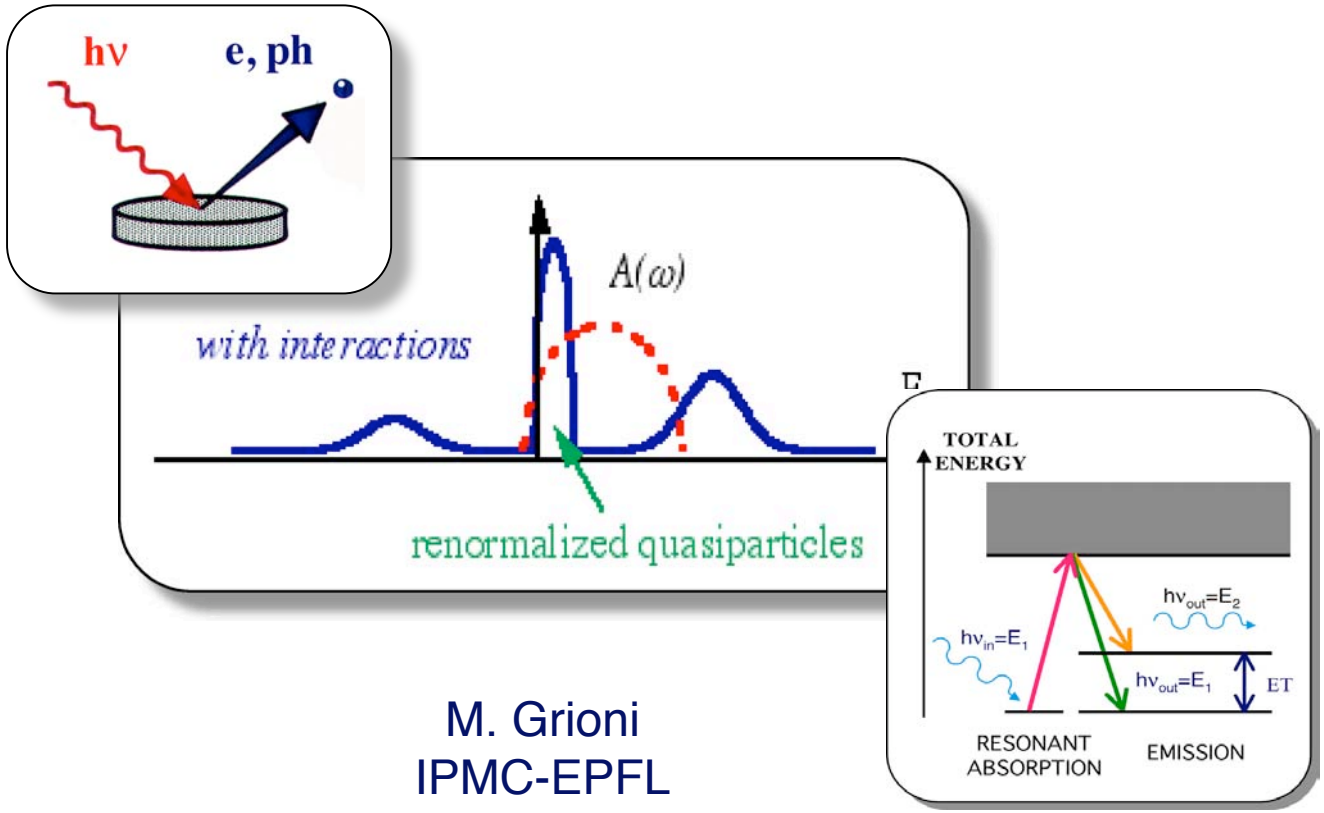
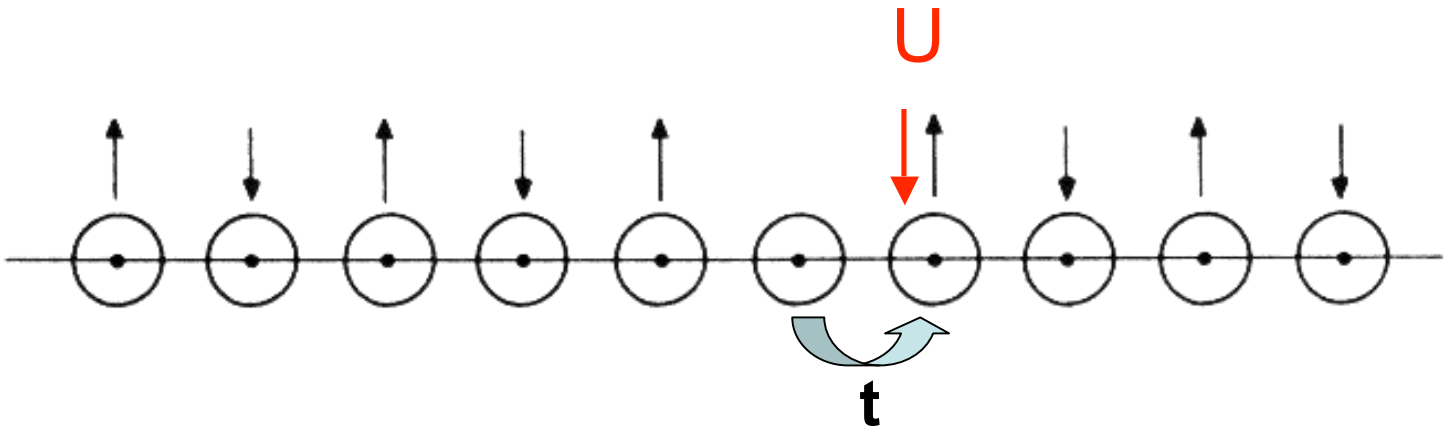
RIXS & strong correlations



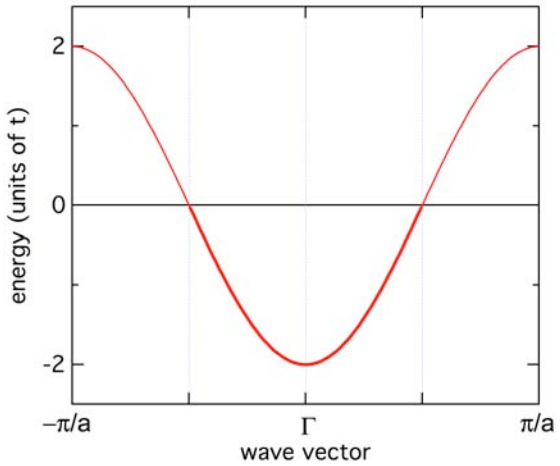
M. Grioni
IPMC-EPFL

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Strong Coulomb interactions

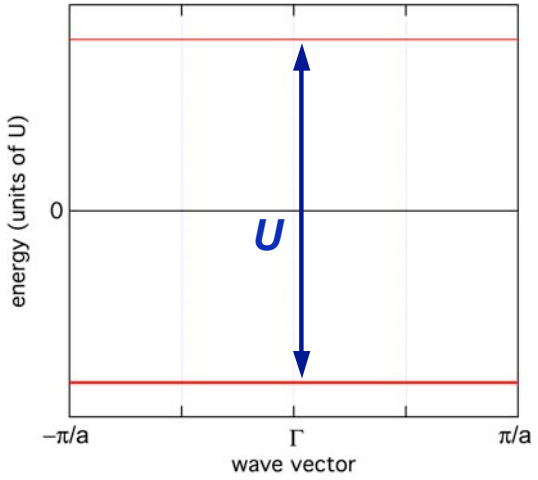


U«t



Metal (boring)

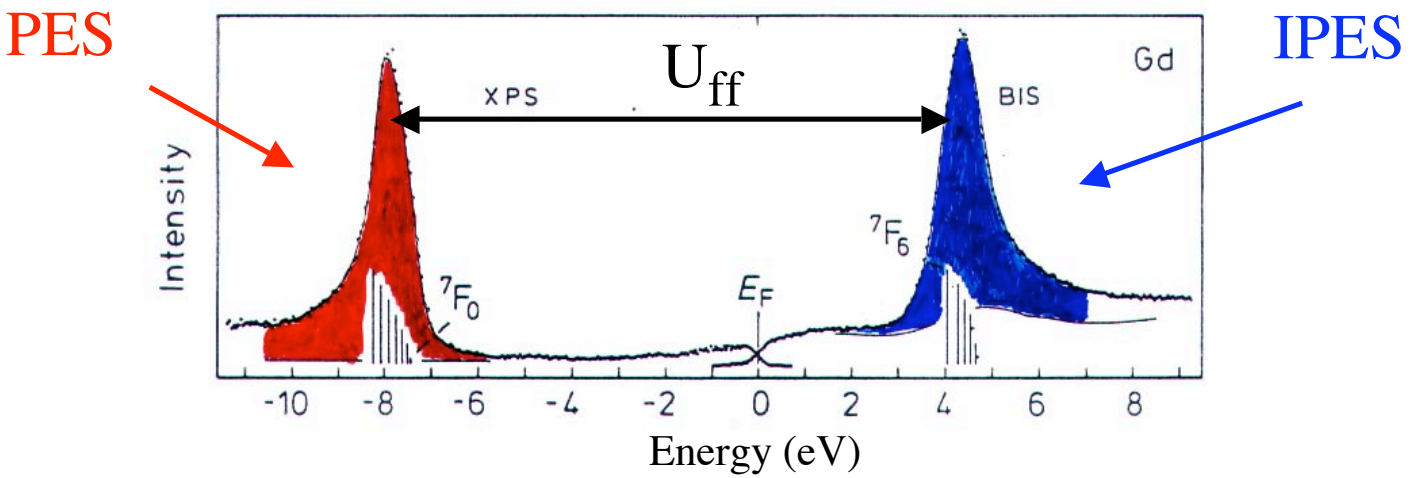
t«U



Mott insulator

Spectral signature of a Mott gap

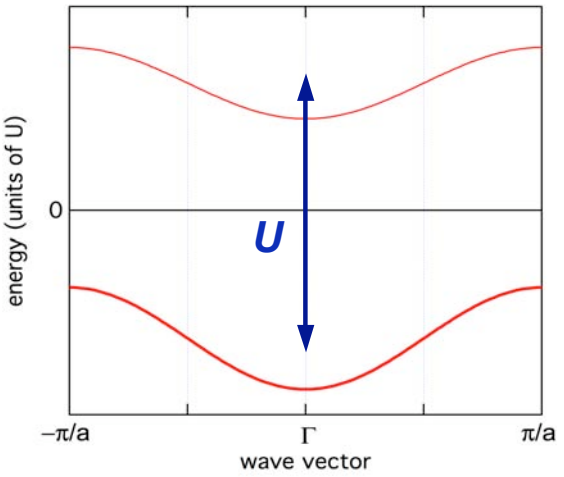
A REAL CASE: 4f ELECTRONS IN THE LANTHANIDES

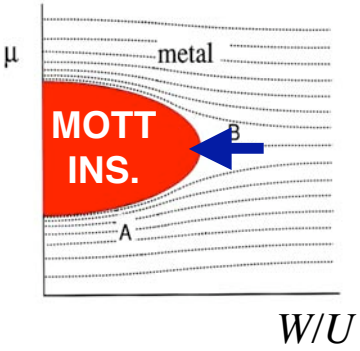


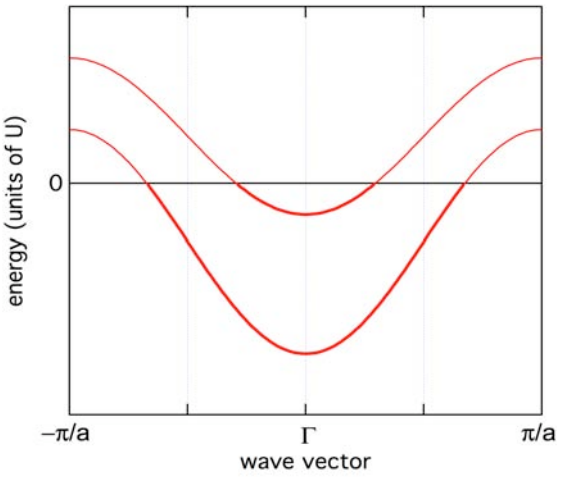
In between...more interesting

From G.Kotliar and D.Vollhardt,
Physics Today, March 2004

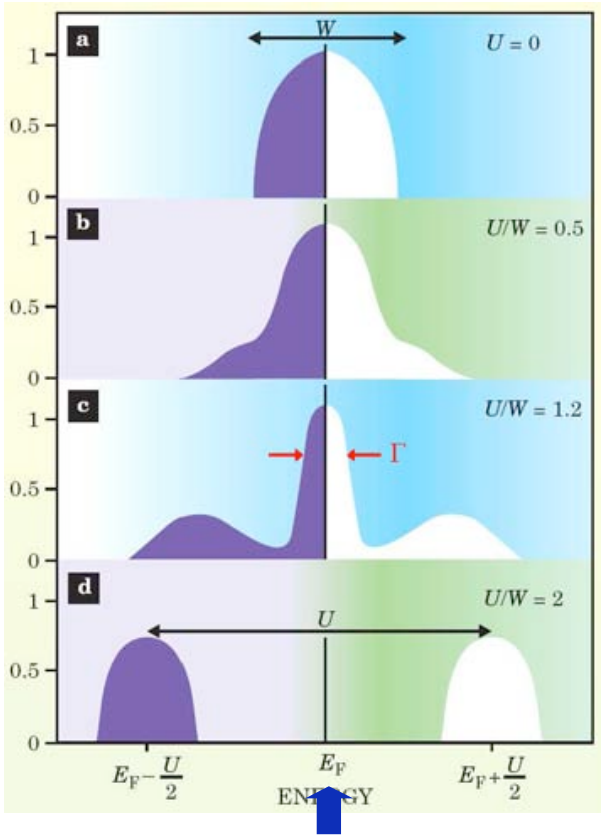
" simple cartoon"







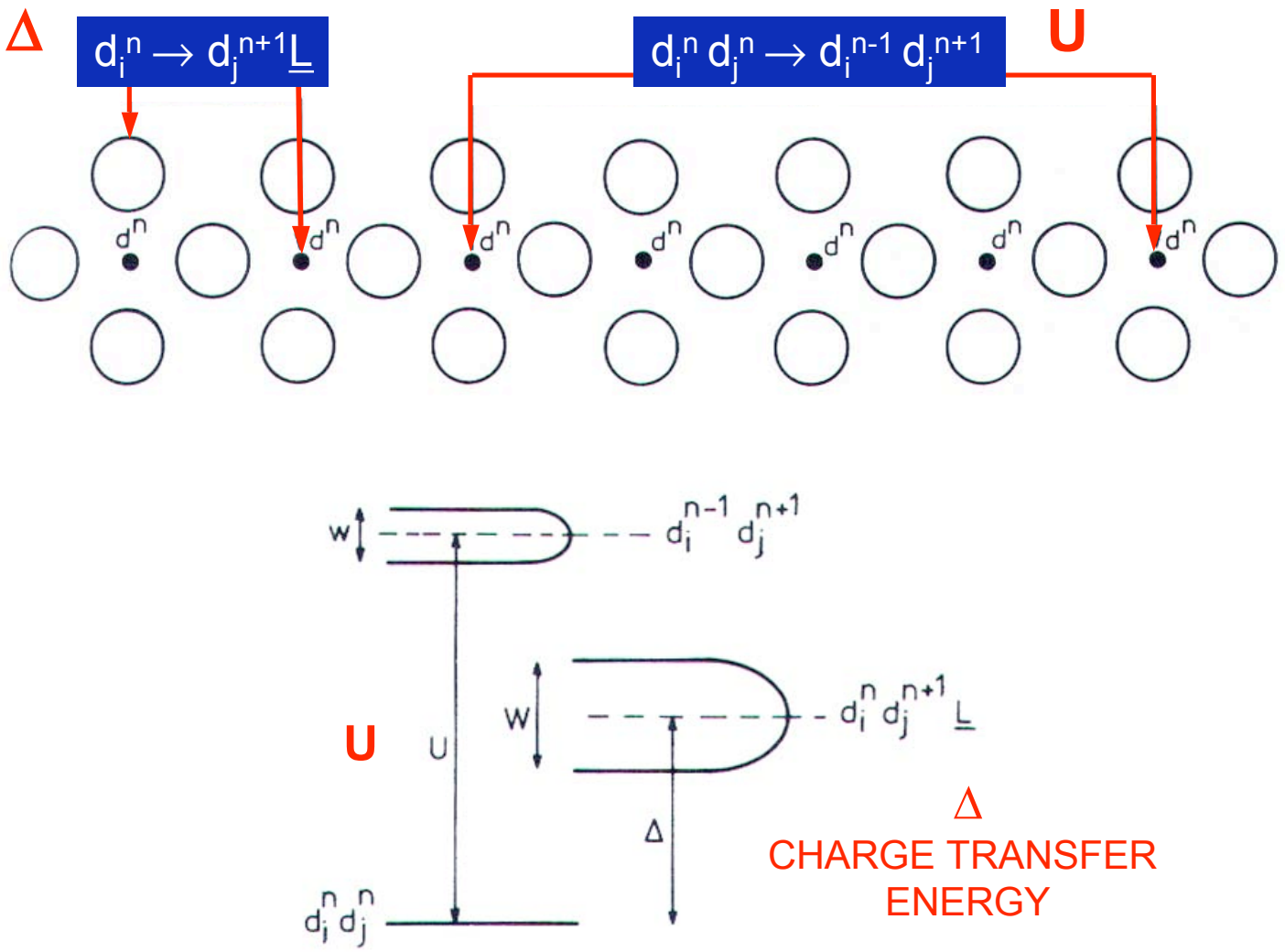
Realistic picture (DMFT)



U

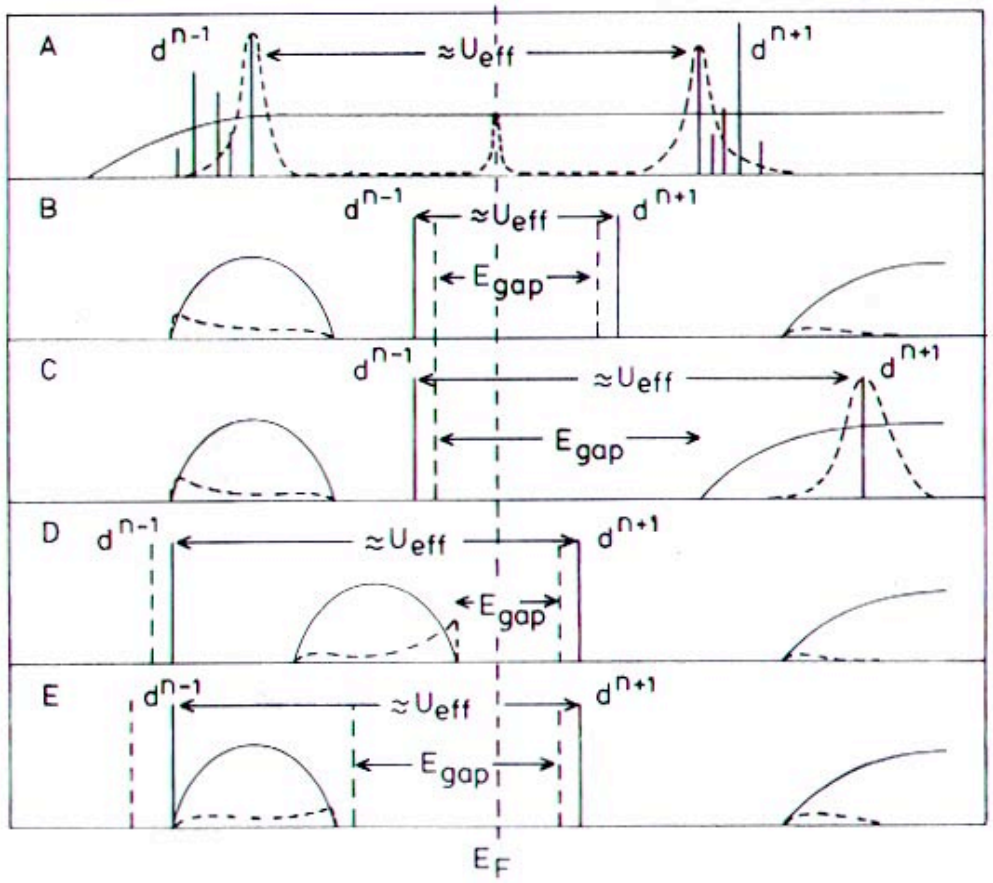
Emergent low-energy scales
(J, δ_K, Δ_{SC})

Two kinds of charge fluctuations



J. Zaanen, G.A. Sawatzky, J.W. Allen, Phys. Rev. Lett. **55**, 418 (1985)

Different regimes of the ZSA scenario



METAL

MOTT

CHARGE TRANSFER

cuprates →

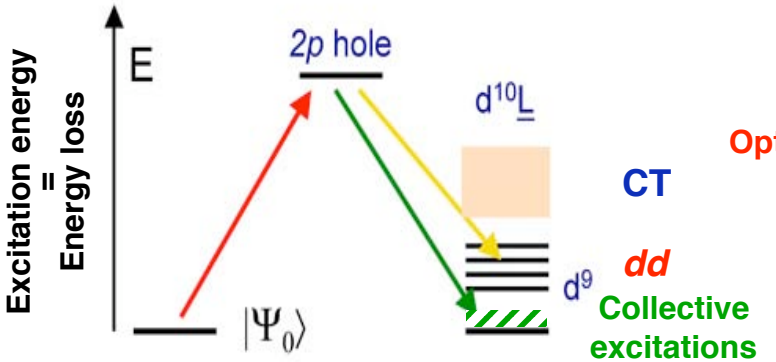
Multiple energy scales

High-T_c superconductors, CMR materials, multiferroics, Kondo, quantum magnets

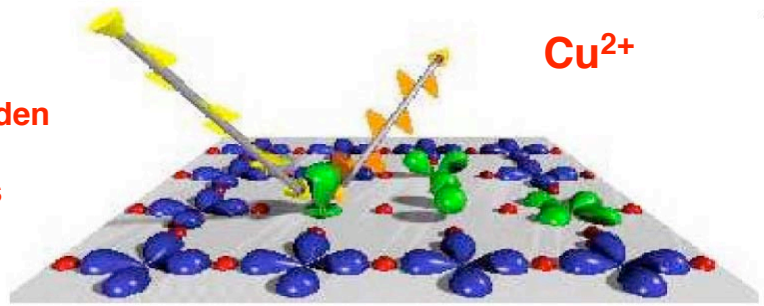
Soft x-rays RIXS: optics with q≠0

Cu L-edge (*2p* → *3d*) RIXS (930 eV)

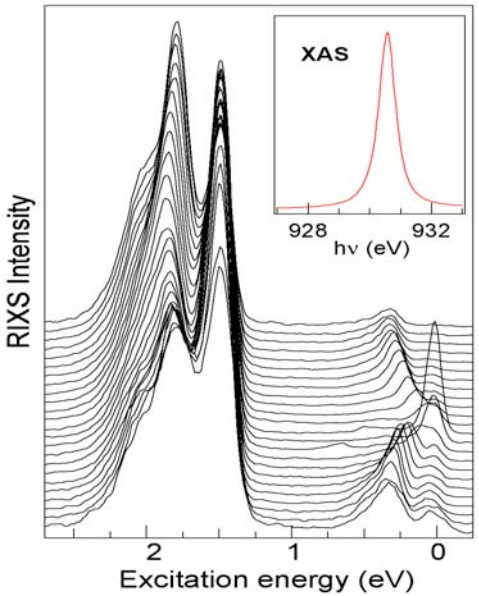
Directly probes *d* states of 3d transition metals ($L_{2,3}$ edges)



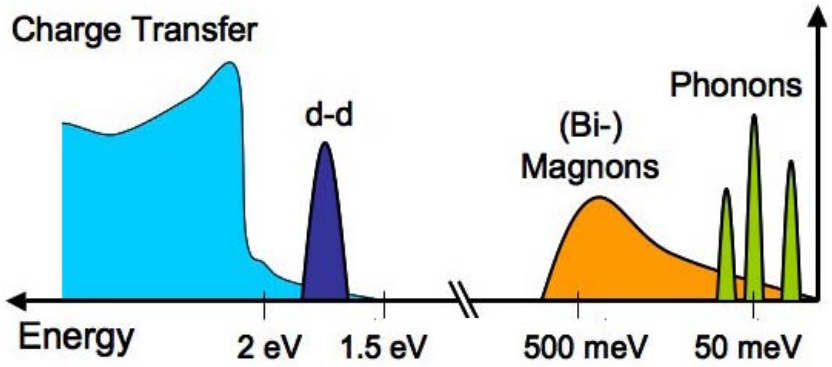
Optically-forbidden
(dipole, spin)
dd transitions



$3d^9 \rightarrow 2p^5 3d^{10} \rightarrow (3d^9)^*$



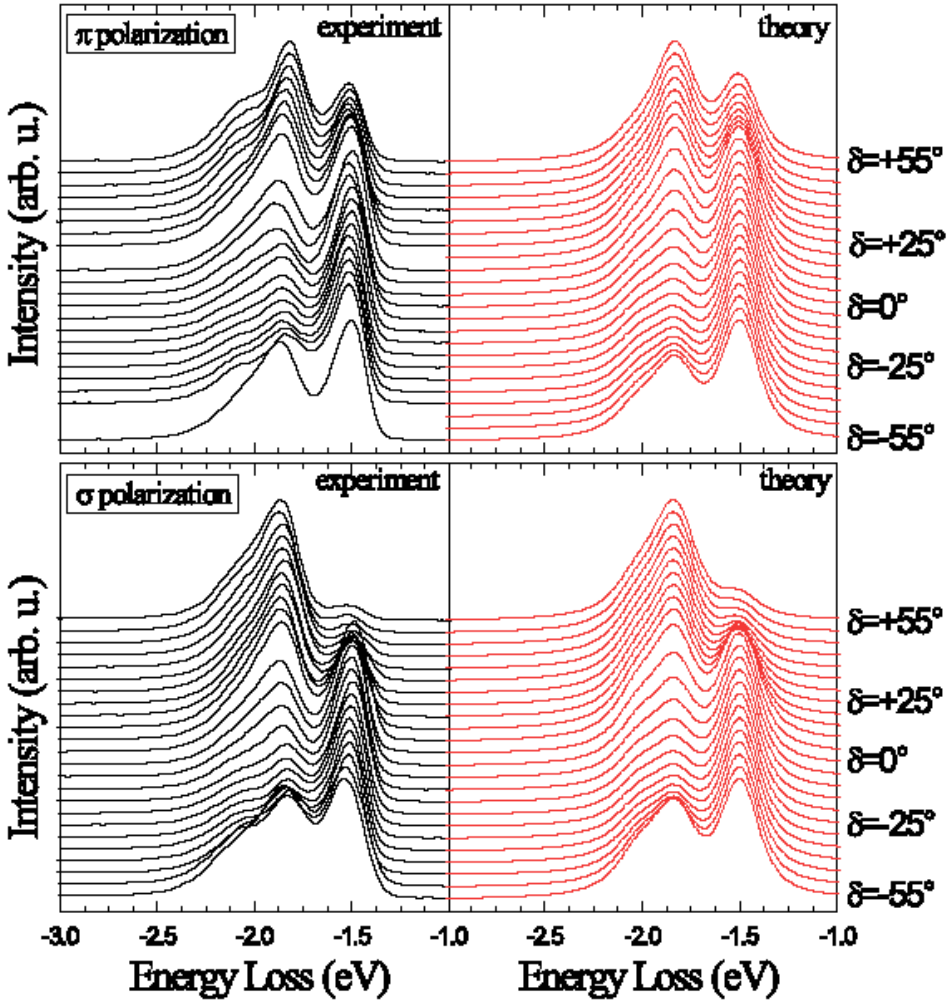
RIXS: probes multiple energy scales

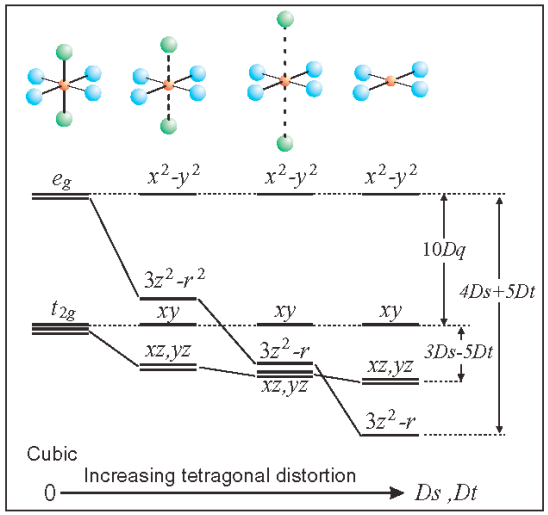


Ament et al.,
Rev. Mod. Phys. (2011)

Charge (*dd*) excitations

Sr_2CuOCl_2 - cluster model

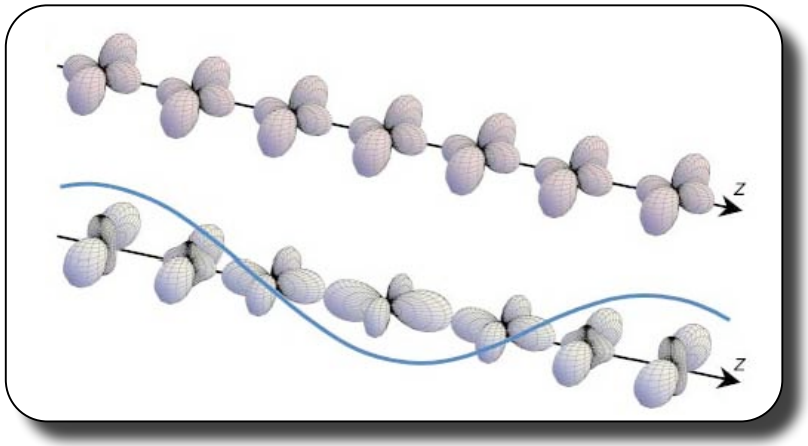




M. Moretti et al, New J. Phys. 13, 043026 (2011)

Orbital excitations

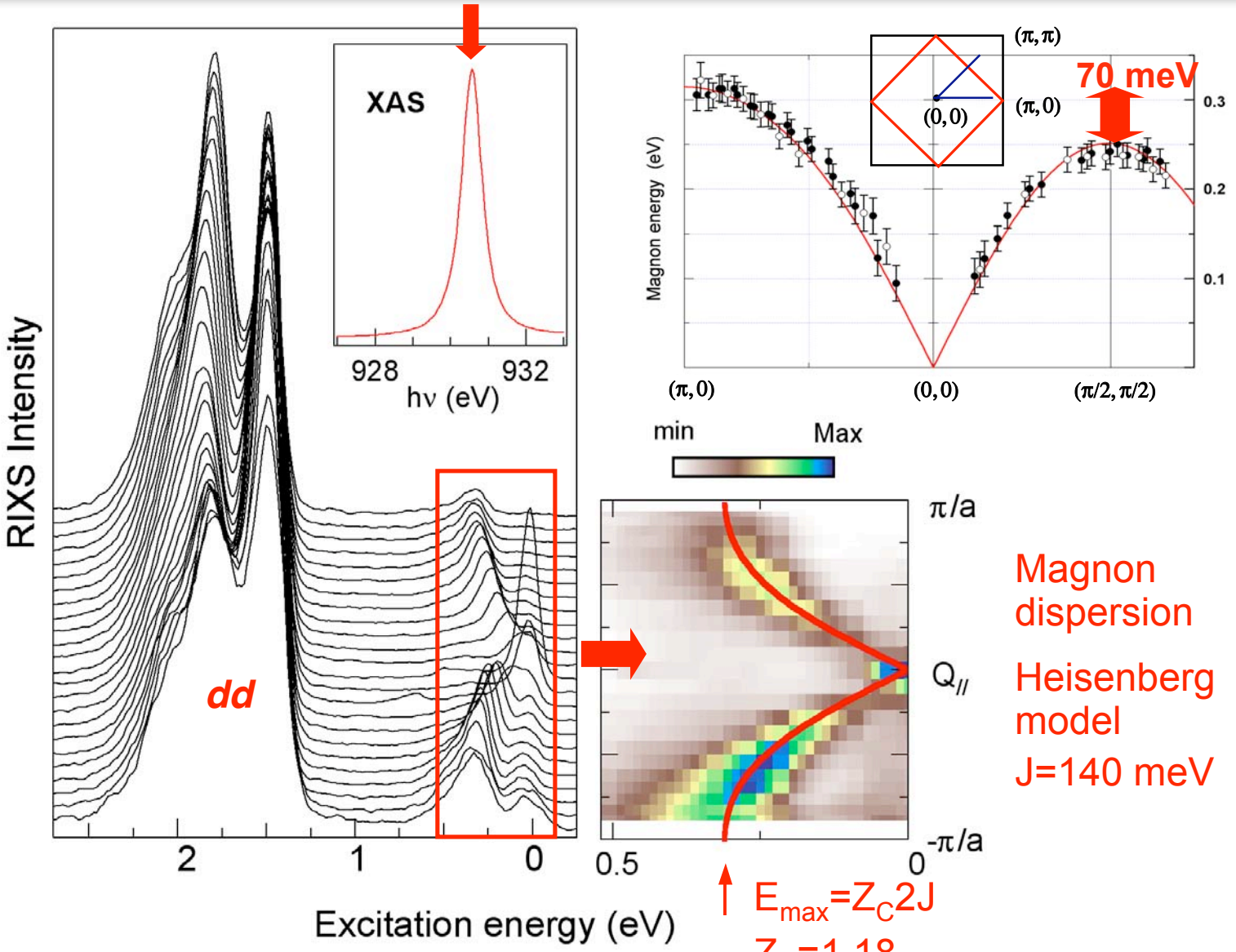
Orbital order



Orbiton

J. Schlappa et al., to be published

Spin excitations: $Sr_2CuO_2Cl_2$



Magnon dispersion

Heisenberg model

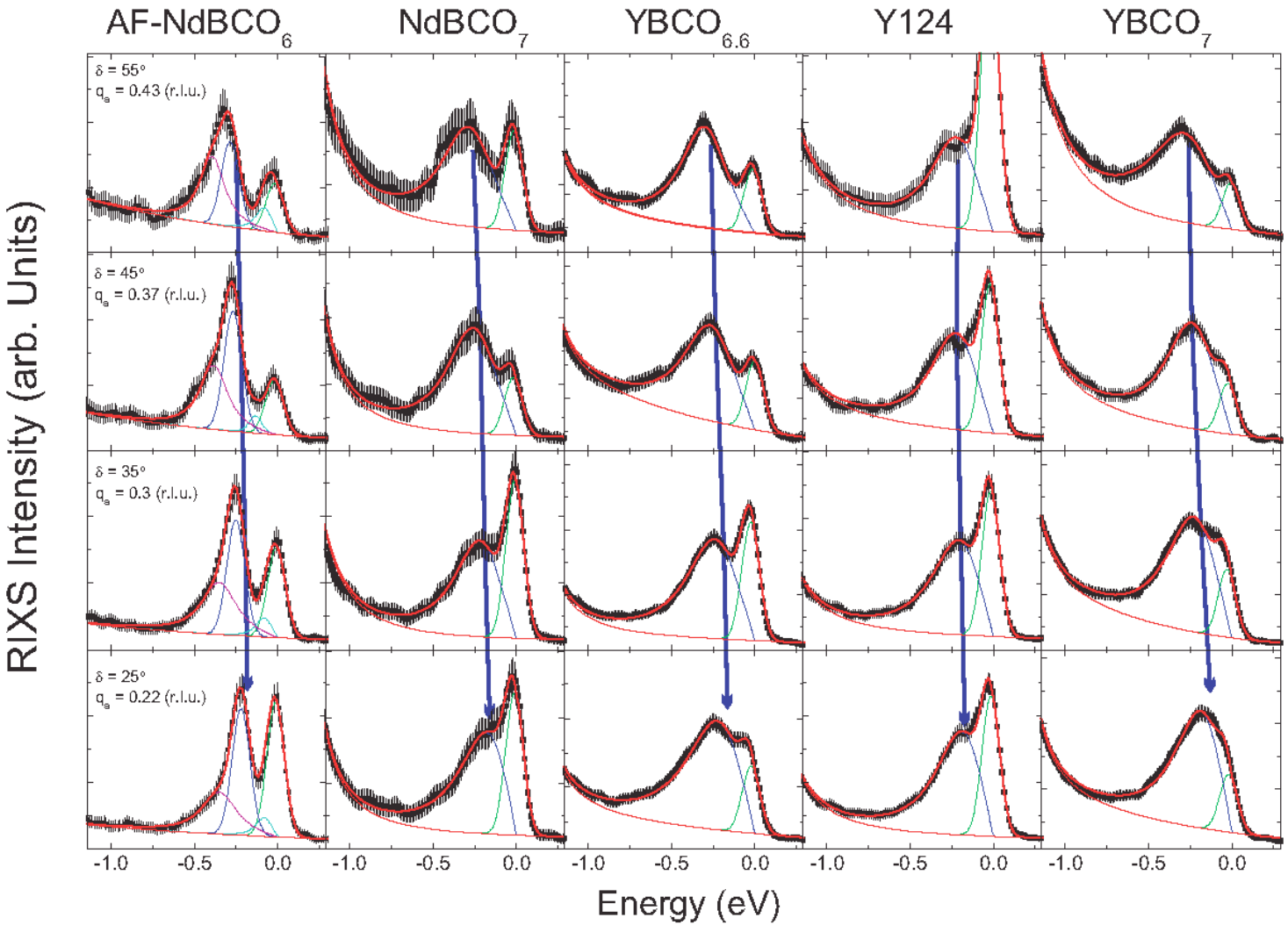
J=140 meV

$E_{max}=Z_C 2J$

$Z_C=1.18$

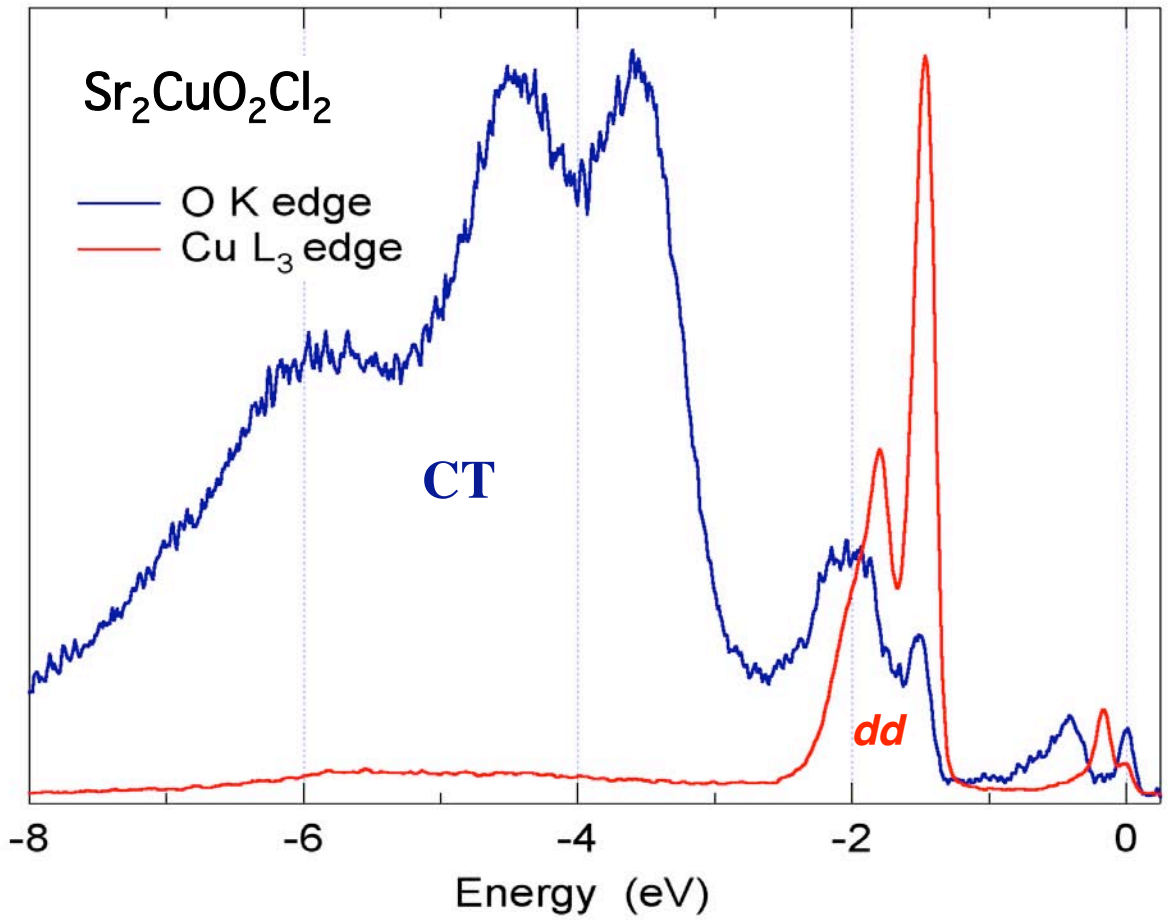
M. Guarise et al., *Phys. Rev. Lett.* **105**, 157006 (2010)

Paramagnons in the doped cuprates

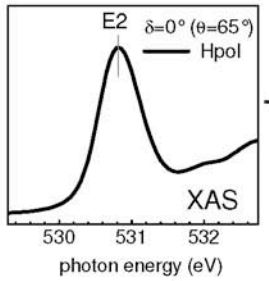


M. Le Tacon et al., *Nature Phys*. **7**, 725 (2011)

Complementary views from the Cu and the O sites



Gap excitations at the the O K-edge



$CuGeO_3$

charge-transfer excitations
strong T dependence

D: ?

C: Zhang-Rice singlet (ZRS) *

B: *d-d* excitations
No T dependence

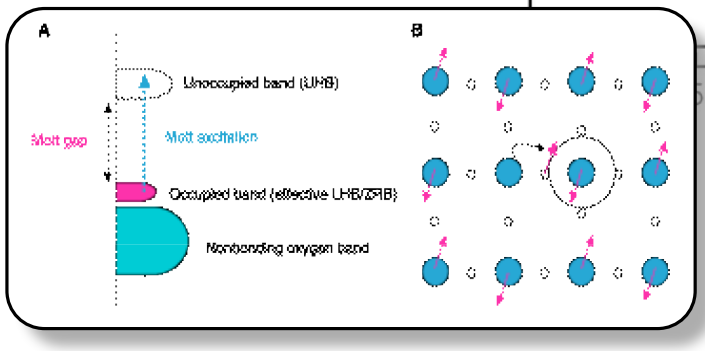
A: ~ elastic line

9 K
40 K
75 K
100 K
150 K
200 K
250 K
300 K

Intensity (a.u.)

4
3
2
1
0
energy loss (eV)

Sensitive to the magnetic structure



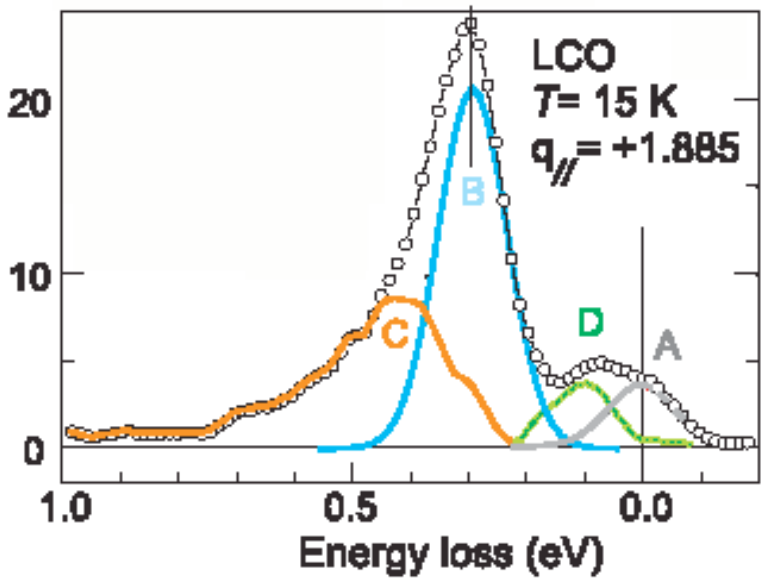
Zhang-Rice singlet

$d^9\underline{L}$

V. Bisogni, C. Monney et al., to be published

Opportunities at XFEL: 1. resolution

More flux = better resolution (up to a point)



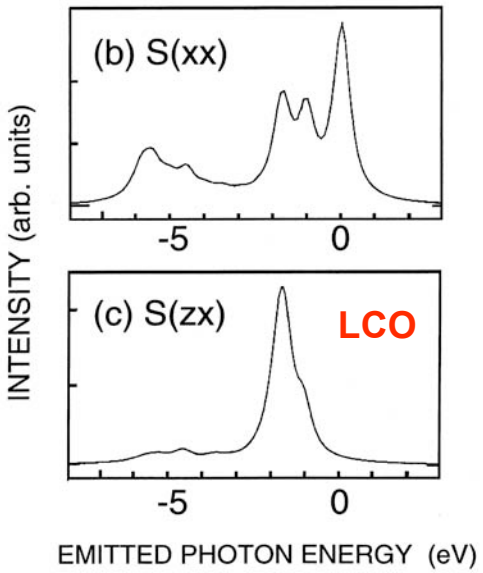
From: L. Braicovich et al., PRL **104**, 077002 (2010)

- Separate the truly elastic response
- Phonons
- single magnon vs. multiple magnons
- Smaller J materials

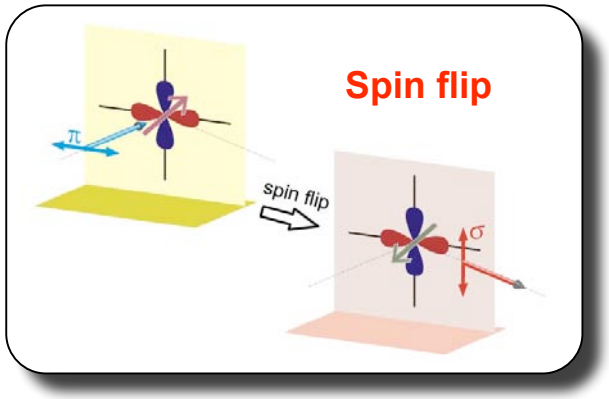
i) beyond cuprates ii) simpler theory)

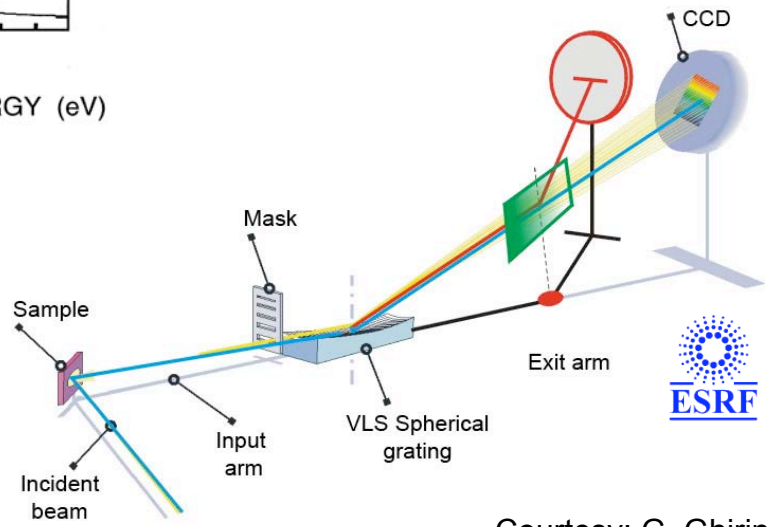
Opportunities at XFEL: 2. polarization analysis

More flux = photons to spare (up to a point)



A.Kotani, JES **110**, 197 (2000)



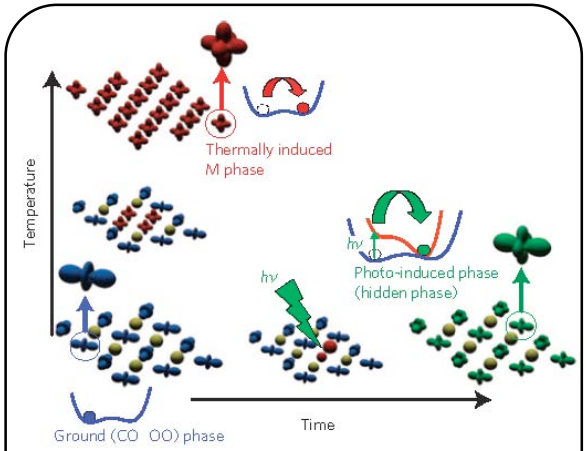


Courtesy: G. Ghiringhelli

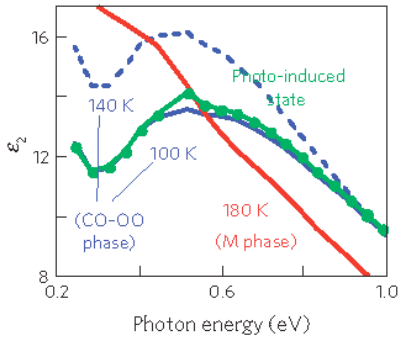
Opportunities at XFEL : 3. time-resolved RIXS

RIXS is a fast probe - NOT limited to q=0

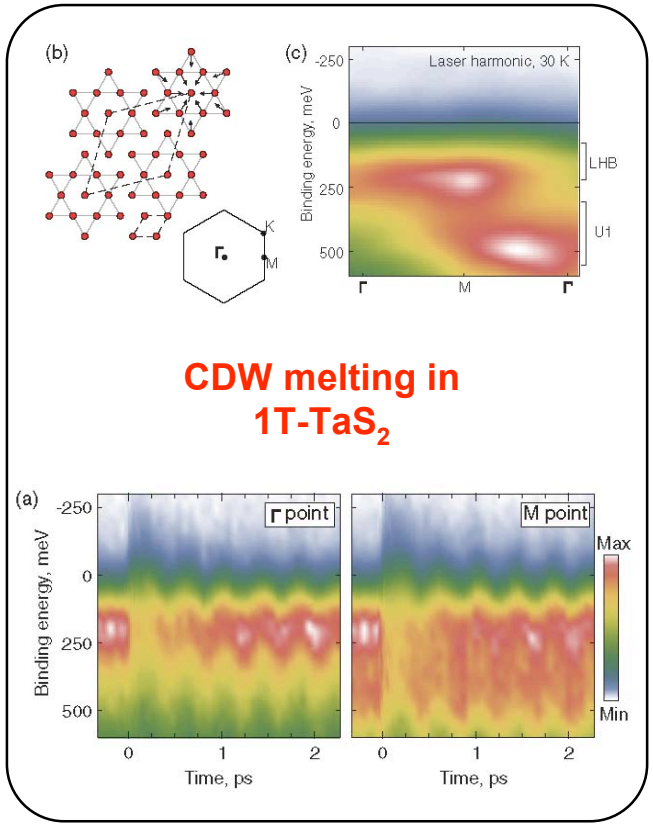
Transient/hidden phases - relaxation dynamics



Hidden insulating phase in $Nd_{0.5}Sr_{0.5}MnO_3$

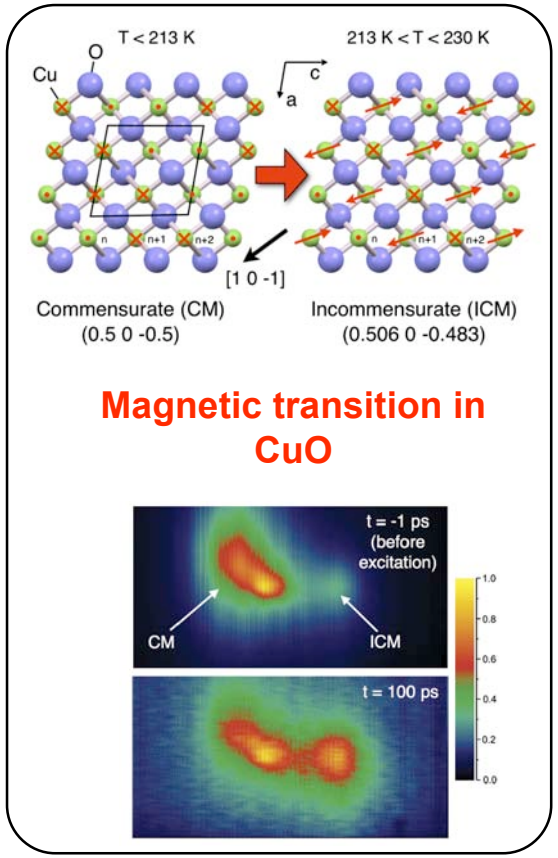


H. Ichikawa et al., Nature Mat. **10**, 101 (2011)



CDW melting in $1T\text{-}TaS_2$

J.C. Petersen et al., PRL **107**, 177402 (2011)

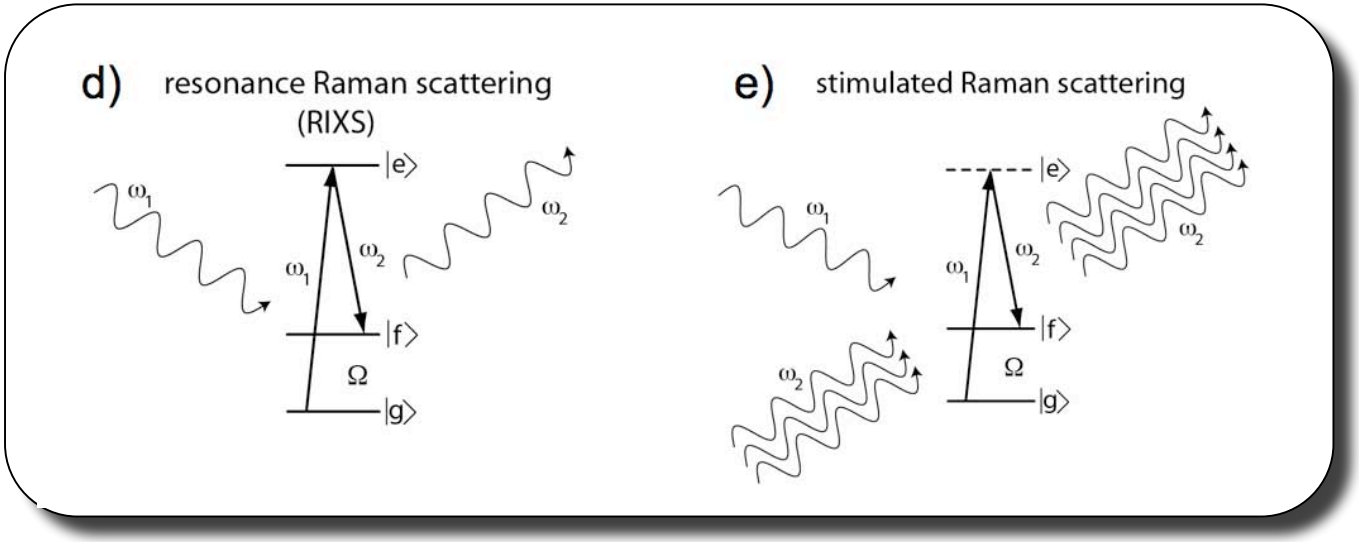


Magnetic transition in CuO

S.L. Johnson et al., PRL **108**, 037203 (2012)

Opportunities at XFEL: out on a limb

Stimulated RIXS and other nonlinear processes



B. Patterson, SLAC-TN-10-026

Potential gain: 10^6 (?)

…yet to be demonstrated

Summary

- RIXS probes charge, spin, orbital degrees of freedom in strongly correlated materials
- New opportunities for hRIXS @ E-XFEL
- A careful analysis of spectrometer design options is (urgently) needed