Resonant Inelastic X-ray Scattering on high Tc cuprates, iron pnictides and magnetic iridates

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Michel van Veenendaal, Tom Devereaux, Ilya Eremin

KITP 30.10.2014

What is

Resonant
Inelastic
X-ray scattering

} ***RIXS***

What is *Resonant* *Inelastic* *X-ray scattering* } *RIXS*

X-ray scattering: photon in → solid → photon out

inelastic: $\omega_{out} < \omega_{in}$

resonant: tune ω_{in} *to an atomic absorption edge*

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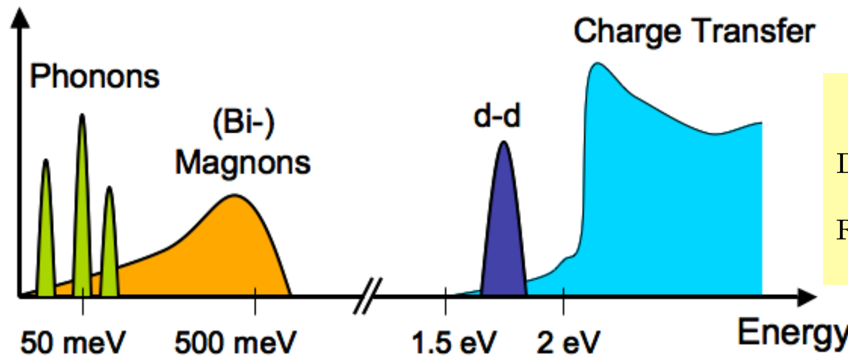

Ament, van Veenendaal, Devereaux, Hill & JvdB
Rev. Mod. Phys. 83, 705 (2011)

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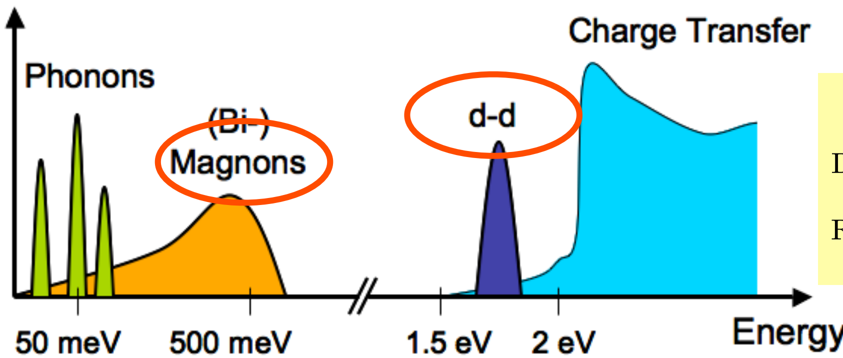

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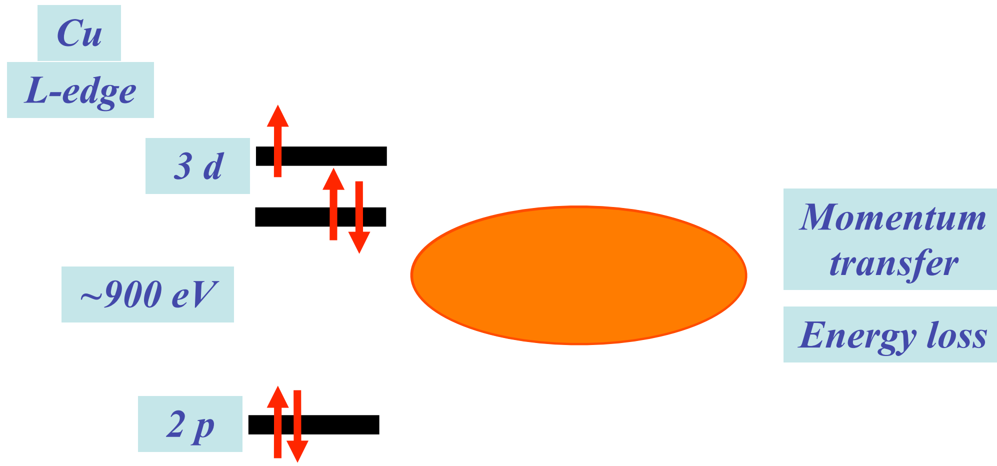
How RIXS works



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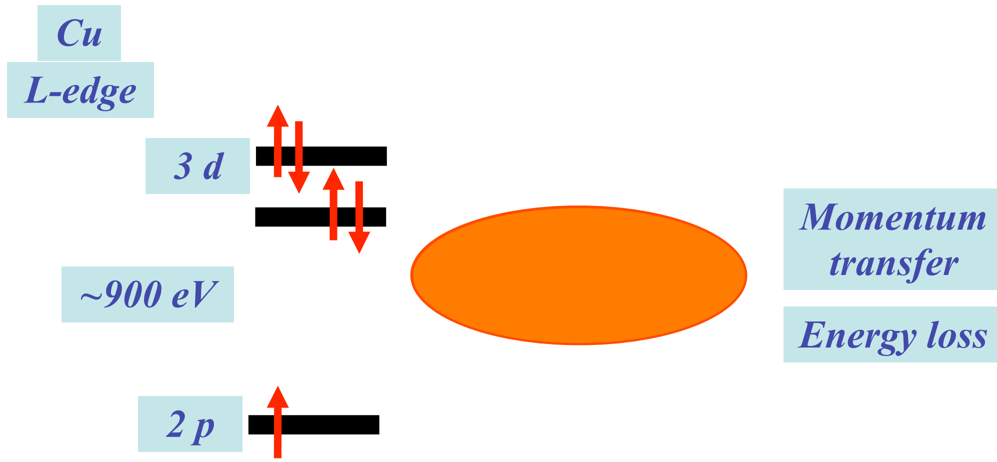

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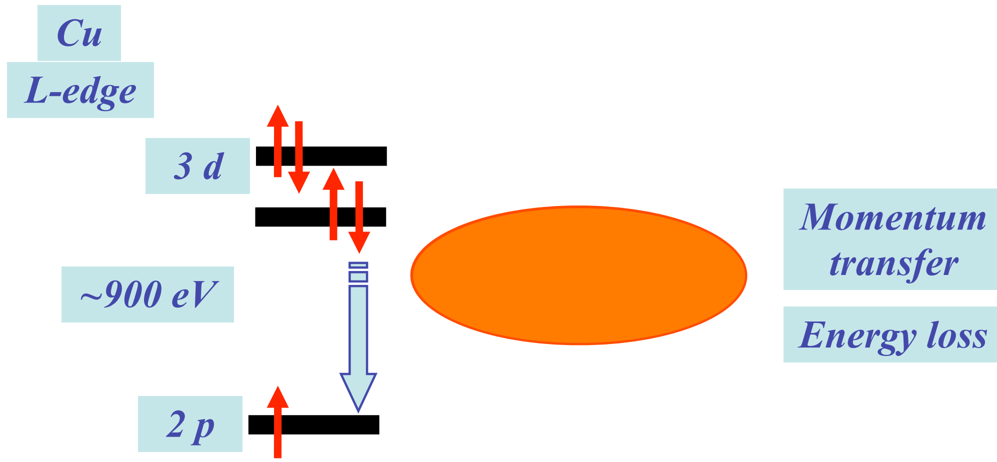

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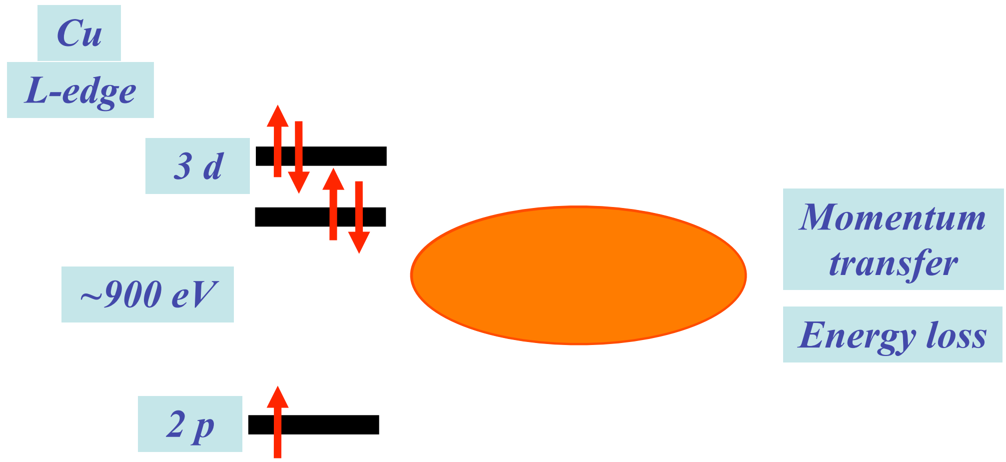

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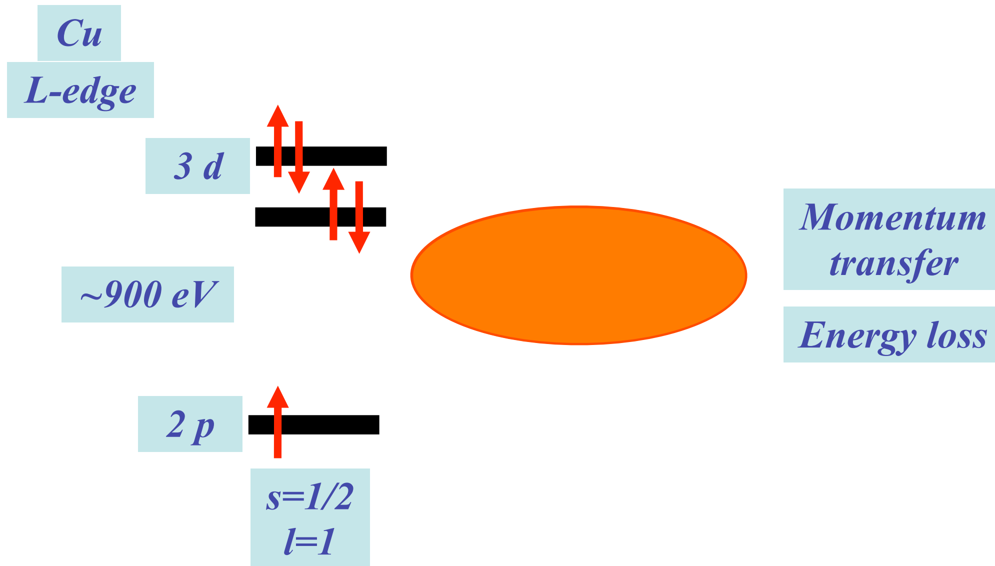

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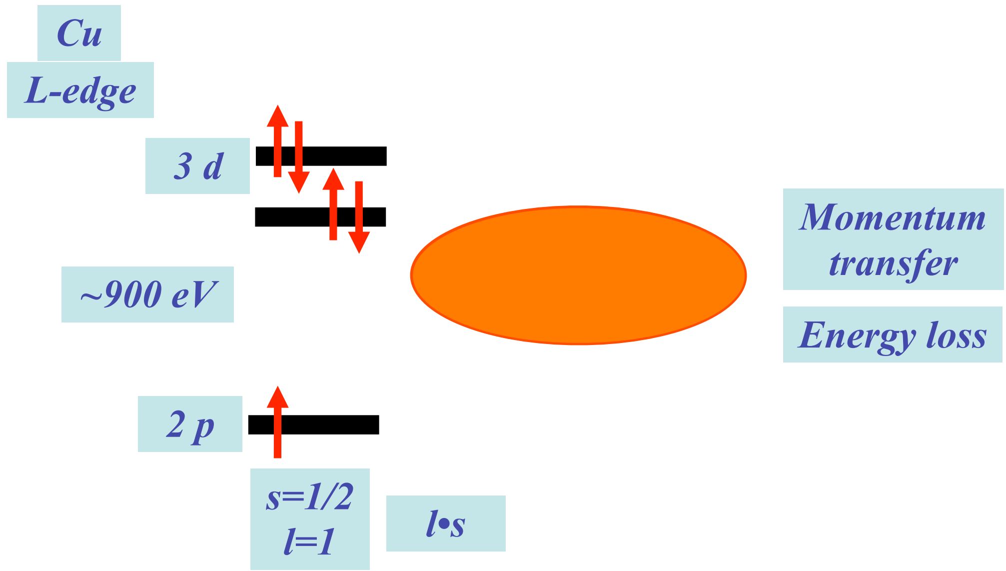

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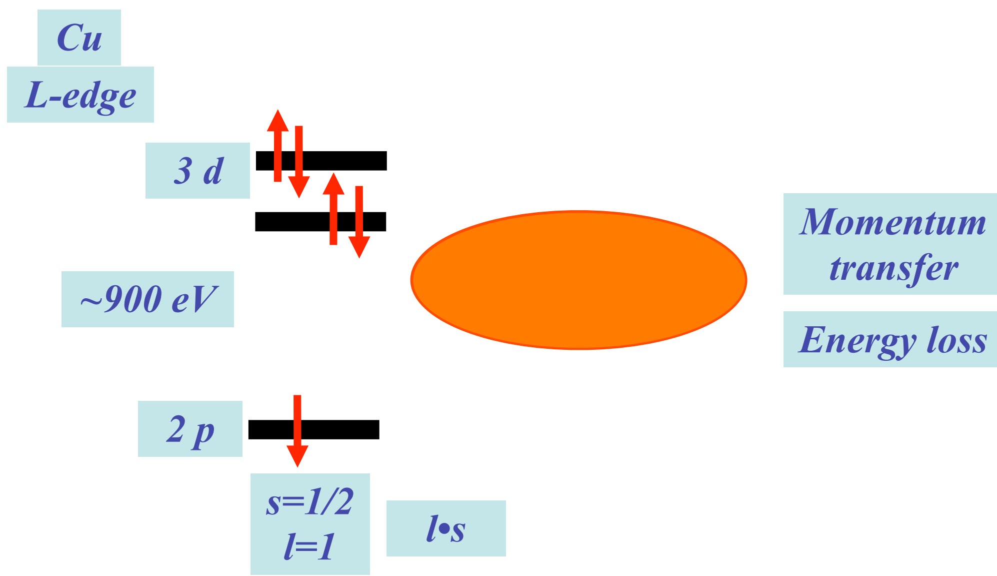

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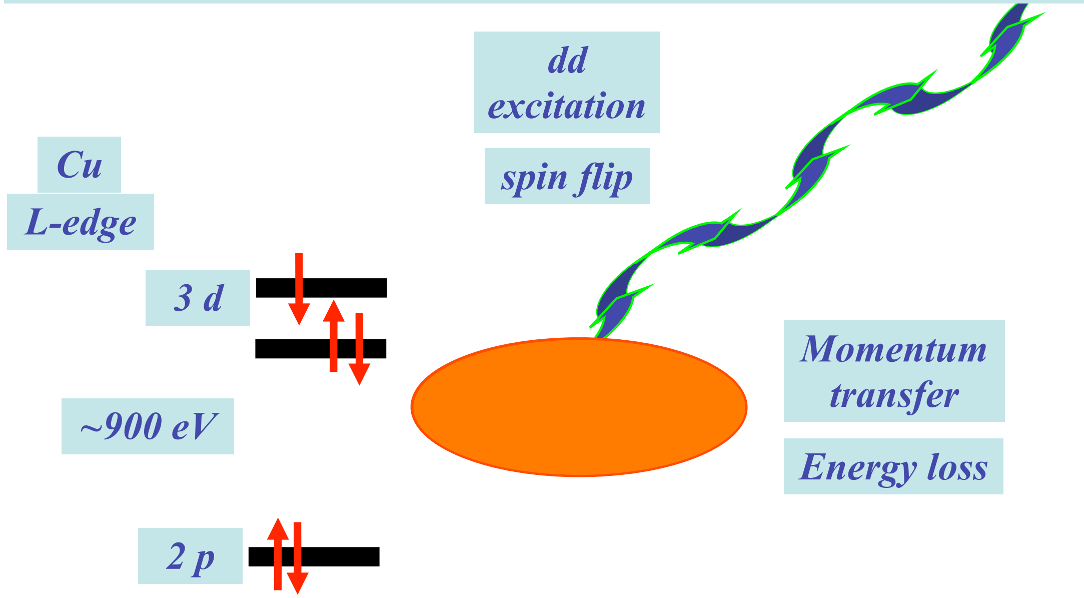

Ament *et al.*, PRL 103, 117003 (2009)

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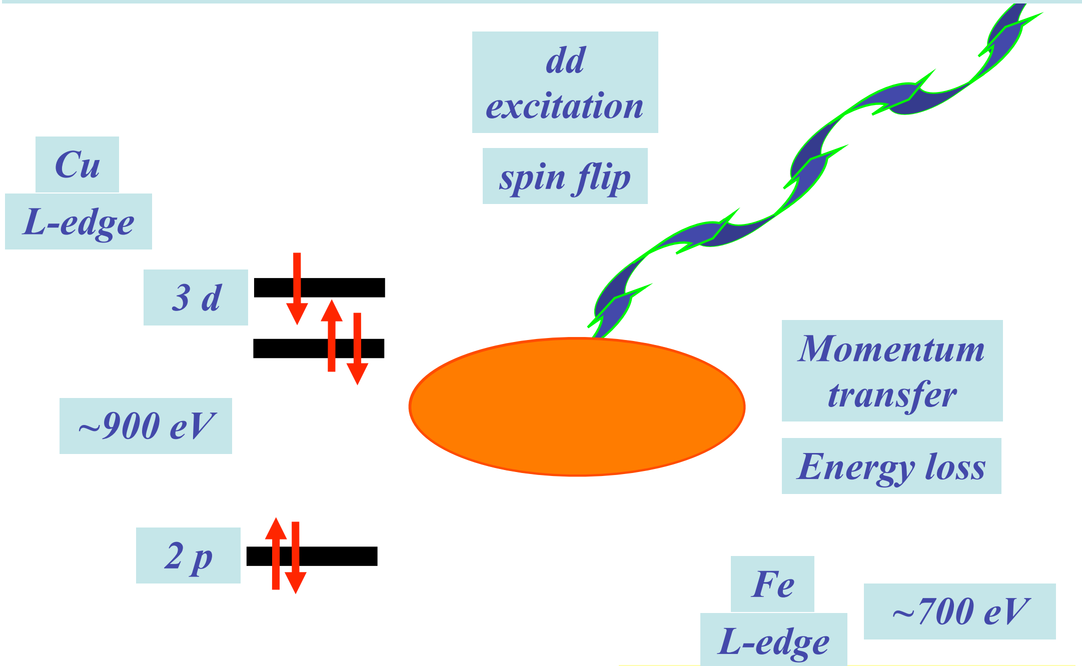

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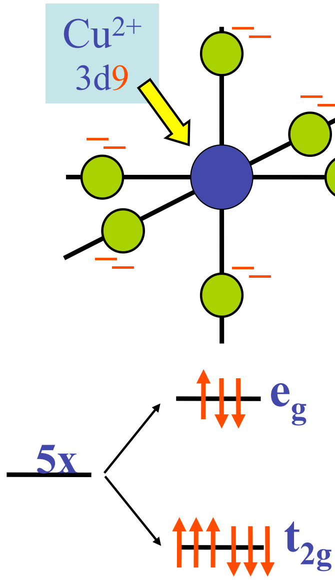
RIXS:

Orbital and Magnetic excitations in quasi-2D and 1D antiferromagnets

Cu oxides & Fe pnictides

Atomic Model: Local d-d orbital splitting: Cu^{2+}

Cubic Crystal field splitting



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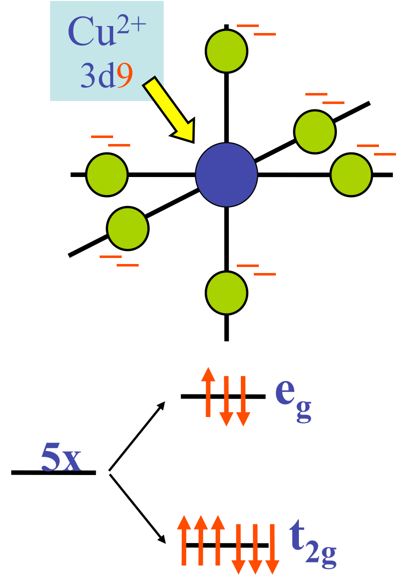

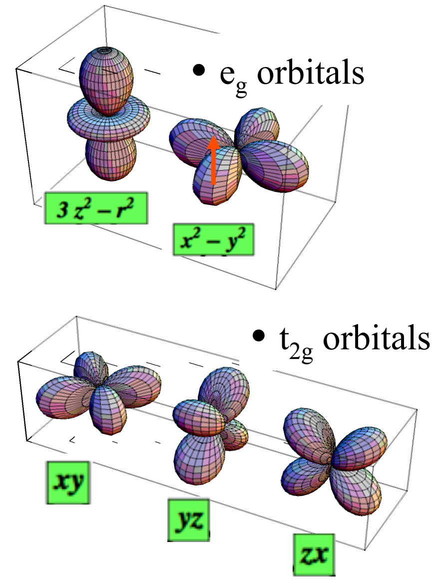

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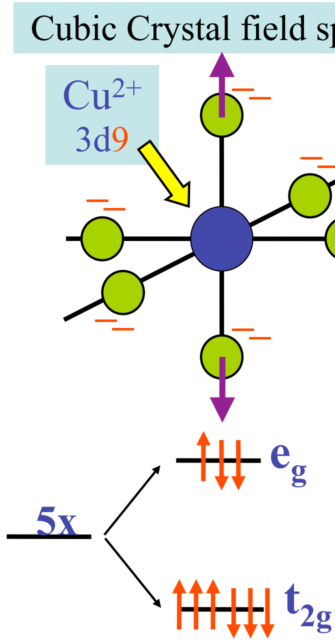

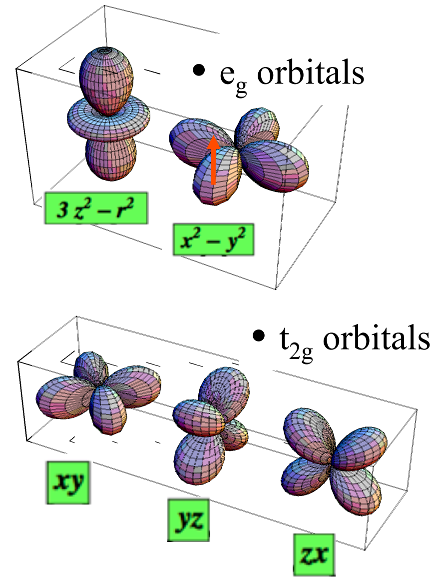

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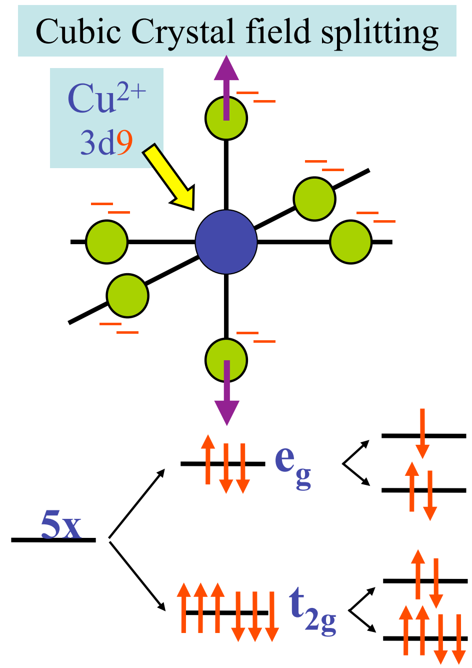
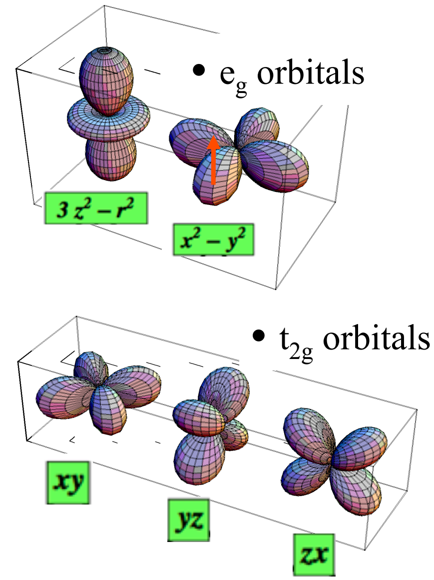
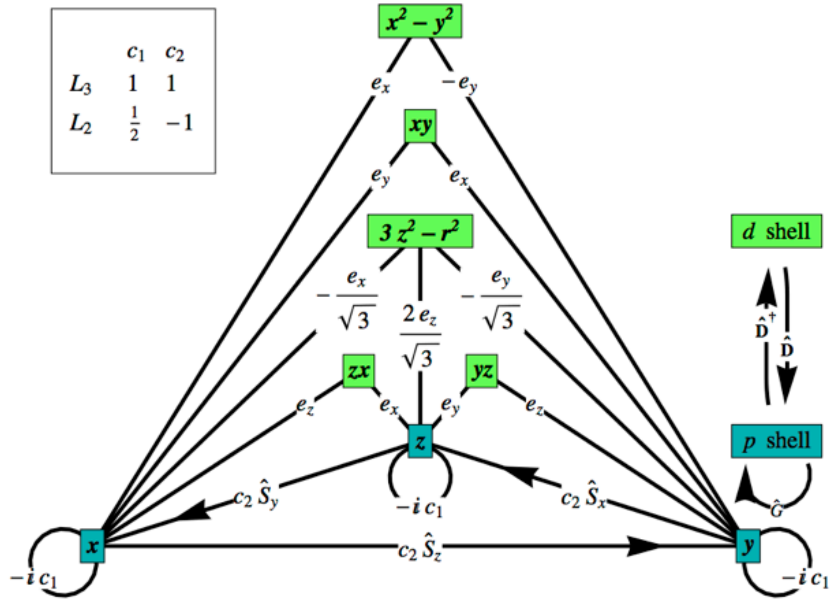




RIXS amplitude @ transition metal L-edge



Ament, Ghiringhelli, Moretti, Braicovich & JvdB, PRL 103, 117003 (2009)

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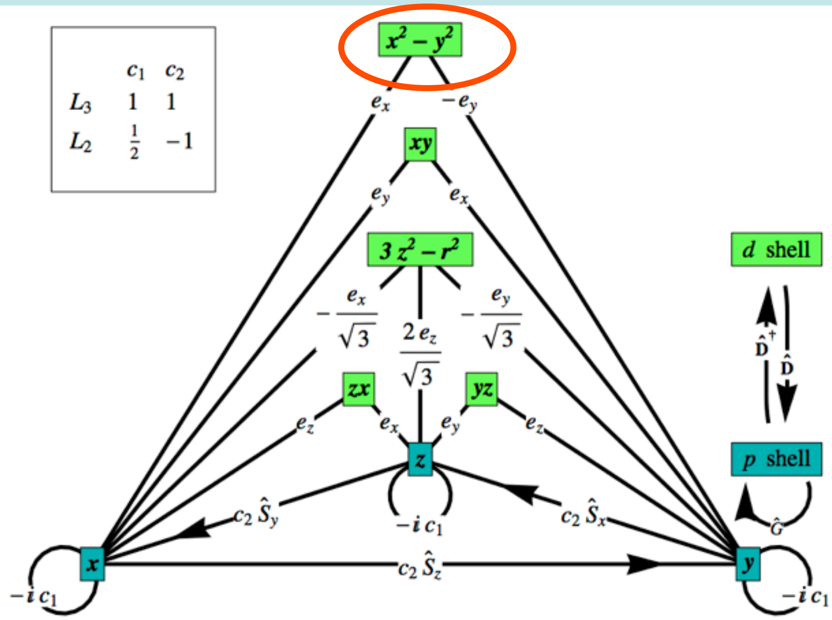

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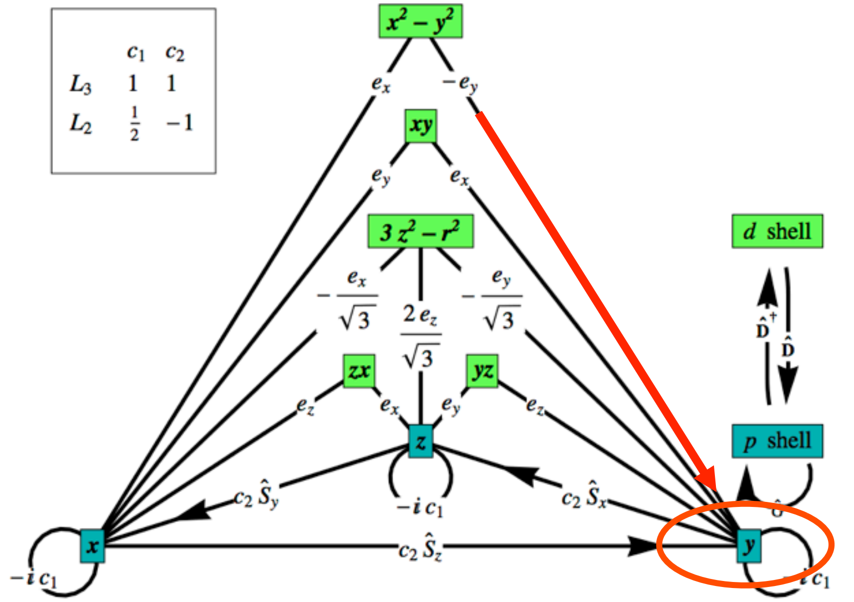

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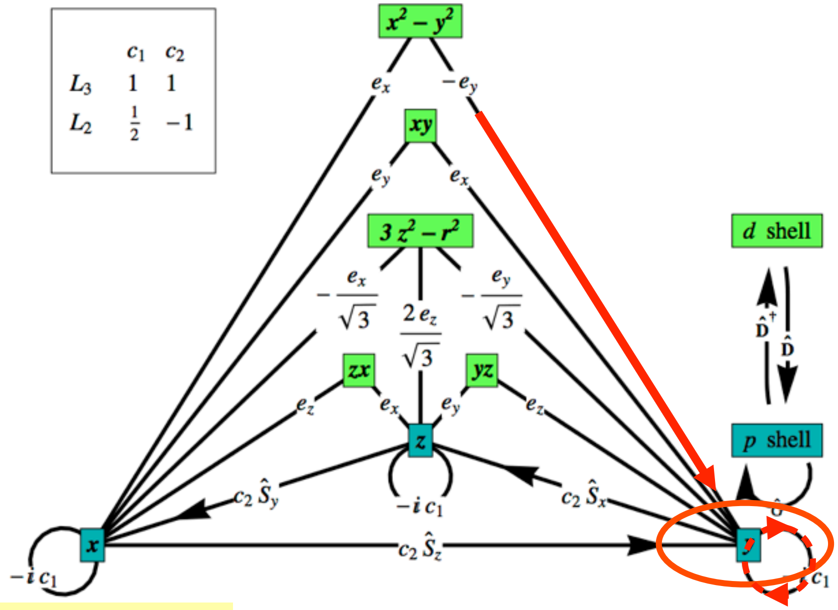

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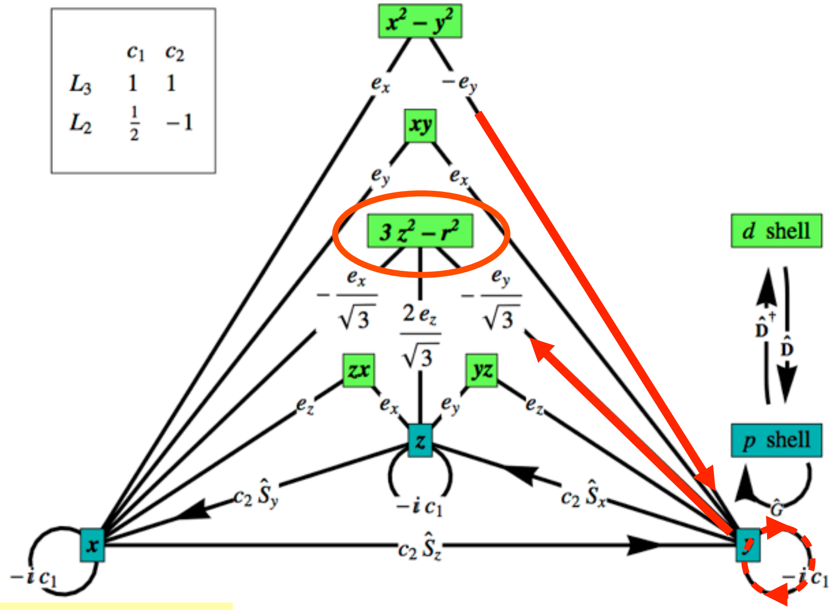

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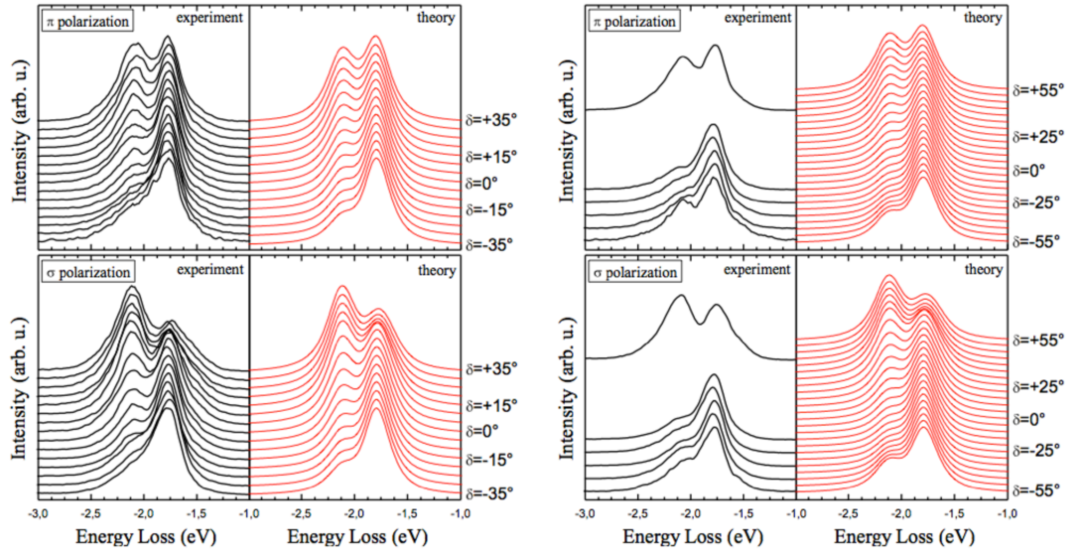
RIXS: Orbital excitations in La_2CuO_4



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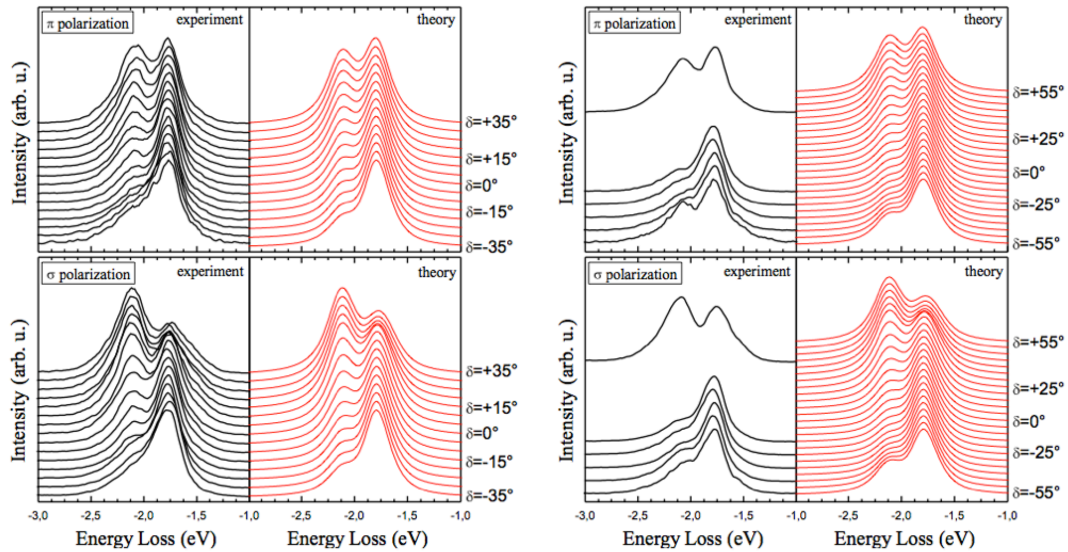

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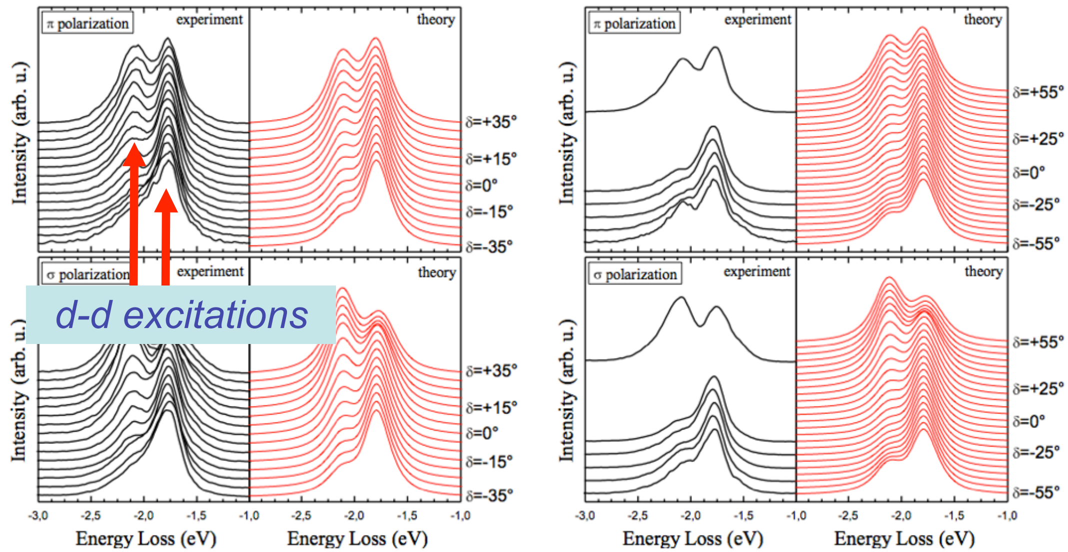

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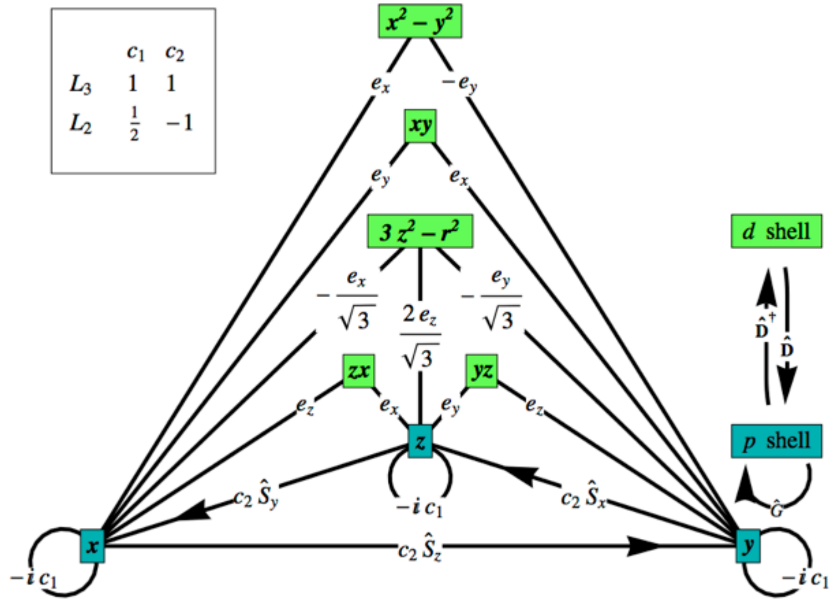

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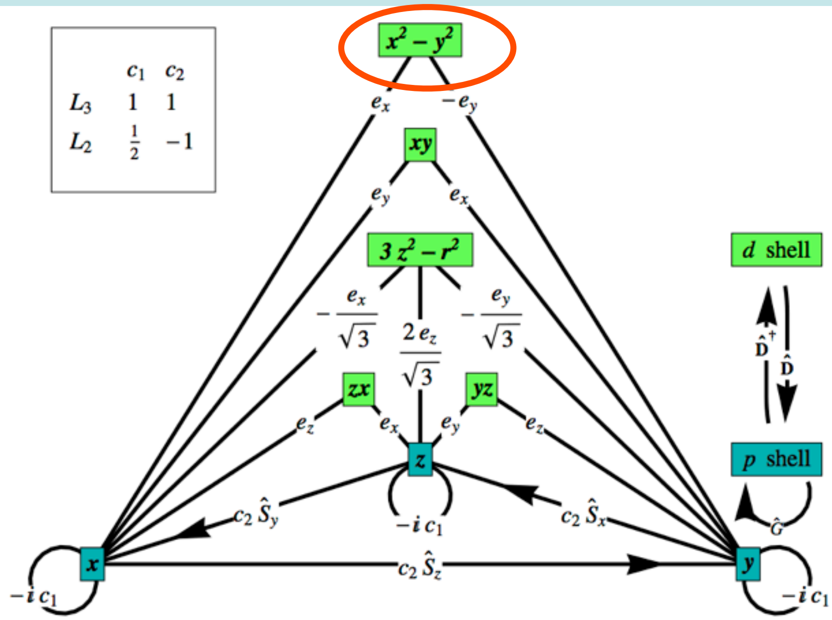

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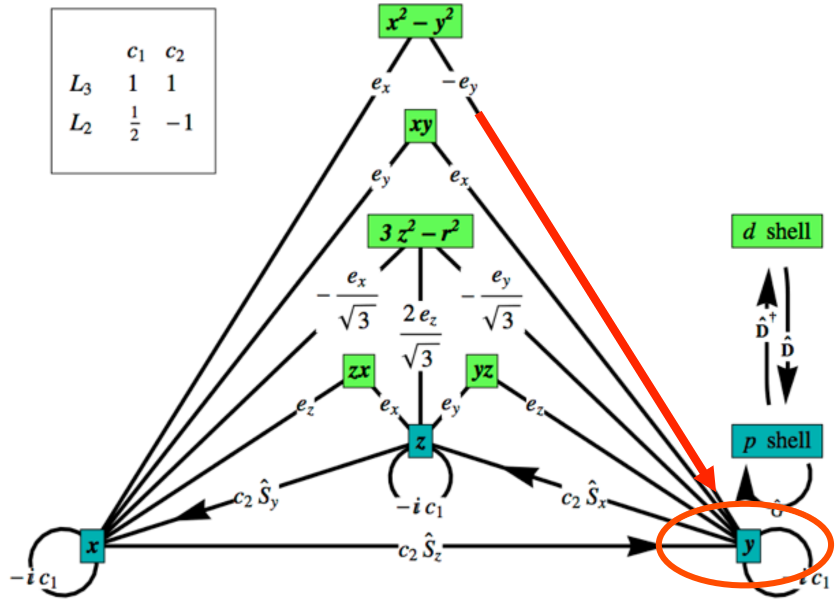

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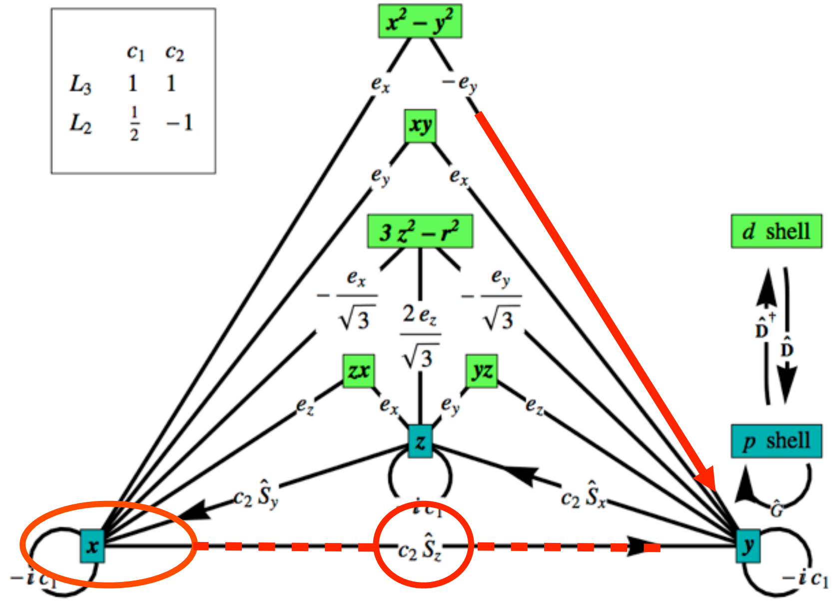

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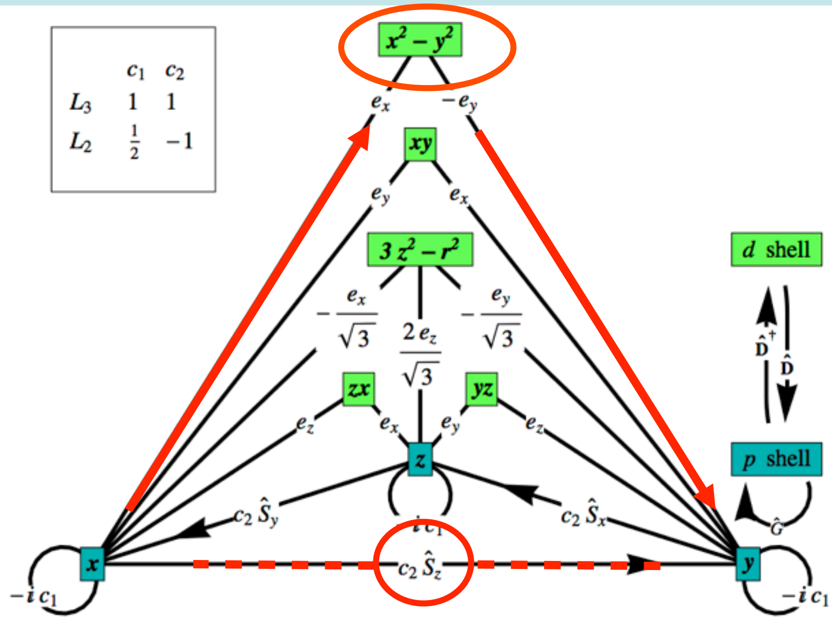

	c_1	c_2
L_3	1	1
L_2	$\frac{1}{2}$	-1

Ament, Ghiringhelli, Moretti, Braicovich & JvdB, PRL 103, 117003 (2009)

x^2-y^2 spin *NOT* // z:
pure spin flip

Marra, Wohlfeld & JvdB, PRL 109, 117401 (2012)

Magnetic RIXS on La_2CuO_4 @ Cu L-edge

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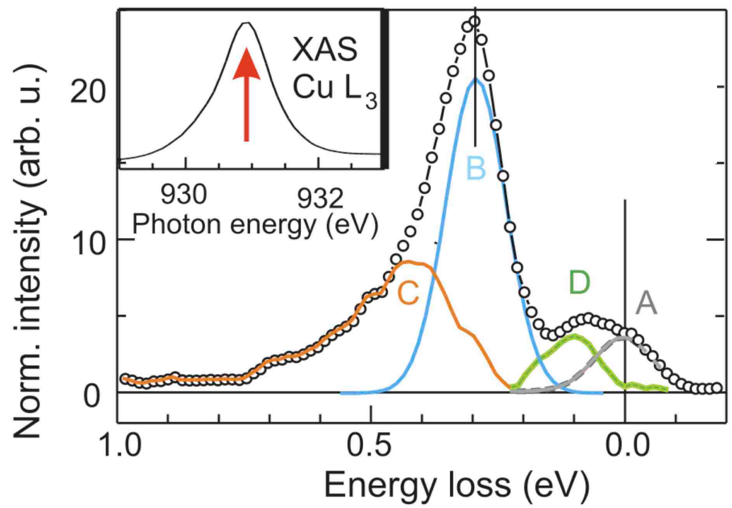

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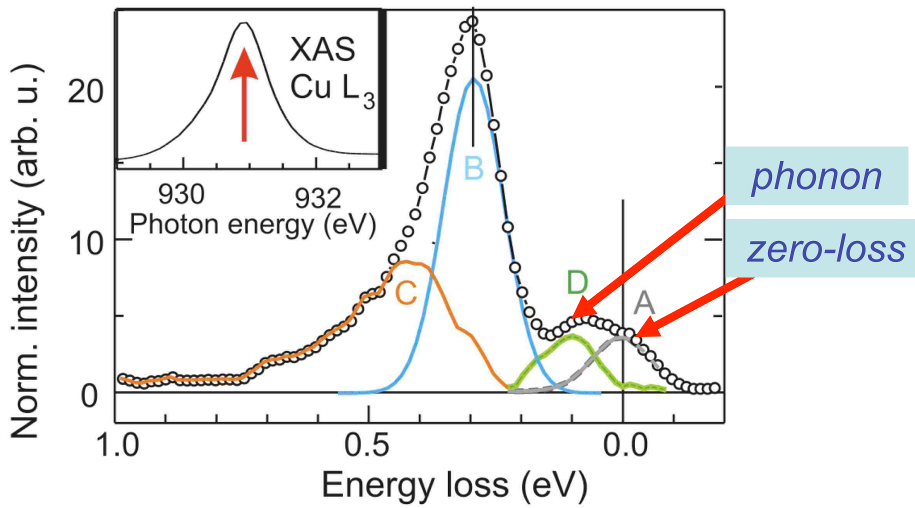

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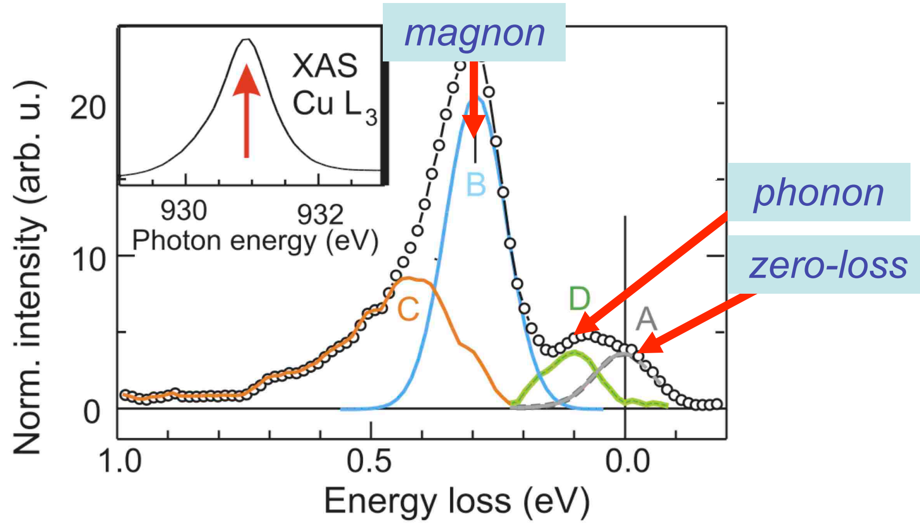

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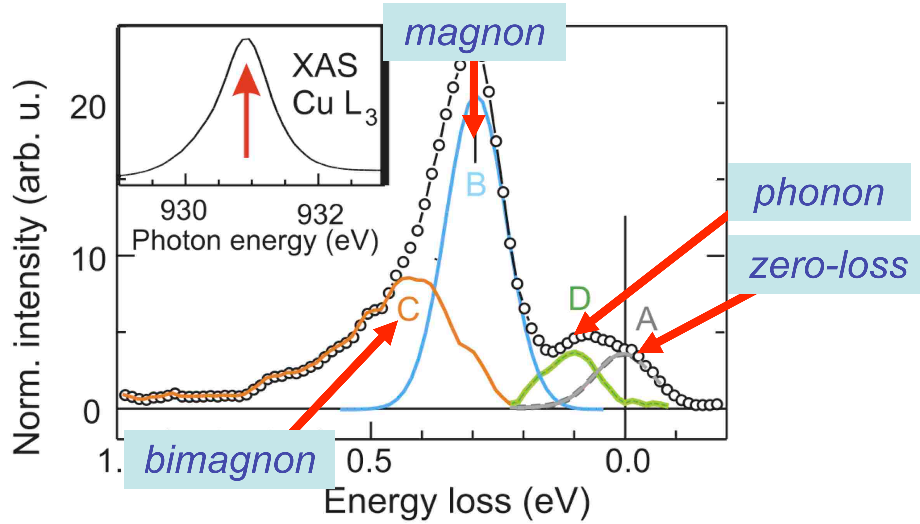

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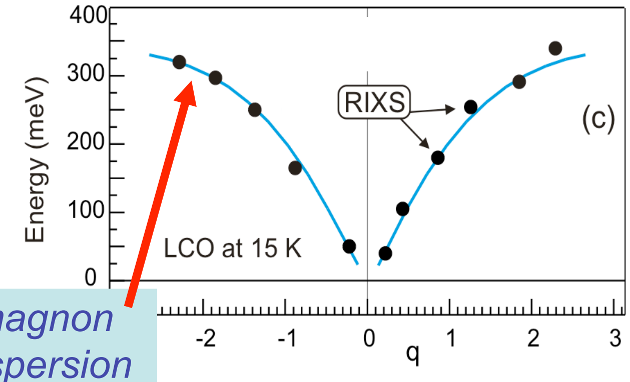

magnon dispersion

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

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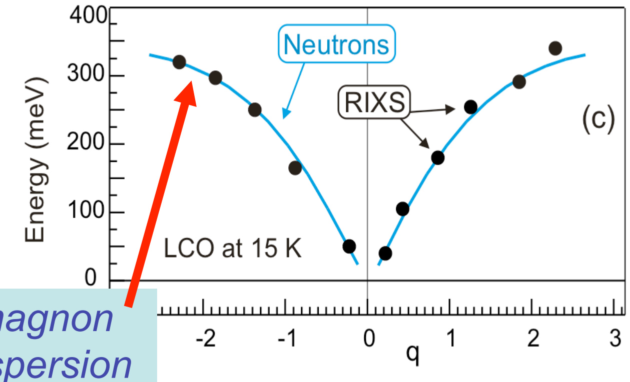

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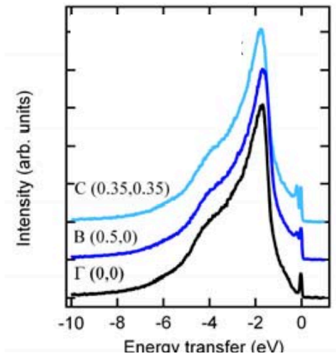
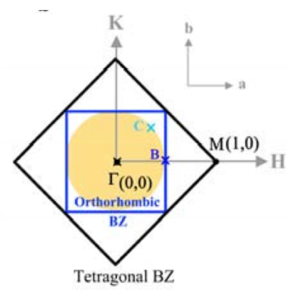
Magnetic RIXS on $BaFe_2As_2$ @ Fe L-edge





Kejin Zhou, Huang, Monney, Dai, Strocov, Wang, Chen, Zhang, Dai, Patthey, JvdB, Ding & Schmitt, Nat. Comm. 4, 1470 (2013)

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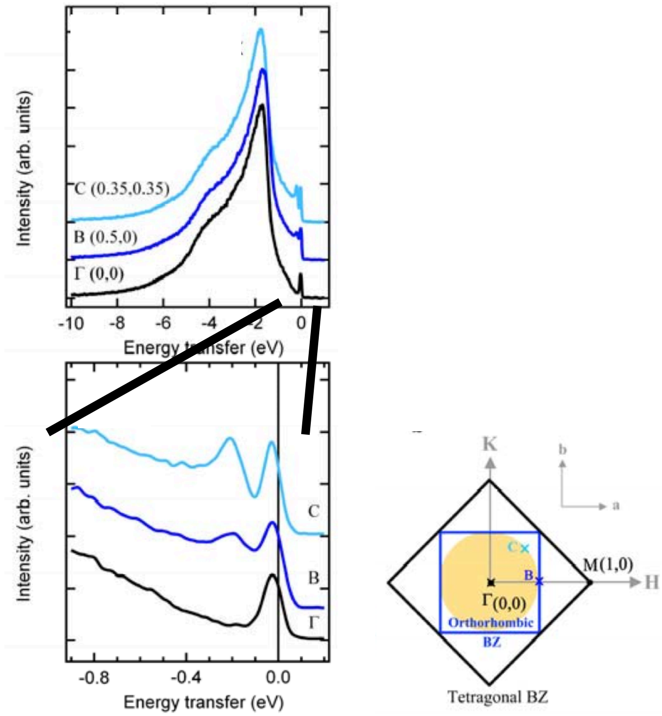

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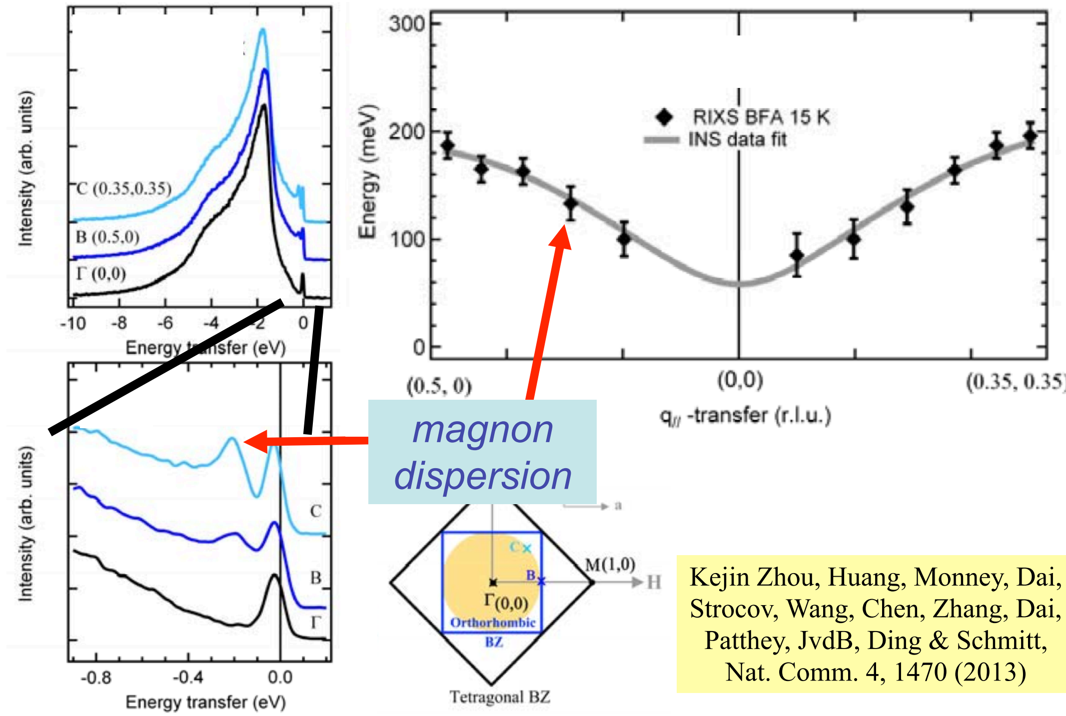

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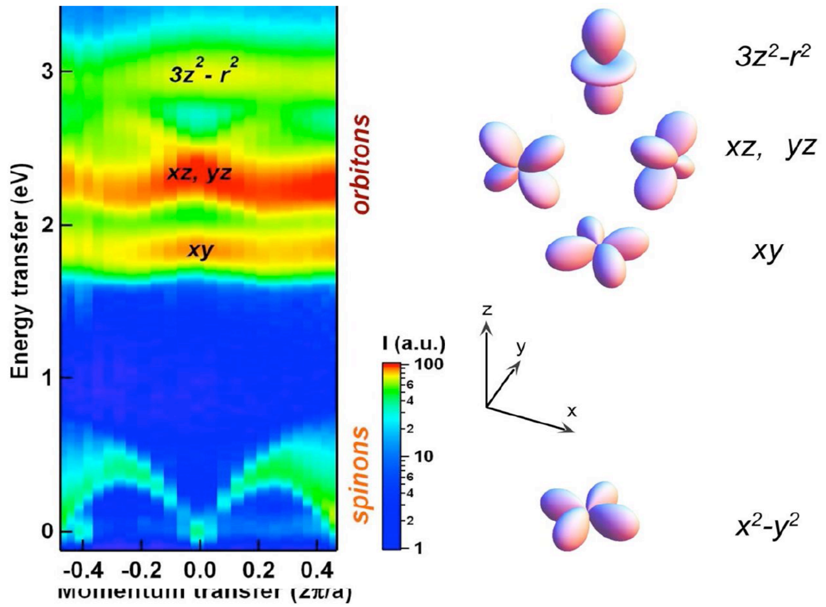
RIXS spectrum of Sr_2CuO_3 spin chain



Schlappa, Wohlfeld, Zhou, Mourigal, Haverkort, Strocov, Hozoi, Monney, Nishimoto, Singh, Revcolevschi, Caux, Patthey, Ronnow, JvdB & Schmitt, Nature 485, 82 (2012)

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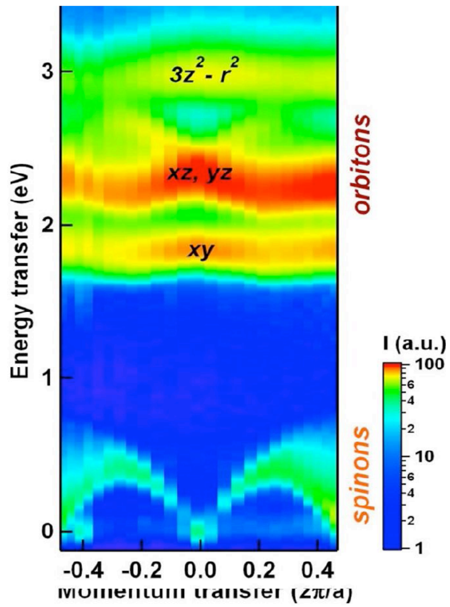

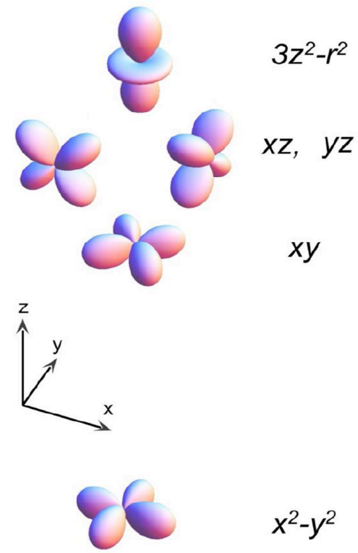

Orbital excitations

Schlappa, Wohlfeld, Zhou, Mourigal, Haverkort, Strocov, Hozoi, Monney, Nishimoto, Singh, Revcolevschi, Caux, Patthey, Ronnow, JvdB & Schmitt, Nature 485, 82 (2012)

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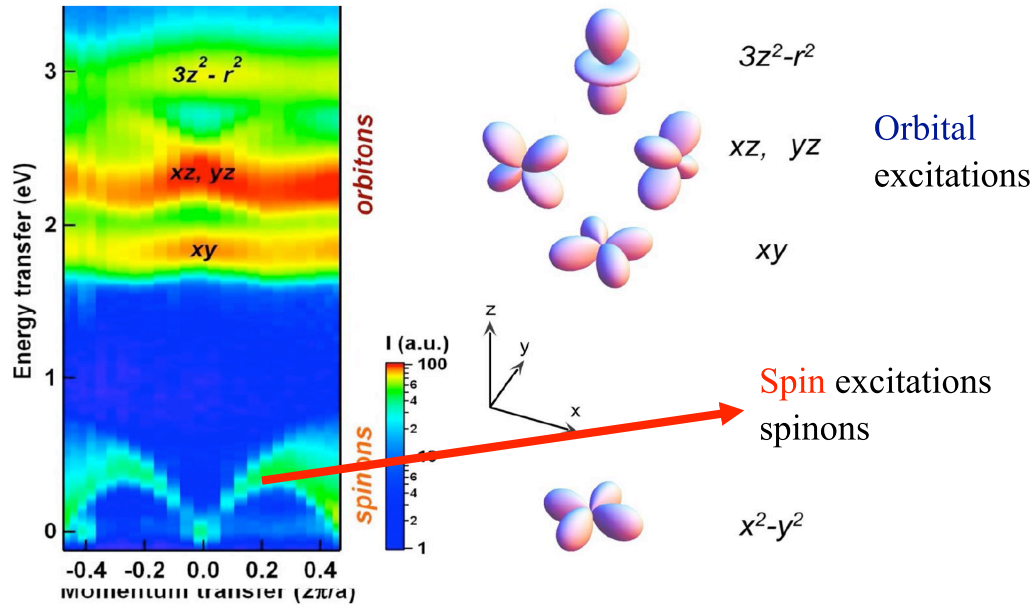

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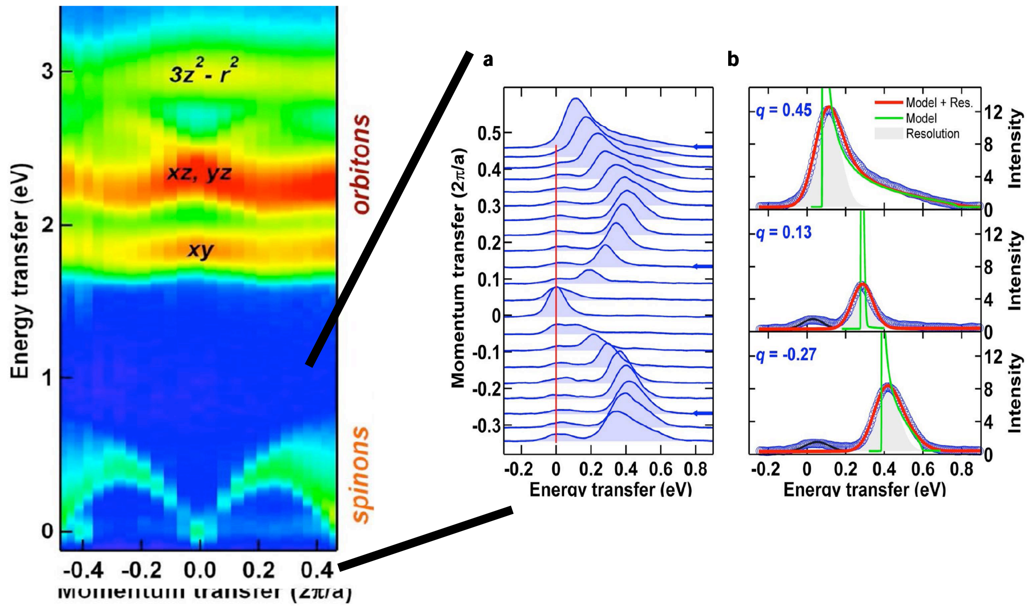

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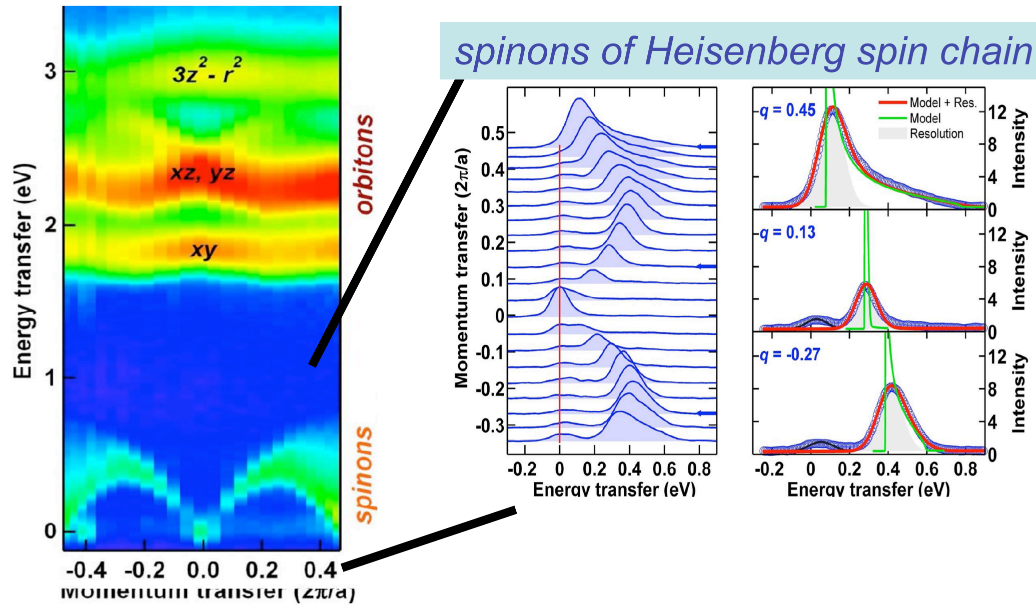

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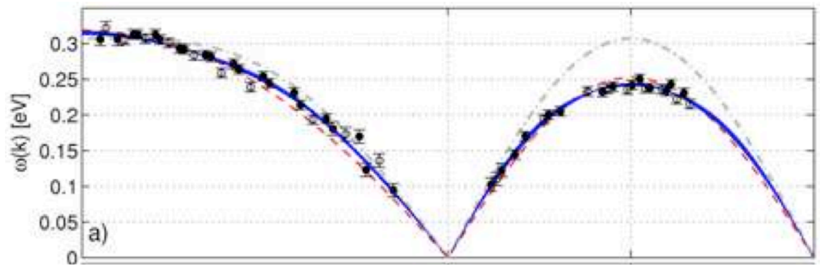
RIXS magnon dispersion of $Sr_2CuO_2Cl_2$

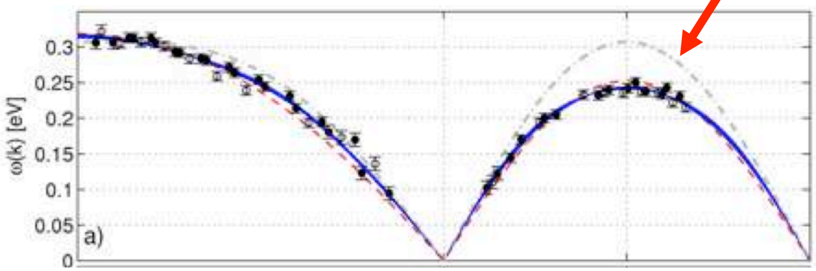


—> transferred momentum q

Guarise *et al*.,
PRL 105, 157006 (2010)

RIXS magnon dispersion of $Sr_2CuO_2Cl_2$

deviation from
simple Heisenberg



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PRL 105, 157006 (2010)

Magnetic RIXS vs. Inelastic Neutron Scattering

	RIXS	*Neutrons*
amount of material needed		
magnon energy accessible		
materials		
momentum range accessible		

Magnetic RIXS vs. Inelastic Neutron Scattering

	RIXS	Neutrons
amount of material needed	small	large
magnon energy accessible		
materials		
momentum range accessible		

Magnetic RIXS vs. Inelastic Neutron Scattering

	RIXS	*Neutrons*
amount of material needed	*small*	*large*
magnon energy accessible	*high (>25 meV)*	*low (<25 meV)*
materials		
momentum range accessible		

Magnetic RIXS vs. *Inelastic Neutron Scattering*

	RIXS	*Neutrons*
amount of material needed	*small*	*large*
magnon energy accessible	*high (>25 meV)*	*low (<25 meV)*
materials	*Cu, Fe ...*	*non-absorbers*
momentum range accessible		

Magnetic RIXS vs. Inelastic Neutron Scattering

	RIXS	Neutrons
amount of material needed	small	large
magnon energy accessible	high (>25 meV)	low (<25 meV)
materials	Cu, Fe ...	non-absorbers
momentum range accessible	soft: < 1 BZ hard: few BZ's	many BZ's

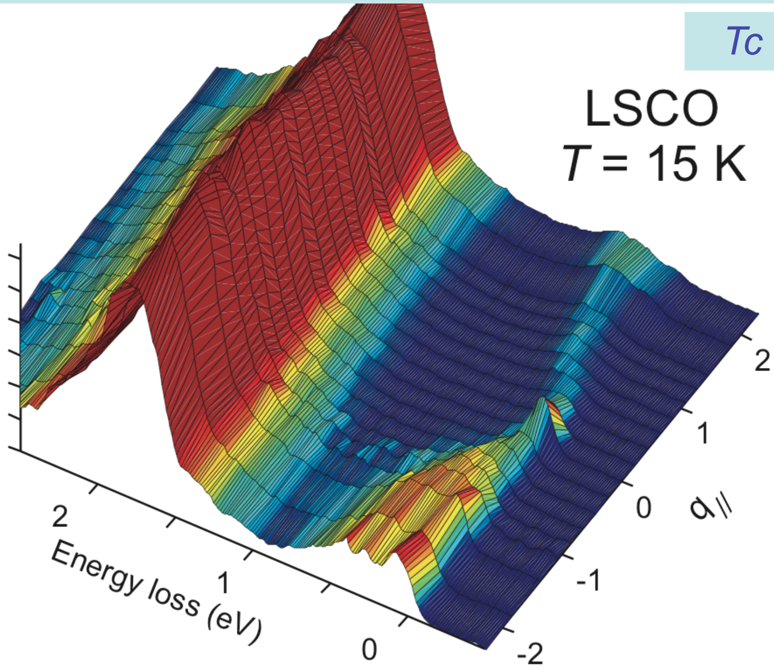
Magnetic RIXS on

doped quasi-2D

Cu-oxides and Fe-pnictides

Magnetic L-edge RIXS on 8% doped $La_{2-x}Sr_xCuO_4$

Tc = 21K



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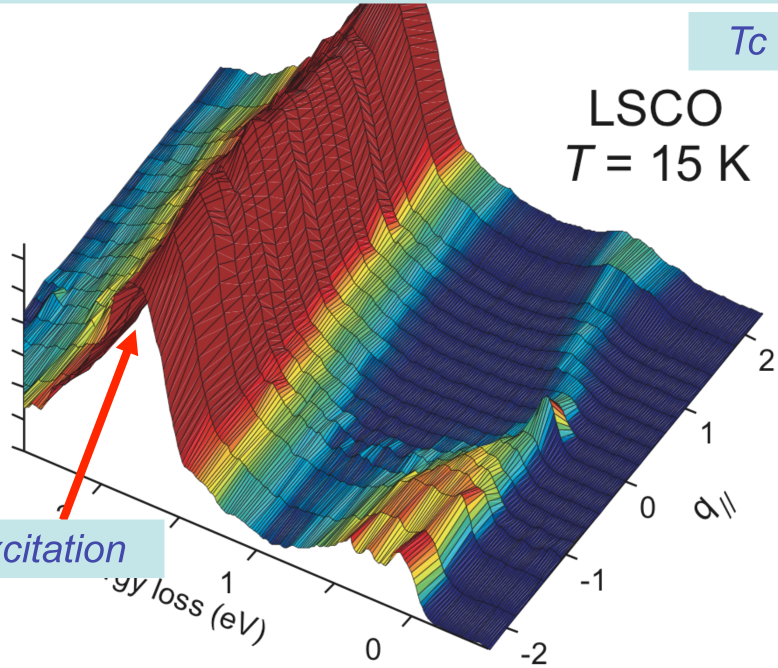

d-d excitation

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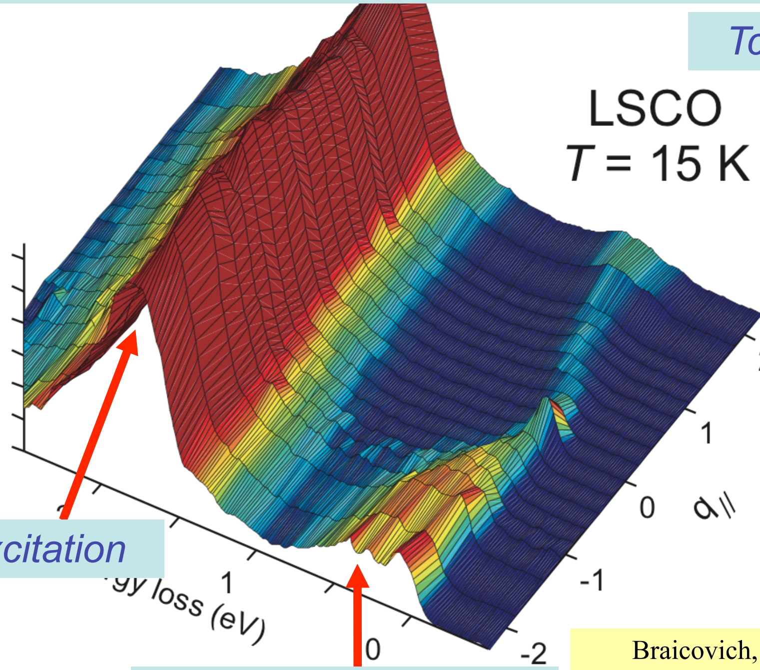


d-d excitation

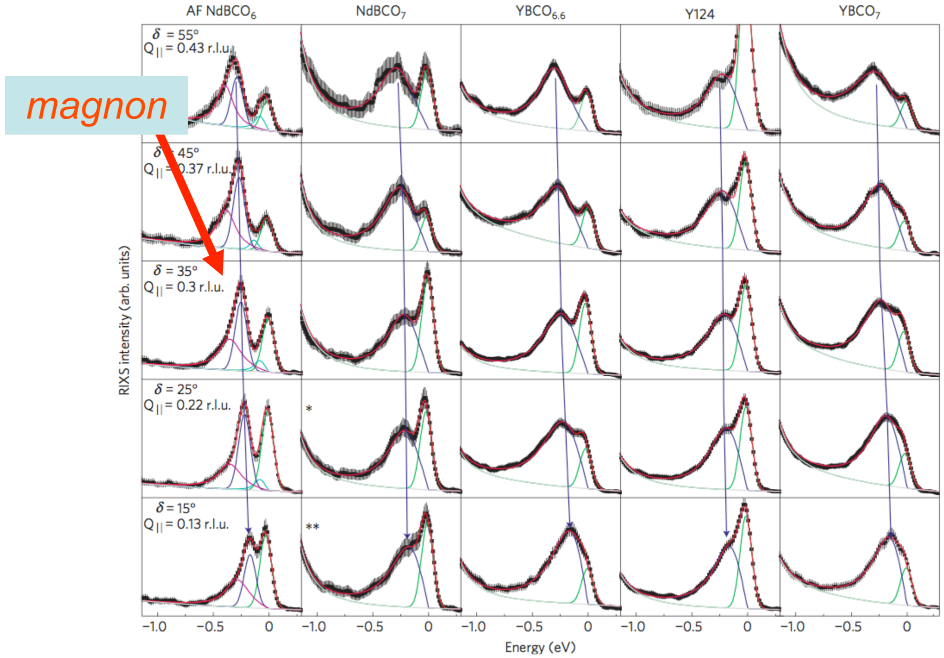
paramagnon

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

nature physics
ARTICLES
PUBLISHED ONLINE: 10 JULY 2011 | DOI: 10.1038/NPHYS2041

Intense paramagnon excitations in a large family of high-temperature superconductors

M. Le Tacon[1]★, G. Ghiringhelli[2], J. Chaloupka[1], M. Moretti Sala[2], V. Hinkov[1,3], M. W. Haverkort[1], M. Minola[2], M. Bakr[1], K. J. Zhou[4], S. Blanco-Canosa[1], C. Monney[4], Y. T. Song[1], G. L. Sun[1], C. T. Lin[1], G. M. De Luca[5], M. Salluzzo[5], G. Khaliullin[1], T. Schmitt[4], L. Braicovich[2] and B. Keimer[1]★



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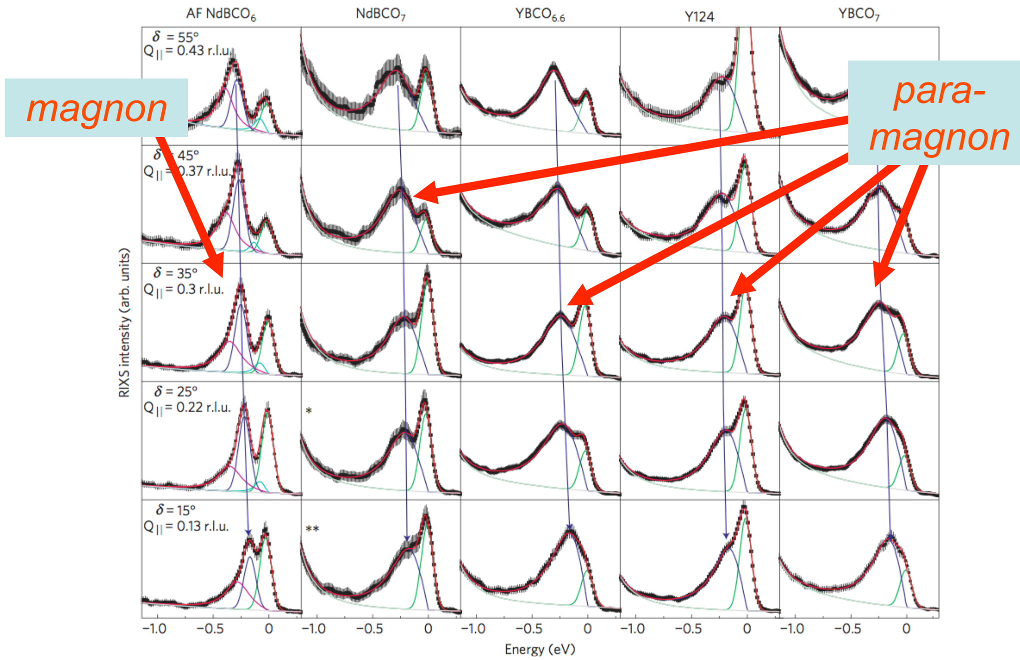

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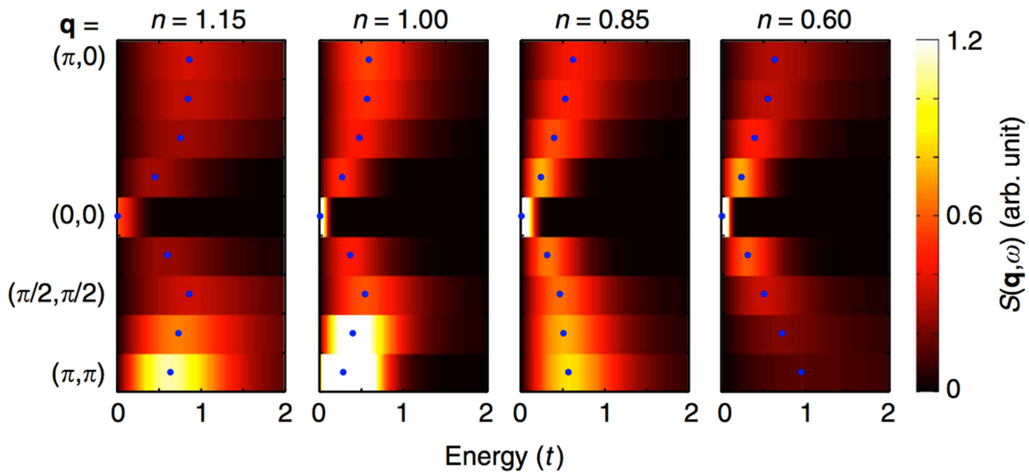
Dynamical structure factor Hubbard model, QMC

U=8t



Jia, Nowadnick, Wohlfeld, Kung, Chen, Johnston, Tohyama, Moritz & Devereaux
Nat. Comm. 5, 3314 (2014)

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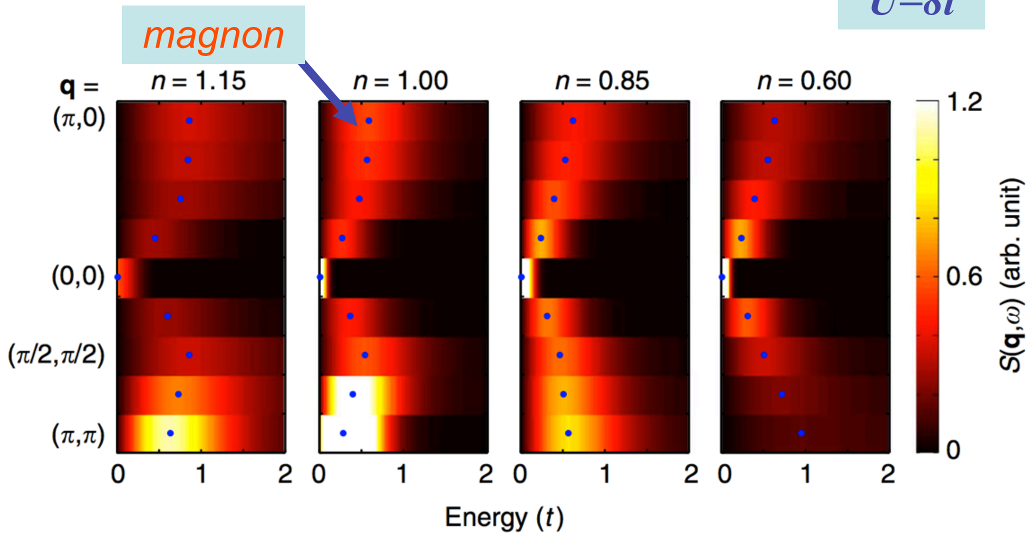

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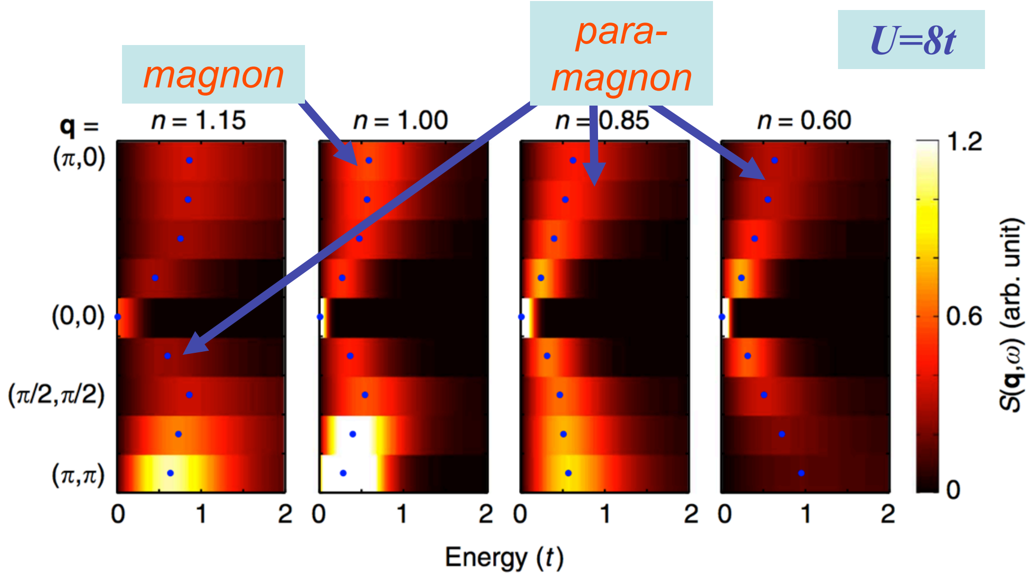

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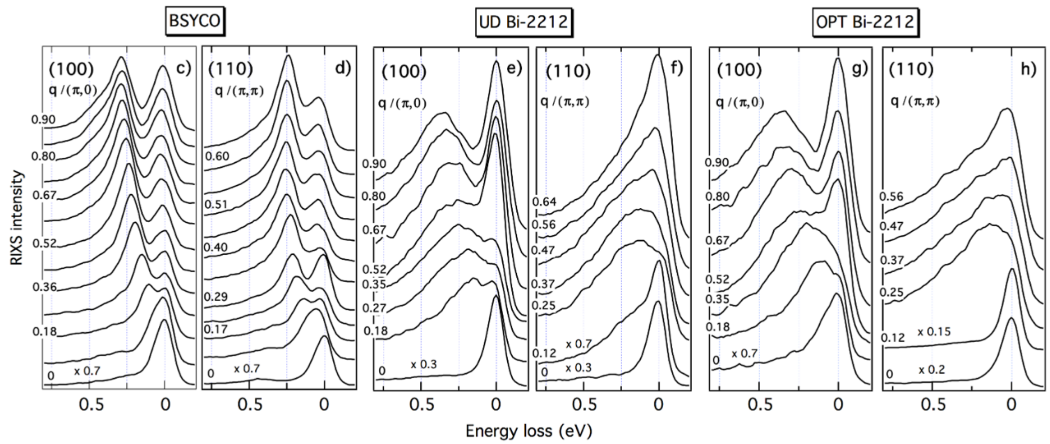
RIXS on Bi-2212 cuprate



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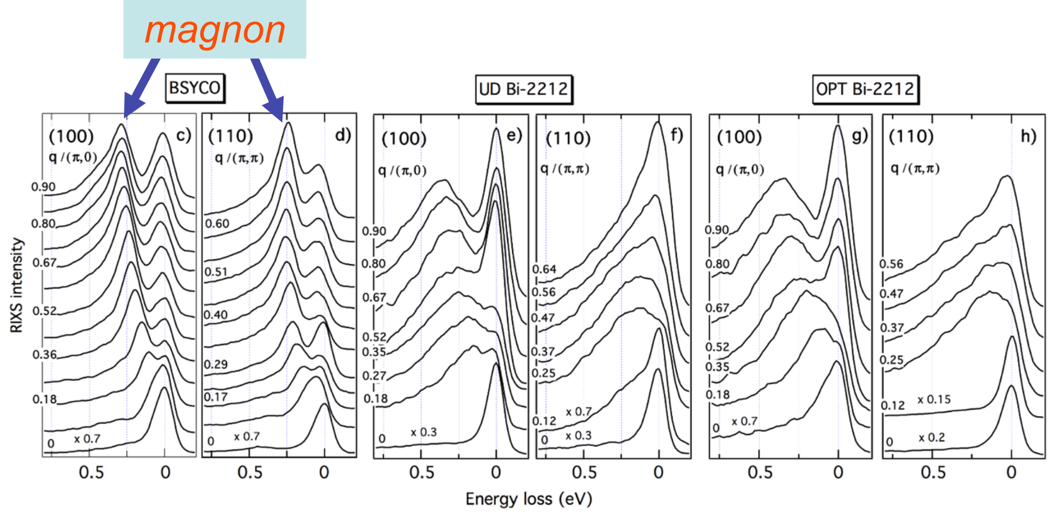

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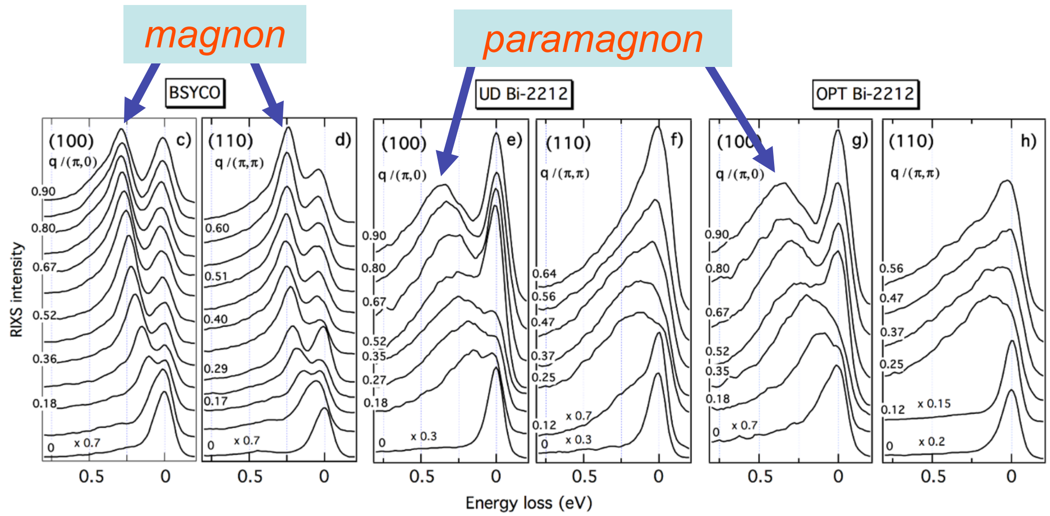

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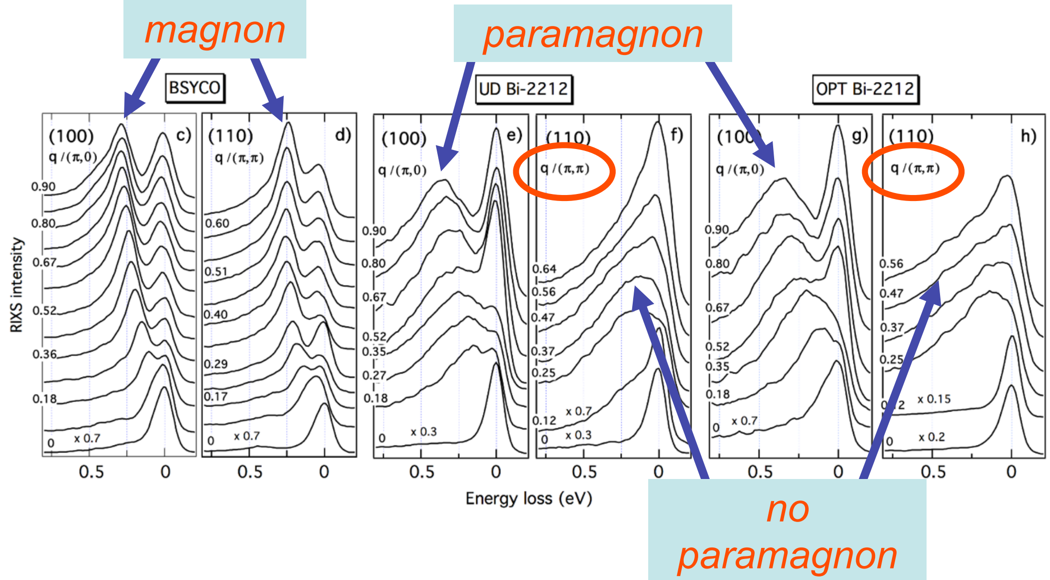

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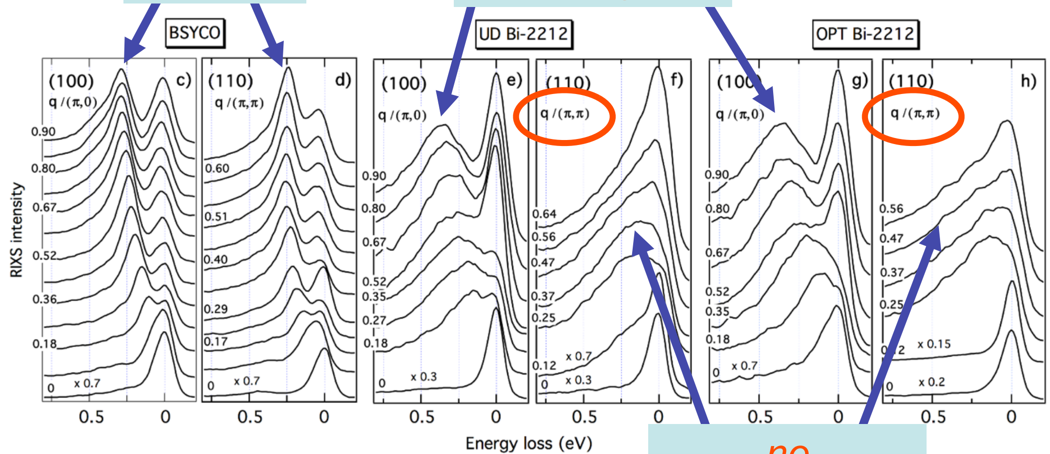
RIXS on Bi-2212 cuprate

magnon

paramagnon



no paramagnon

Related to presence of e-h continuum?

Benjamin, Klich & Demler
PRL 112, 247002 (2014)

Guarise, Piazza, Berger, Giannini, Schmitt, Rønnow, Sawatzky, JvdB, Altenfeld, Eremin & Grioni,
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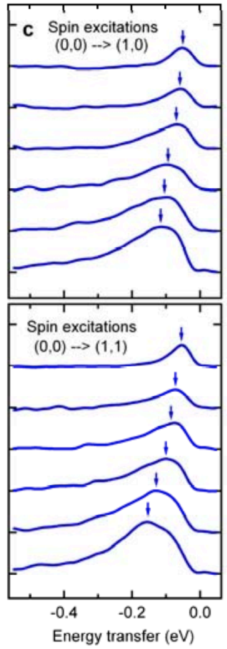
Magnetic RIXS on $Ba_{0.6}K_{0.4}Fe_2As_2$



Zhou, Huang, Monney, Dai, Strocov, Wang, Chen, Zhang, Dai, Patthey, JvdB, Ding & Schmitt, Nat. Comm. 4, 1470 (2013)

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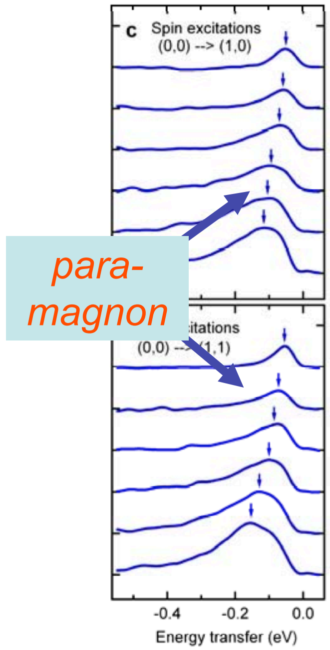

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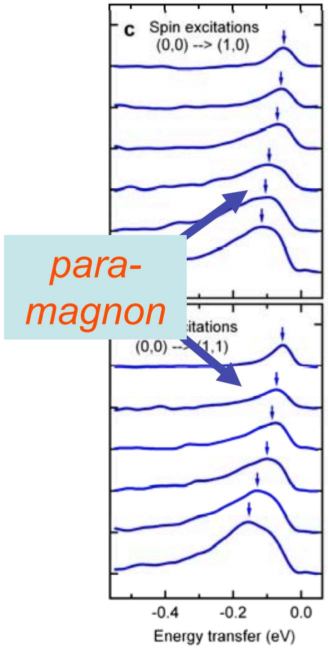

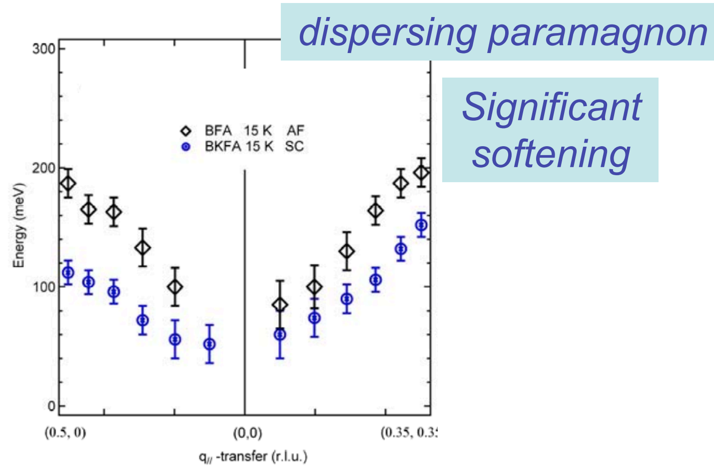

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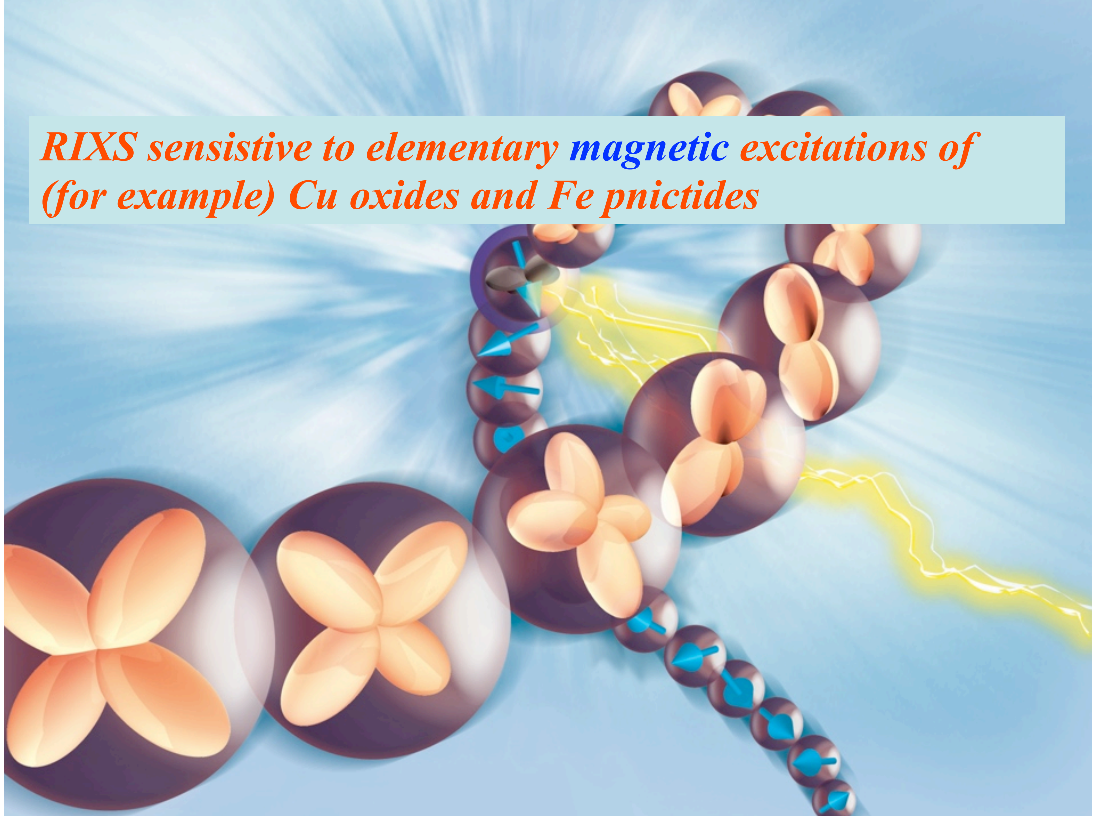
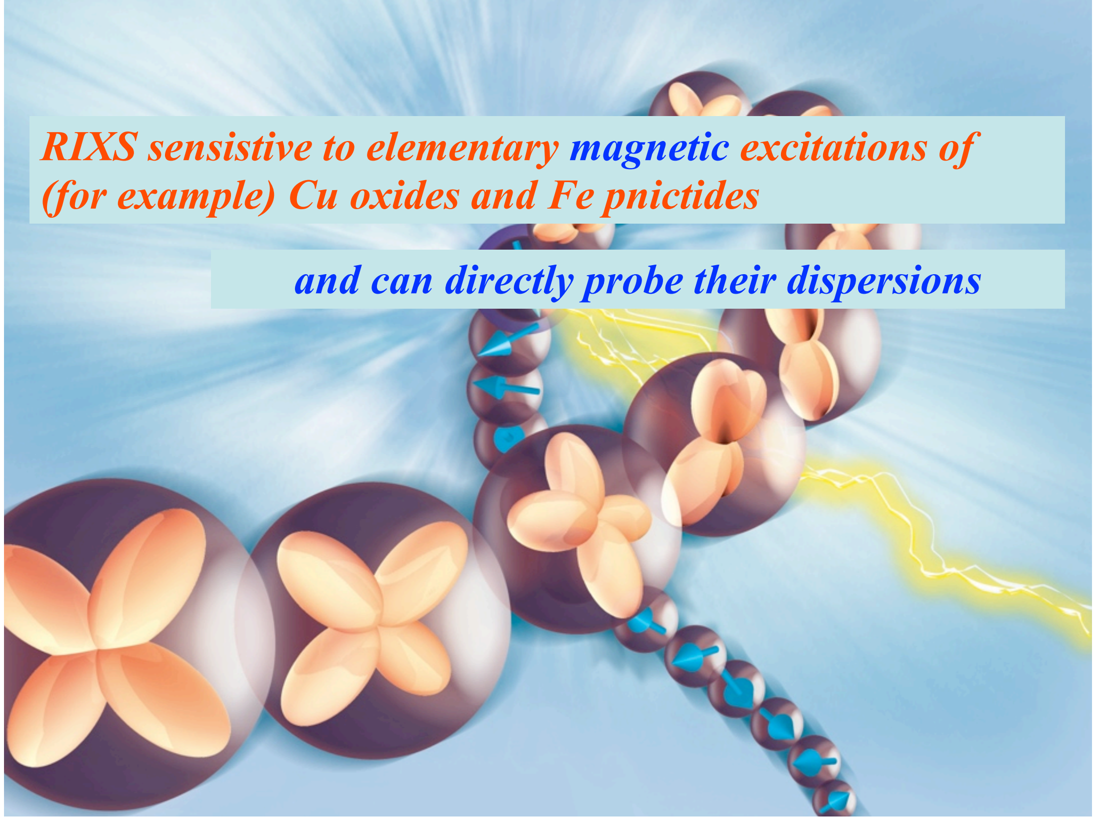
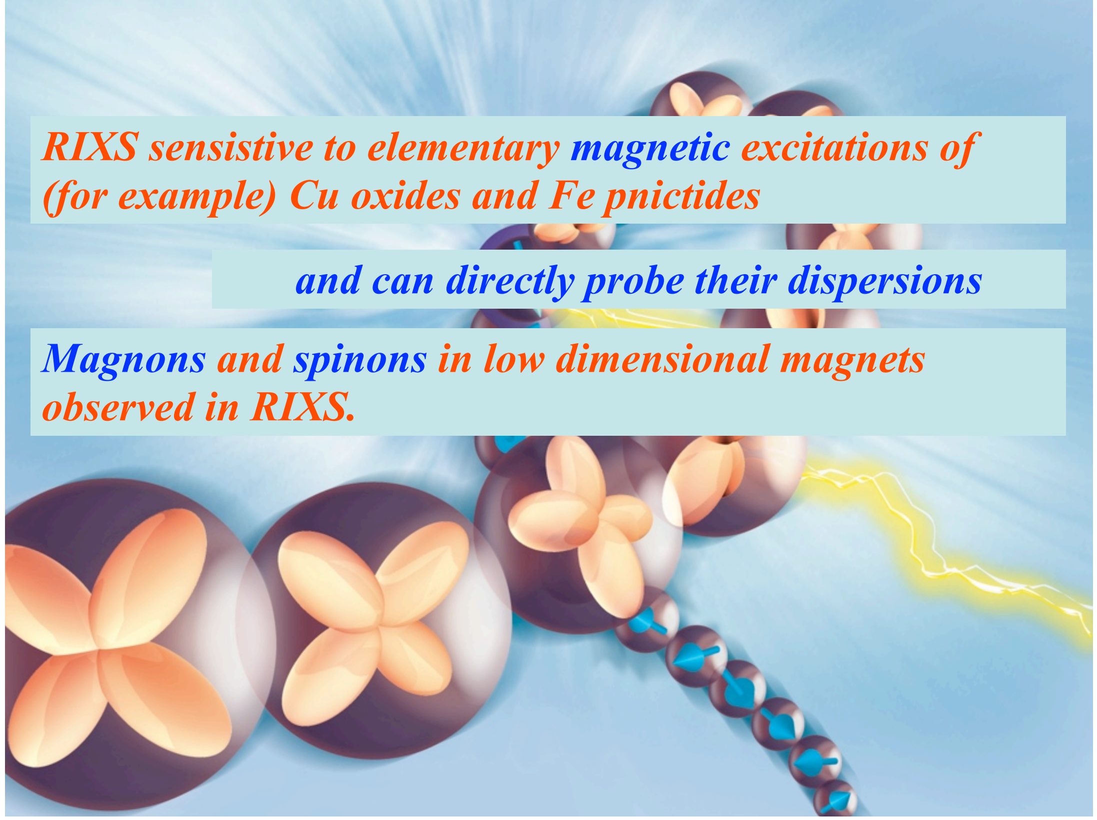
RIXS sensistive to elementary magnetic excitations of (for example) Cu oxides and Fe pnictides




RIXS sensistive to elementary magnetic excitations of
(for example) Cu oxides and Fe pnictides
and can directly probe their dispersions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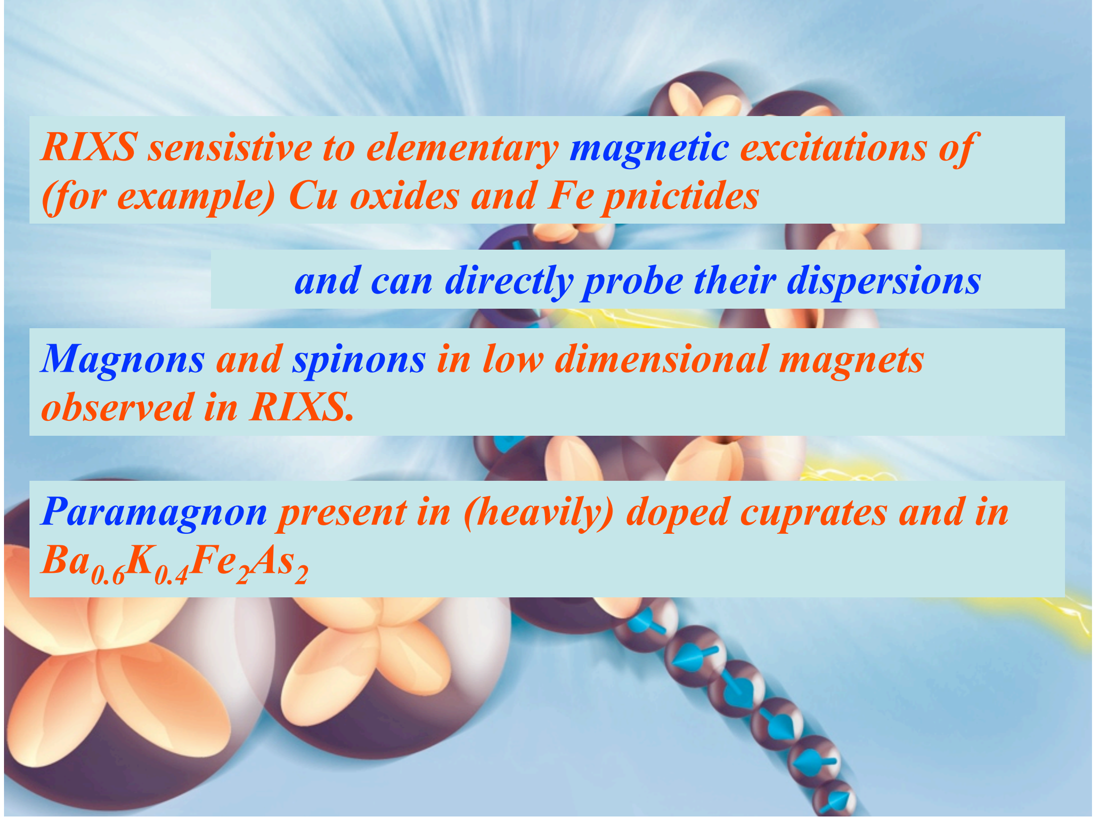
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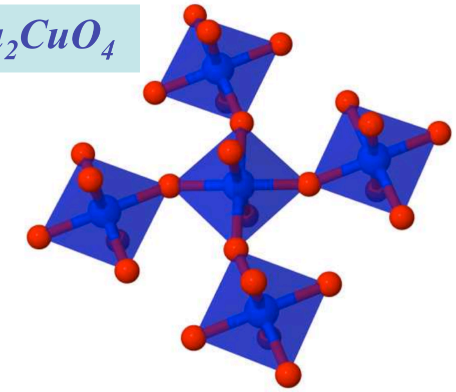
Magnons and spinons in low dimensional magnets observed in RIXS.
Paramagnon present in (heavily) doped cuprates and in $Ba_{0.6}K_{0.4}Fe_2As_2$

Magnetic Iridium Oxides

Sr_2IrO_4 : *equivalent of cuprate* La_2CuO_4



Jackeli & Khaliullin, PRL 102,017205 (2009)

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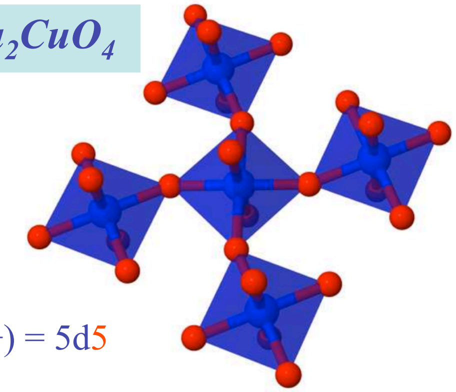

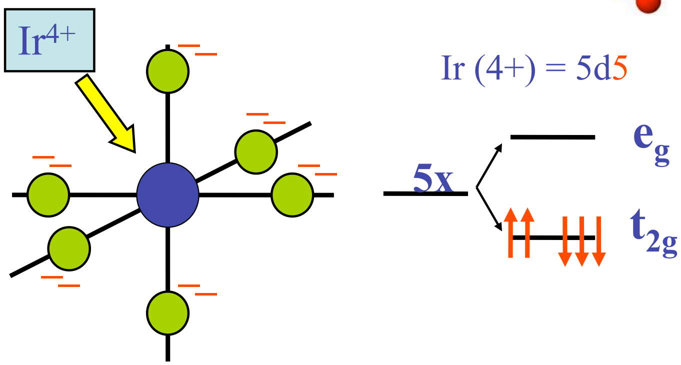

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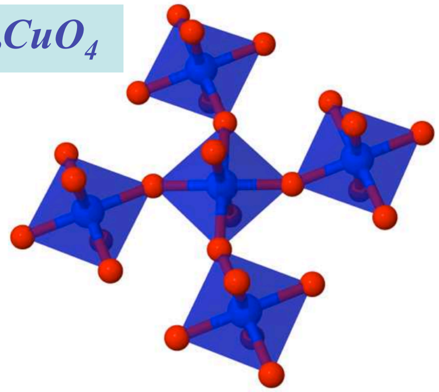
t_{2g}^5: single hole s=1/2 in 3-fold degenerate l=1 state



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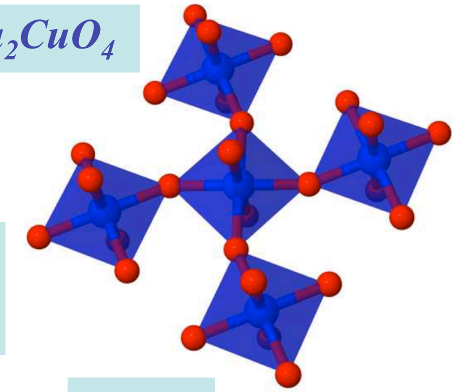

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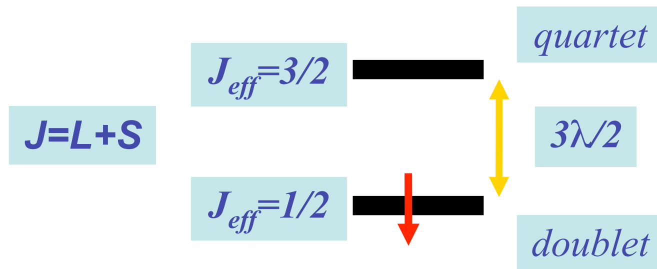
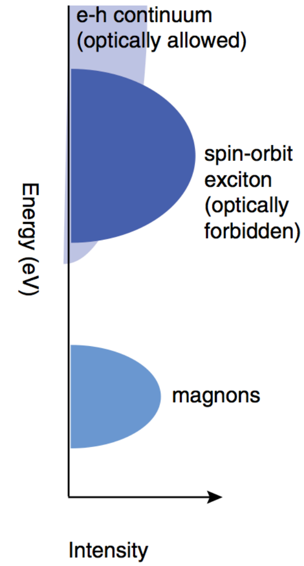


Direct RIXS on Sr_2IrO_4



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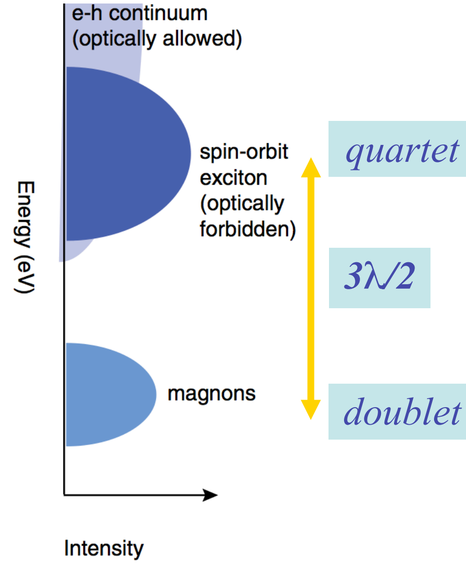

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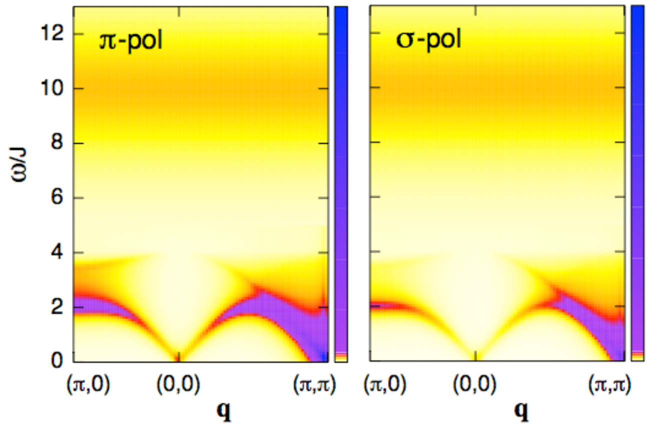
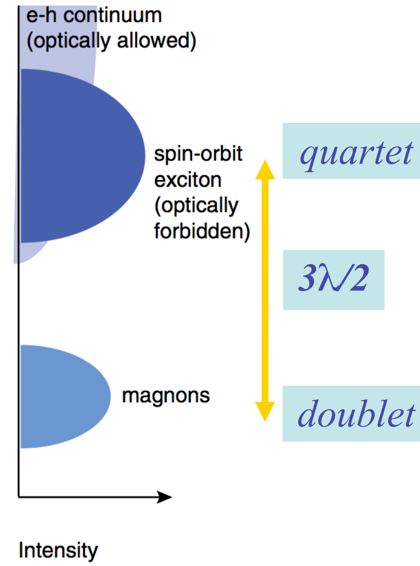


Ament, Khaliullin & JvdB
PRB 84, 020403 (2011)



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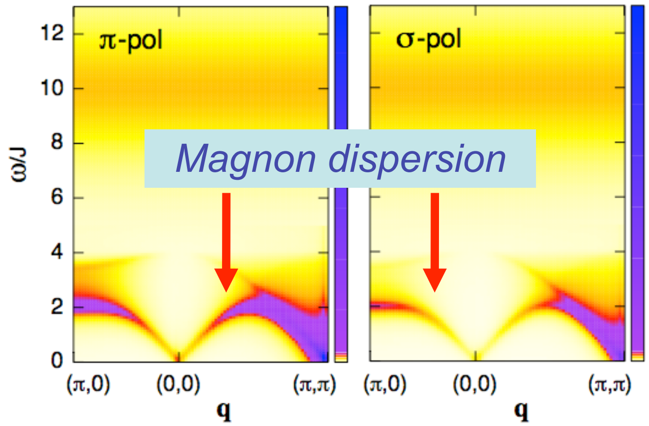

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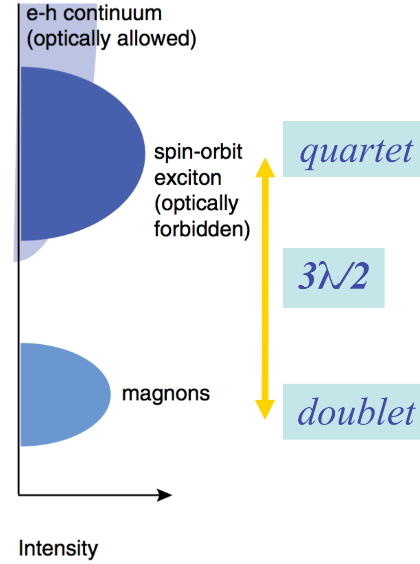

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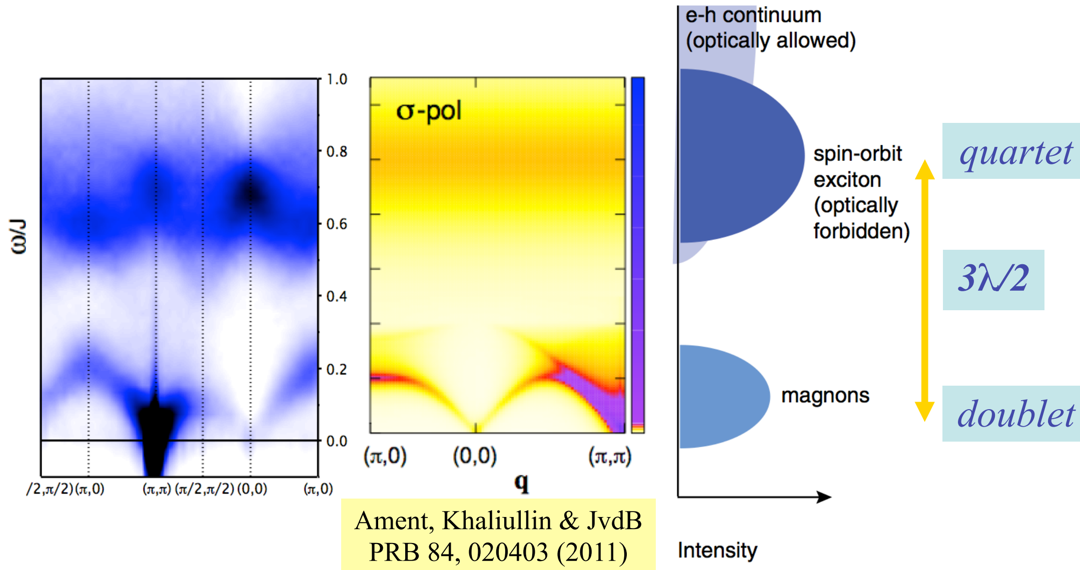

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Jungho Kim,[1] D. Casa,[1] M. H. Upton,[1] T. Gog,[1] Young-June Kim,[2]
J. F. Mitchell,[3] M. van Veenendaal,[1,4] M. Daghofer, [5] J. van den Brink,[5]
G. Khaliullin,[6] B. J. Kim[3,*]

PRL 108, 177003 (2012)

RIXS determines orbital energies + magnetic interactions directly

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Can J / orbital energies be calculated from first principles?

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Can J / orbital energies be calculated from first principles?

Density functional theory (DFT)

Of limited use for d/f electrons

In strict sense a ground state theory

RIXS determines orbital energies + magnetic interactions directly

Can J / orbital energies be calculated from first principles?

Density functional theory (DFT)

Of limited use for d/f electrons

In strict sense a ground state theory

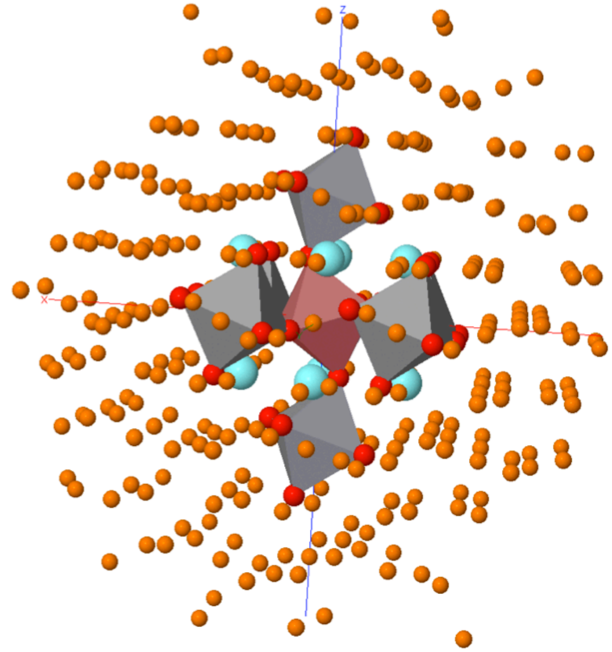
DFT+ (LDA+U, LDA+DMFT)

Not ab initio, parameters ad hoc, not always well-known or sometimes not well-defined

Hybrid uncorrelated - correlated approach

QC: wavefunction-based correlation methods

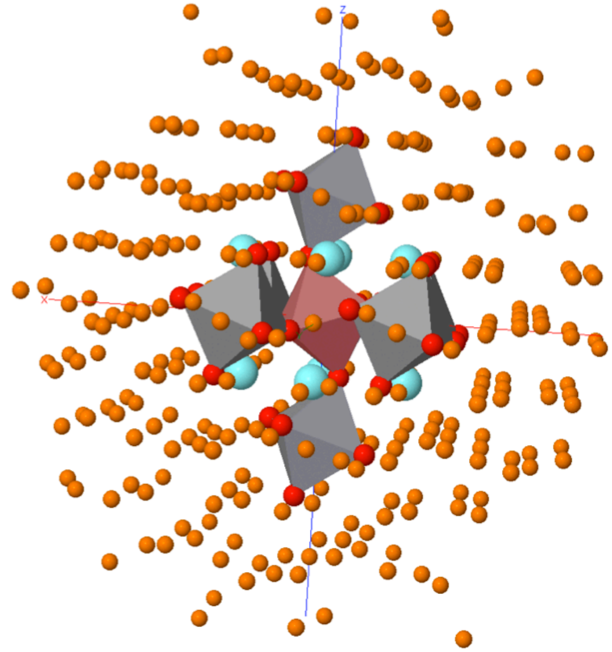
Finite embedded clusters



QC: wavefunction-based correlation methods

Fully ab initio for ground and excited states

Finite embedded clusters

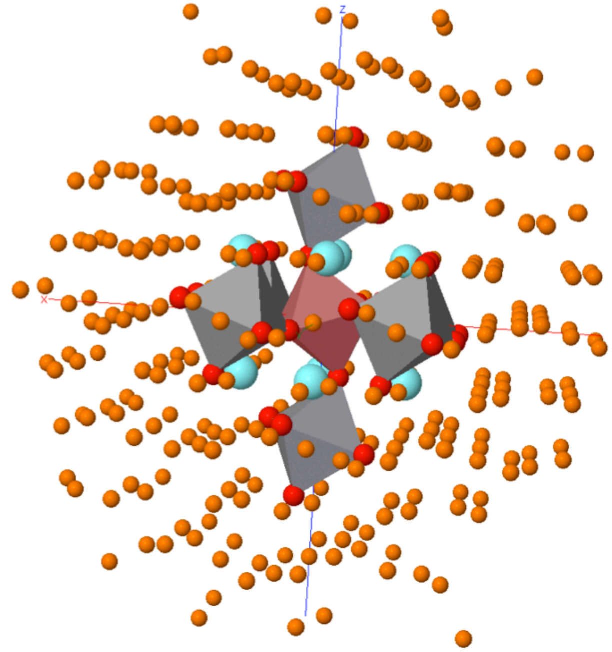


QC: wavefunction-based correlation methods

Fully ab initio for ground and excited states

Fully correlated: multi-configuration wave-functions

Finite embedded clusters



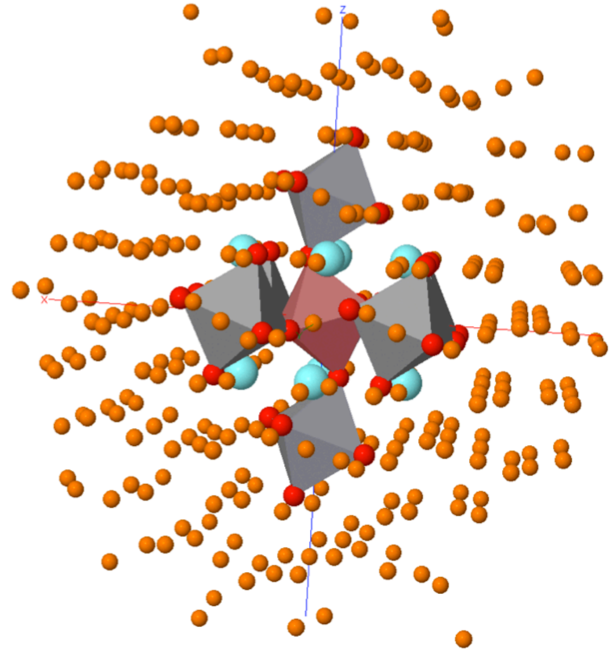
QC: wavefunction-based correlation methods

Fully ab initio for ground and excited states

Fully correlated: multi-configuration wave-functions

Heavy machinery

Finite embedded clusters



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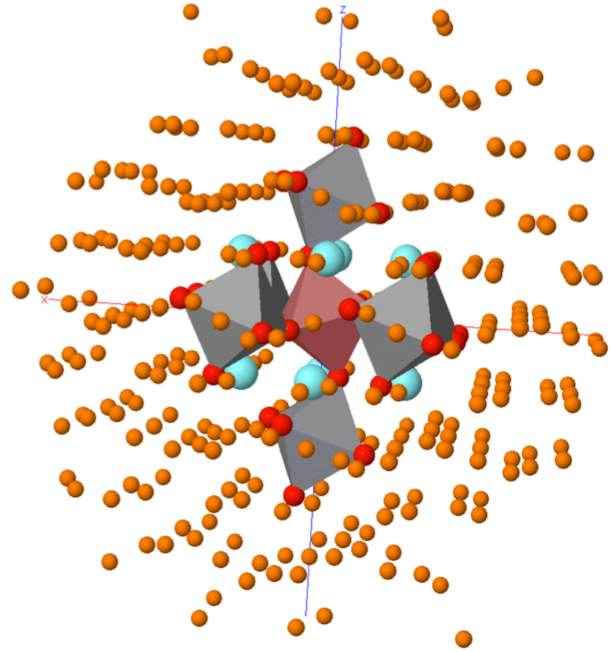
Heavy machinery

Excellent for systems with localized electrons

Finite embedded clusters



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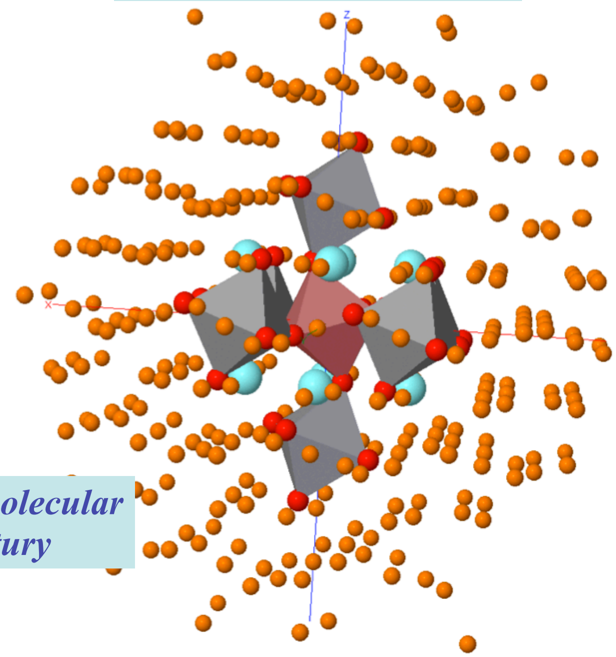


Fully ab initio for ground and excited states

Fully correlated: multi-configuration wave-functions

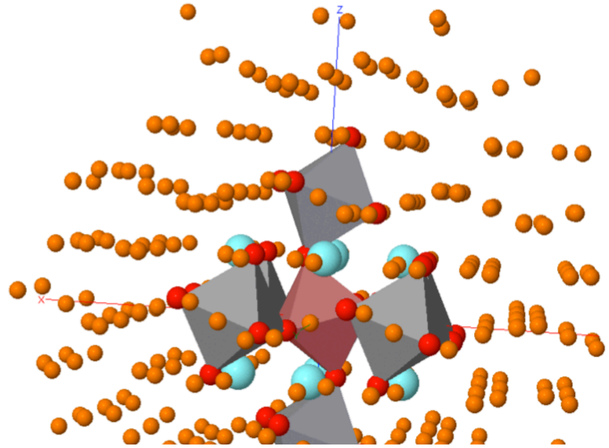
Heavy machinery

Excellent for systems with localized electrons

Approximations tested in molecular systems since half century

QC: wavefunction-based correlation methods

Finite embedded clusters



Fully ab initio for ground and excited states

Fully correlated: multi-configuration wave-functions

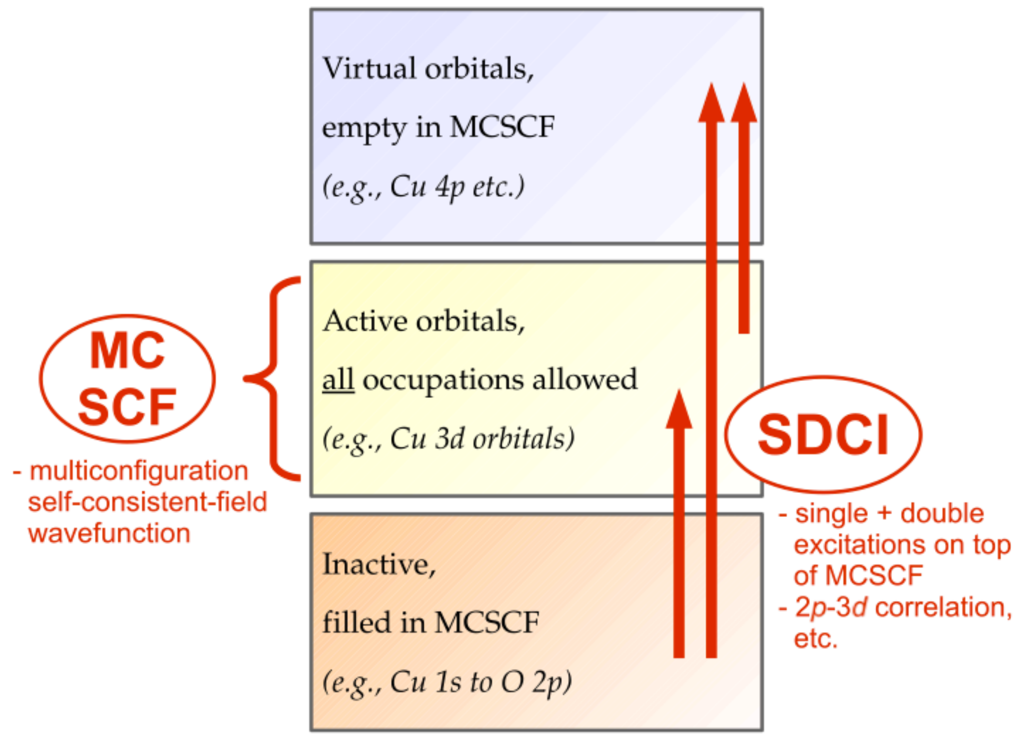
Heavy machinery

Excellent for systems with localized electrons

Our scheme : direct-space multireference CI, finite embedded clusters

The infinite solid-state environment : one-electron embedding potential

- simplest: point-charge array
- more advanced: based on prior periodic Hartree-Fock

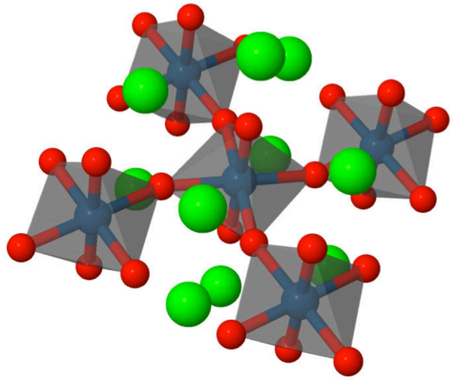

Virtual orbitals,
empty in MCSCF
(e.g., Cu 4p etc.)
Active orbitals,
all occupations allowed
(e.g., Cu 3d orbitals)
Inactive,
filled in MCSCF
(e.g., Cu 1s to O 2p)
MC SCF
- multiconfiguration self-consistent-field wavefunction
SDCI
- single + double excitations on top of MCSCF
- 2p-3d correlation, etc.

tetravalent iridates

quasi-0D	Sr_3IrCuO_6
quasi-1D	*postperovskite* $CaIrO_3$
quasi-2D	*perovskite* Sr_2IrO_4 *and* Ba_2IrO_4
2D/3D	*honeycomb:* A_2IrO_3, *A=Na/Li*
	hyper-honeycomb: β-Li_2IrO_3
3D	*pyrochlore* $Y_2Ir_2O_7$

quasi-2D iridates: Sr_2IrO_4 and Ba_2IrO_4

Sr_2IrO_4

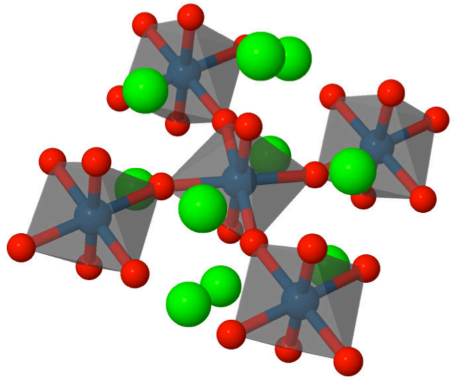
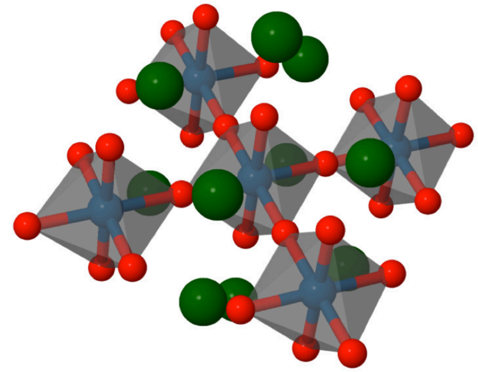


Elongated octahedra

distortion 3.8%

Rotation of octahedra 11^o

quasi-2D iridates: Sr_2IrO_4 and Ba_2IrO_4

Sr_2IrO_4	Ba_2IrO_4
	
Elongated octahedra	*Elongated octahedra*
distortion 3.8%	*distortion 6.6%*
Rotation of octahedra 11^o	*No rotation of octahedra*

dd excitations of Sr_2IrO_4 and Ba_2IrO_4

Hole config.	Rel. Energy (eV)	
	Sr_2IrO_4	Ba_2IrO_4
t_{2g}^1 (+SOC)		
$j = 1/2$	0	0
$j = 3/2$	$0.65 - 0.81$	$0.69 - 0.82$
$t_{2g} \rightarrow e_g$	2.8-5.9	2.0-5.0
O $p \rightarrow$ Ir d	3.0-6.0	1.7-4.5

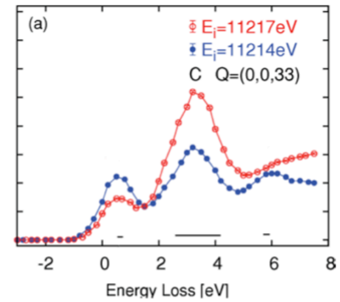
Katukuri, Stoll, JvdB & Hozoi
PRB 85, 220402(R) (2012)

dd excitations of Sr_2IrO_4 and Ba_2IrO_4

Hole config.	Rel. Energy (eV) Sr_2IrO_4	Rel. Energy (eV) Ba_2IrO_4
t_{2g}^1 (+SOC)		
$j = 1/2$	0	0
$j = 3/2$	$0.65-0.81$	$0.69-0.82$
$t_{2g} \rightarrow e_g$	2.8-5.9	2.0-5.0
O $p \rightarrow$ Ir d	3.0-6.0	1.7-4.5

Katukuri, Stoll, JvdB & Hozoi
PRB 85, 220402(R) (2012)

RIXS[1] for Sr_2IrO_4



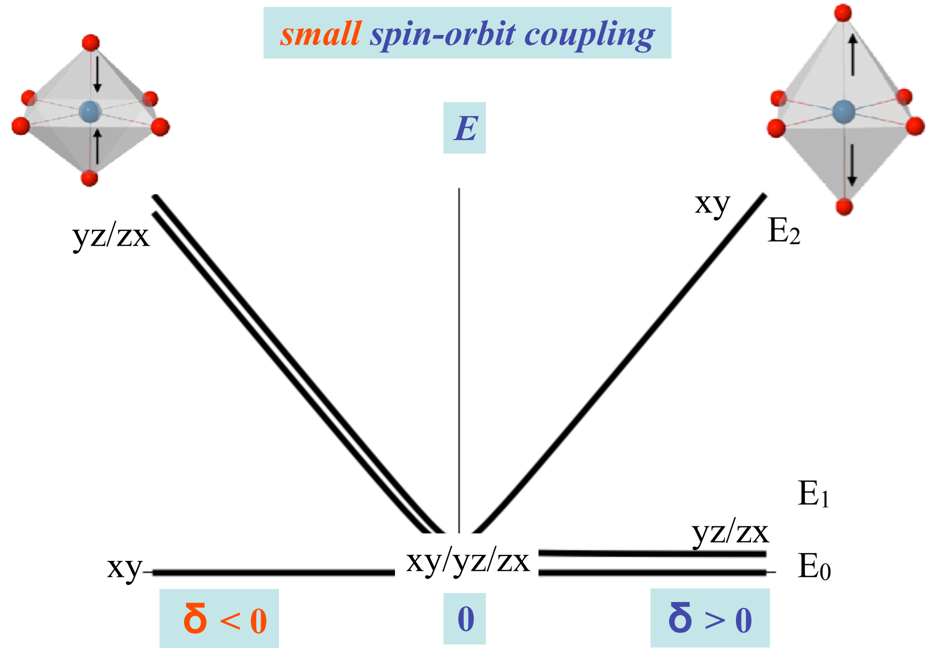
$\lambda_{SOC} = \frac{2\Delta}{3}$ (eV)

$Sr_2IrO_4 \approx 0.46$

$Ba_2IrO_4 \approx 0.43$

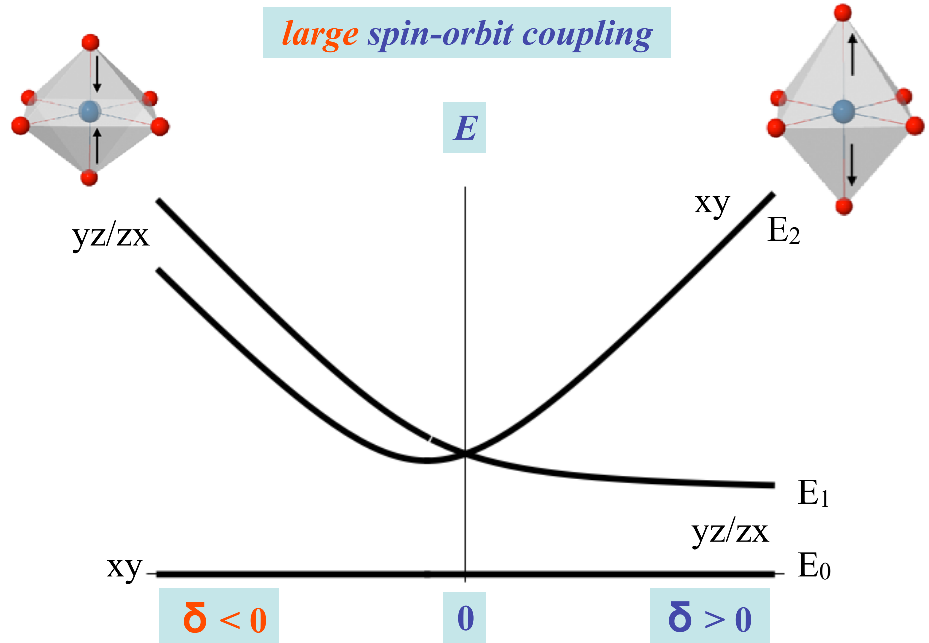
Ishii, Jarrige, Yoshida, Ikeuchi, Mizuki,
Ohashi, Takayama, Matsuno & Takagi
PRB 83, 115121 (2011)

Tetragonal distortion δ

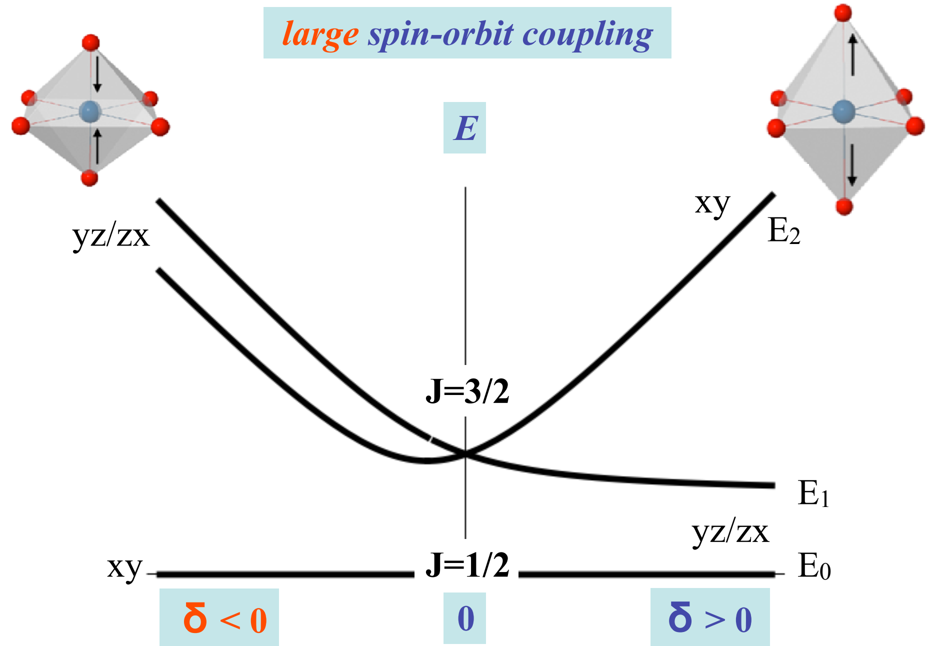


Tetragonal distortion δ

large spin-orbit coupling



Tetragonal distortion δ



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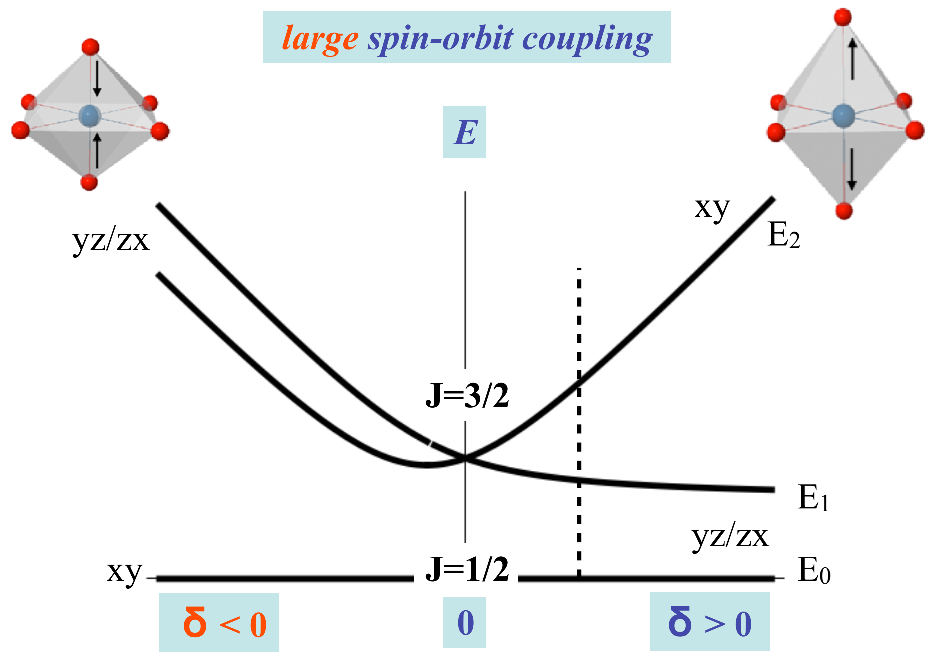

CF splittings in Sr_2IrO_4 and Ba_2IrO_4

Table 4. Relative Energies (meV) for the Split Ir $^2T_{2g}(t_{2g}{}^5)$ States in Sr_2IrO_4 and Ba_2IrO_4[a]

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CASSCF	0	−120
MRCI	0	−155
Ba_2IrO_4		
CASSCF	0	70
MRCI	0	65

[a]SOC is not accounted for.

Katukuri, Stoll, JvdB & Hozoi
PRB 85, 224002(R) (2012)

Katukuri, Roszeitis, Yushankhai, Mitrushchenkov, Stoll, van Veenendaal, Fulde, JvdB & Hozoi, Inorg. Chem. 53, 4833 (2014)

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PRB 85, 224002(R) (2012)

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Katukuri, Stoll, JvdB & Hozoi
PRB 85, 224002(R) (2012)

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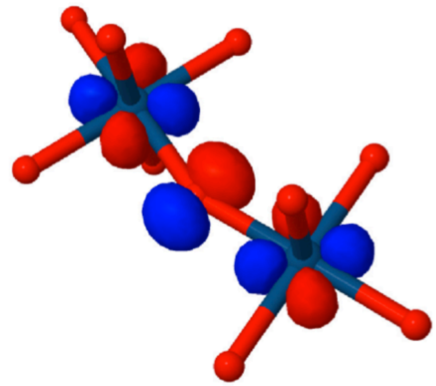
Negative splitting for Sr214

Katukuri, Stoll, JvdB & Hozoi
PRB 85, 224002(R) (2012)

Katukuri, Roszeitis, Yushankhai, Mitrushchenkov, Stoll, van Veenendaal, Fulde, JvdB & Hozoi, Inorg. Chem. 53, 4833 (2014)

Super-exchange J in Sr_2IrO_4 and Ba_2IrO_4

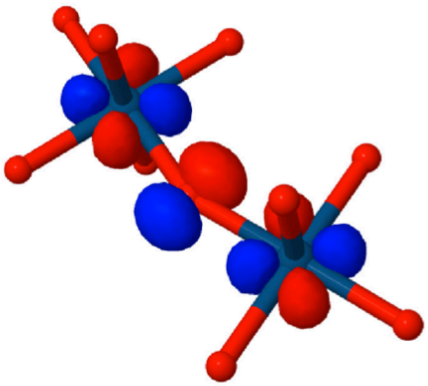
- Two active Ir sites



Super-exchange J in Sr_2IrO_4 and Ba_2IrO_4

- Two active Ir sites
- Small splittings between triplet states (< 3meV), Heisenberg model appropriate

J(meV)$< 0 \rightarrow$ FM	Sr_2IrO_4	Ba_2IrO_4
CASSCF	-19.2	15.4
CASSCF+SOC	28.8	35.7
SDCI+SOC	51.3	58.0
Experiment[1]	60	



With SOC, J is not so sensitive to the Ir-O-Ir angle

Katukuri, Stoll, JvdB & Hozoi
PRB 85, 224002(R) (2012)

Jungho Kim, Casa, Upton, Gog, Y-J Kim, Mitchell, Veenendaal, Daghofer, JvdB, Khaliullin & B.J. Kim
PRL 108, 177003 (2012)

Magnetic interactions in Sr_2IrO_4 and Ba_2IrO_4

$$\mathcal{H}_{\rm S}^{i,j} = J\tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j + \mathbf{D}\cdot\tilde{\mathbf{S}}_i \times \tilde{\mathbf{S}}_j + \tilde{\mathbf{S}}_i \cdot \bar{\bar{\mathbf{\Gamma}}} \cdot \tilde{\mathbf{S}}_j + \mu_{\rm B}\sum_{k=i,j} \mathbf{h}\cdot\bar{\bar{\mathbf{g}}}_k \cdot \tilde{\mathbf{S}}_k$$

J	D	Γ_{xx}	Γ_{yy}	Γ_{zz}
47.8	±11.9	0.42	–0.84	0.42

Bogdanov, Romhanyi, Katukuri, Yushankhai, Kataev, Buchner, JvdB & Hozoi, unpublished

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Number of states	CASSCF		MRCI	
	$g_\perp$	$g_\parallel$	$g_\perp$	$g_\parallel$
Sr_2IrO_4 ($\Delta_{t_{2g}} = -155$ meV):				
1D (3 KD's with SOC)	1.67	2.25	1.60	2.35
5D, 2Q, 1S (27 KD's)	1.81	2.27	**1.76**	**2.31**
Ba_2IrO_4 ($\Delta_{t_{2g}} = 65$ meV):				
1D (3 KD's)	2.00	1.61	2.01	1.60
5D, 2Q, 1S (27 KD's)	2.09	1.77	**2.10**	**1.76**

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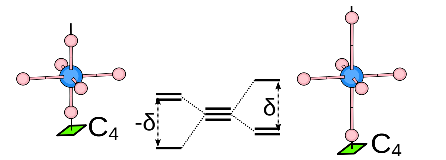

compresed

$\delta<0$, $g_\perp<2<g_\parallel$

elongated

$\delta>0$, $g_\parallel<2<g_\perp$

Bogdanov, Romhanyi, Katukuri, Yushankhai, Kataev, Buchner, JvdB & Hozoi, unpublished

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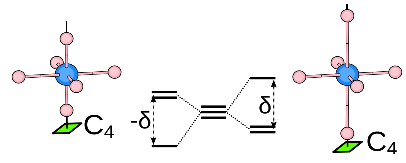

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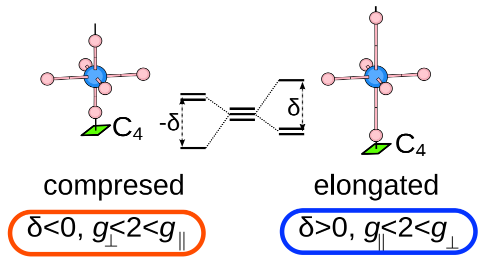
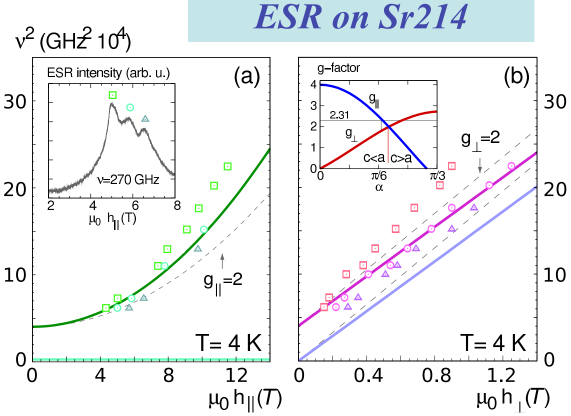


Bogdanov, Romhanyi, Katukuri, Yushankhai, Kataev, Buchner, JvdB & Hozoi, unpublished

Longer range crystal fields in Sr_2IrO_4 and Ba_2IrO_4

ESR on Sr214



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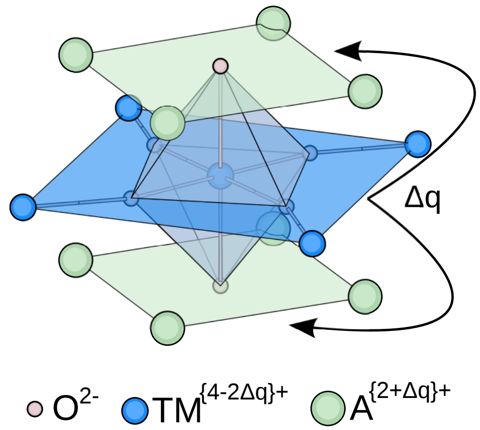

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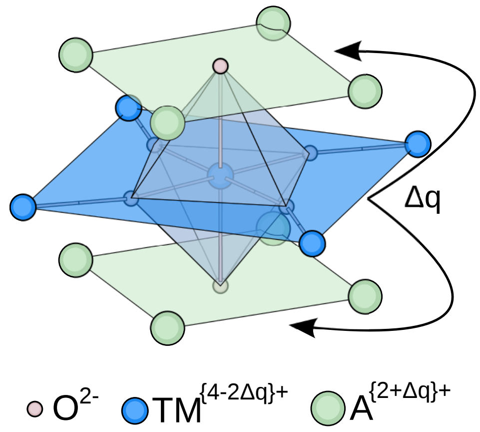

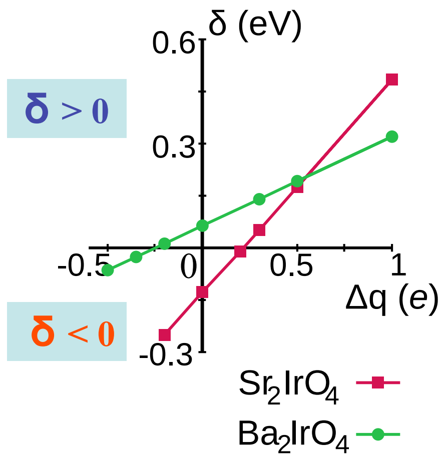

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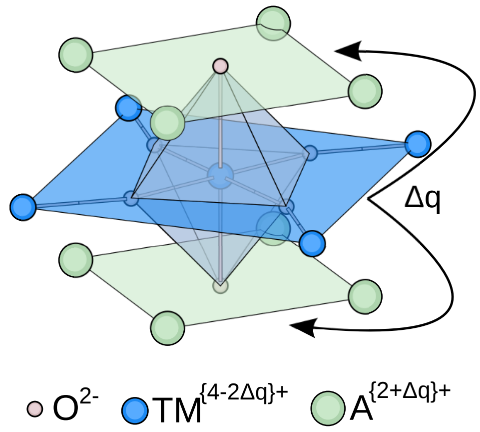
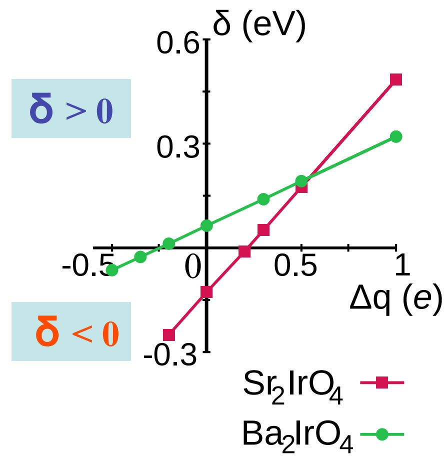
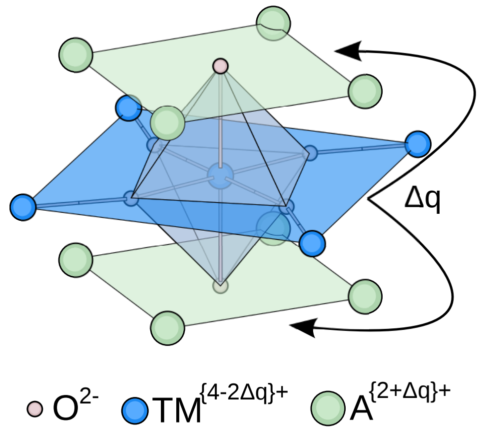


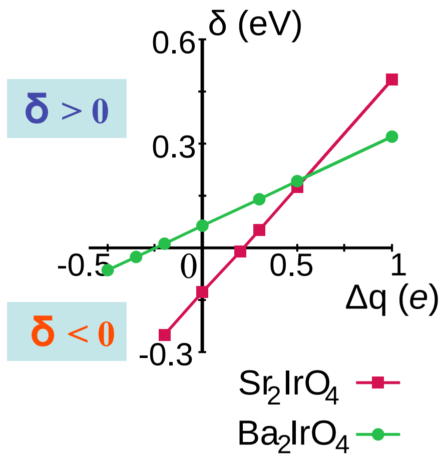


Highly charged Ir^{4+} causes strong longe range CF

Bogdanov, Romhanyi, Katukuri, Yushankhai, Kataev, Buchner, JvdB & Hozoi, unpublished

Longer range crystal fields in Sr_2IrO_4 and Ba_2IrO_4



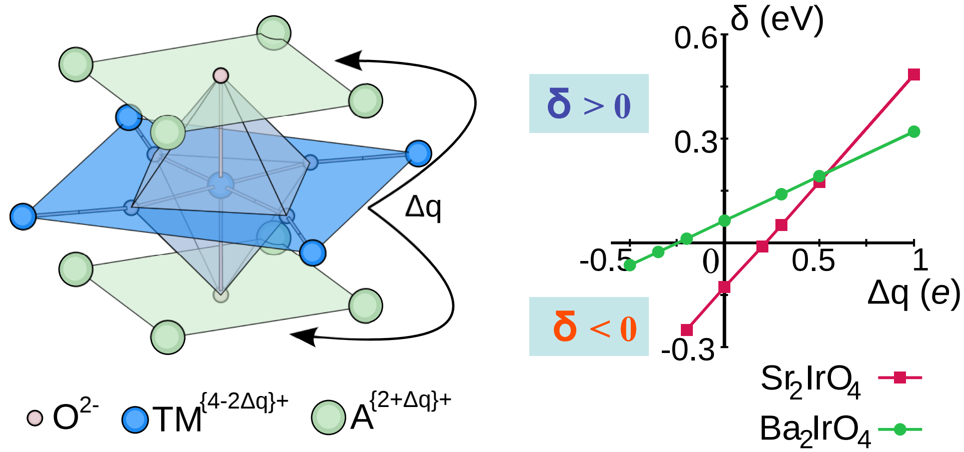


Highly charged Ir^{4+} causes strong longe range CF

This CF counter-acts δ of oxygen cage

Bogdanov, Romhanyi, Katukuri, Yushankhai, Kataev, Buchner, JvdB & Hozoi, unpublished

Longer range crystal fields in Sr_2IrO_4 and Ba_2IrO_4



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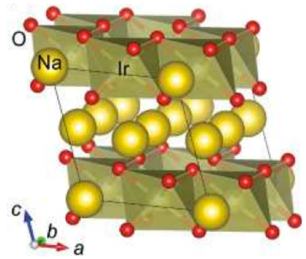
This CF counter-acts δ of oxygen cage

Causes level inversion in less-elongated Sr214

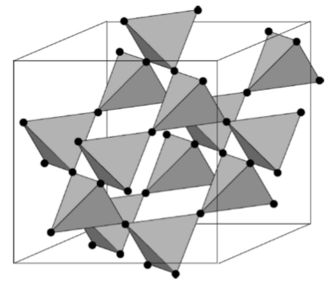
Bogdanov, Romhanyi, Katukuri, Yushankhai, Kataev, Buchner, JvdB & Hozoi, unpublished

More iridates ...

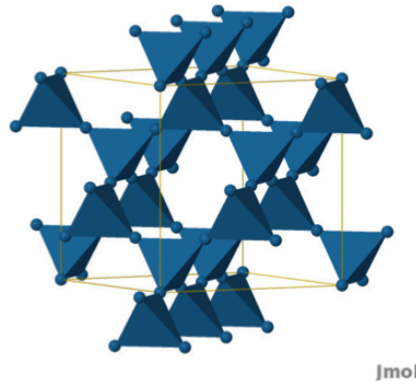
honeycomb A_2IrO_3

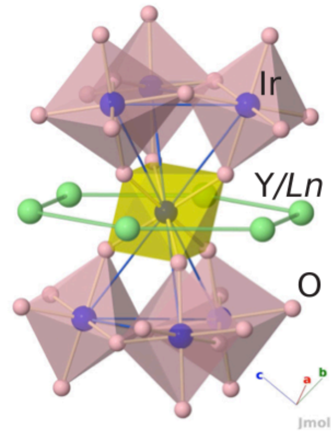


pyrochlore $A_2Ir_2O_7$



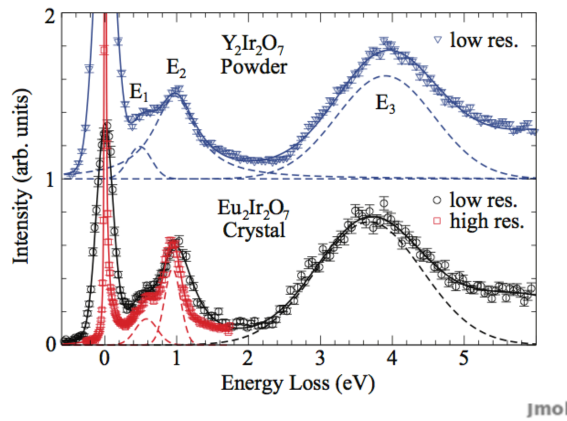
pyrochlore $Y_2Ir_2O_7$

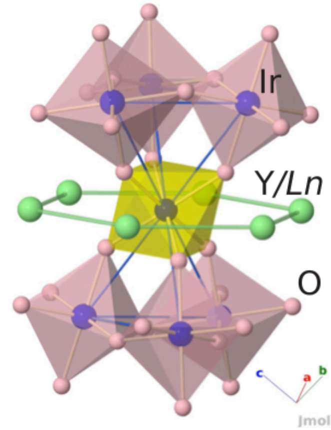




Hozoi, Gretarsson, Clancy, Jeon, Lee, K.H. Kim, Yushankhai, Fulde, Y.-J. Kim & JvdB PRB 89, 115111 (2014)

pyrochlore $Y_2Ir_2O_7$





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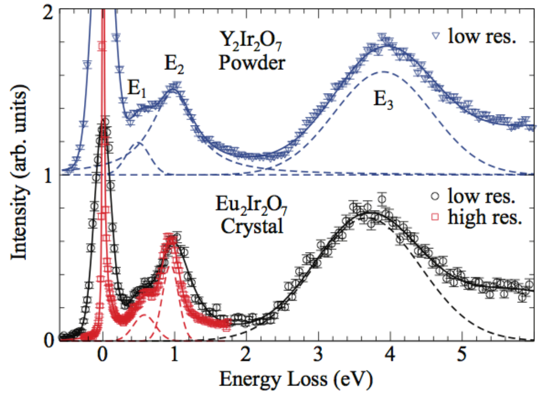

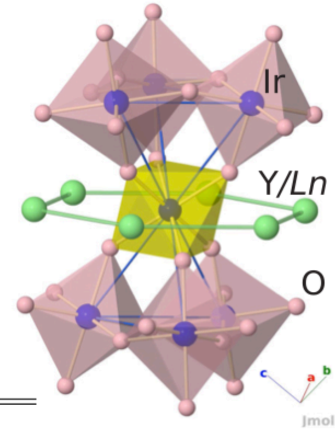

	E_1	E_2	$t_{2g}^4 e_g^1$
$Sm_2Ir_2O_7$	0.61	0.91	3.41–4.75
$Eu_2Ir_2O_7$	0.60 (**0.59**)	0.91 (**0.95**)	3.39–4.72 (**3.70**)
$Lu_2Ir_2O_7$	0.57	0.92	3.49–4.88
$Y_2Ir_2O_7$	0.58 (**0.53**)	0.94 (**0.98**)	3.48–4.84 (**3.90**)

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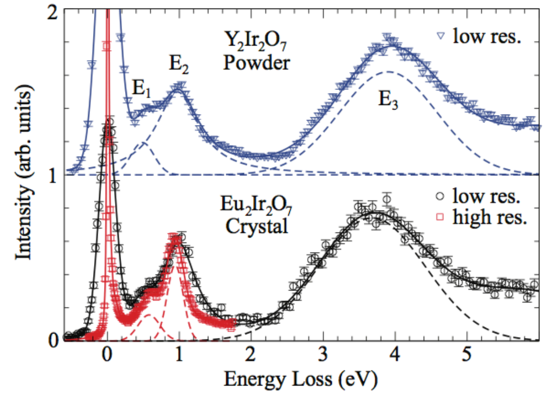

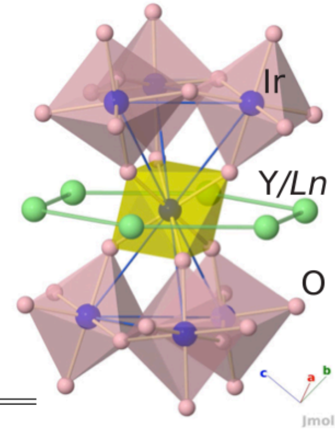

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	Undistorted Octahedron	
	E_1^0	E_2^0
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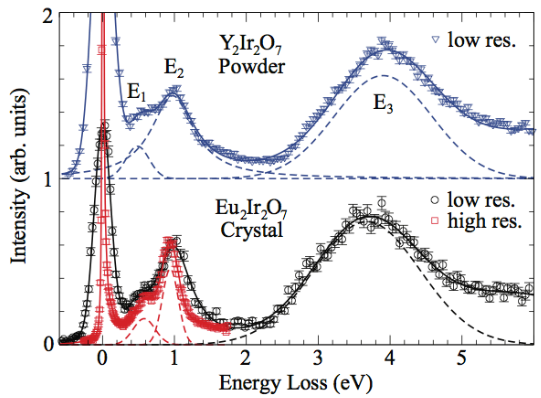

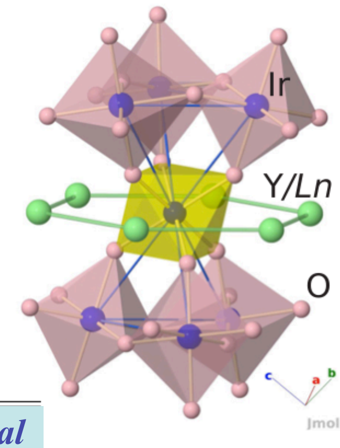

- ***Y coordination causes non-cubic crystal field***
- ***J=3/2 states split also when IrO_6 octahedron is undistorted***

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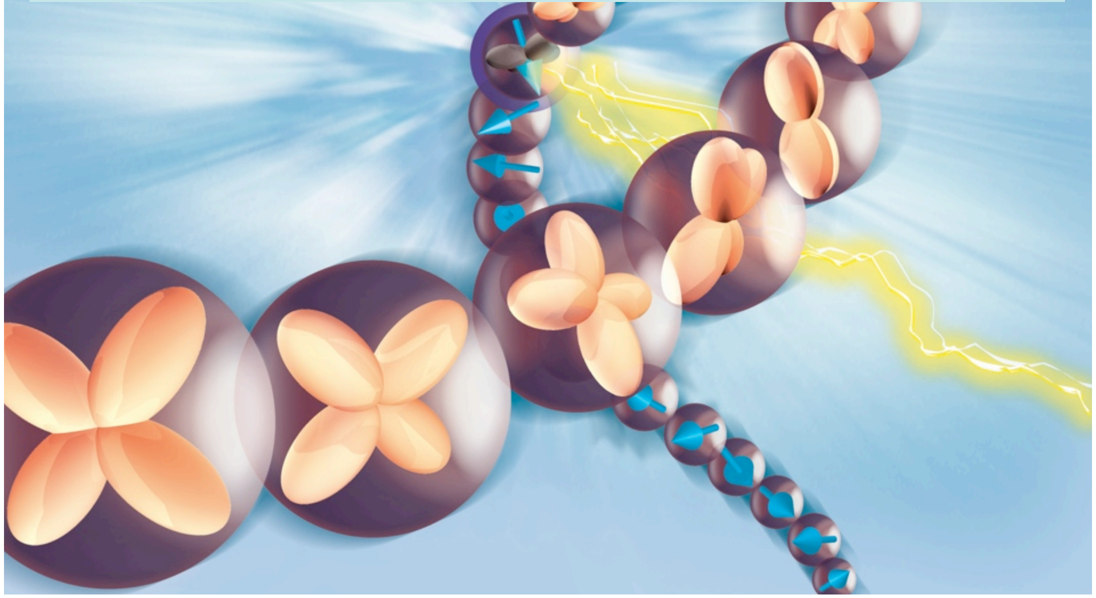
RIXS sensistive to elementary electronic and magnetic excitations of (for example) cuprates and iridates



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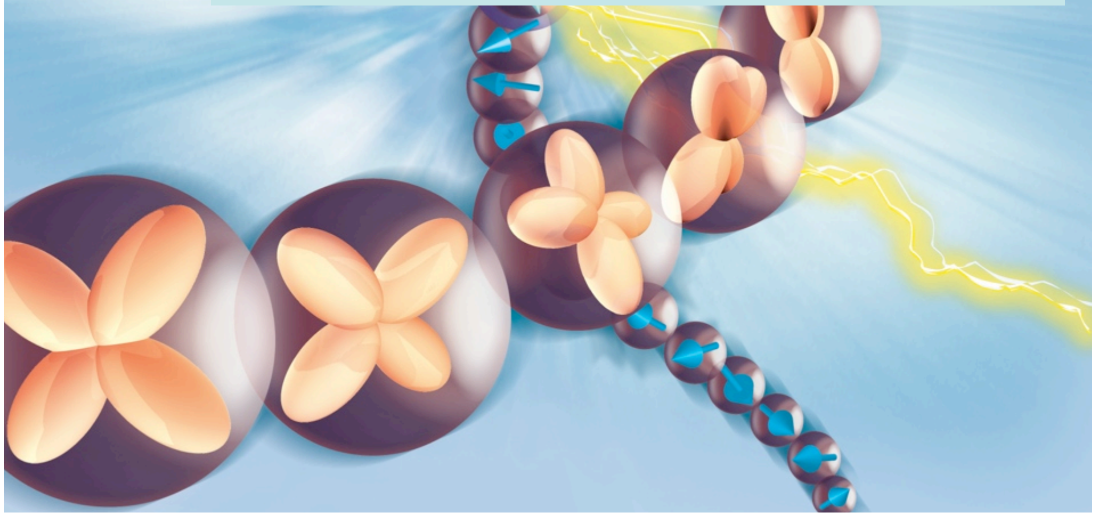

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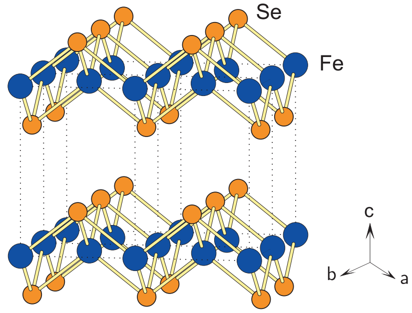
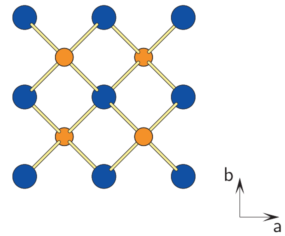
Superconductivity in FeSe





Baek, Efremov, Ok, Kim, JvdB & Buchner, ArXiv:1408.1875

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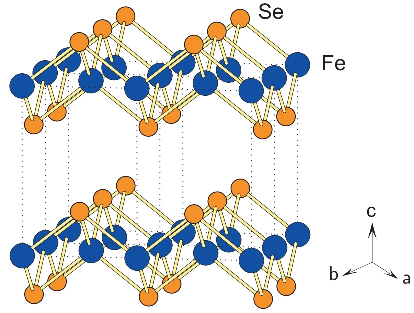

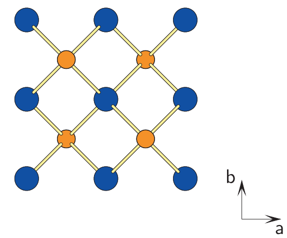

FeSe: (one of the) simplest iron based SC with T_c=9K

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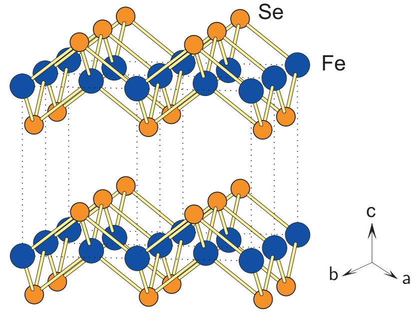

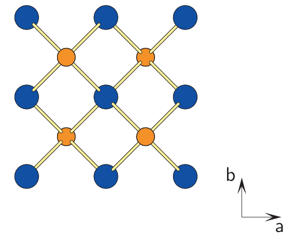

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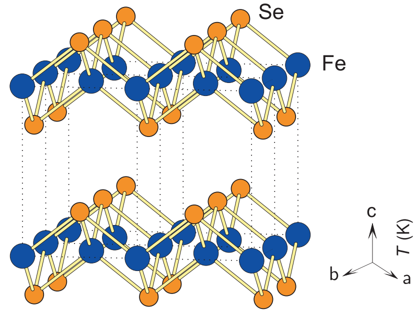

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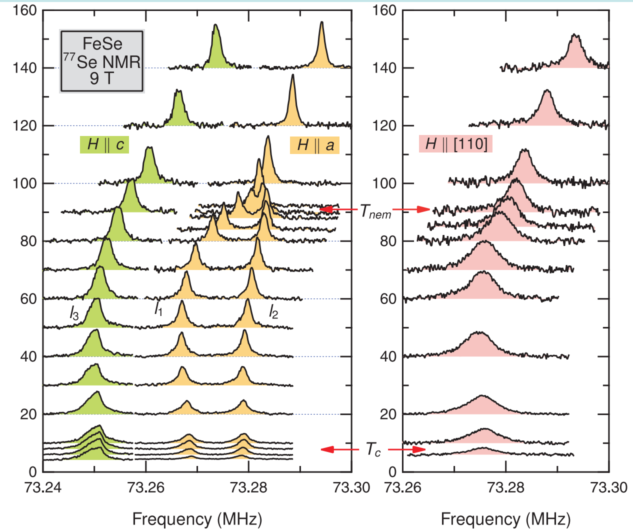
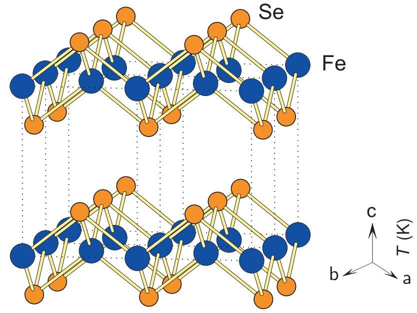


Se^{77} NMR: nematic order at 90 K

Baek, Efremov, Ok, Kim, JvdB & Buchner, ArXiv:1408.1875

Superconductivity in FeSe: orbitals set the stage



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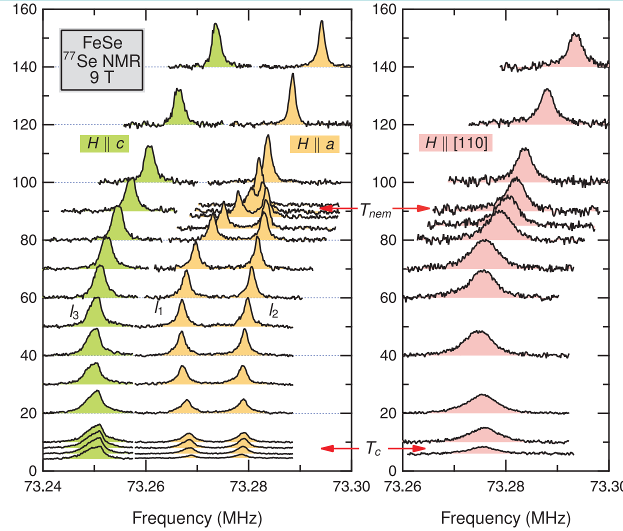

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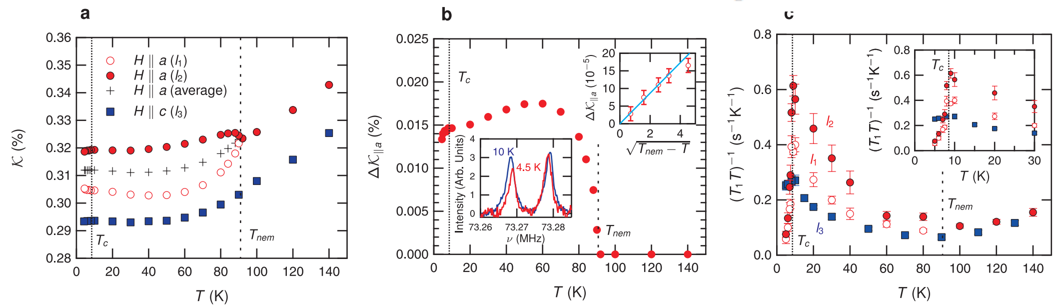
$$\mathcal{K} = A_{\mathrm{hf}}\chi_{\mathrm{spin}} \qquad (T_1T)^{-1} \propto \sum_{\mathbf{q}} A_{\mathrm{hf}}^2(\mathbf{q})\chi''(\mathbf{q},\omega)/\omega$$



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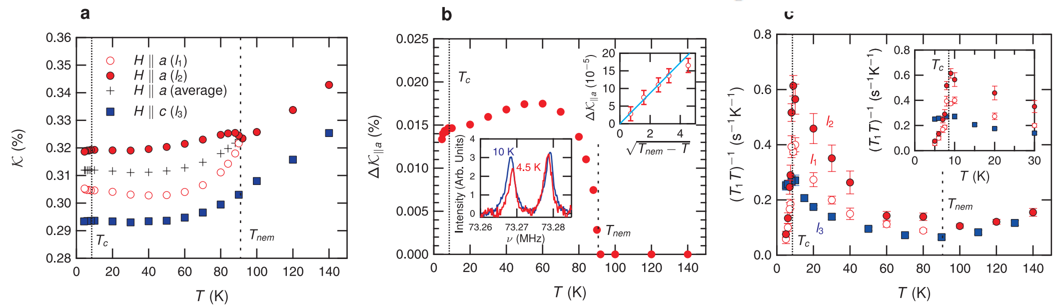

Orbital order parameter $\psi = (n_x - n_y)/(n_x + n_y)$

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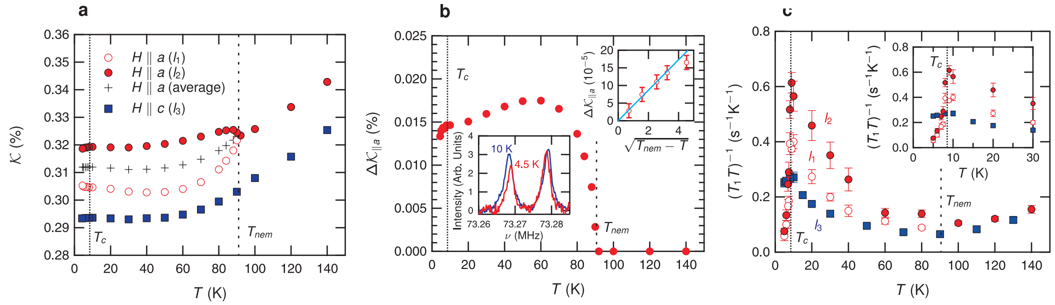

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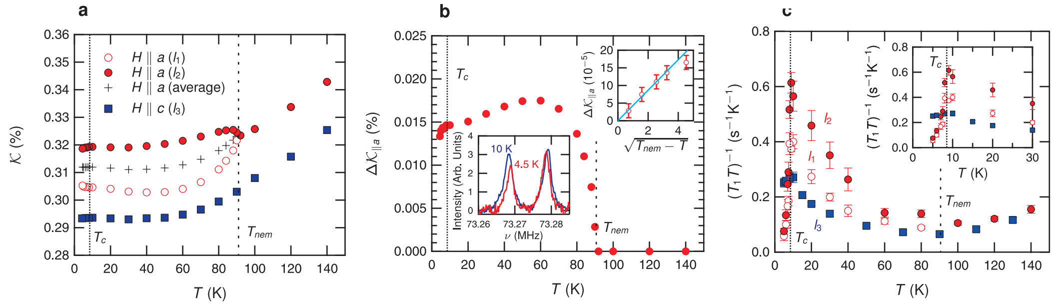

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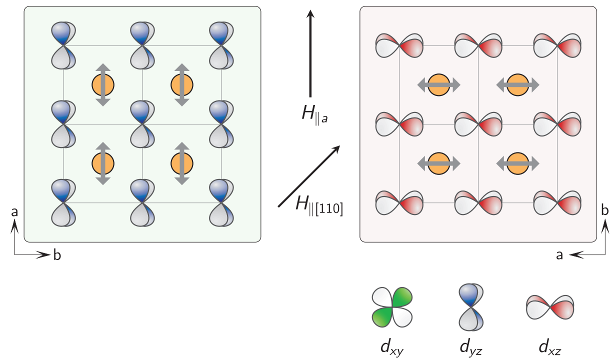
...from which follows $\Delta\mathcal{K}_{\|a} \propto \psi \propto \sqrt{T_{OO} - T}$

Orbital nematicity in FeSe



Orbital nematic order parameter and superconductivity compete