



novel SuperConductors and Synchrotron Radiation:
state of the art and perspectives
Adriatico Guesthouse, Trieste, Italy / 10-11 December 2014



Elettra Sincrotrone Trieste

10 December, 2014

Charge density order and magnetic fluctuations in cuprate superconductors studied with Resonant (Inelastic) X-ray Scattering



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Summary

- ◇ The case of high T_c superconductors for resonant x-ray scattering
- ◇ Persistence of magnetic excitations in HTcS
- ◇ Charge Density Waves in HTcS
- ◇ New instrumentation, new experiments

Acknowledgements



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D. G. Schlom

Cornell

Mark Dean, John Hill, Stuart Wilkins, I. Bozovic, R. M. Konik, G. D. Gu, X. Liu, Y.-J. Sun, J. Strle,

Brookhaven Natl. Lab.

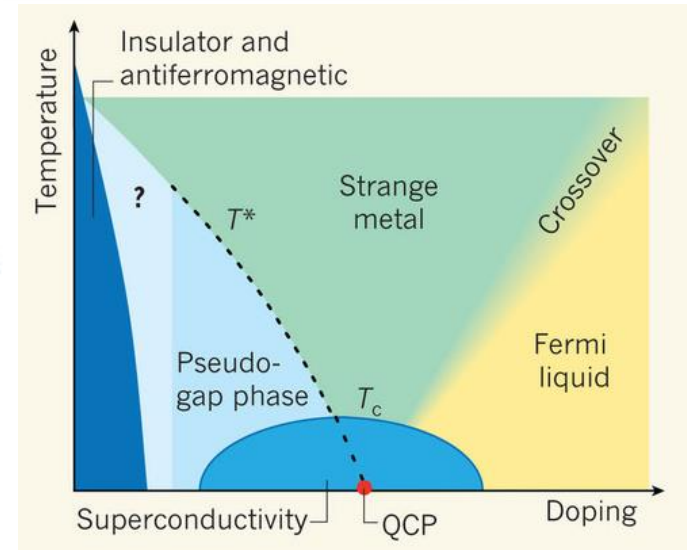
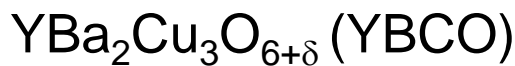
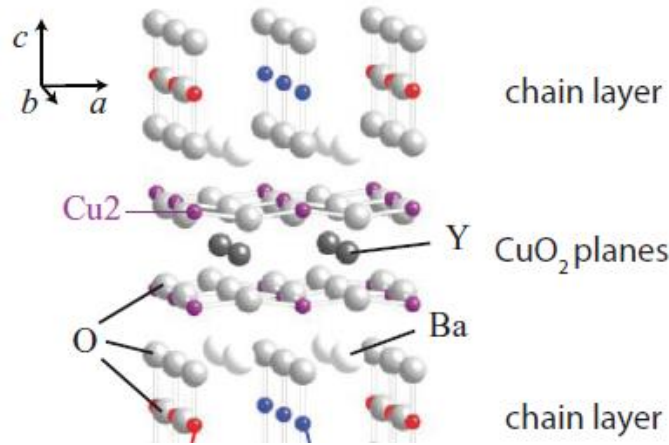
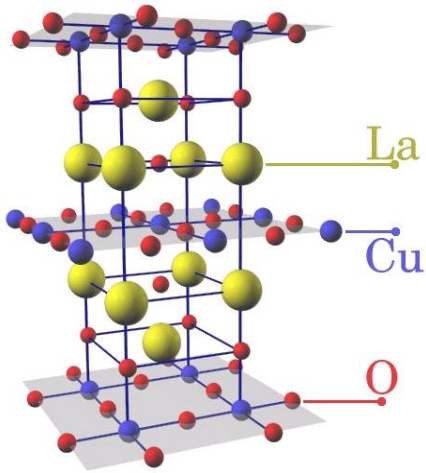
Makoto Hashimoto, W.-S. Lee, Z.X. Shen, Tom Devereaux, Chunjin Jia, Brian Moritz

Stanford

K. Ishii, M. Fujita, T. Tohyama,

Spring8, Tohoku, Kyoto

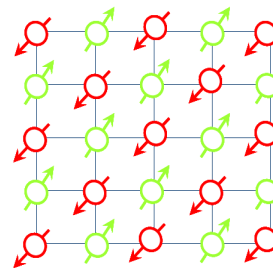
High T_c superconducting cuprates



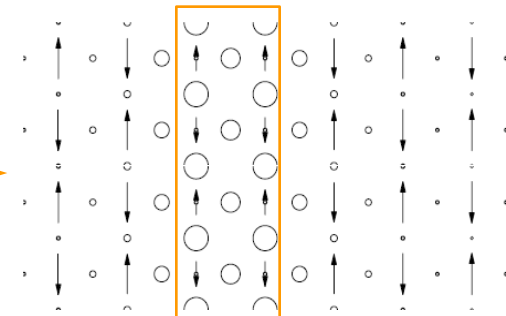
CuO_2 planes \rightarrow Doping (by substitution) \rightarrow High- T_c superconductivity

Evidence of **ordering phenomena**:

- **Uniform 2D AntiFerroMagnetism (AFM)** \rightarrow in undoped insulating samples



- **Uniaxially modulated spin and charge order (stripes)** \rightarrow in the 214-family: $\text{La}_{2-x-y}(\text{Sr},\text{Ba})_x(\text{Nd},\text{Eu})_y\text{CuO}_4$

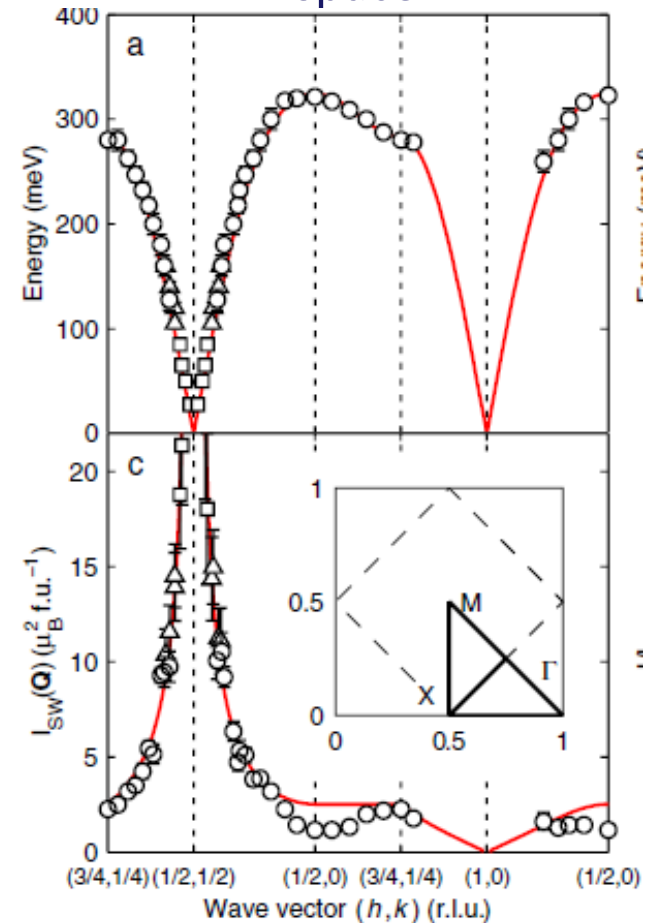
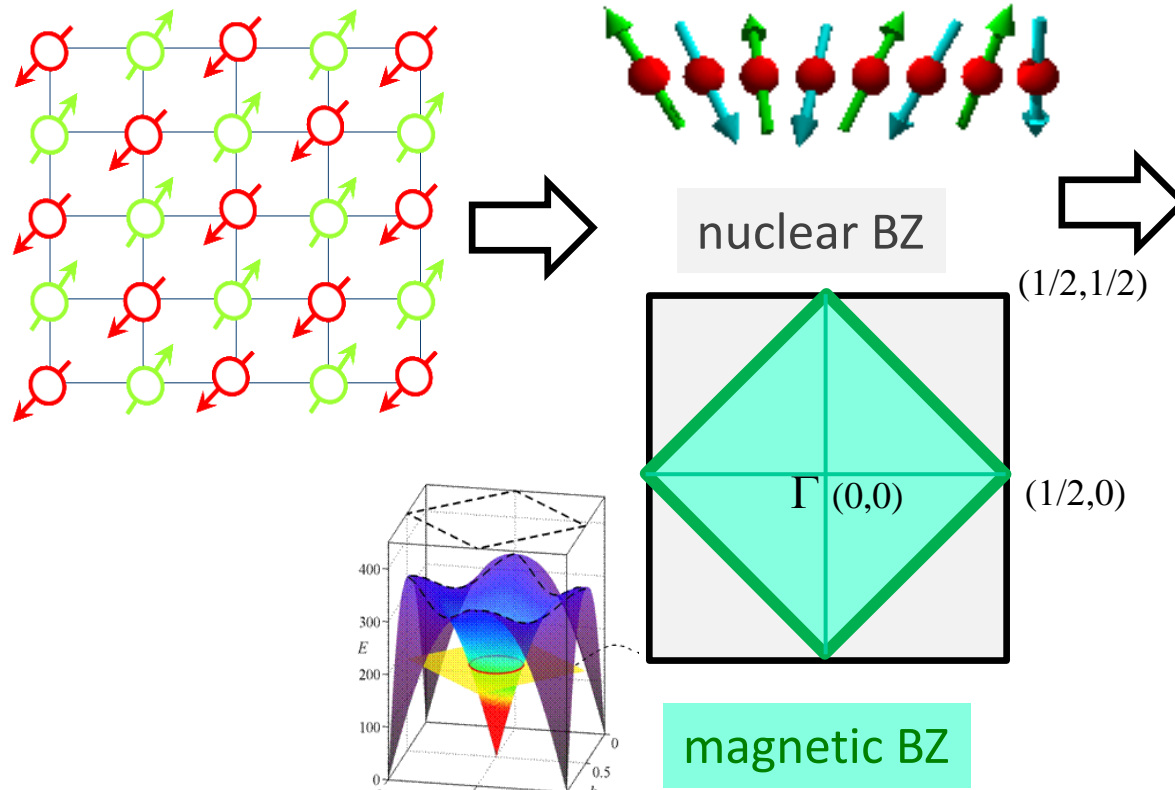


Cuprates: spin waves in the 2D AF lattice

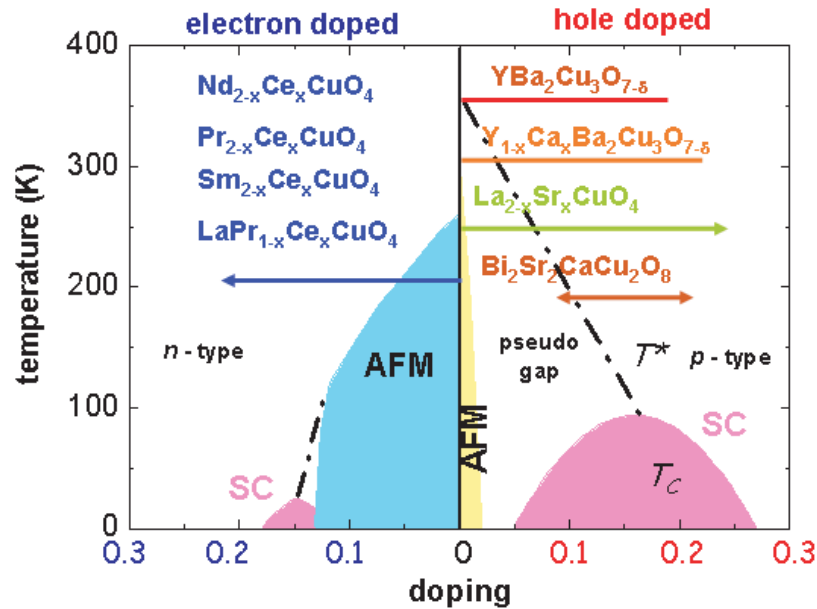
Undoped AF square lattice,
long range order due to large
superexchange interaction J

Flipping one spin gives rise
to a spin wave (magnon)...

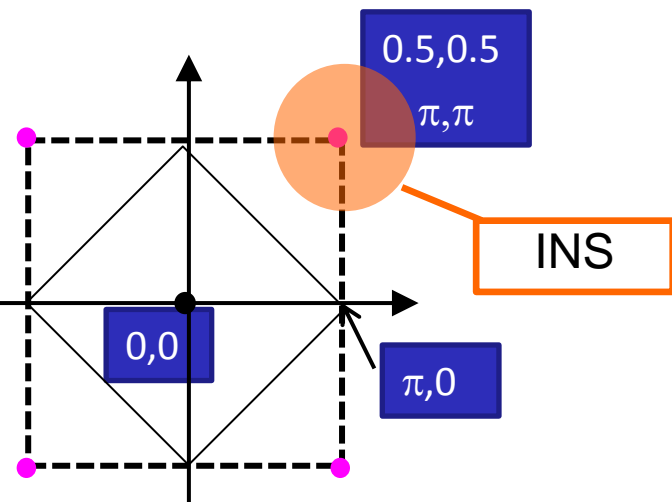
... with a well defined
dispersion in reciprocal
space



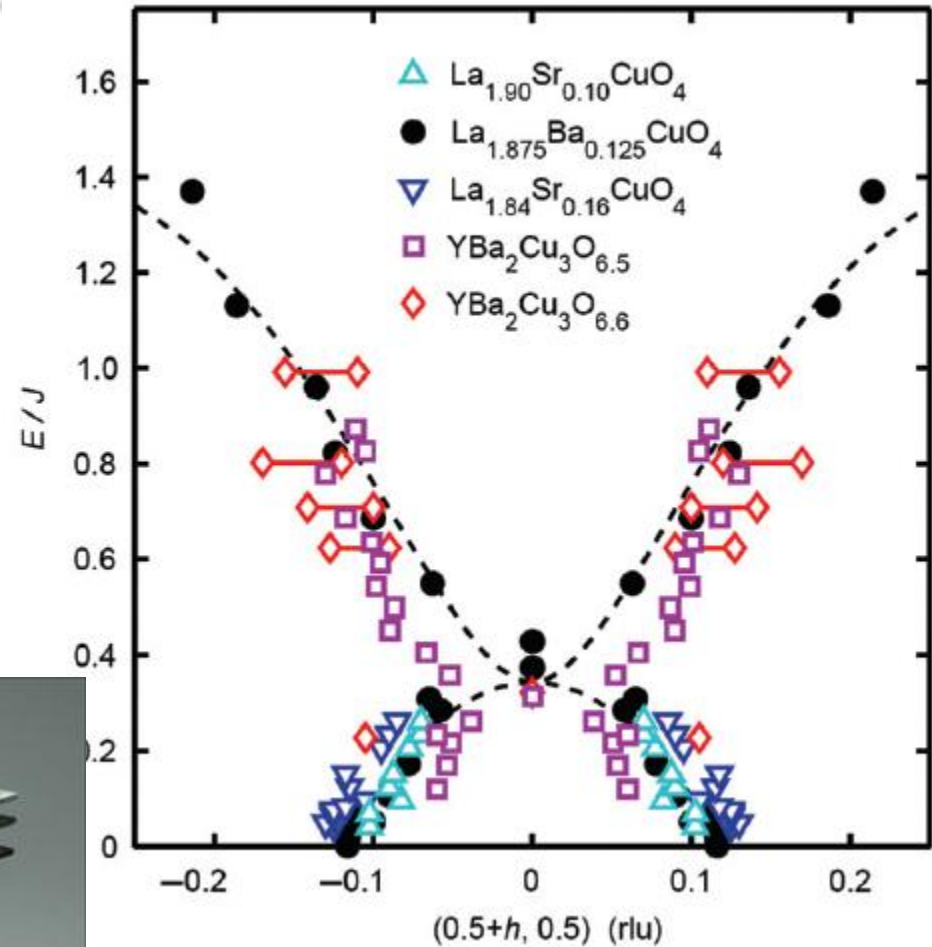
Spin excitations in HTcS: doped SC



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

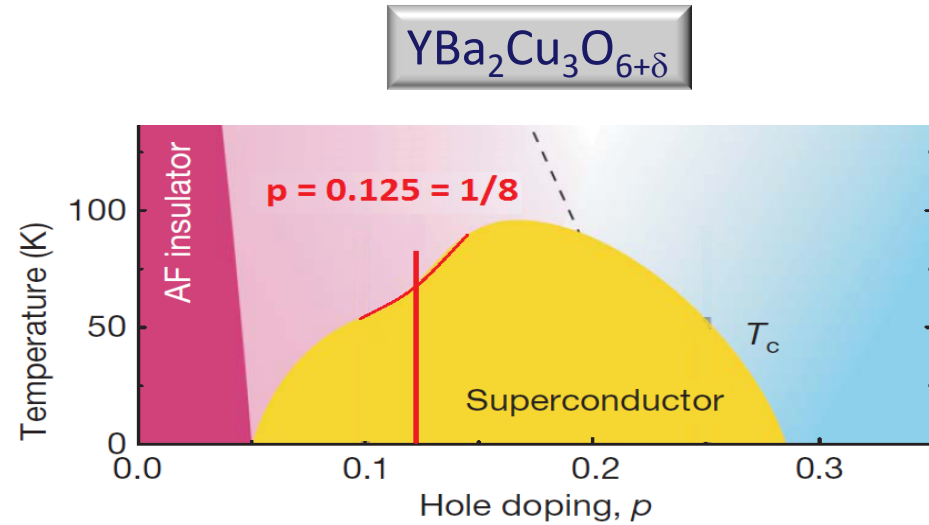
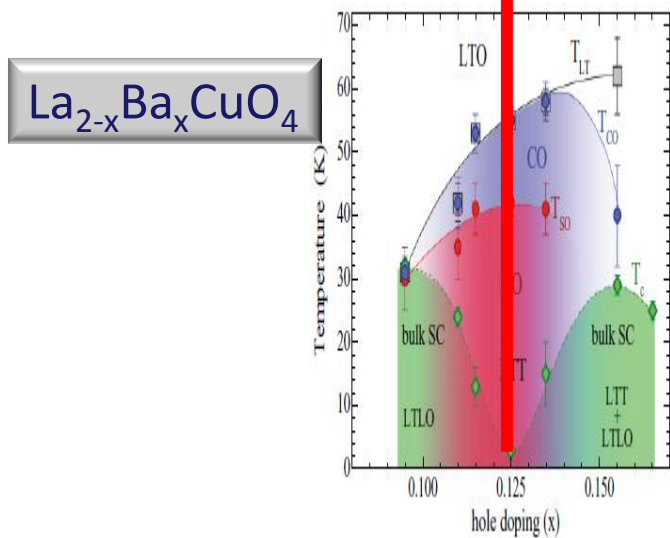
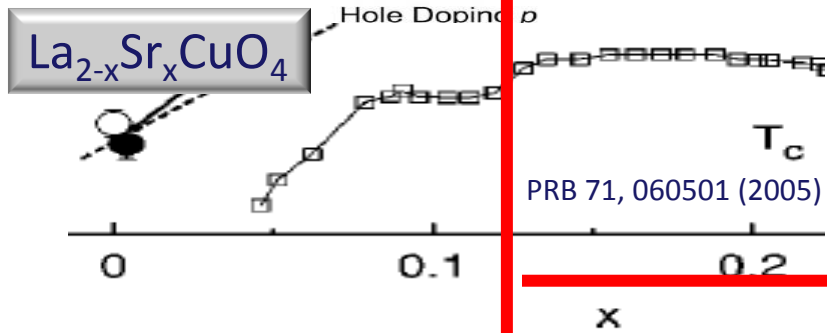
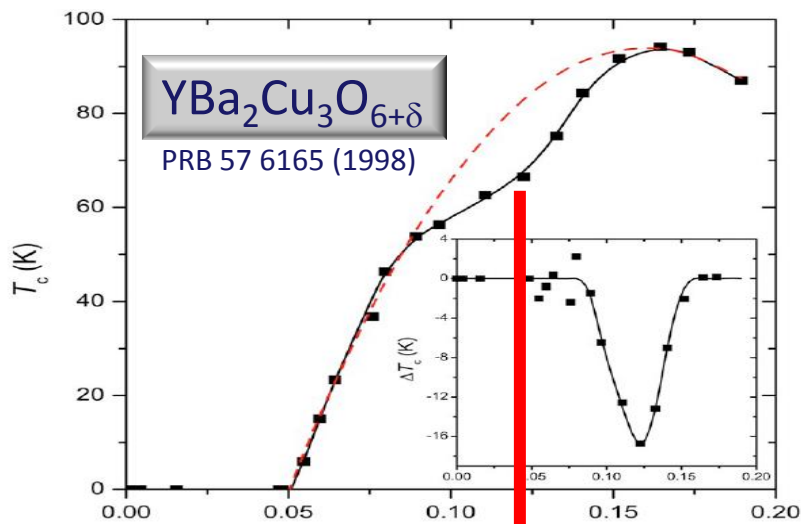


V. Hinkov et al, Eur. Phys. J. Special Topics 188, 113–129 (2010)



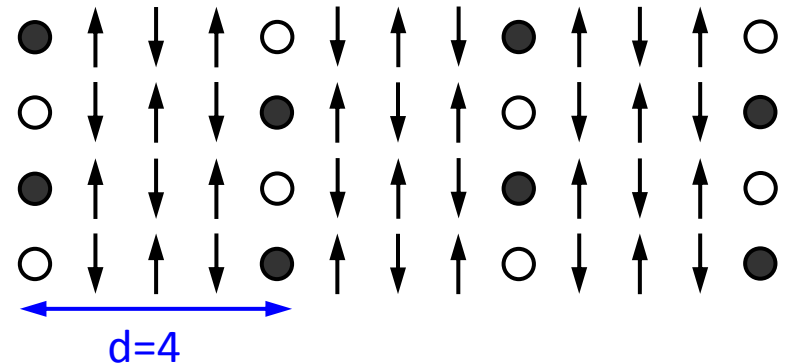
J.M. Tranquada, in *Handbook of High-Temperature Superconductivity: Theory and Experiment*, J.R. Schrieffer and J.S. Brooks, eds., Springer, 2007,

LSCO vs YBCO (214 vs 123)



$p = 0.125 = 1/8$

Static stripes in LXCO, period 4,
suppress SC



Resonant (Inelastic) soft X-ray Scattering

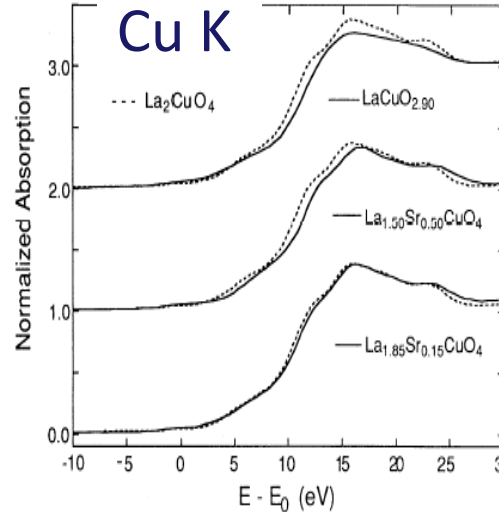
Soft RIXS: exploiting the 2p-3d resonant absorption

Resonant Inelastic X-ray Scattering:

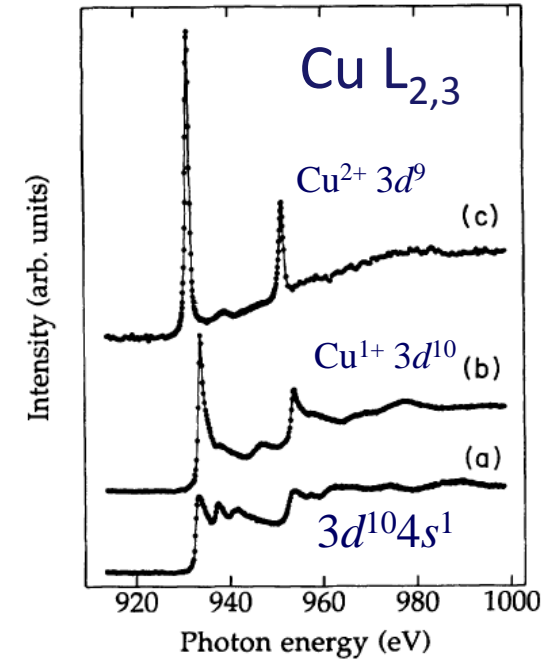
- an energy loss experiment
- made with photons of high energy
- at a core absorption resonance

Conservation laws:

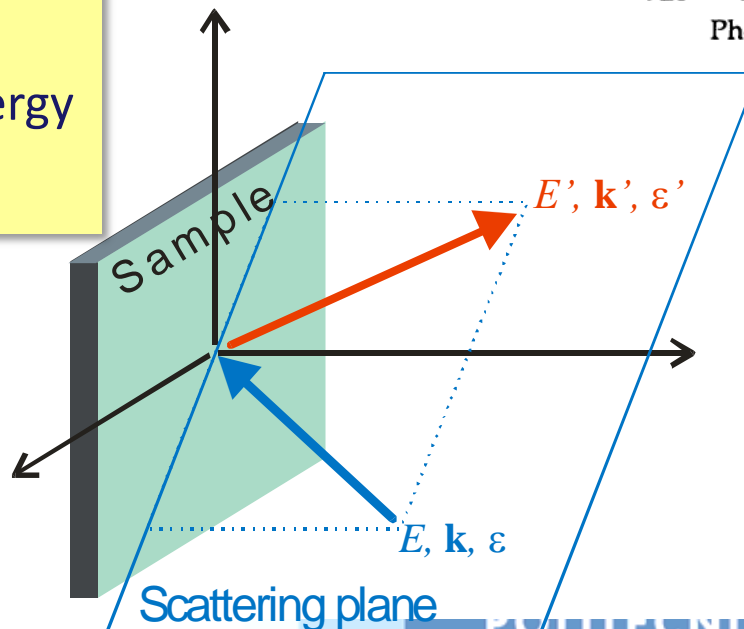
- Energy
- Momentum
- "Angular momentum"



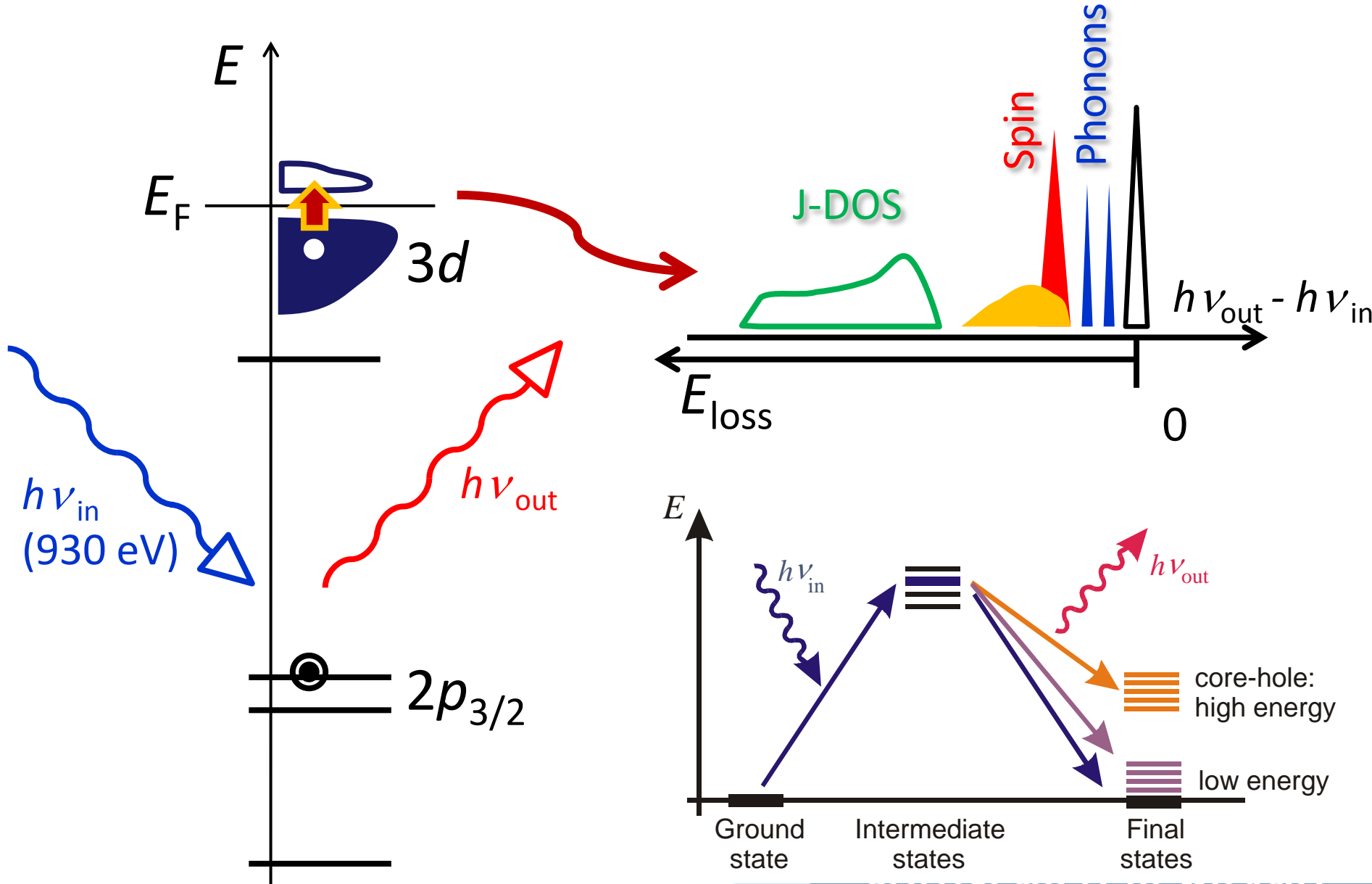
Z. Tan *et al* Phys. Rev. B **47**, 12365 (1993)



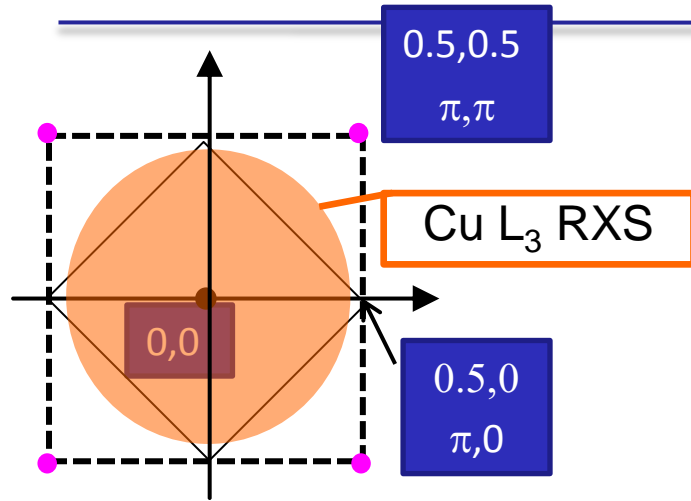
M. Grioni *et al* PRB **45**, 3309 (1992)



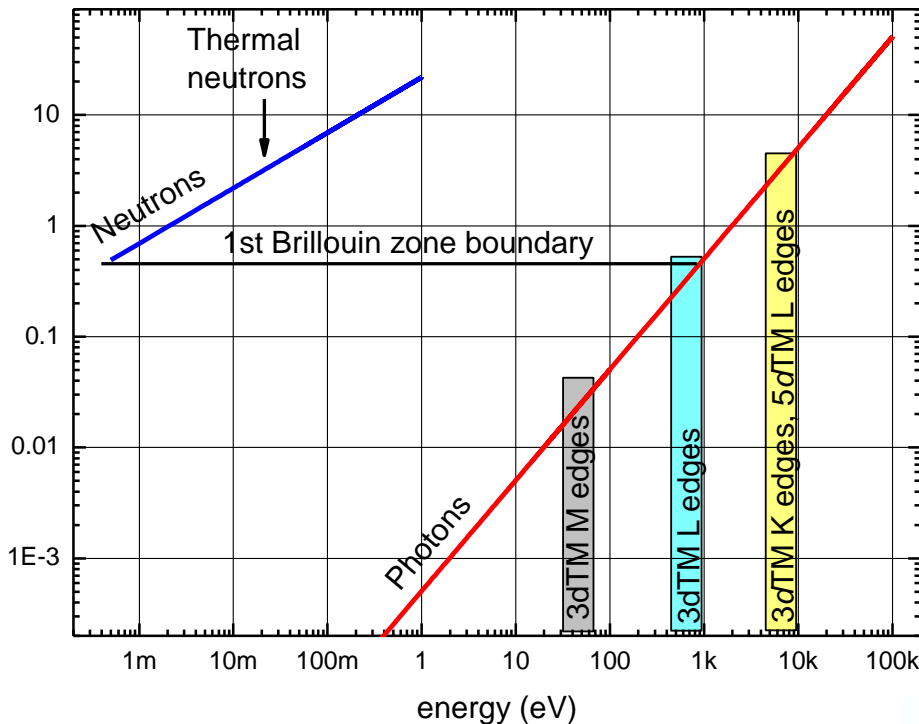
Cu L₃ RIXS



Cu L₃ RIXS: Experimental conditions

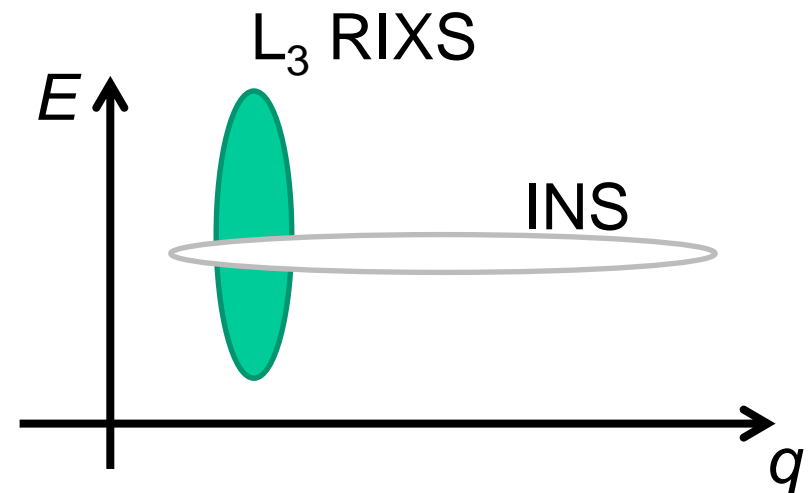


Wavevector of particles used in inelastic scattering

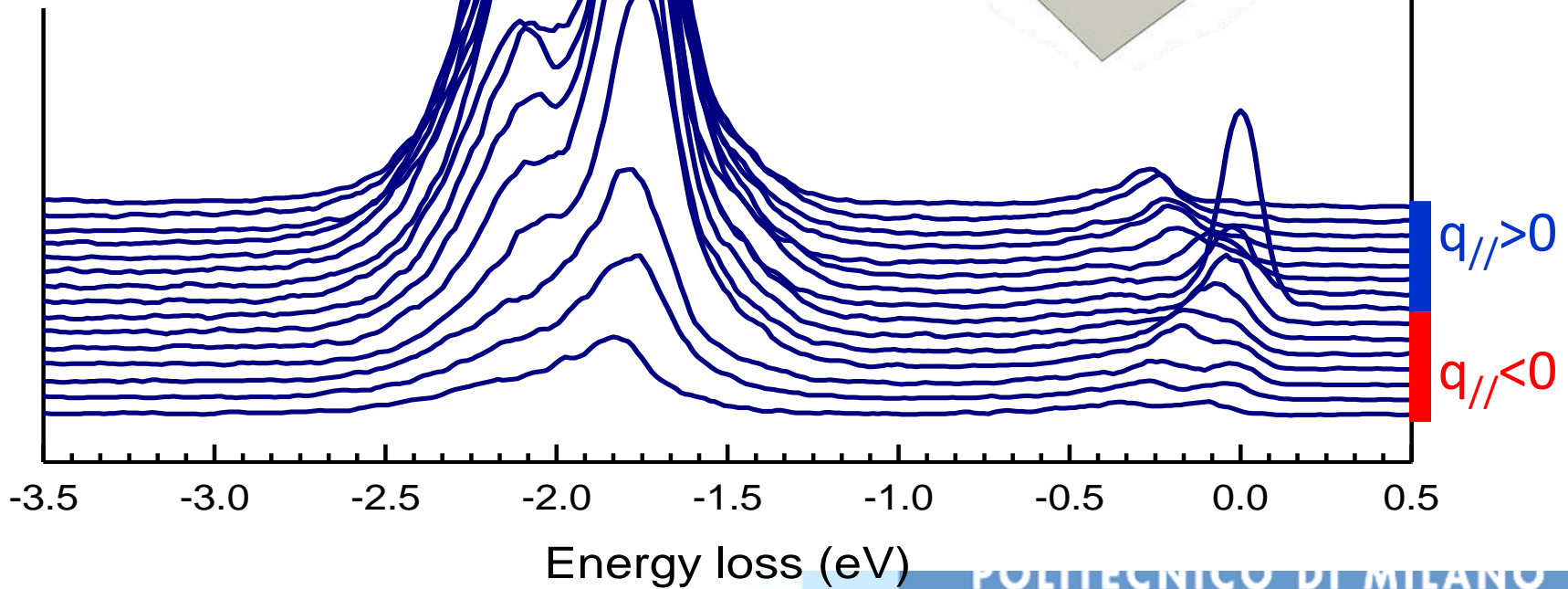
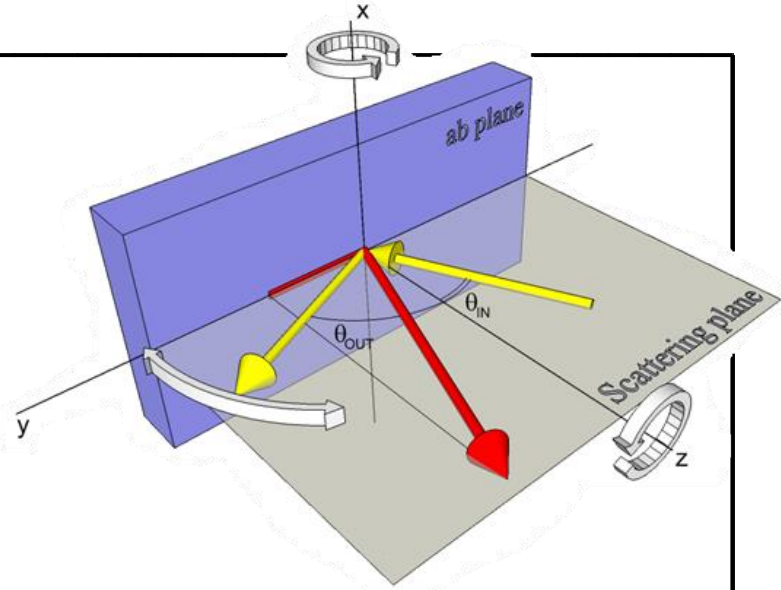
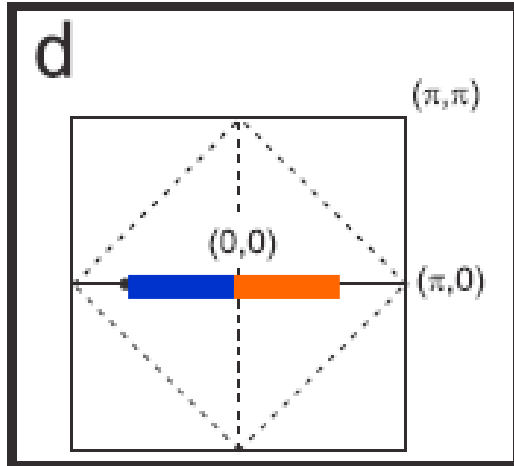


Cu L₃ resonance:

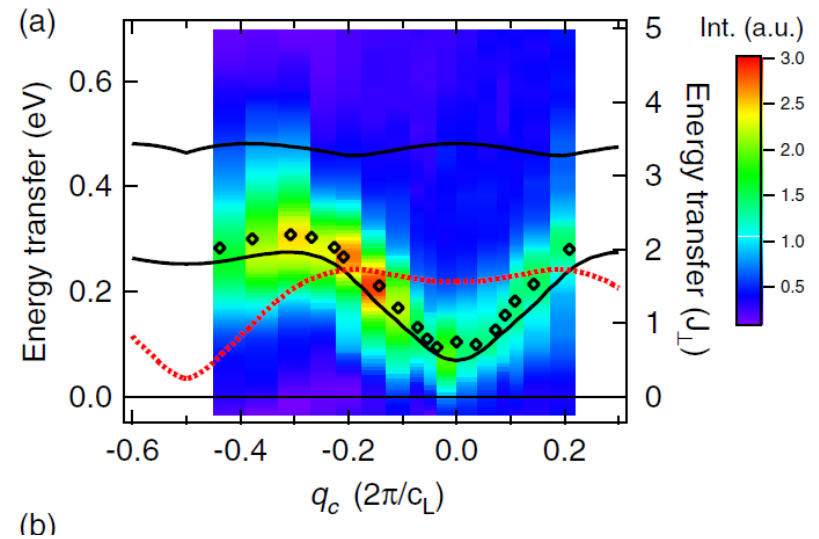
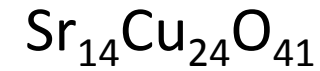
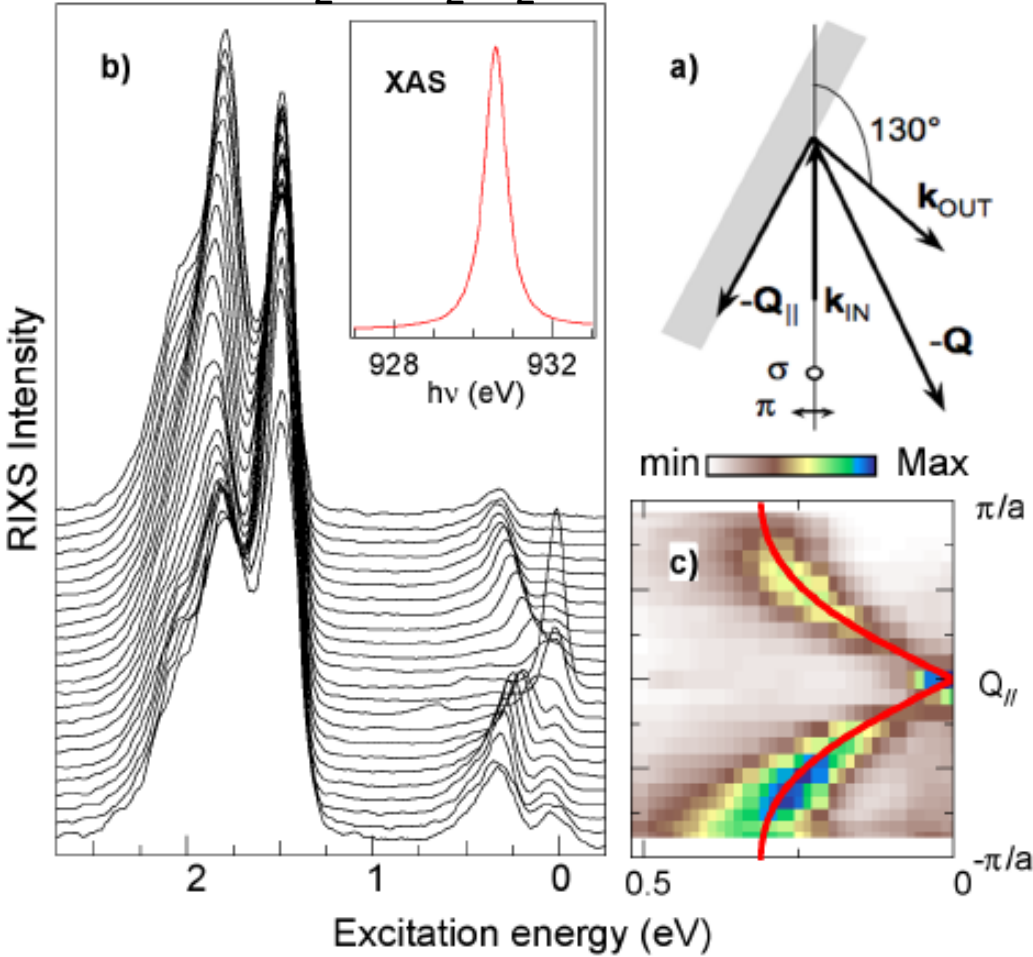
- $E_0 = 930 \text{ eV}$
- $q_{\text{max}} = 0.86 \text{ Ang}^{-1}$
- confined inside a region around Γ
- 2p core hole: spin-orbit interaction
- E resolution: 120-240 meV
- q resolution: 0.005 rlu
- $\frac{1}{2}$ - 1 hour per spectrum



Dispersing peaks in the MIR...



Undoped compounds

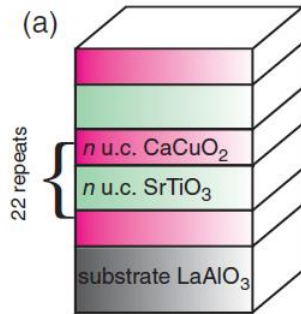


J. Schlappa et al, PRL 103, 047401 (2009)

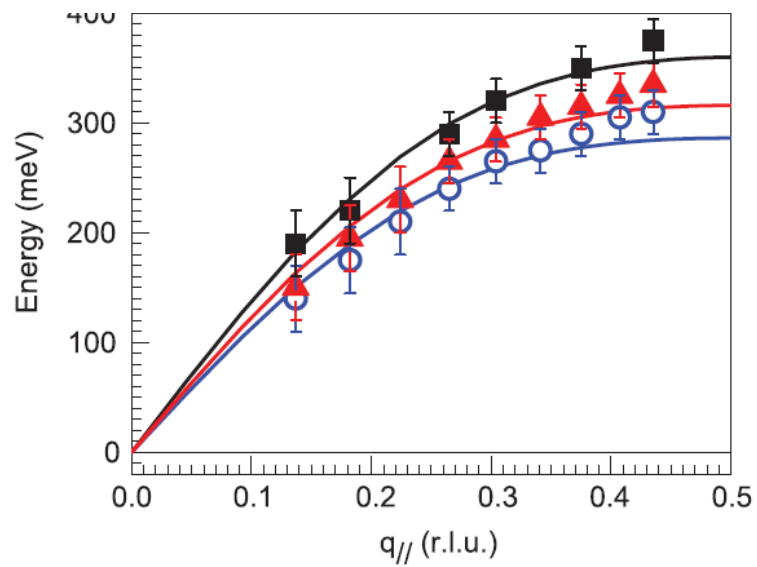
M. Guarse et al, PRL 105 157006 (2009)

Magnetic and ligand field properties of copper at the interfaces of $(\text{CaCuO}_2)_n/(\text{SrTiO}_3)_n$ superlattices

M. Minola,¹ D. Di Castro,² L. Braicovich,³ N. B. Brookes,⁴ D. Innocenti,² M. Moretti Sala,^{3,*} A. Tebano,² G. Balestrino,² and G. Ghiringhelli³

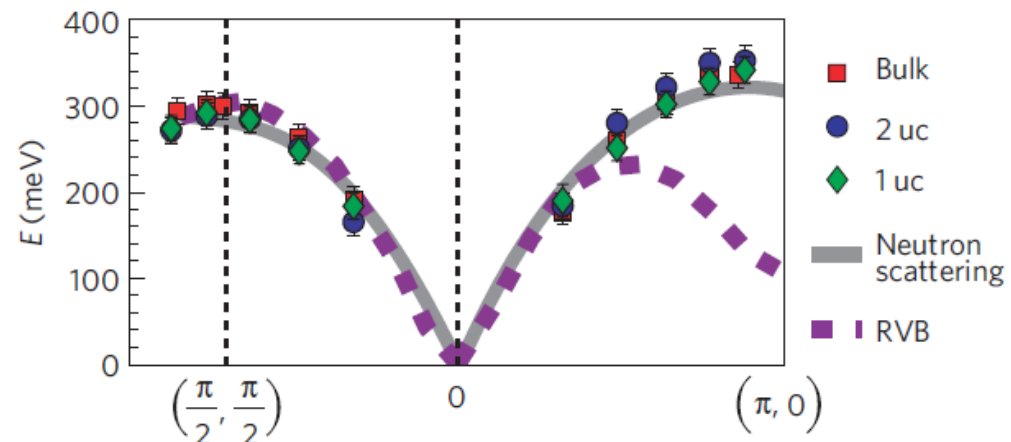
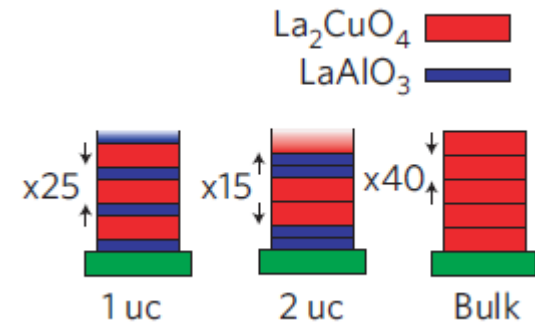


	SL ($n = 2$)	SL ($n = 3$)	CaCuO_2	La_2CuO_4
U	1970	2720	3010	2200
t	250	320	360	300
J	127	138	157	138
J_c	41	42	49	38
$J' = J''$	2	2	2	2

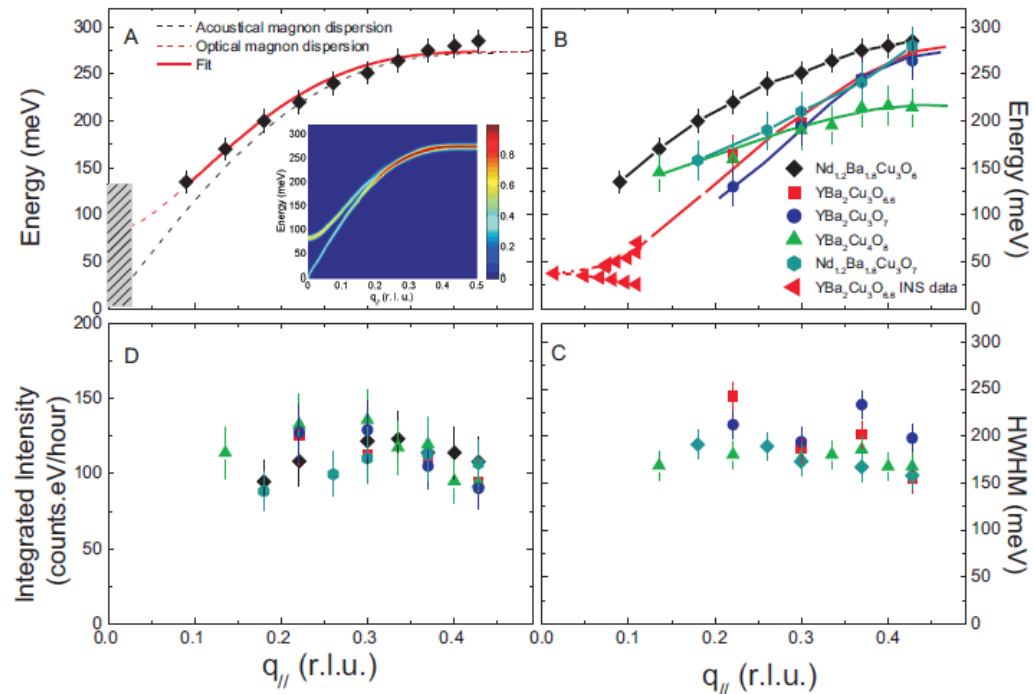
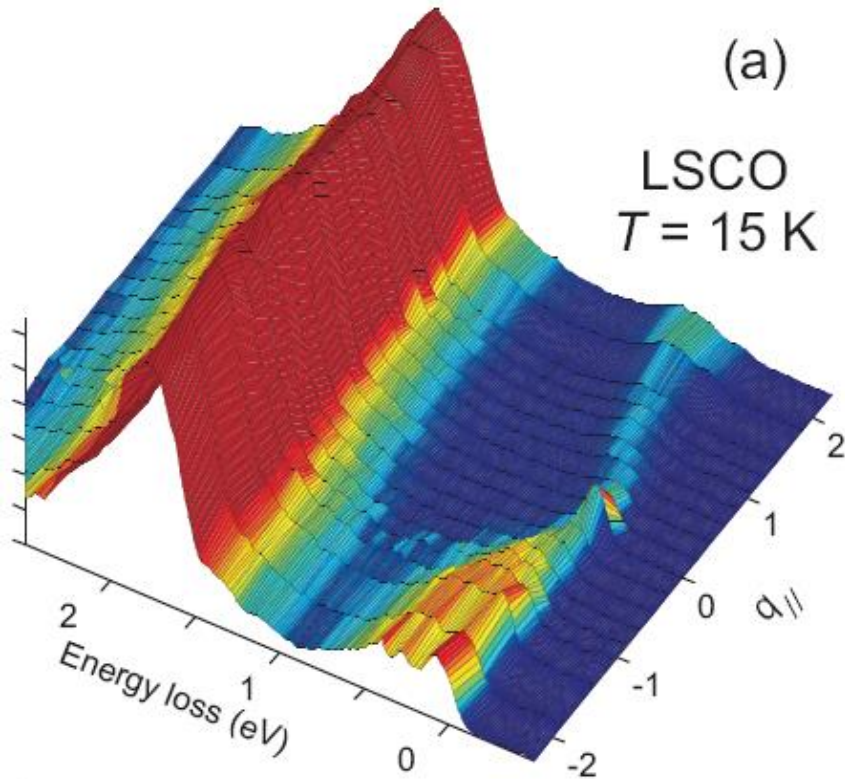


Spin excitations in a single La_2CuO_4 layer

M. P. M. Dean^{1*}, R. S. Springell^{2,3}, C. Monney⁴, K. J. Zhou^{4†}, J. Pereira^{1†}, I. Božović¹, B. Dalla Piazza⁵, H. M. Rønnow⁵, E. Morenzoni⁶, J. van den Brink⁷, T. Schmitt⁴ and J. P. Hill^{1*}



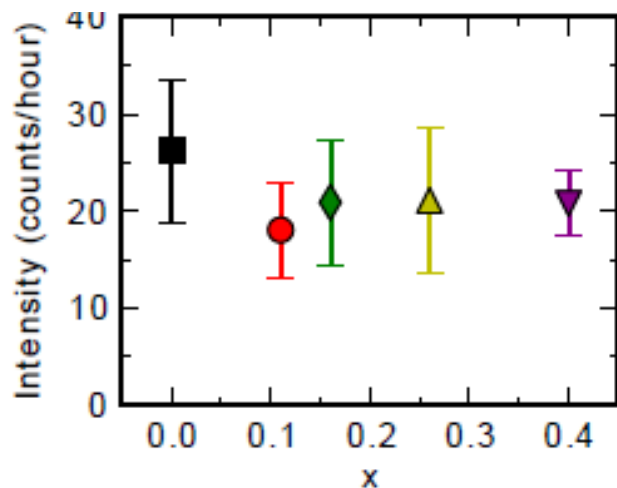
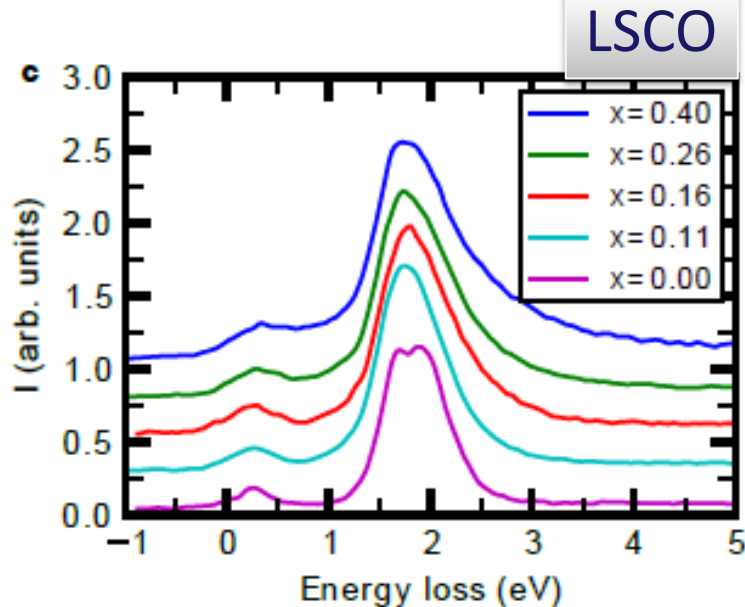
LSCO, YBCO and NdBCO



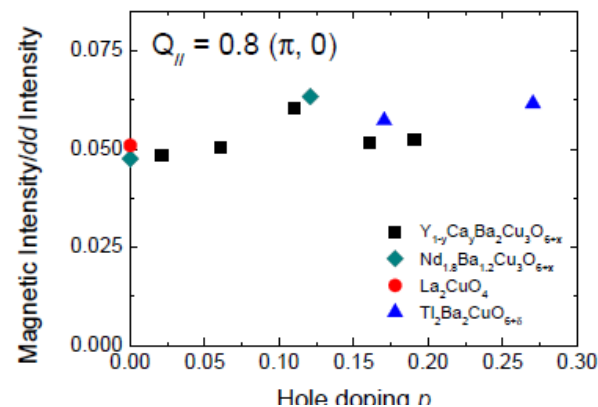
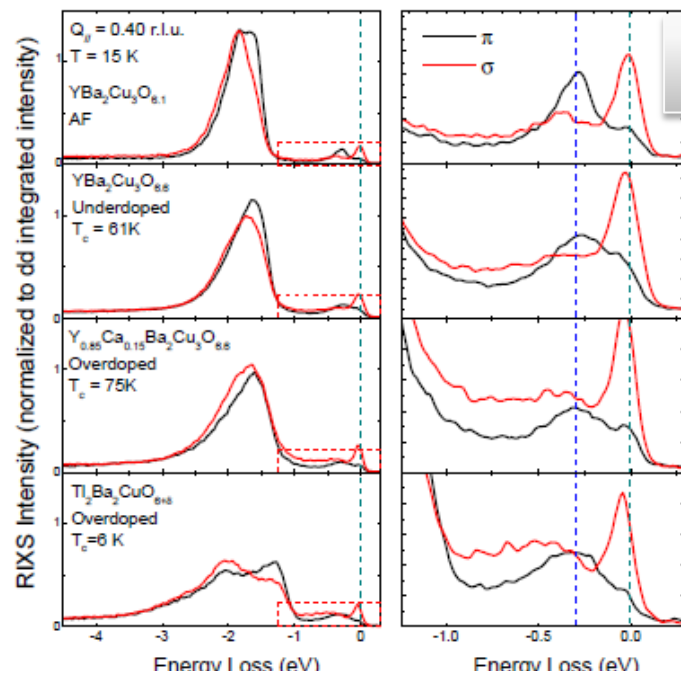
LSCO & NdBCO: 100 nm films on STO. YBCO: detwinned single crystals

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)



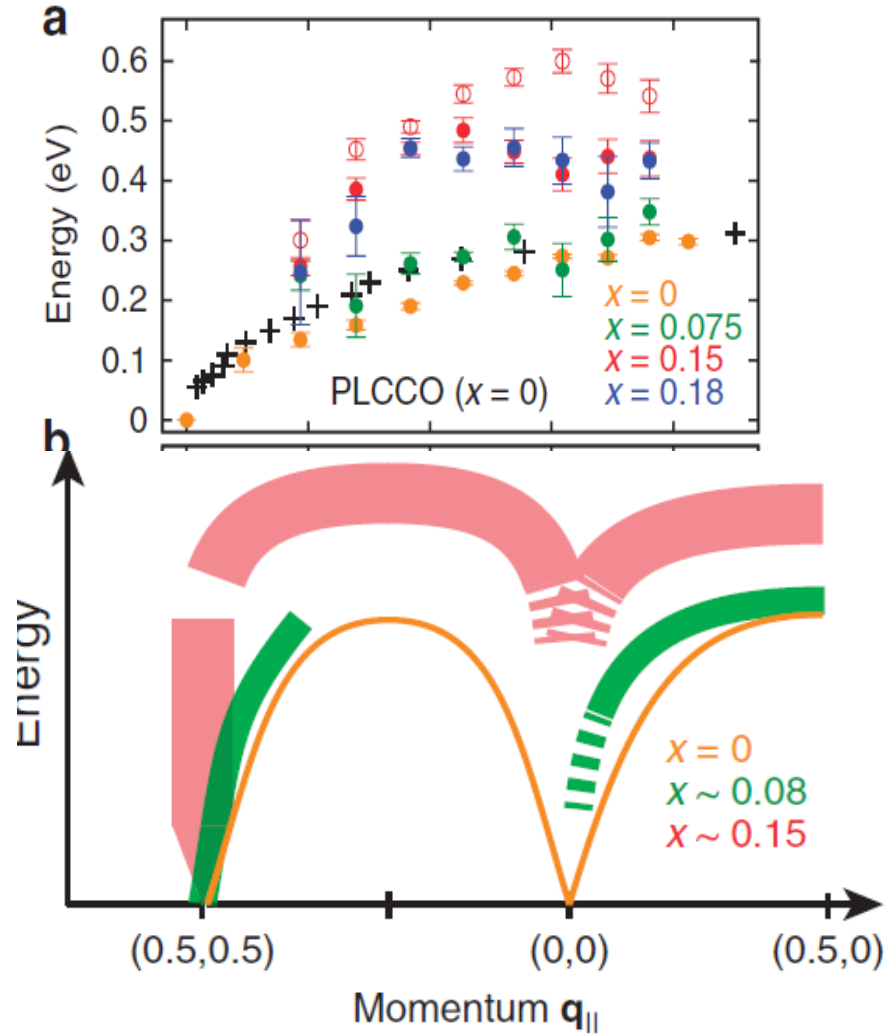
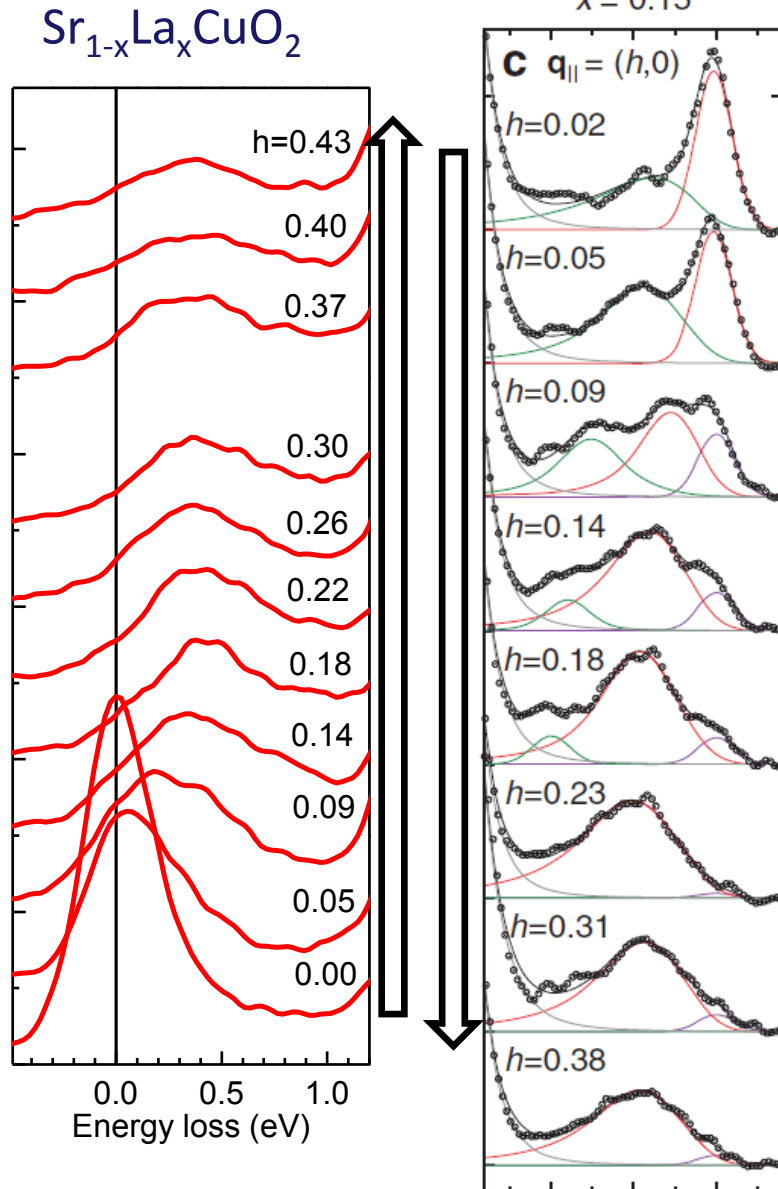
π pol



M. P. M. Dean, G. Dellea, R. S. Springell, F. Yakhov-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)

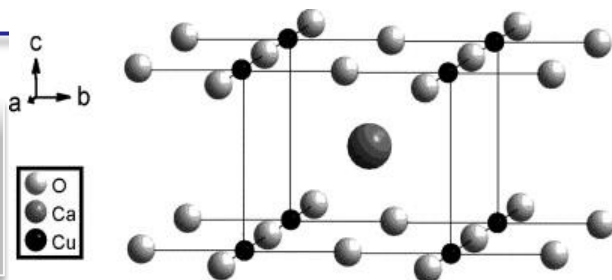
Spin excitations in e-doped SC



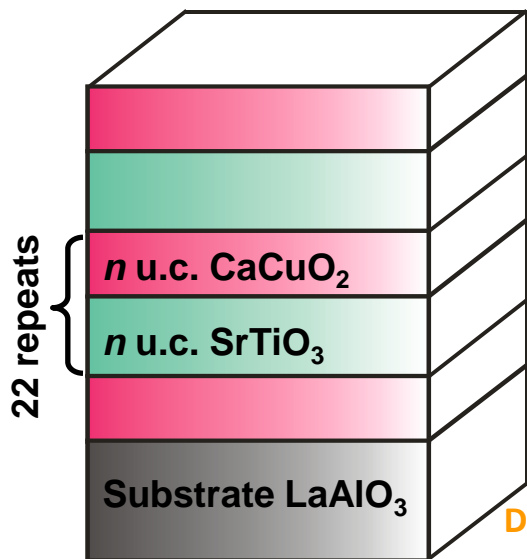
K. Ishii, M. Fujita, T. Sasaki, M. Minola, G. Dellea, C. Mazzoli, K. Kummer, G. Ghiringhelli, L. Braicovich, T. Tohyama, K. Tsutsumi, K. Sato, R. Kajimoto, K. Ikeuchi, K. Yamada, M. Yoshida, M. Kurooka & J. Mizuki, Nat. Comm. **5**, 3714 (2014)

Paramagnons in e- and h-doped infinite layers

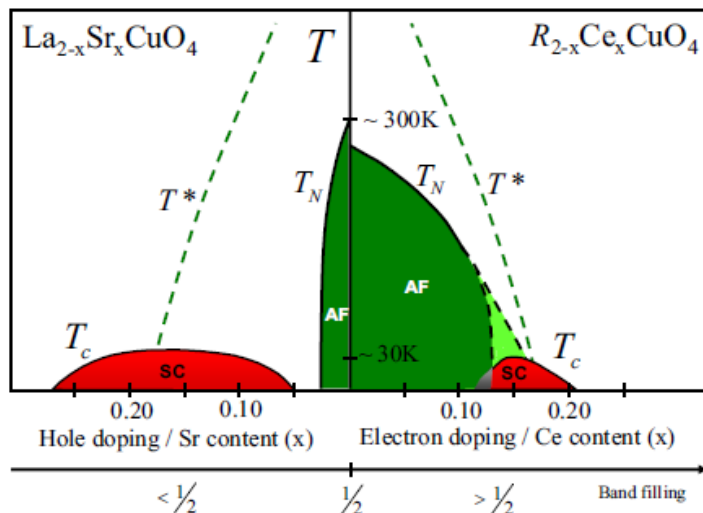
Hole-doped CCO/STO superlattices



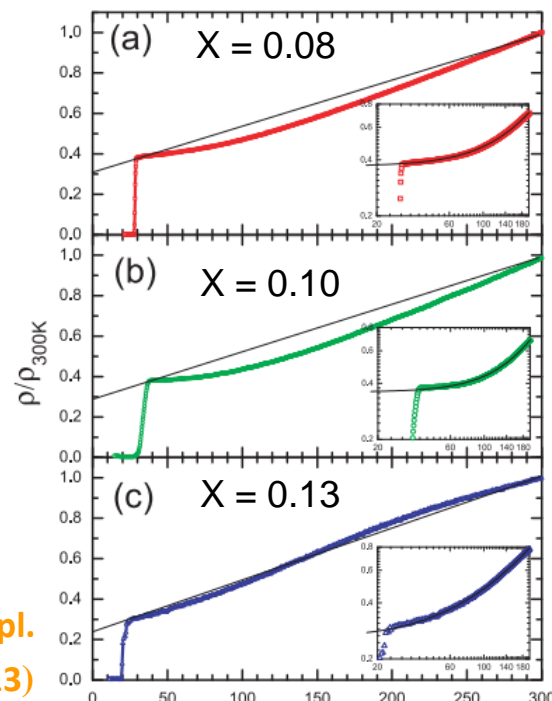
Electron-doped:
 $\text{Sr}_{1-x}\text{La}_x\text{CuO}_2/\text{GdScO}_3$



D. Di Castro et al., *Phys. Rev. B* 86, 134524 (2012)



L. Maritato et al., *J. Appl. Phys.* 113, 053911 (2013)



$\text{Sr}_{1-x}\text{La}_x\text{CuO}_2$ epitaxial films: $T(K)$
 grown on a GdScO_3 s \rightarrow strain
 annealing \rightarrow oxygen content
 $x \rightarrow$ La stoichiometry

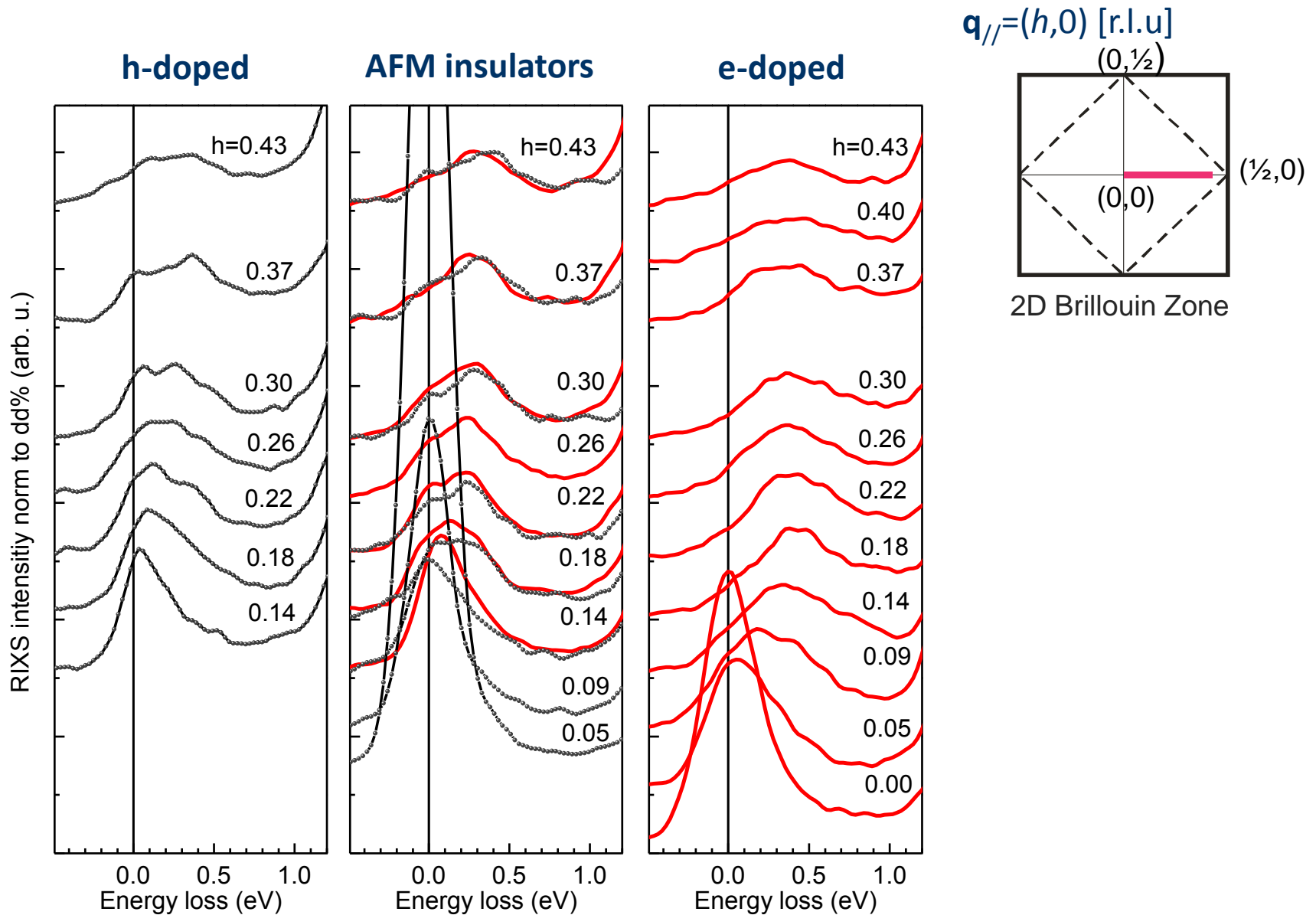
SLs grown in a highly oxidizing atmosphere

\rightarrow SC

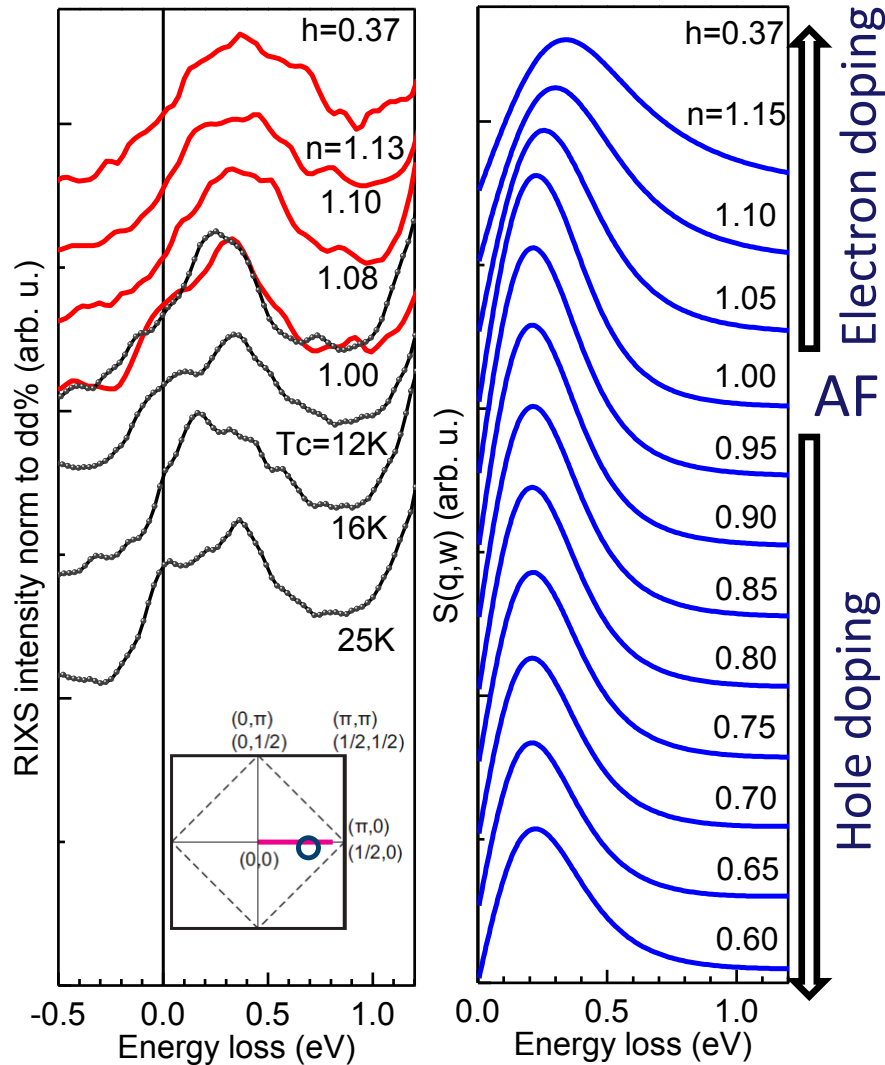
Extra oxygen ions at interfaces \rightarrow charge reservoir \rightarrow hole doping CuO_2 planes

SC confined within few unit cells at interface.

Paramagnon dispersion along (1,0) direction

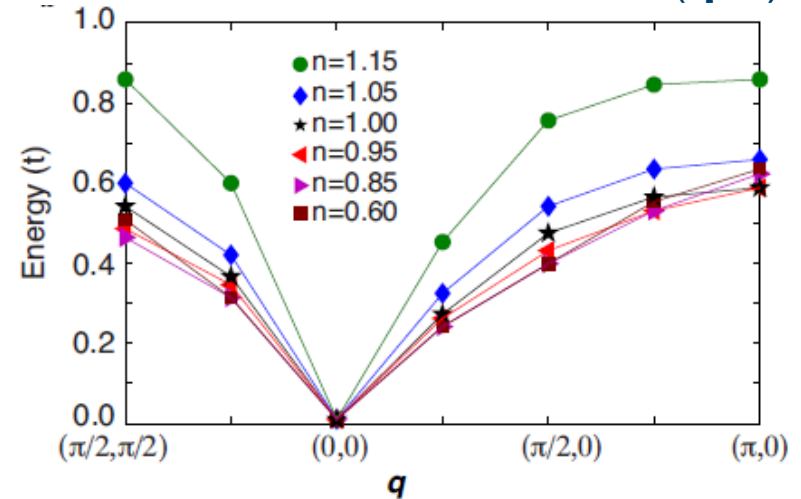


Doping dependence in exp. and theory



Single band Hubbard model in a 12-site cluster

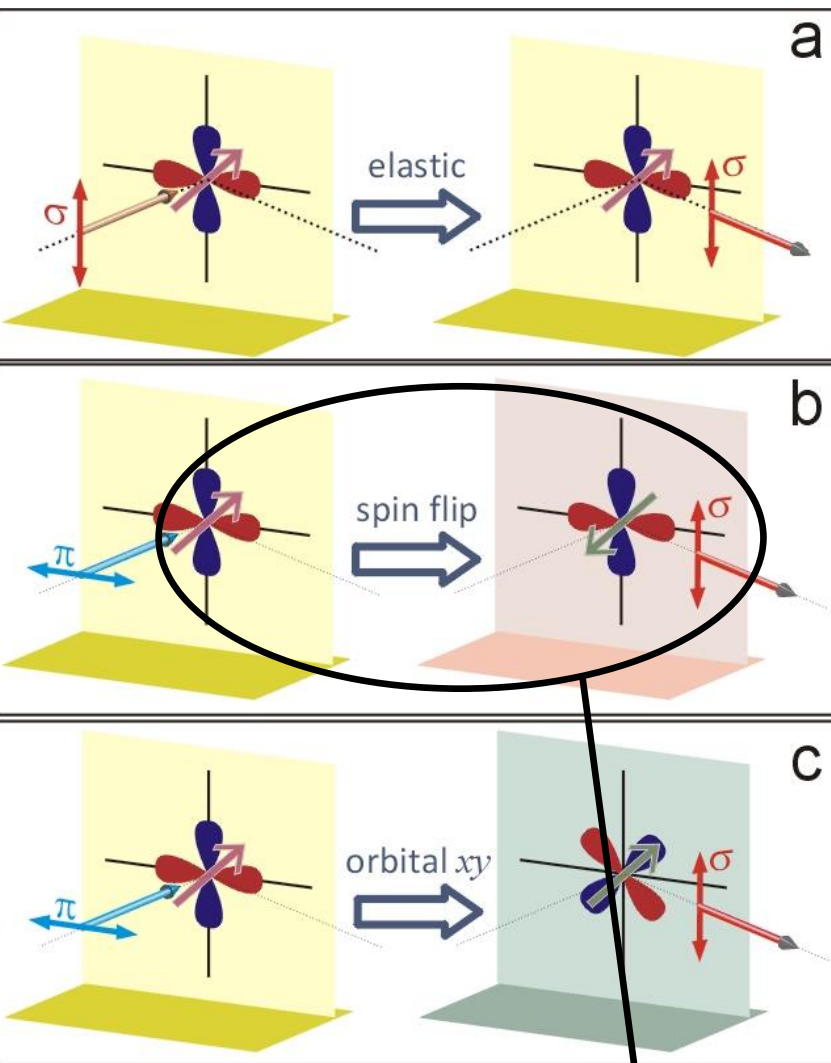
DQMC simulations used for $S(\mathbf{q}, \omega)$



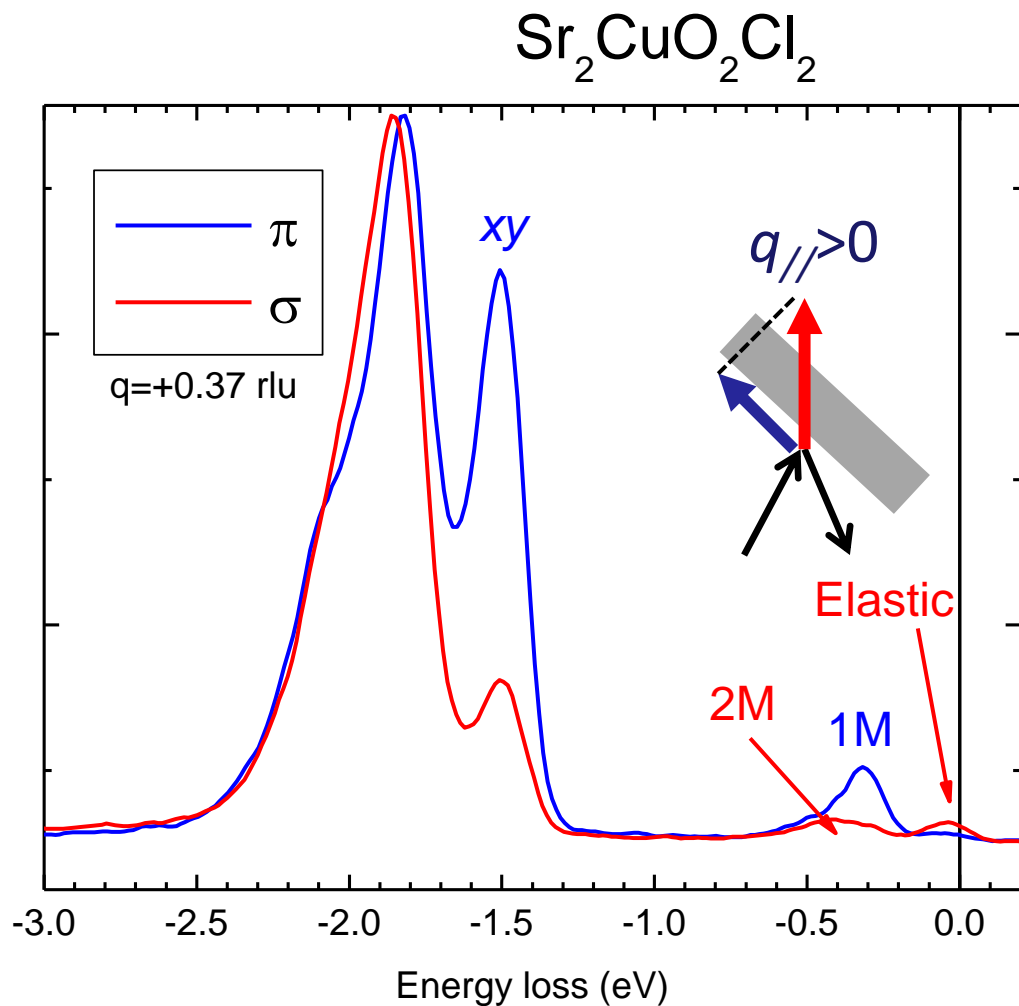
C. J. Jia, E. A. Nowadnick, K. Wohlfield, Y. F. Kung, C.-C. Chen, S. Johnston, T. Tohyama, B. Moritz & T. P. Devereaux, Nat. Comm. 5, 3314 (2014)

G. Dellea, M. Minola, C. Mazzoli, L. Braicovich, A. Galdi, P. Orgiani, L. Maritato, D. Di Castro, A. Tebano, G. Balestrino, C. Aruta, M. Moretti Sala, C. Jia, B. Moritz, T. Devereaux, N. B. Brookes, D.G. Schlom and G. Ghiringhelli, unpublished

Polarization dep. of Cu L₃ RIXS intensity

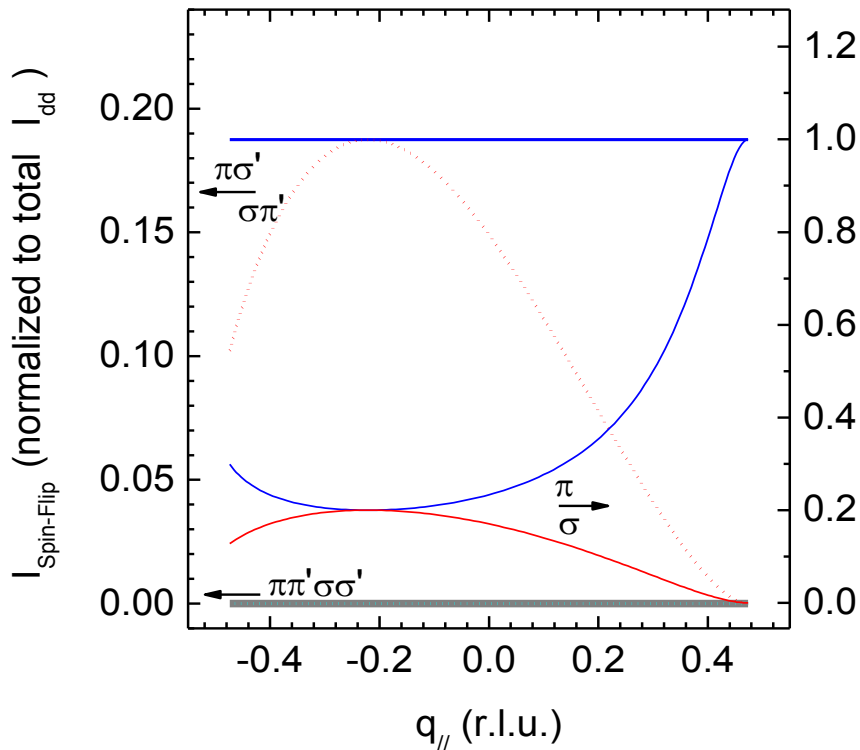


Crossed polarizations

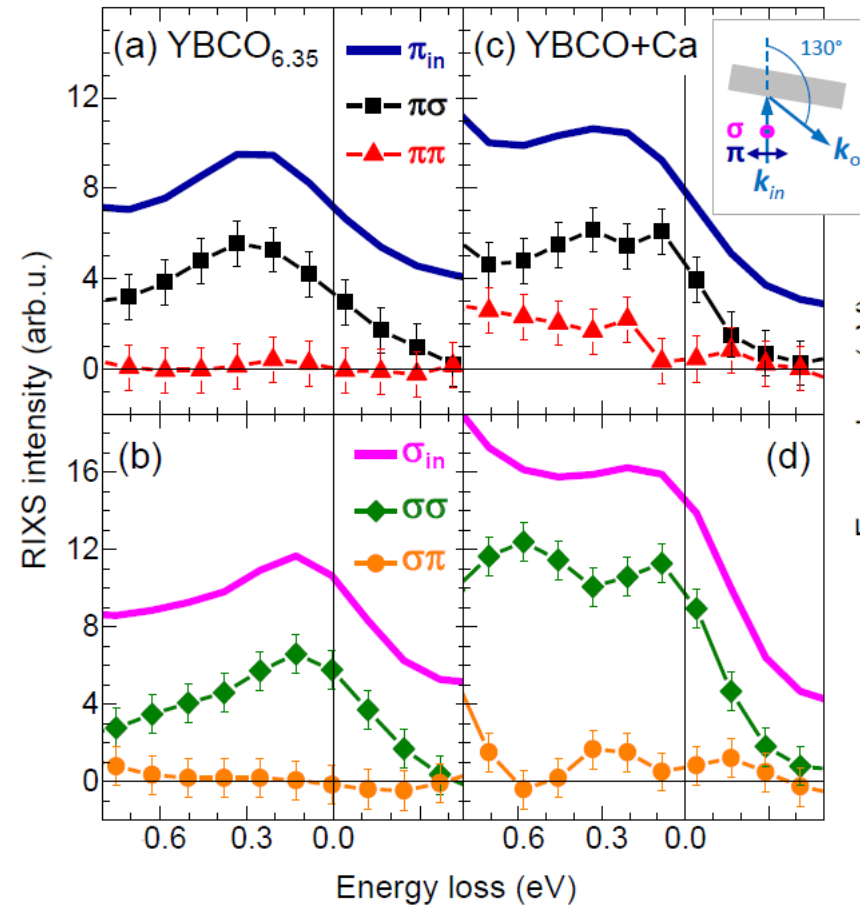


The spin-flip cross section in doped compounds

Single ion X-sections with full polarization control: only crossed polarization can give SF

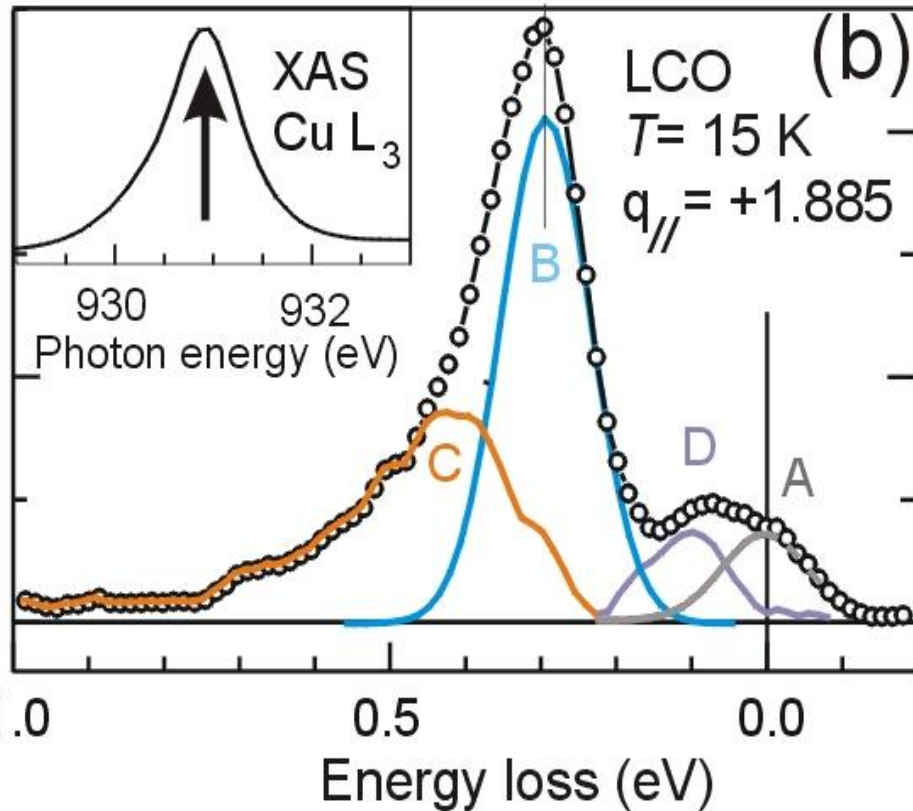


Relative spin-flip fraction
in non-dd channel

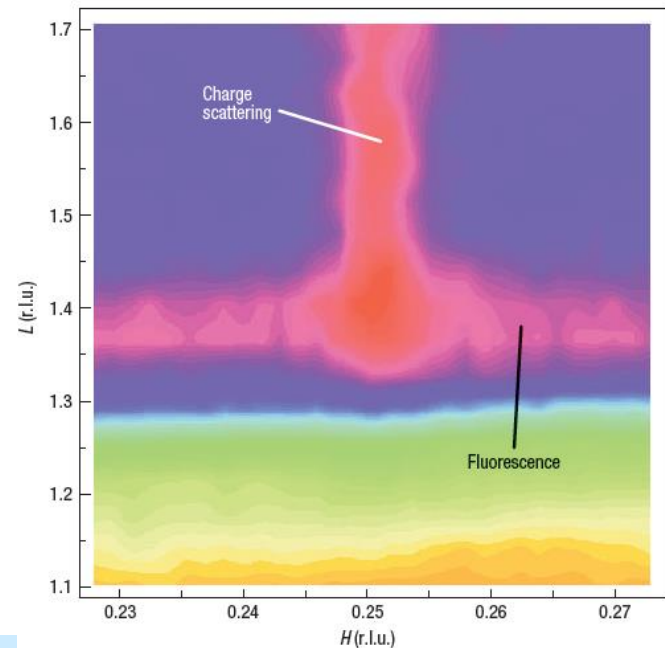


Polarimeter on AXES@ID08:
ionic selection rules are
confirmed for UD and OD
YBCO

How about the elastic peak in RIXS?



The elastic peak is usually small at Cu L_3 , and in principle the elastic intensity should all be in the Bragg peaks, i.e. in what is usually measured by RIXS, without energy resolution...



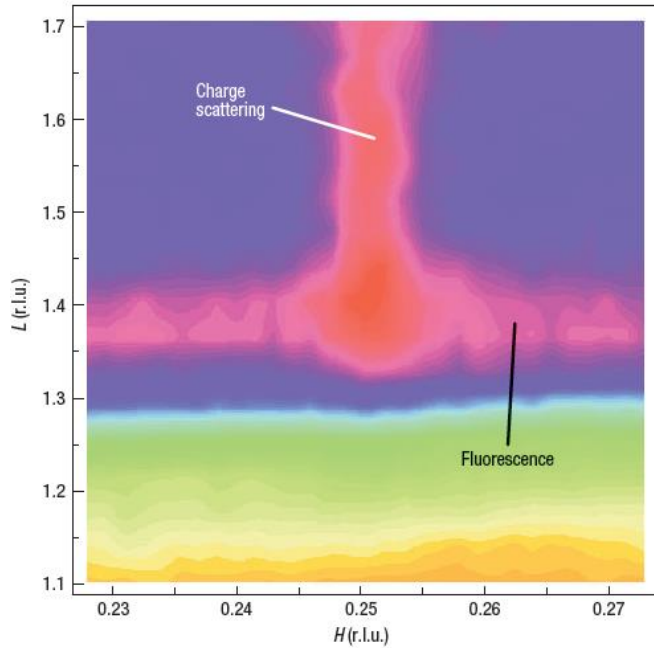
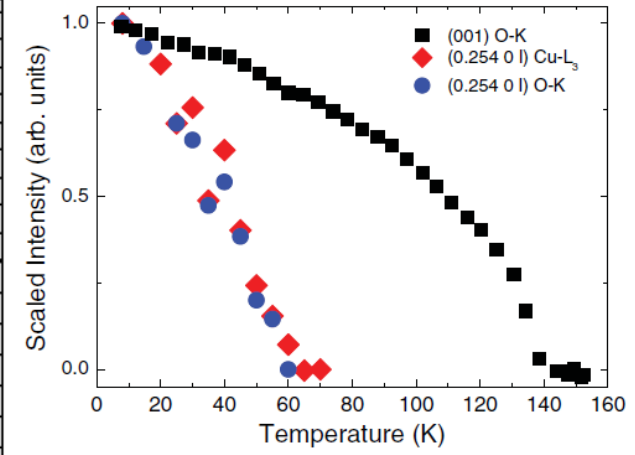
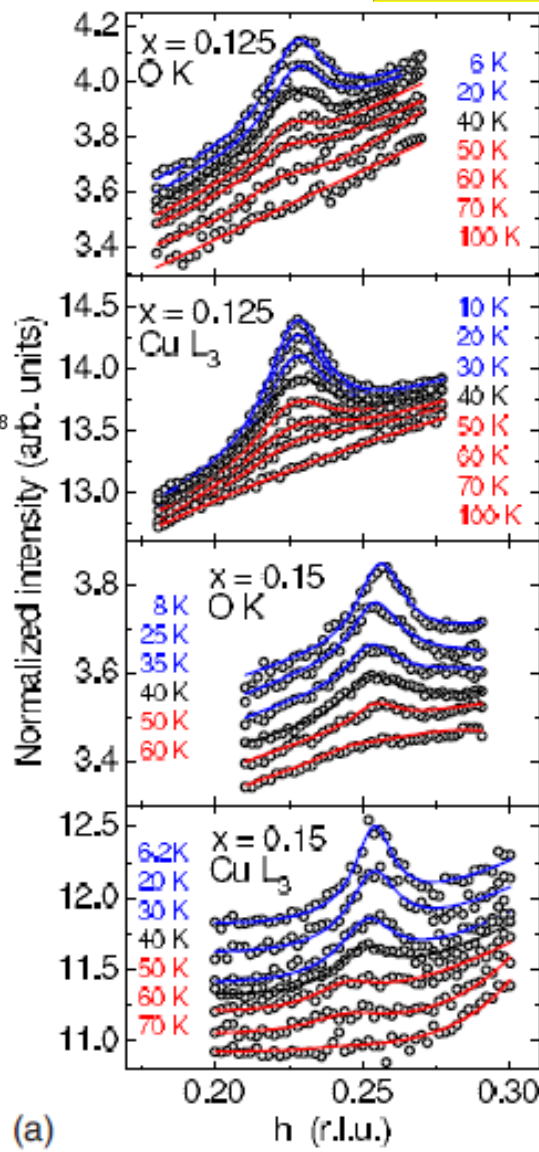
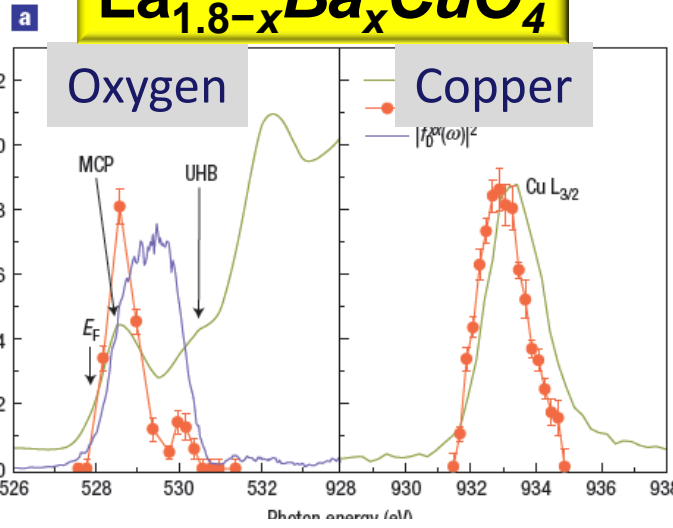
L. Braicovich, et al PRL **104** 077002 (2010)

P. Abbamonte et al, Nat. Phys. **1**, 155 (2005)

Cu L₃ RXS from stripes in striped cuprates

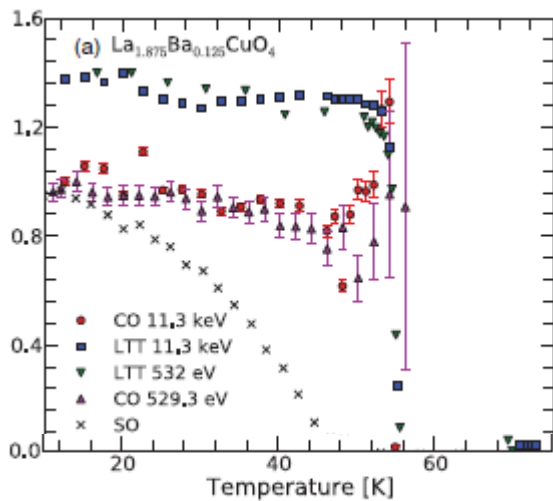
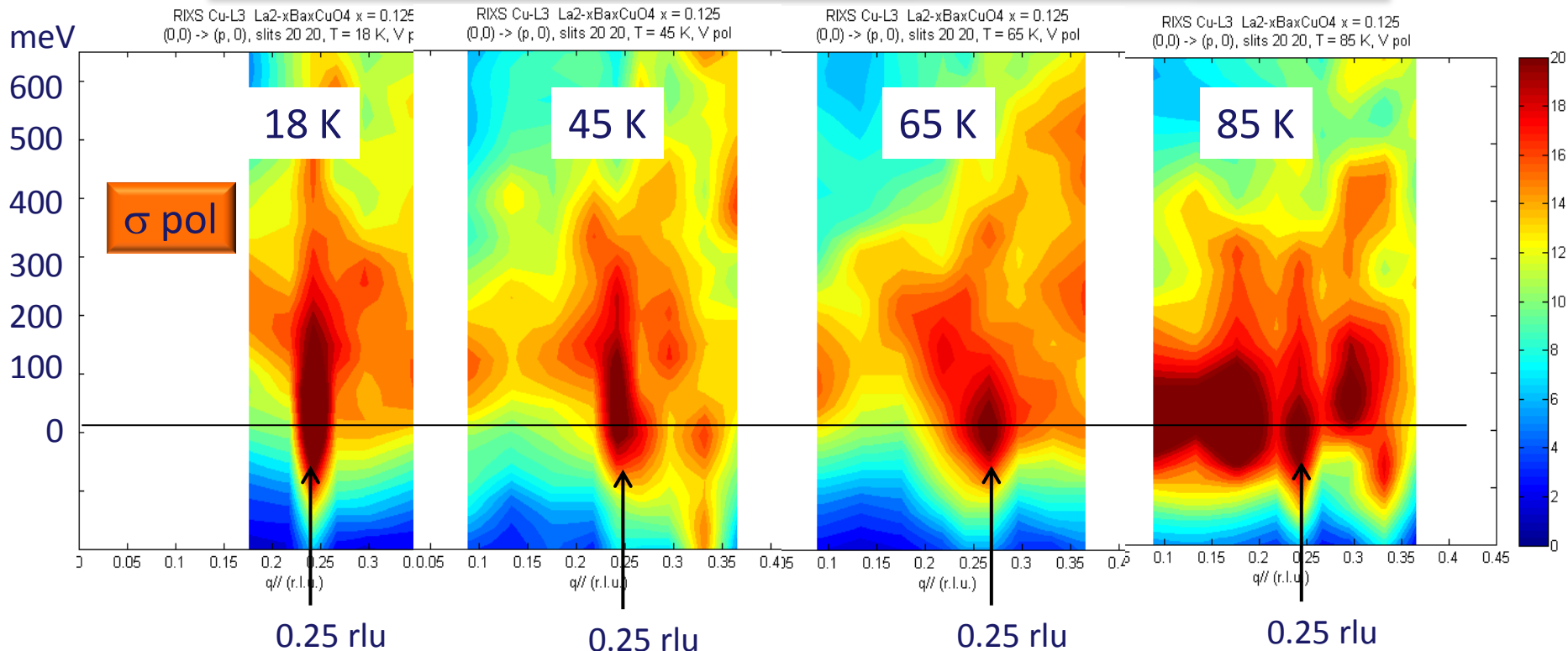
La_{1.8-x}Ba_xCuO₄

La_{1.8-x}Eu_{0.2}Sr_xCuO₄



J. Fink et al, Phys Rev B 79, 100502 (2009); 83 092503 (2011)

Cu L₃ RIXS of LBCO

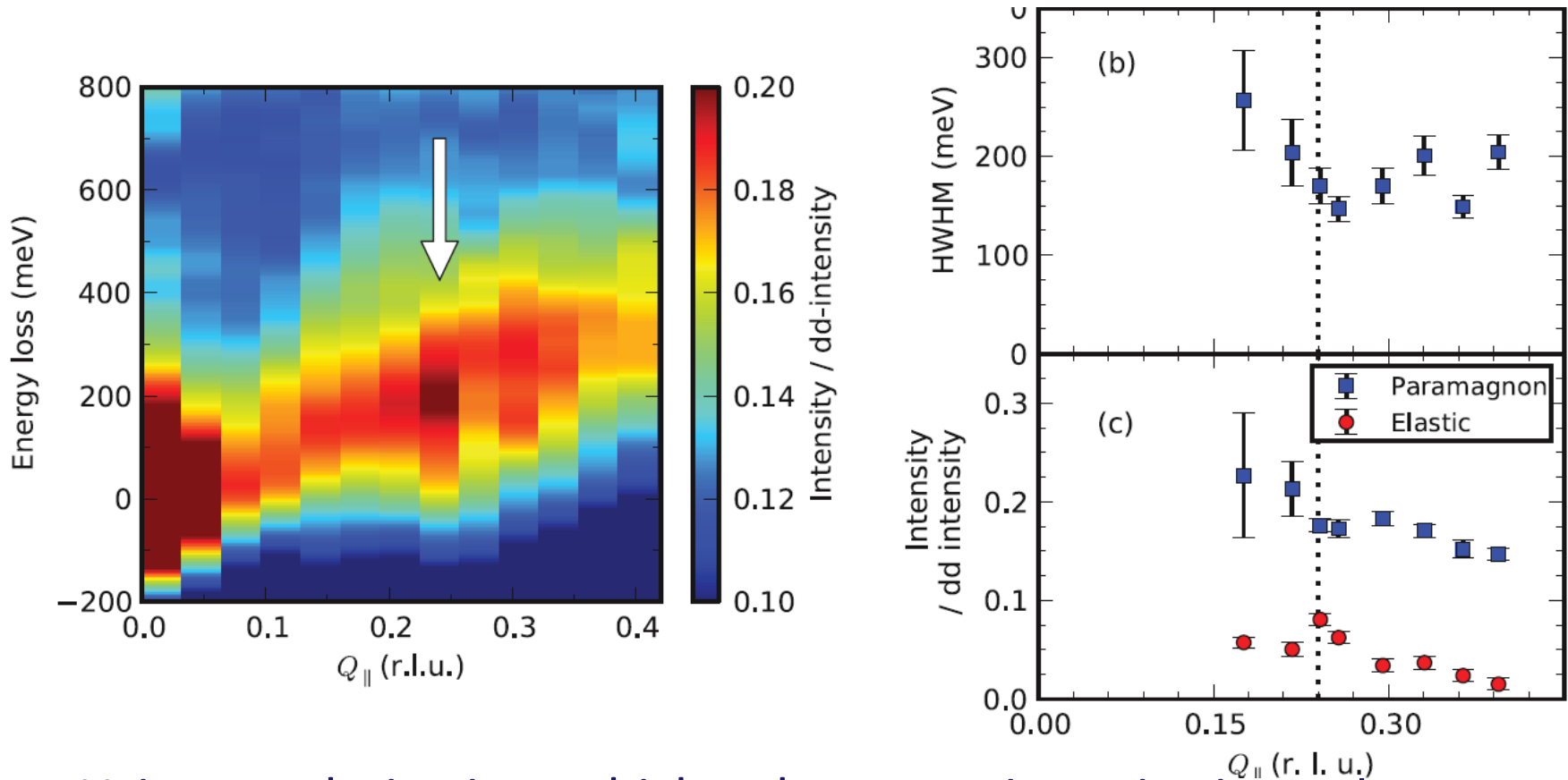


G. Dellea, M.P.M. Dean, M. Minola, N. B. Brookes, M. Le Tacon, S.B. Wilkins, L. Braicovich, J.P. Hill, G. Ghiringhelli, et al
unpublished

The charge ordering peak persists above T_{struct}

S.B: Wilkins et al, Phys Rev B 84, 145111 (2011)

Cu L₃ RIXS of LBCO, x=0.125 (striped)



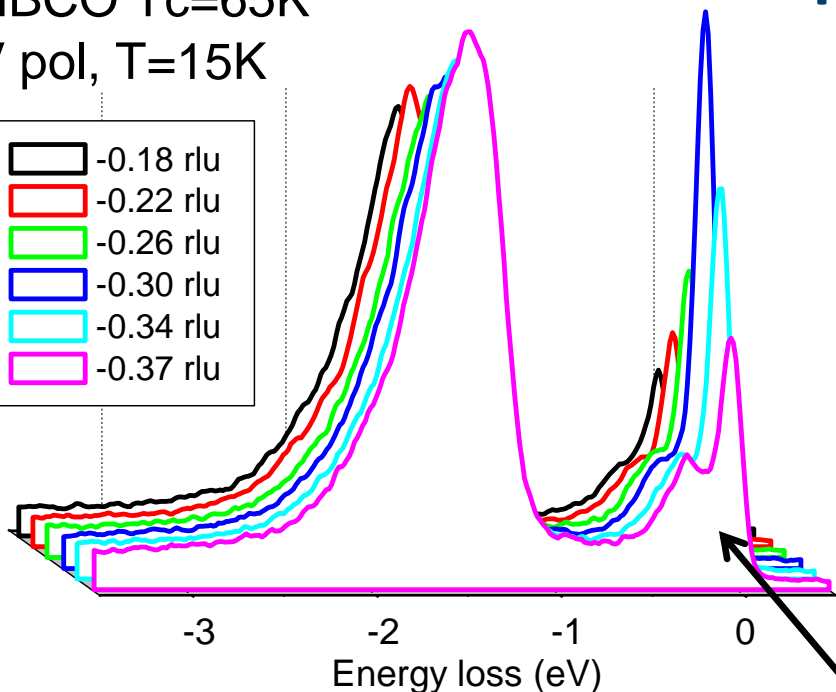
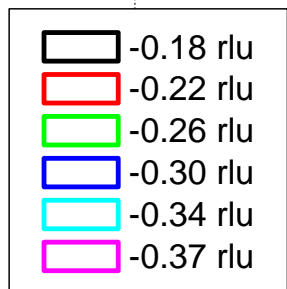
Using π polarization, which enhances spin excitations, the charge ordering wave vector remains significant. However we see no indications of spin order peaks.

Spin excitation dispersion is visibly modified by stripes.

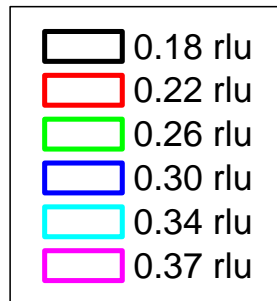
NdBa₂Cu₃O_{6+y}: elastic peak enhancement around 0.3 rlu

NBCO T_c=65K

V pol, T=15K

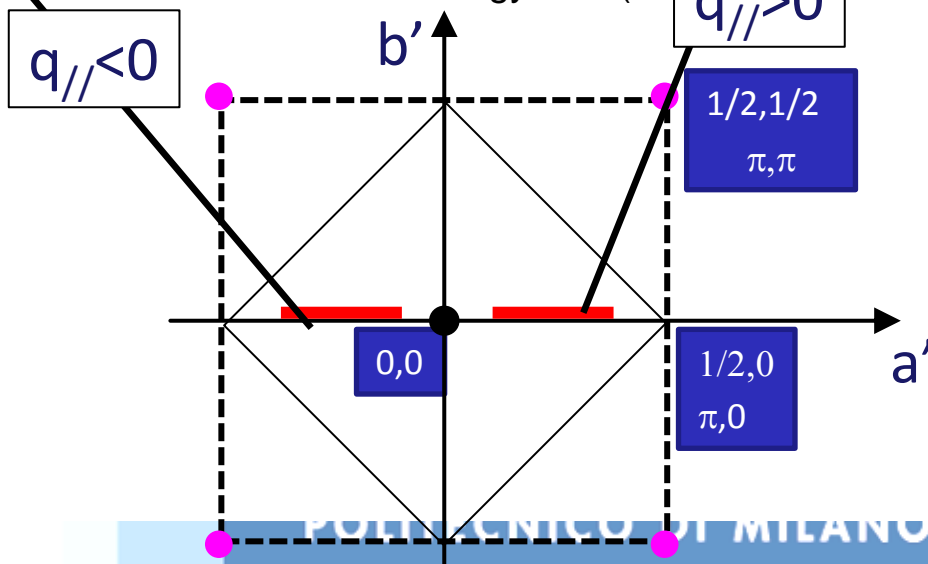
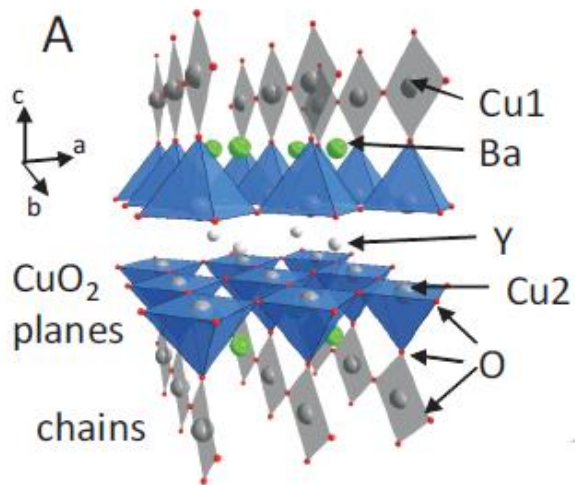
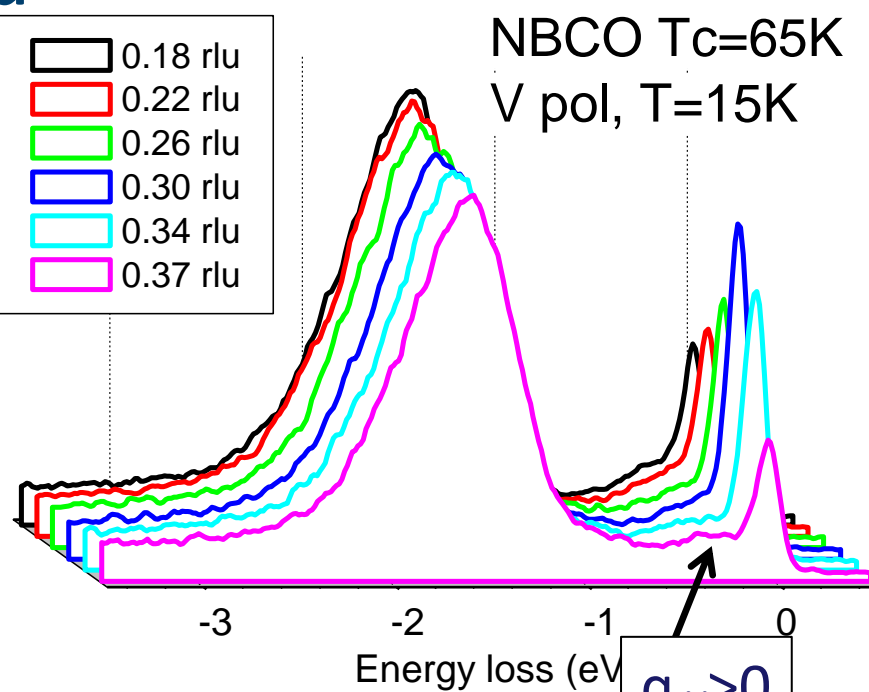


rlu

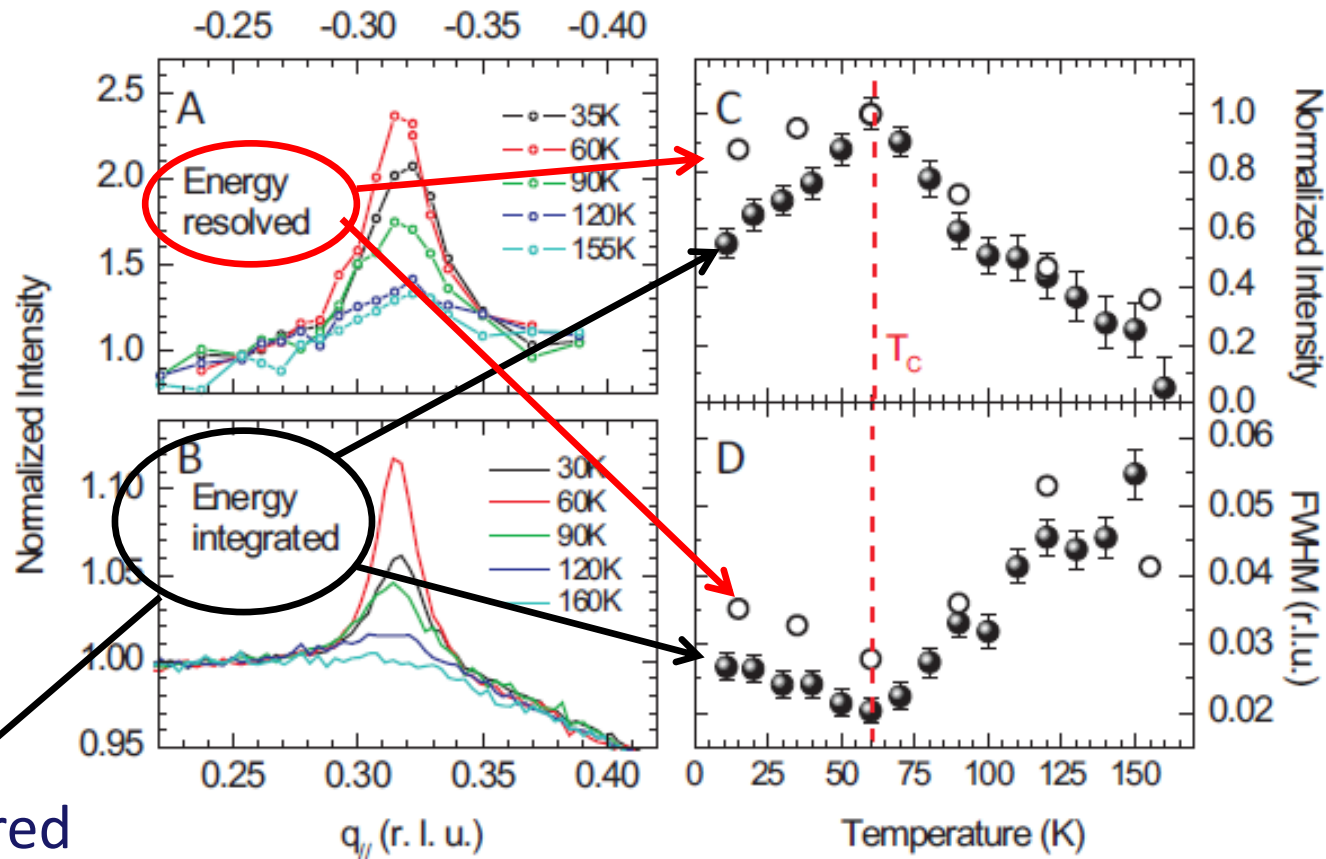


NBCO T_c=65K

V pol, T=15K



T dependence



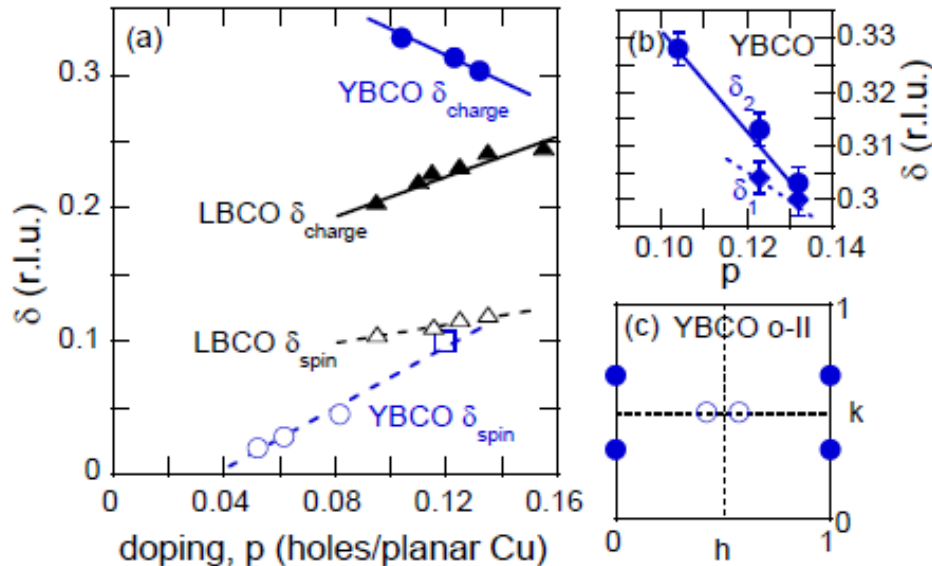
Measured
at Bessy

Max intensity at T_c : CDW competes with SC

YBCO: doping dependence

Direct observation of charge density wave order at zero magnetic field in ortho-II $\text{YBa}_2\text{Cu}_3\text{O}_{6.54}$

E. Blackburn,¹ J. Chang,^{2,3,*} M. Hücker,⁴ A. T. Holmes,¹ N. B. Christensen,⁵ Ruixing Liang,^{6,7}
D. A. Bonn,^{6,7} W. N. Hardy,^{6,7} M. v. Zimmermann,⁸ E. M. Forgan,¹ and S. M. Hayden⁹



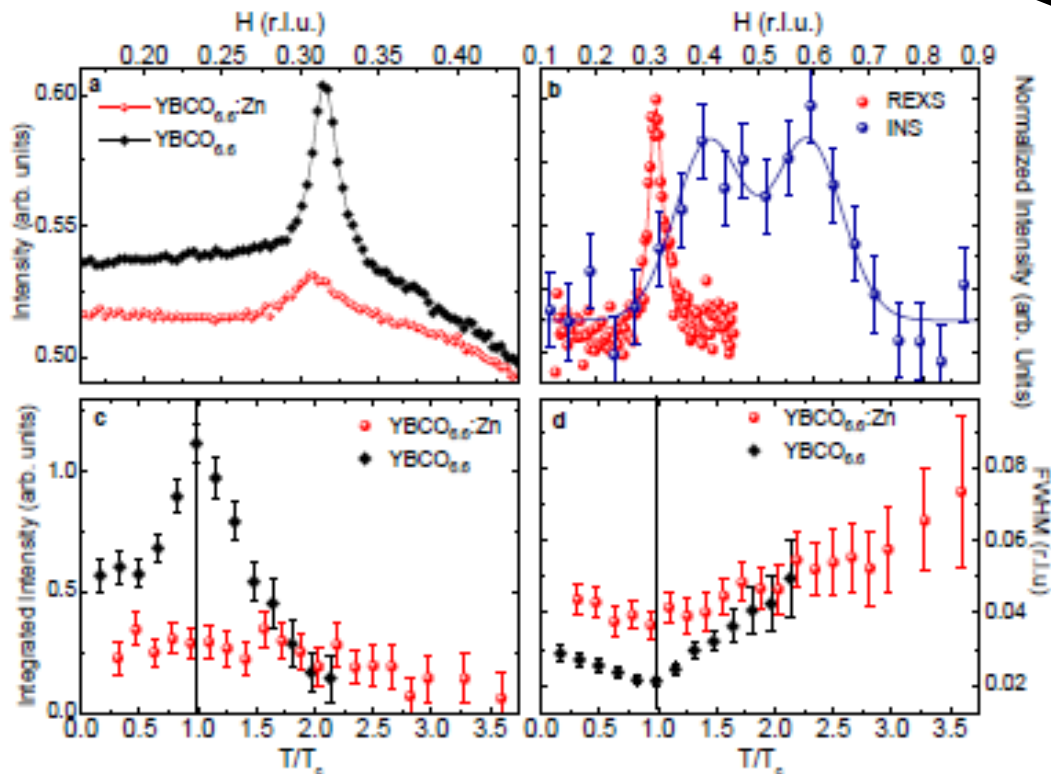
y in YBCO	Oxygen ordering	Doping level p	T_c (K)	T_{CDW} (K)
6.54	o-II	0.104	58	155(10)
6.67	o-VIII	0.123	67	140(10)
6.75	o-III	0.132	74	140(10)

arXiv:1212.3836v1

... and independence of charge and spin ordering WV

Three-phase competition in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$

S. Blanco-Canosa,¹ A. Frano,^{1,2} T. Loew,¹ Y. Lu,¹ J. Porras,¹ G. Ghiringhelli,³ M. Minola,³ C. Mazzoli,³ L. Braicovich,³ E. Schierle,² E. Weschke,² M. Le Tacon,¹ and B. Keimer¹



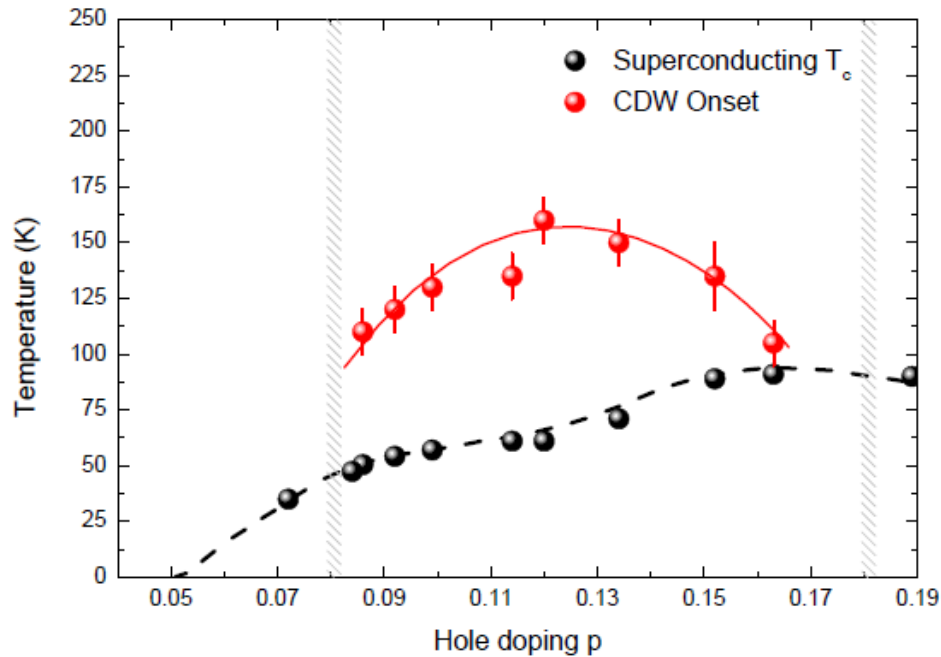
Charge ordering
Spin ordering
Superconductivity

YBCO6.6

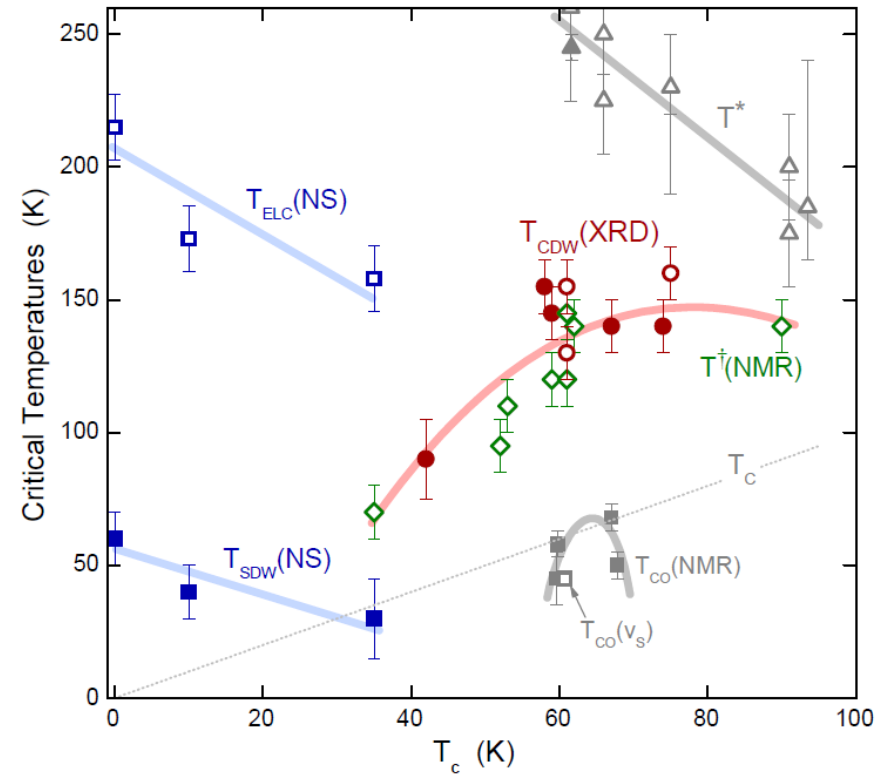
Blanco-Canosa, A. Frano, T. Loew, Y. Lu, J. Porras, G. Ghiringhelli, M. Minola, C. Mazzoli, L. Braicovich, E. Schierle, E. Weschke, M. Le Tacon, and B. Keimer, *Phys. Rev. Lett.* **110**, 187001 (2013)

tures. Rather than forming a coherent spin- and charge-modulated “striped” state, as in the 214 system, [3, 10–14] spin and charge order are strongly competing in $\text{YBCO}_{6+\delta}$. Stripe order is thus not a universal feature of the underdoped cuprates. We further show that

YBCO doping dependence, up to optimal doping



S. Blanco-Canosa, A. Frano, E. Schierle, J. Porras, T. Loew, M. Minola, M. Bluschke, E. Weschke, B. Keimer, and M. Le Tacon, arXiv 1406.1595v1



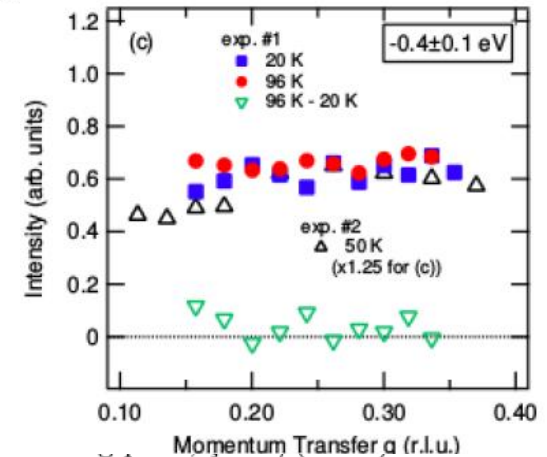
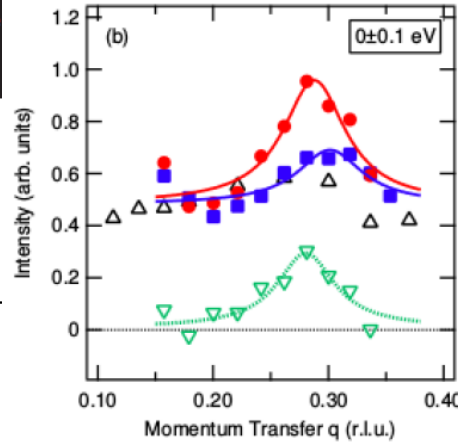
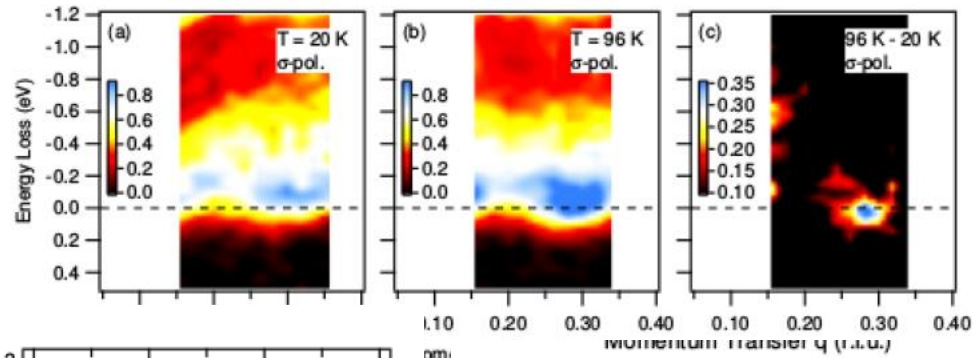
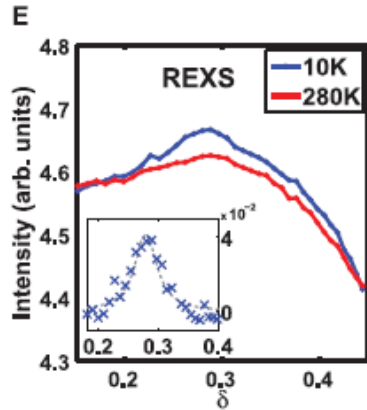
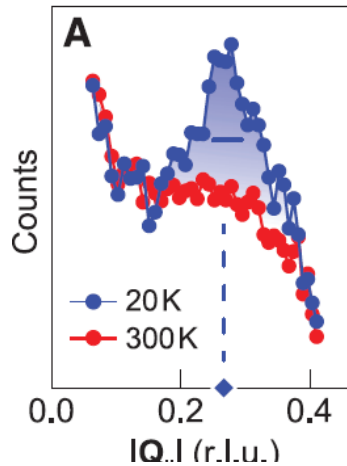
M. Hücker, N. B. Christensen, A. T. Holmes, E. Blackburn, M. Forgan, Ruixing Liang, D. A. Bonn, W. N. Hardy, O. Gutowski, M. v. Zimmermann, S. M. Hayden, and J. Chang, arXiv:1405.7001v1

UD Bi2201, Bi2212, Hg1201 and OPD Bi2212

Bi2201 and Bi2212 underdoped

Bi2212 optimally doped

REXS - UD15K

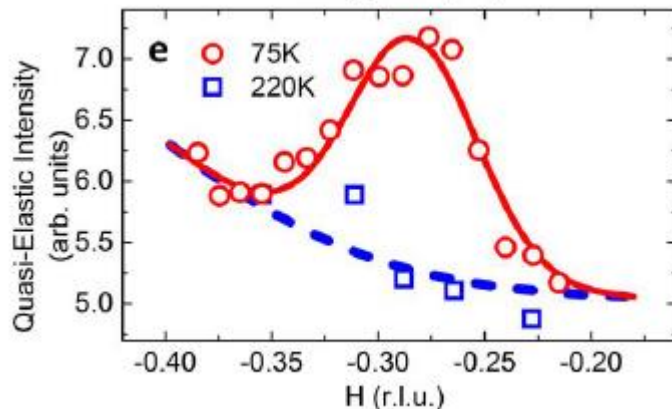


R. Comin et al, Science 343, 390 (2014);

Eduardo H. da Silva Neto et al, Science 343, 393 (2014)

Hg1201 underdoped

energy loss (eV)

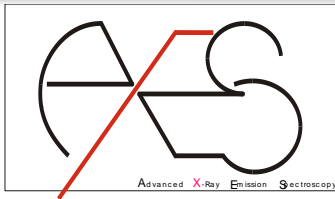


Sample	p	T_c	$q_{ }$ (r.l.u.)	ξ (Å)	refs.
Bi2201	0.115	15	0.265	26	[16]
Bi2201	0.130	22	0.257	23	[16]
Bi2201	0.145	30	0.243	21	[16]
Bi2212	0.09	45	0.30	24	[15]
Bi2212	0.160	98	0.28	<24 (at T_c)	this work
YBCO	0.115	61	0.32	~60 (at T_c)	[8, 10]
LBCO	0.125	2.5	0.236	~200	[4, 6-8]
LBCO	0.155	30	0.244	~240 (15 - 25 K)	[4, 6-8]

W. Tabis et al, Nat. Comm. In press (2014)

M. Hashimoto, G. Ghiringhelli et al, PRB Rapid 89 220511 (2014)

AXES (ESRF, ID08) and SAXES (SLS, ADRESS)



Since 1994: AXES at beam line ID08 of the ESRF

$L = 2.2 \text{ m}$

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

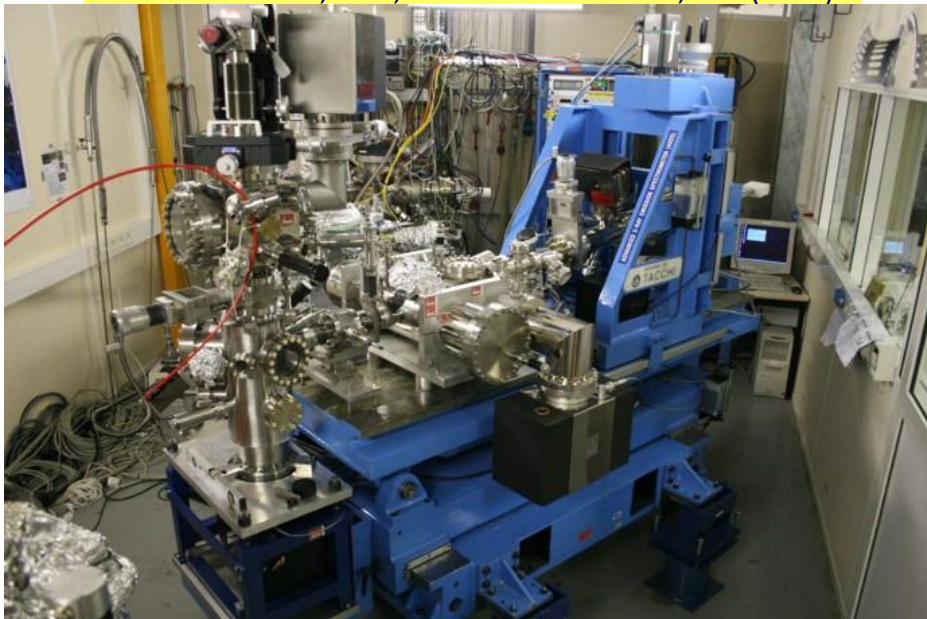
$L = 5.0 \text{ m}$

Design: $E/\Delta E = 12,000$ at Cu L_3

2008: $E/\Delta E = 10,000$ at Cu L_3

C. Dallera *et al.* J. Synchrotron Radiat. **3**, 231 (1996)
G. Ghiringhelli *et al.*, Rev. Sci. Instrum. **69**, 1610 (1998)
M. Dinardo *et al.*, Nucl. Instrum. Meth A **570**, 176 (2007)

G. Ghiringhelli, et al Rev. Sci. Instrum. **77**, 113108 (2006)
V. Strocov, T. Schmitt, L. Patthey et al, J. Synch. Rad., **17**, 631 (2010).

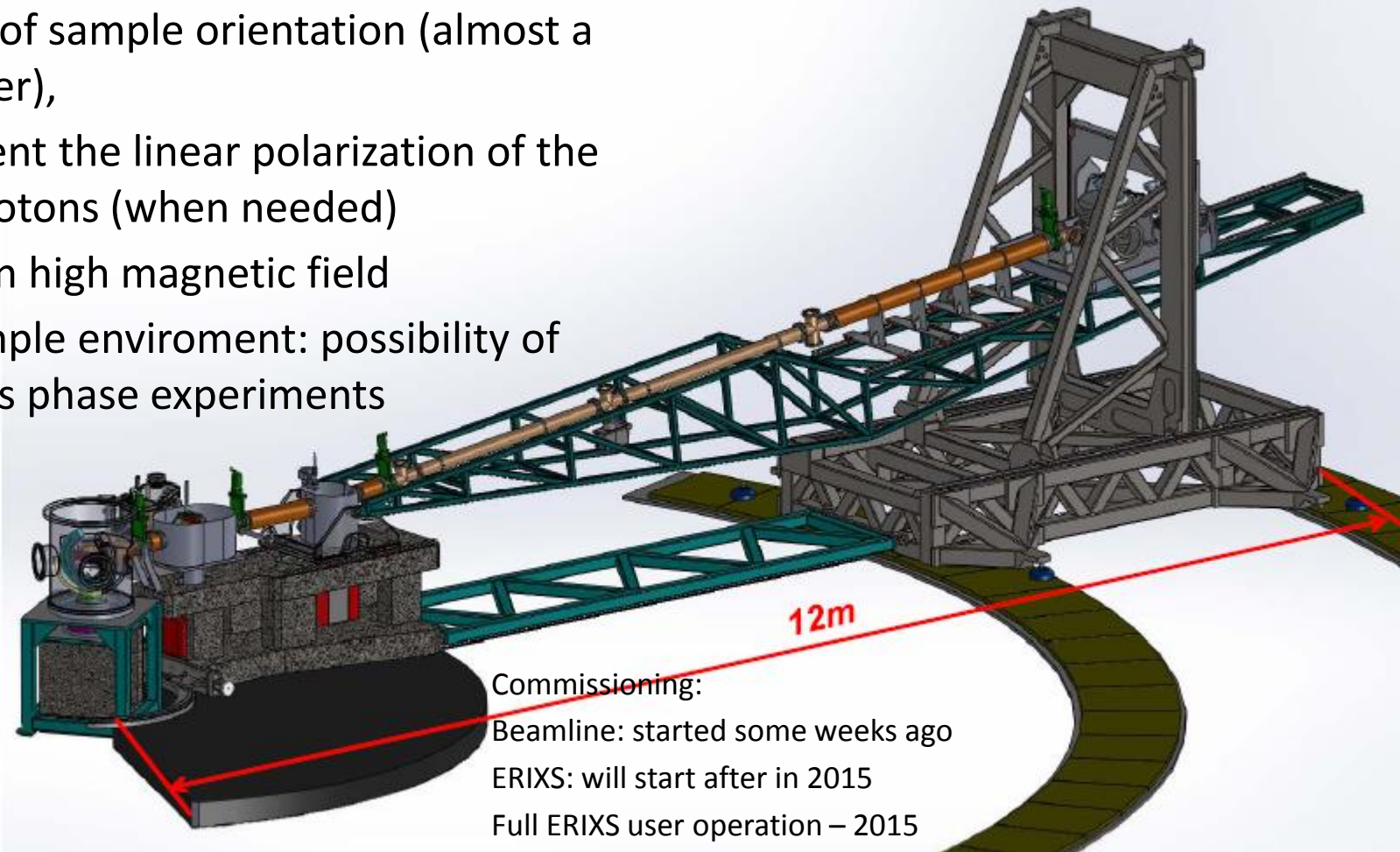


ERIXS spectrometer at the new ID32

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
- continuous 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 environment: possibility of liquid and gas phase experiments

ESRF Upgrade programme,
N.B. Brookes, F. Yakhou, GG



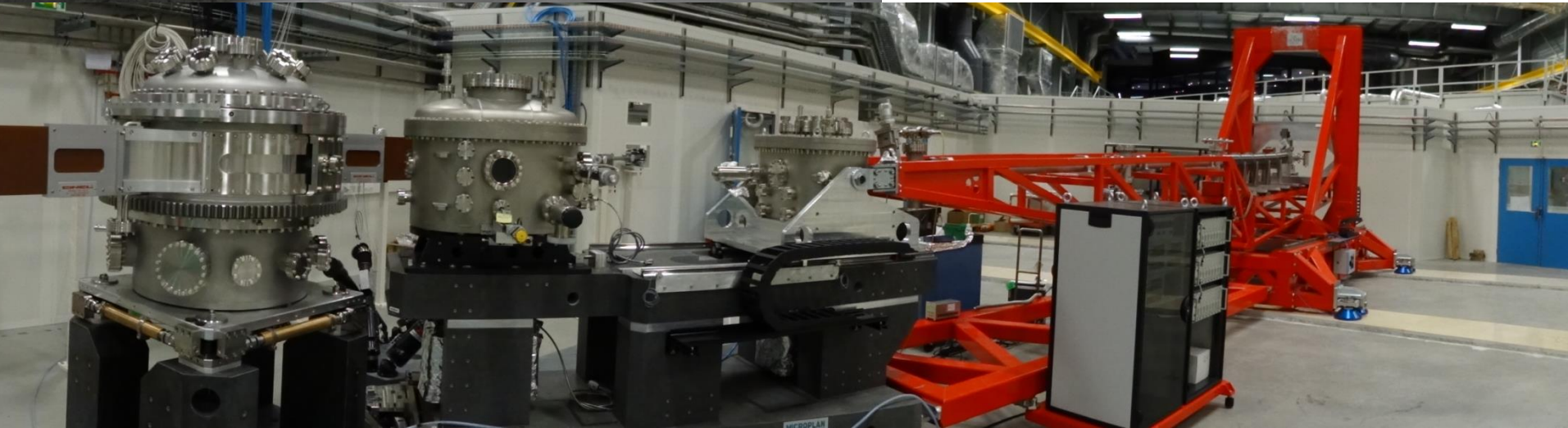
Commissioning:

Beamline: started some weeks ago

ERIXS: will start after in 2015

Full ERIXS user operation – 2015

ERIXS, 21/10/2014



The European Users Consortium Heisenberg RIXS at XFEL

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Simo Huotari, Oulu, Finland

Maurits W. Haverkort, Max-Planck-Institut für Festkörperforschung

Frank de Groot, Utrecht University

Stefan Eisebitt, Technische Universität Berlin

Andrea Cavalleri, CFEL Hamburg, Oxford U.

Marc Simon, Laboratoire Chimie-Physique-Matière et Rayonnement

Alexei Erko, Helmholtz-Zentrum Berlin

Alexander Föhlisch, Helmholtz-Zentrum Berlin and Uni Potsdam

Recent expression of interest by
STFC and UK scientific
community

Working Group DESY/HZB/POLIMI/XFEL:

A. Foehlich

Giacomo Ghiringhelli

Tim Laarmann

Simone Techert

Andreas Scherz

Wilfried Wurth

XFEL SASE3: Andreas Scherz, Serguei Molodtsov

hRIXS: RIXS at the European XFEL

5-6 m scattering arm

Continuous rotation in backscattering ($2\theta = 60^\circ - 150^\circ$)

Possibility of full forward scattering ($2\theta = 0^\circ - 20^\circ$)

Up to 20,000 resolving power

TR-RIXS non-linear RIXS

Conclusions

Cu L₃ RIXS tells us that:

- Magnetic excitations persist up to very OVD regime
- Their dependence on E_{in} indicate they are collective excitations, rather than SF particle-hole excitations
- Charge ordering in HTS is rather ubiquitous, but difficult to observe
- RXS can be used to learn more on CO, but some info can come only from XRD
- Spin-order modulations are even more difficult to detect with x-rays, but signatures might be found in the paramagnon dispersion measured by RIXS
- RIXS can probe the relevant phonons too: we will study them with higher resolution

Thanks