\zeta_{SO} \sim 0.4$ eV

L_3 at 11.2 keV

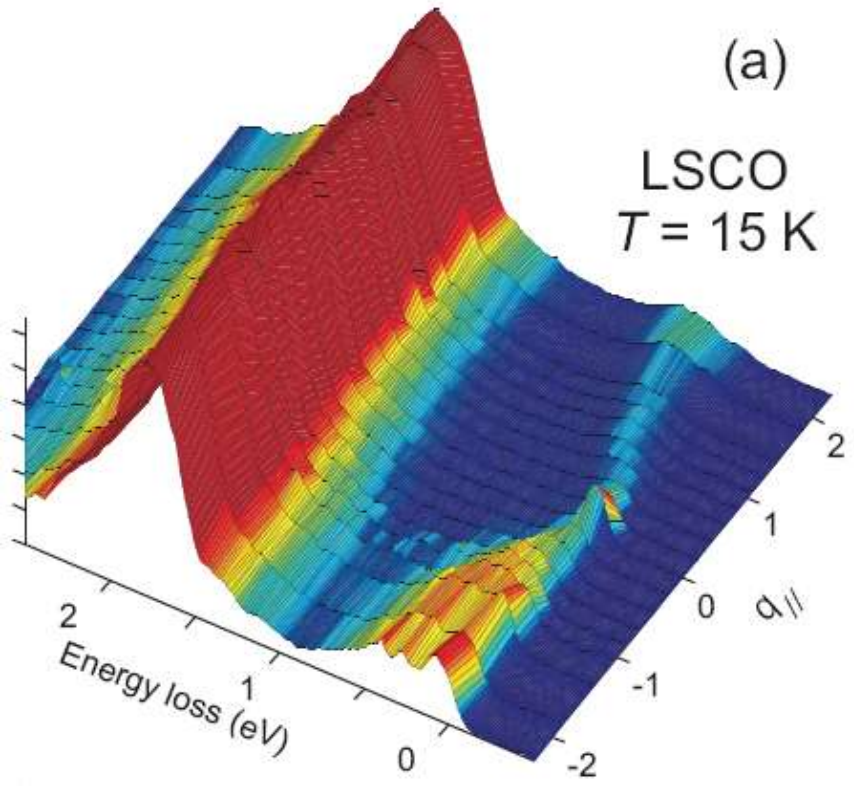


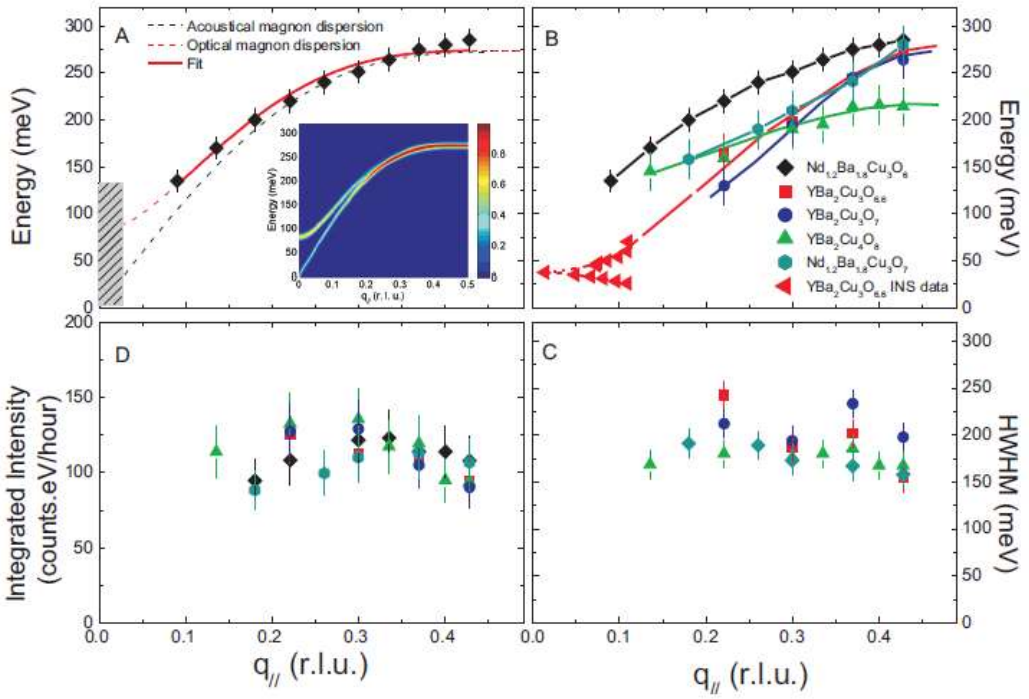




Jungho Kim, D. Casa, M. H. Upton, T. Gog, Young-June Kim, J. F. Mitchell, M. van Veenendaal, M. Daghofer, J. van den Brink, G. Khaliullin, and B. J. Kim, Phys. Rev. Lett. **108**, 177003 (2012)

Superconductors: LSCO, YBCO and NdBCO





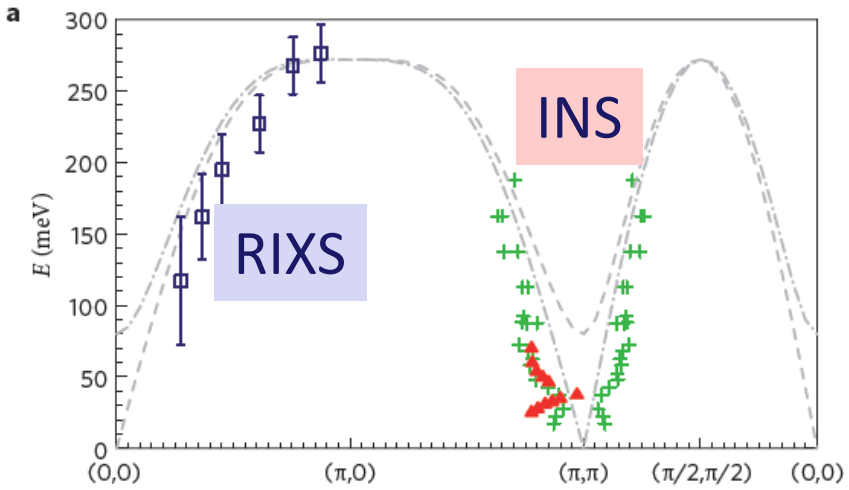
LSCO & NdBCO: 100 nm films on STO. YBCO: detwinned single crystals

Dispersing magnetic excitations are almost as strong in SC as in the AF parent compounds: they can be involved in Cooper pairing

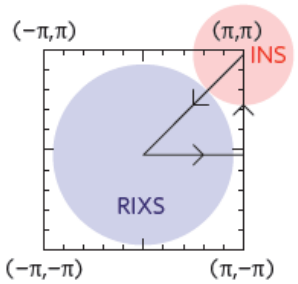
L. Braicovich, J. van den Brink, V. Bisogni, M. Moretti Sala, L. Ament, N.B. Brookes, G.M. de Luca, M. Salluzzo, T. Schmitt, and G. Ghiringhelli PRL **104** 077002 (2010)

M. Le Tacon, G. Ghiringhelli, J. Chaloupka, M. Moretti Sala, V. Hinkov, M.W. Haverkort, M. Minola, M. Bakr, K. J. Zhou, S. Blanco-Canosa, C. Monney, Y. T. Song, G. L. Sun, C. T. Lin, G. M. De Luca, M. Salluzzo, G. Khaliullin, T. Schmitt, L. Braicovich and B. Keimer, Nat. Phys. **7**, 725 (2011)

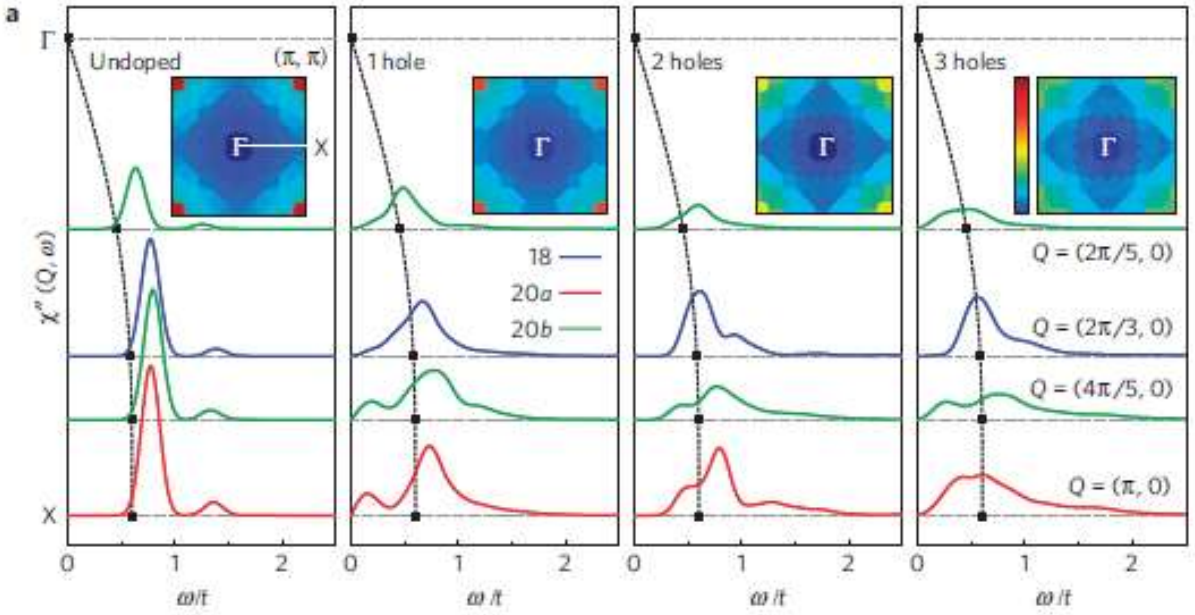
YBCO: doping dependence of χ''



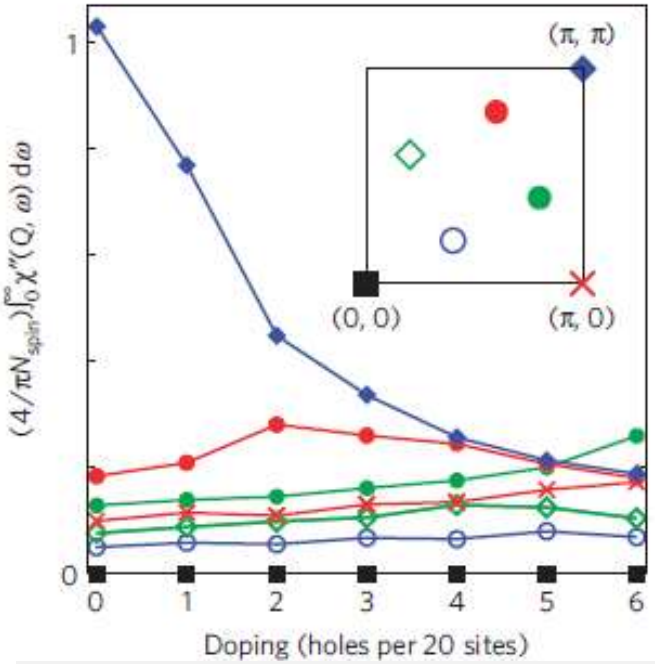
Matthias Vojta, *News and Views*, Nature Physics **7,** 674 (2011)



$YBa_2Cu_3O_{6.6}$



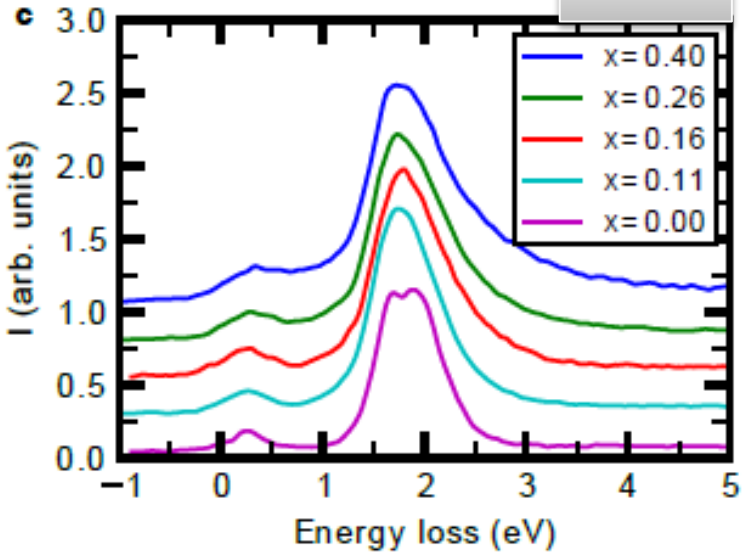
Imaginary part of the spin susceptibility $\chi''(Q;w)$ *resulting from exact diagonalization of the t–J model with J/t=0.3 on small cluster. (G. Khaliullin)*

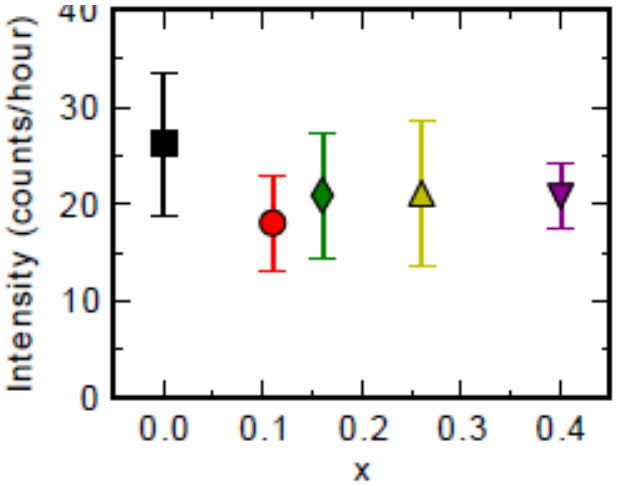


Energy-integrated $\chi''$of the 20-site cluster (normalized) for 7 accessible non-equivalent Q vectors. *(G. Khaliullin)*

Peristent magnetic excits in overdoped cuprates

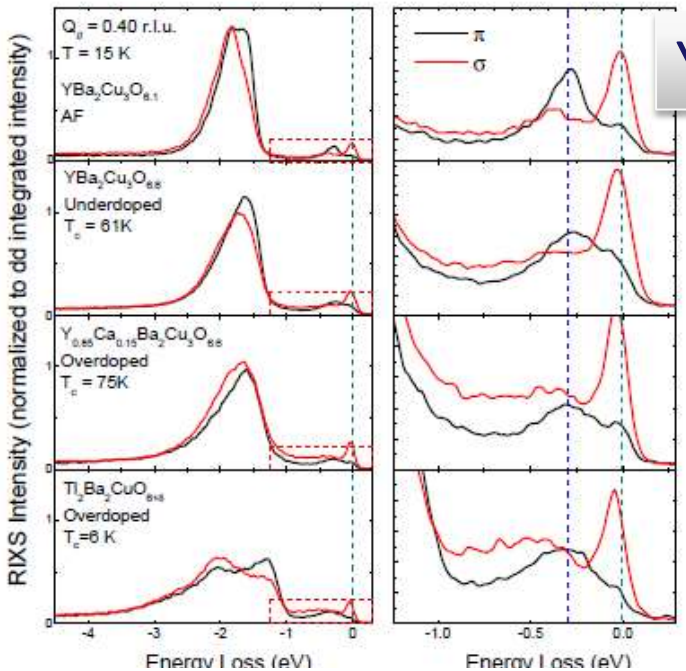
LSCO

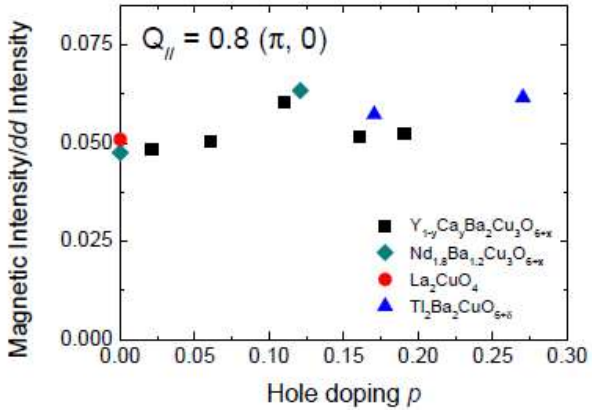




π pol

YBCO

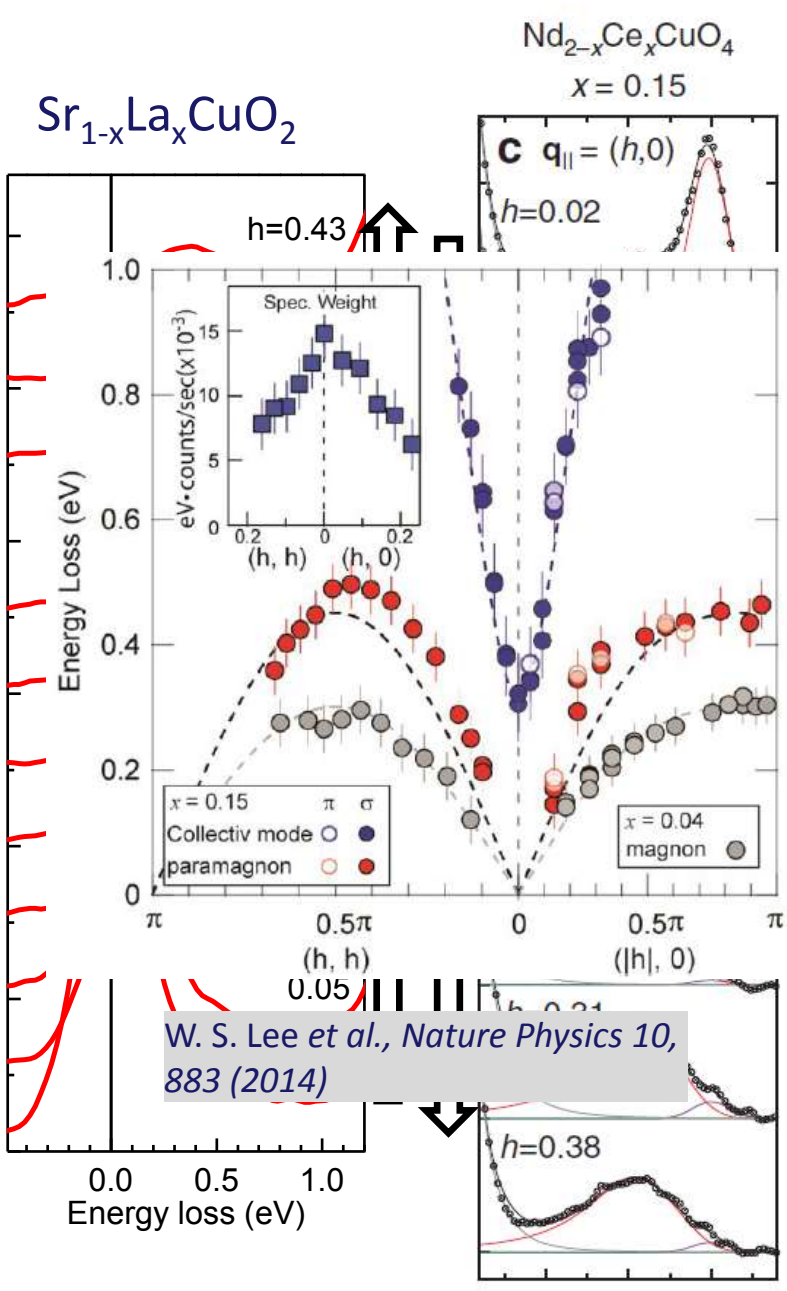




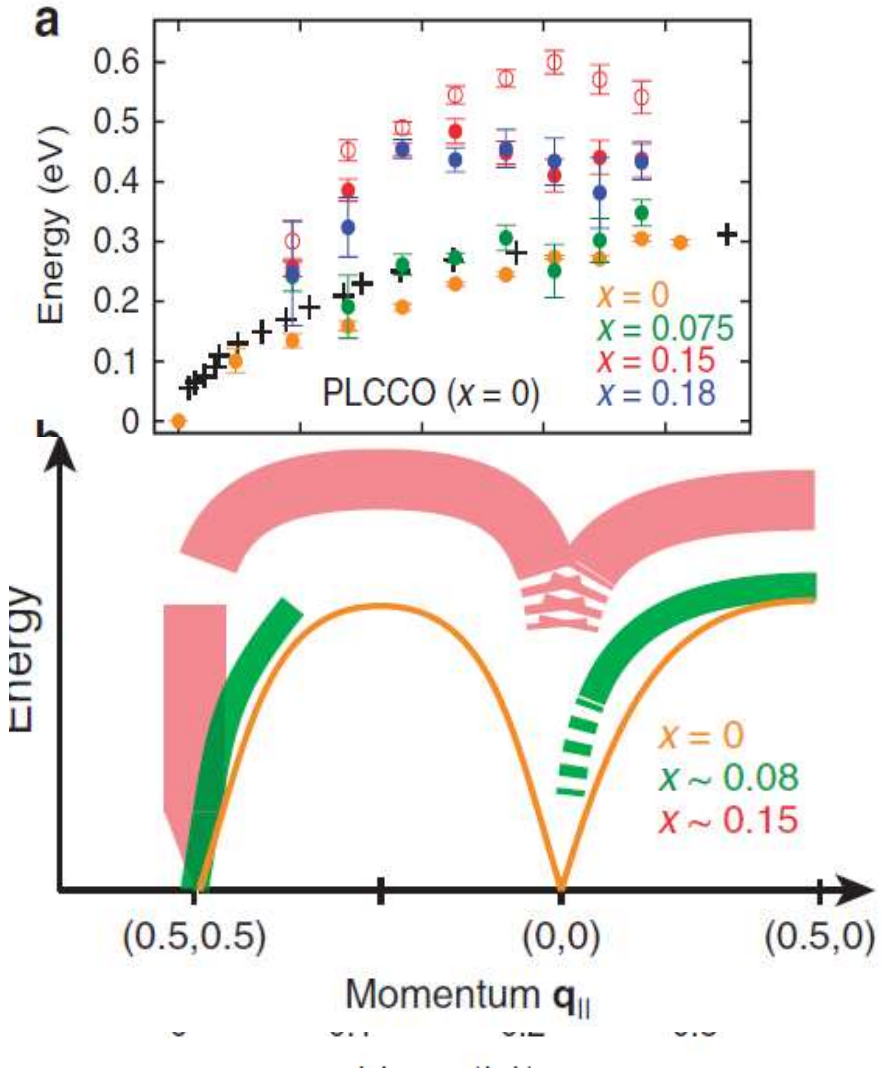
M. P. M. Dean,, . G. Dellea, R. S. Springell, F. Yakhou-Harris, K. Kummer, N. B. Brookes, X. Liu, Y.-J. Sun, J. Strle, T. Schmitt, L. Braicovich, G. Ghiringhelli, I. Bozovic, and J. P. Hill, Nat. Mater. **12**, 1019 (2013)

M. Le Tacon, M. Minola, D. C. Peets, M. Moretti Sala, S. Blanco-Canosa, V. Hinkov, R. Liang, D. A. Bonn, W. N. Hardy, C. T. Lin, T. Schmitt, L. Braicovich, G. Ghiringhelli, and B. Keimer, Phys. Rev. B 88, 020501 (2013)

Spin excitations in e-doped SC

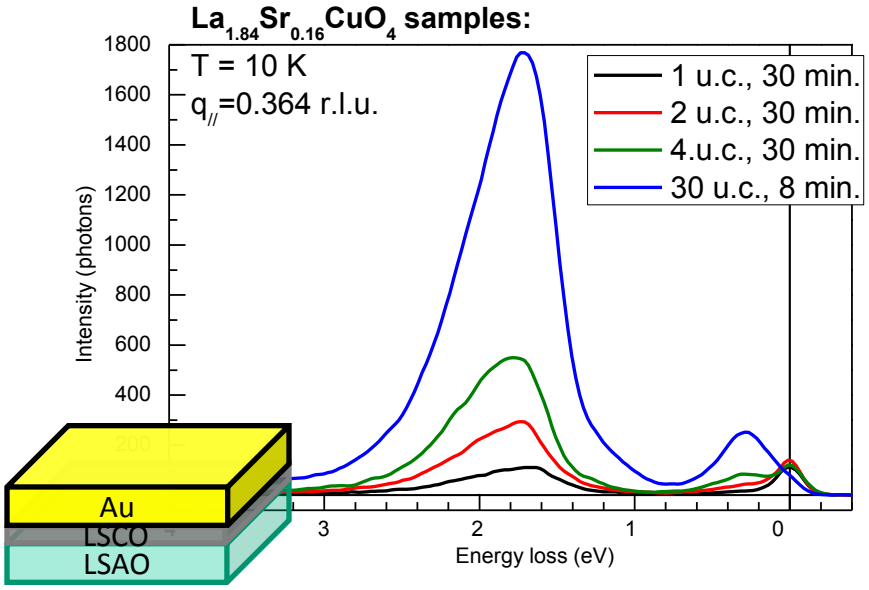


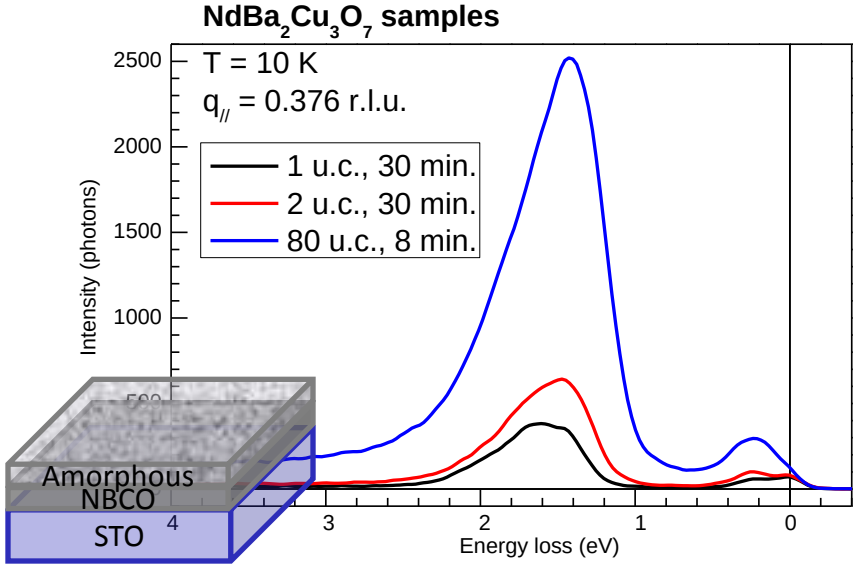
W. S. Lee *et al., Nature Physics 10, 883 (2014)*

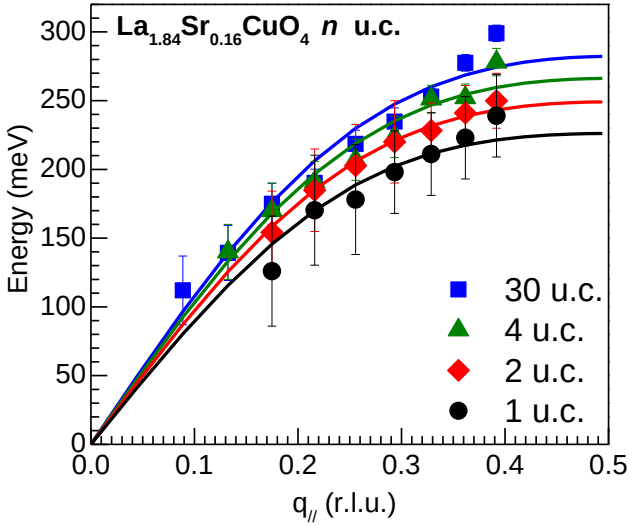


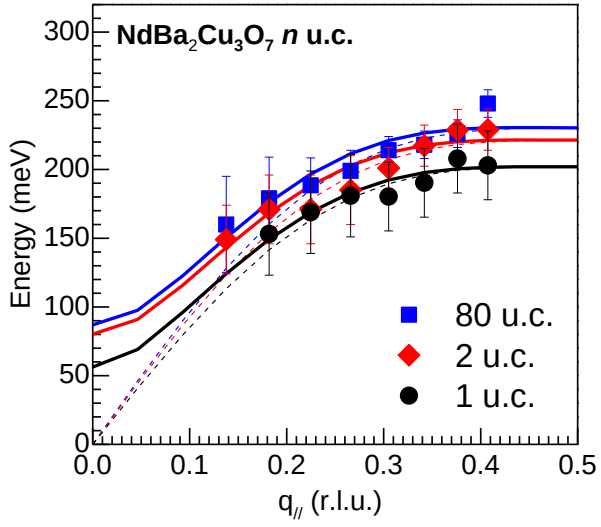
K. Ishii, M. Fujita, T. Sasaki, M. Minola, G. Dellea, C. Mazzoli, K. Kummer, G. Ghiringhelli, L. Braicovich, T. Tohyama, K. Tsutsumi, K. Sato, R. Kajimoto, K. Ikeuchi, K. Yamada, M. Yoshida, M. Kurooka & J. Mizuki, Nat. Comm. **5**, 3714 (2014)

Exceptional sensitivity of RIXS



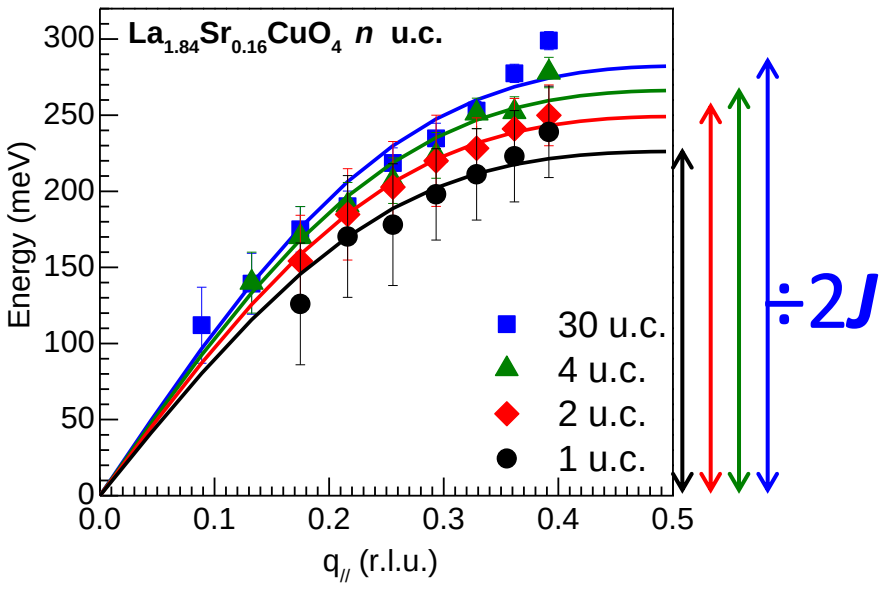


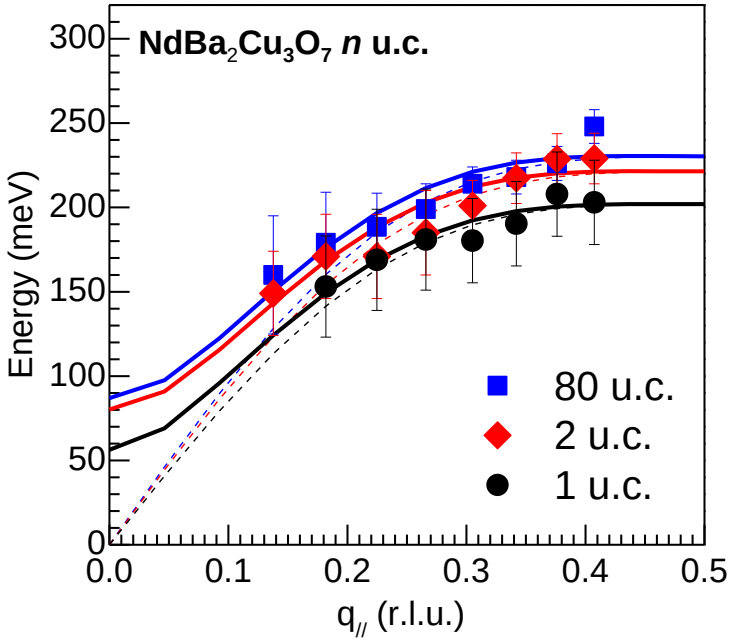


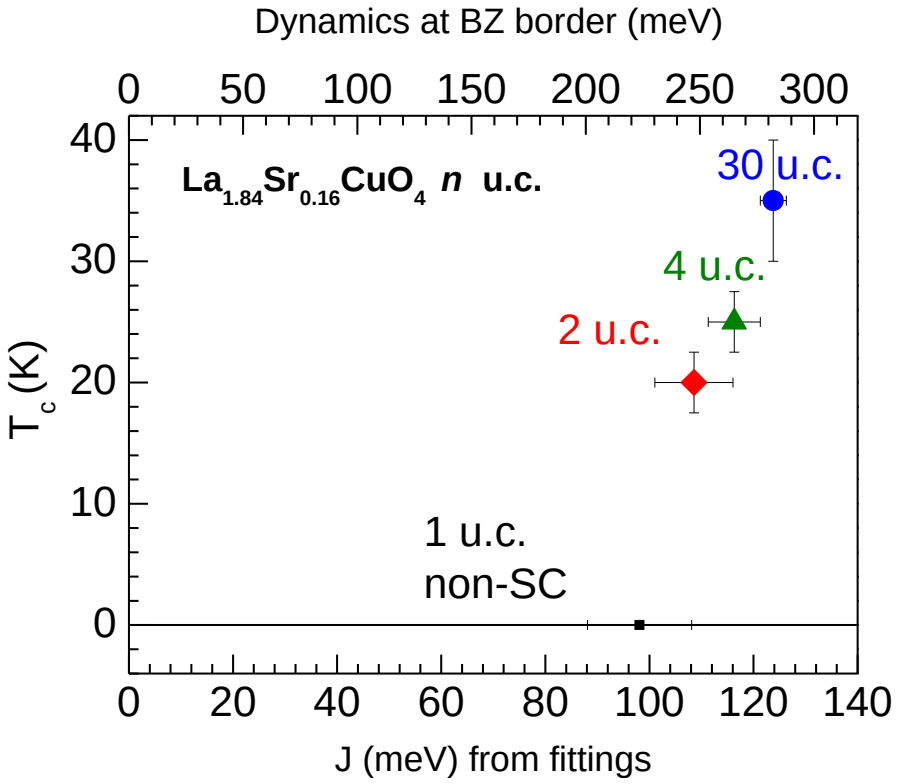


Experiment at ADRESS beam line of SLS: **M. Minola**, G. Dellea, M. Salluzzo, V. Bisogni, T. Schmitt, M. Le Tacon, G. Logvenov, G. Cristiani, F. Baiutti, B. Keimer, L. Braicovich, G. Ghiringhelli, unpublished

Small effect of thickness on *J*





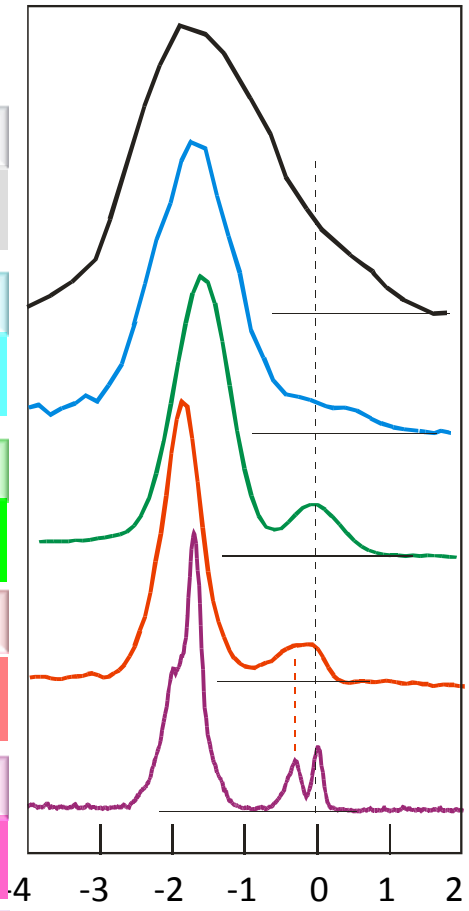


Linear spin-wave theory fittings

J decreases at lower film thickness, but only by 20% from bulk to 1 uc

ENERGY RESOLUTION: progress in the last 20 years

La_2CuO_4
Cu 2*p* → 3*d*
Photon energy ~ 931 eV



Δ*E* ~1.6 eV

K. Ichikawa *et al.*, J. Electron Spectrosc. Relat. Phenom.**78**, 183 (1996).

Δ*E* ~1.2 eV

L. C. Duda *et al.*, J. Electron Spectrosc. Relat. Phenom. **110–111**, 275 (2000).

2000 Uppsala

Δ*E* ~0.8 eV

AXES @ ID08, 2003. G. Ghiringhelli *et al.*, Phys Rev Lett. **92**, 117406 (2004).

2003

Δ*E* ~0.45 eV

AXES @ ID08, 2007. L. Braicovich *et al.*, arXiv:0807:1140v1, (2008).

2007

ESRF + AXES

Δ*E* ~0.13 eV

SAXES @ SLS, 2008. G. Ghiringhelli, L. Braicovich, T. Schmit *et al.*, unpublished

2008 SLS + SAXES

Δ*E* ~0.050 eV

2015

Δ*E* ~0.030 eV

2016

ESRF + ERIXS

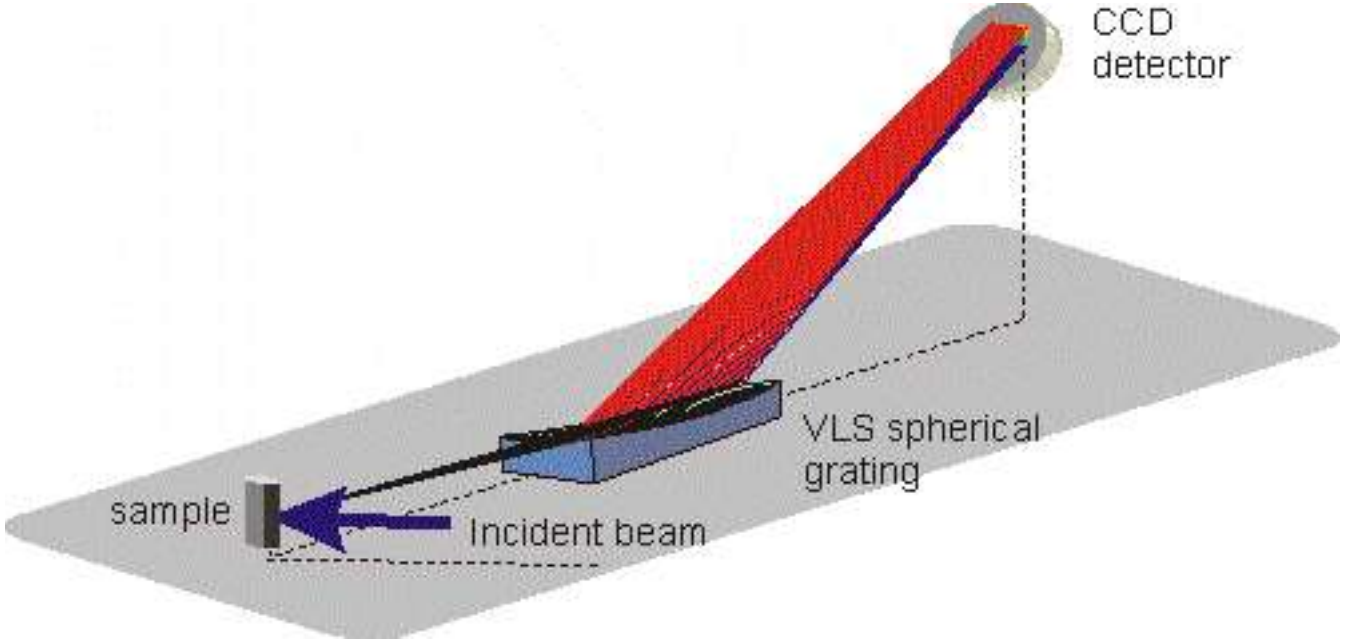
Combined resolving power has increased by a factor 30

Soft x-ray RIXS instrumentation

High resolution mono, small x-ray spot on the sample

Grating spectrometer: optimized efficiency, high resolution

The main limiting factor is INTENSITY!!!!



From AXES (ESRF, ID08) to SAXES (SLS, ADRESS)

Since 1994: AXES at beam line
ID08 of the ESRF
L = 2.2 m
Design: $E/\Delta E$ = 2,000 at Cu L_3 (930 eV)
2010: $E/\Delta E$ = 5,000 at Cu L_3

Since 2007: SAXES at beam line
ADRESS of the SLS
L = 5.0 m
Design: $E/\Delta E$ = 12,000 at Cu L_3
2011: $E/\Delta E$ = 11,000 at Cu L_3

C. Dallera *et al*. J. Synchrotron Radiat. **3**, 231 (1996)
G. Ghiringhelli *et al.*, Rev. Sci. Instrum. **69**, 1610 (1998)
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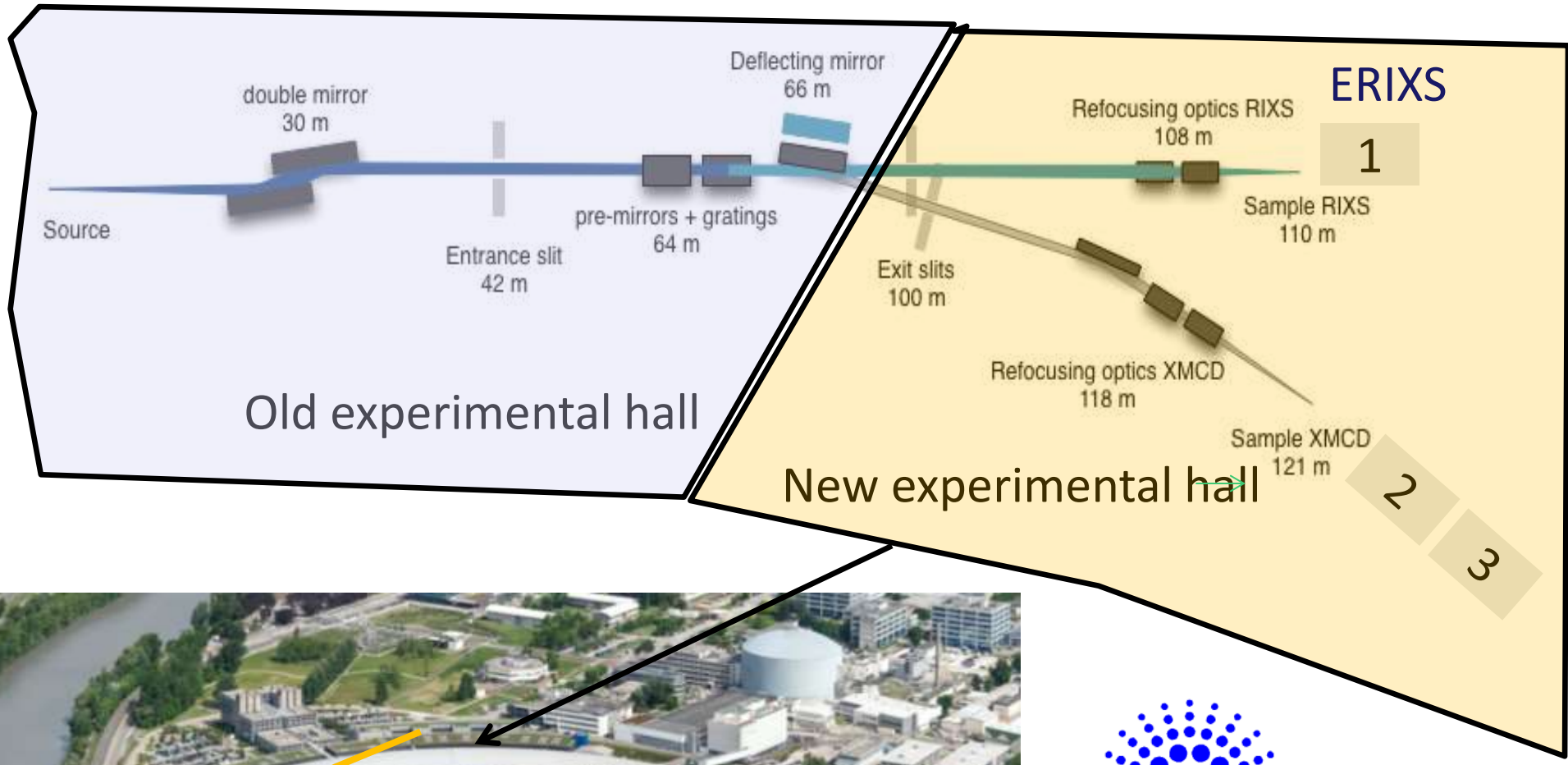
V. Strocov, T. Schmitt, L. Patthey et al, J. Synch. Rad., 17, 631 (2010).

New ID32 at the ESRF



ESRF

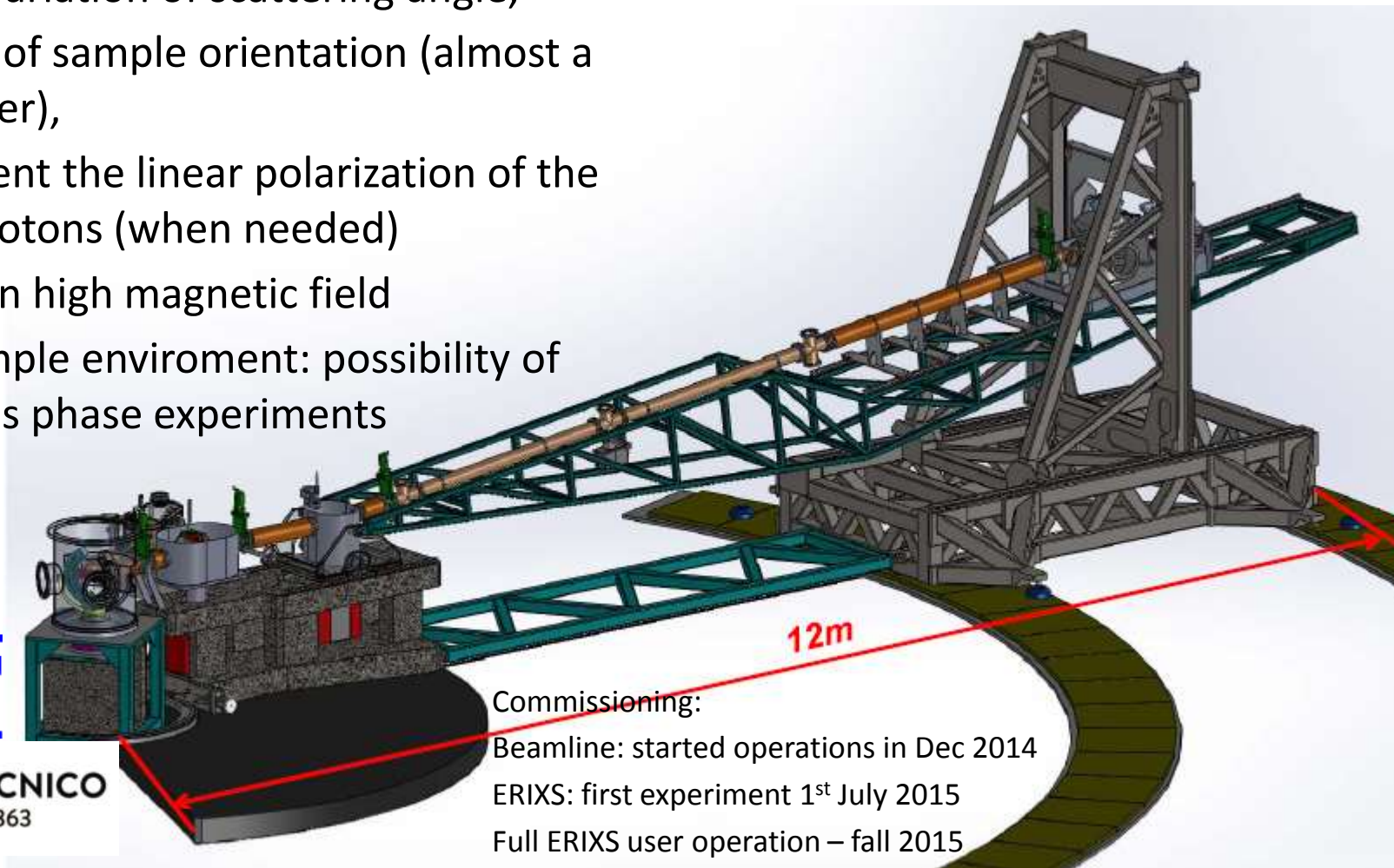
ERIXS spectrometer at the new ID32

FEATURES:

- $E/\Delta E$ > 20,000 below 1000 eV from day one (50 meV at Cu L_3) and $E/\Delta E$ > 30,000 ultimate
- continous variation of scattering angle,
- full control of sample orientation (almost a diffractometer),
- measurement the linear polarization of the scattered photons (when needed)
- optionally in high magnetic field
- flexible sample enviroment: possibility of liquid and gas phase experiments

ESRF Upgrade program,

N.B. Brookes, F. Yakhou, GG et al



ESRF

POLITECNICO MILANO 1863

Commissioning:

Beamline: started operations in Dec 2014

ERIXS: first experiment 1st July 2015

Full ERIXS user operation – fall 2015

ERIXS and the other HR soft-RIXS projects

SR FACILITY	E/ΔE (combined)	Length	YEAR	NOTES
ESRF, ERIXS@ID32	30,000	11 m	2015	With Polarimeter
DIAMOND, IXS	40,000	14 m	2017	
MAX IV, Veritas	40,000	?	2017	Rowland Geometry
NSLS II, Centurion@SIX	70,000	15 m	2017	Hettrick-Underwood, 50 nrad slope error, 1 um spot on sample
European XFEL	20,000	5 m	2017	For non linear RIXS and pump-probe time-resolved RIXS

Bibliography

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Resonant inelastic x-ray scattering studies of elementary excitations

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Insights into the high temperature superconducting cuprates from resonant inelastic X-ray scattering

M.P.M. Dean

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