Summerschool – MPG-UBC-UTokyo Center

X-rays for the study of quantum materials

High resolution RIXS for the study of strongly-correlated and novel materials

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ACCADEMIA NAZIONALE DEI LINCEI

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SPIN

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Summary

RIXS: resonant inelastic x-ray scattering

1. From XAS to RIXS: a second order process
2. RIXS instrumentation
3. Orbital (*dd*) excitations
4. Magnetic excitations
5. Phonons and charge order
6. REXS: the elastic part of RIXS spectra
7. Time resolved RIXS

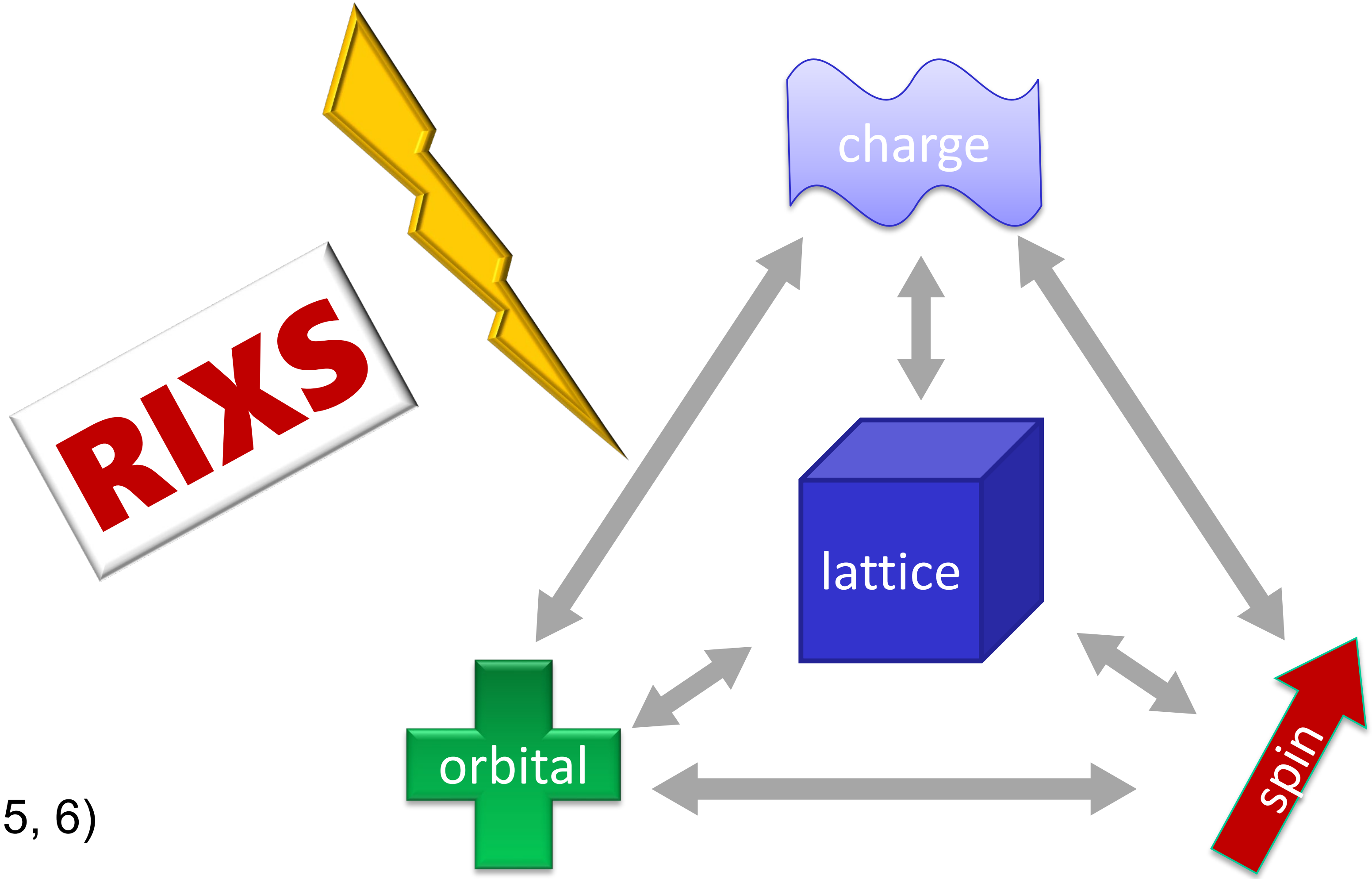
One probe for several degrees of freedom

1. Energy loss spectroscopy
2. Momentum resolution
3. Coupling to
    a. Charge
    b. Spin
    c. Orbital
    d. Lattice
4. Bulk sensitivity
5. Good energy resolution
6. Decent count rate

electrons (1, 2, 3, 5, 6)

neutrons (1, 2, 3b, 3d, 4, 5)

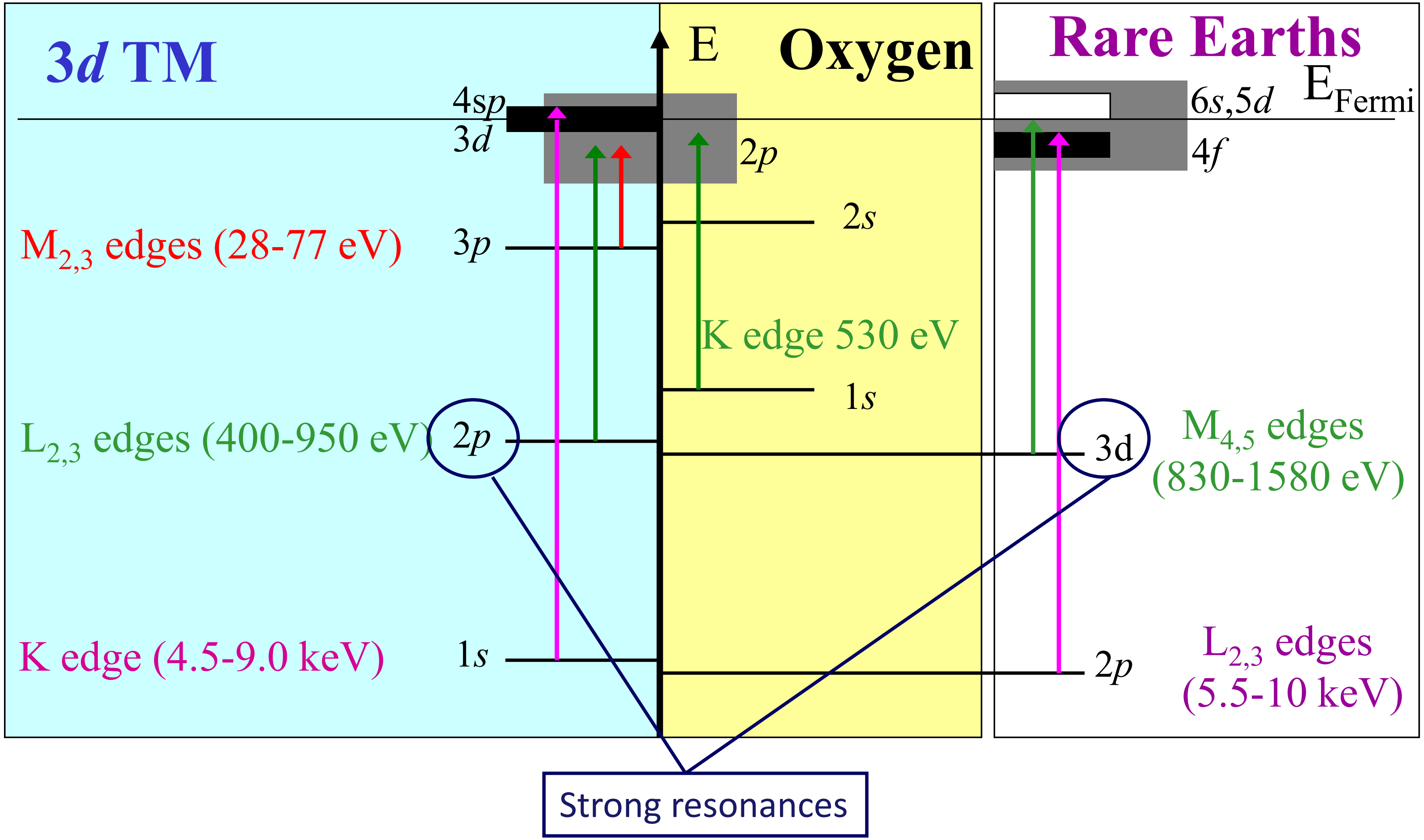
photons (1, 2, 3a,3c, 3d, 4, 5, 6)



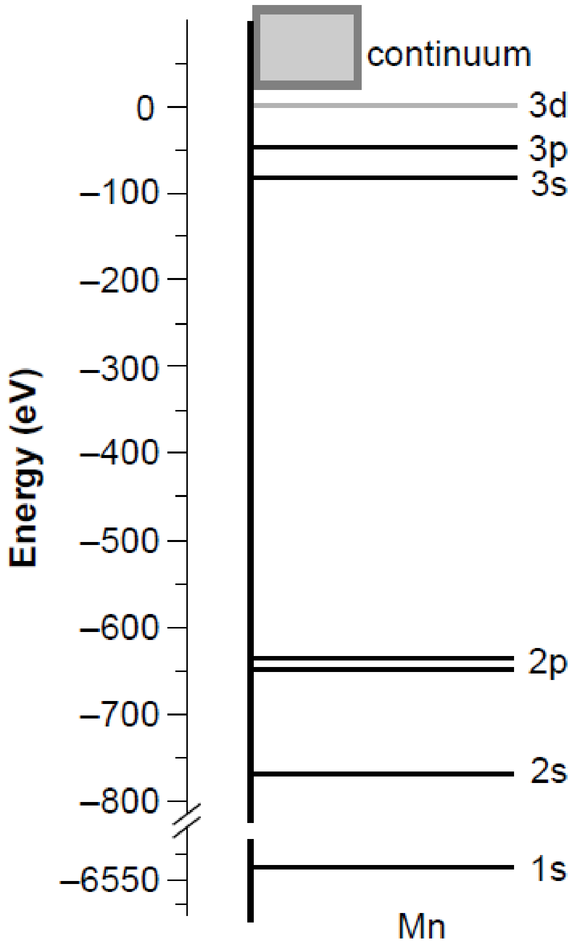
Part 1

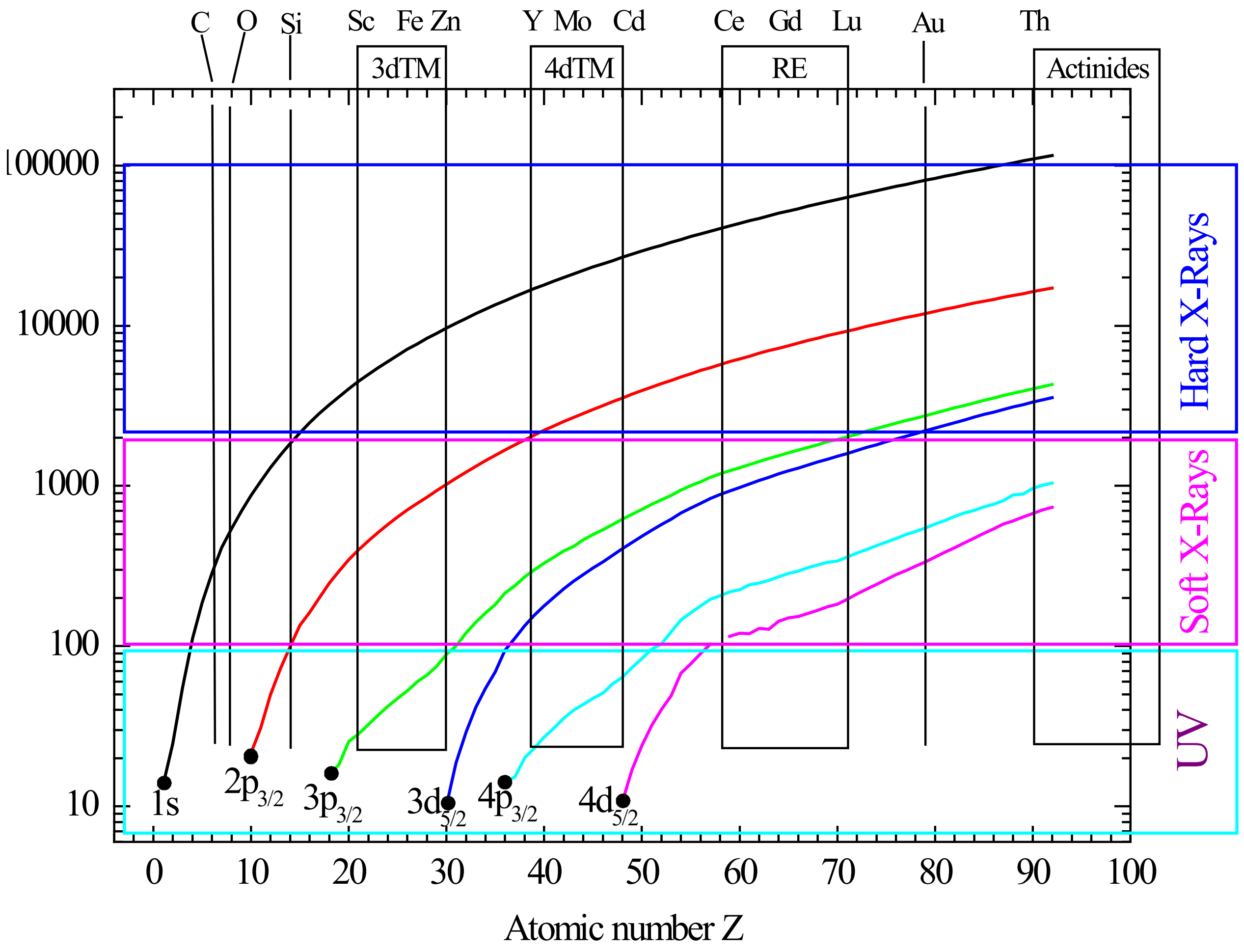
FROM XAS TO RIXS

Resonances in the XAS



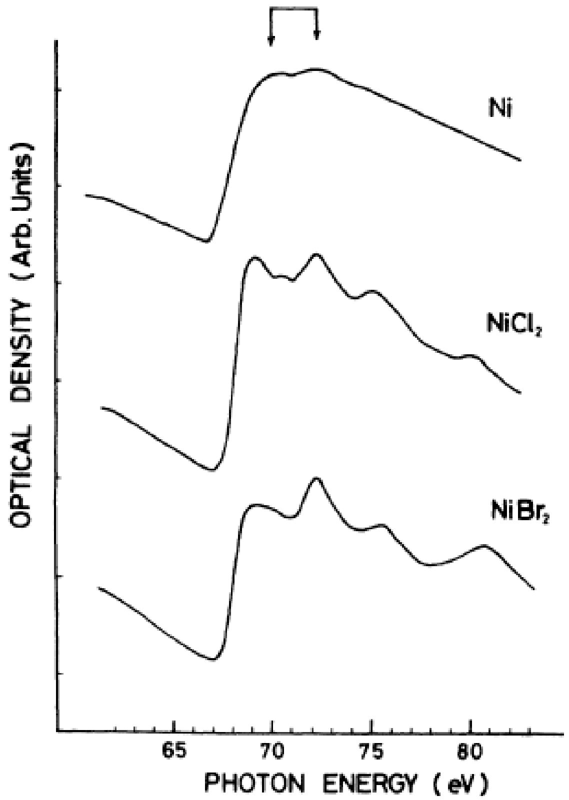
Core level binding energies and edges



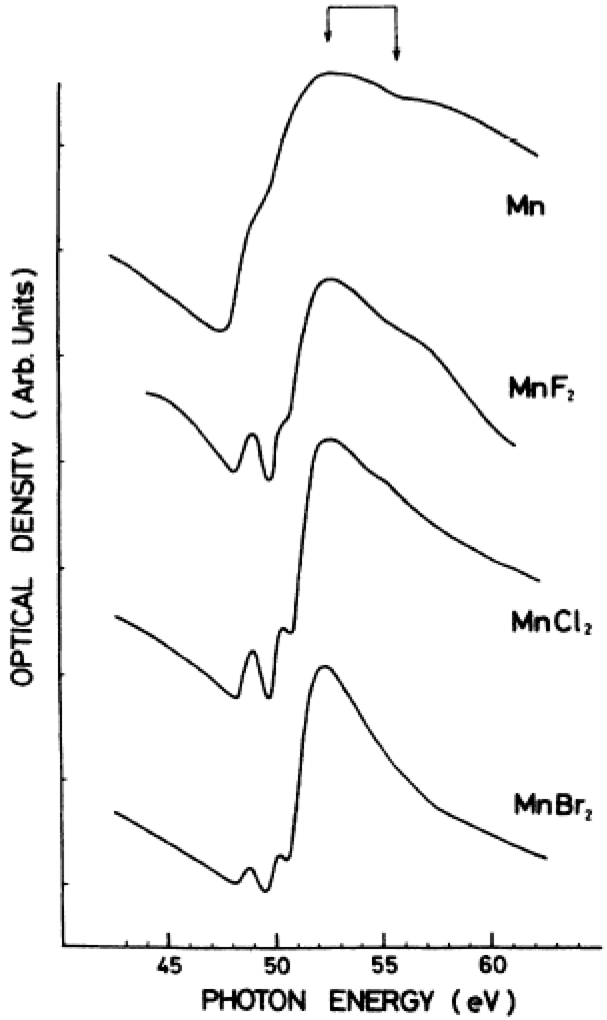


3*p*: $M_{2,3}$ edge XAS

Spin-Orbit splitting

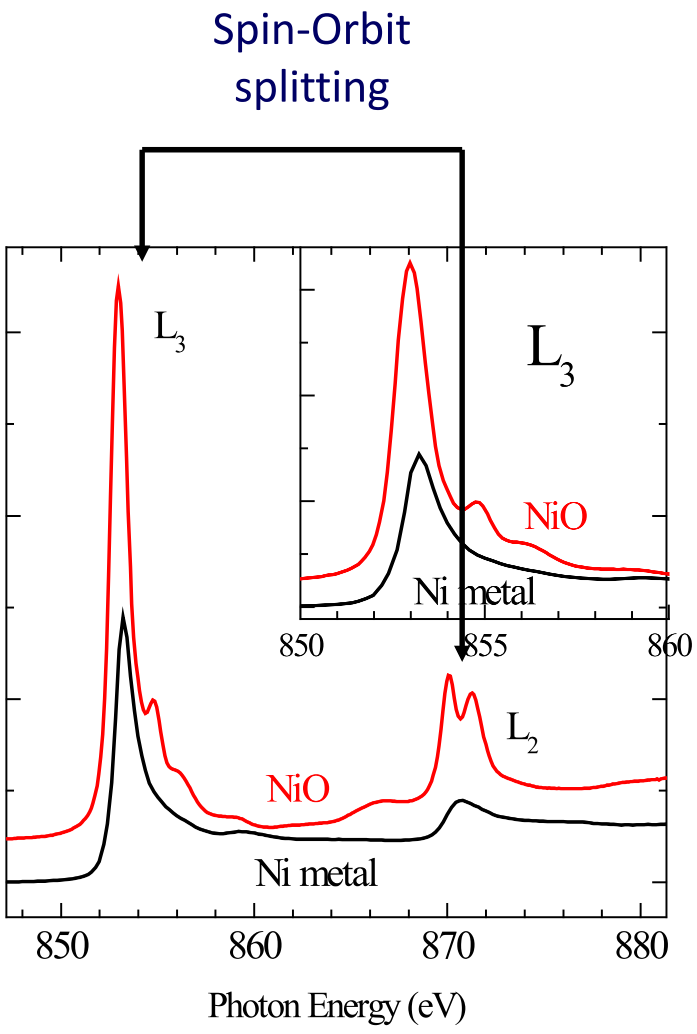


Spin-Orbit splitting

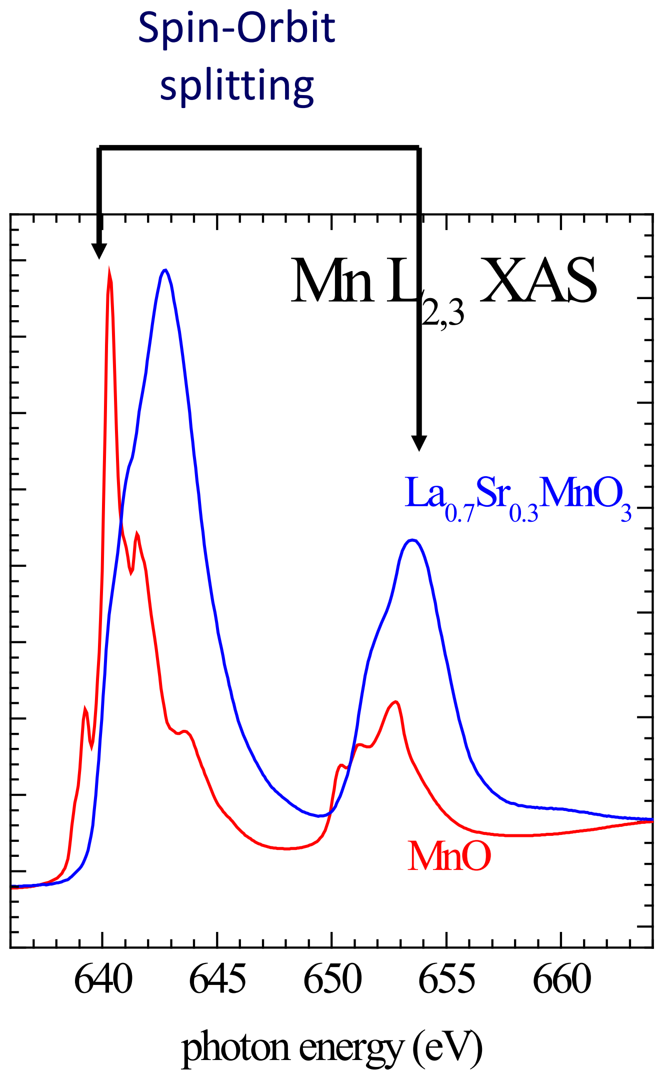


Source: S. Nakai, *et al* PRB **9**, 1870 (1974)

2*p*: $L_{2,3}$ edge XAS



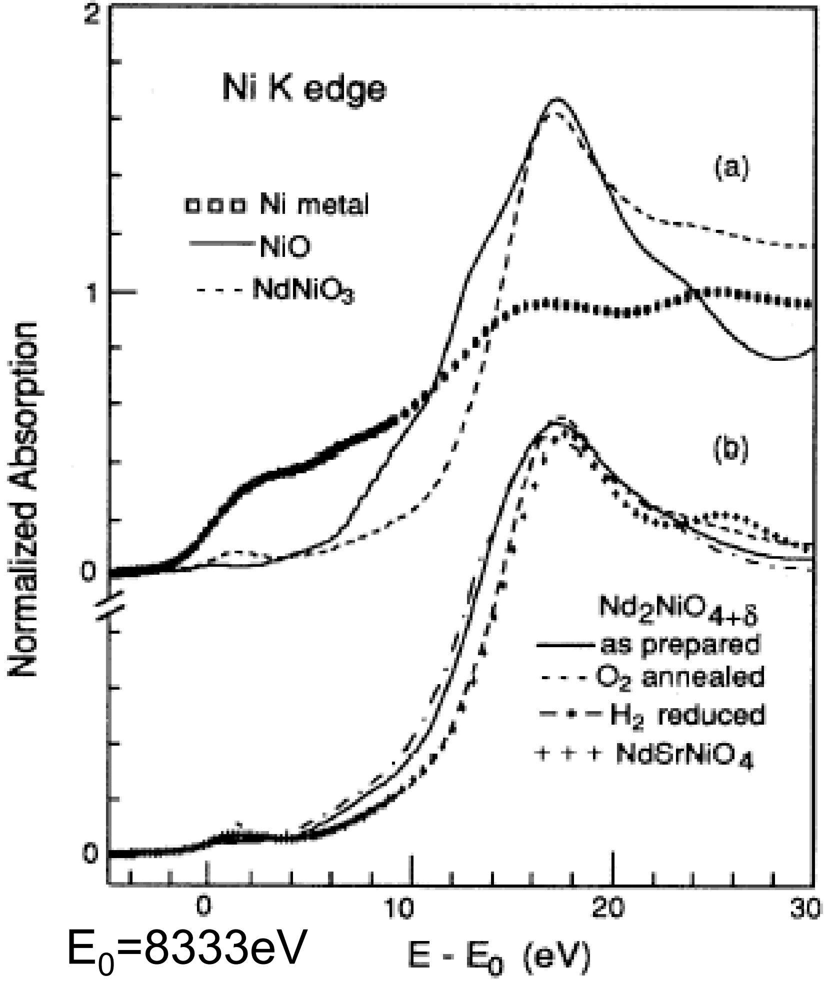
Source: G. Ghiringhelli, N.B. Brookes *et al* unpublished



Source: C. Aruta, G. Ghiringhelli *et al* unpublished

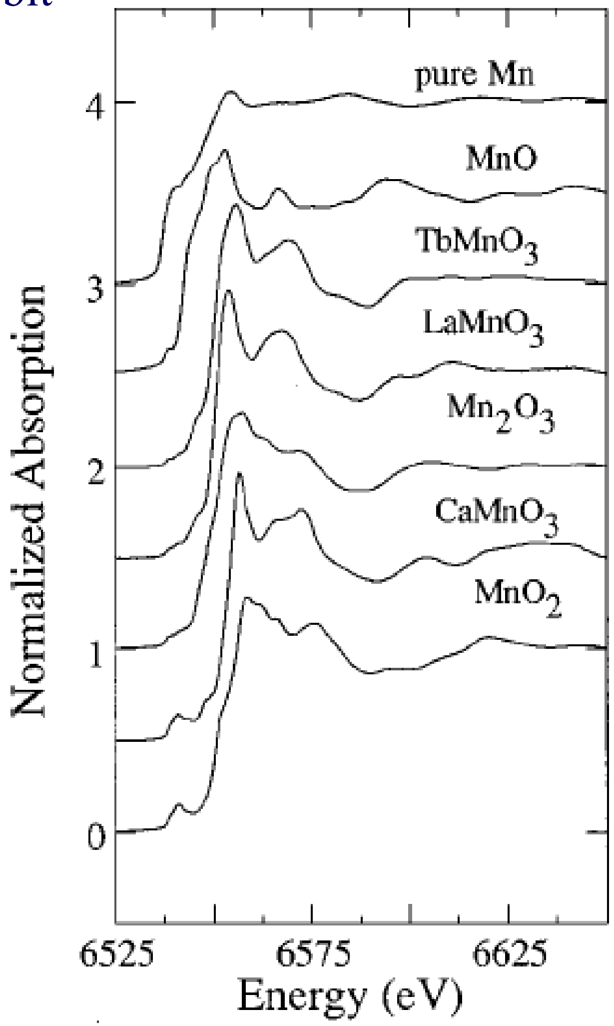
1*s*: Ni and Mn K edge XAS

NO Spin-Orbit splitting



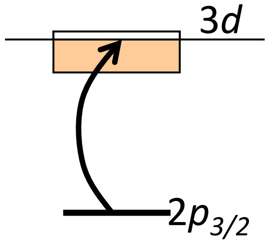
E_0=8333eV

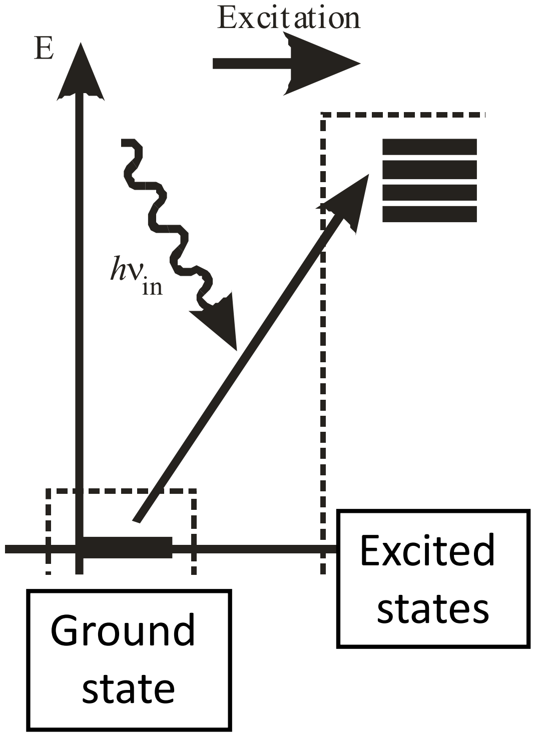
Source: Z. Tan *et al* Phys. Rev. B **47**, 12365 (1993)



Source: G. Subìas, et al PRB **56**, 8183 (1997)

L_3 XAS and multiplets





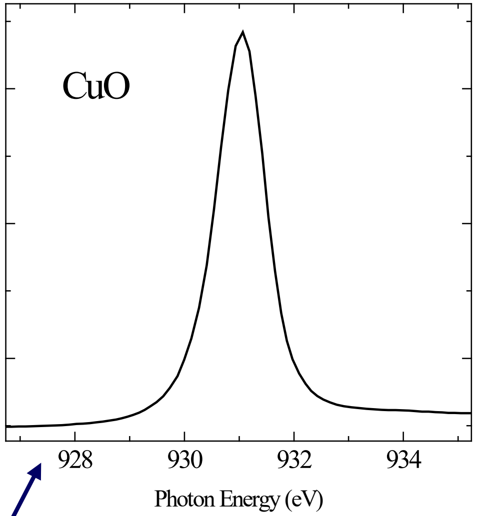
$$3d^{\,n} \longrightarrow 2p^5 3d^{\,n+1}$$

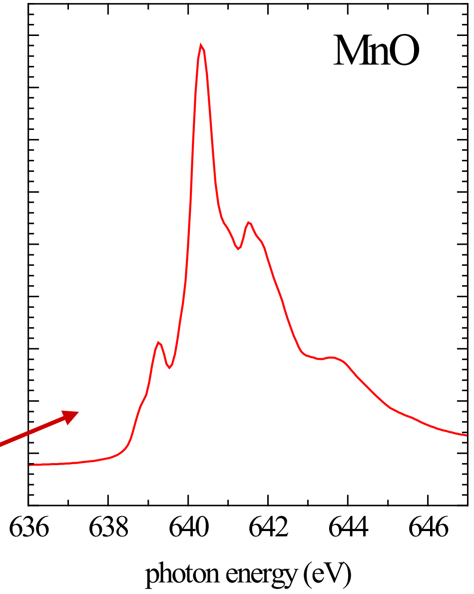
CuO: $3d^9 \rightarrow 3d^{10}$

One single peak

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

Many peaks





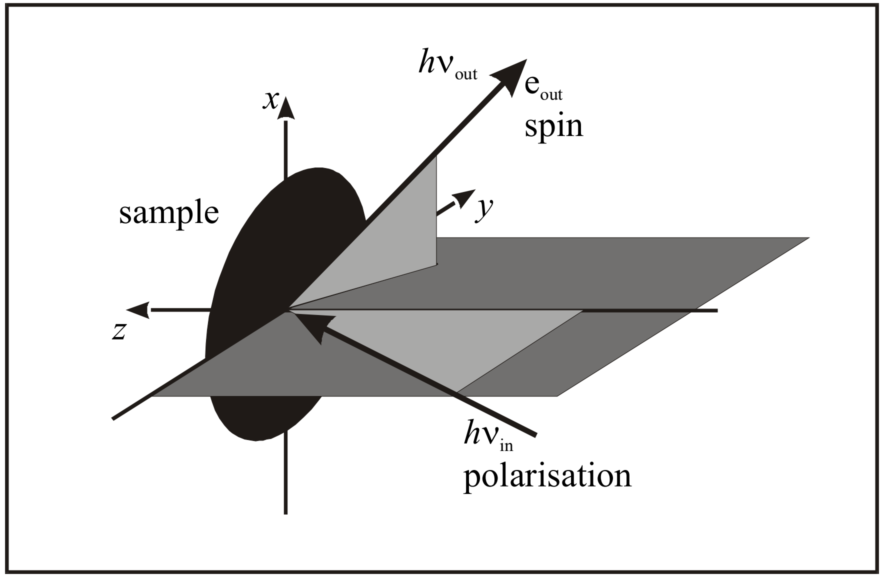
Second order processes: what after XAS?

What about looking at the emitted x-rays
after a resonant absorption?

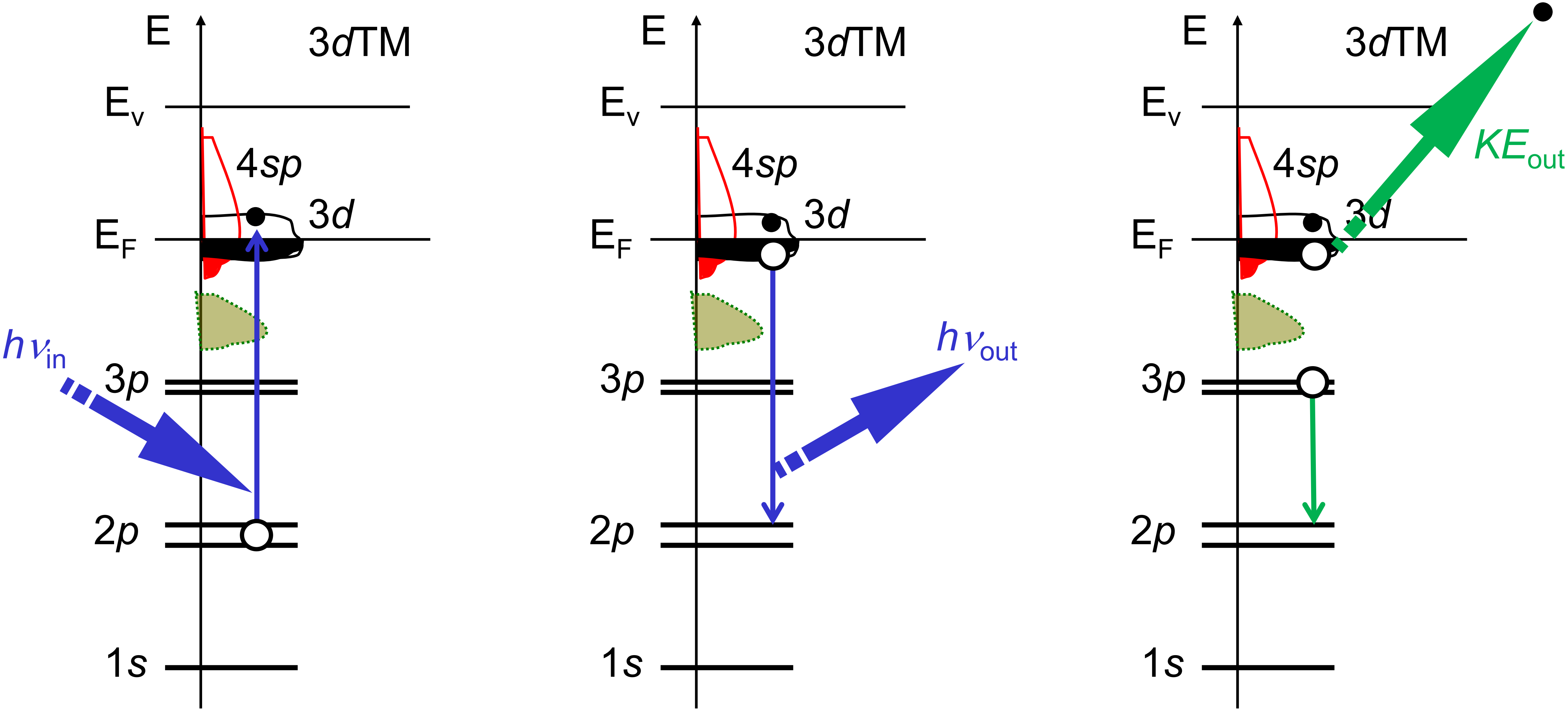
We can access local and collective excitations.

Electric dipole selection rules are not a limitation.

Photon momentum can be used to probe dispersion.



Decay of the core hole after a resonant absorption

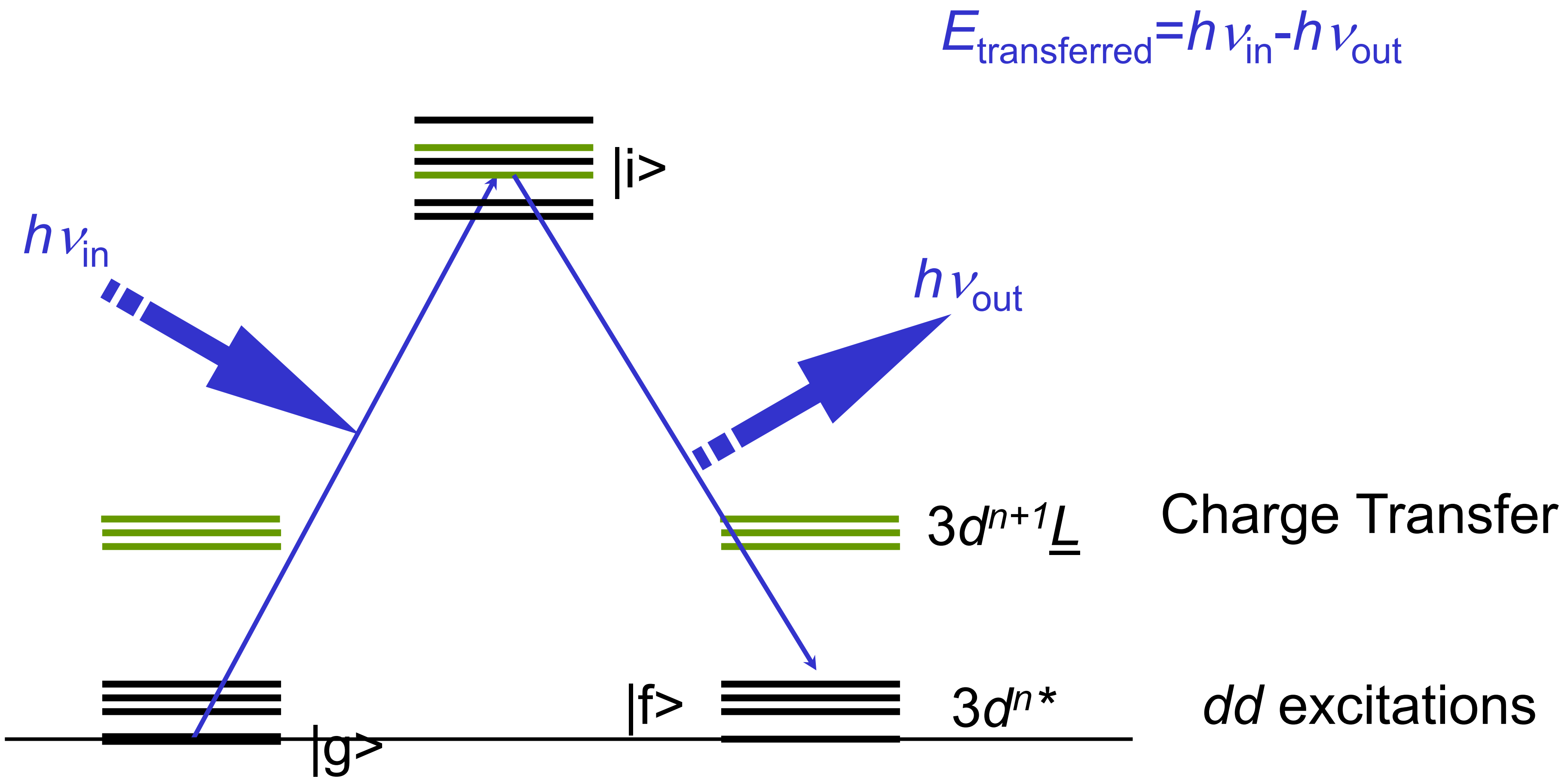


Absorption

Radiative decay (XES, RIXS)

Auger decay (ResAuger, ResPES)

RIXS: a resonant inelastic scattering



RIXS probes charge neutral local excitations

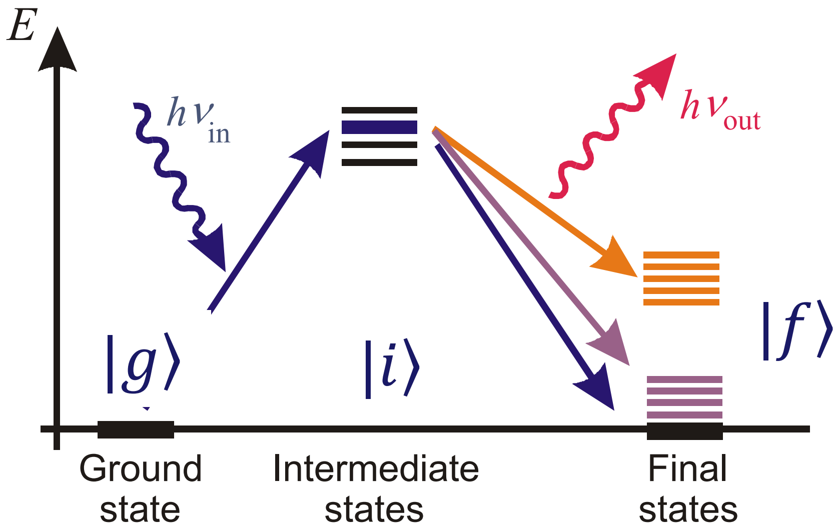
RIXS: a 2nd order process decribed by Kramers-Heisenberg formula

Several spectral features coming from different final states via the same set of intermediate states

2 steps: emission and absorption

The intermediate state is not known: we sum over amplitudes given by different intermediate states

Intensity : $$\sum_f \left| \sum_i \frac{\langle f|T^{(e)}|i\rangle\langle i|T^{(a)}|g\rangle}{E_g + h\nu_{\text{in}} - E_i - i\Gamma_i} \right|^2 \times \frac{\Gamma_f/\pi}{(E_g + h\nu_{\text{in}} - E_f - h\nu_{\text{out}})^2 + \Gamma_f^2},$$

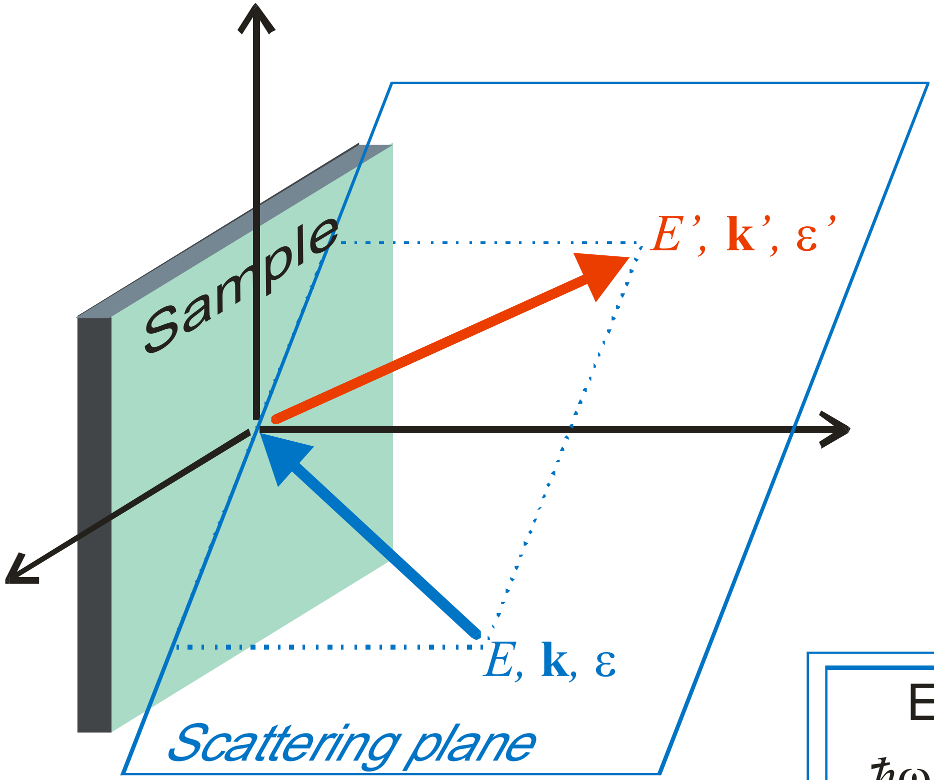


Resonance in the excitation step

Energy transfer from photon to sample

Lorentzian broadening due to final state lifetime

L edge RIXS : energy and momentum transfer

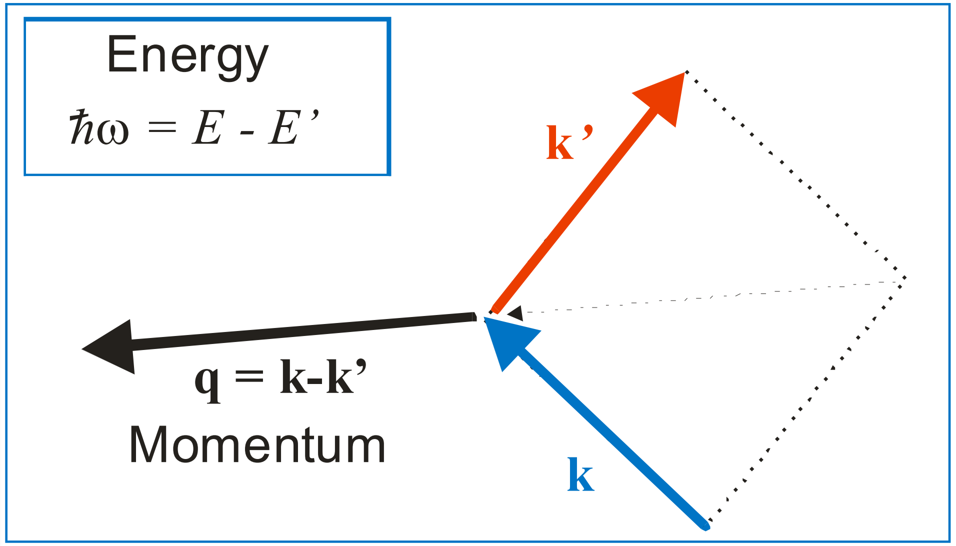


Resonant Inelastic X-ray Scattering:

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

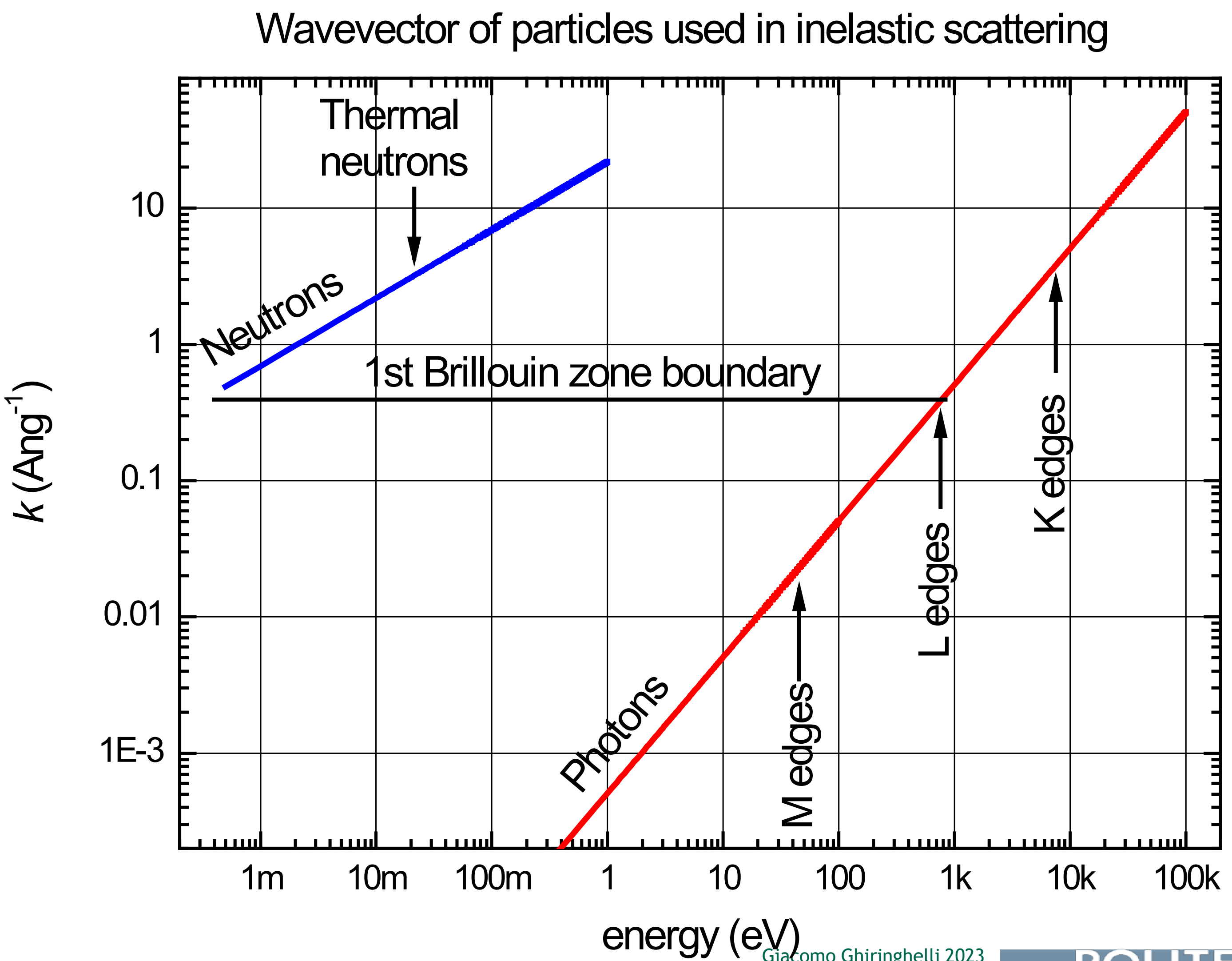
Conservation laws:

- Energy
- Momentum
- “Angular momentum”

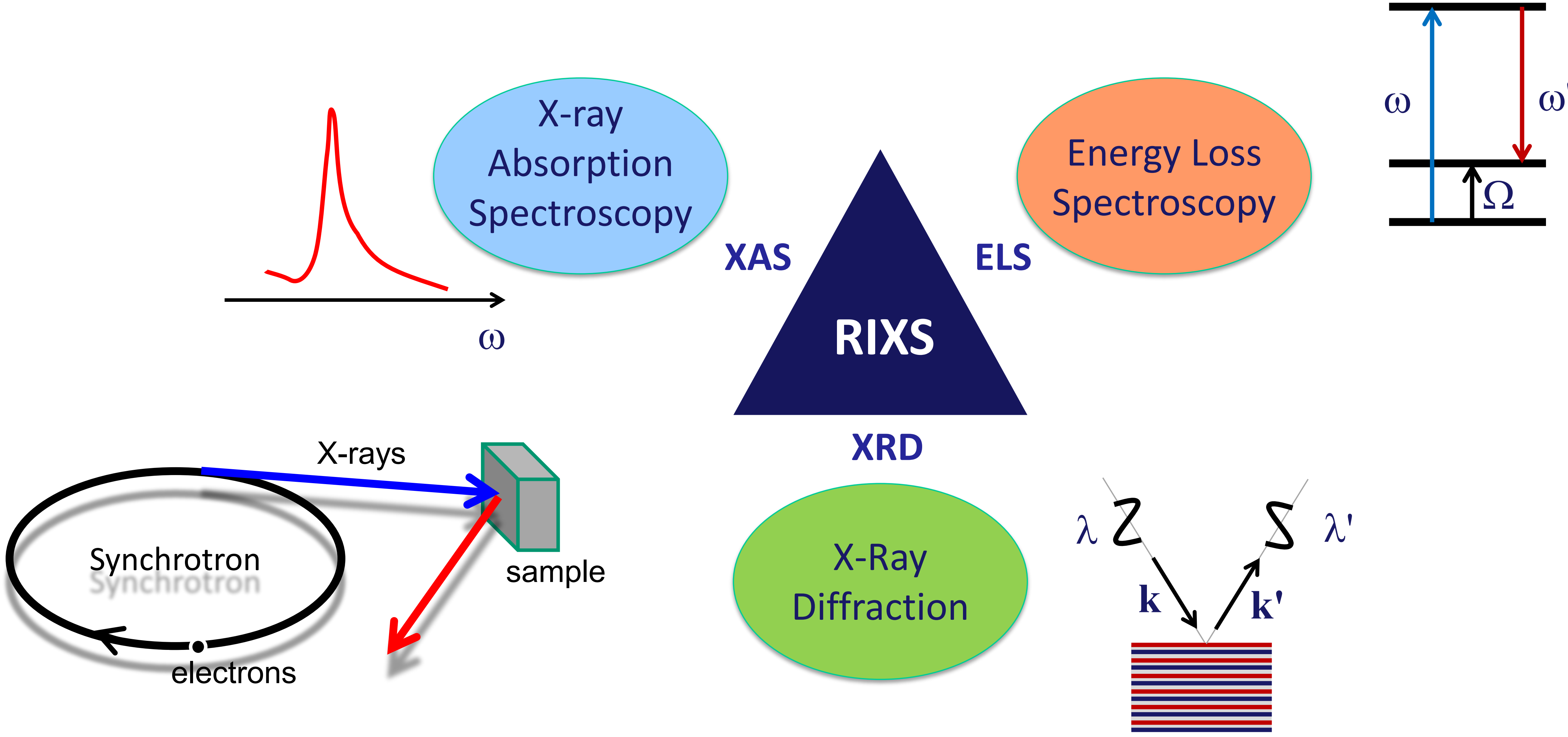


Photon momentum and kinematics

Photons vs Neutrons: energy and momentum



Resonant Inelastic X-ray Scattering

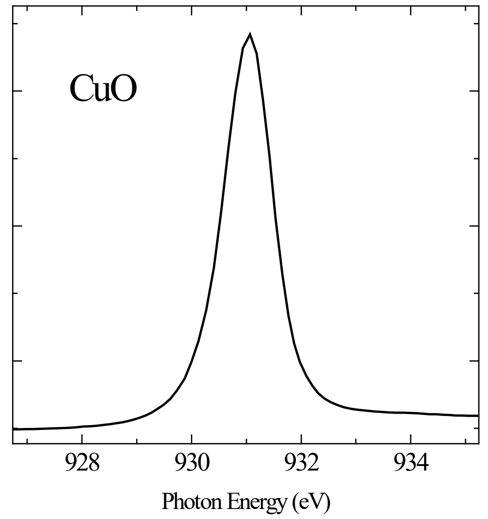


Cuprates: the "easy" case

In cuprates Cu is divalent: $Cu^{2+} \Longleftrightarrow 3d^9$

This makes XAS almost trivial: 1 peak only

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

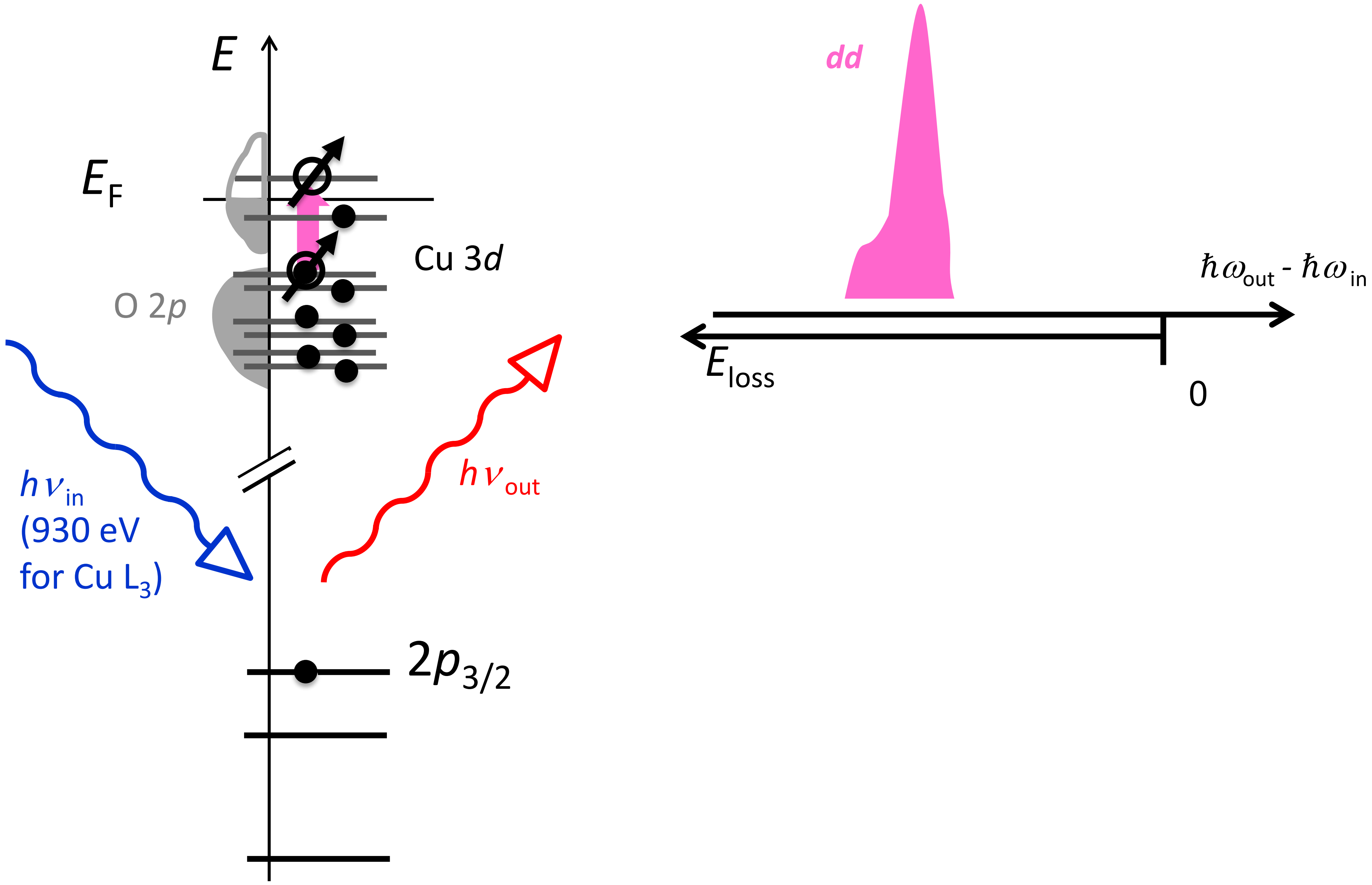


RIXS can be calculated even by hand:

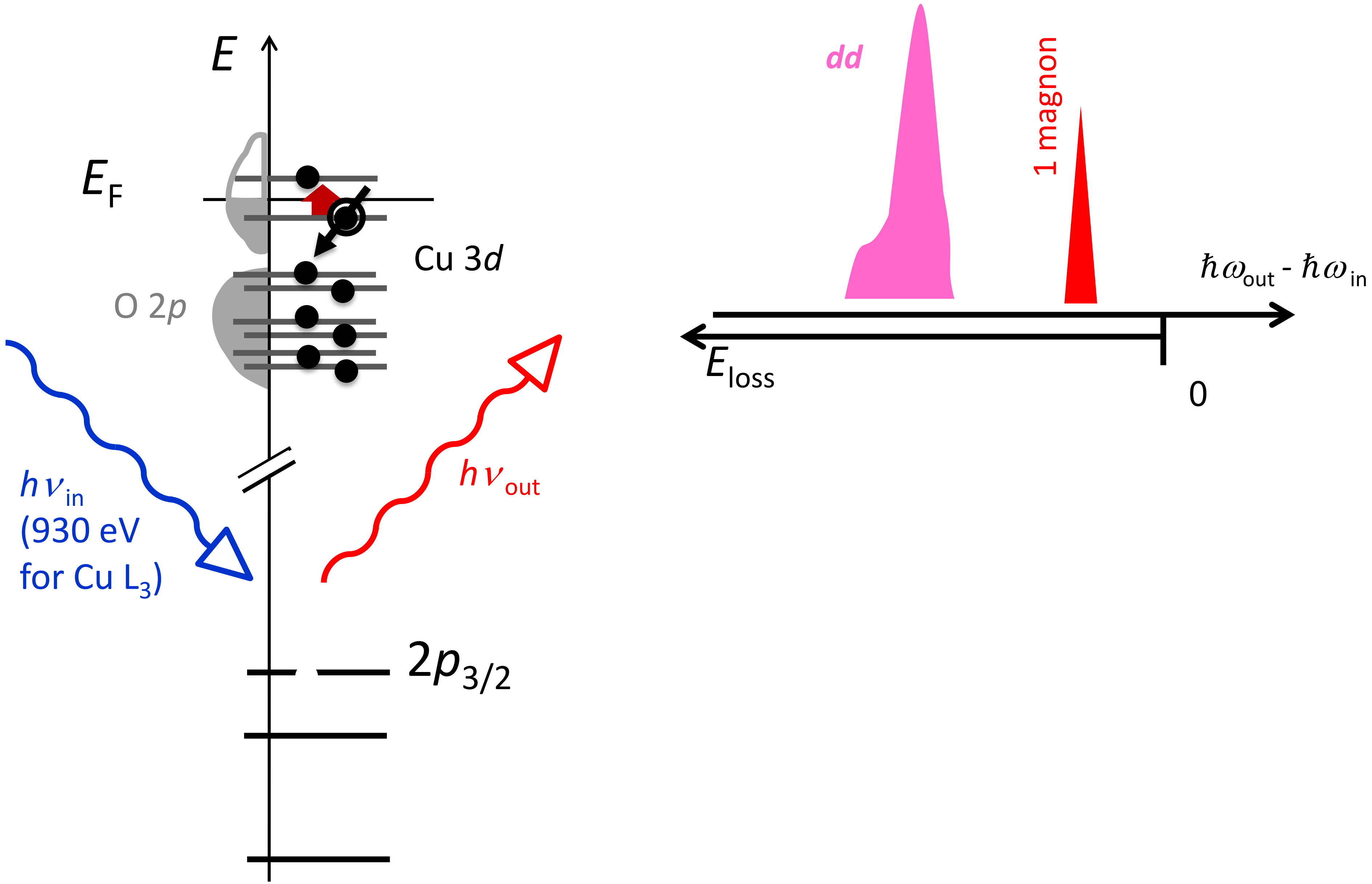
$$3d^9 \longrightarrow (2p_{3/2})^3 3d^{10} \longrightarrow (3d^9)^*$$

Even for magnetic excitations (spin waves), because fast collision approximation is a very good approximation

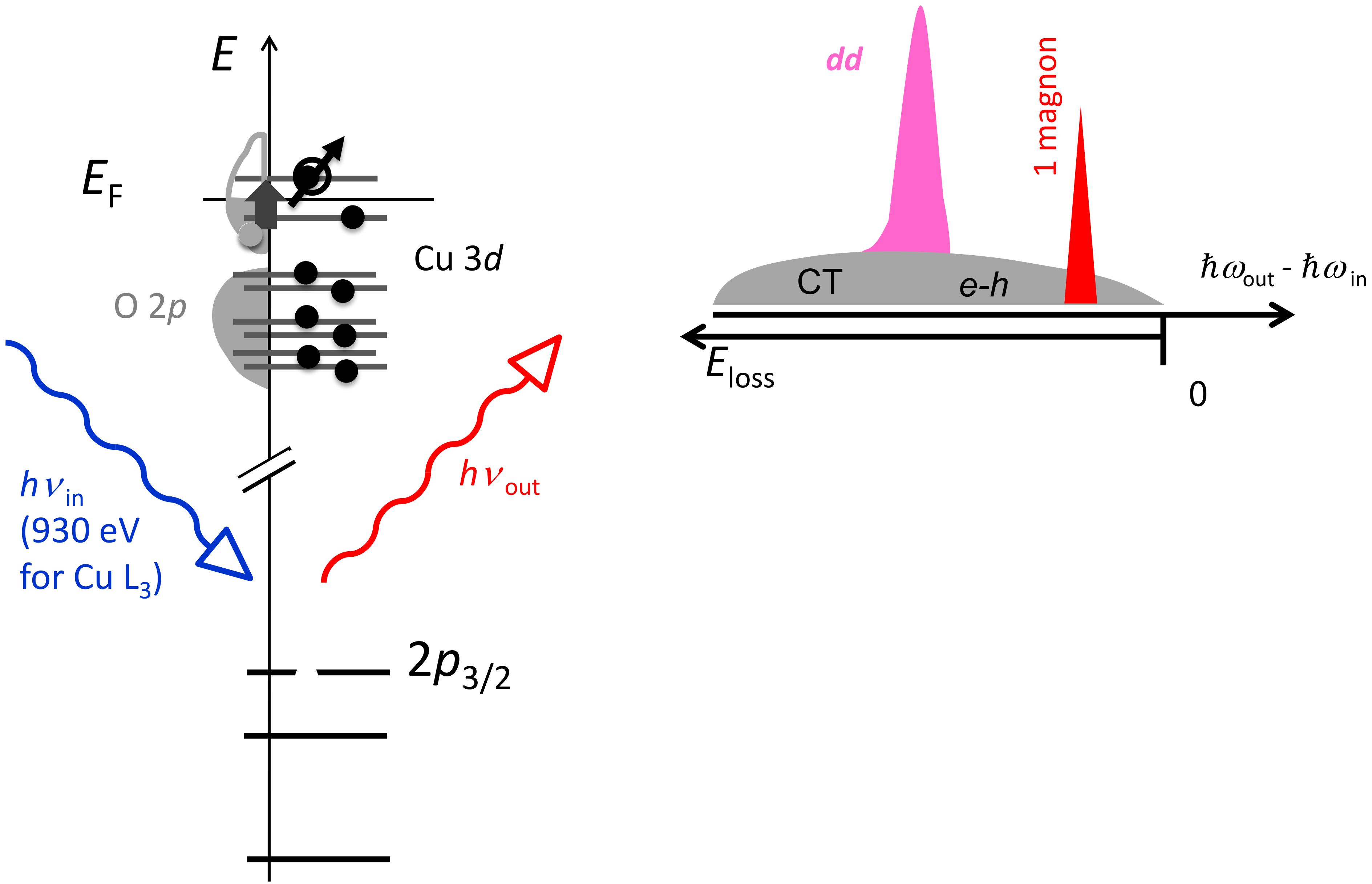
RIXS at the Cu L_3 resonance



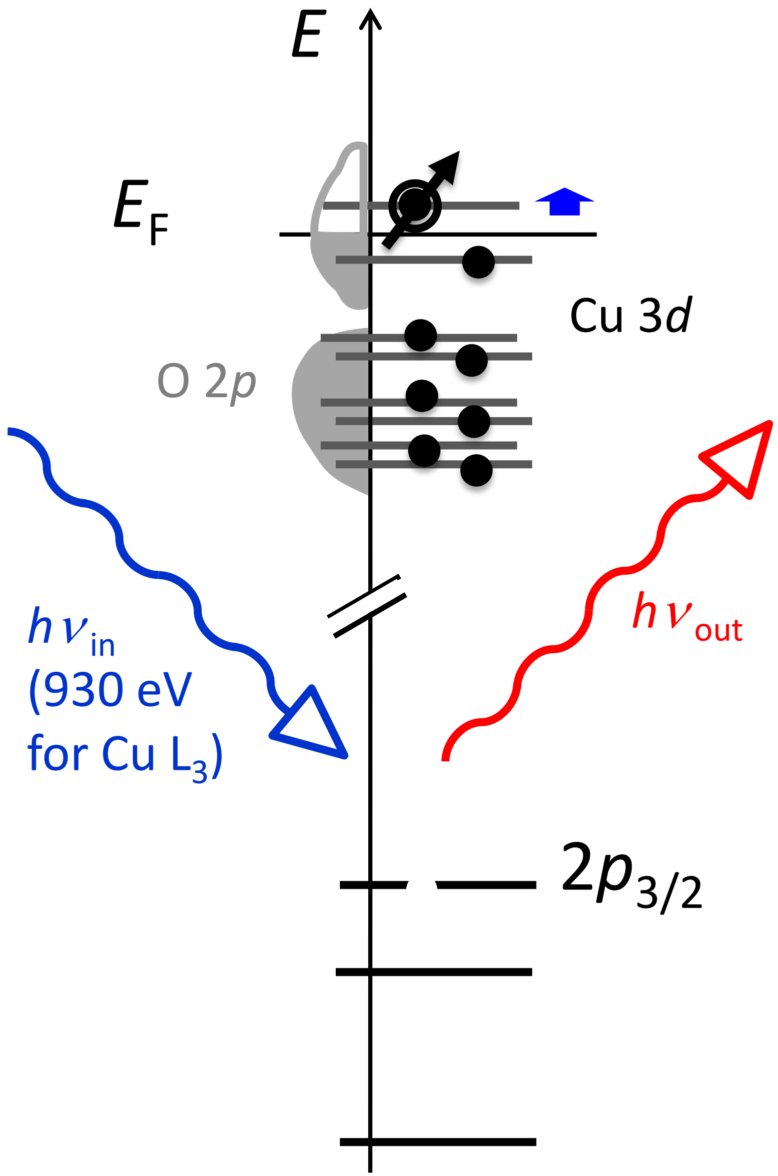
Cu L_3 RIXS: magnon excitations

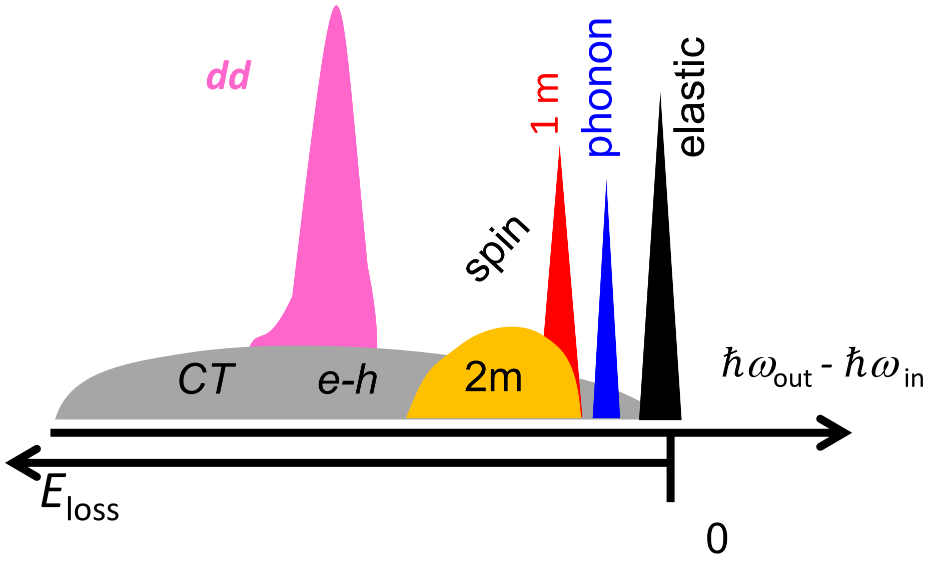


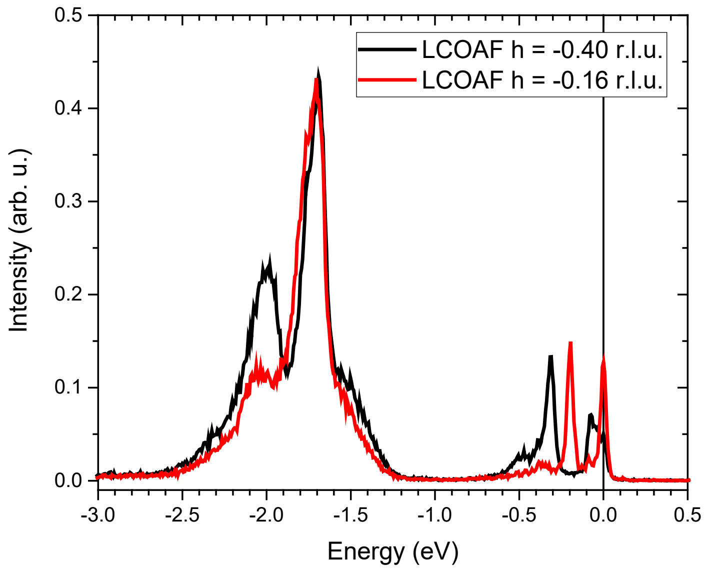
Cu L_3 RIXS: charge transfer and *e-h* excitations



Cu L_3 RIXS: elastic, phonon, 2-magnon



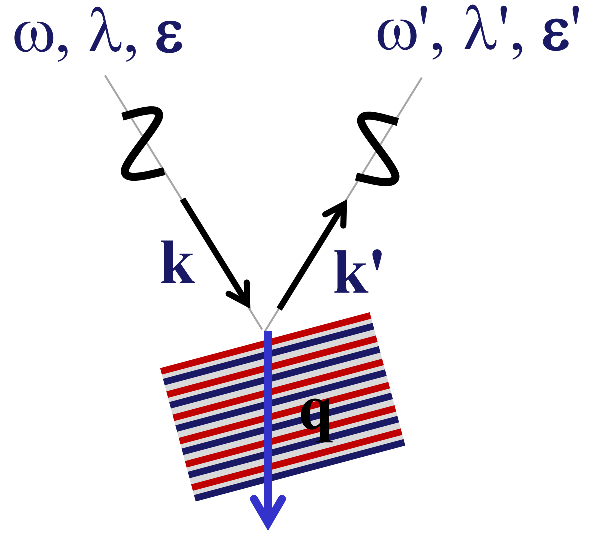




$\Omega=\omega-\omega'$

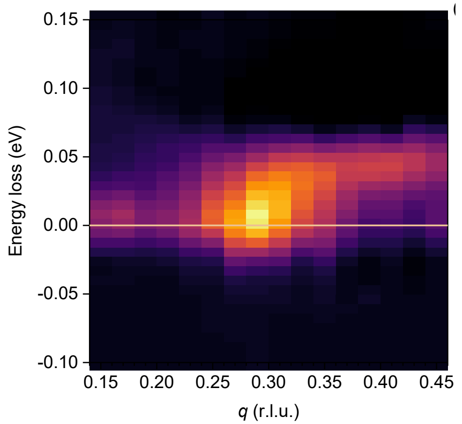
$\mathbf{q} = \mathbf{k}' - \mathbf{k}$

ε, ε': polarization

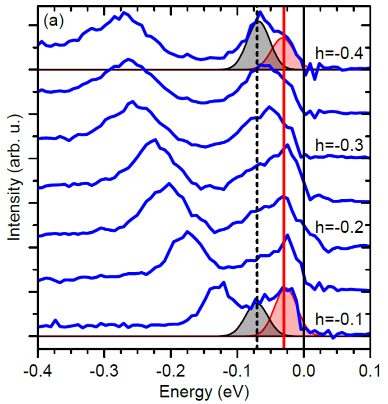


RIXS catalogue

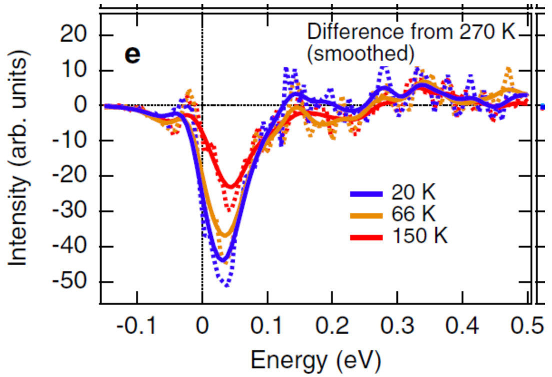
Charge Order
(CDW, CDF)

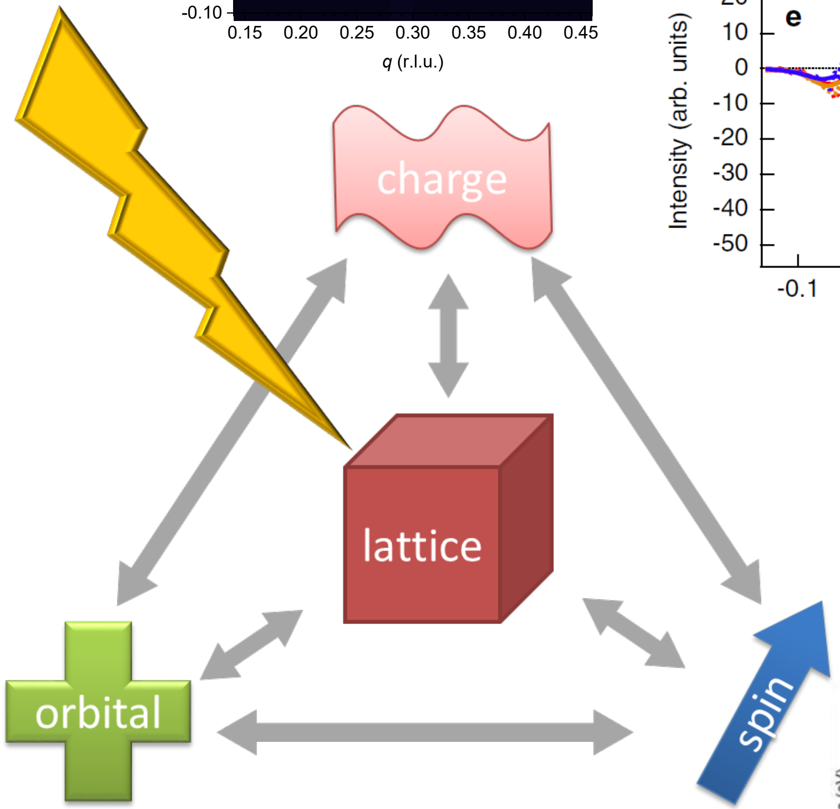


Lattice excitations
(phonons)

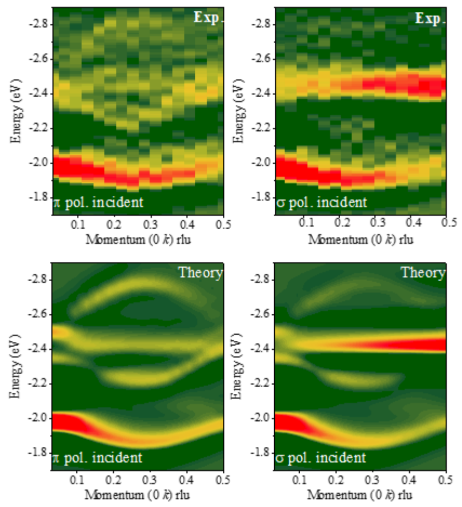


Charge excitations
(SC gap, pseudogap)

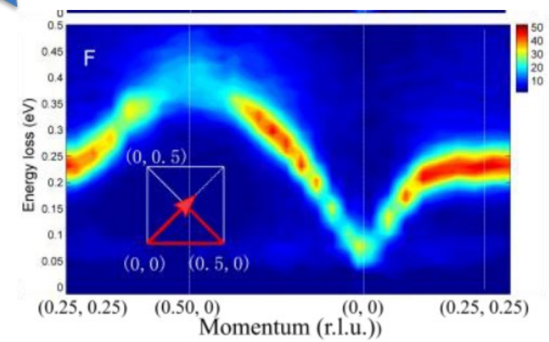




dd excitations



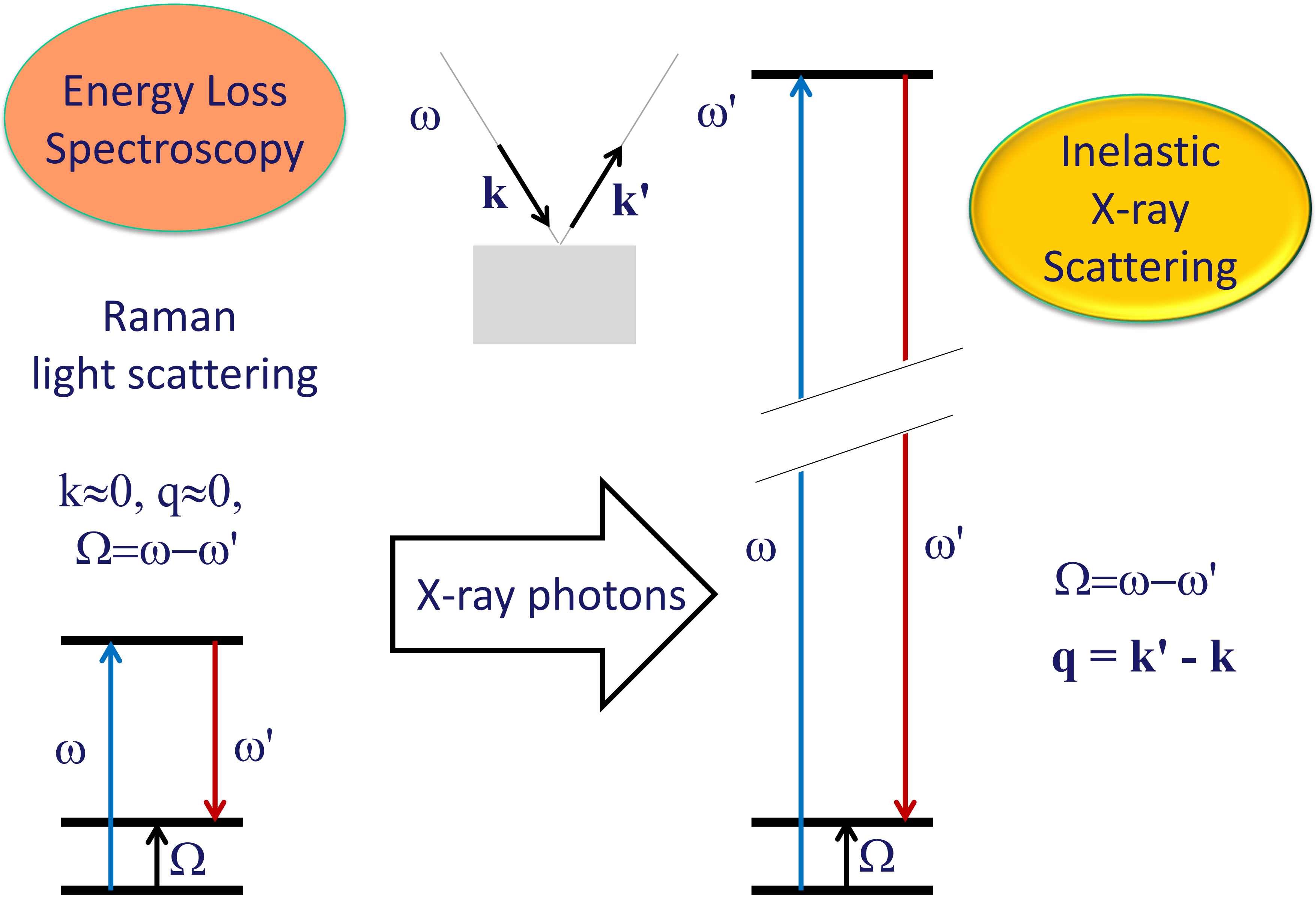
Spin excitations (magnons)



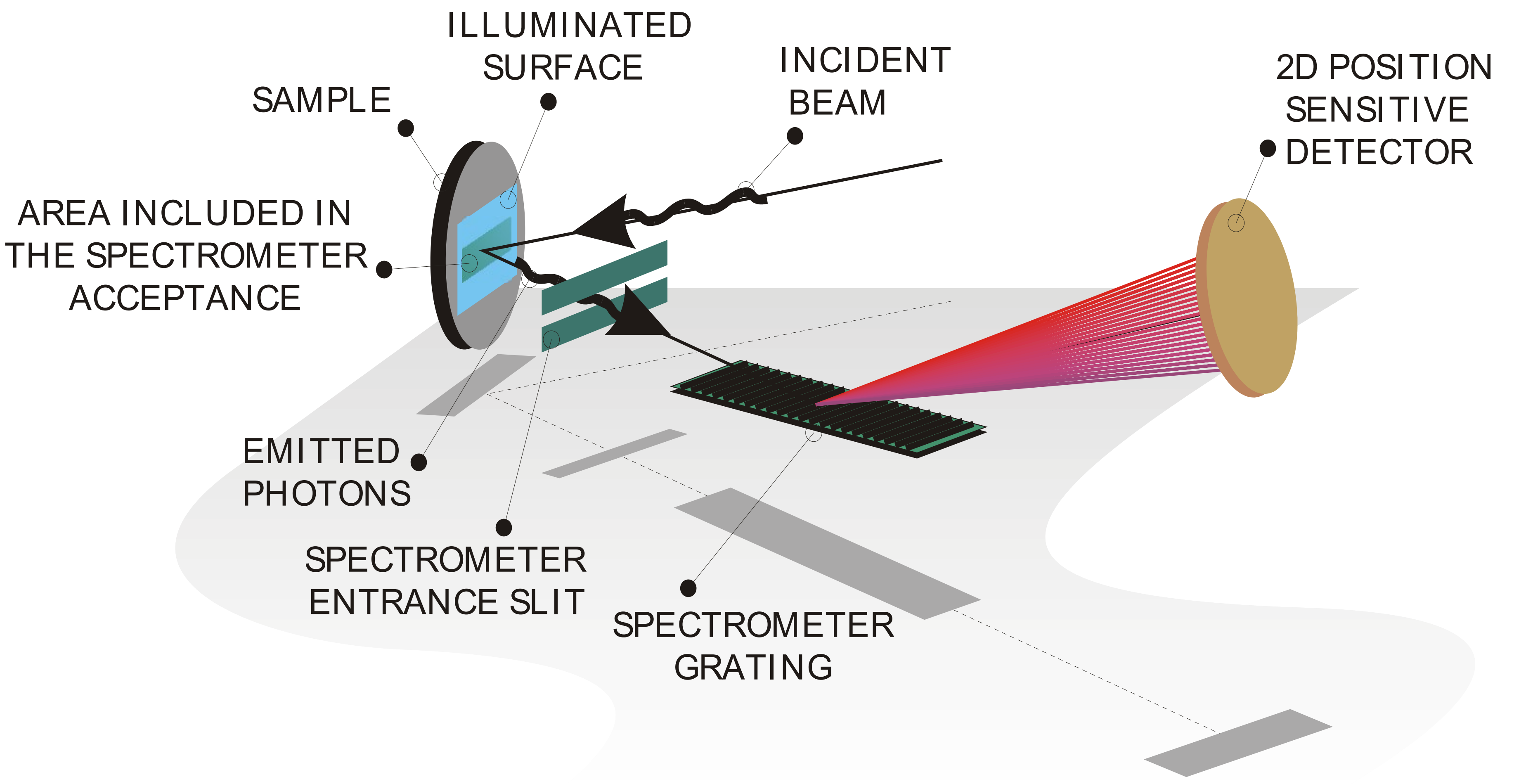
Part 2

INSTRUMENTATION FOR RIXS (MOSTLY SOFT X-RAY REGIME)

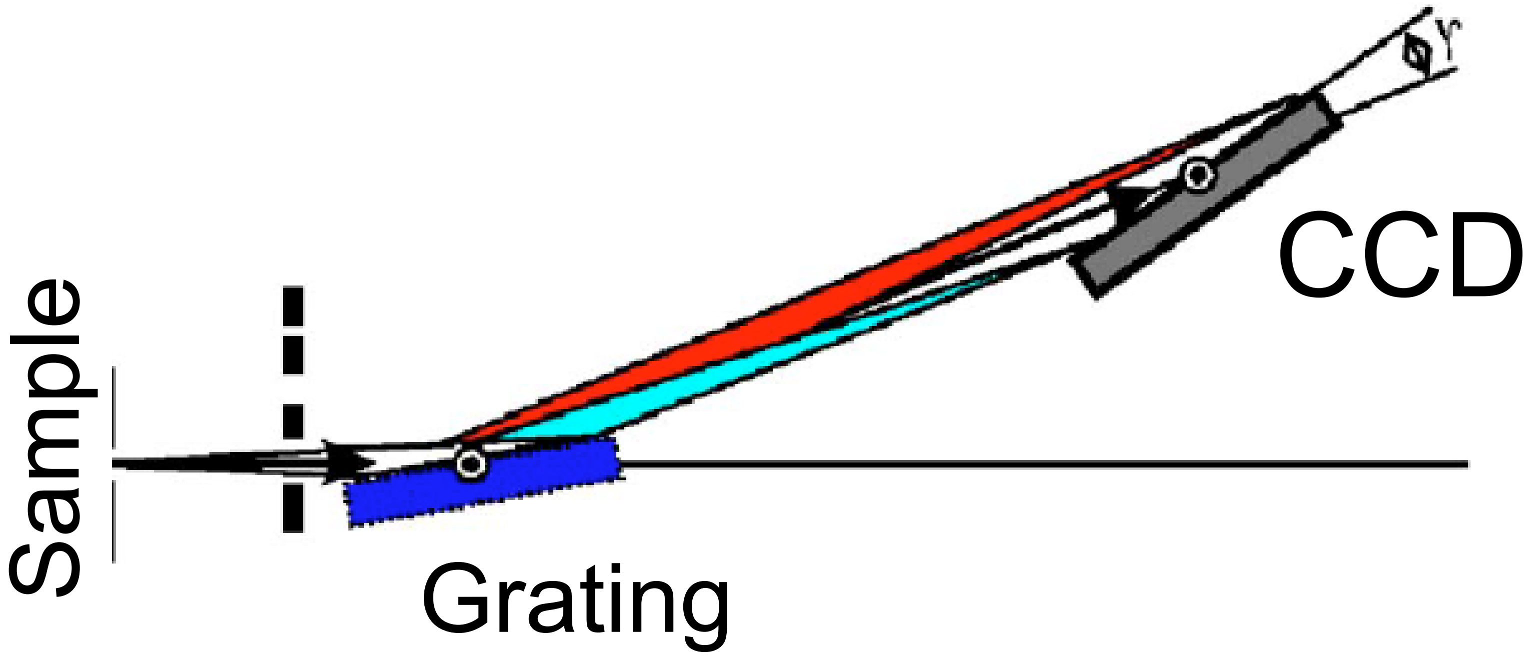
RIXS: a sort of resonant Raman spectroscopy

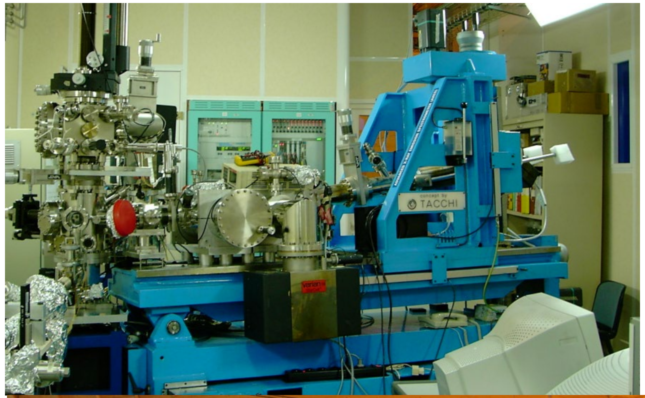


Soft x-ray spectrometer



Longer instruments for better resolution





AXES, ESRF: **2.2 m**
1994 – 2012
$E/\Delta E \sim 3000$

The progress in instrumentation has been the key of the RIXS success: discoveries were enabled by better resolution.

SAXES, SLS: **5 m**
Since 2007
$E/\Delta E \sim 10{,}000$

Similar instruments:

- TPS Taiwan
- European XFEL
- Bessy II

ERIXS, ID32: **10 m,**
Since 2015
$E/\Delta E \sim 50{,}000$
Polarization Analysis

- Diamond I21
- NSLS II SIX

ERIXS at ID32

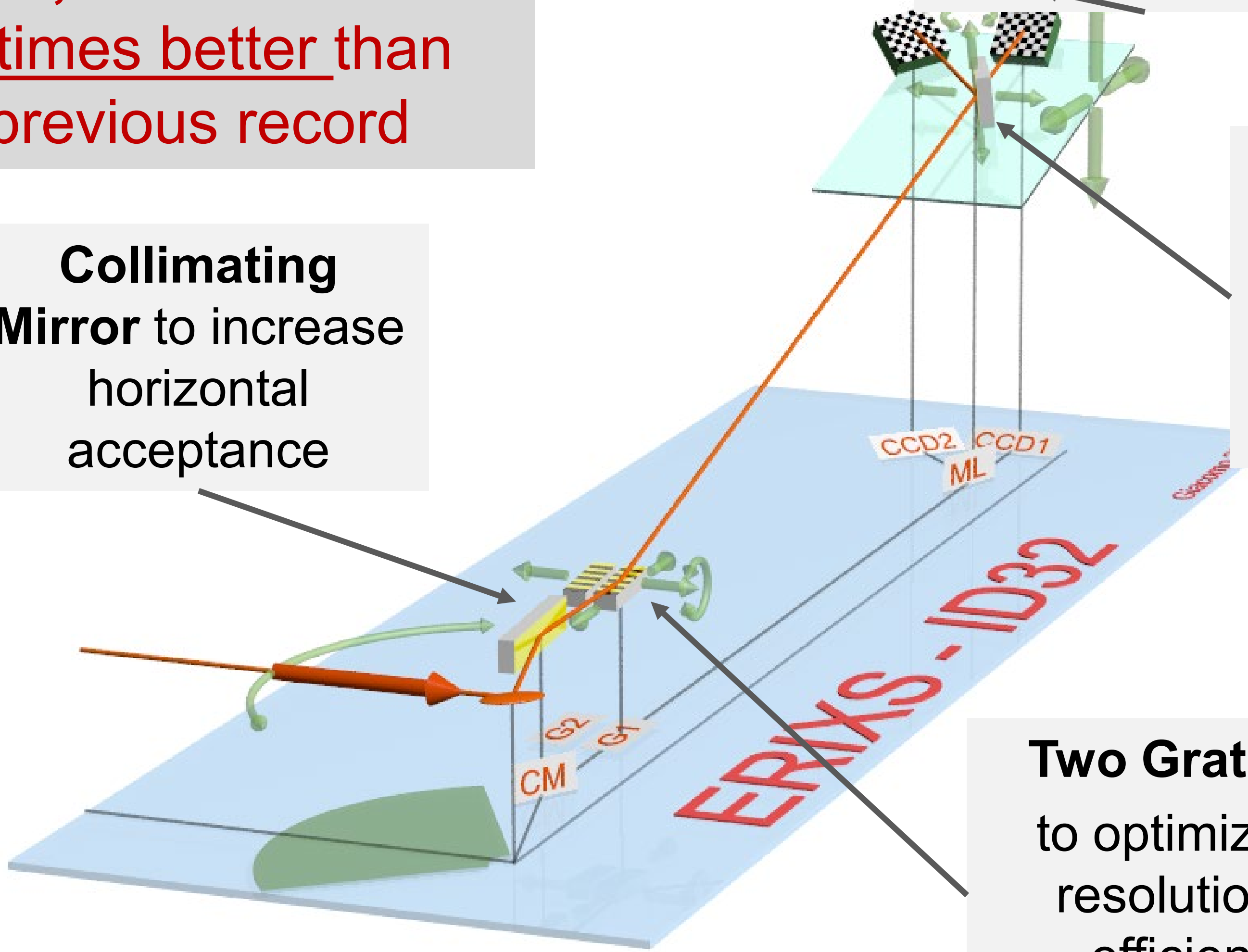
Resolving power:
40,000 at 1 keV
3 times better than
previous record

Collimating Mirror to increase horizontal acceptance

Two CCD detectors

Multi-layer mirror, to measure polarization of scattered photons

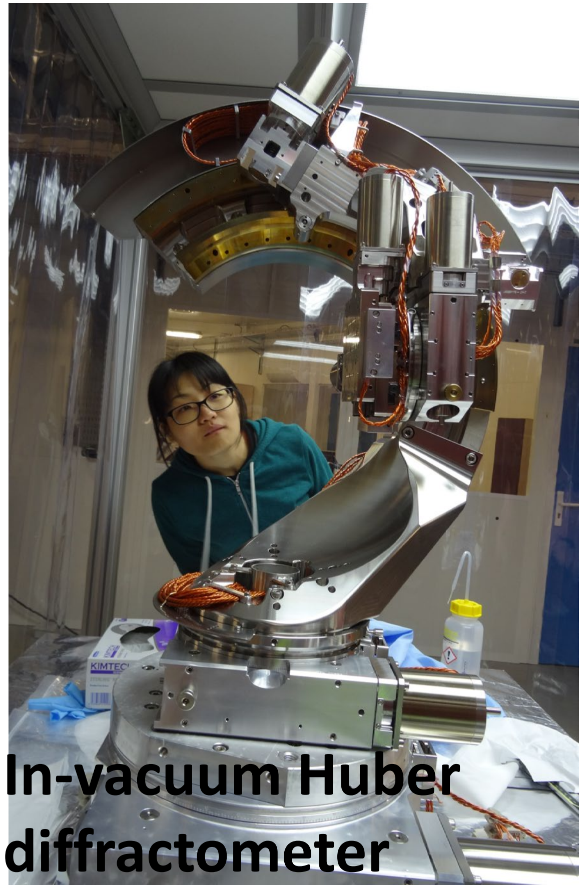
Two Gratings, to optimize for resolution or efficiency



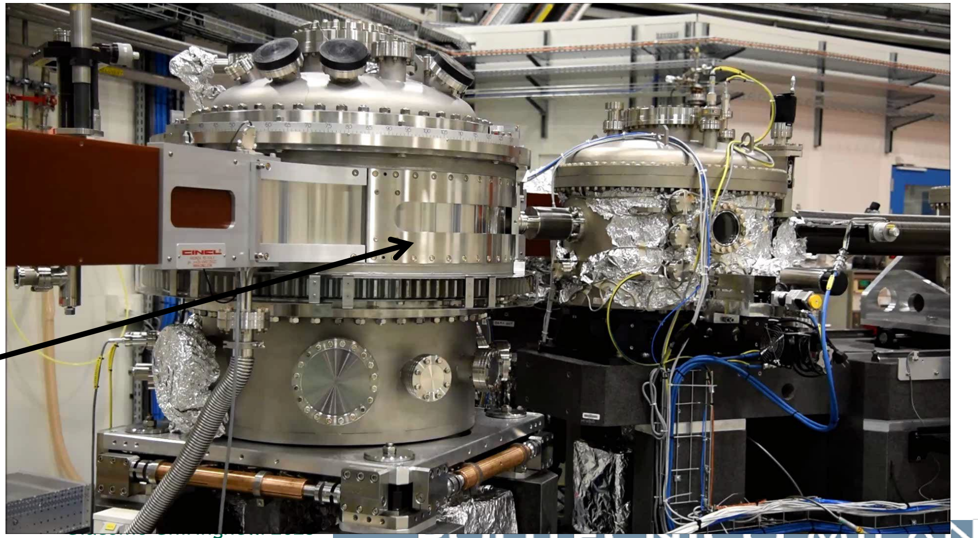
ERIXS Spectrometer

Continuously rotating scattering arm

Speed
x8.6



In-vacuum Huber diffractometer



Sample chamber
CINEL – Italy

ESRF

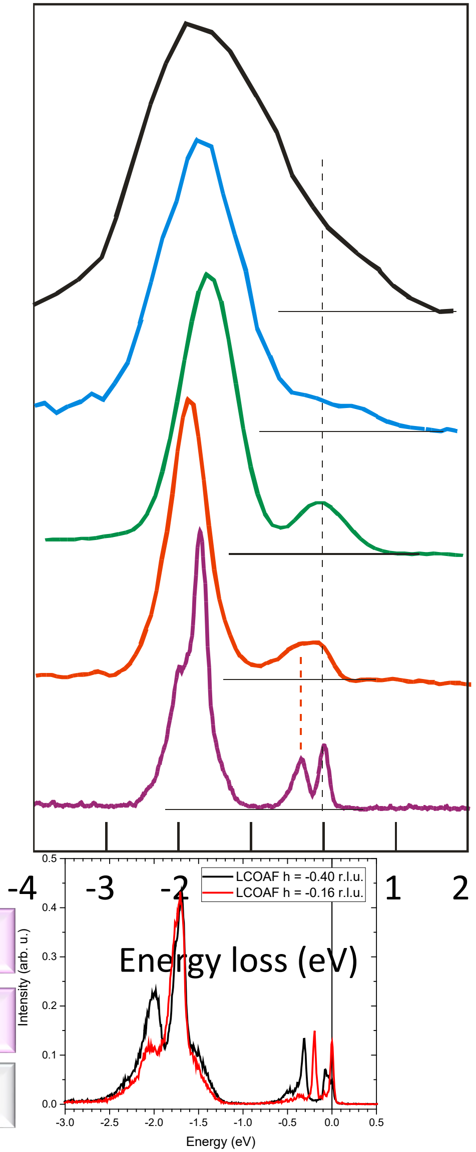
ID32@ESRF and I21@DLS

ERIXS at ID32

I21 at Diamond

ENERGY RESOLUTION: progress in 20 years

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



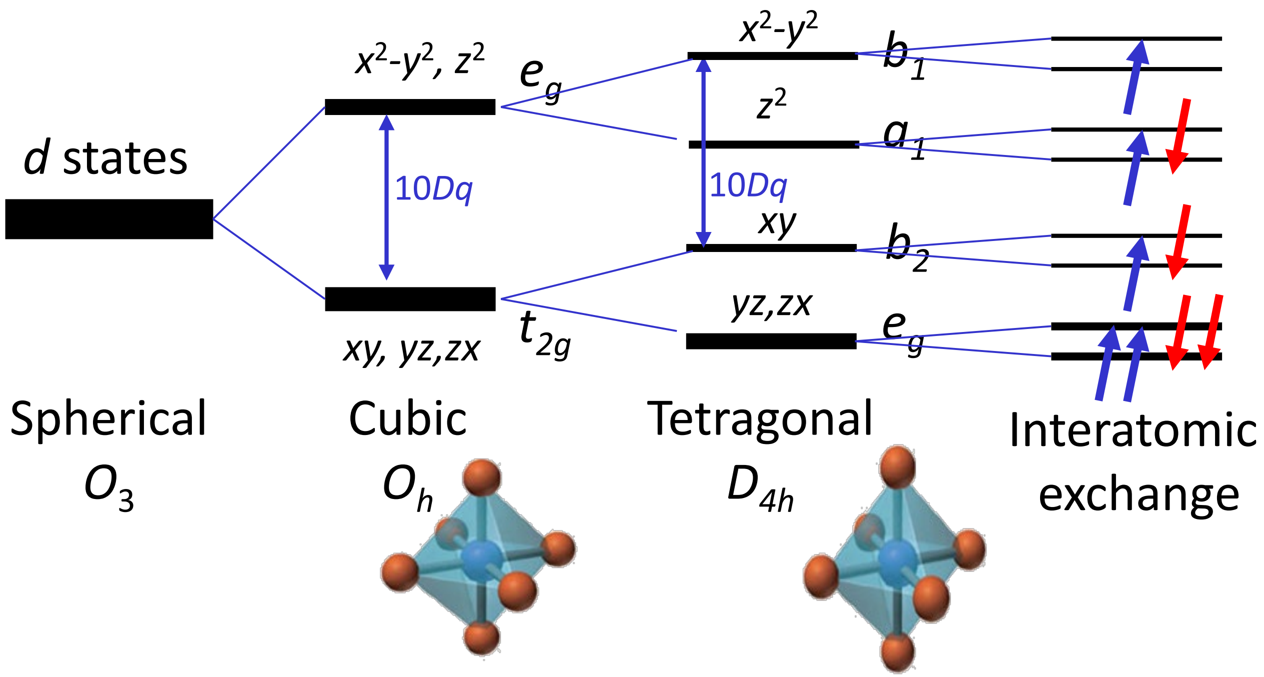
Δ*E* ~1.6 eV		
Δ*E* ~1.2 eV	2000	Uppsala
Δ*E* ~0.8 eV	2003	ESRF + AXES
Δ*E* ~0.45 eV	2007	ESRF + AXES
Δ*E* ~0.13 eV	2008	SLS + SAXES
Δ*E* ~0.050 eV	2015	ESRF + ERIXS
Δ*E* ~0.030 eV	2016	ESRF + ERIXS
Δ*E* ~0.023 eV	2019	NSLS II + SIX
	2021	ESRF + ERIXS

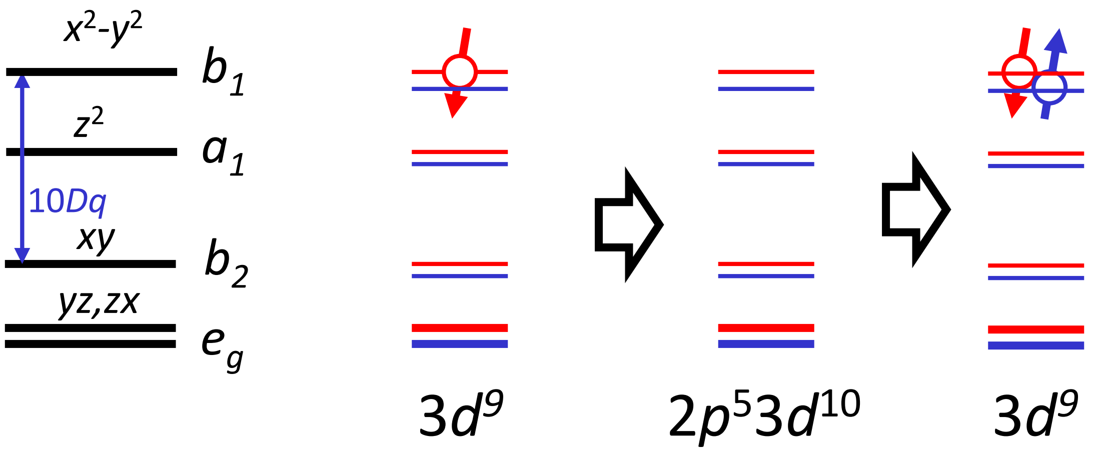
Combined resolving power has increased by a factor 70

Part 3

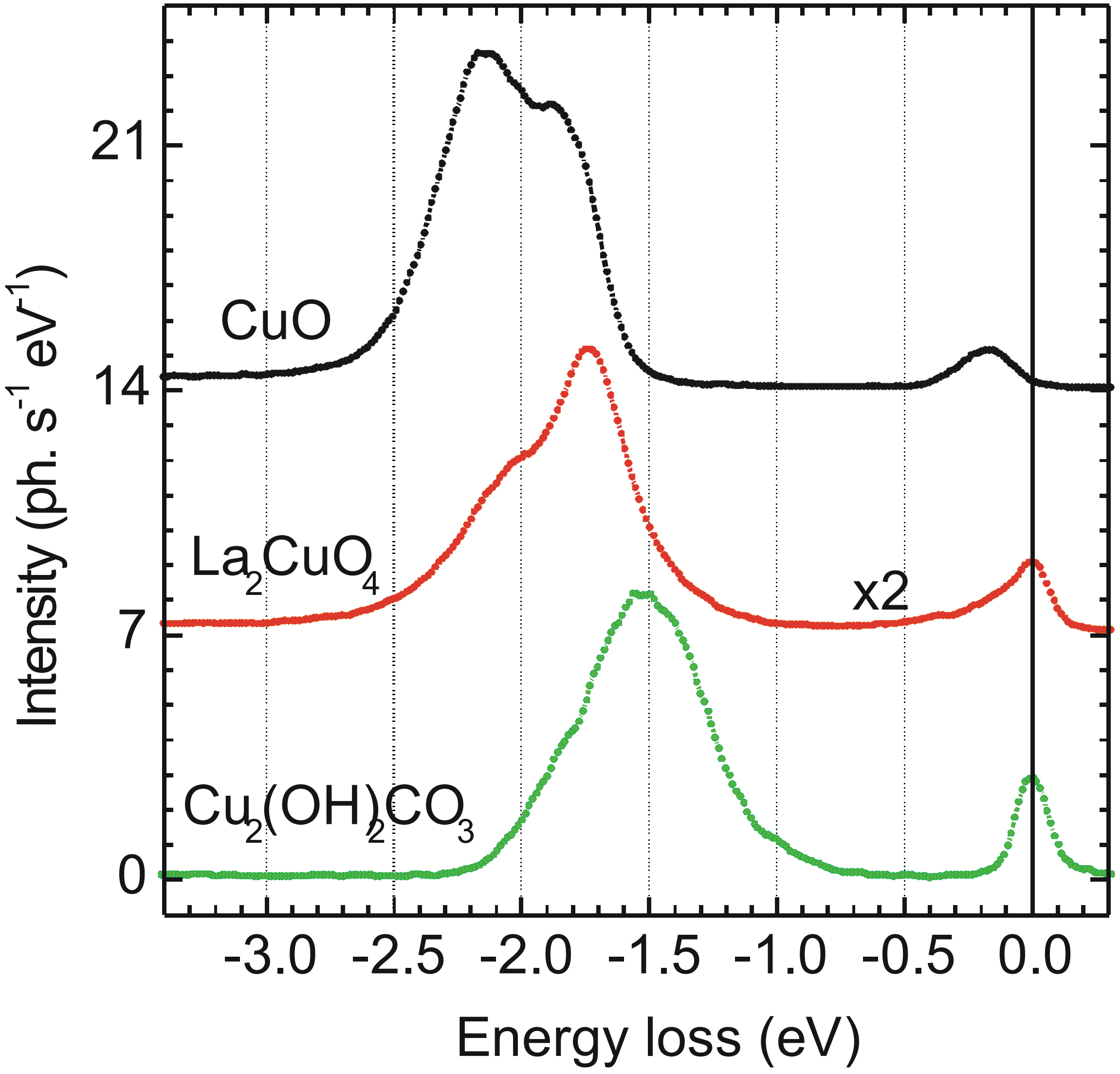
ORBITAL EXCITATIONS

dd excitations in Cu^{2+} systems





Cu L_3 edge RIXS: CuO, La_2CuO_4, Malachite



Cu^{2+} in square approximately planar coordination

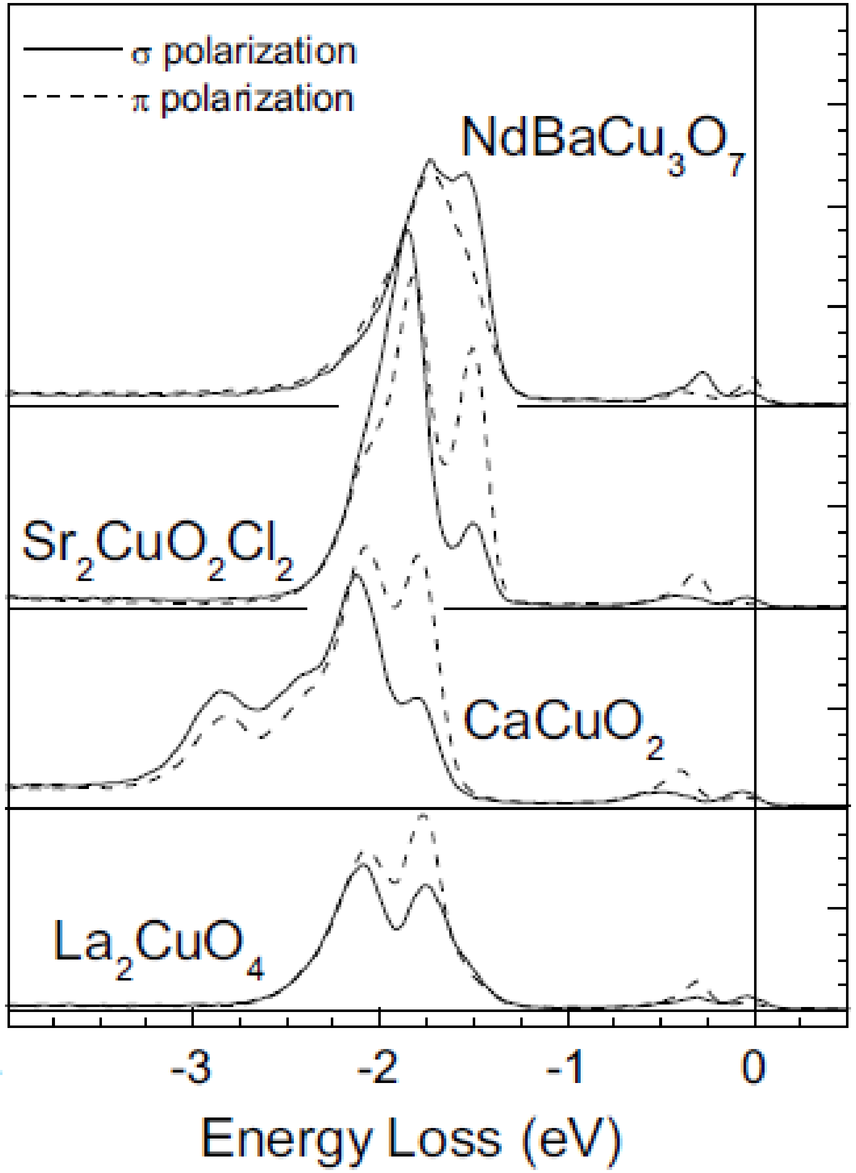
Cu-O distances:
CuO 1.7 – 2-2 Ang
LCO 1.9 – 2.4 Ang
Malachite 1.9 – 2.6 Ang

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

⇩

Different *dd* excitations

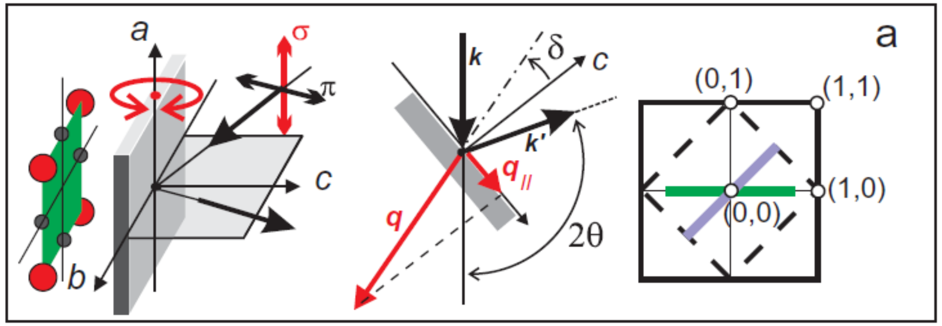
This is a very direct way of measuring the *dd*-excitation energies



New Journal of Physics
The open-access journal for physics

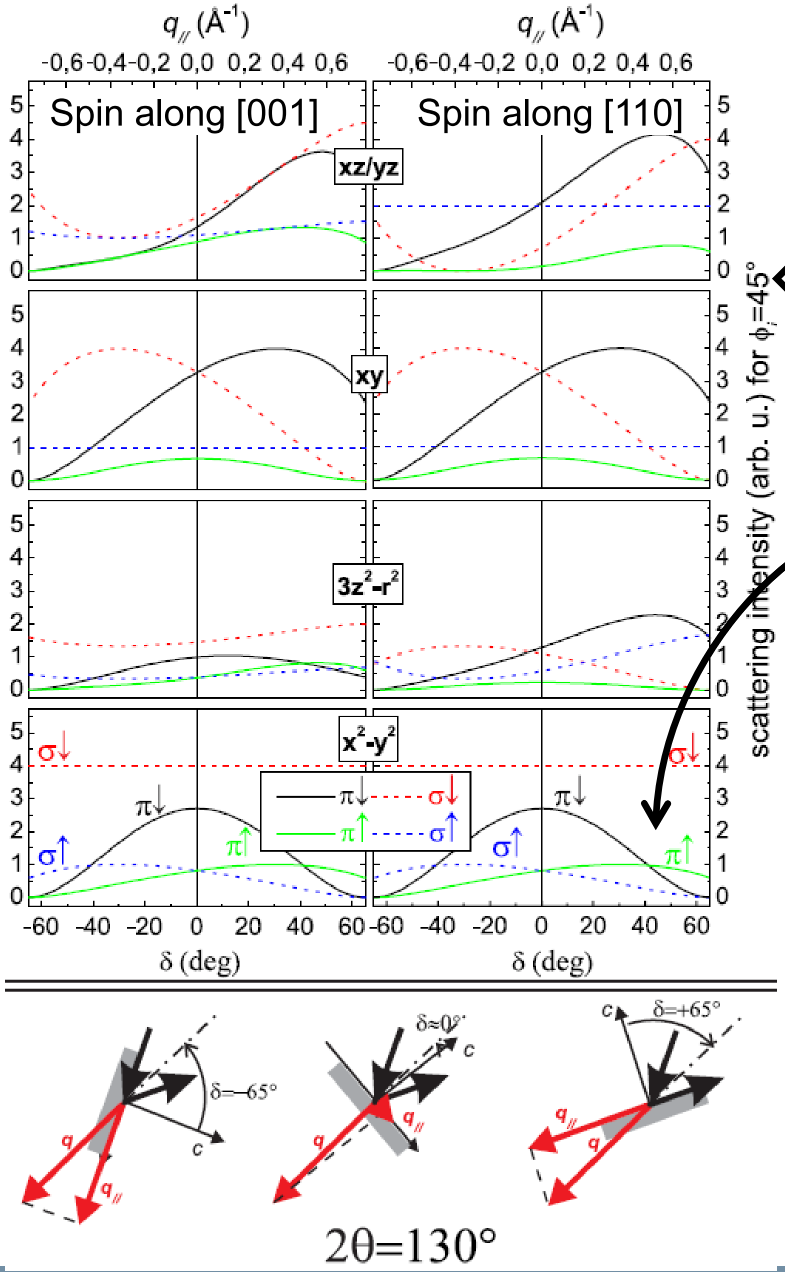
Energy and symmetry of dd excitations in undoped layered cuprates measured by Cu L_3 resonant inelastic x-ray scattering

M Moretti Sala[1,8,9], V Bisogni[2,10], C Aruta[3], G Balestrino[4], H Berger[5], N B Brookes[2], G M de Luca[3], D Di Castro[4], M Grioni[5], M Guarise[5], P G Medaglia[4], F Miletto Granozio[3], M Minola[1], P Perna[3], M Radovic[3,11], M Salluzzo[3], T Schmitt[6], K J Zhou[6], L Braicovich[7] and G Ghiringhelli[7]



M. Moretti Sala, et al New J. Phys. **13**, 043026 (2011)

dd-excitation energies from fitting using atomic cross sections

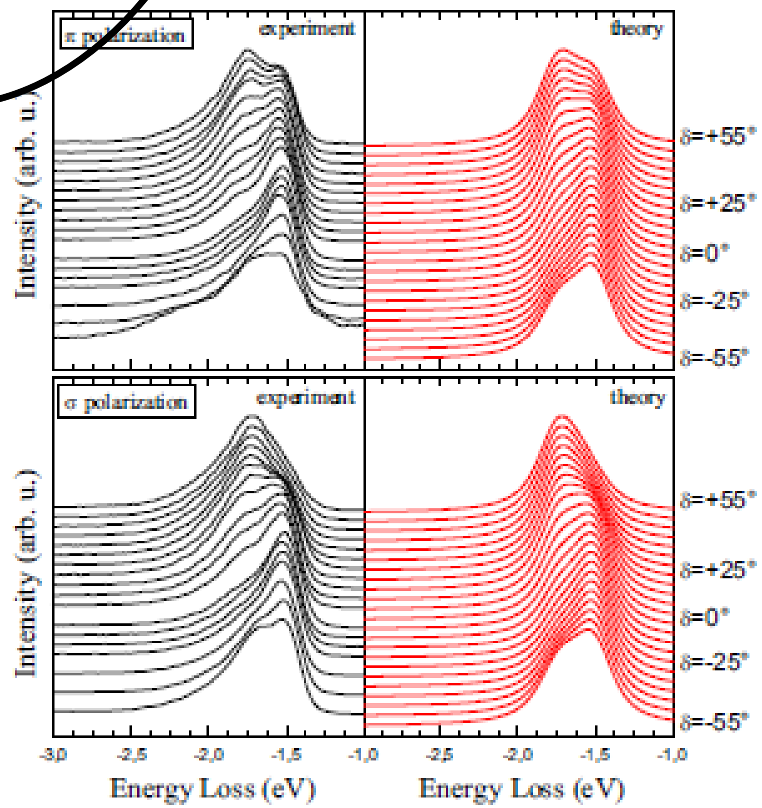


Ground state: $\underline{3d}^{\downarrow}{}_{x^2-y^2}$

Spin flip: $\underline{3d}^{\uparrow}{}_{x^2-y^2}$

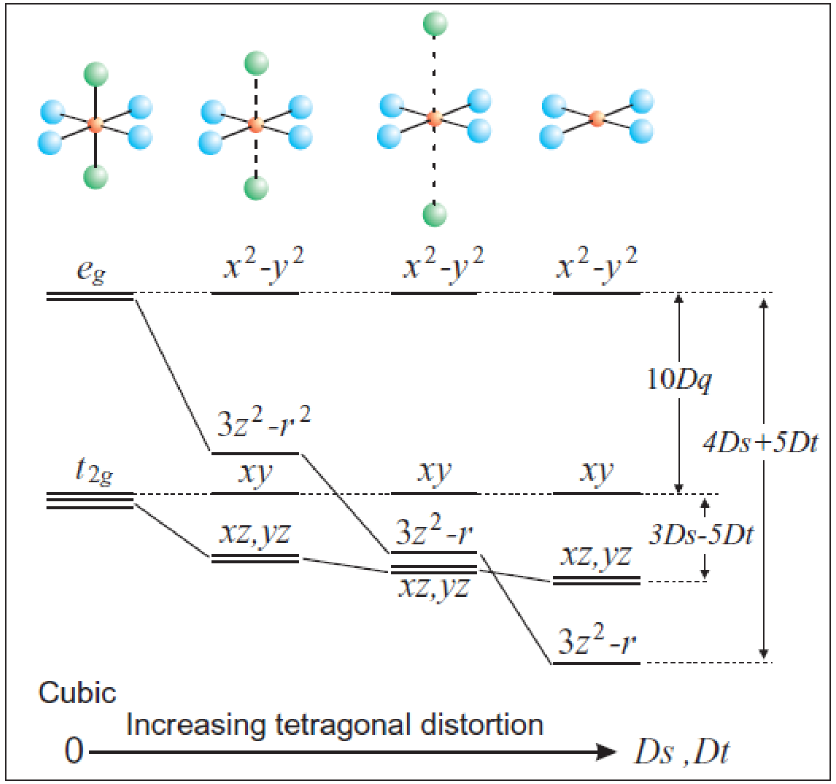
$F(\theta_{in},\phi_{in},\theta_{out},\phi_{out},\theta_{spin},\phi_{spin},\varepsilon_{in},\varepsilon_{out})$

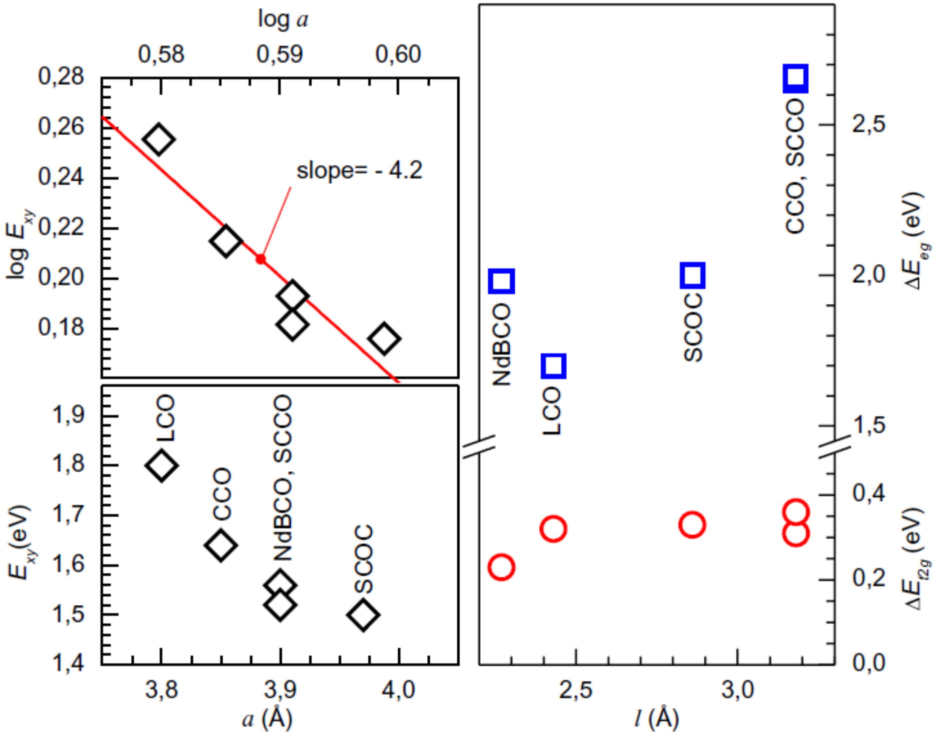
NdBCO



M. Moretti Sala, et al New J. Phys. **13**, 043026 (2011)

Crystal field trends in cuprates

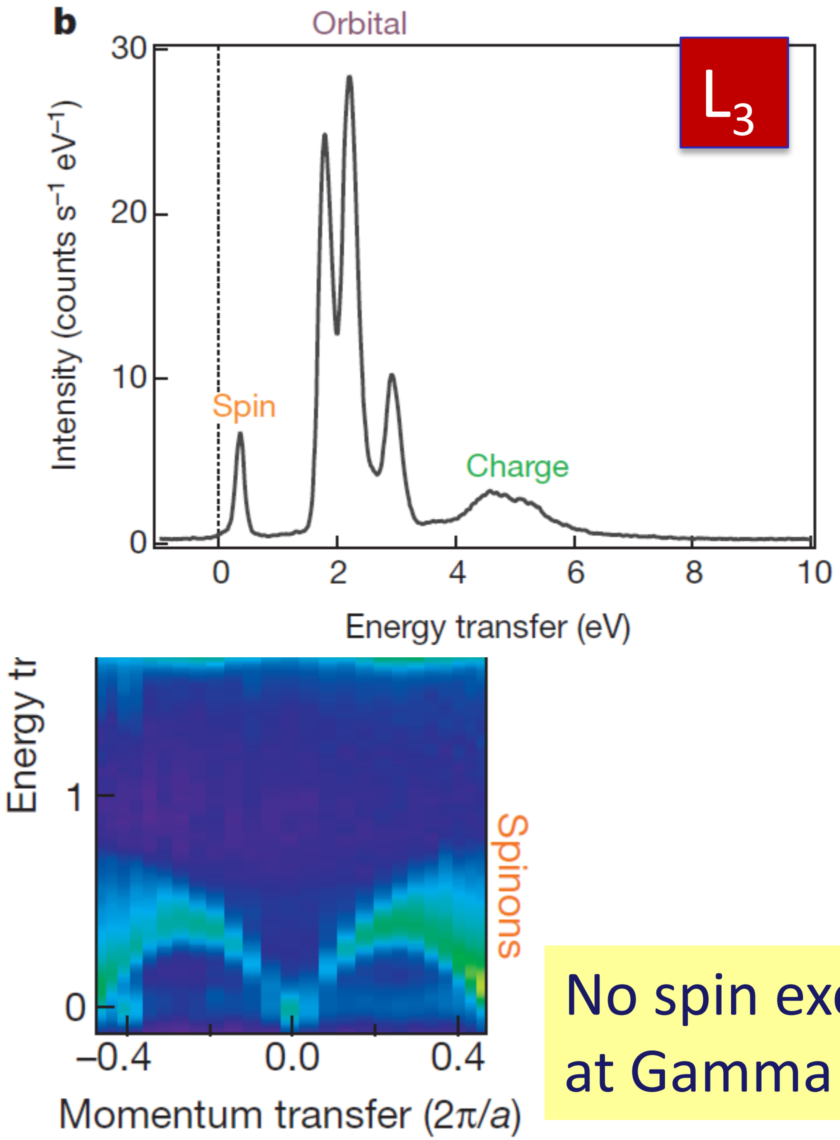


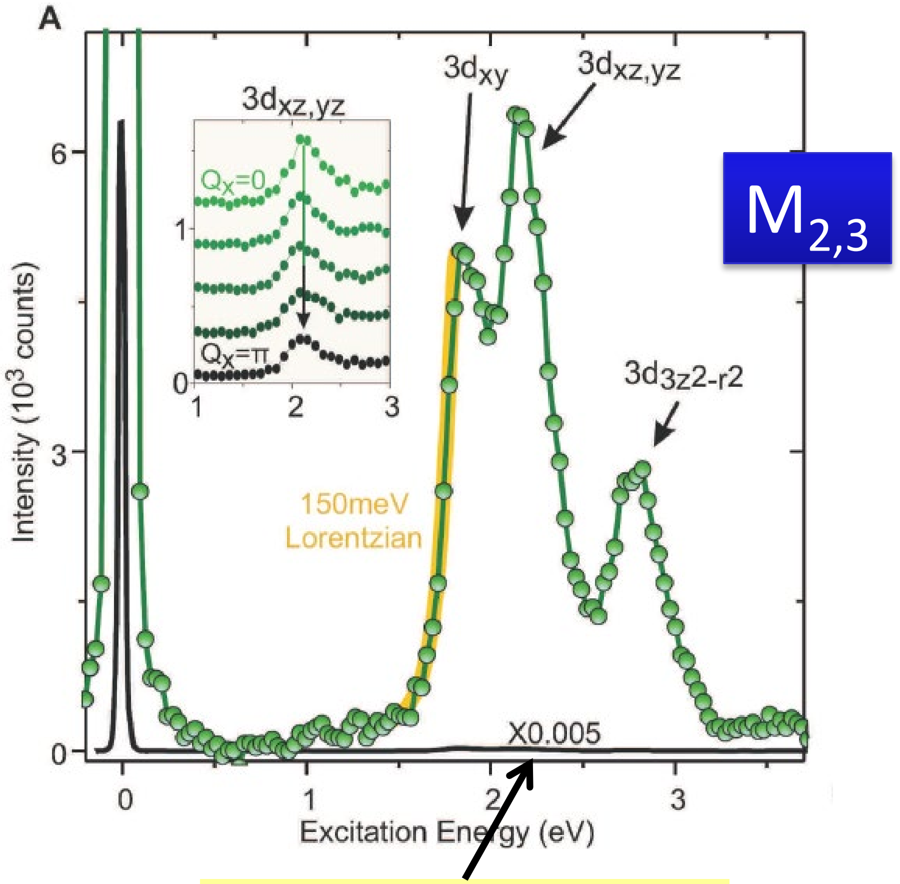


	La_2CuO_4	$Sr_2CuO_2Cl_2$	$CaCuO_2$
J [meV]	130[34,35]	130[35]	130[35]
$E_{3z^2-r^2}$ $(\Gamma_{3z^2-r^2})$ [eV]	1.70 (.14)	1.97 (.10)	2.72 (.12)
E_{xy} (Γ_{xy}) [eV]	1.80 (.10)	1.50 (.08)	1.75 (.09)
$E_{xz/yz}$ $(\Gamma_{xz/yz})$ [eV]	2.12 (.14)	1.84 (.10)	2.10 (.18)

M. Moretti Sala, et al New J. Phys. **13**, 043026 (2011)

dd excitations and absorption edge: Cu L_3 vs $M_{2,3}$ edges





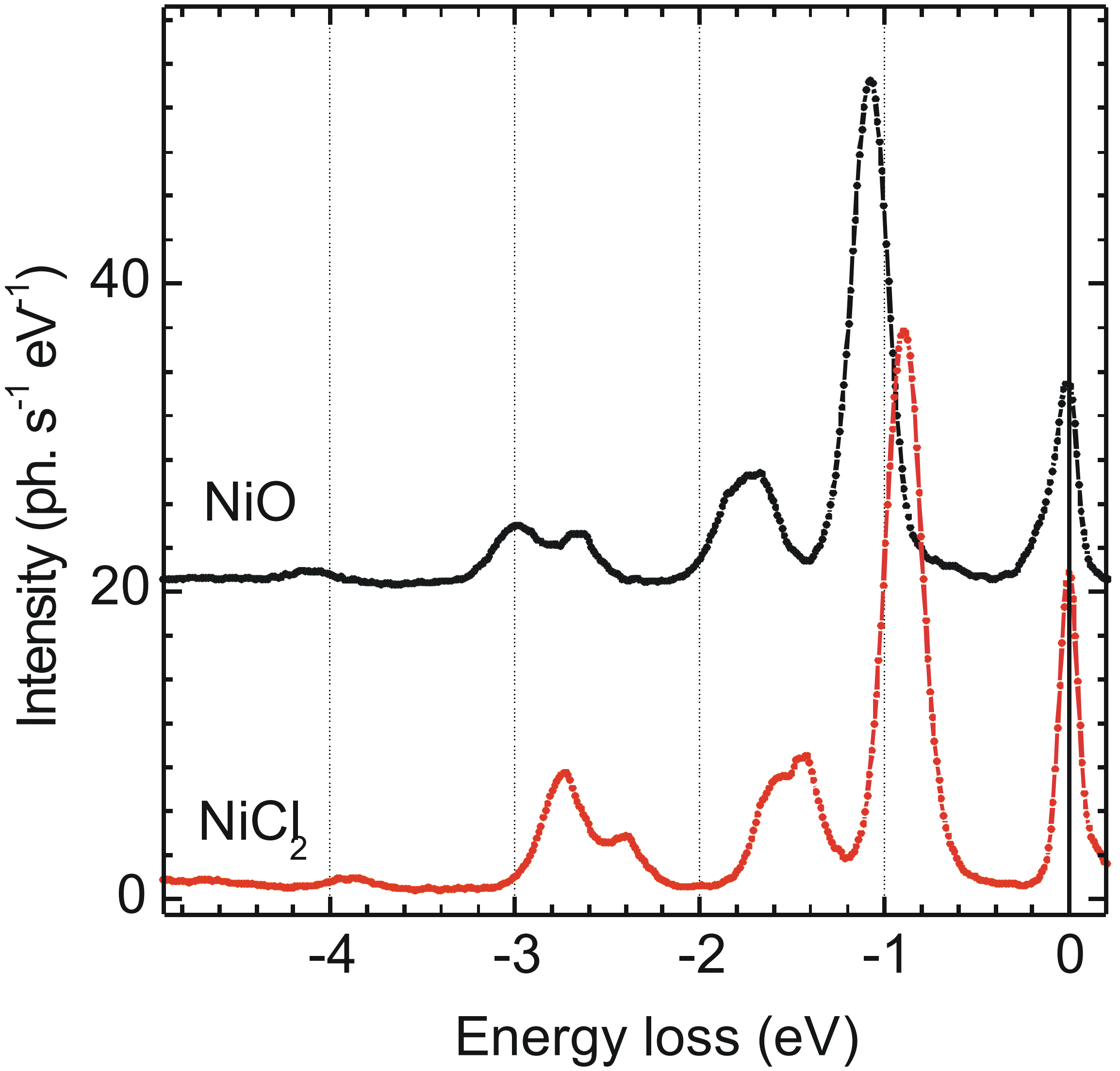
No spin excitations at Gamma point

Very weak signal with respect to the elastic peak

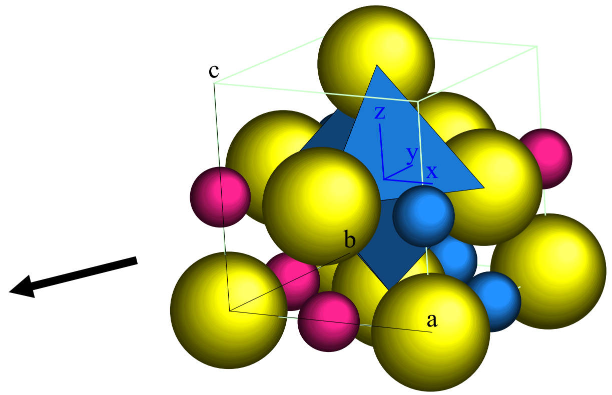
J. Schlappa et al NATURE 485, 82 (2012)

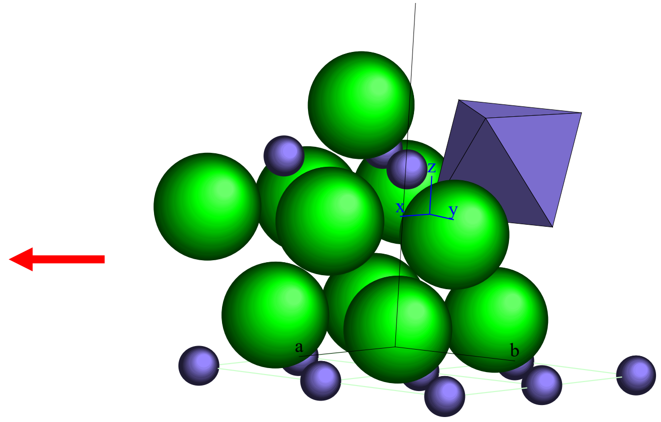
L.A. Wray et al arXiv:1203.2397v1

Ni L_3 edge: NiO, $NiCl_2$

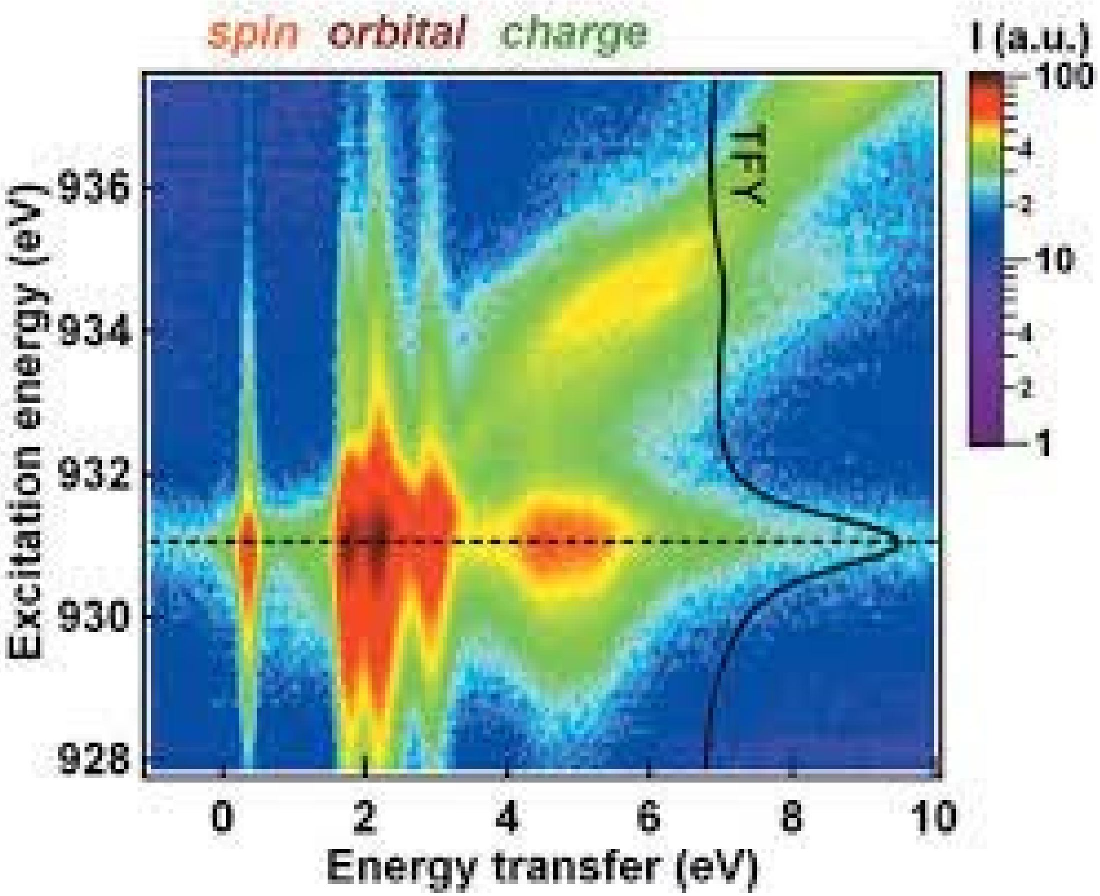


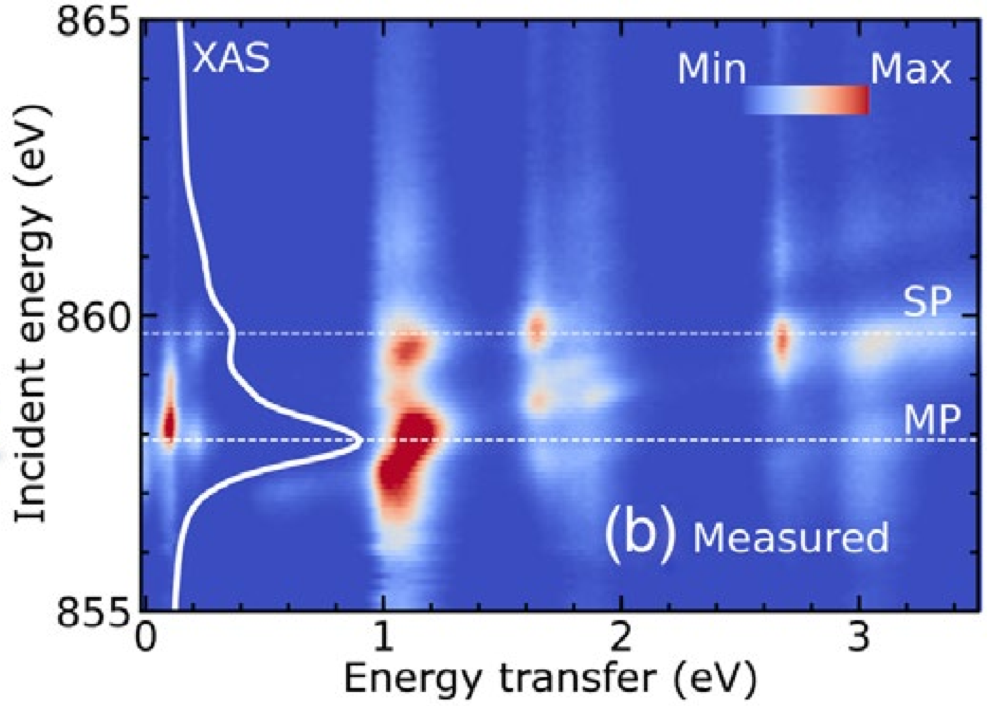
Ni^{2+} ($3d^8$) in octahedral coordination

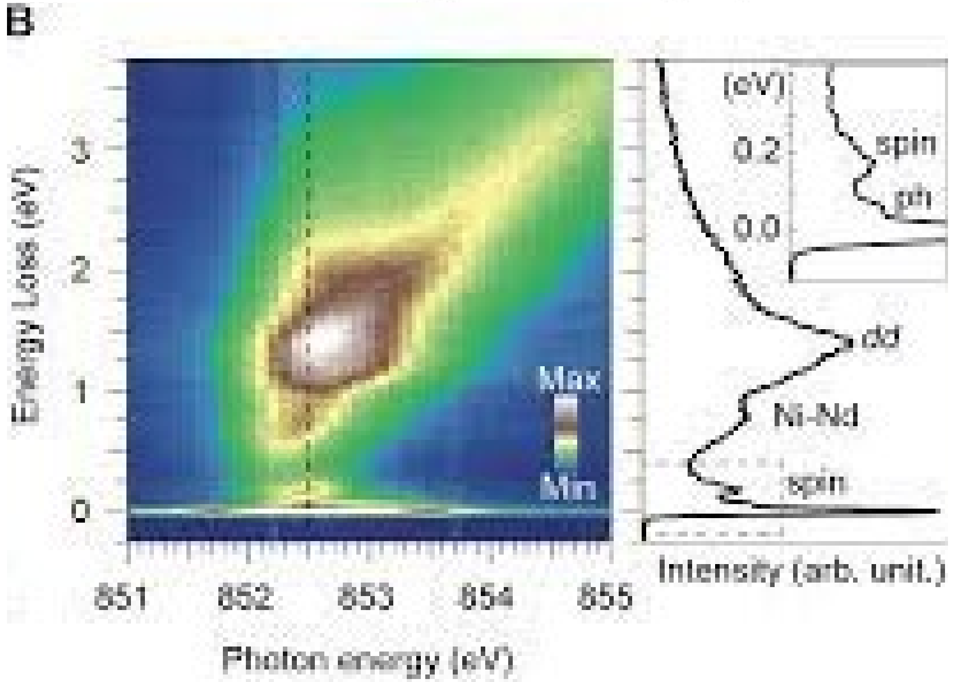




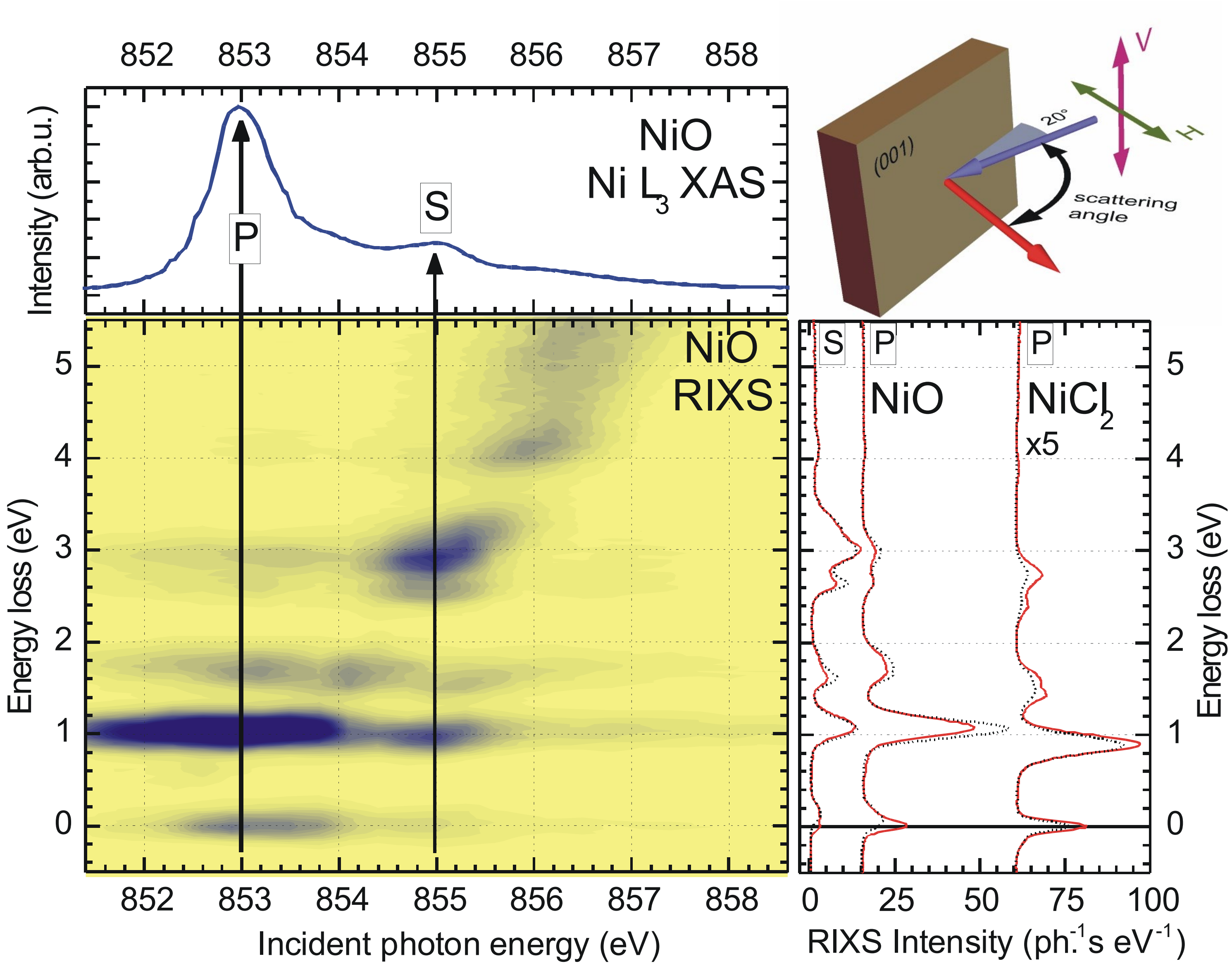
RIXS maps


spin orbital charge
I (a.u.)
100
10
1
TFY
Excitation energy (eV)
936
934
932
930
928
0
2
4
6
8
10
Energy transfer (eV)


865
860
855
Incident energy (eV)
XAS
Min
Max
SP
MP
(b) Measured
0
1
2
3
Energy transfer (eV)


B
Energy Loss (eV)
Max
Min
851
852
853
854
855
Photon energy (eV)
spin
ph
dd
Ni-Nd
spin
Intensity (arb. unit.)

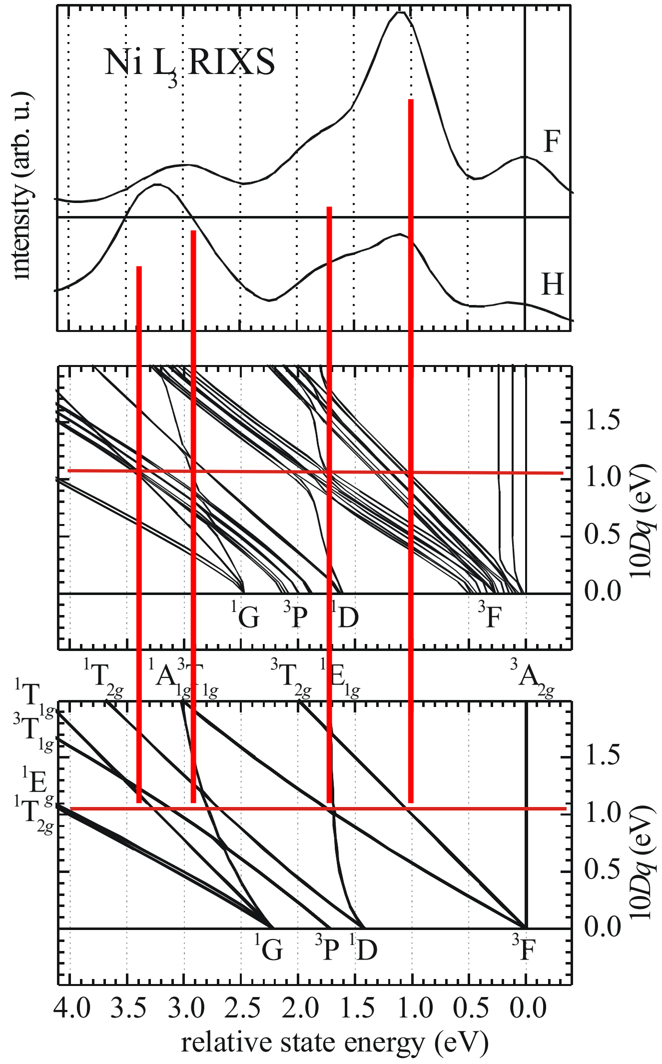
Ni^{2+} in NiO: dependence on incident photon energy

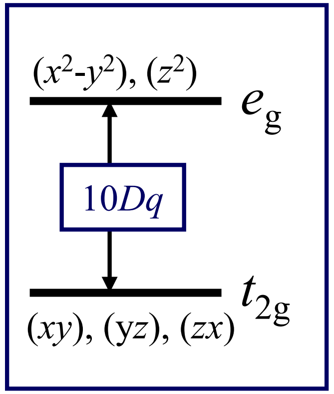


G. Ghiringhelli et al , Phys Rev Lett **102**, 027401 (2009)

Many excited states

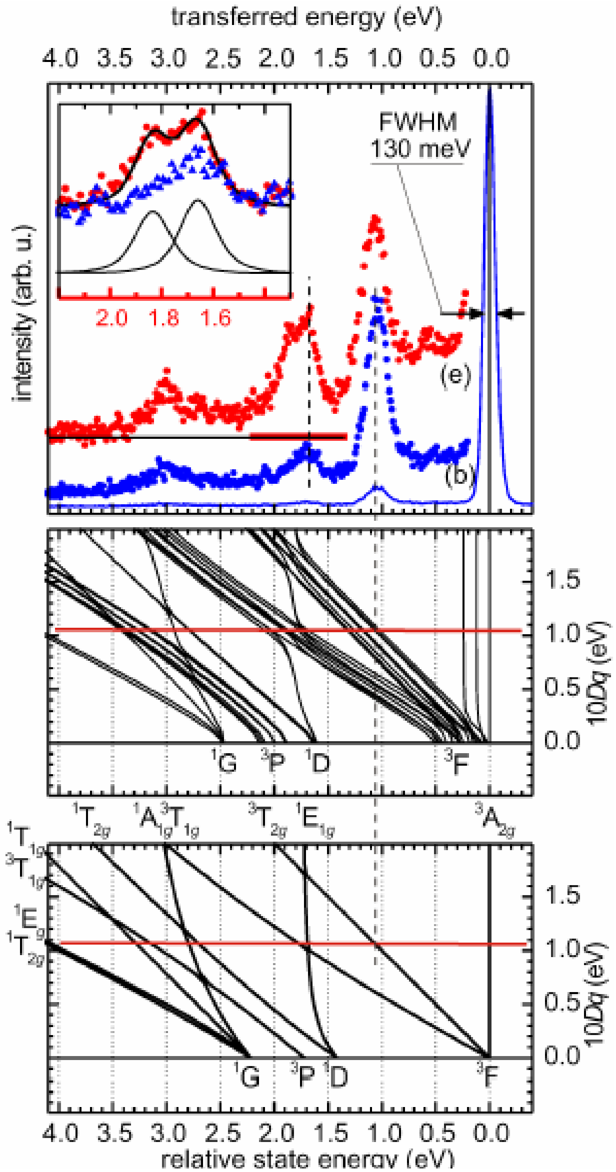
Crystal field model: Sugano-Tanabe diagrams





Single ion
Octahedral C.F.
3*d* spin-orbit
Exchange

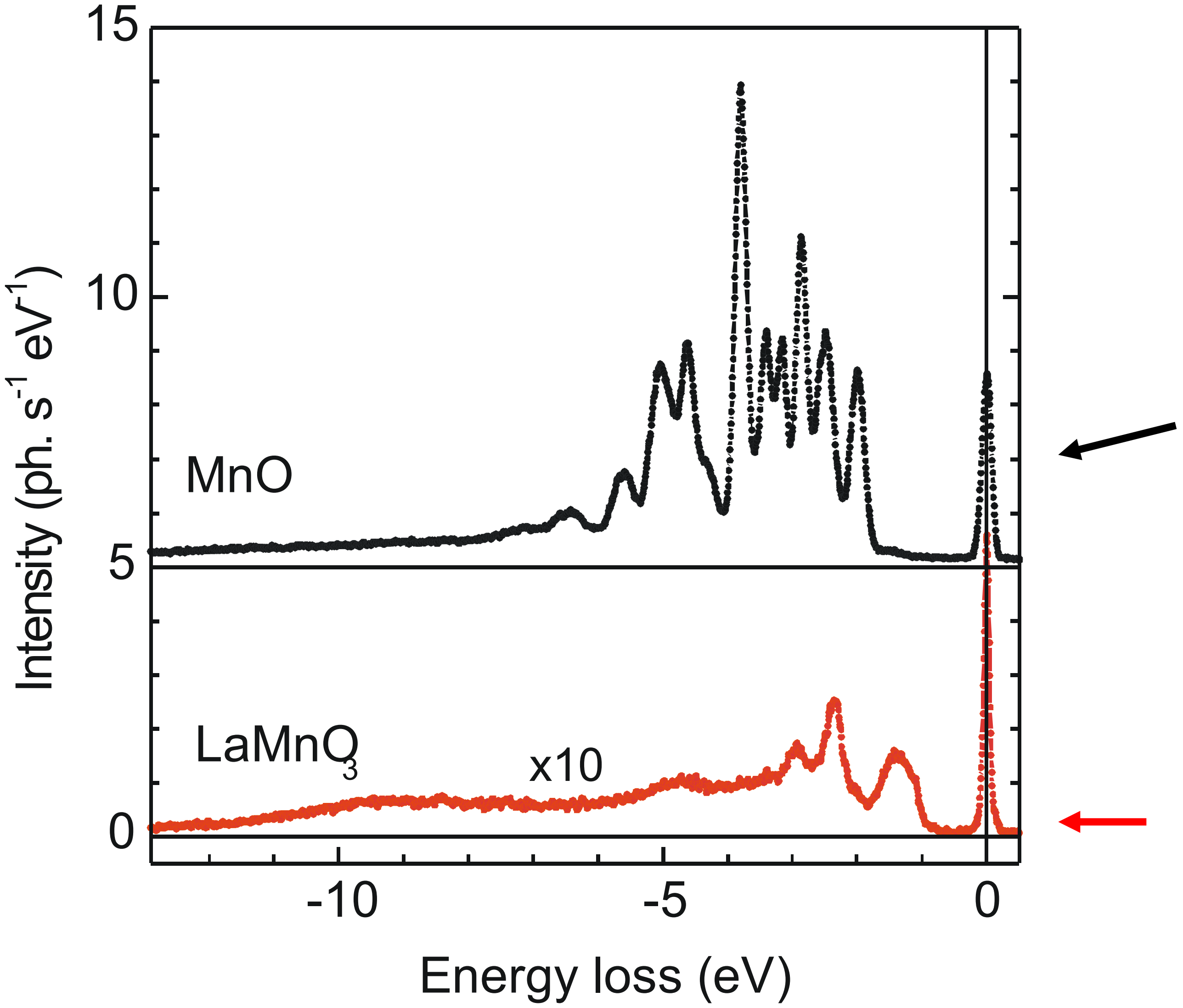
Single ion
Octahedral C.F.



G. Ghiringhelli *et al*, J. Phys. Cond. Mat. **17**, 5397 (2005)

S.G.Chiuzbaian, G. Ghiringhelli *et al*, Phys. Rev. Lett. **95**, 197402 (2005)

Mn L_3 edge: MnO, $LaMnO_3$



Mn^{2+} and Mn^{3+} in octahedral coordination

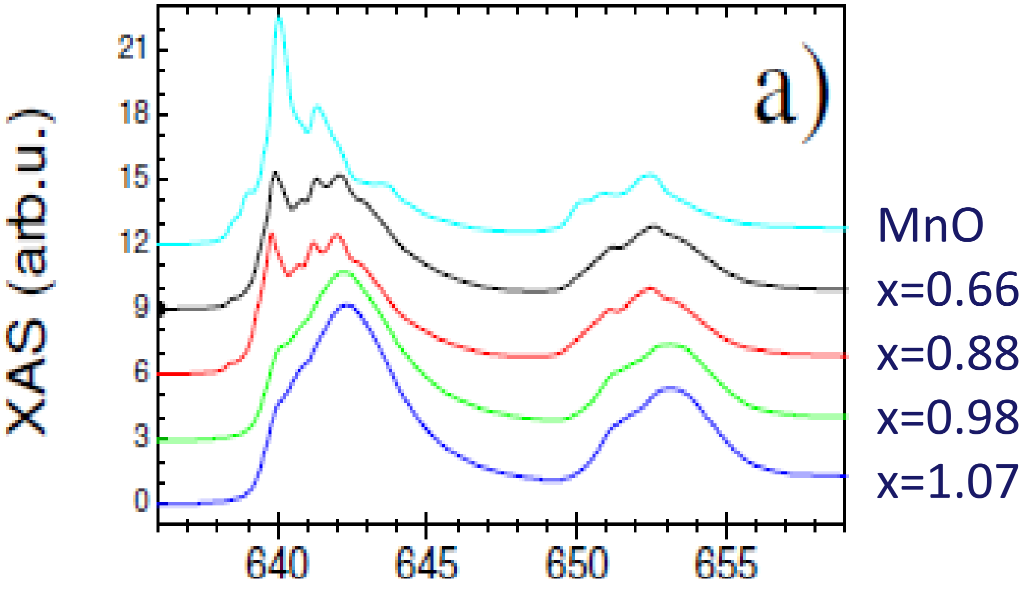
Mn^{2+}: $3d^5$

Mn^{3+}: $3d^4$

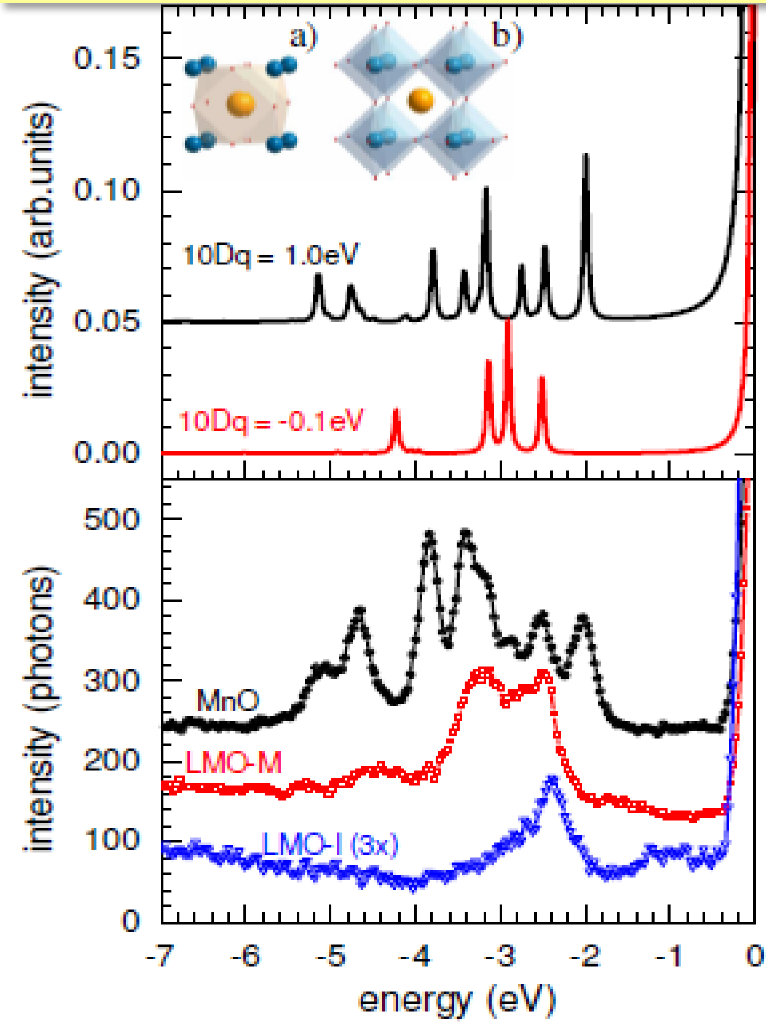
An application to thin film: Mn^{2+} in La_xMnO_3

La_xMnO_{3-d}/STO films
x=La/Mn ratio
for x<1 becomes FM (self doping)

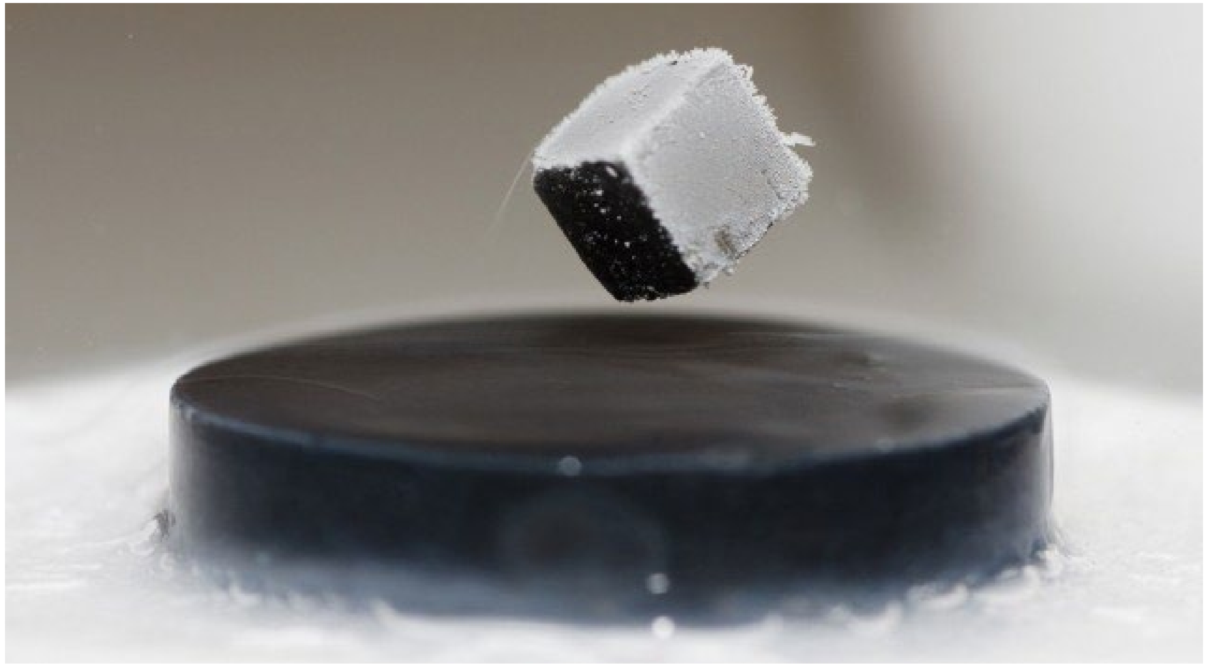
XAS reveals the presence of Mn^{2+} for x<1



RIXS shows that Mn^{2+} is at site A, ie, it replaces La^{3+}



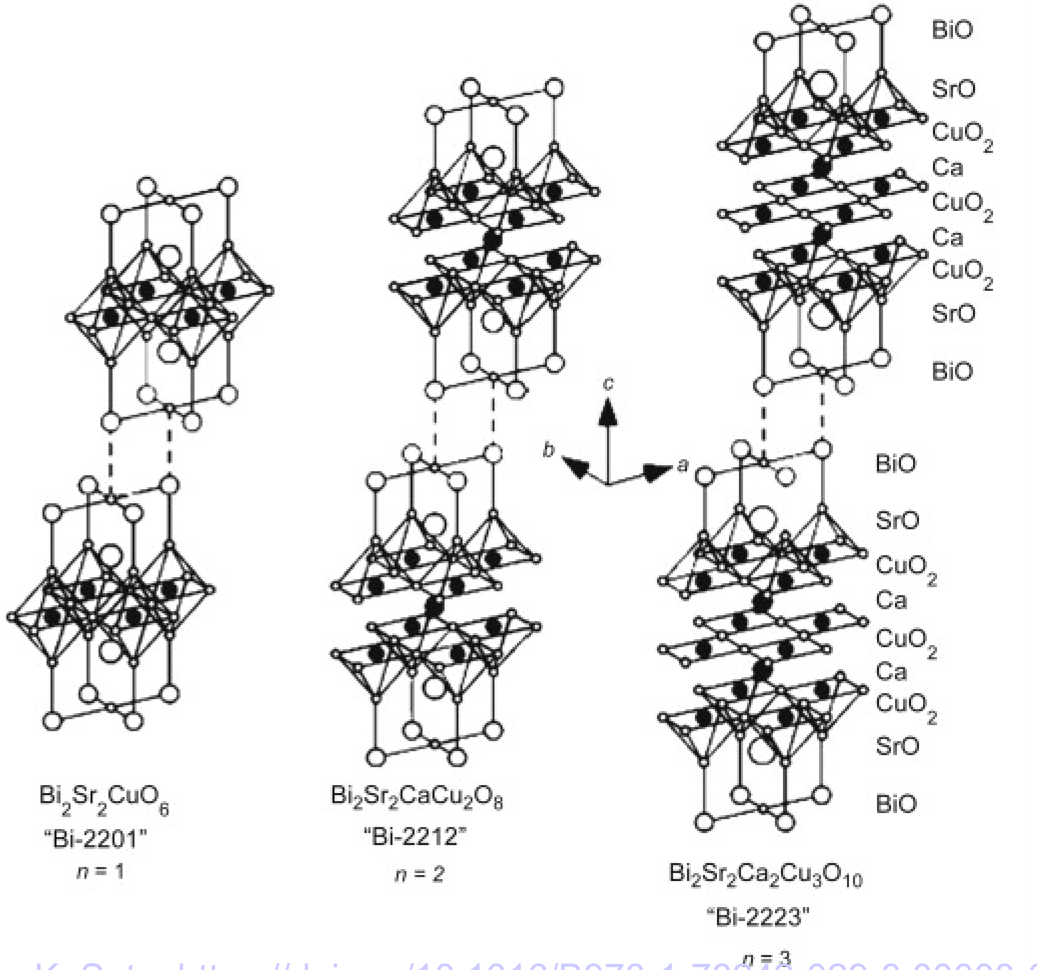
P. Orgiani, A. Galdi, C. Aruta, V. Cataudella, G. De Filippis, C.A. Perroni, V. Marigliano Ramaglia, R. Ciancio, N.B. Brookes, M. Moretti Sala, G. Ghiringhelli, and L. Maritato, Phys. Rev. B **82**, 205122 (2010)



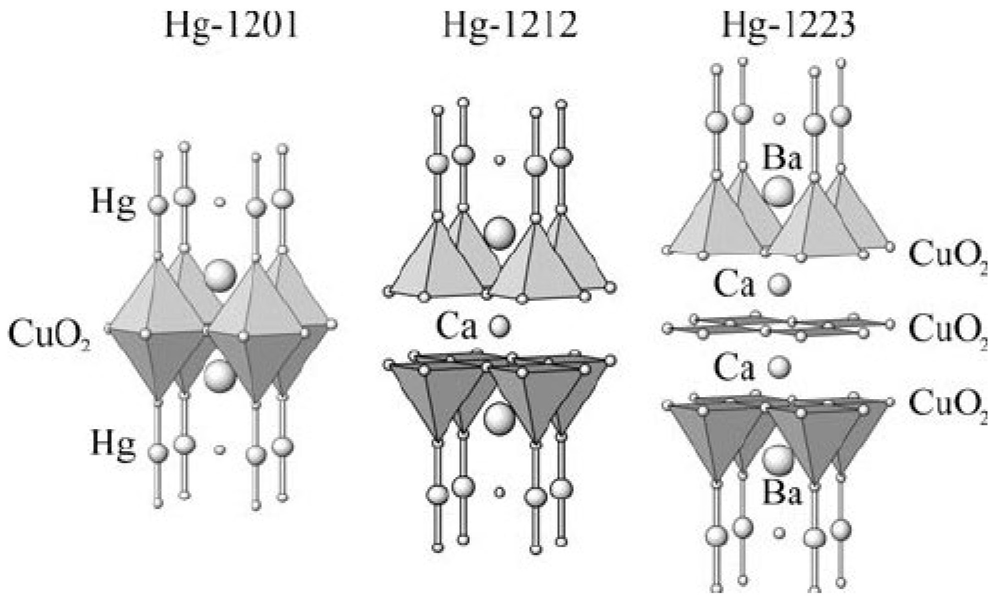
HIGH TC SUPERCONDUCTING CUPRATES

Quasi 2D materials: single layer, bi-layer, tri-layer

$Bi_2Sr_2CuO_{6+X}$ (Bi-2201)	$Bi_2Sr_2CaCu_2O_{8+X}$ (Bi-2212)	$(Bi, Pb)_2Sr_2Ca_2Cu_3O_{10+X}$ (Bi-2223)
T_c: ~20 K	T_c: ~90 K	T_c: 110-120 K

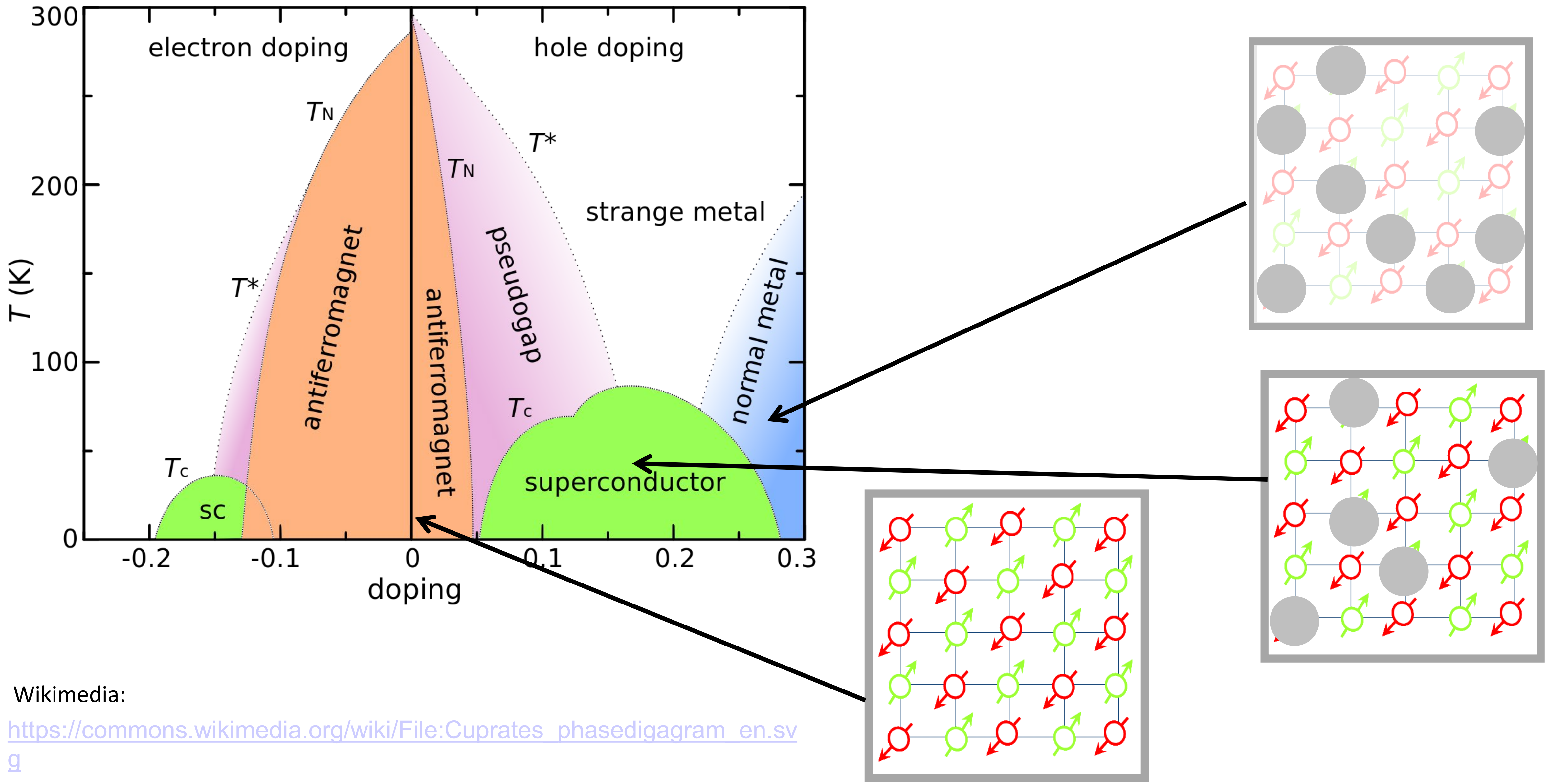


K. Sato, https://doi.org/10.1016/B978-1-78242-029-3.00003-0



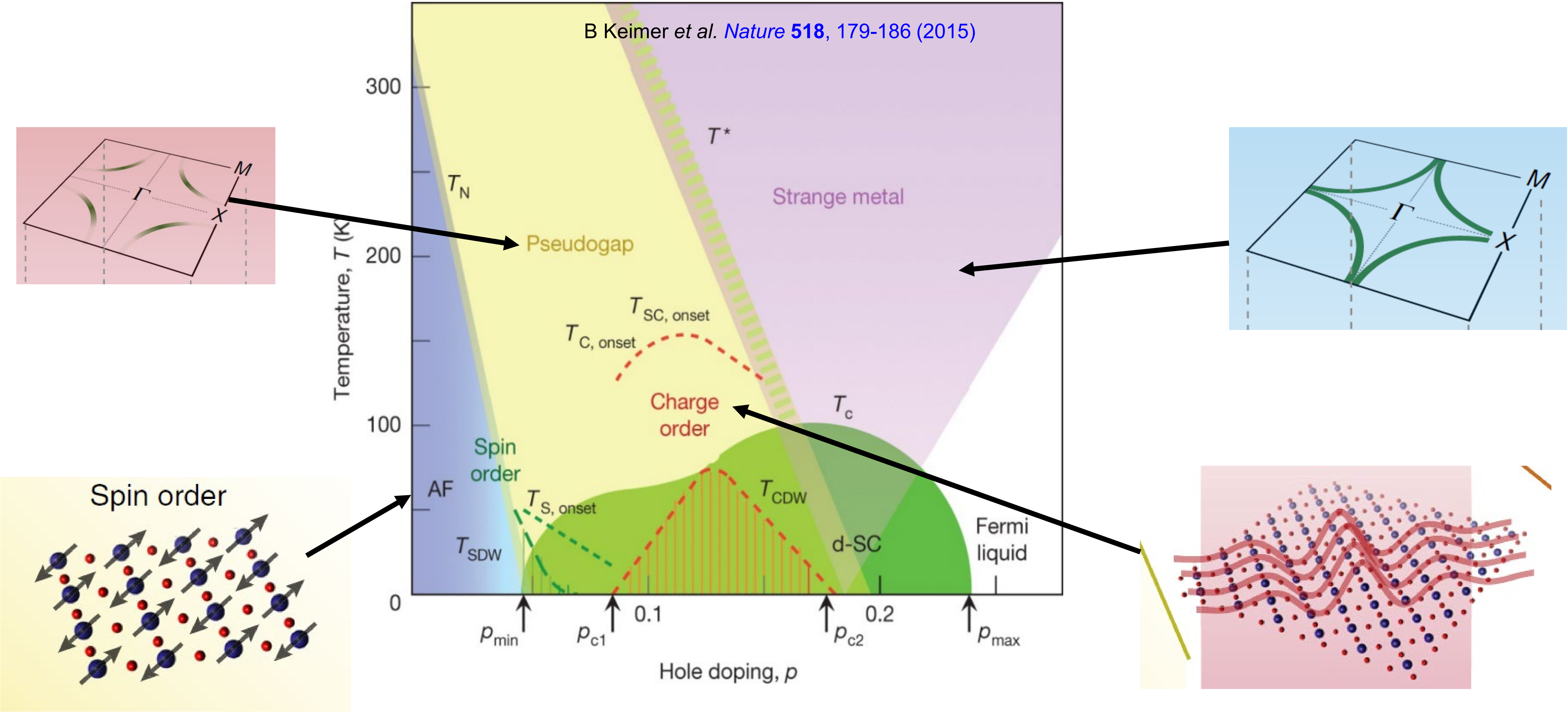
Antipov et al. : http://dx.doi.org/10.1088/0953-2048/15/7/201

The doping of the CuO_2 planes



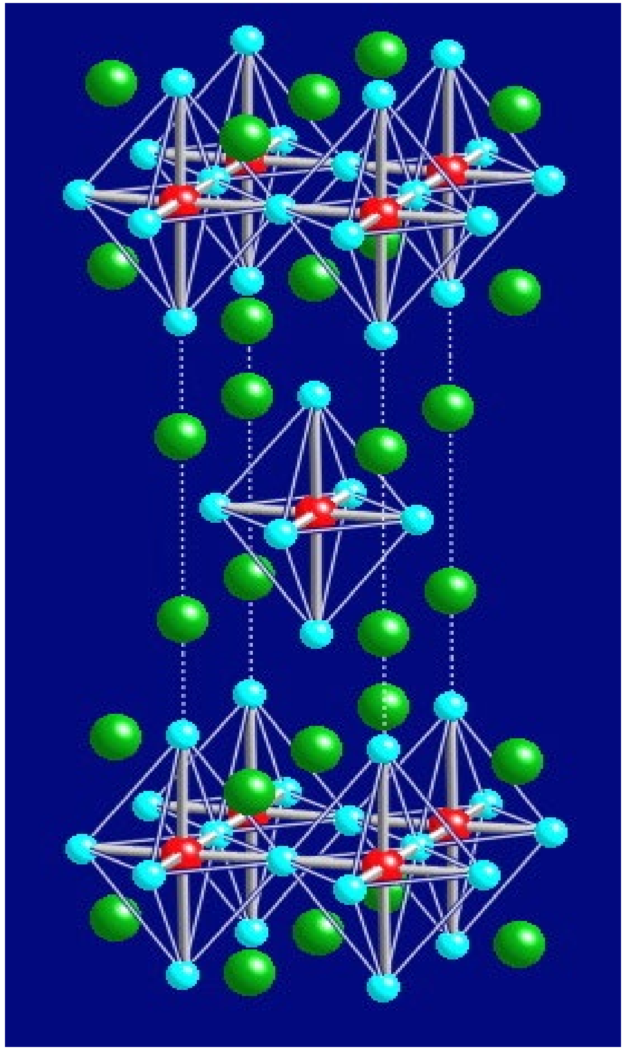
Wikimedia:
https://commons.wikimedia.org/wiki/File:Cuprates_phasedigagram_en.svg

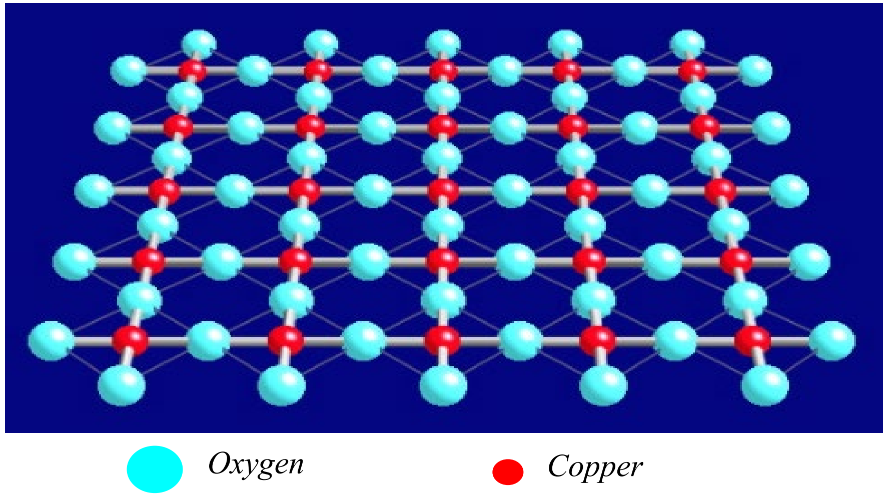
Cuprates: Magnetism, Charge Order and Superconductivity



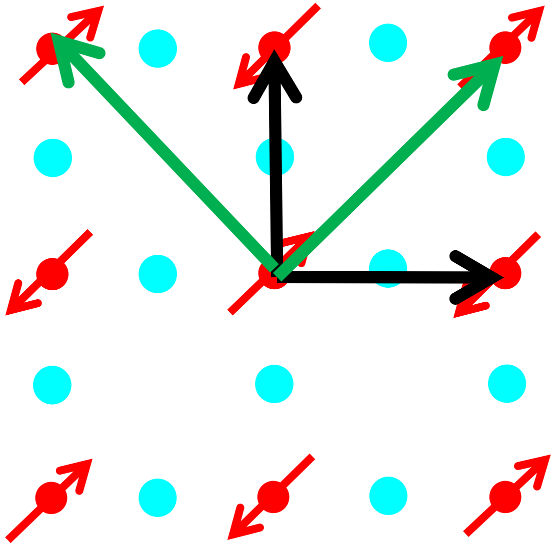
J. Pelliciari and R. Comin *Nature Materials* **17**, 661 (2018)

La_2CuO_4: 2D spin ½ Heisenberg AF insulator

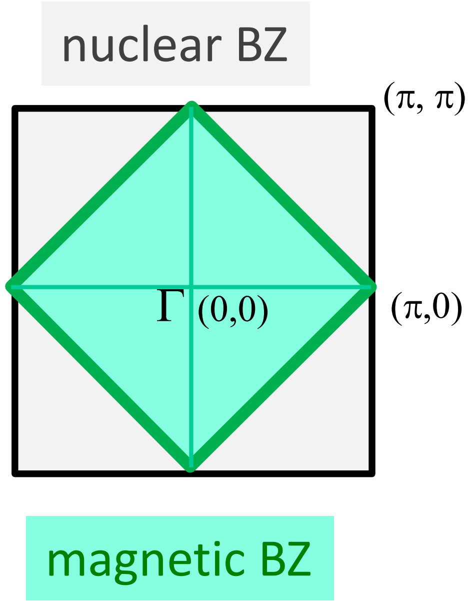




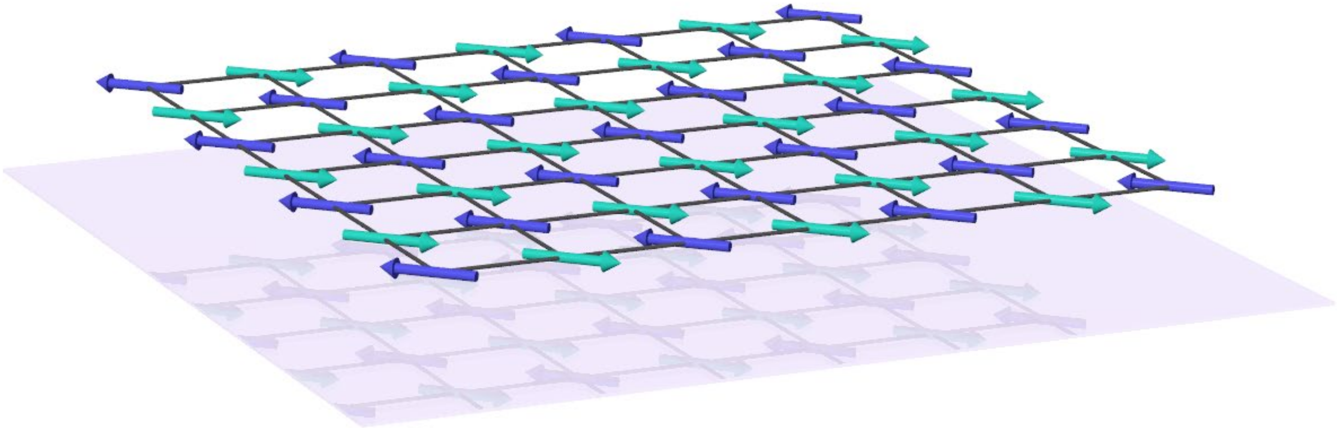
DIRECT SPACE

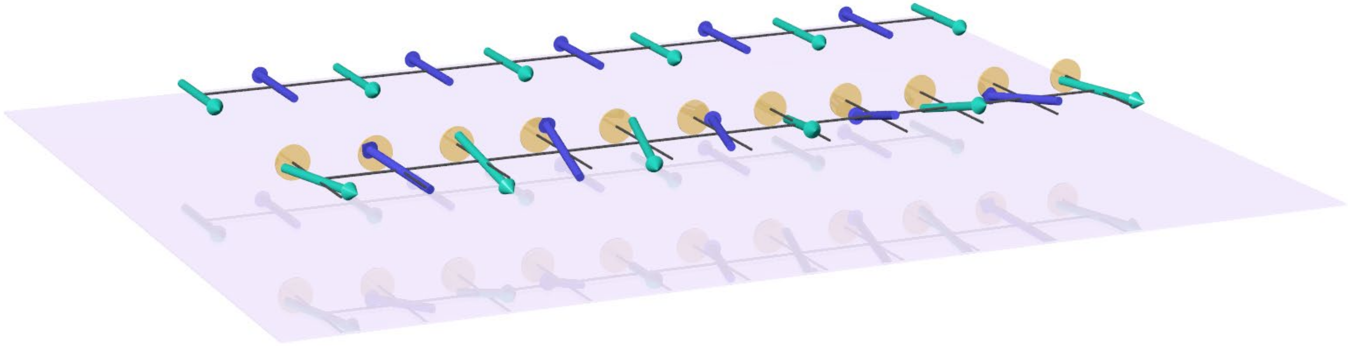


RECIPROCAL SPACE



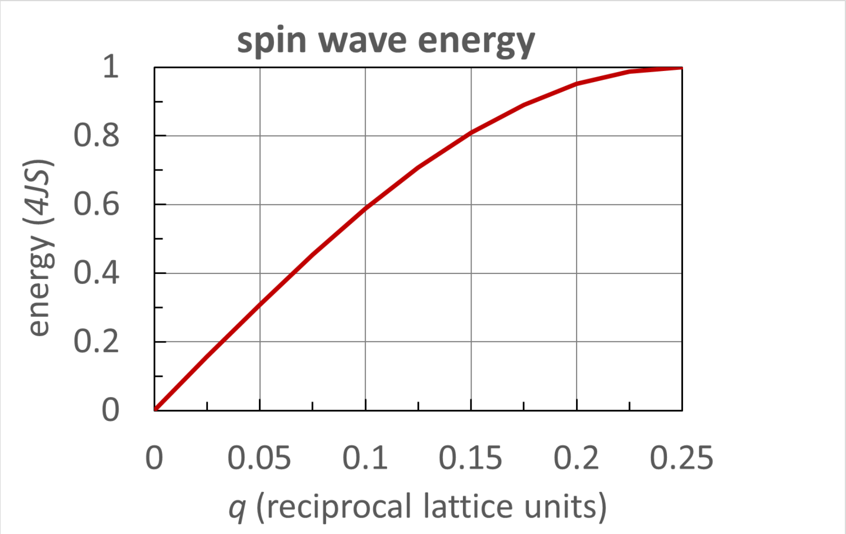
Elementary magnetic excitations are spin waves



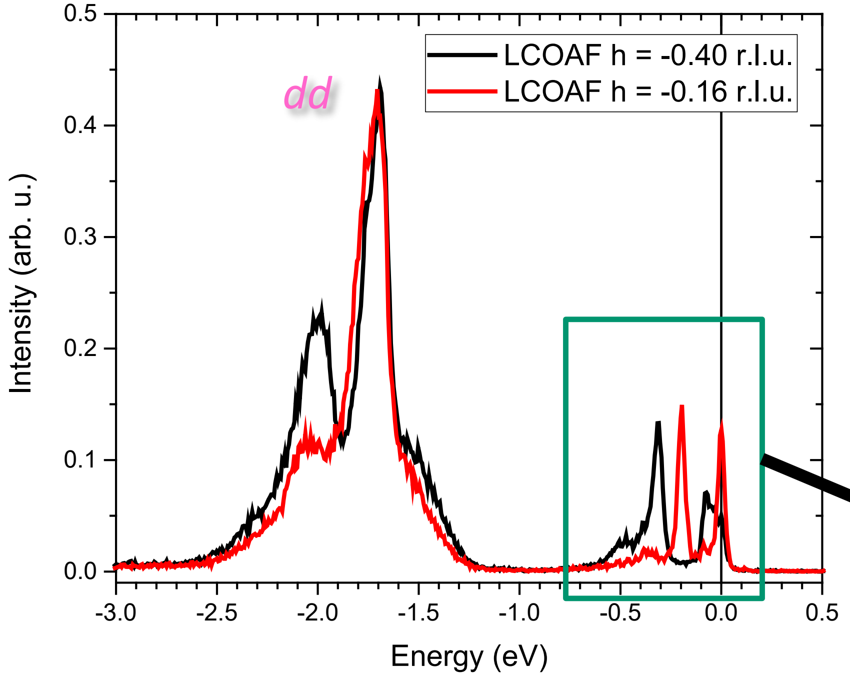


Part 4

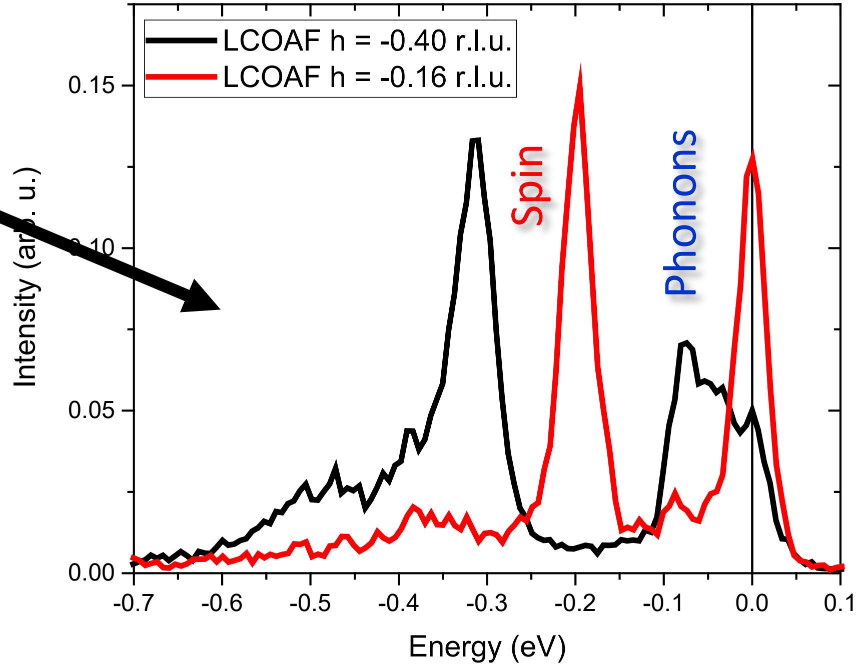
SPIN EXCITATIONS



High energy resolution is needed to look at spin excitations



La_2CuO_4
40 meV resolution
30 min accumulation

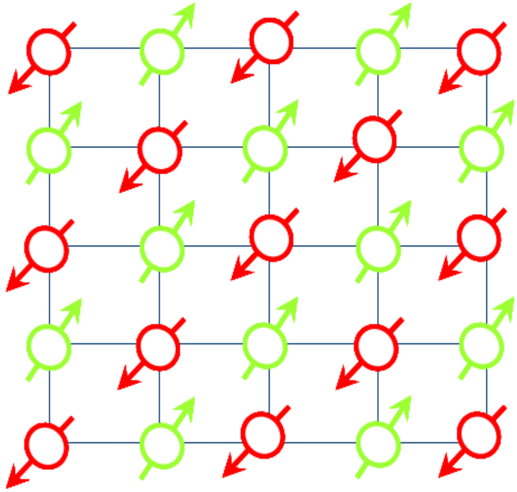


Instrumental BW of RIXS today: ~30 meV (at ESRF ID32, DLS I21, NSLS II SIX)

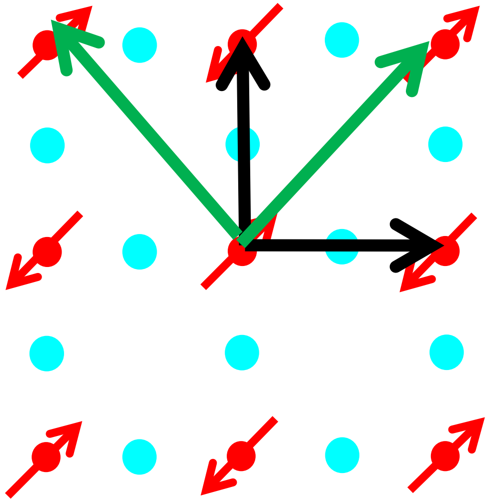
Spin excitations in cuprates: neutron scattering

2D AF

Square lattice

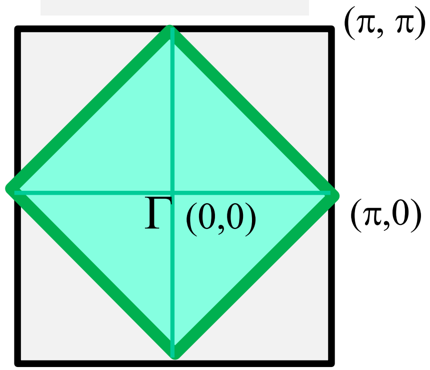


DIRECT SPACE



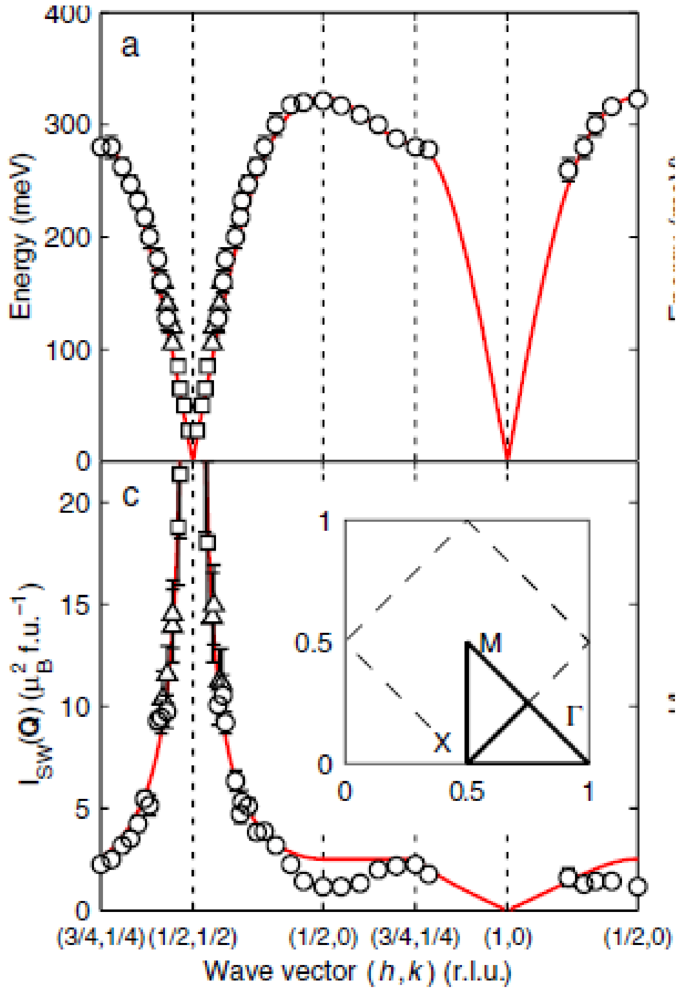
RECIPROCAL SPACE

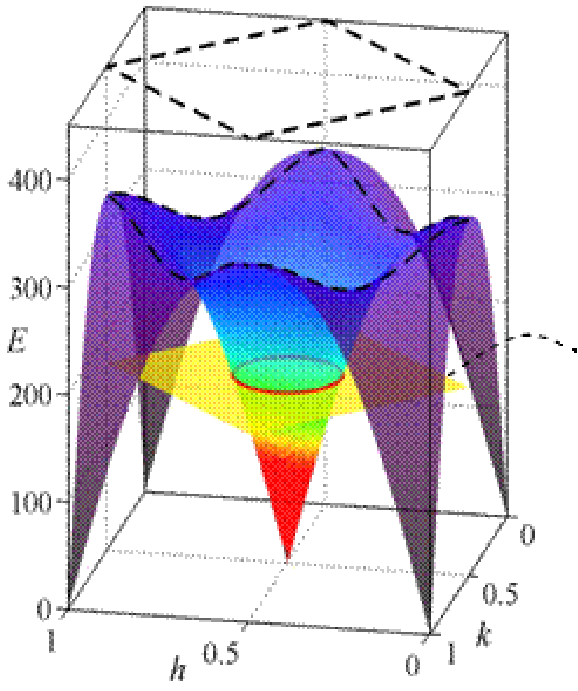
nuclear BZ



magnetic BZ

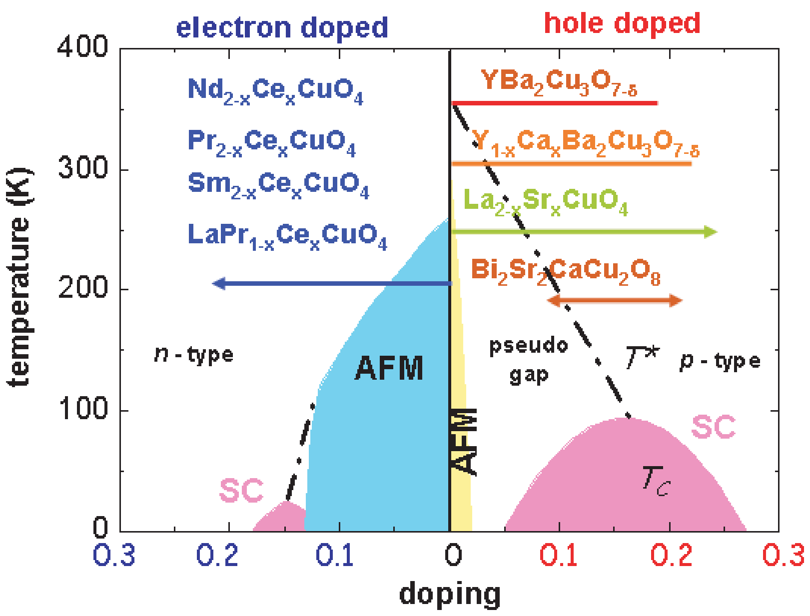
INS: La_2CuO_4



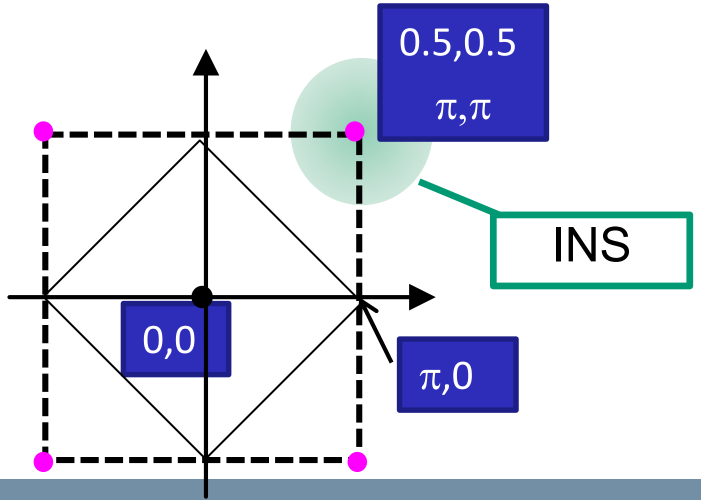


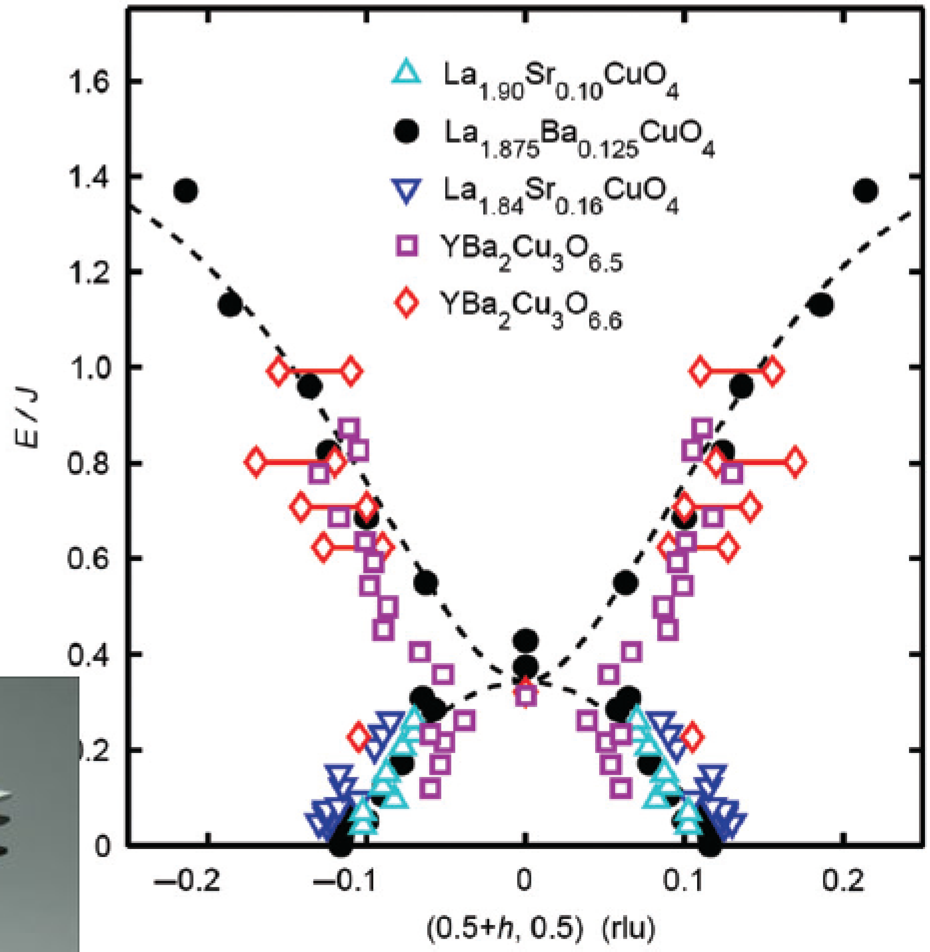
N. S. Headings, S. M. Hayden, R. Coldea, and T. G. Perring, Phys Rev Lett. **105** 247001 (2011)

Spin excitations in HTcS: doped SC



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

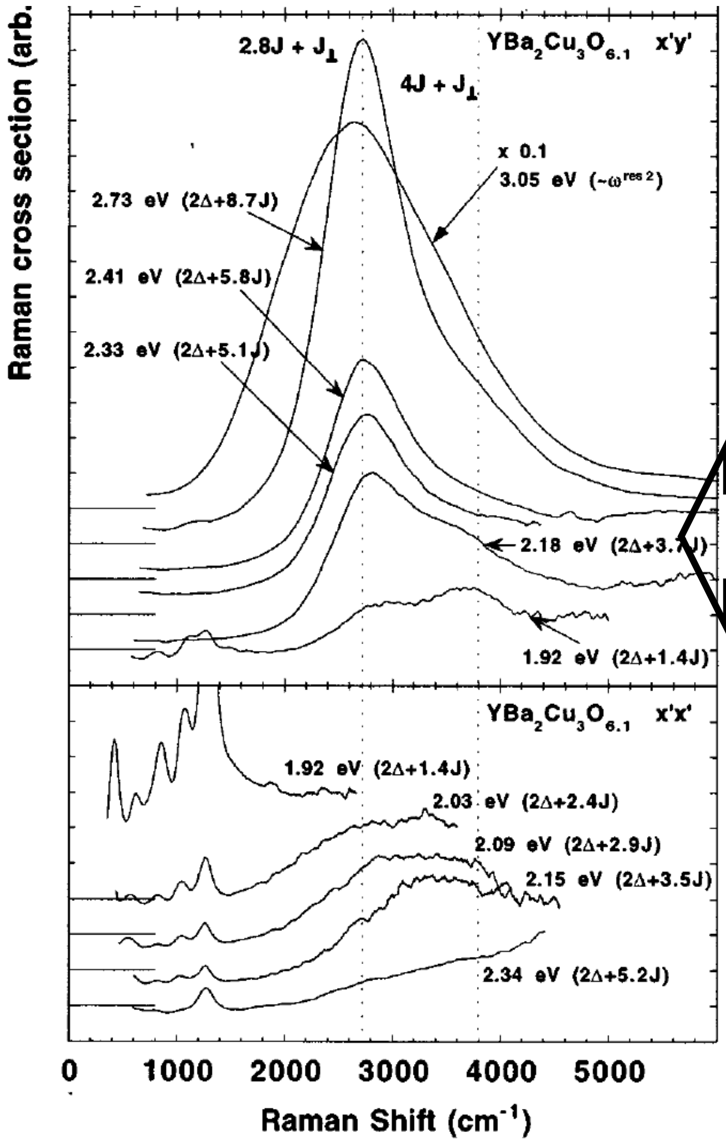




J.M. Tranquada, in *Handbook of High-Temperature Superconductivity: Theory and Experiment*, J.R. Schrieffer and J.S. Brooks, eds., Springer, 2007,

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

RIXS for spin excitations

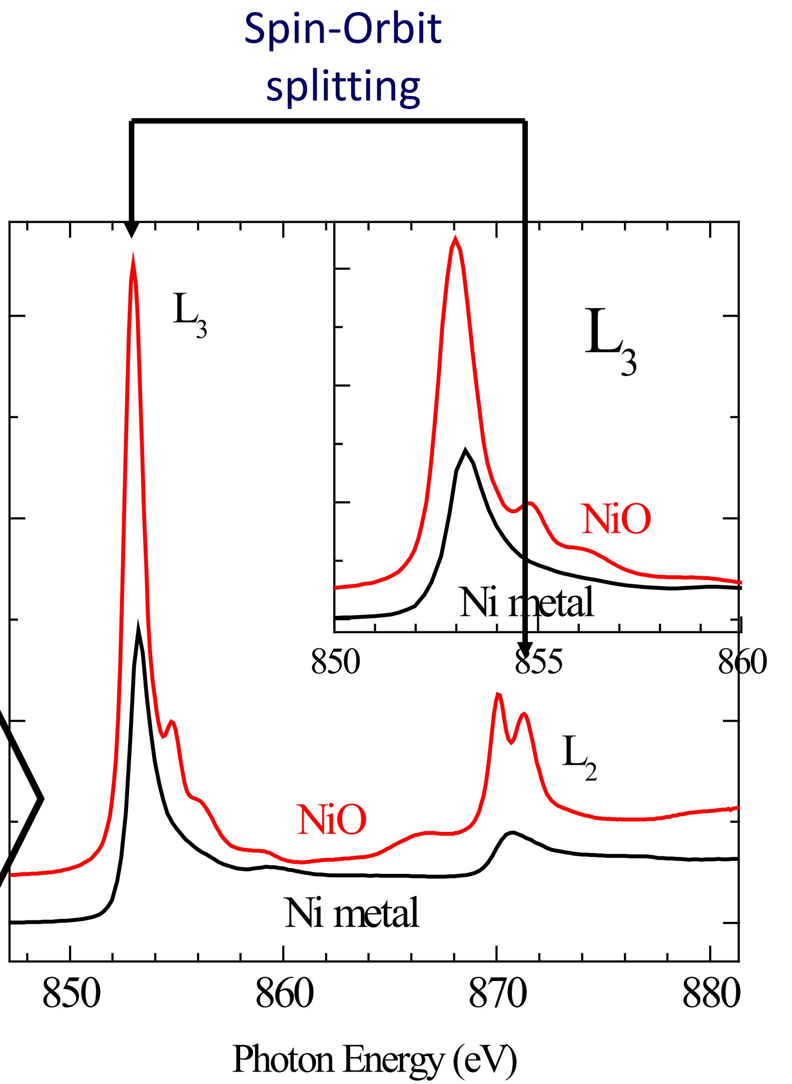


How can an x-ray photon reverse an electron spin, $\Delta S=1$?

We have learned that in radiative transitions the spin is conserved: $\Delta s_i=0$.

Indeed in Raman light scattering and optical absorption only bimagnons can be probed: $\Delta S=0$.

The secret is in the large spin-orbit interaction of 2*p* states of the 3dTM (Cu, Ni, etc), 10-20 eV.



G. Blumberg, P. Abbamonte, M. V. Klein, W. C. Lee, D. M. Ginsberg, L. L. Miller, and A. Zibold, Phys. Rev. B **53**, R11930 (1996).

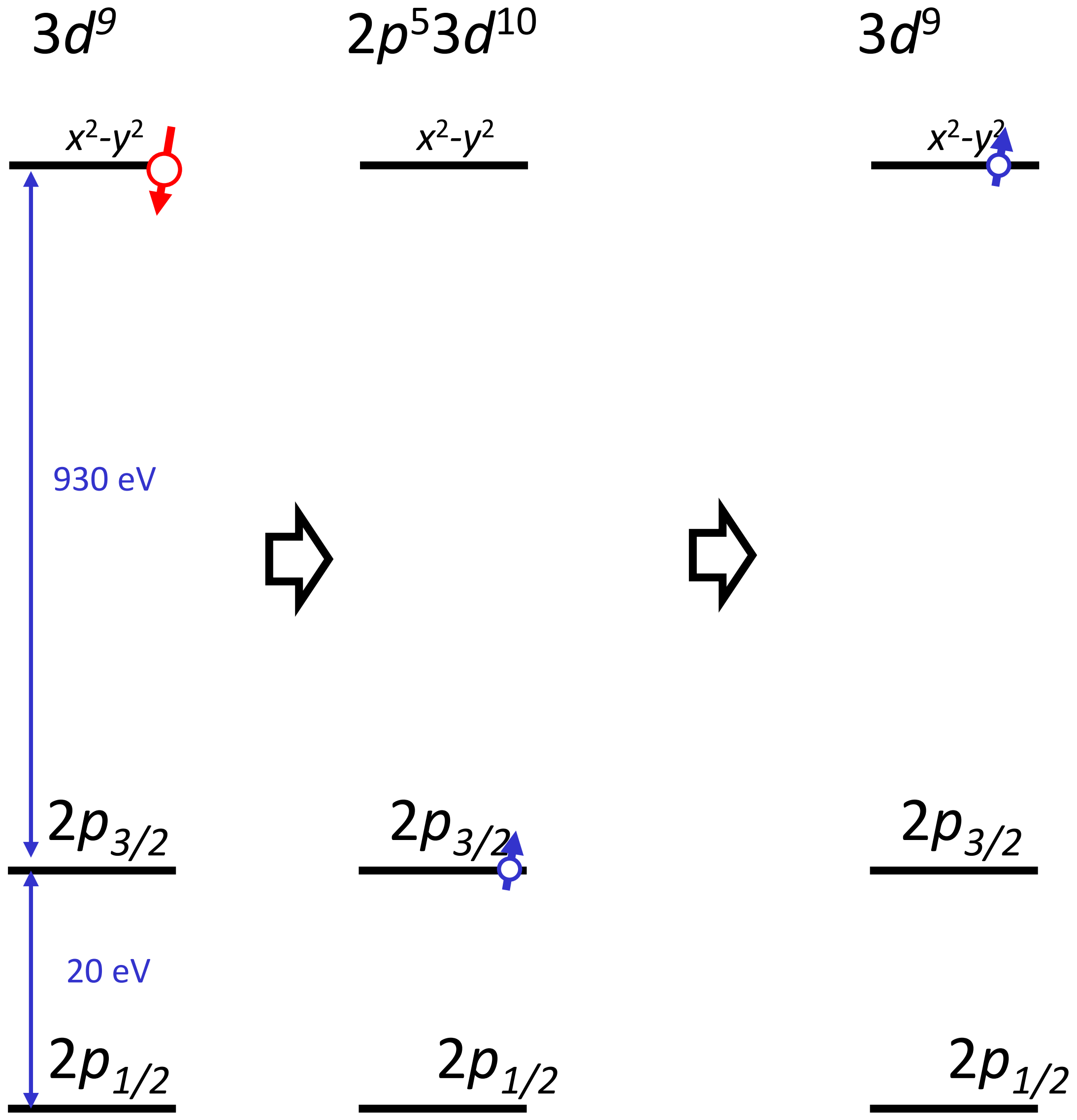
spin-flip excitations and the 2p S-O coupling

$3d$	E_g	$d_{3z^2-r^2}$	$Y_{2,0}$
		$d_{x^2-y^2}$	$\frac{Y_{2,2}+Y_{2,-2}}{\sqrt{2}}$
	T_{2g}	d_{xy}	$-i\frac{Y_{2,2}-Y_{2,-2}}{\sqrt{2}}$
		d_{yz}	$i\frac{Y_{2,1}+Y_{2,-1}}{\sqrt{2}}$
		d_{zx}	$-\frac{Y_{2,1}-Y_{2,-1}}{\sqrt{2}}$

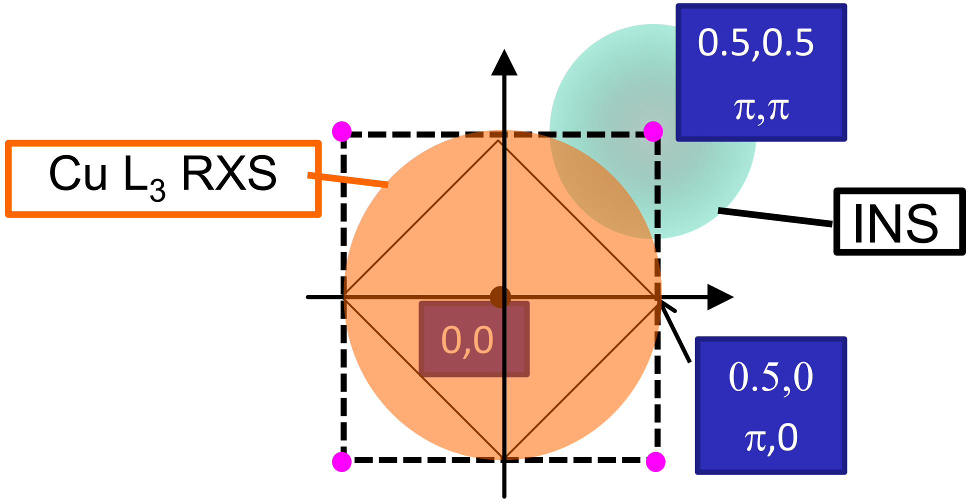
The 3d spin must not be pure UP or DOWN

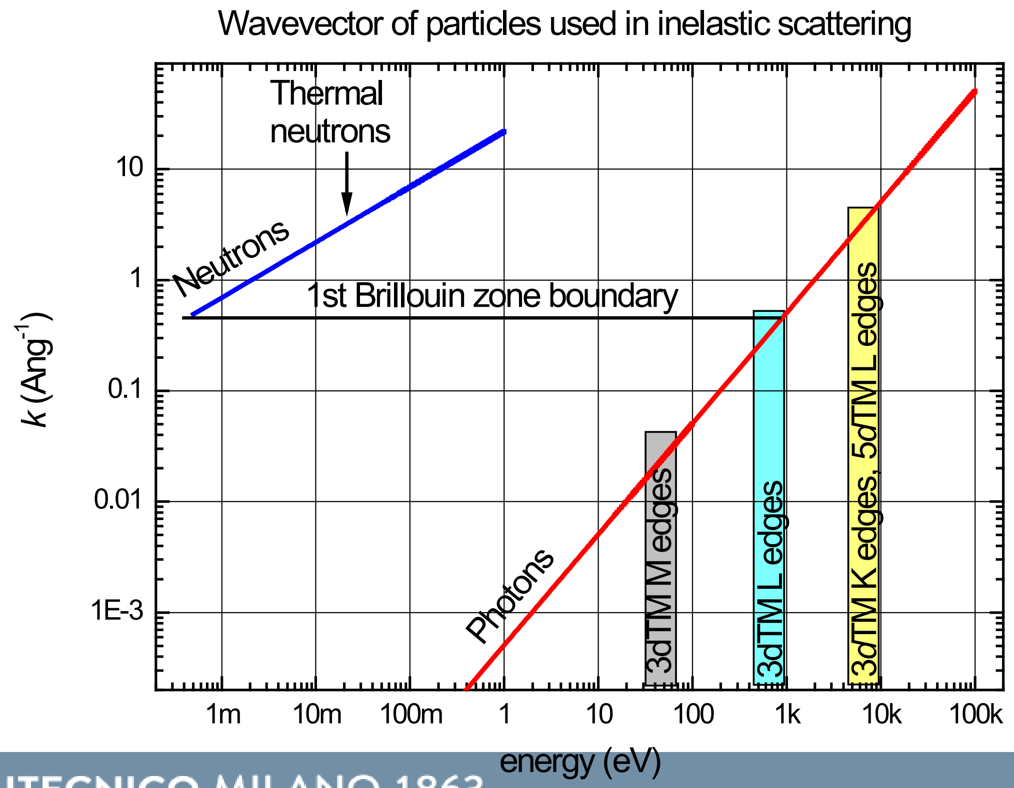
$2p_{3/2}$			
$\lvert\frac{3}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},\frac{1}{2}\rangle$	$\lvert\frac{3}{2},-\frac{1}{2}\rangle$	$\lvert\frac{3}{2},-\frac{3}{2}\rangle$
$Y^{\uparrow}_{1,1}$	$\frac{\sqrt{2}}{\sqrt{3}}Y^{\uparrow}_{1,0}+\frac{1}{\sqrt{3}}Y^{\downarrow}_{1,1}$	$\frac{1}{\sqrt{3}}Y^{\uparrow}_{1,-1}+\frac{\sqrt{2}}{\sqrt{3}}Y^{\downarrow}_{1,0}$	$Y^{\downarrow}_{1,-1}$

$2p_{1/2}$	
$\lvert\frac{1}{2},\frac{1}{2}\rangle$	$\lvert\frac{1}{2},-\frac{1}{2}\rangle$
$-\frac{1}{\sqrt{3}}Y^{\uparrow}_{1,0}+\frac{\sqrt{2}}{\sqrt{3}}Y^{\downarrow}_{1,1}$	$-\frac{\sqrt{2}}{\sqrt{3}}Y^{\uparrow}_{1,-1}+\frac{1}{\sqrt{3}}Y^{\downarrow}_{1,0}$



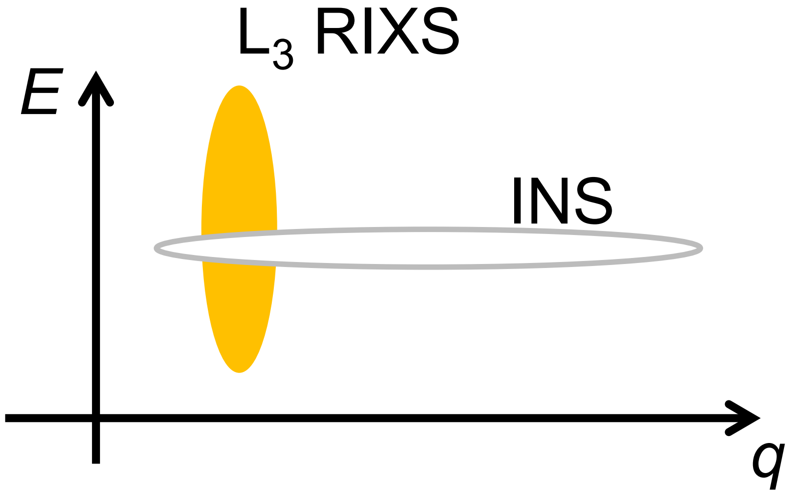
RIXS: Experimental conditions



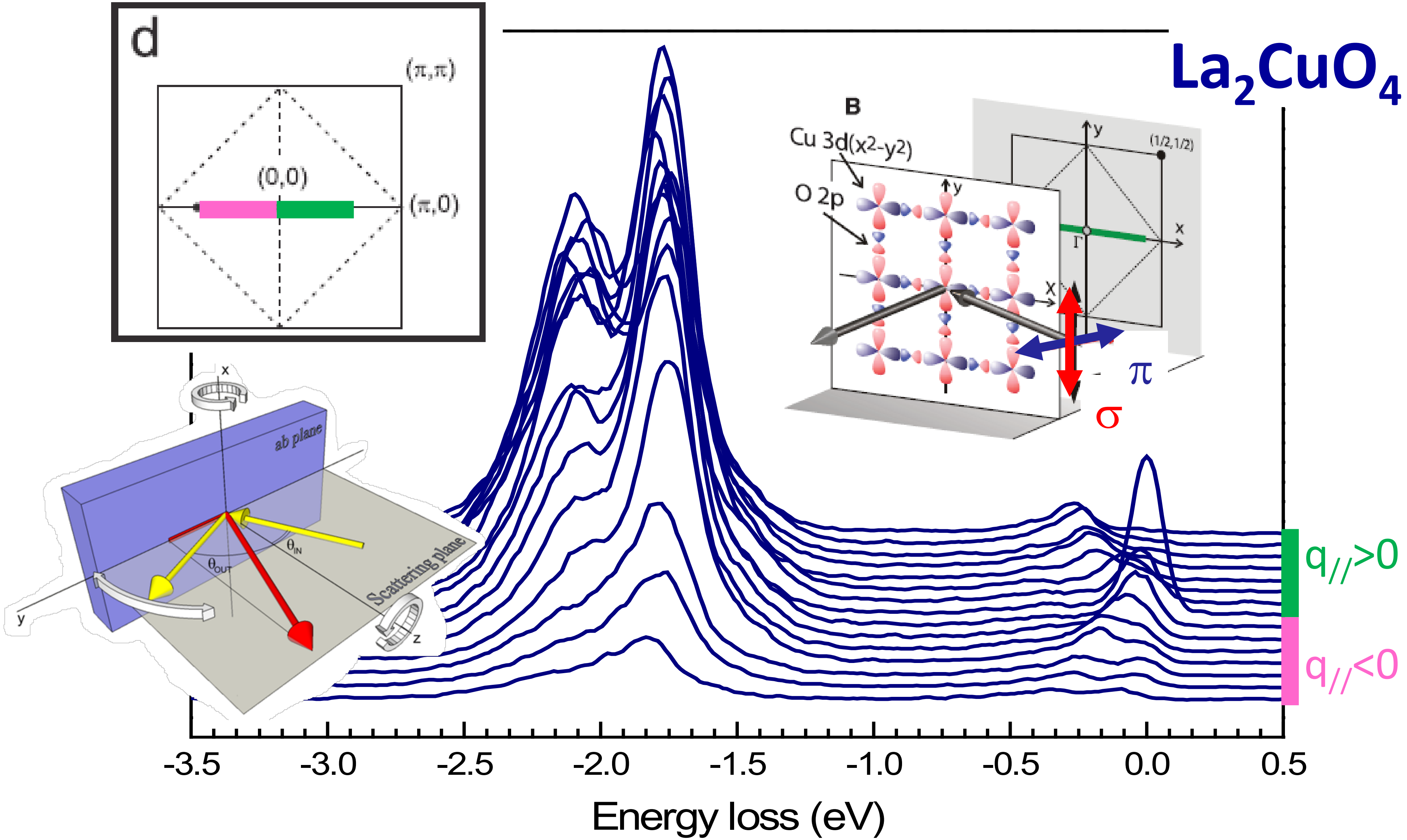


Cu L_3 resonance:

- E_0 = 930 eV
- q_{max} = 0.86 Ang^{-1}
- confined inside a region around Γ
- 2p core hole: spin-orbit interaction
- E resolution: 30-50 meV
- *q* resolution: 0.005 rlu
- 5-15 min per spectrum



First demonstration: La_2CuO_4



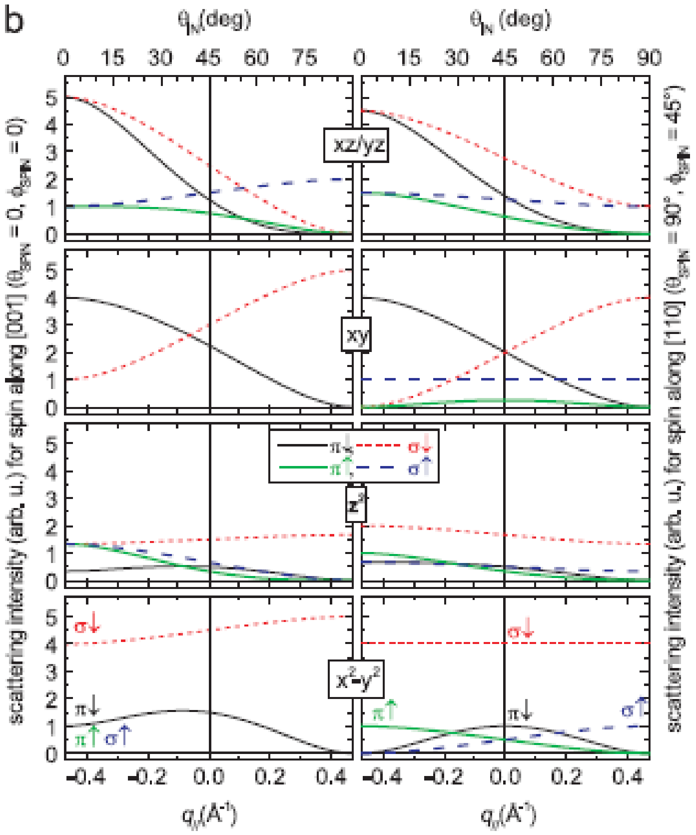
L. Braicovich, J. van den Brink, V. Bisogni, M. Moretti Sala, L. Ament, N.B. Brookes, G.M. de Luca, M. Salluzzo, T. Schmitt, and G. Ghiringhelli PRL **104** 077002 (2010)

Theory of magnetic RIXS (1)

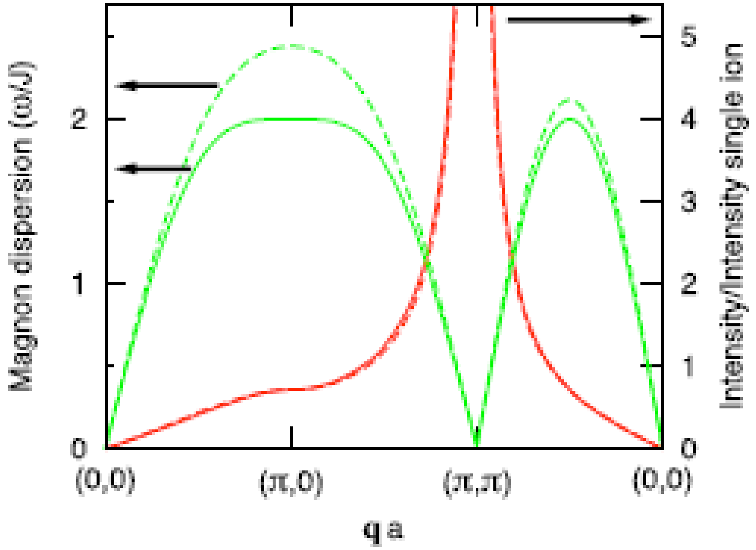
PRL 103, 117003 (2009) PHYSICAL REVIEW LETTERS week ending 11 SEPTEMBER 2009

Theoretical Demonstration of How the Dispersion of Magnetic Excitations in Cuprate Compounds can be Determined Using Resonant Inelastic X-Ray Scattering

Luuk J. P. Ament,[1,4] Giacomo Ghiringhelli,[2] Marco Moretti Sala,[2] Lucio Braicovich,[2] and Jeroen van den Brink[1,3,4]



Single ion cross section



Linear spin wave theory

Theory of magnetic RIXS (2)

PRL **105**, 167404 (2010) PHYSICAL REVIEW LETTERS week ending 15 OCTOBER 2010

Theory of Resonant Inelastic X-Ray Scattering by Collective Magnetic Excitations

M. W. Haverkort

Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart Germany

(Received 9 October 2009; published 15 October 2010)

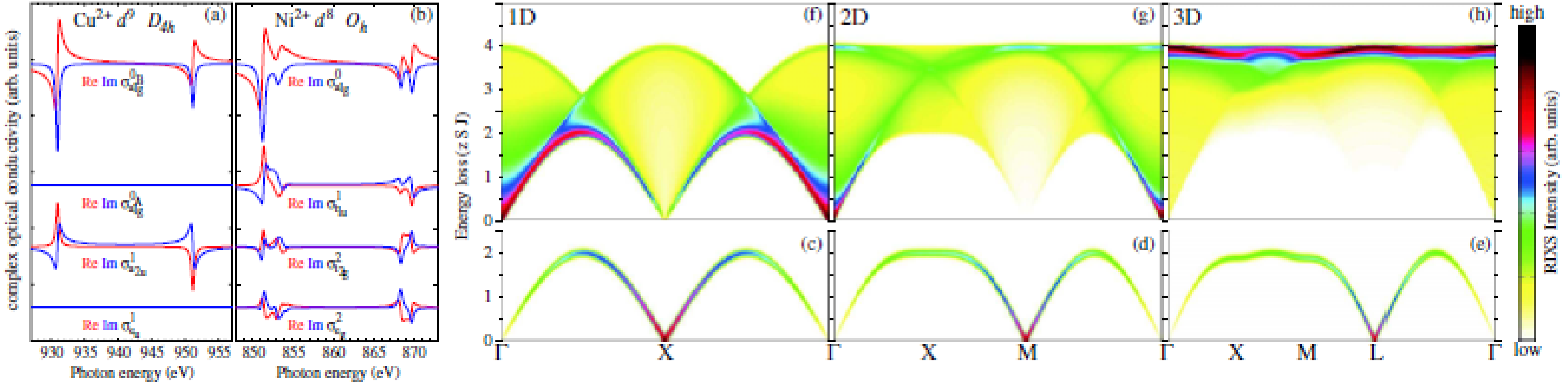
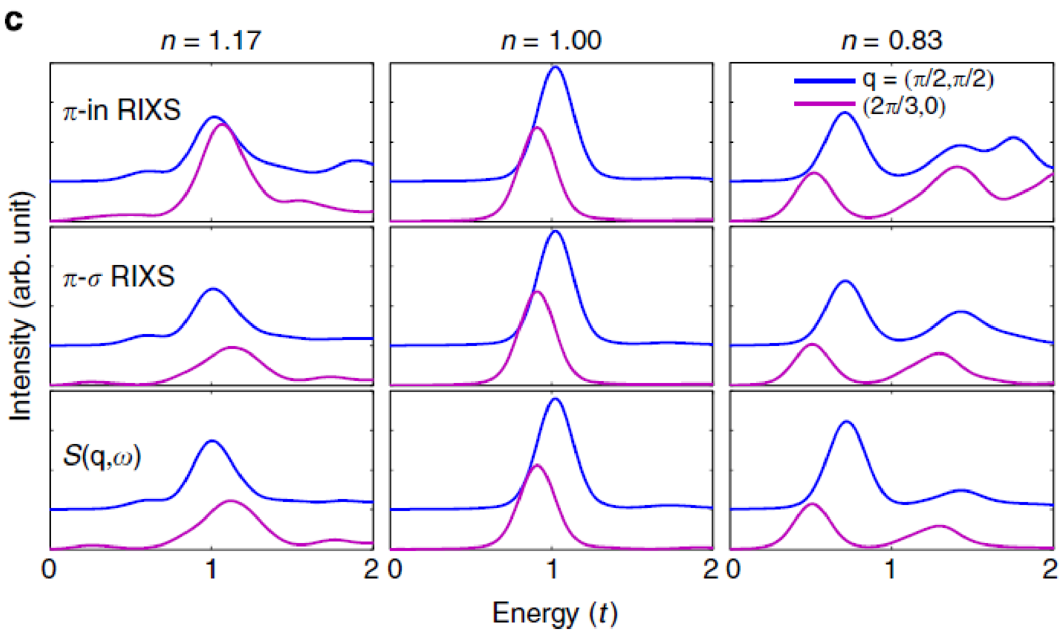


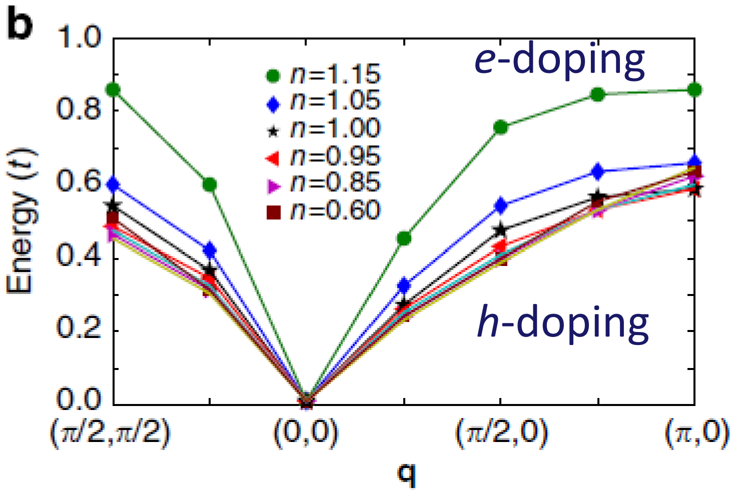
FIG. 1 (color online). Left: Fundamental x-ray absorption spectra that enter into the RIXS transition operator as energy dependent complex matrix elements calculated for (a) Cu^{2+} and (b) Ni^{2+}. Right: The Cu^{2+} and Ni^{2+} one magnon (c)–(e) and Ni^{2+} two magnon (f)–(h) RIXS spectral function, calculated using linear spin-wave theory for a 1D chain (c),(f), a 2D square (d),(g), and a 3D cubic (e),(h) Heisenberg model in energy loss units of zSJ (number of neighbors × spin × exchange constant).

Theory of magnetic RIXS (3)

What is the relation between RIXS and $S(\mathbf{q},\omega)$?

$S(\mathbf{q},\omega)$ vs p





RIXS measures $S(\mathbf{q},\omega)$ quite well

Spin excitations harden with *e*-doping, and change very little with *h*-doping.

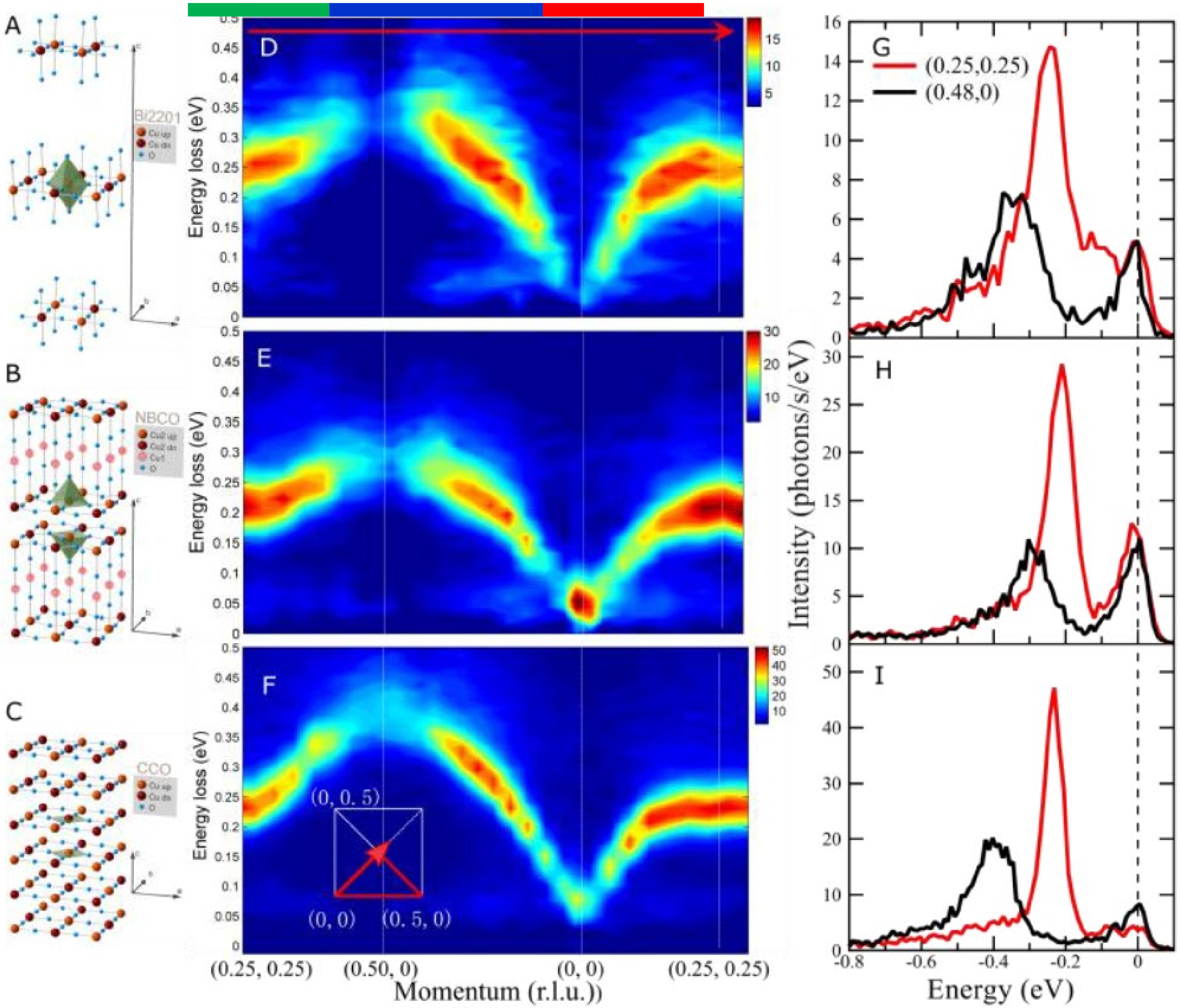
C.J. Jia, E.A. Nowadnick, K. Wohlfeld, Y.F. Kung, C.-C. Chen, S. Johnston, T. Tohyama, B. Moritz & T.P. Devereaux, NATURE COMMUNICATIONS , 5:3314 (2014)

Spin-waves with Cu L_3 RIXS

$Bi_2Sr_2CuO_6$

$NdBa_2Cu_3O_{6.1}$

$CaCuO_2$



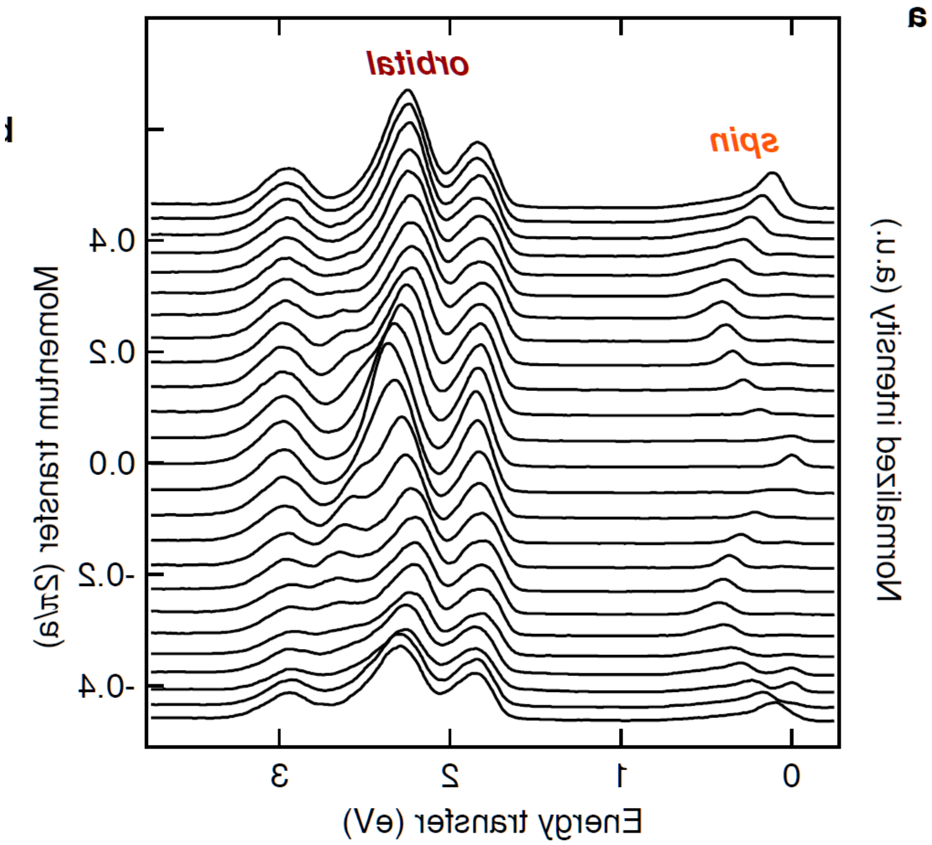
Y. Y. Peng, G. Dellea, M. Minola, M. Conni, A. Amorese, D. Di Castro, G. M. De Luca, K. Kummer, M. Salluzzo, X. Sun, X. J. Zhou, G. Balestrino, M. Le Tacon, B. Keimer, L. Braicovich, N. B. Brookes and G. Ghiringhelli, *Nature Physics* **13** 1201

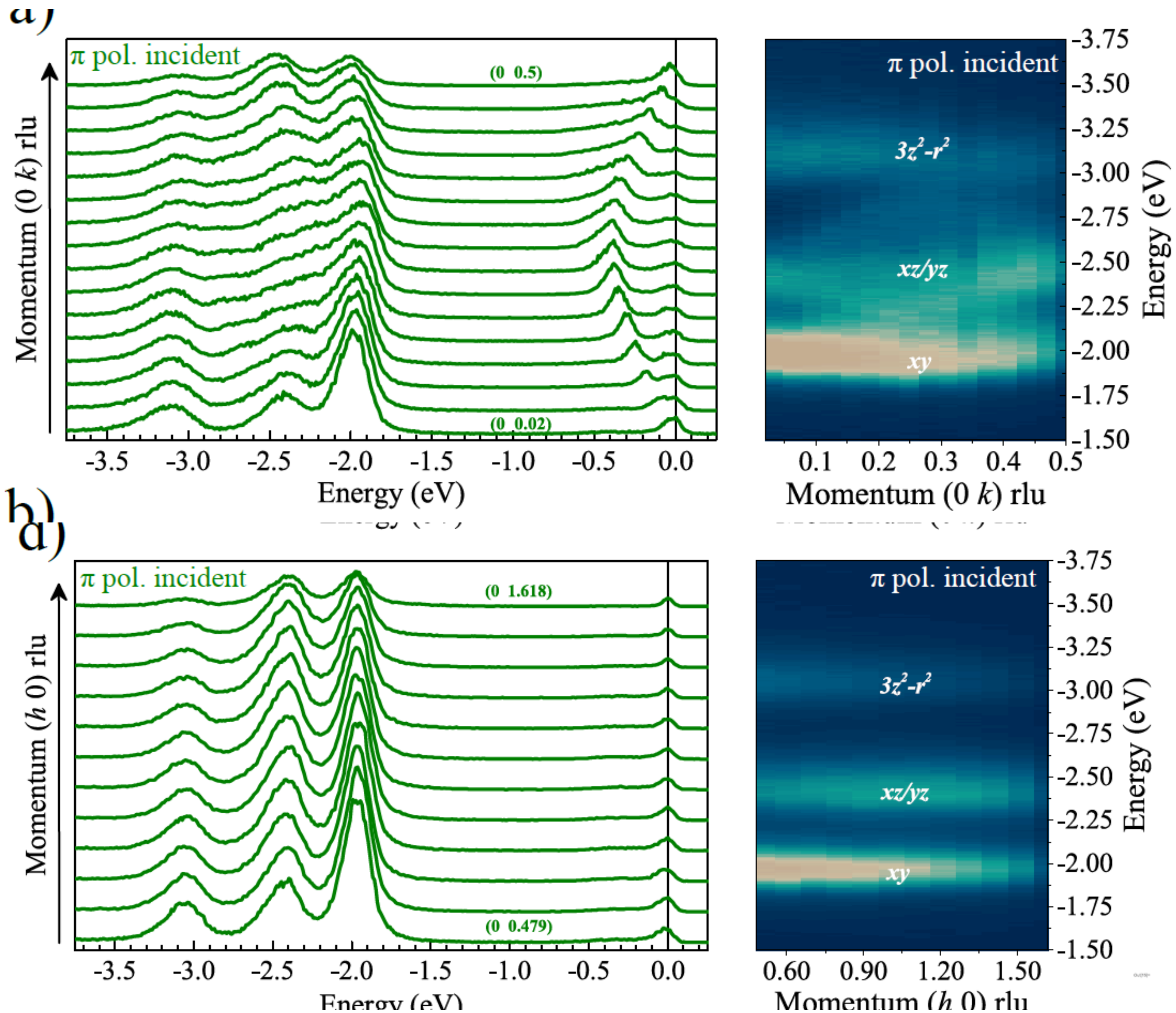
Quasi 1D cuprates: spin and orbital excitations

Ca_2CuO_3

Dispersion along chain direction

Sr_2CuO_3



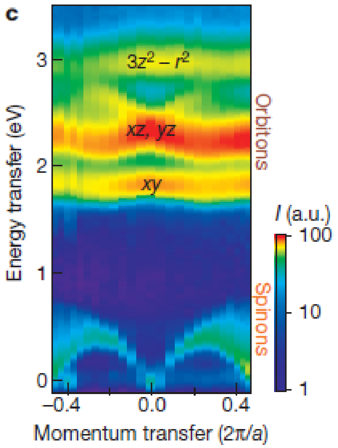


Haverkort, V. N. Strocov, L. Hozoi, C. Monney, S. Nishimoto, S. Singh, A. Revcolevschi, J.-S. Caux, L. Patthey, H. M. Rønnow, J. van den Brink & T. Schmitt, *Nature* **485** 82 (2012)

R. Fumagalli, J. Heverhagen, D. Betto, R. Arpaia, M. Rossi, D. Di Castro, N.B. Brookes, M. Moretti Sala, M. Daghofer, L. Braicovich, K. Wohlfeld, and G. Ghiringhelli, *Phys. Rev. B* **101** 205117 (2020)

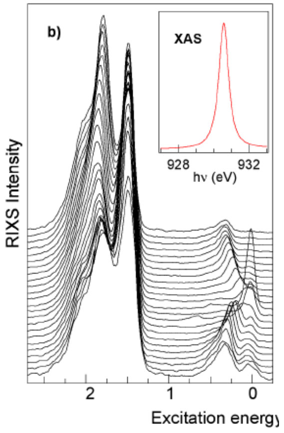
RIXS selected Highlights: spin excitations

Sr_2CuO_3



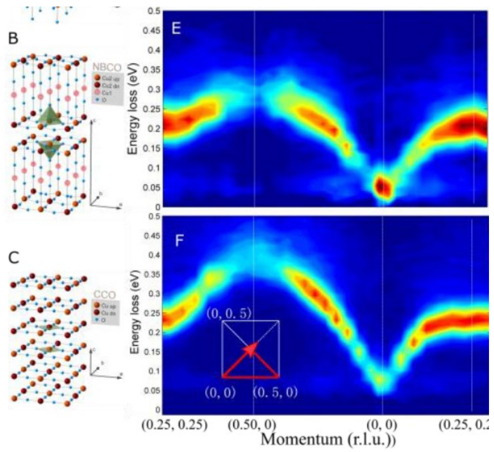
J Schlappa *et al*, Nature (2012)

$Sr_2CuO_2Cl_2$



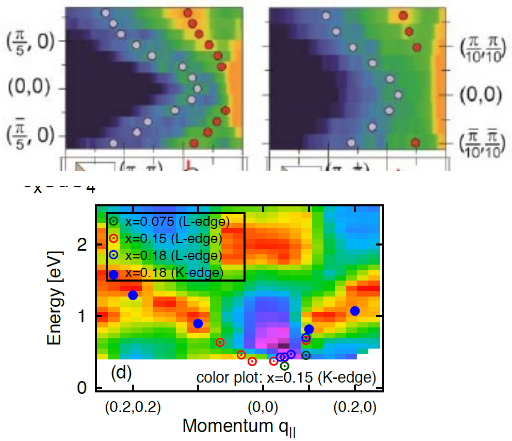
M Guarise, *et al*. PRL (2010)

$Bi_2Sr_2CuO_6$, $NdBa_2Cu_3O_{6.1}$, $CaCuO_2$



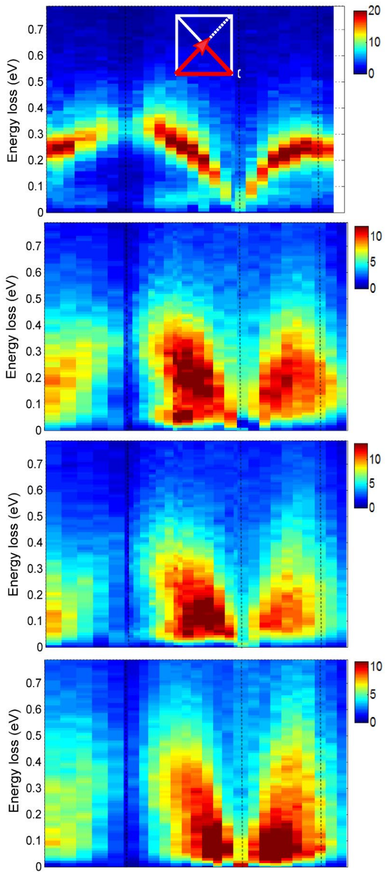
YY Peng, *et al*. Nat. Phys. (2017)

$Nd_{2-x}Ce_xCuO_4$



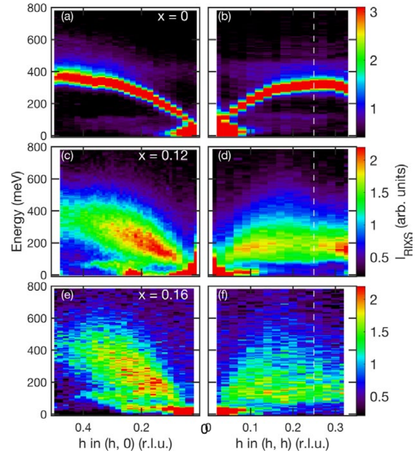
WS Lee, *et al*. Nat. Phys. (2014)
KIshii, *et al*, Nat Comm. (2014)

$Pb\text{-}Bi_2Sr_2CuO_{6+\delta}$



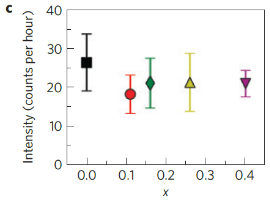
YY Peng, *et al*. PRB. (2018)

$La_{2-x}Sr_xCuO_4$



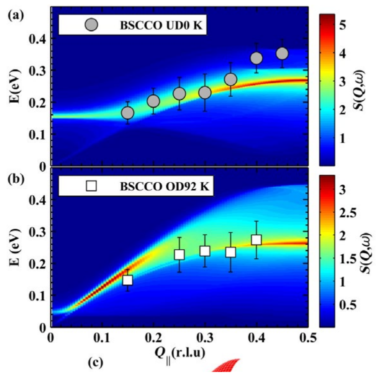
HC Robarts, *et al*. PRB (2019)

$La_{2-x}Sr_xCuO_4$



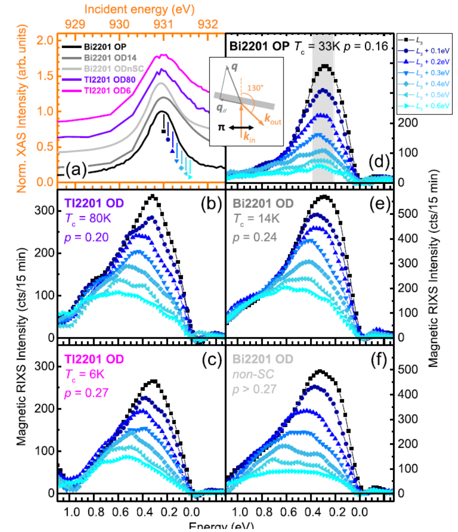
MPM Dean *et al*.
Nat Materials (2013)

$Bi_2Sr_2CaCuO_8$



MPM Dean *et al*. PRL (2013)

$Pb\text{-}Bi_2Sr_2CuO_{6+\delta}$ $Tl_2Ba_2CuO_{6+\delta}$



M Minola *et al*. PRL (2017)

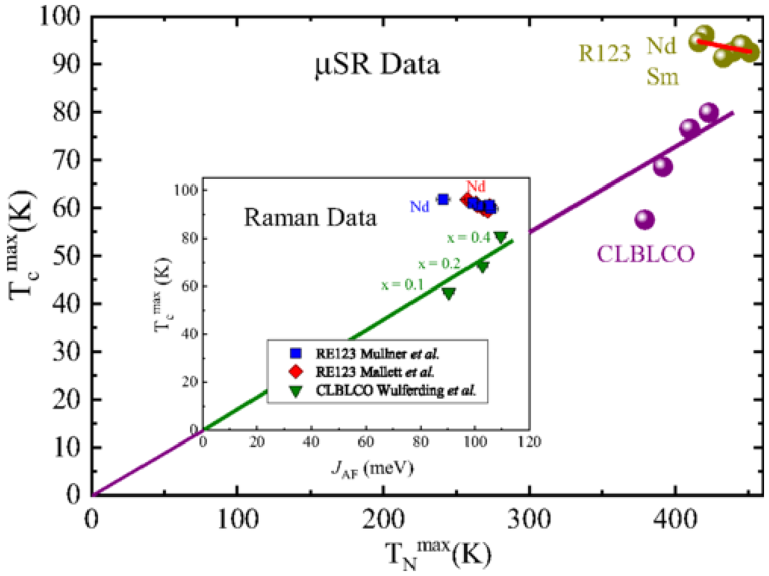
Exchange interaction and superconductivity

REVIEWS OF MODERN PHYSICS, VOLUME 84, OCTOBER–DECEMBER 2012

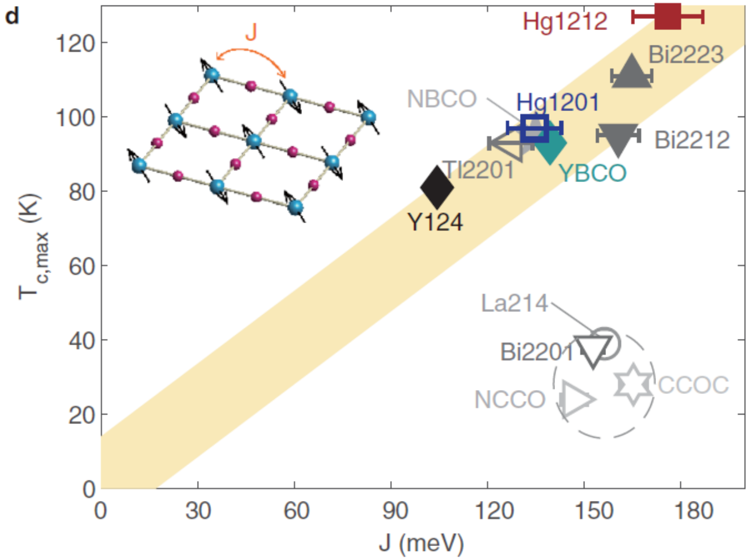
A common thread: The pairing interaction for unconventional superconductors

D. J. Scalapino*

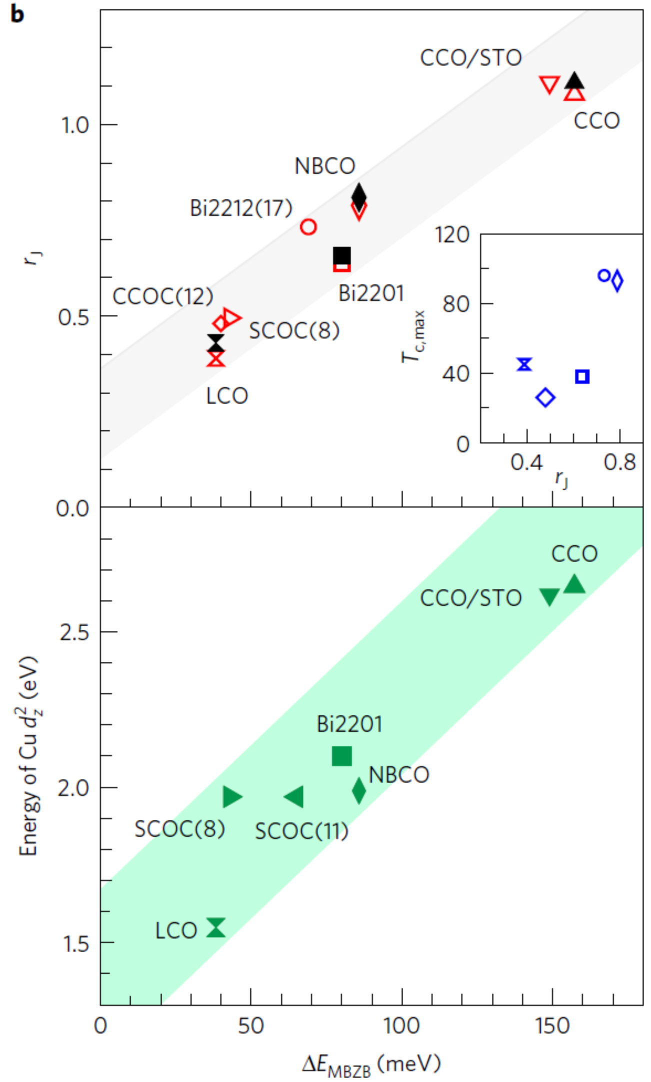
interaction for Hubbard-like models, it is proposed that spin-fluctuation mediated pairing is the common thread linking a broad class of superconducting materials.



Amit Keren, Wayne Crump, Ben P. P. Mallett, Shen V. Chong, Itai Keren, Hubertus Luetkens, and Jeffery L. Tallon, *Phys. Rev. B* **100**, 144512

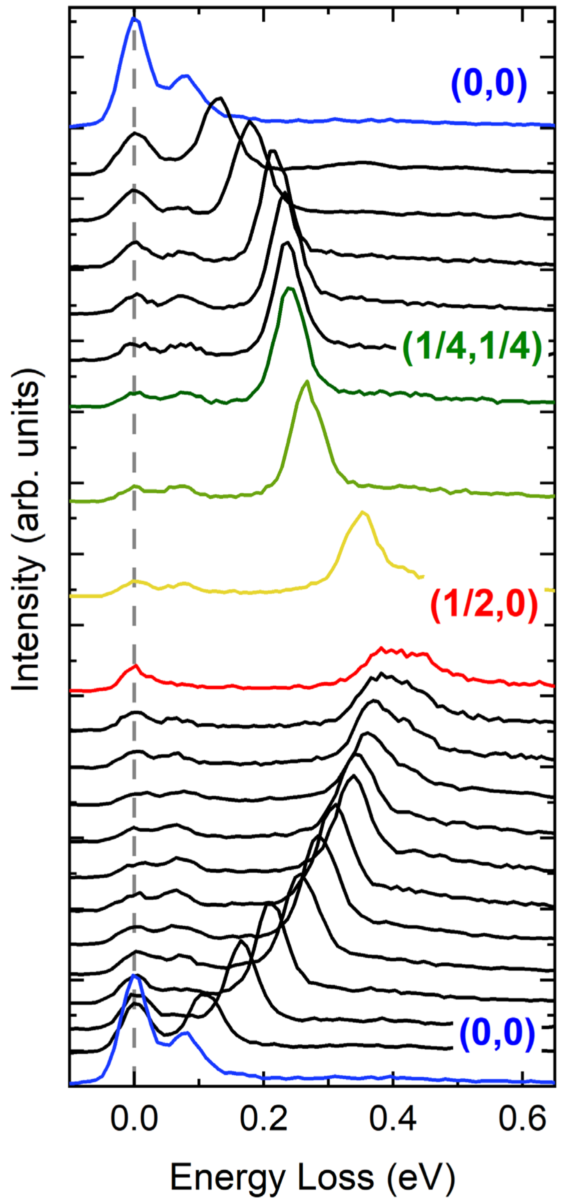


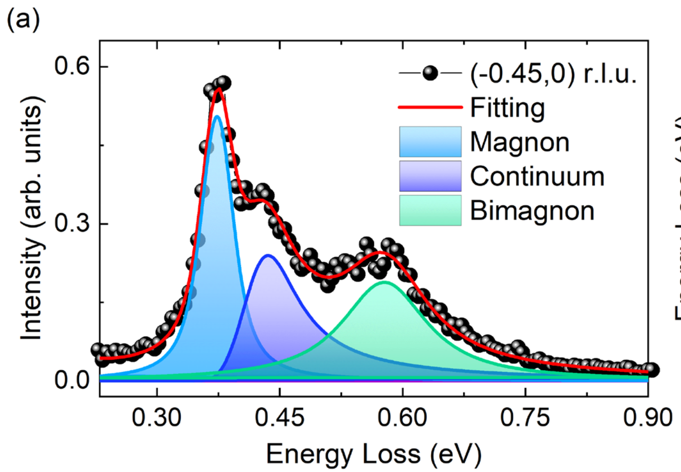
Lichen Wang, Guanhong He, Zichen Yang, Mirian Garcia-Fernandez, Abhishek Nag, Ke-Jin Zhou, Matteo Minola, Matthieu Le Tacon, Yingying Peng, Yuan Li, *Nature Communications* **13**, 3163 (2022)

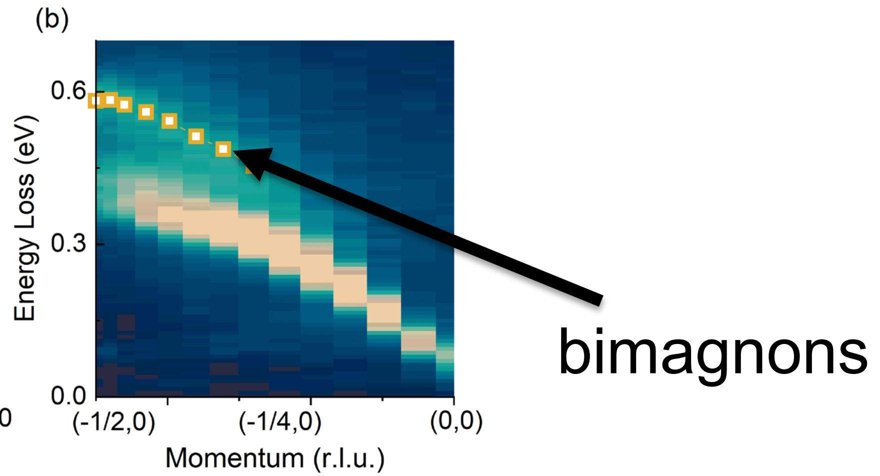


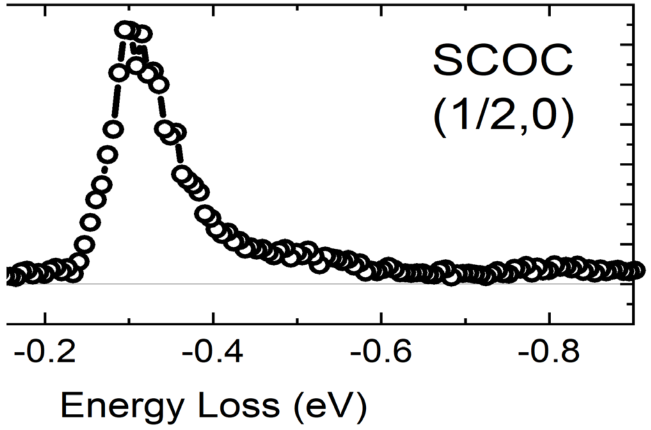
Y. Y. Peng, G. Dellea, M. Minola, M. Conni, A. Amorese, D. Di Castro, G. M. De Luca, K. Kummer, M. Salluzzo, X. Sun, X. J. Zhou, G. Balestrino, M. Le Tacon, B. Keimer, L. Braicovich, N. B. Brookes and G. Ghiringhelli, *Nature Physics* **13** 1201 (2017)

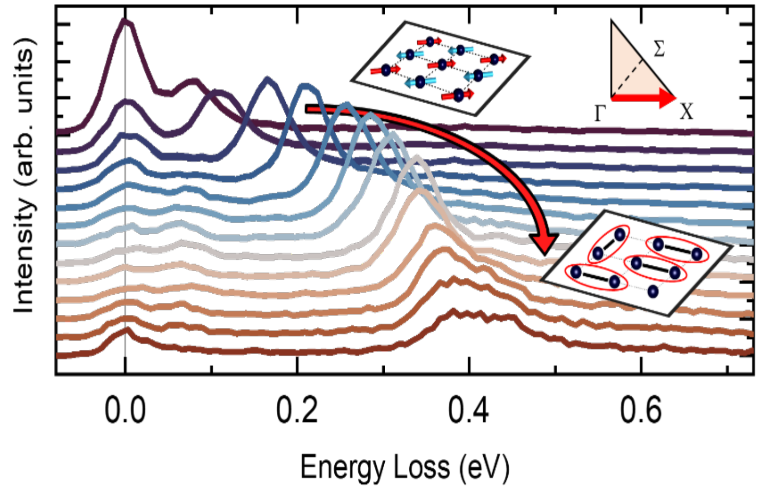
Deconfined spinon pairs in $CaCuO_2$









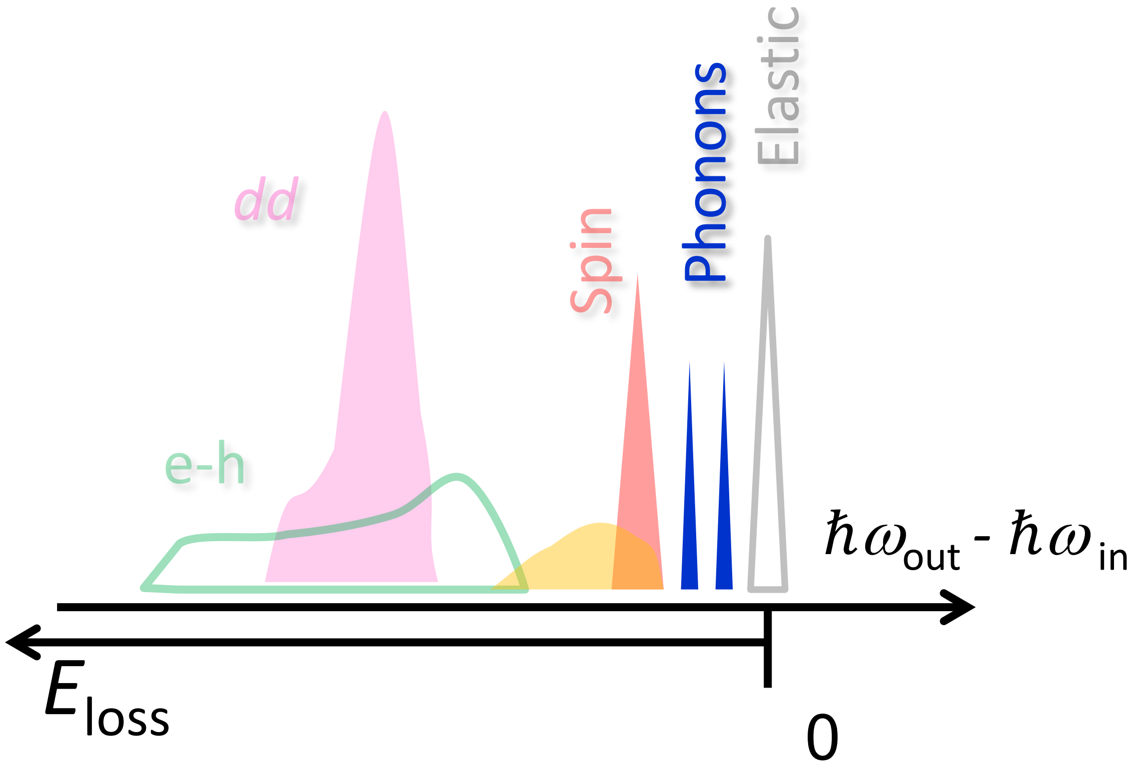


Leonardo Martinelli, Davide Betto, Kurt Kummer, Riccardo Arpaia, Lucio Braicovich, Daniele Di Castro, Nicholas B. Brookes, Marco Moretti Sala, and Giacomo Ghiringhelli, Phys Rev. X **12**, 021041 (2022)

Part 5

PHONONS

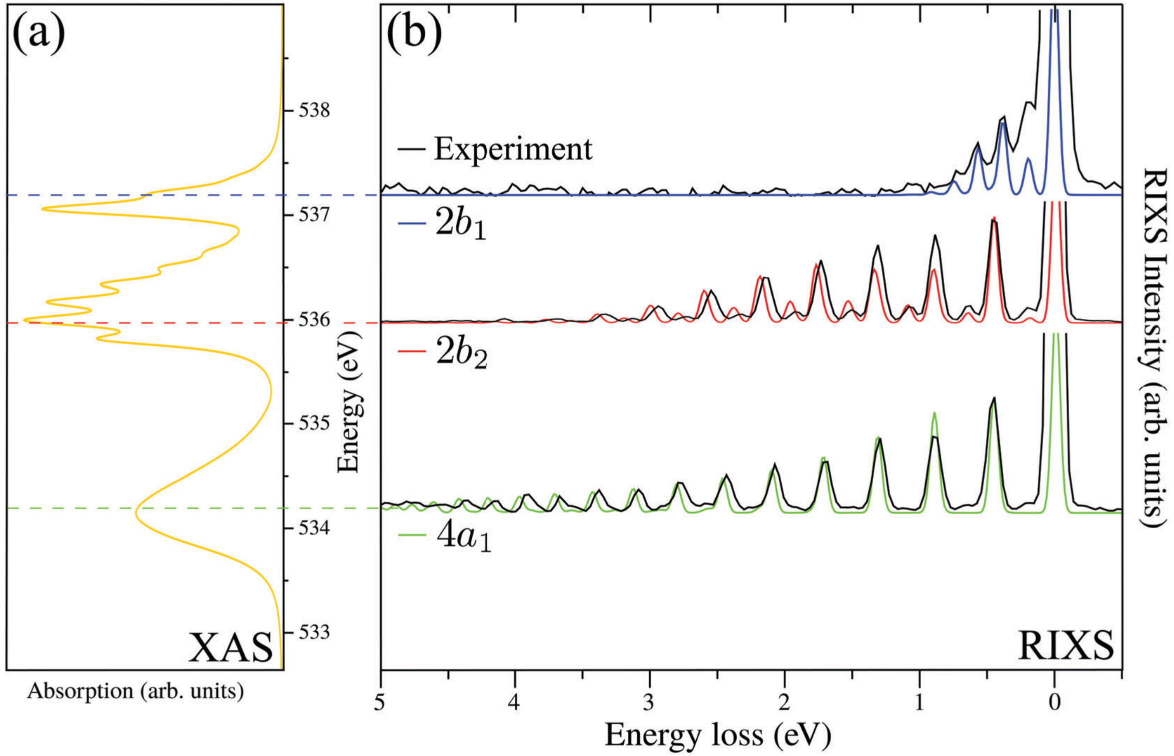
Phonons



Why do we see phonons in RIXS?

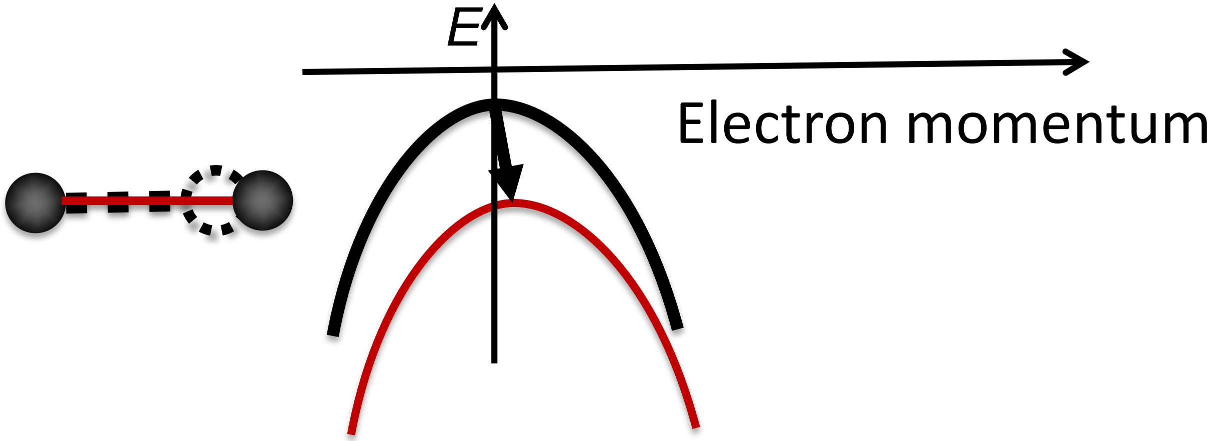
How can we use the phonon signal?

RIXS of water



Vinıcius Vaz da Cruz, Emelie Ertan, Rafael C. Couto, Sebastian Eckert, Mattis Fondell, Marcus Dantz, Brian Kennedy, Thorsten Schmitt, Annette Pietzsch, Freddy F. Guimaraes, Hans Ågren, Faris Gel'mukhanov, Michael Odelius, Alexander Fohlisch and Victor Kimberg, *PCCP* **19**, 19573 (2017)

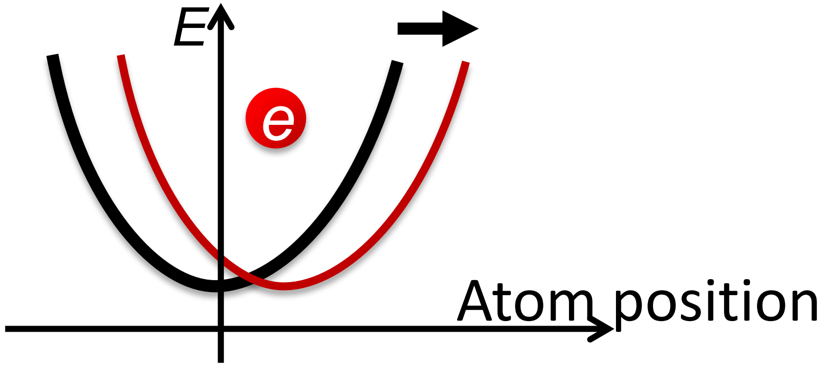
Electron phonon coupling

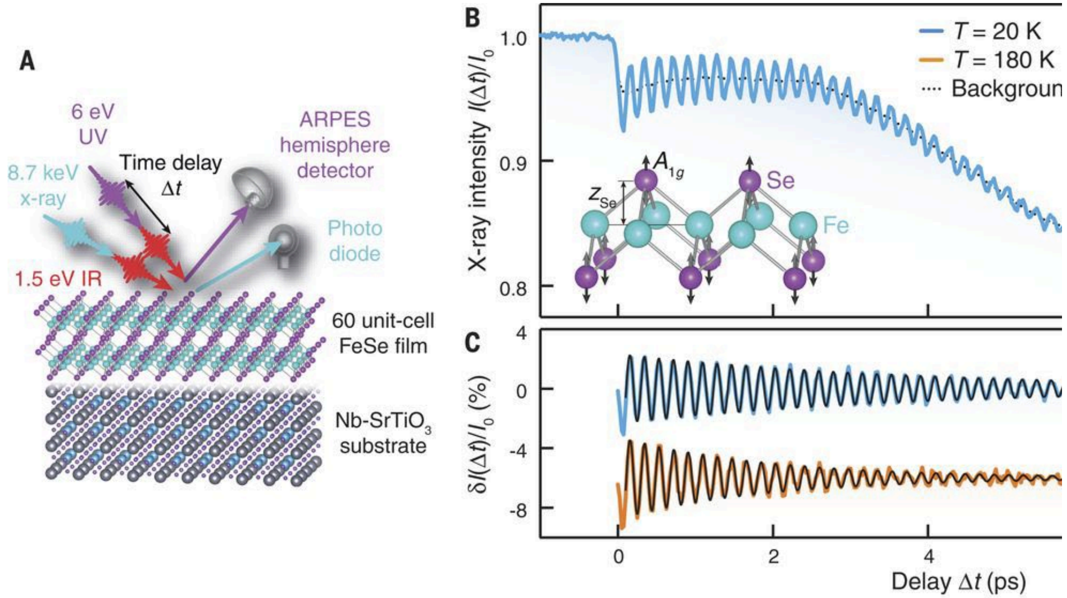


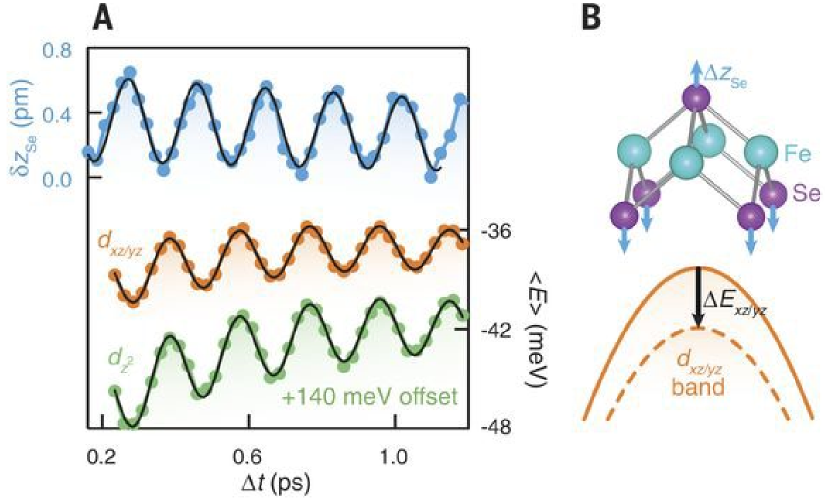
How $\mathcal{H}$ is modified by an atomic displacement

≡

How lattice is deformed by the presence of a valence electron







S. Gerber, S.-L. Yang, D. Zhu, H. Soifer, J. A. Sobota, S. Rebec, J. J. Lee, T. Jia, B. Moritz, C. Jia, A. Gauthier, Y. Li, D. Leuenberger, Y. Zhang, L. Chaix, W. Li, H. Jang, J.-S. Lee, M. Yi, G. L. Dakovski, S. Song, J. M. Glownia, S. Nelson, K. W. Kim, Y.-D. Chuang, Z. Hussain, R. G. Moore, T. P. Devereaux, W.-S. Lee, P. S. Kirchmann, and Z.-X. Shen, *Science* **357,** 71(2017)

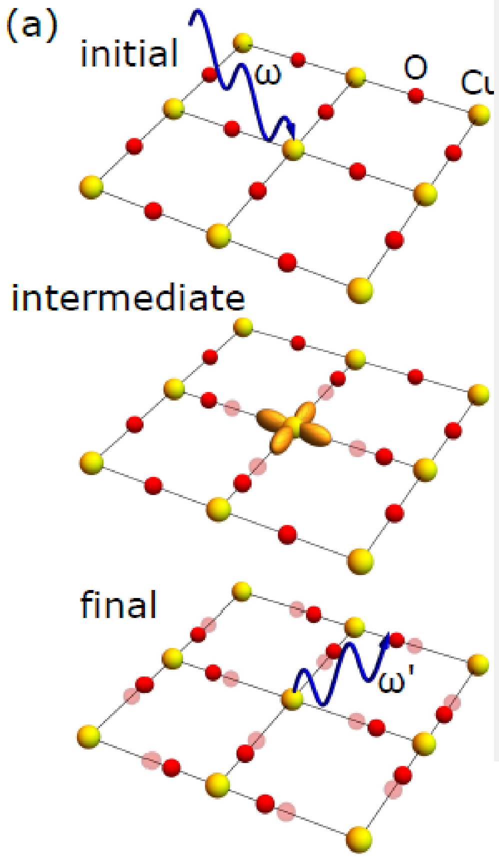
Measuring EPC with RIXS: mechanism

Theory by Ament, van den Brink

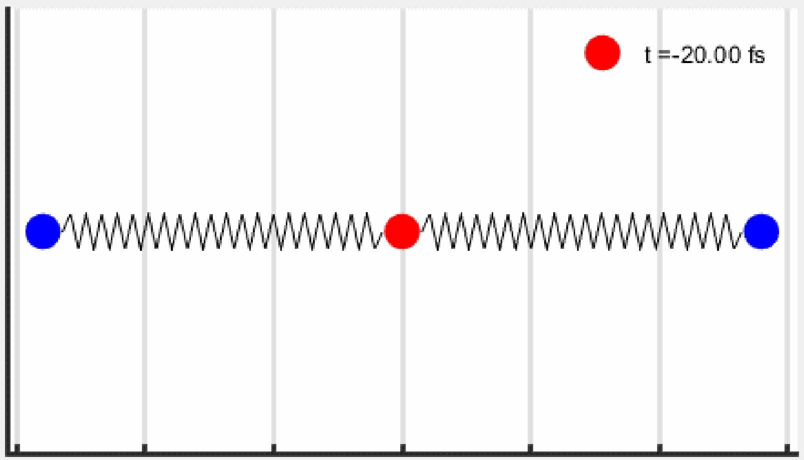
Phonon peak intensity grows with:

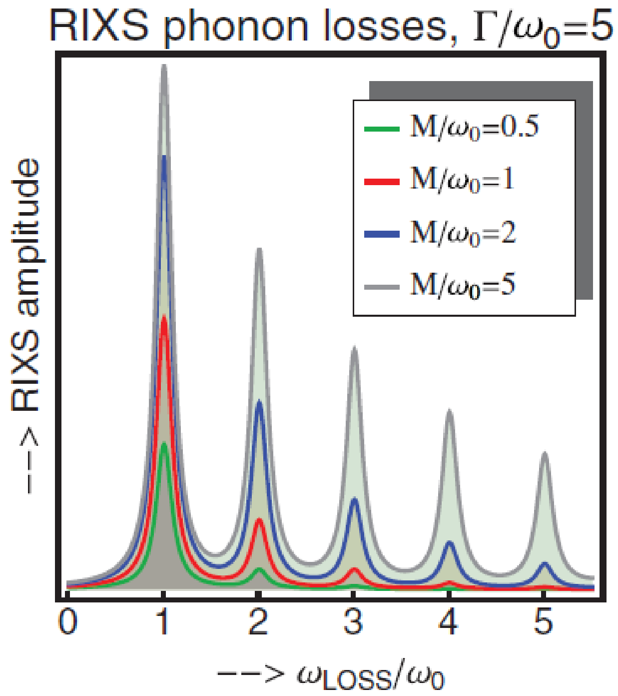
- EPC, i.e., M or $g = (M/w_0)^2$
- Intermediate state lifetime

2ph, *3ph* peaks

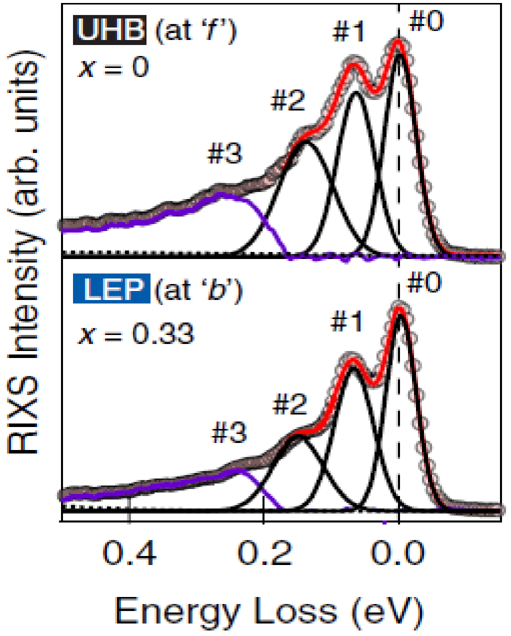


Harmonic oscillator analogy





~~Application to 1D~~ system (O K edge)



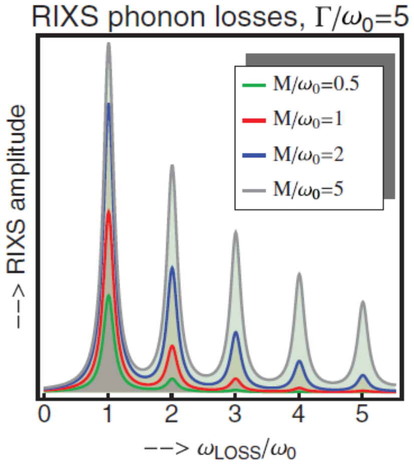
Matteo Rossi, Riccardo Arpaia, Roberto Fumagalli, Marco Moretti Sala, Davide Betto, Gabriella M. De Luca, Kurt Kummer, Jeroen van den Brink, Marco Salluzzo, Nicholas B. Brookes, Lucio Braicovich, Giacomo Ghiringhelli, PRL **123**, 027001 (2019)

L. J. P. Ament, M. van Veenendaal and J. van den Brink, EPL **95** (2011) 27008

W-S Lee et al, PRL **110**, 265502 (2013)

Phonons in RIXS spectra

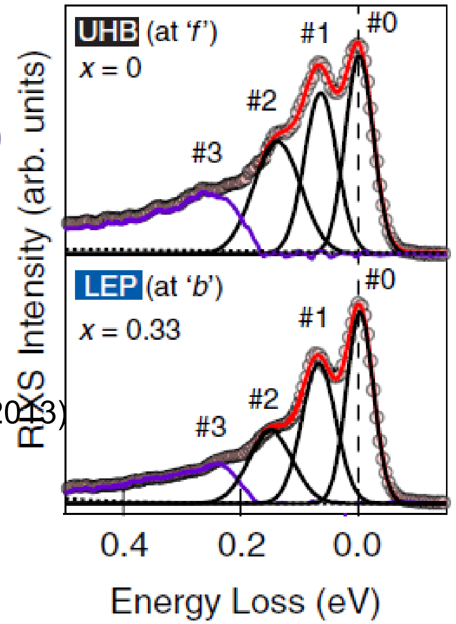
Signal is directly related to *e-ph* interaction



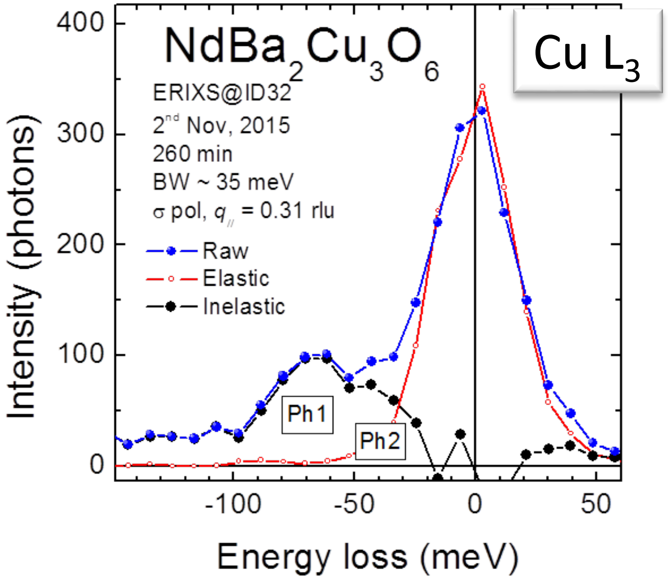
Theory

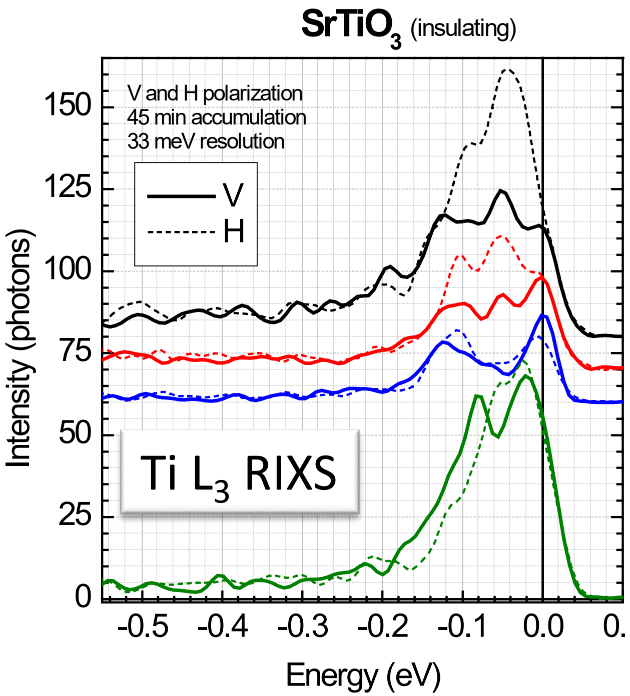
L. J. P. Ament, M. van Veenendaal and J. van den Brink, EPL **95** (2011) 27008

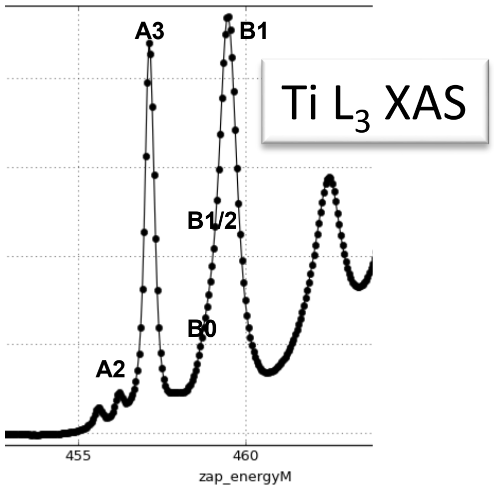
Application to 1D system (O K edge)



W-S Lee et al, PRL **110**, 265502 (2013)



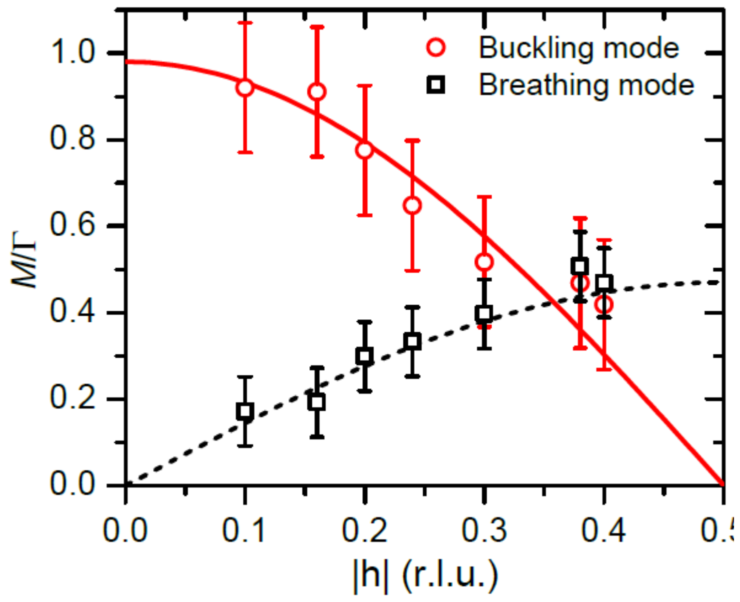


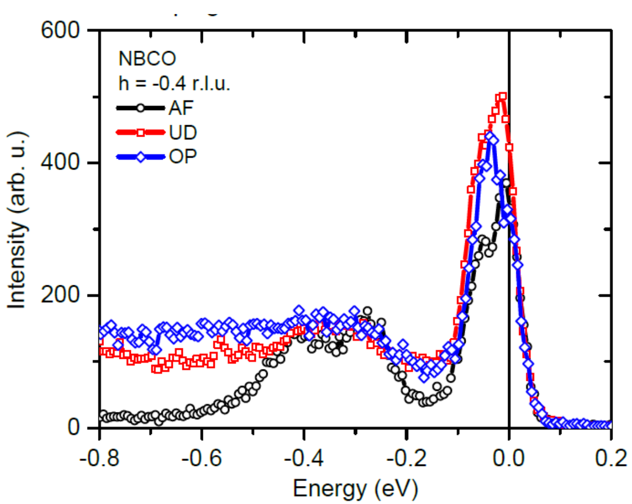


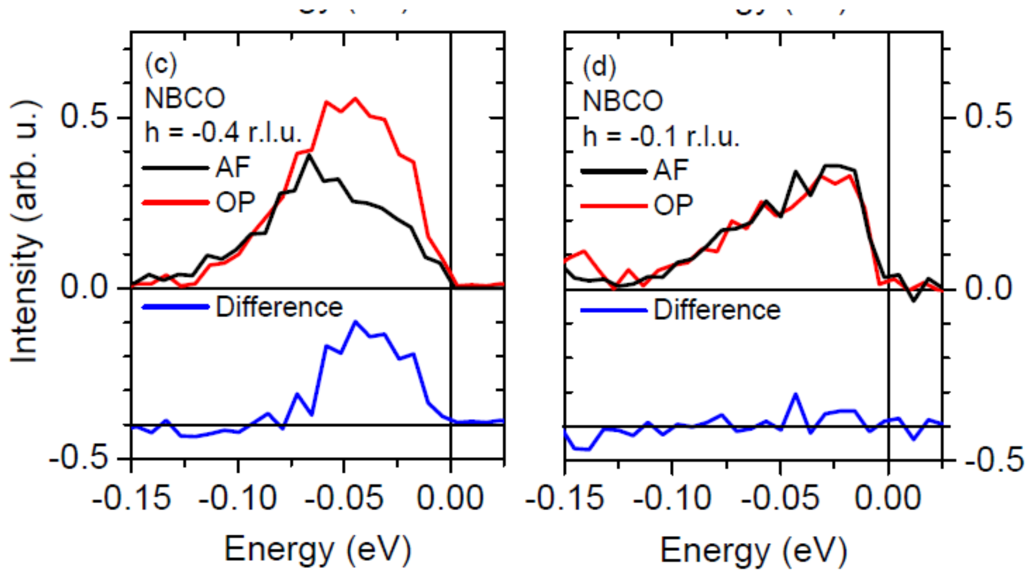
EPC in $NdBa_2Cu_3O_{7-\delta}$

Doping dependence: interplay with CDW at large *q* in (10)

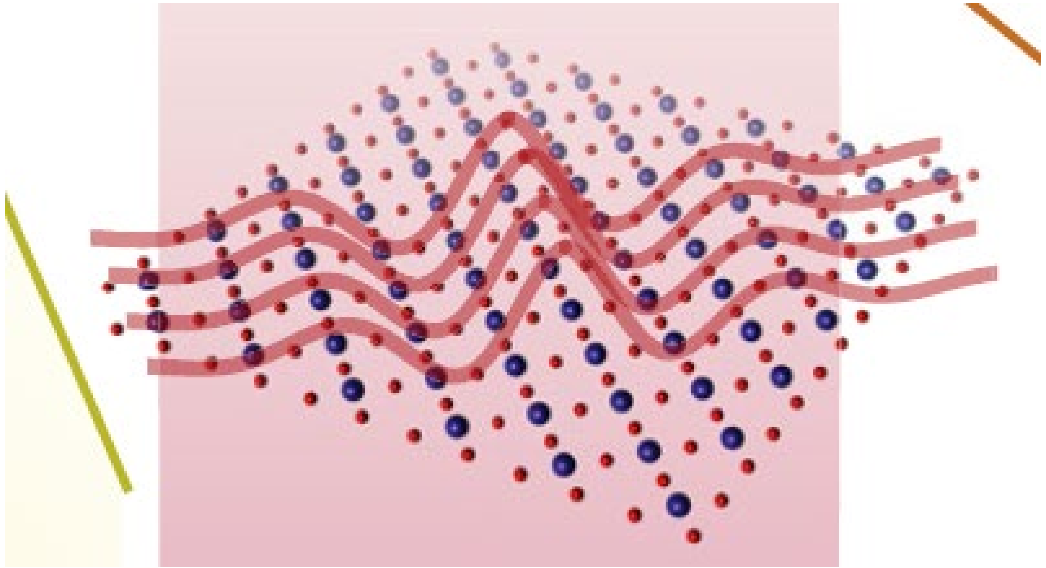
q dependence







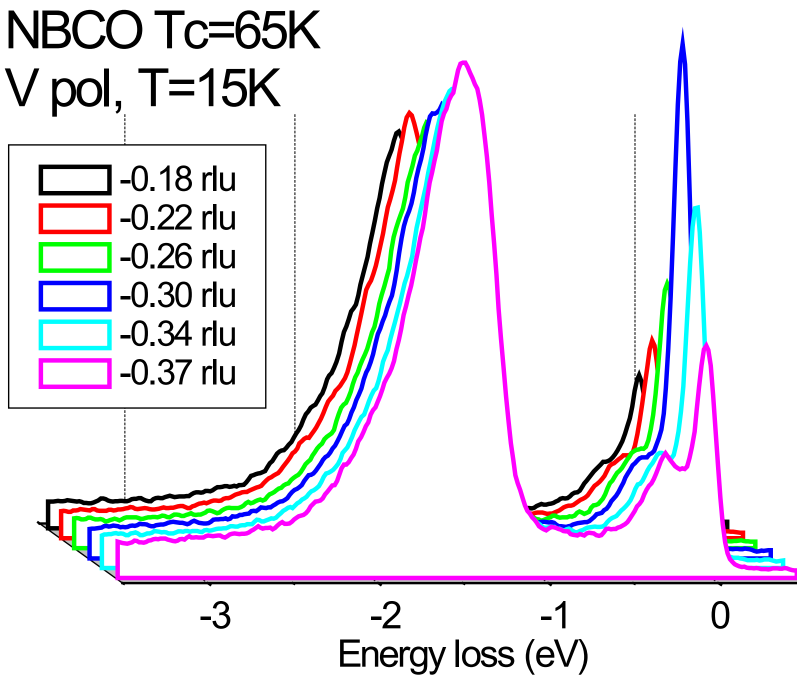
Lucio Braicovich, Matteo Rossi, Roberto Fumagalli, Yingying Peng, Yan Wang, Riccardo Arpaia, Davide Betto, Gabriella M. De Luca, Daniele Di Castro, Kurt Kummer, Marco Moretti Sala, Mattia Pagetti, Giuseppe Balestrino, Nicholas B. Brookes, Marco Salluzzo, Steven Johnston, Jeroen van den Brink, Giacomo Ghiringhelli, *Phys. Rev. Research* **2**, 023231 (2020)

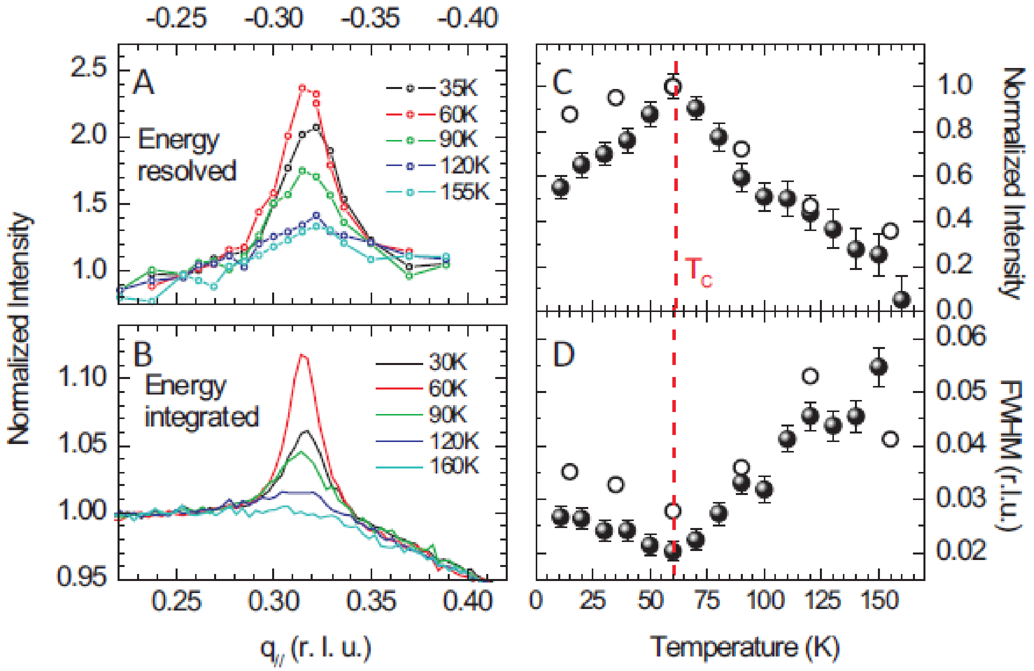


Part 5

CHARGE ORDER AND CHARGE DENSITY FLUCTUATIONS

First observation of CDW in YBCO with R(I)XS





G. Ghiringhelli, M. Le Tacon, M. Minola, S. Blanco-Canosa, C. Mazzoli, N.B. Brookes, G.M. De Luca, A. Frano, D. G. Hawthorn, F. He, T. Loew, M. Moretti Sala, D.C. Peets, M. Salluzzo, E. Schierle, R. Sutarto,G. A. Sawatzky, E. Weschke, B. Keimer, L. Braicovich, *Science* **337**, 821 (2012)

Other evidences of CDW in YBCO

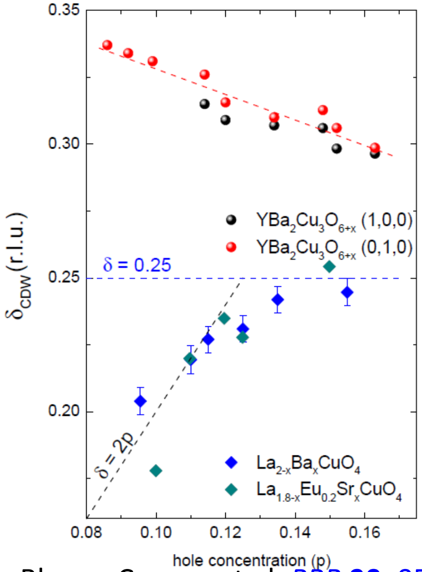
NMR, Charge modulation at low T, high field
Wu et al. *Nature* **477** 191 (2011)

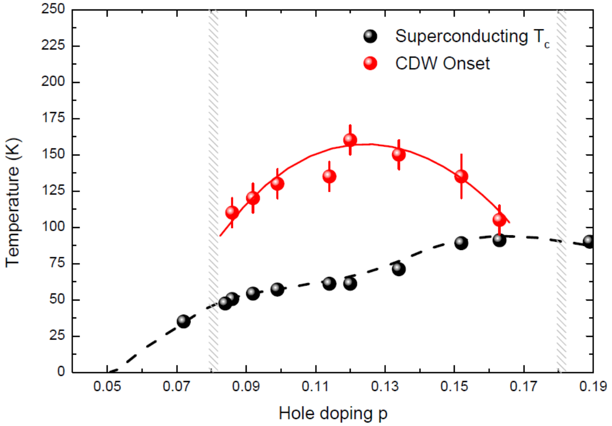
L = 0.5: Doubling of unit cell along c-axis
Field enhancement of the CDW (HXRD)
Chang et al. *Nat.Phys.* **8** 871 (2012)

Bi-axial, Static order under high field.
Leboeuf et al. *Nat.Phys.* **9** 79 (2013)

Ubiquitous CDW in cuprates

YBCO

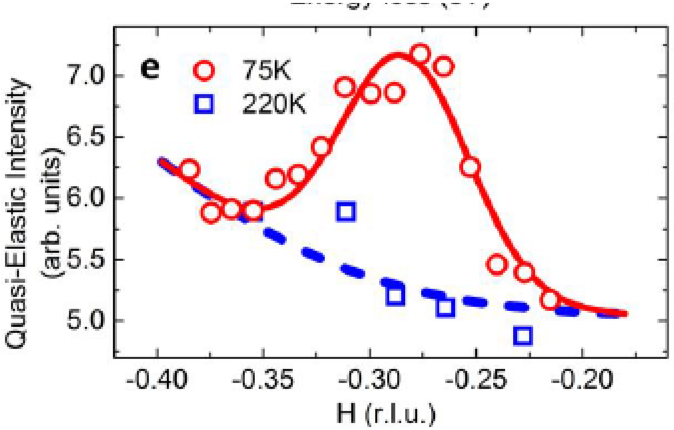




Blanco-Canosa et al. *PRB* **90**, 054513 (2014)

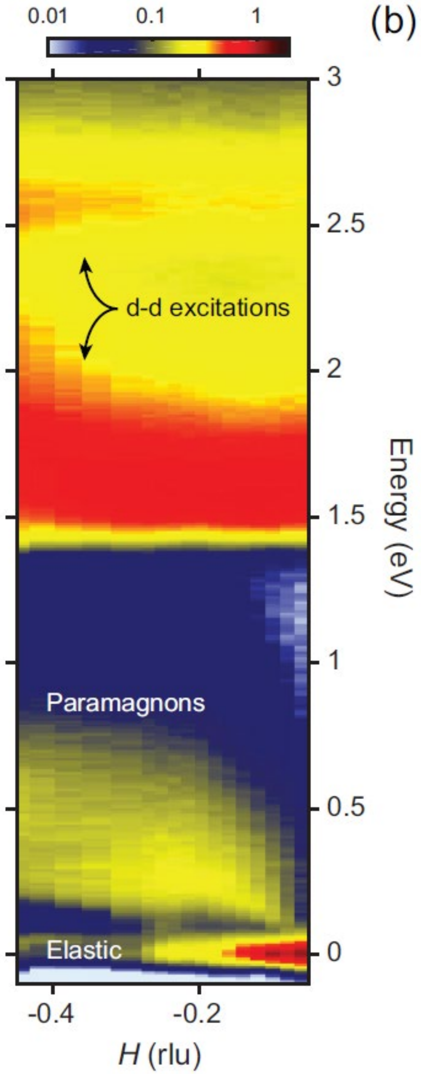
Huecker et al. *PRB* **90**, 054514 (2014)

Hg1201 underdoped



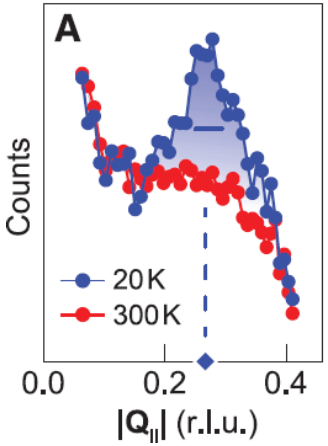
W. Tabis et al, *Nat. Comm.* **5**, 5875 (2014)

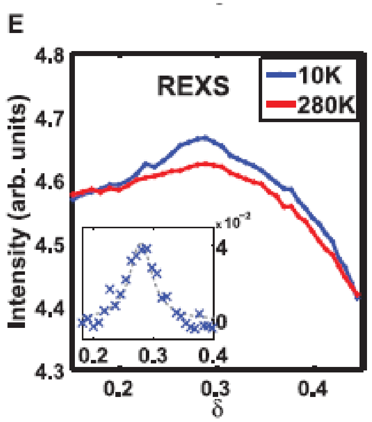
NCCO e-doped



M. E. H. da Silva Neto et al, *PRB* **98** 161114 (2018)

Bi2201 and Bi2212 underdoped

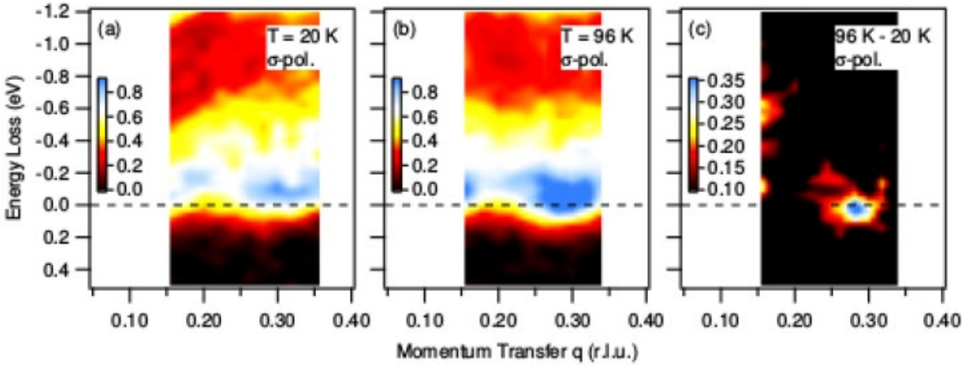




R. Comin et al, Science 343, 390 (2014;

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

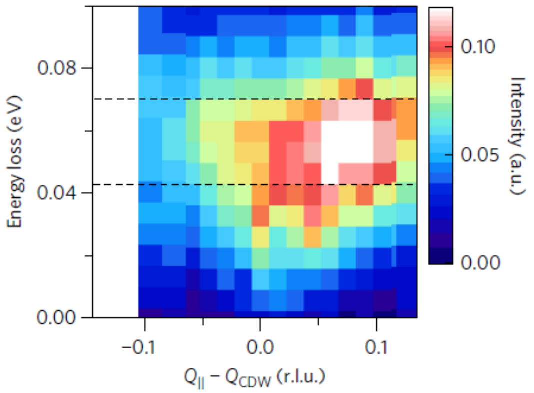
Bi2212 optimally doped

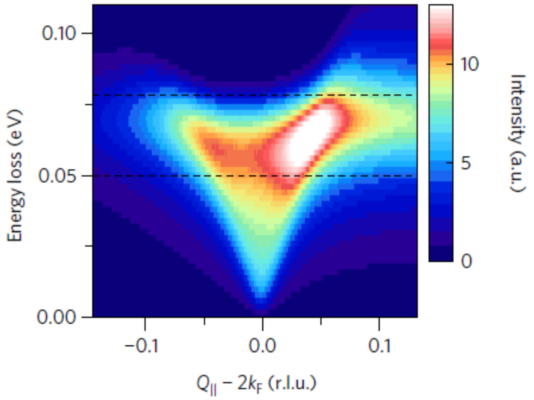


M. Hashimoto, G. Ghiringhelli et al, *PRB* Rapid 89 220511 (2014)

Charge order and phonons

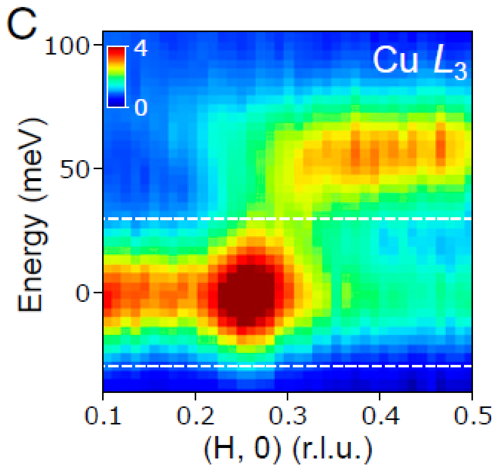
$Bi_2Sr_2CaCuO_8$





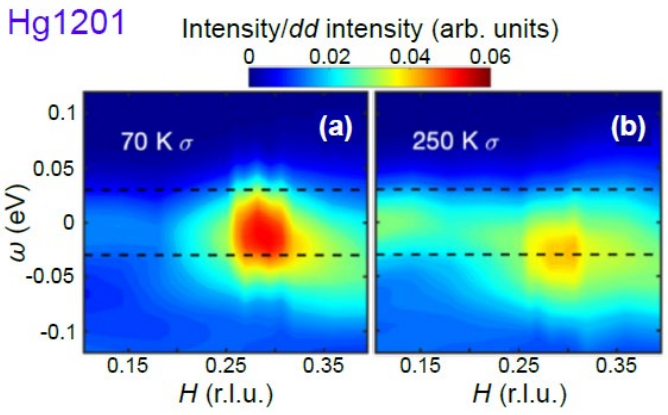
L Chaix *et al*, Nat Phys (2017)

$La\text{-}Bi_2Sr_2CuO_{6+\delta}$



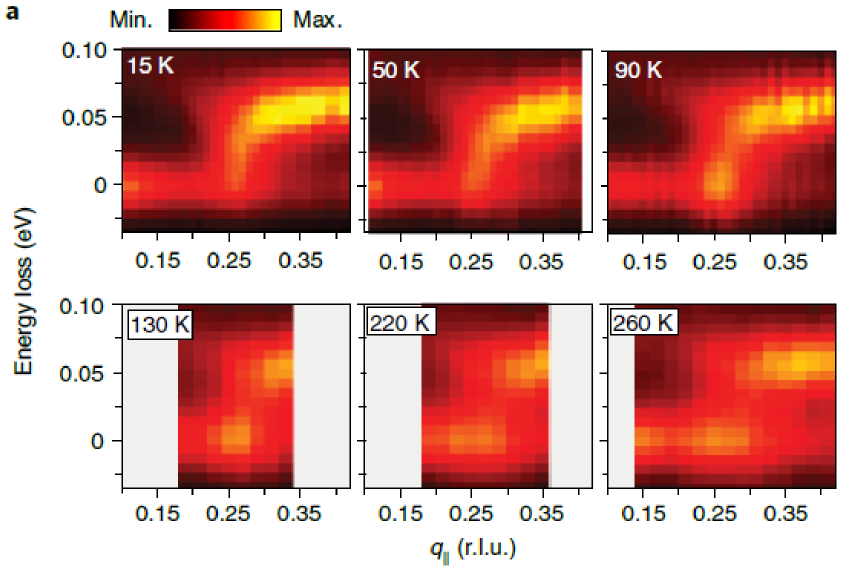
J Li *et al*, PNAS (2020)

$HgBa_2CuO_{4+\delta}$



B Yu, *et al*. PRX. (2020)

$Bi_2Sr_2CaCuO_8$



WS Lee *et al*, Nat Phys (2021)

The RIXS phase diagram of cuprates

Before RIXS, *circa* 2007