RIXS beyond cuprates: An overview

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IXS2019, June 24

Physics
UNIVERSITY OF TORONTO

Outline

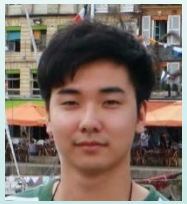
- RIXS snapshot
- Part I: Magnons
  - Curpates
  - Iridates
    - Square lattice iridates – comparison with cuprates
    - Other iridates – magnons at lower energy scale
- Part II: Orbital excitations
  - Non-dispersive dd excitations
  - Collective spin-orbit excitations
  - Future
- Conclusions

Acknowledgements

B. Lebert

W. Jin

Bo Yuan


S. Kim

S. H. Chun

J. P. Clancy

A. Lupascu

K. Plumb

H. Gretarsson

Argonne: Diego Casa, Jungho Kim, Mary Upton, Thomas Gog

Toronto: H.Y. Kee, A. Paramekanti

CLS: Changyong Kim, Ning Chen, Yongfeng Hu

Dresden: Jeroen van den Brink, Liviu Hozoi, V. Katukuri

U Tokyo: Zhaoming Tian, Yang Qiu, Satoru Nakatsuji

Kentucky/Colorado: G. Cao, S. S. A. Seo

SNU/Inha: Namjung Hur, Kee Hoon Kim, T. W. Noh

Gottingen/IISER: Y. Singh, P. Gegenwart

NSLS II: V. Bisogni, I. Jarrige

Advanced Photon Source

UNIVERSITY OF TORONTO

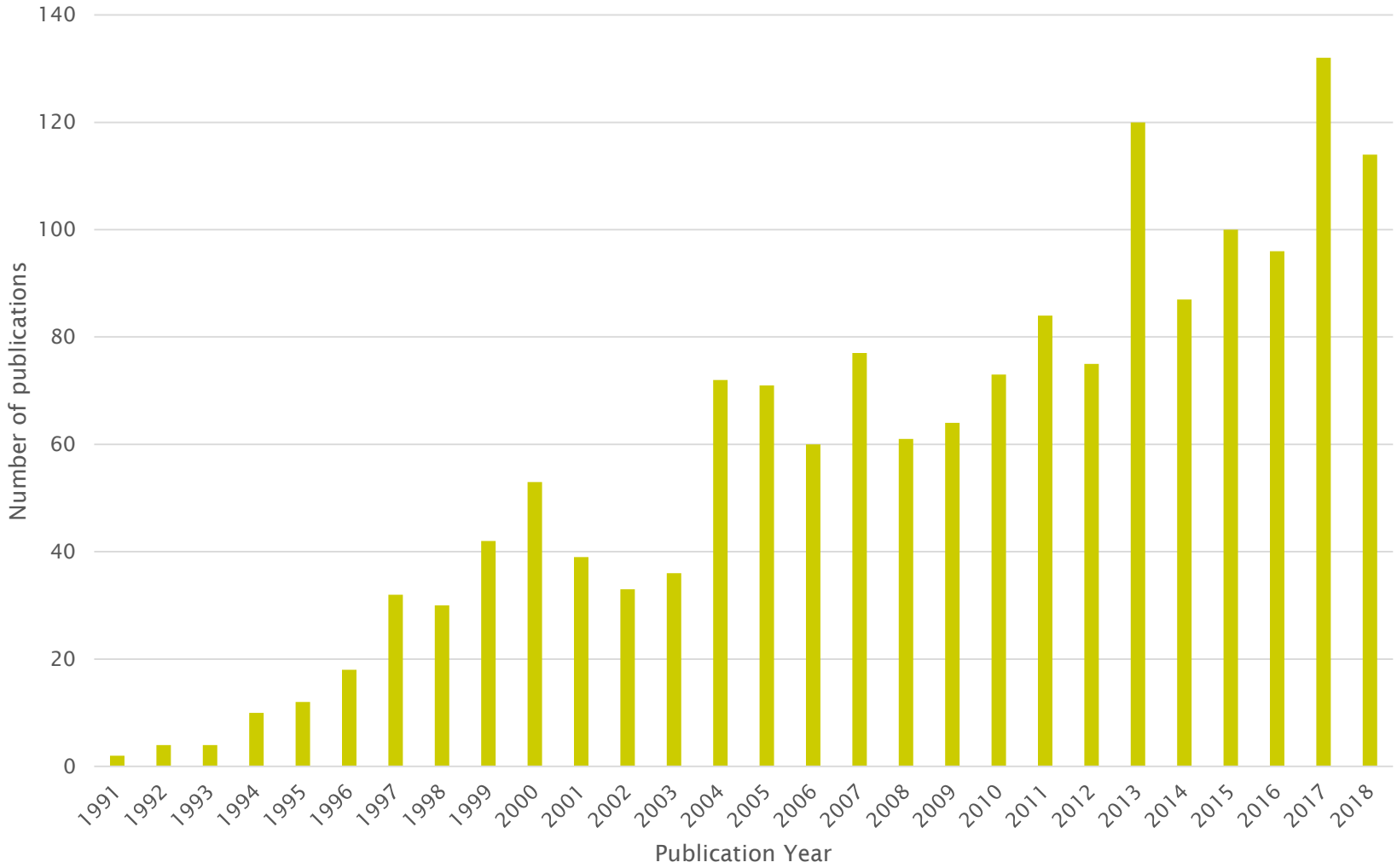
Ontario

NSERC CRSNG

Canada Foundation for Innovation

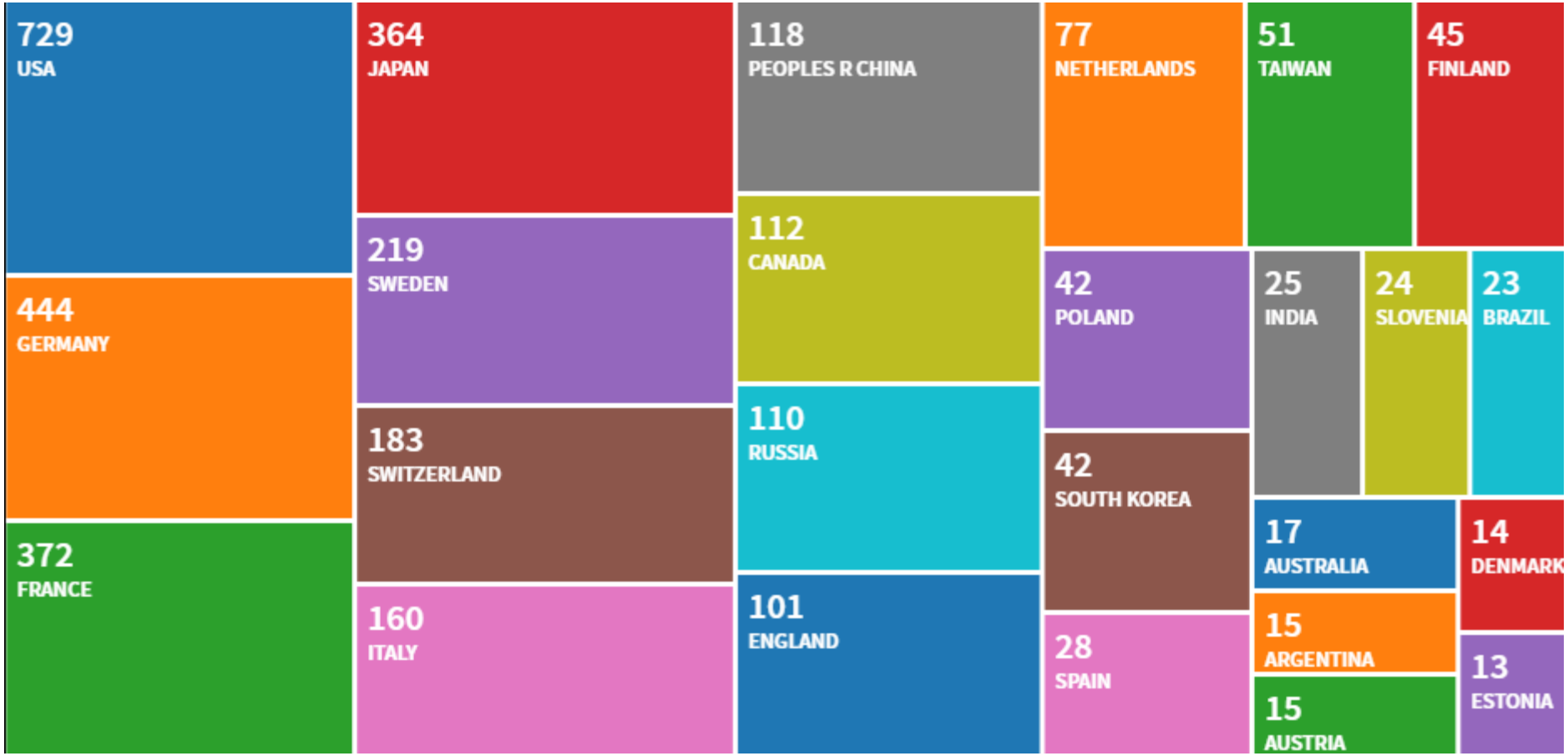
Fondation canadienne pour l'innovation

RIXS is growing

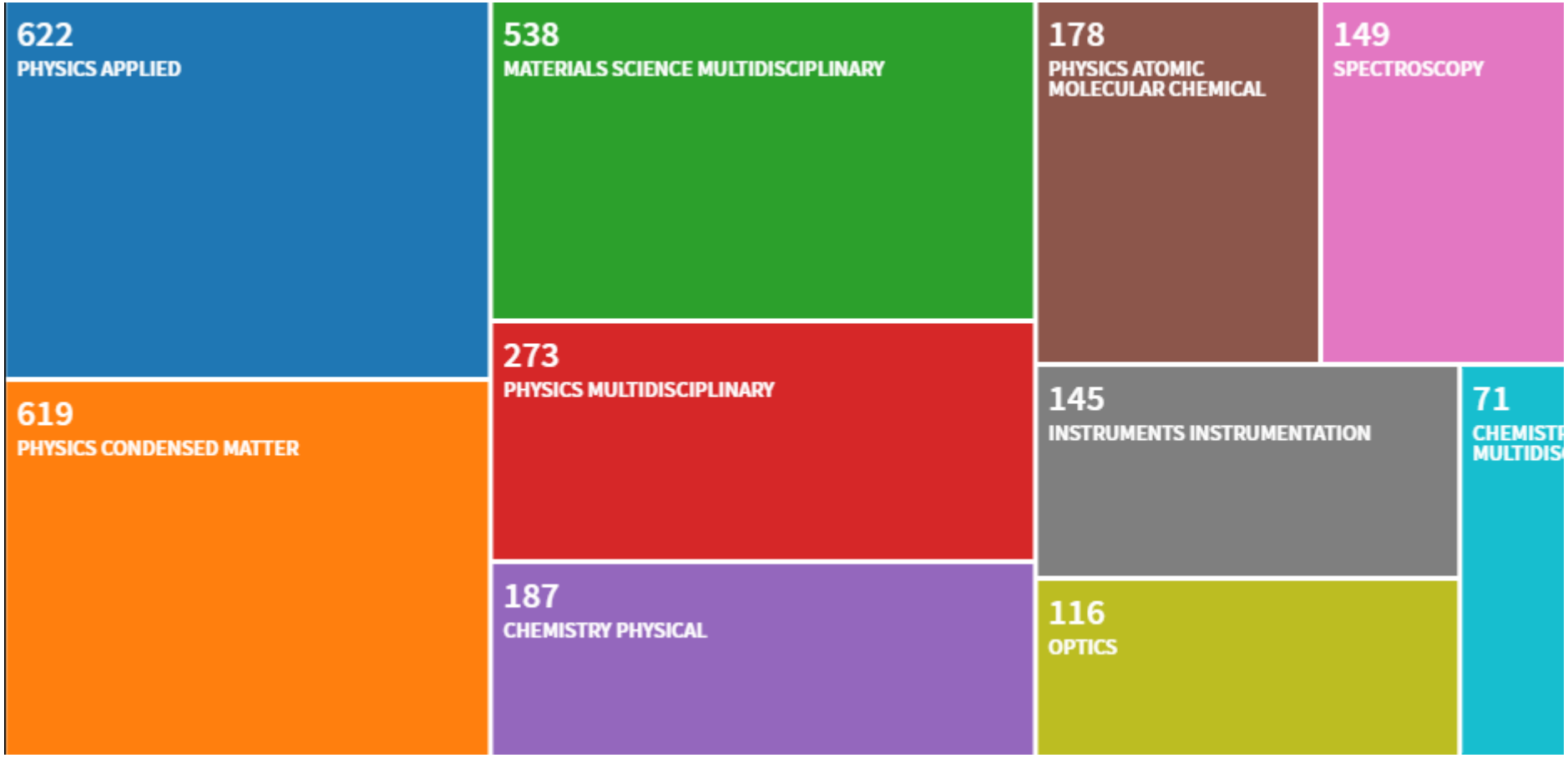


Web of Science Search: RIXS or Resonant Inelastic X-ray Scattering

RIXS is global



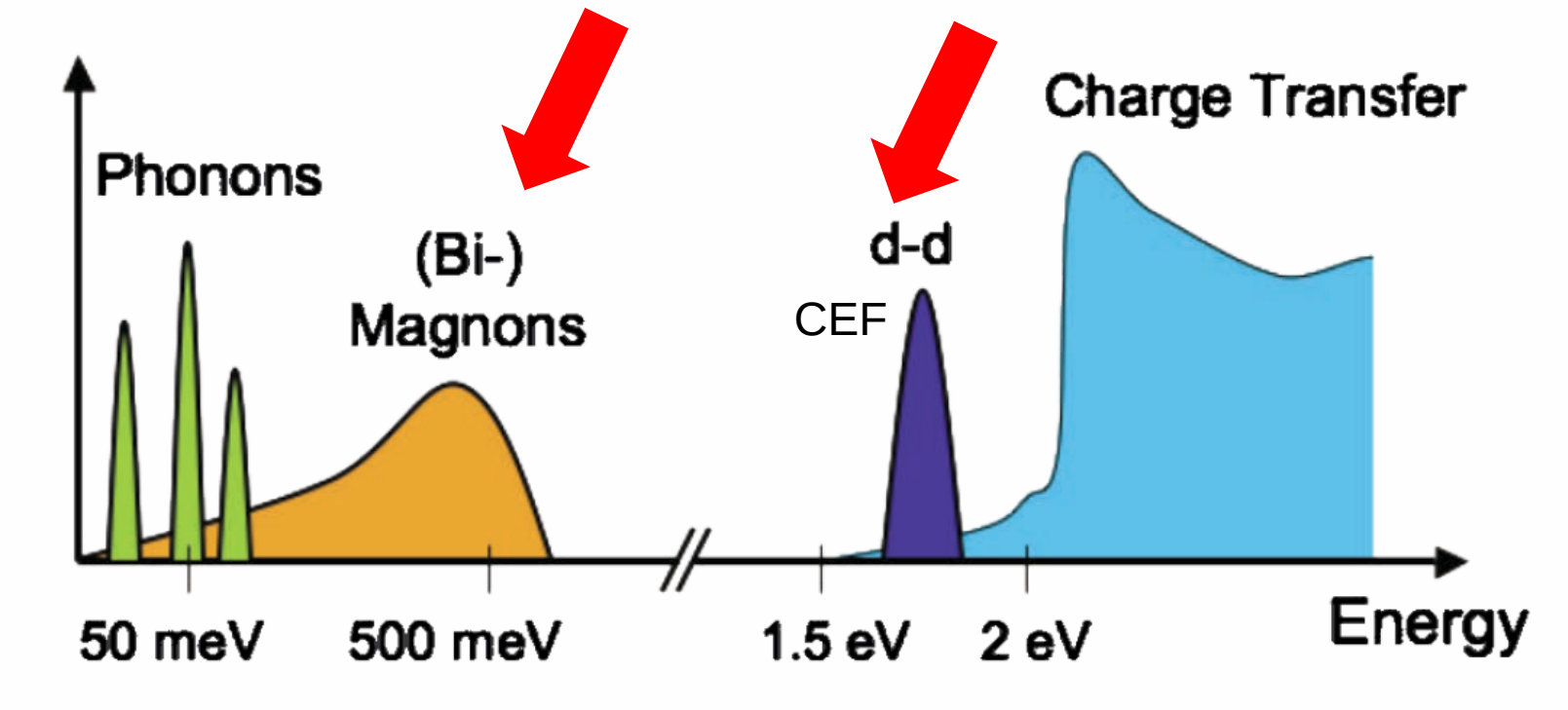
RIXS is diverse



- Total 1656 publications
- “Copper” or “Cuprates” mentioned in 226 pubs (still many more than anything else.

RIXS is useful

- Core-level RIXS useful for studying electronic structure
- Valence RIXS – collective excitations (momentum dependence)



Ament et al. Reviews of Modern Physics 2011

Overview (incomplete)

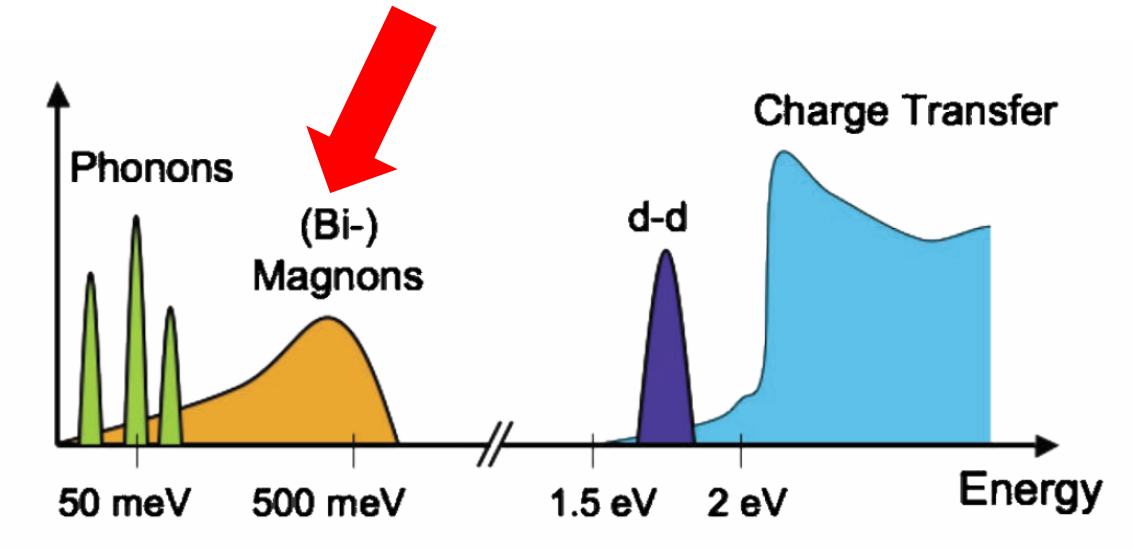
Soft | Hard | Tender | Ligand

1 H 1.00794																	2 He 4.002602
3 Li 6.941	4 Be 9.012182											5 B 10.811	C 12.0107	7 N 14.00674	8 O 15.9994	9 F 18.9984032	10 Ne 20.1797
11 Na 22.989770	12 Mg 24.3050											13 Al 26.581538	14 Si 28.0855	15 P 30.973761	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.955910	22 Ti 47.867	23 V 50.9415	24 Cr 51.9961	25 Mn 54.938049	26 Fe 55.845	27 Co 58.933200	28 Ni 58.6534	29 Cu 63.545	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.92160	34 Se 78.96	35 Br 79.504	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.90585	40 Zr 91.224	41 Nb 92.90638	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.90550	46 Pd 106.42	47 Ag 196.56655	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.760	52 Te 127.60	53 I 126.90447	54 Xe 131.29
55 Cs 132.90545	56 Ba 137.327	57 La 138.9055	72 Hf 178.49	73 Ta 180.94.79	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.217	78 Pt 195.078	79 Au 196.56655	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.58038	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 (269)	111 (272)	112 (277)		114 (289) (287)		116 (289)		118 (293)

Following talk by Kurt Kummer

58 Ce 140.116	59 Pr 140.50765	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.964	64 Gd 157.25	65 Tb 158.92534	66 Dy 162.50	67 Ho 164.93032	68 Er 167.26	69 Tm 168.93421	70 Yb 173.04	71 Lu 174.967
90 Th 232.0381	91 Pa 231.035888	92 U 238.0289	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

Magnons



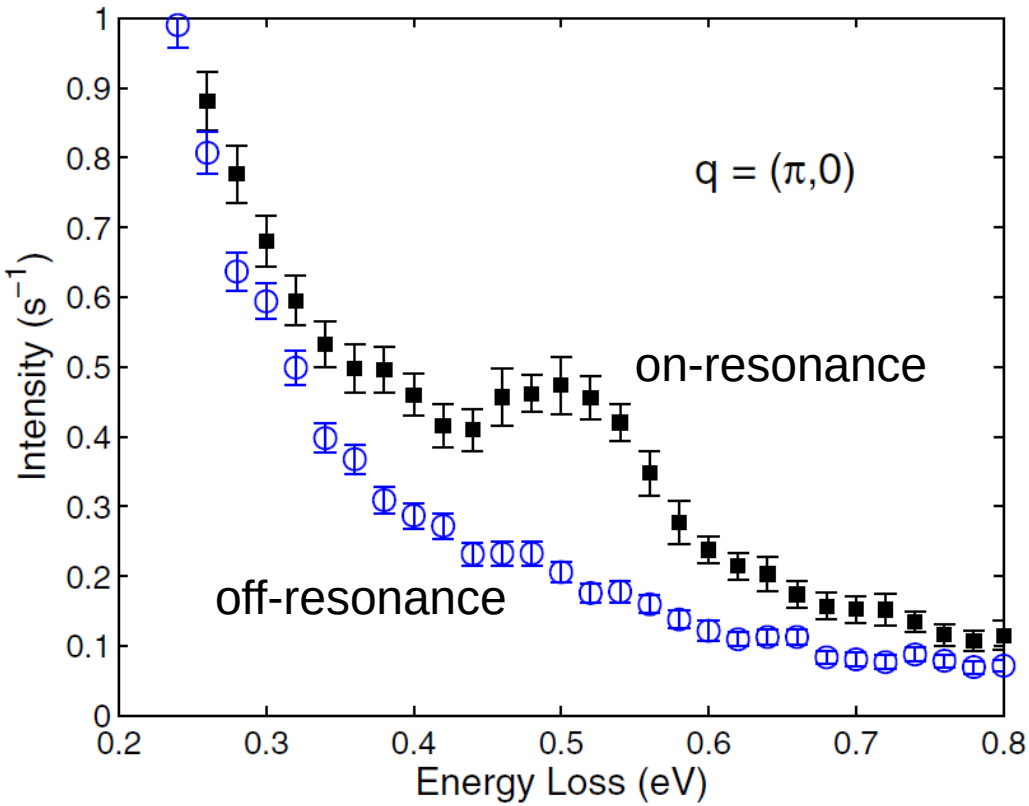
Ament et al. Reviews of Modern Physics 2011

First, Bimagnon

PRL 100, 097001 (2008) PHYSICAL REVIEW LETTERS week ending 7 MARCH 2008

Observation of a 500 meV Collective Mode in $La_{2-x}Sr_xCuO_4$ and Nd_2CuO_4 Using Resonant Inelastic X-Ray Scattering

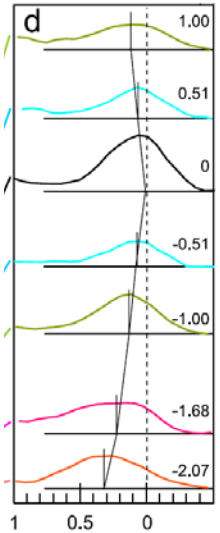
J. P. Hill,[1,2] G. Blumberg,[3] Young-June Kim,[4] D. S. Ellis,[4] S. Wakimoto,[4] R. J. Birgeneau,[4] Seiki Komiya,[5] Yoichi Ando,[5,*] B. Liang,[6] R. L. Greene,[6] D. Casa,[7] and T. Gog[7]



PRL **102,** 167401 (2009) PHYSICAL REVIEW LETTERS week ending 24 APRIL 2009

Dispersion of Magnetic Excitations in the Cuprate La_2CuO_4 and $CaCuO_2$ Compounds Measured Using Resonant X-Ray Scattering

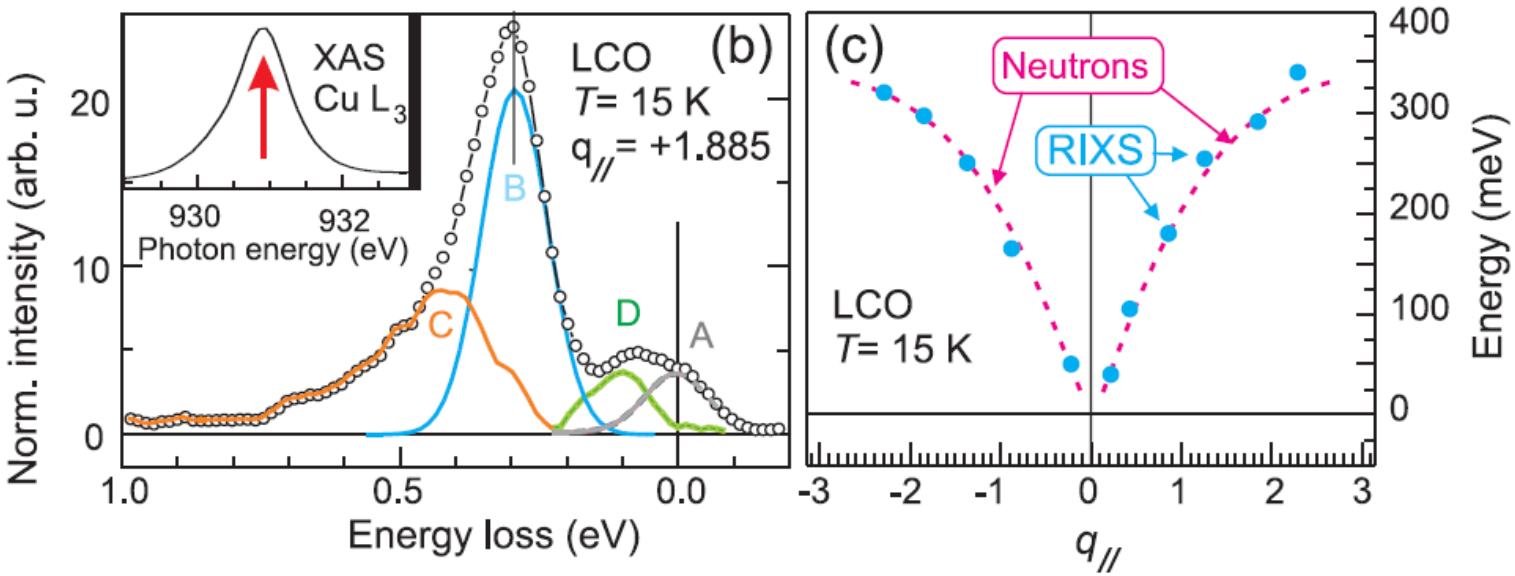
L. Braicovich,[1] L. J. P. Ament,[2] V. Bisogni,[3] F. Forte,[2,4] C. Aruta,[5] G. Balestrino,[6] N. B. Brookes,[3] G. M. De Luca,[5] P. G. Medaglia,[6] F. Miletto Granozio,[5] M. Radovic,[5] M. Salluzzo,[5] J. van den Brink,[2,7] and G. Ghiringhelli[1]



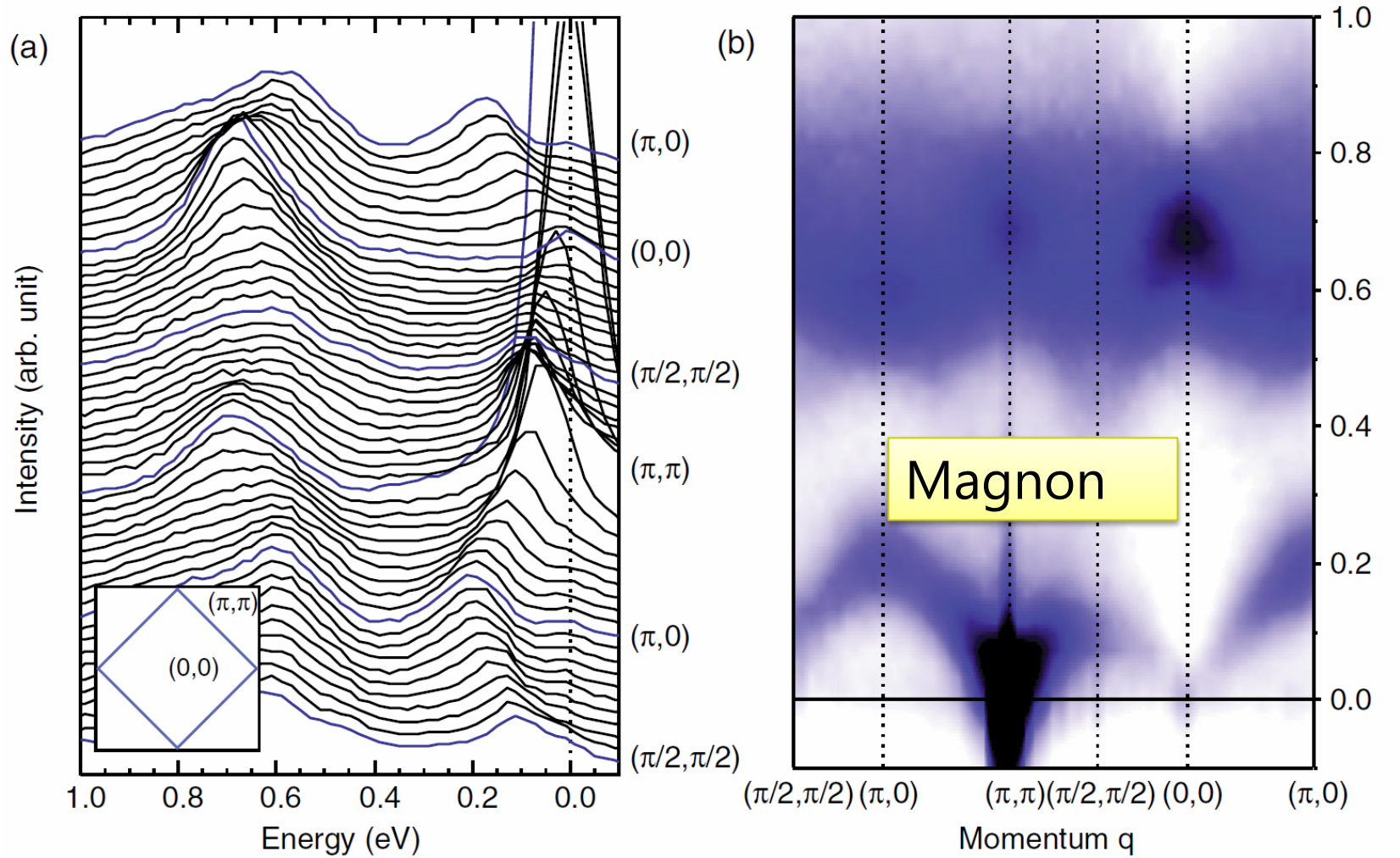
PRL **104,** 077002 (2010) PHYSICAL REVIEW LETTERS week ending 19 FEBRUARY 2010

Magnetic Excitations and Phase Separation in the Underdoped $La_{2-x}Sr_xCuO_4$ Superconductor Measured by Resonant Inelastic X-Ray Scattering

L. Braicovich,[1] J. van den Brink,[2,3,4] V. Bisogni,[5] M. Moretti Sala,[1] L. J. P. Ament,[2,3] N. B. Brookes,[5] G. M. De Luca,[6] M. Salluzzo,[6] T. Schmitt,[7] V. N. Strocov,[7] and G. Ghiringhelli[1]

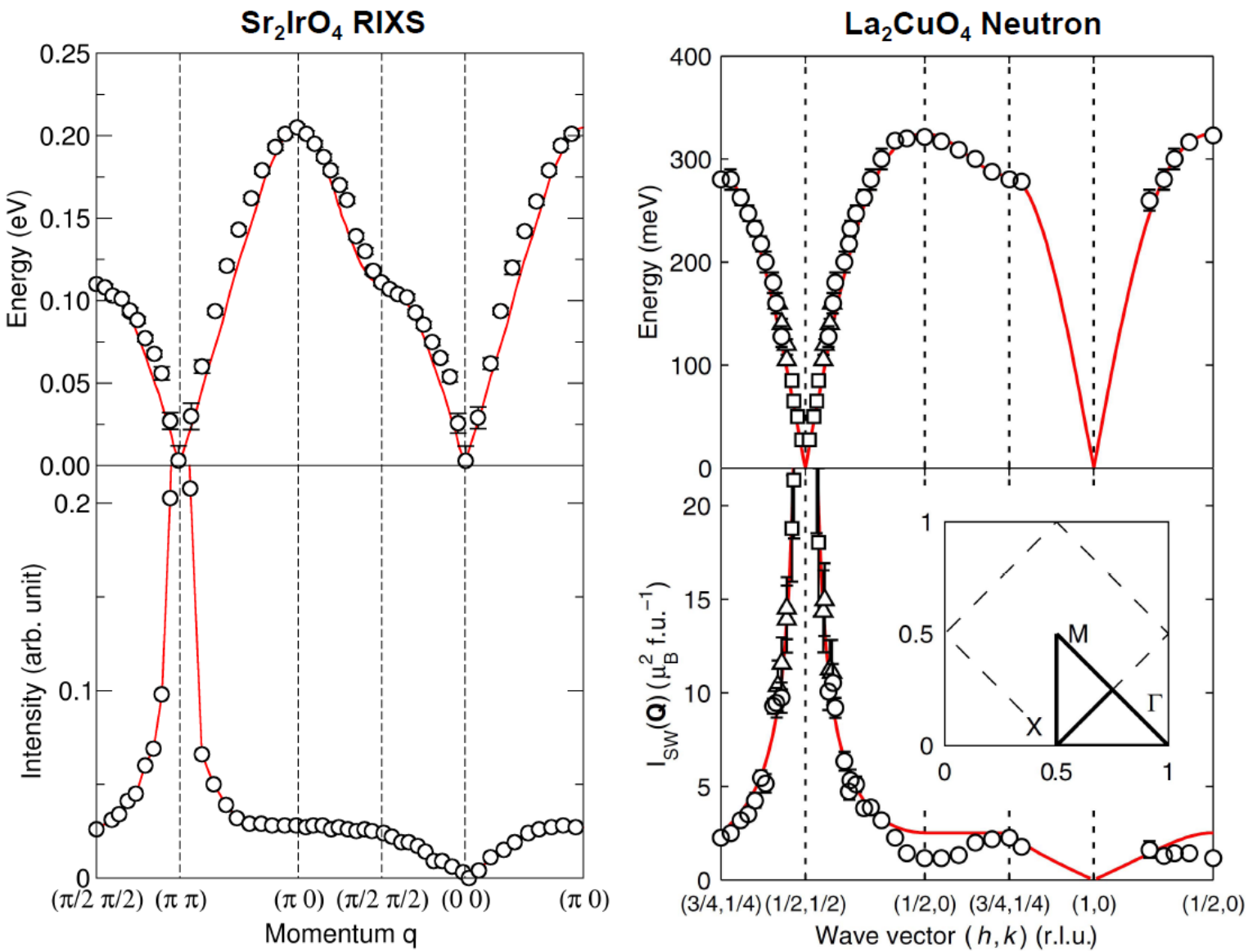


Sr_2IrO_4 – magnons with hard RIXS



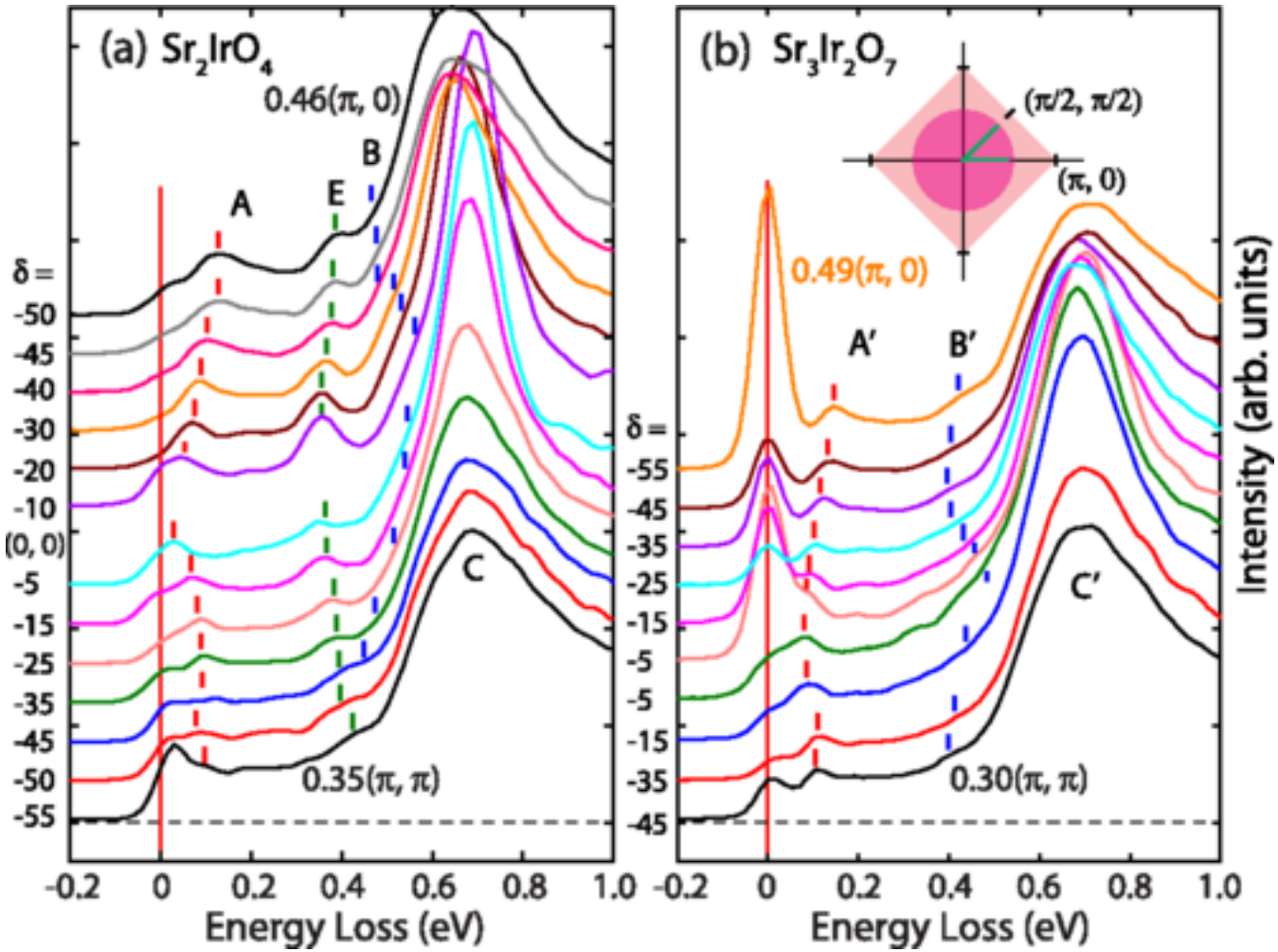
Jungho Kim et al. PRL 108, 177003 (2012)

INS/RIXS Comparison - magnons



YJK et al. Synch. Rad. News 2012

Ligand RIXS – magnons

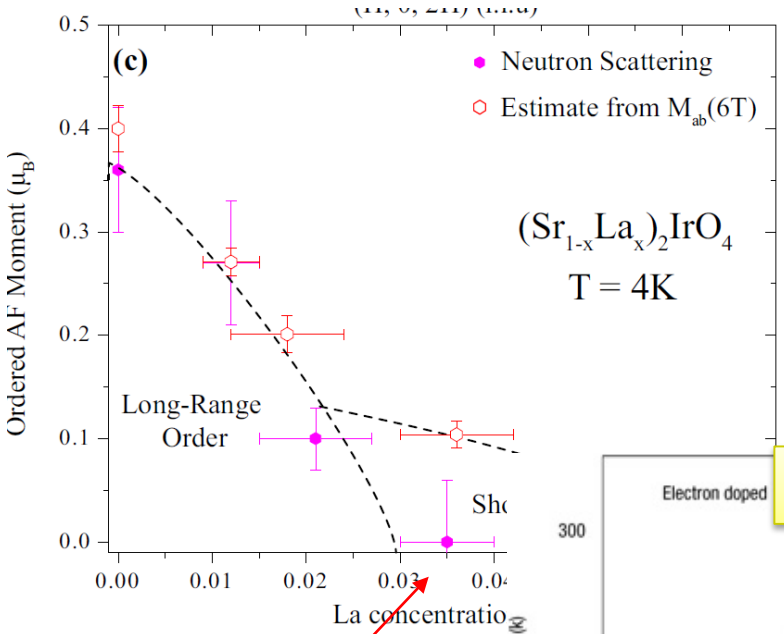


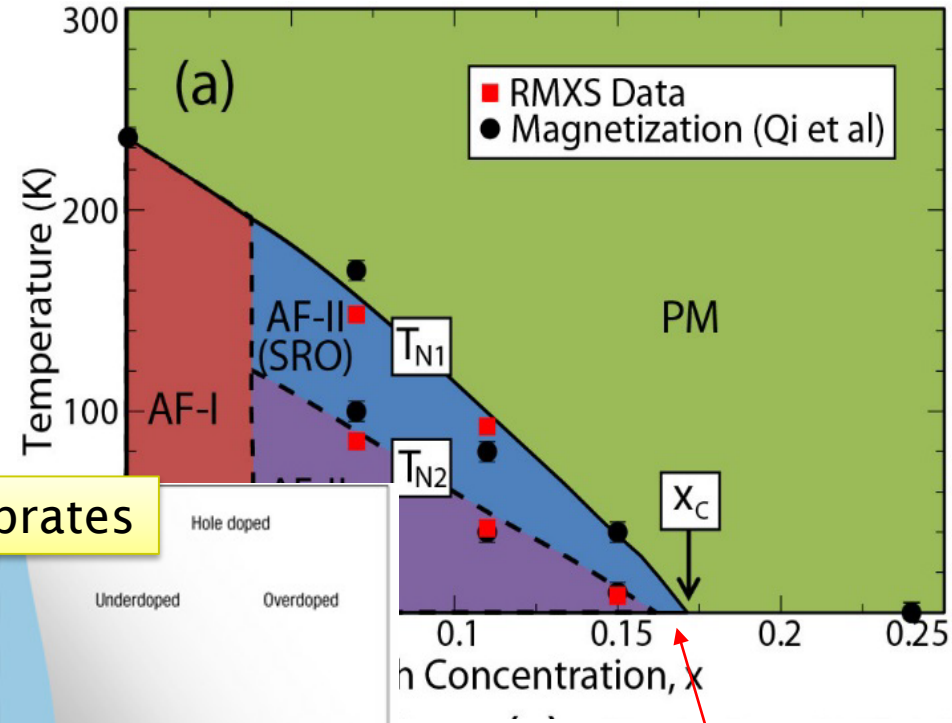
X. Lu, T. Schmitt et al. PRB 2018

Magnetic phase diagram

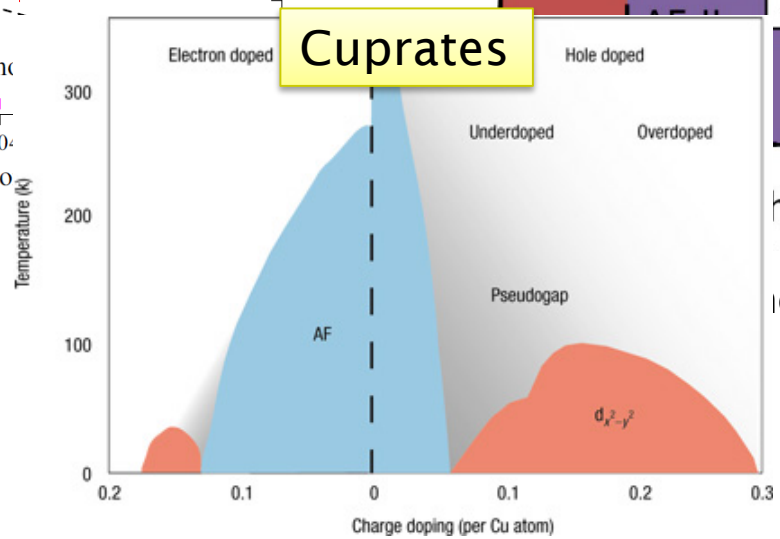
Electron doping
$Sr_{2-x}La_xIrO_4$

Hole doping
$Sr_2Ir_{1-x}Rh_xO_4$





Cuprates



X. Chen, S. Wilson et al.

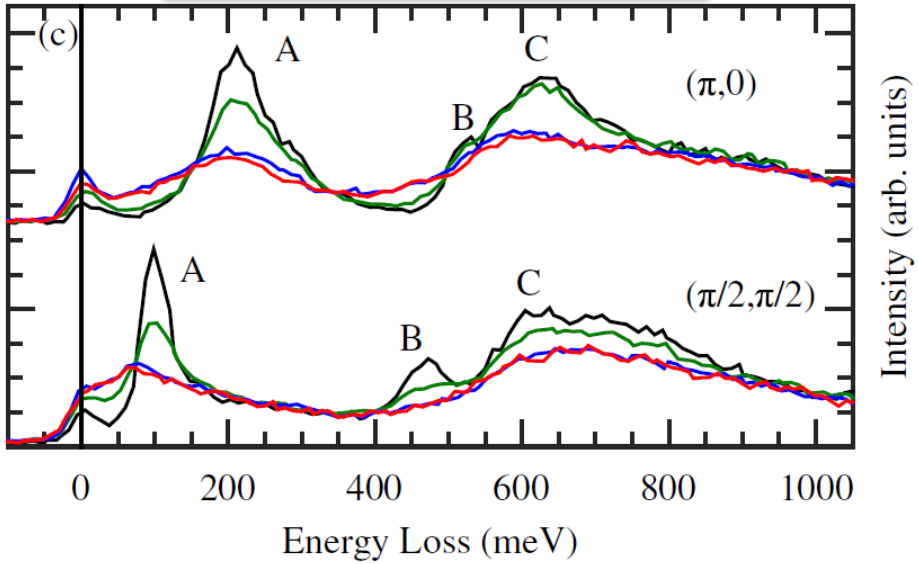
ıcy et al. PRB 2014

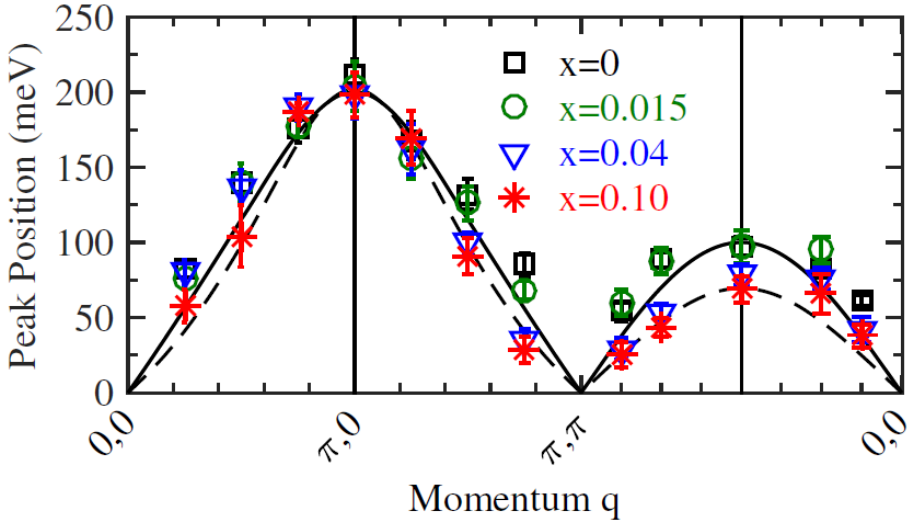
$x_c \sim 0.04$

$x_c \sim 0.17$

Magnon doping dependence

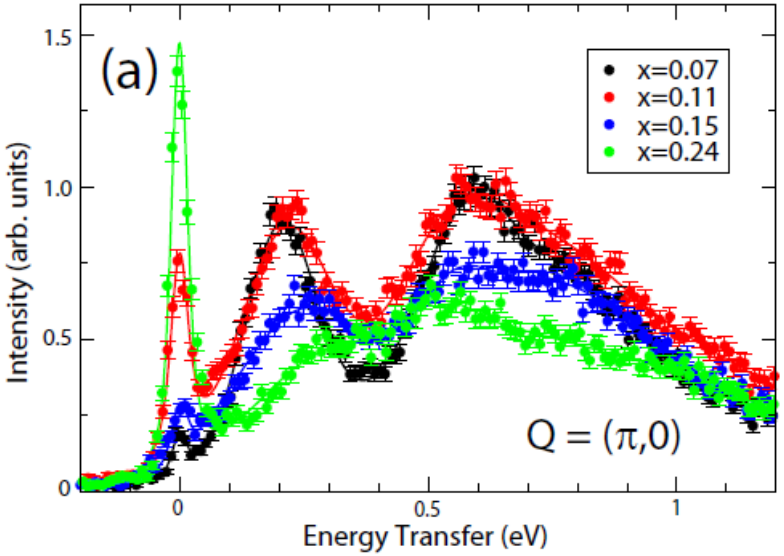
e-doping $Sr_{2-x}La_xIrO_4$

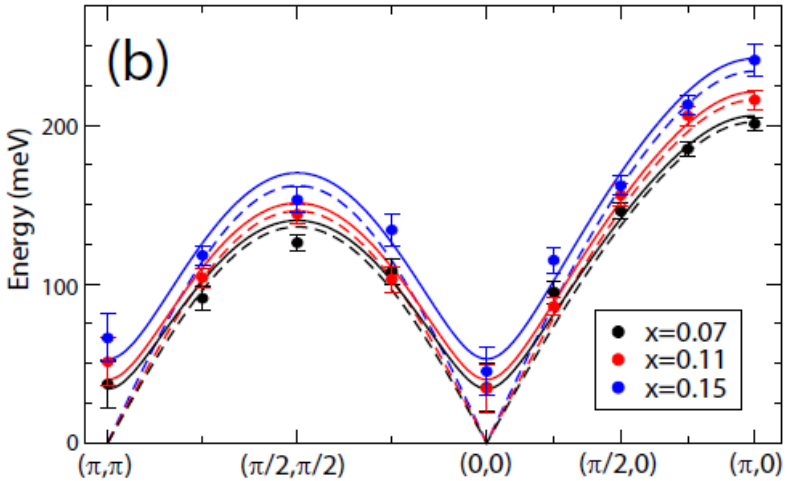




Gretarsson, BJ Kim et al. PRL 2016

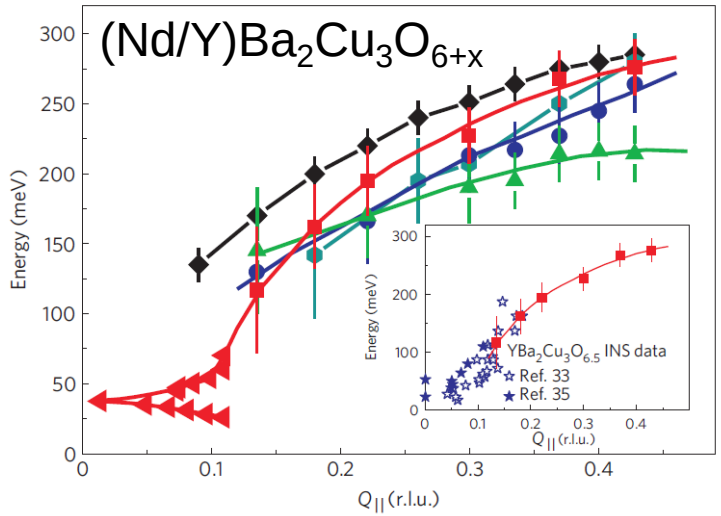
Hole doping $Sr_2Ir_{1-x}Rh_xO_4$



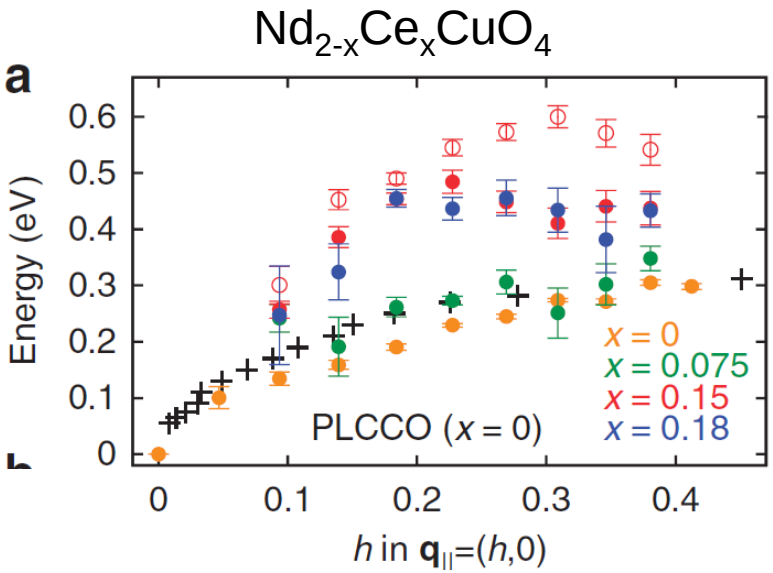


J. P. Clancy, YJK et al. arXiv:1904.06402

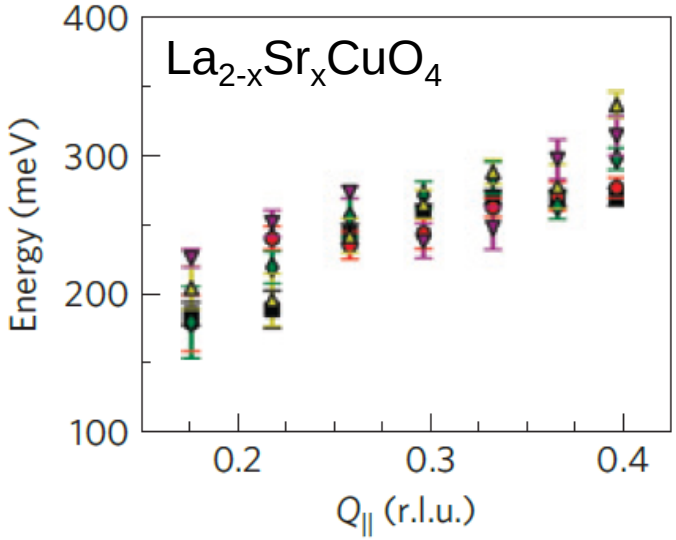
Comparison with Doped Cuprates



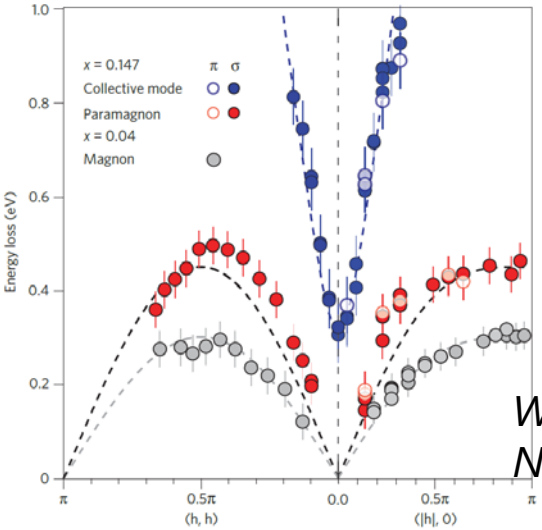
Le Tacon et al, Nat. Phys. (2011)



Ishii et al, Nat. Comm. (2014)



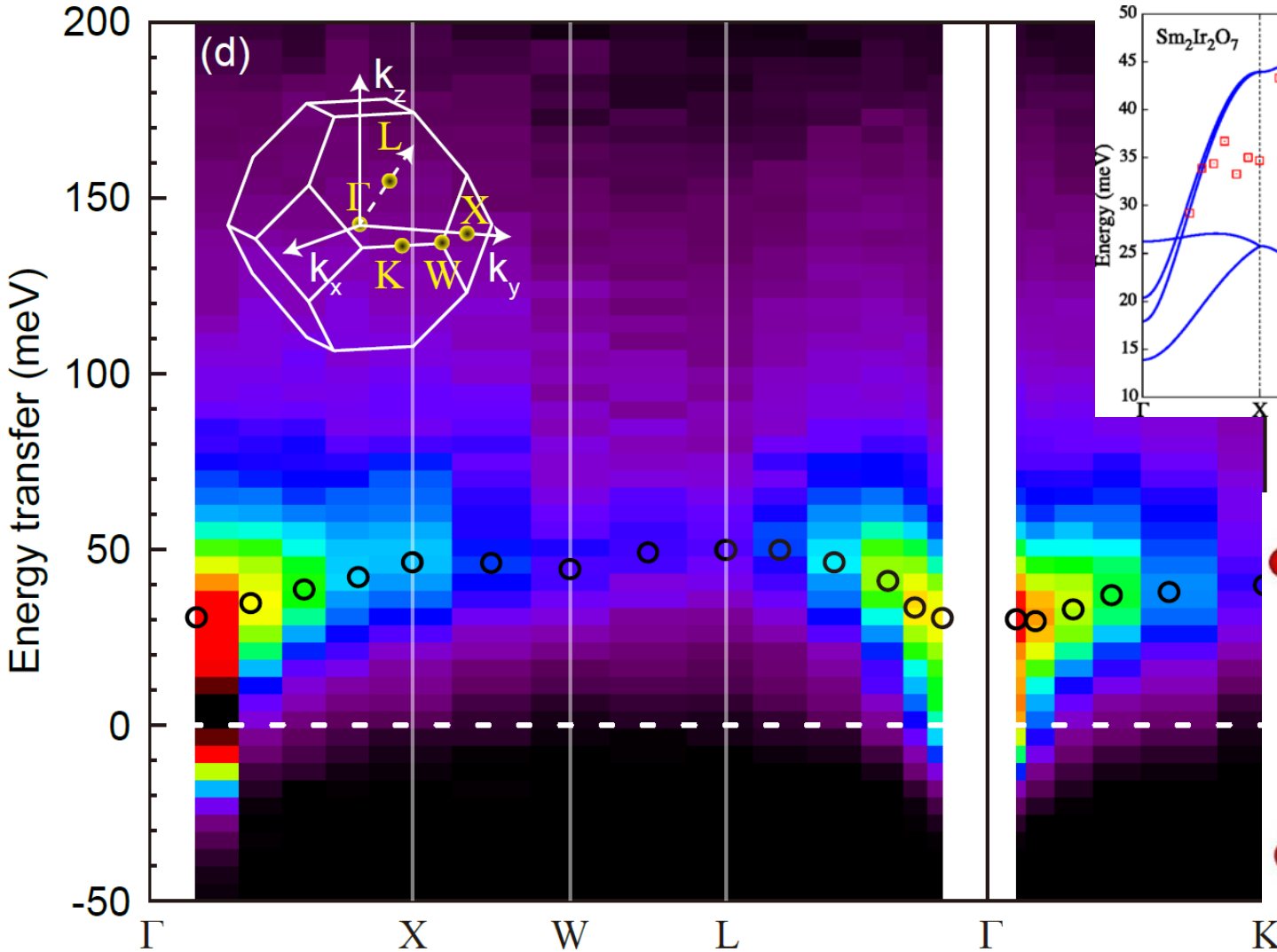
M. Dean et al, Nat. Mater. (2011)

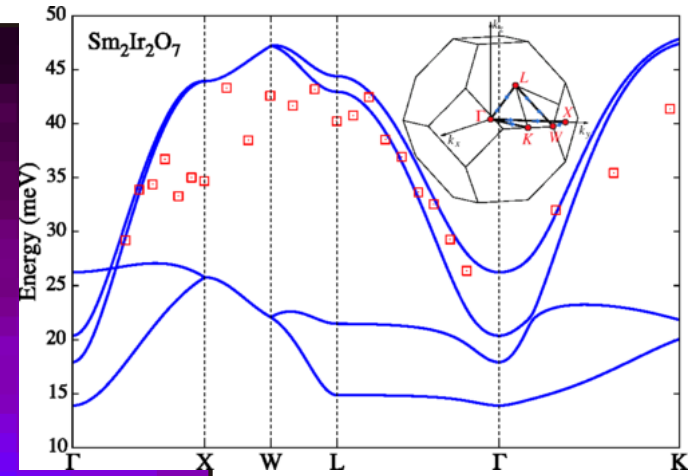


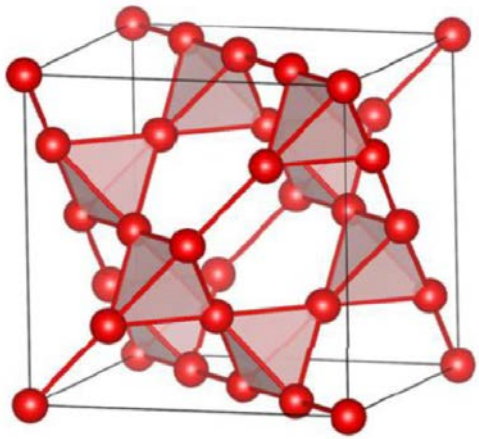
W. S. Lee et al. Nat. Phys. (2015)

Magnetic excitations $Eu_2Ir_2O_7$

Radav et al. PRMater. 2018



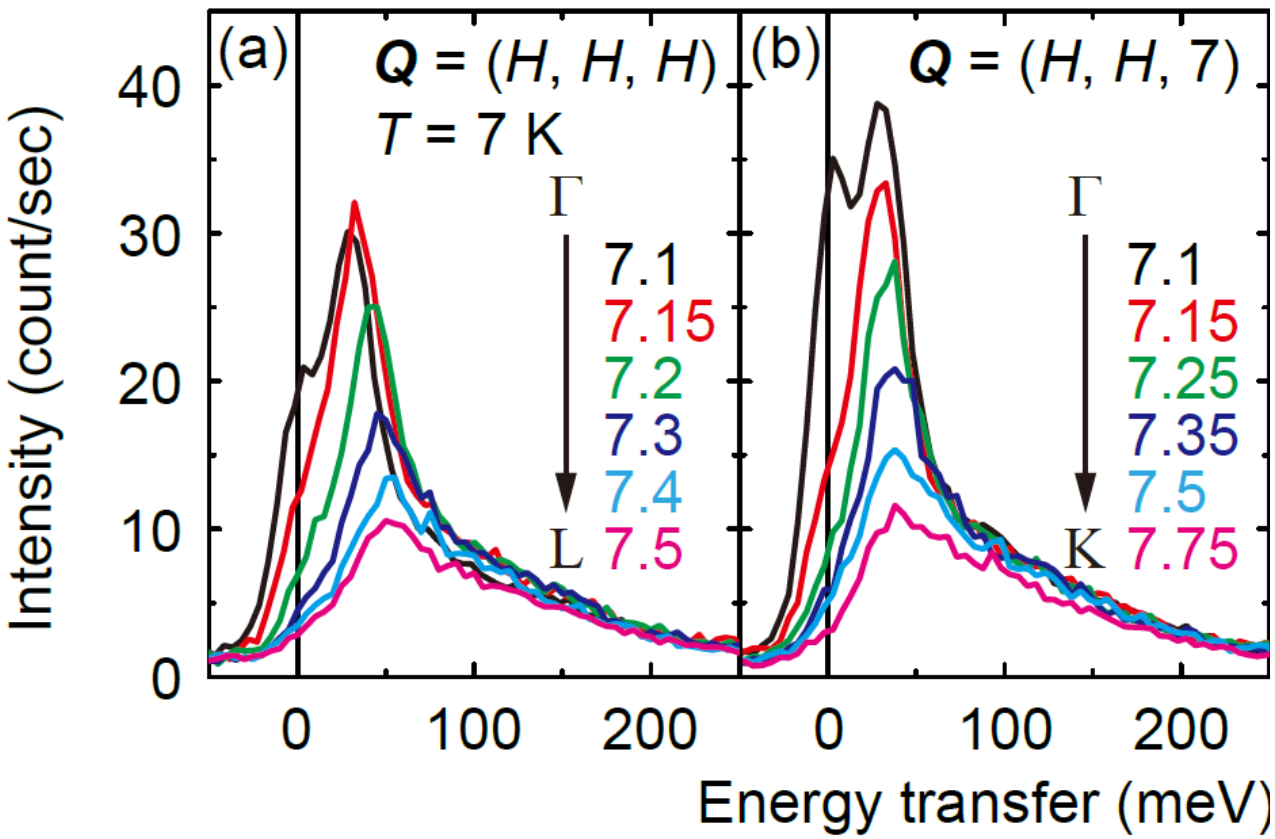


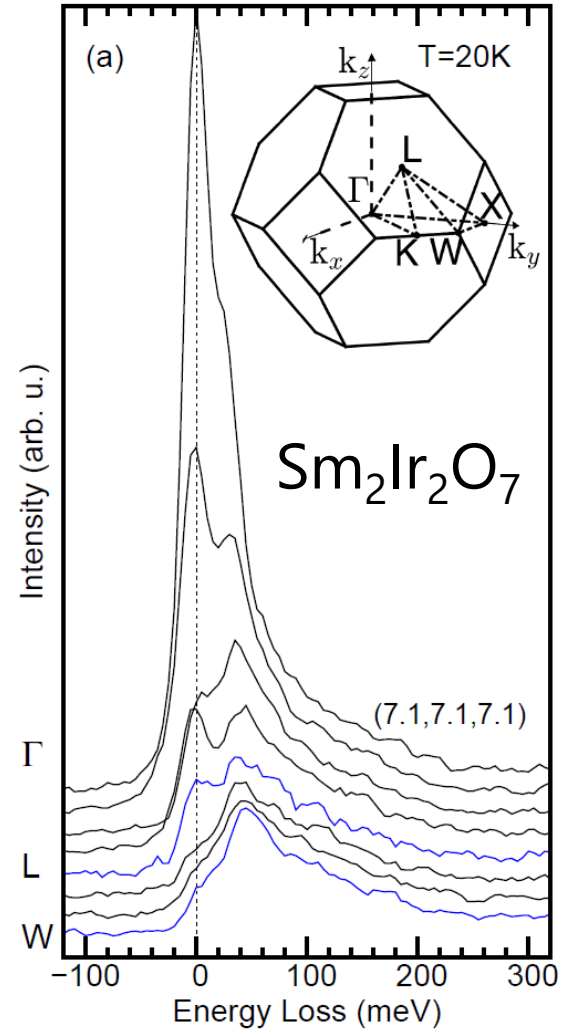


S. H. Chun, YJK et al. PRL 2018

Momentum dependence

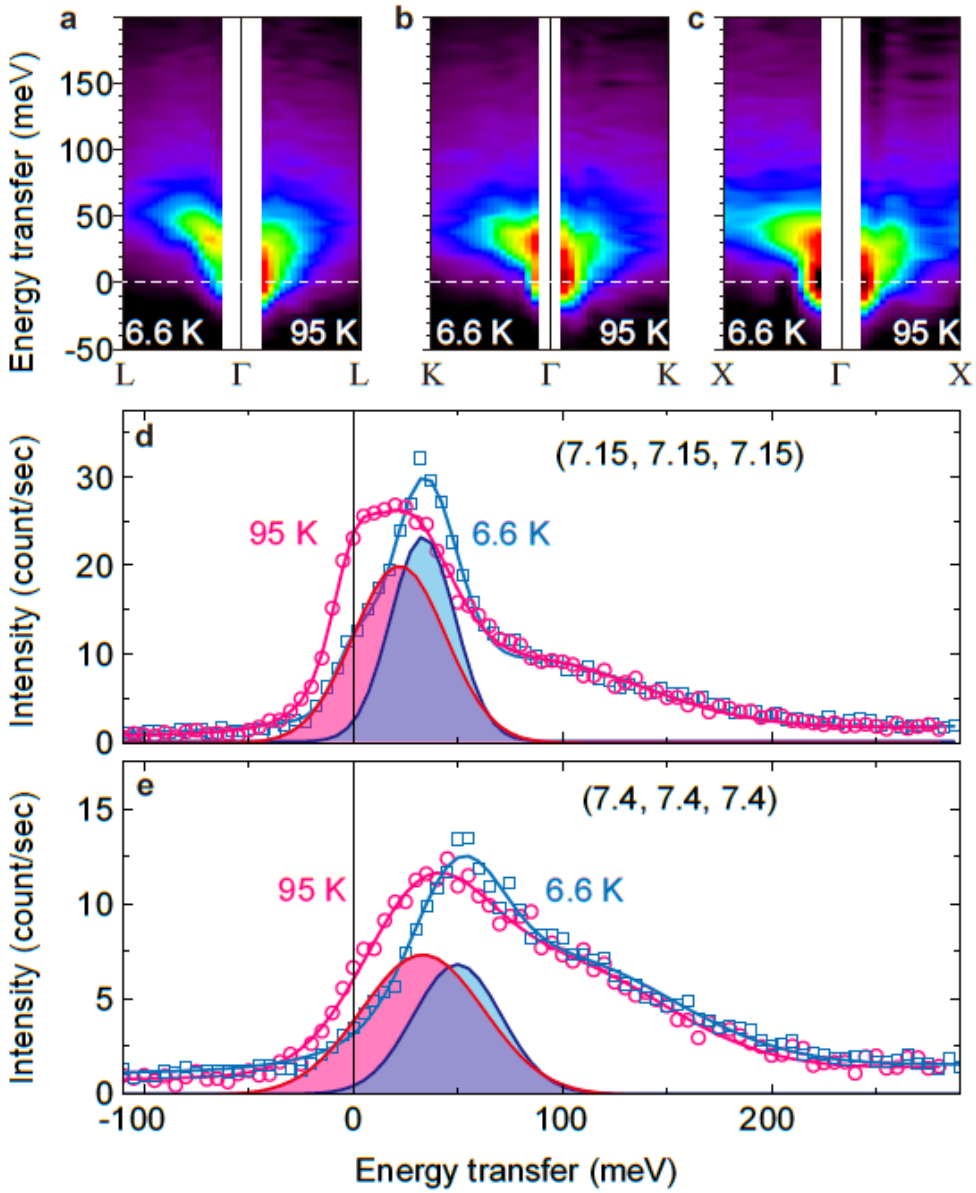
Donnerer et al. PRL (2016)

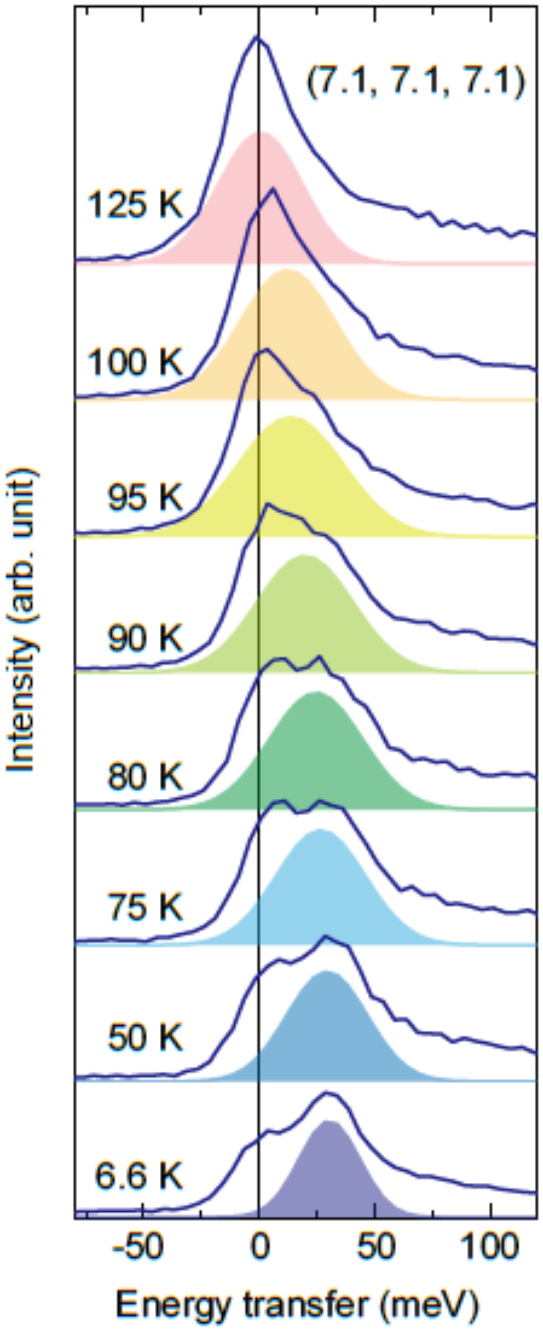




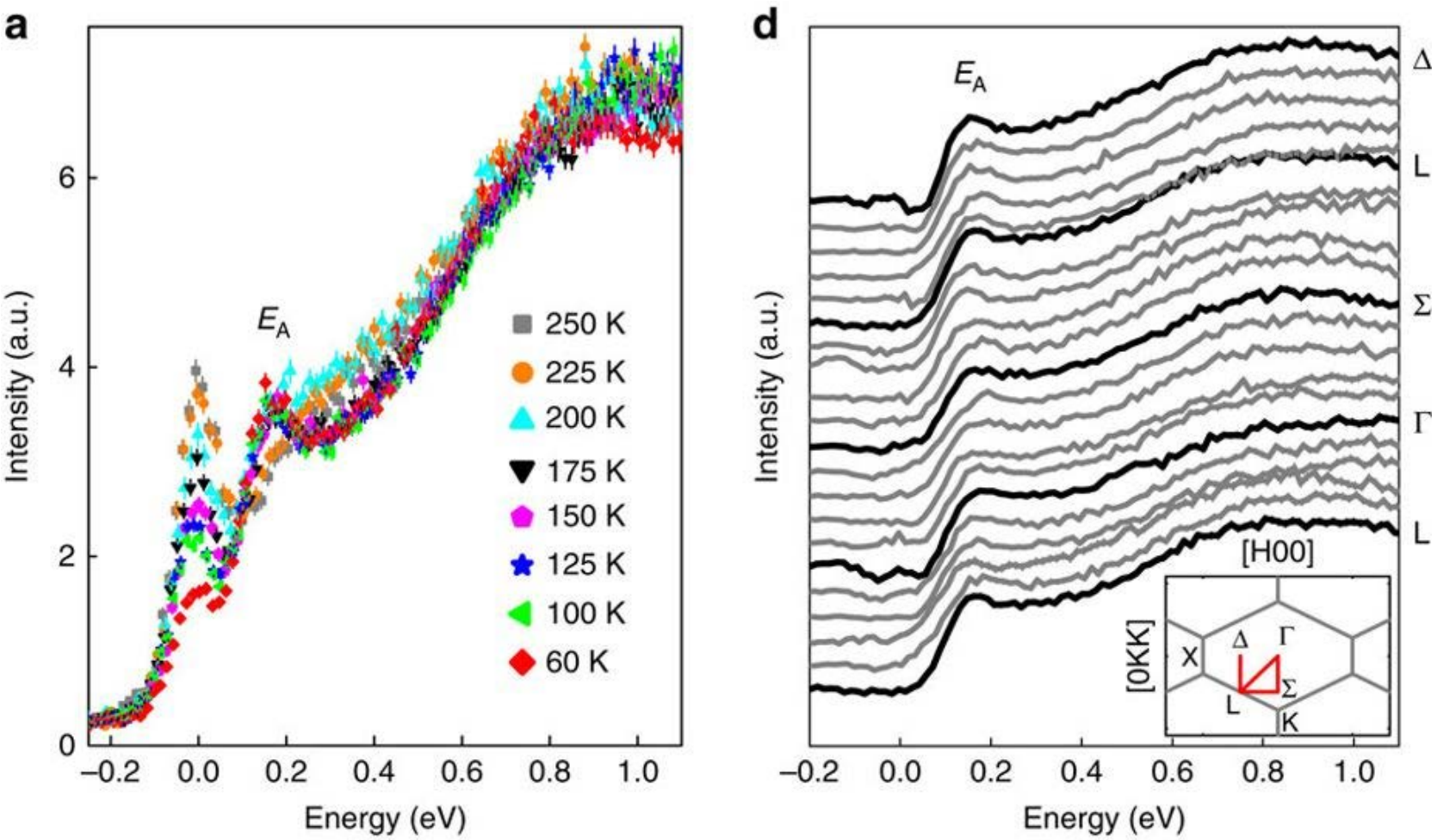
S. H. Chun et al. PRL 2018

Temperature Dependenc





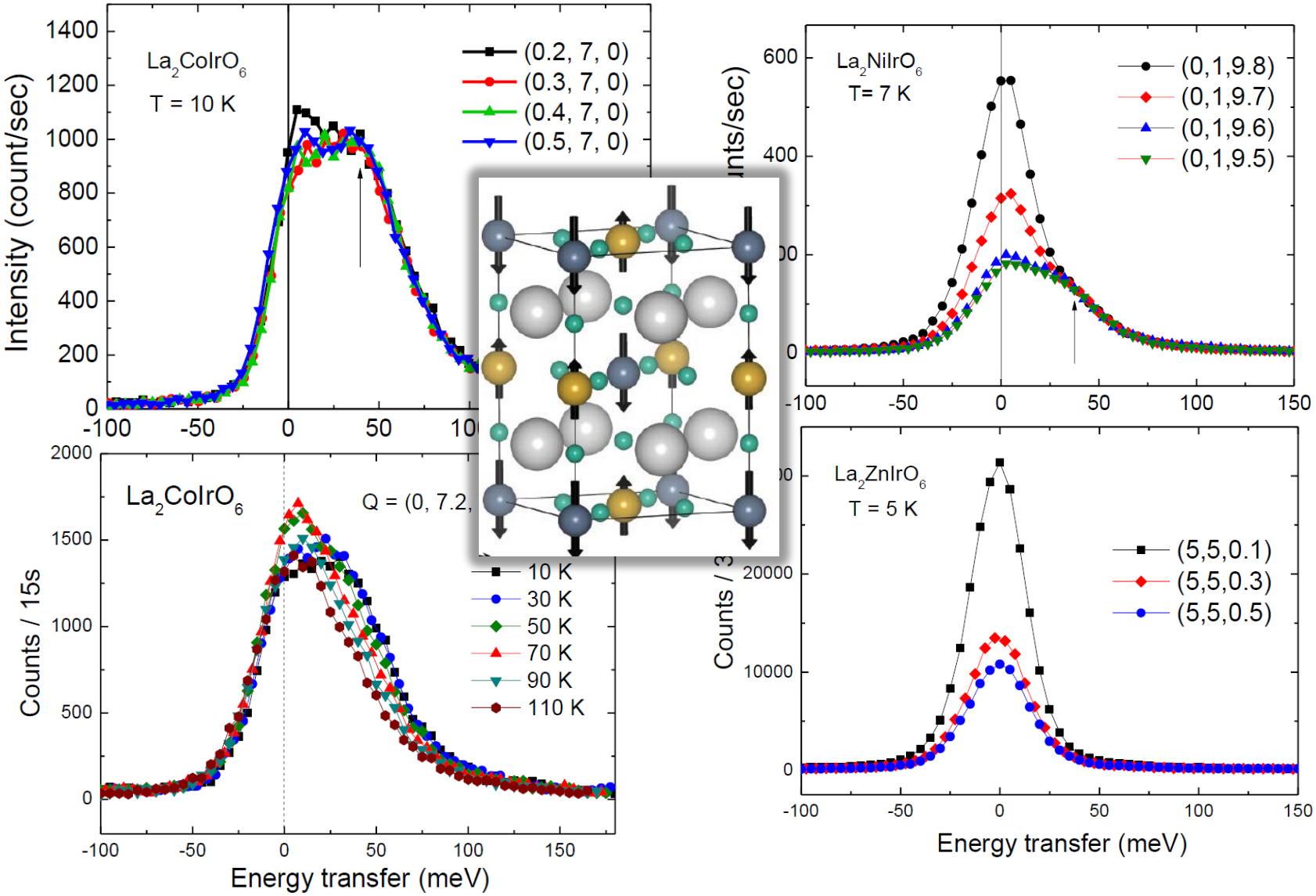
Temperature dep. – $Cd_2Os_2O_7$



S. Calder et al. Nat. Comm. 2016

Double perovskite iridates

W. Jin, YJK et al. unpublished

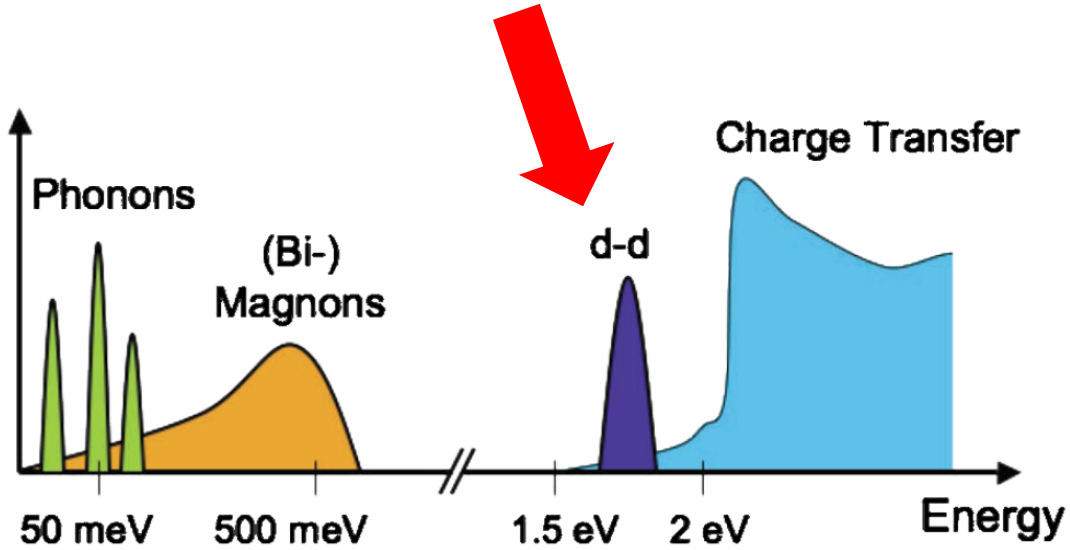


Magnon summary

- Magnon dispersion can be measured with RIXS
- Square lattice materials easier due to large energy scales
- Low energy magnetic excitations are challenging
  - Usually not enough resolution to resolve different modes
  - Temperature dependence often used to show magnetic nature – not always straightforward to understand
  - Background can have different origins and some depend on temperatures
- Need a better strategy for magnon studies
  - A better energy resolution – e.g. flat crystal spectrometer design by Jungho Kim and Thomas Gog
  - Polarization analysis (hard x-ray) ?

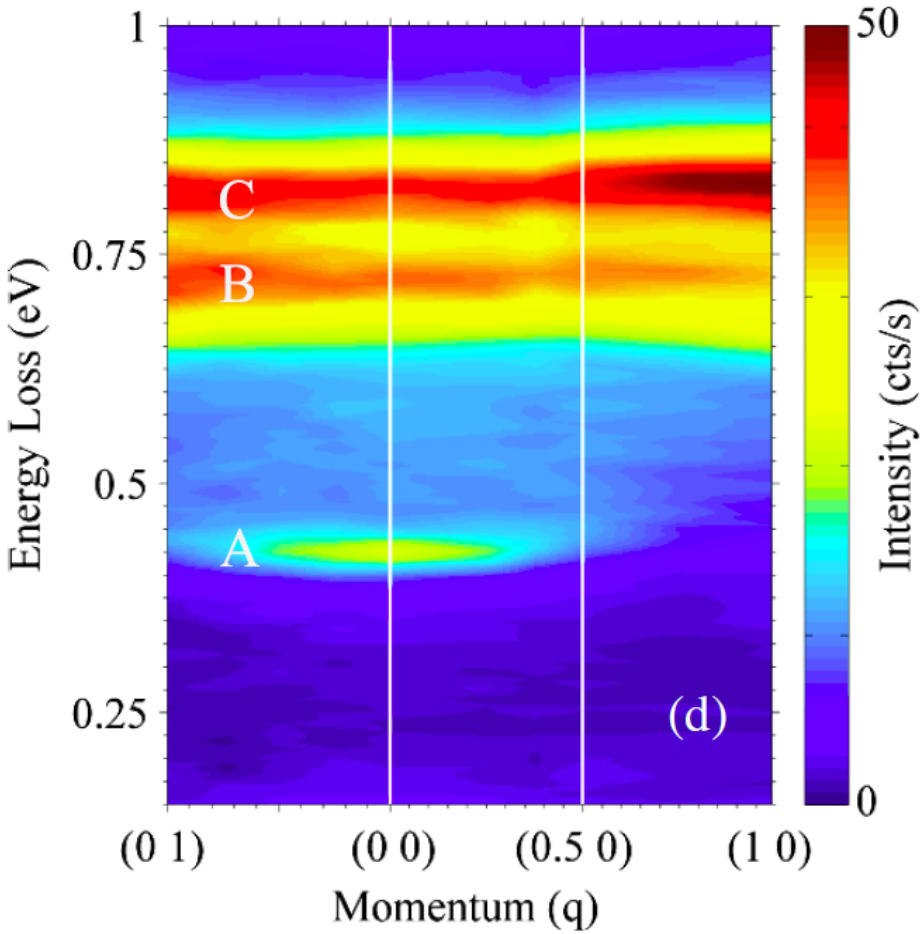
dd
Orbital
Spin-orbit
CEF

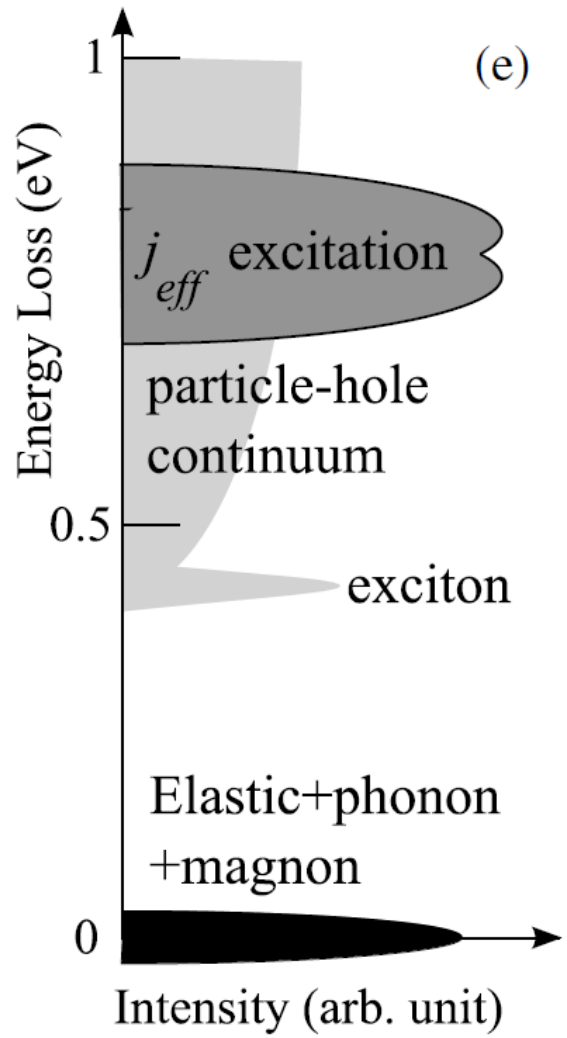
} Excitations



Ament et al. Reviews of Modern Physics 2011

Momentum dependence

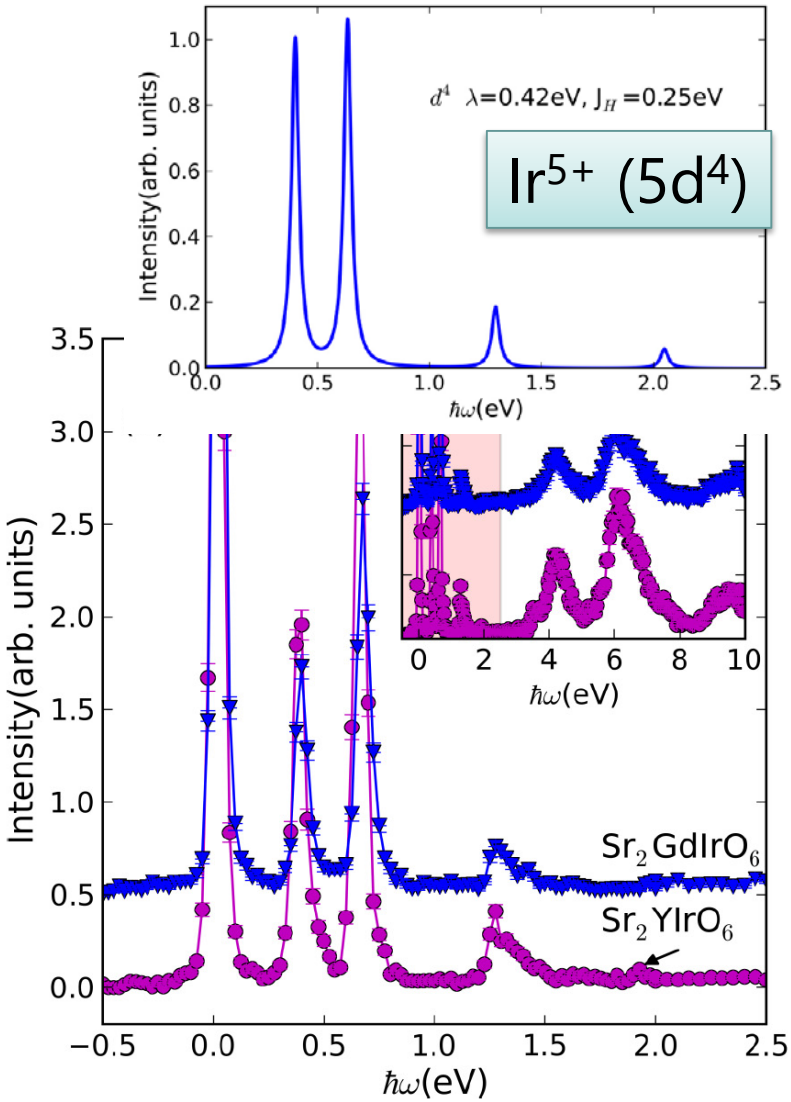


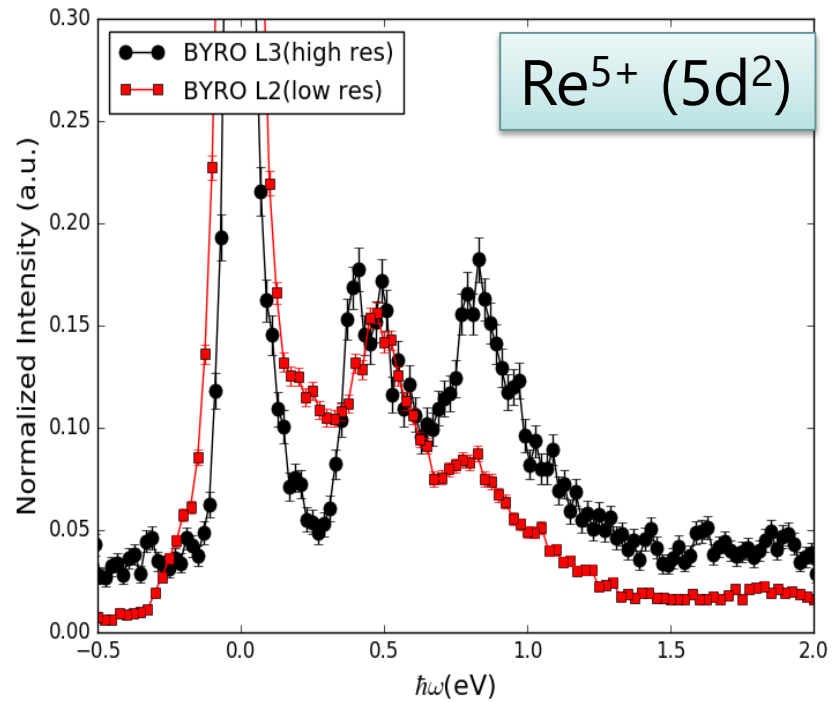


Gretarsson et al. PRL 2013

Iridium and Rhenium DP

Talk by A. Paramekanti at 17:55 today

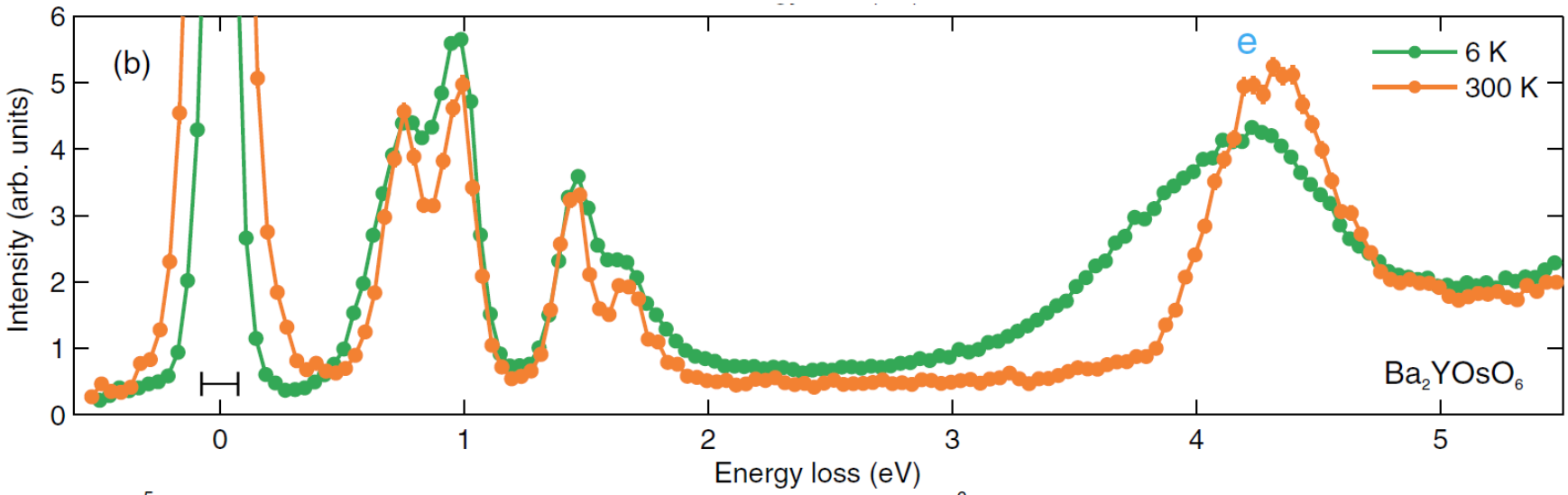


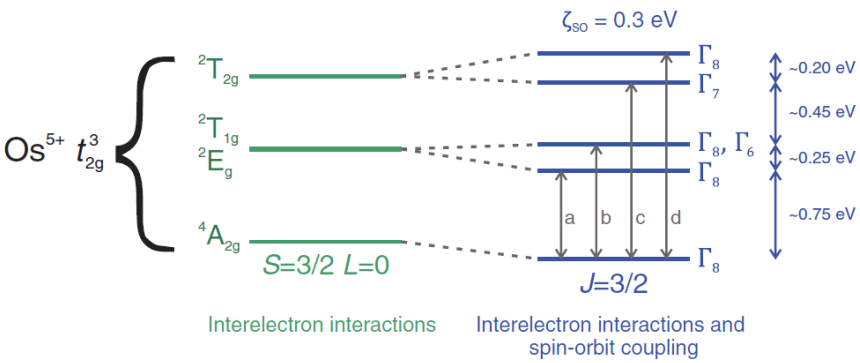


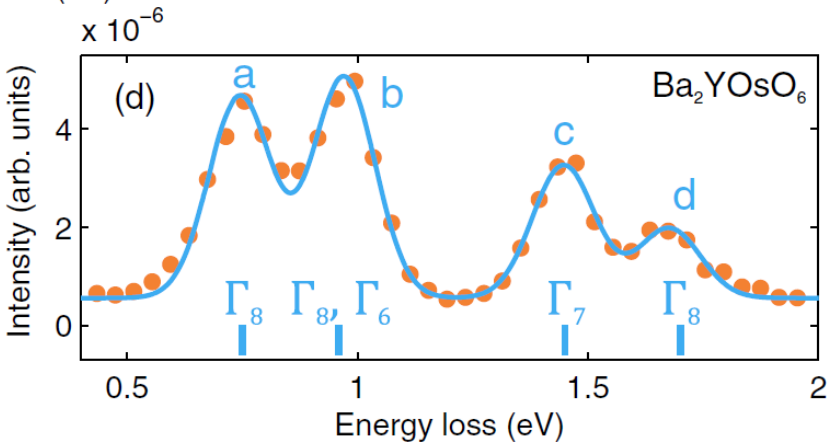
B. Yuan et al. PRB 2017

A. Paramekanti et al. PRB 2018

Osmium double perovskite (DP)







Os^{5+} ($5d^3$)

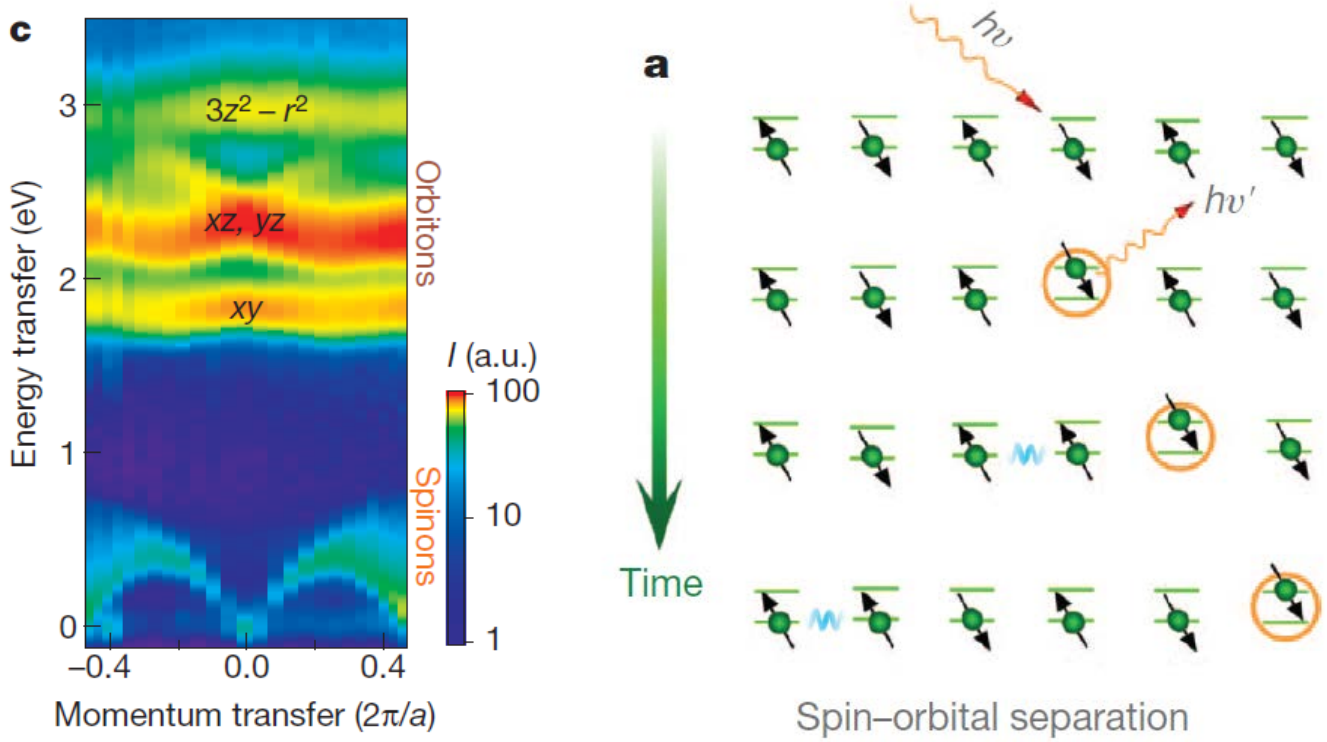
A. E. Taylor, A. D. Christianson et al. PRL 2017

Special Case I: spin chain

Nature 482, 82 (2012)

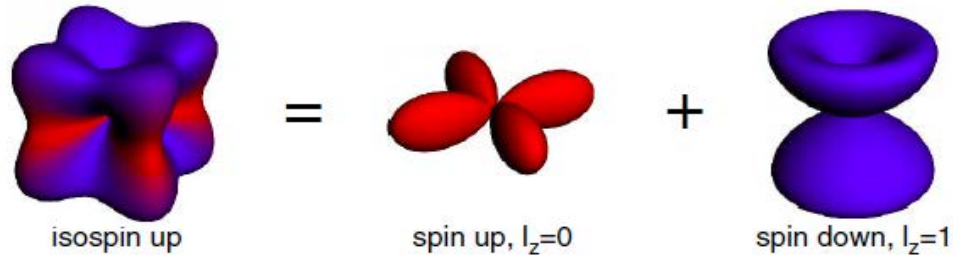
Spin–orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3

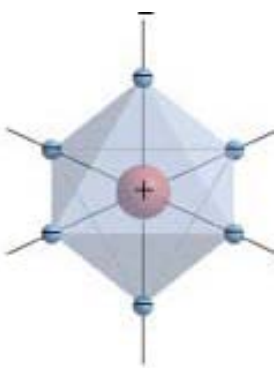
J. Schlappa[1,2], K. Wohlfeld[3], K. J. Zhou[1]†, M. Mourigal[4], M. W. Haverkort[5], V. N. Strocov[1], L. Hozoi[3], C. Monney[1], S. Nishimoto[3], S. Singh[6]†, A. Revcolevschi[6], J.-S. Caux[7], L. Patthey[1,8], H. M. Rønnow[4], J. van den Brink[3] & T. Schmitt[1]

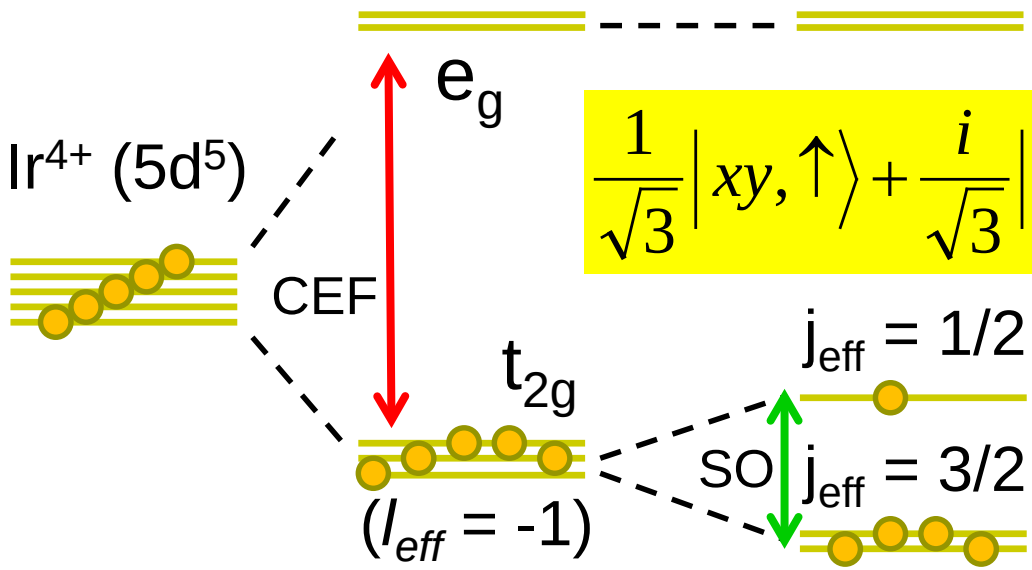


Special Case II: Strong SOC

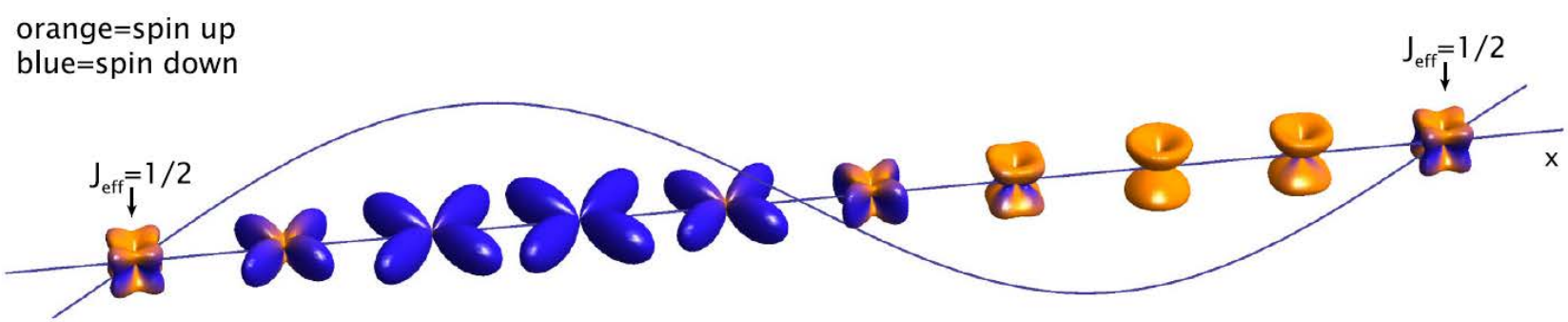
Jackeli and Khaliullin PRL 2009



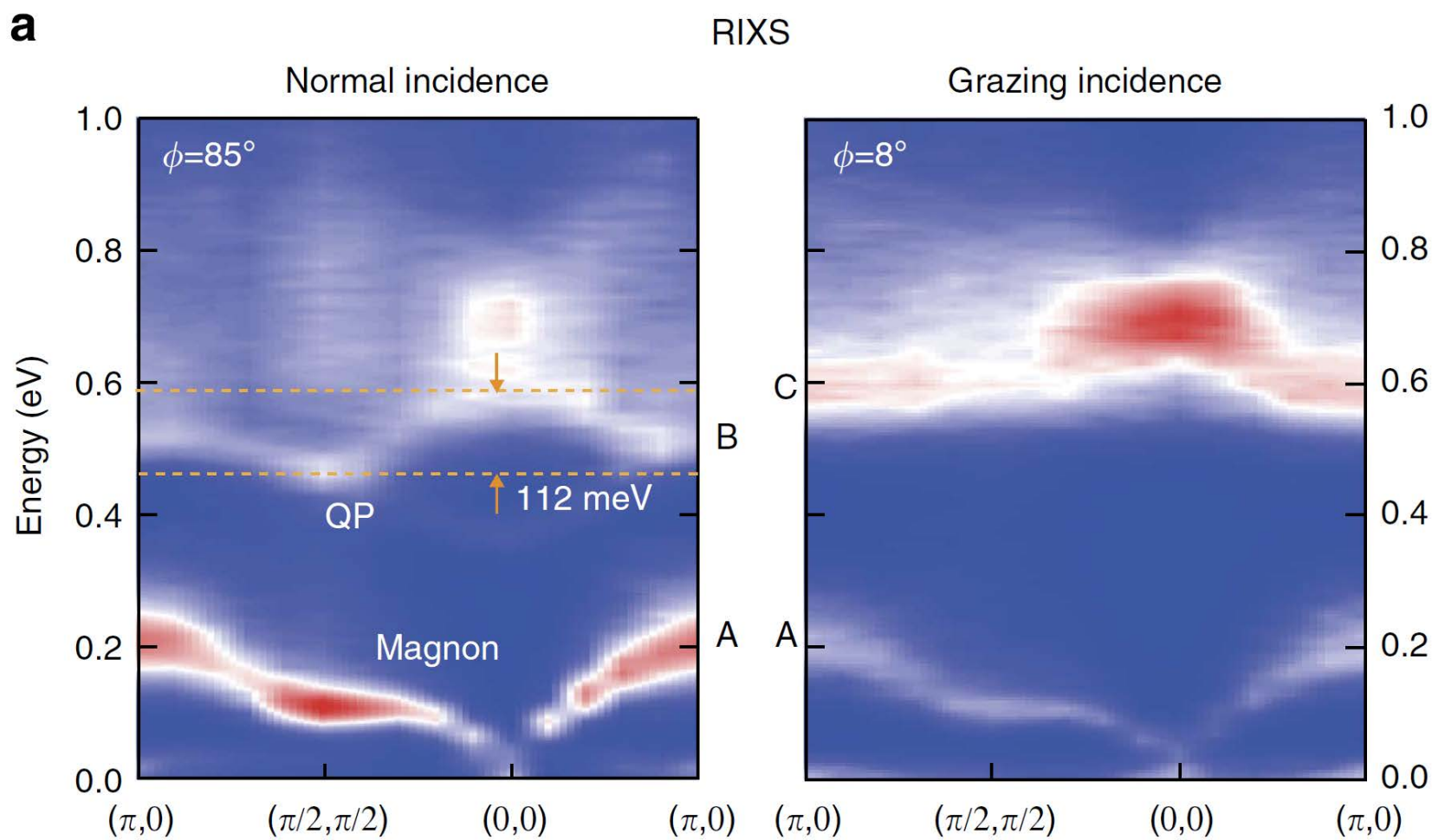




$$\frac{1}{\sqrt{3}}\left|xy,\uparrow\right\rangle+\frac{i}{\sqrt{3}}\left|xz,\downarrow\right\rangle+\frac{i}{\sqrt{3}}\left|yz,\downarrow\right\rangle$$



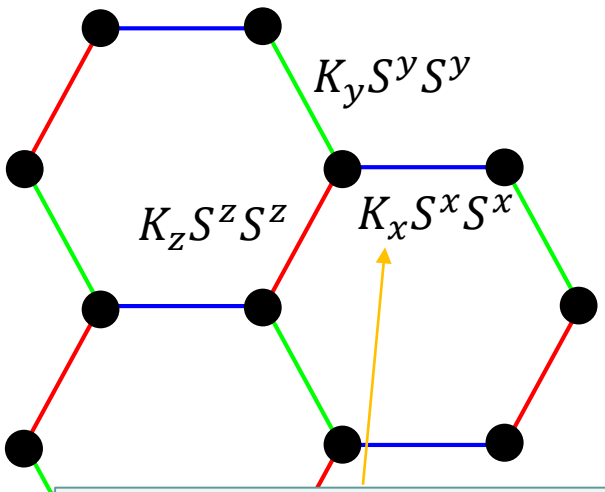
Sr_2IrO_4



Jungho Kim et al. Nature Communications, 2014

Kitaev's honeycomb model

Alexei Kitaev, Ann. Phys. 2006



Kitaev interaction
– bond dependent Ising interaction

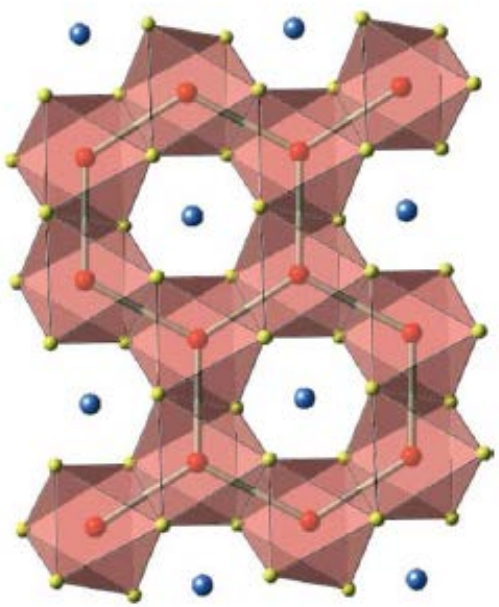
$$\mathcal{H}^{Kitaev} = -\sum_{i,\gamma} K_\gamma S_i^\gamma S_{i+\vec{e}_\gamma}^\gamma$$

- Exactly solvable model
- Ground state: Quantum Spin Liquid

Chaloupka, Jackeli and Khaliullin PRL 2010

- Proposed Honeycomb lattice of Ir^{4+} as a realization of Heisenberg-Kitaev model

$$\mathcal{H}_{ij}^{(\gamma)} = -J_1\ S_i^\gamma S_j^\gamma + J_2\ \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

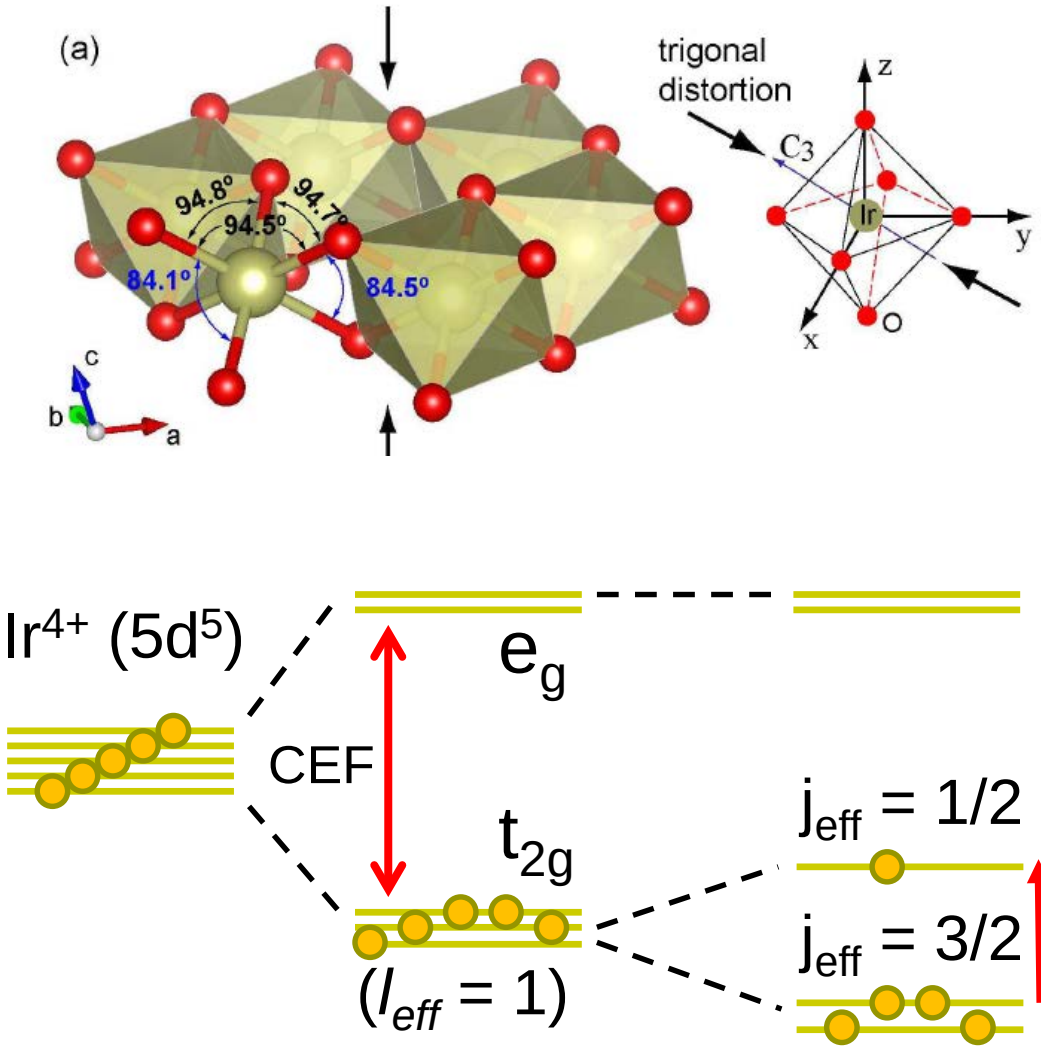


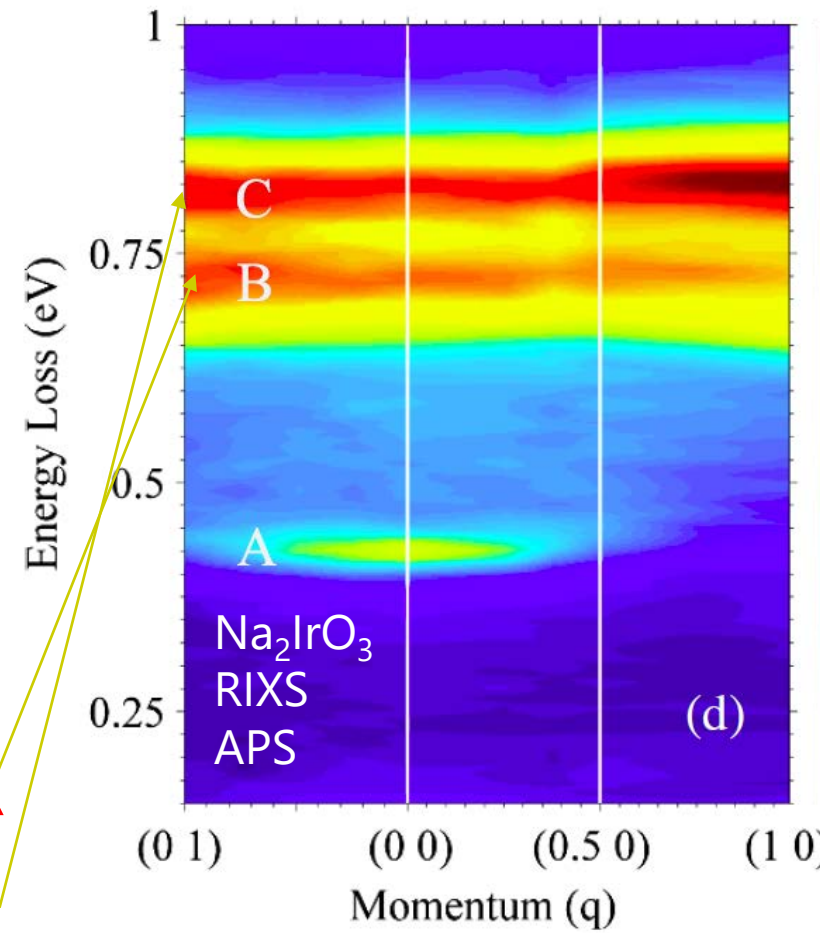
Na_2IrO_3

Yogesh Singh, P. Gegenwart PRB 2010

SOC too small?

F. Ye et al., PRB 85 180403 (2012)

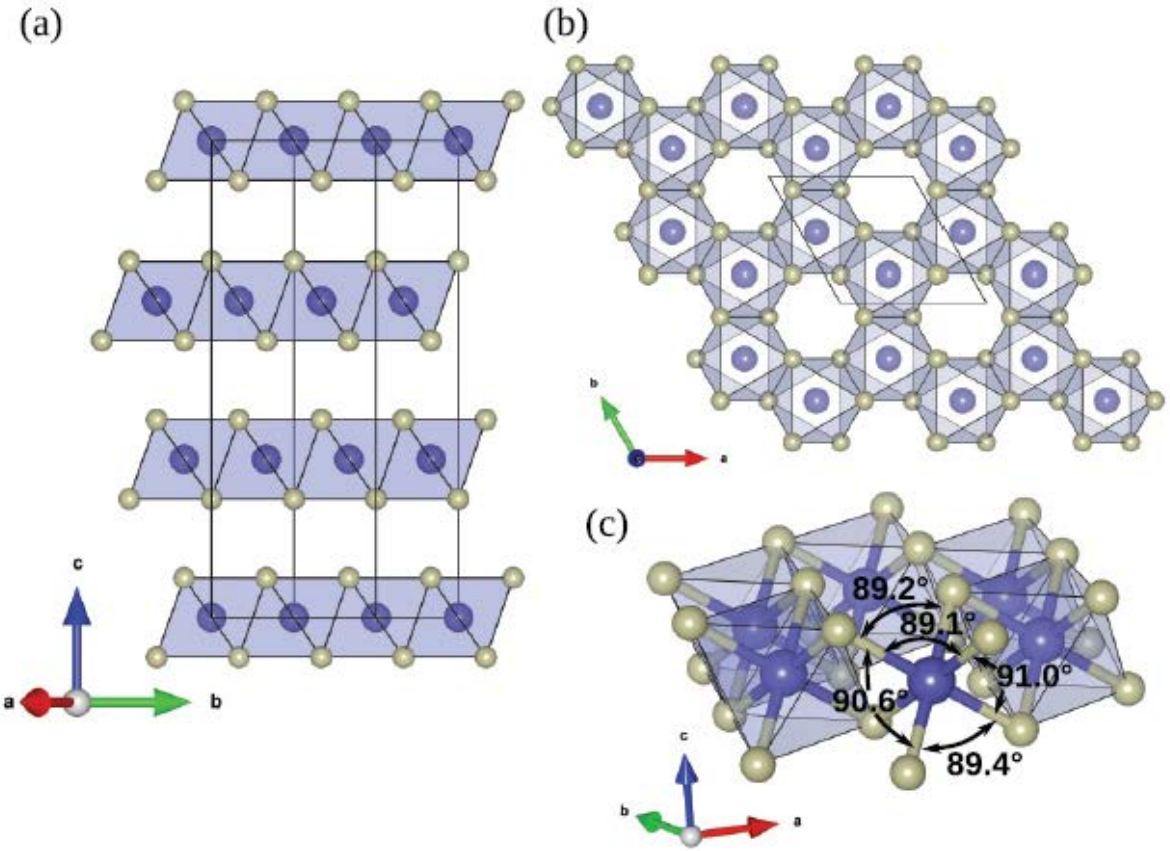


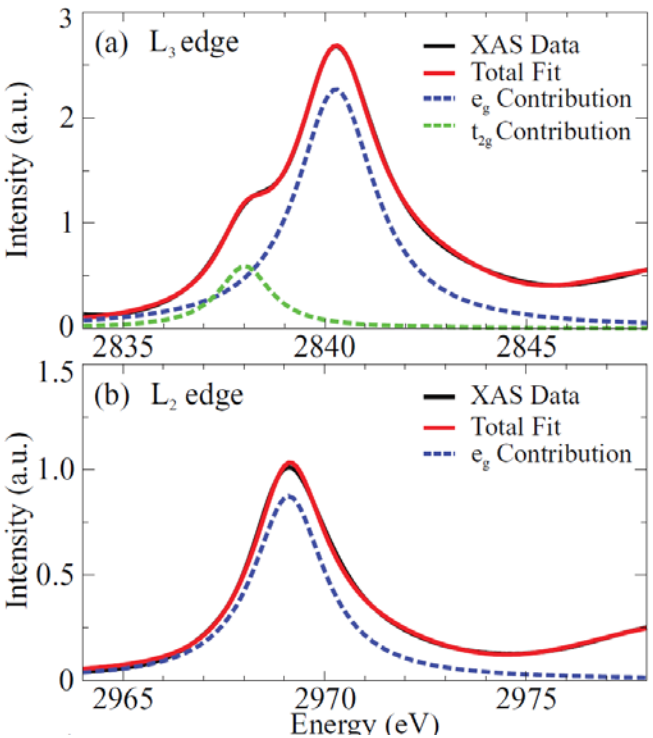


Gretarsson et al. PRL 2013

α-$RuCl_3$

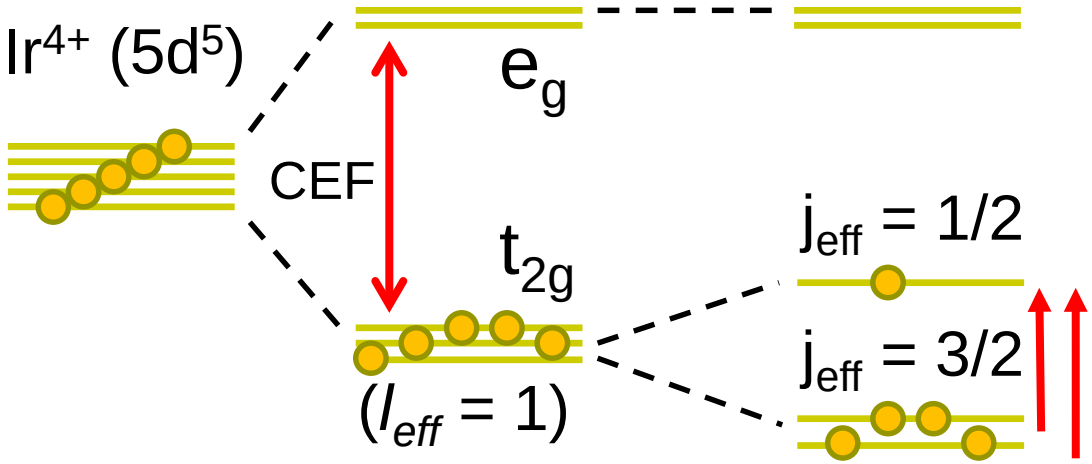
- Well-known semiconductor since 1960's.
- Used as a catalyst

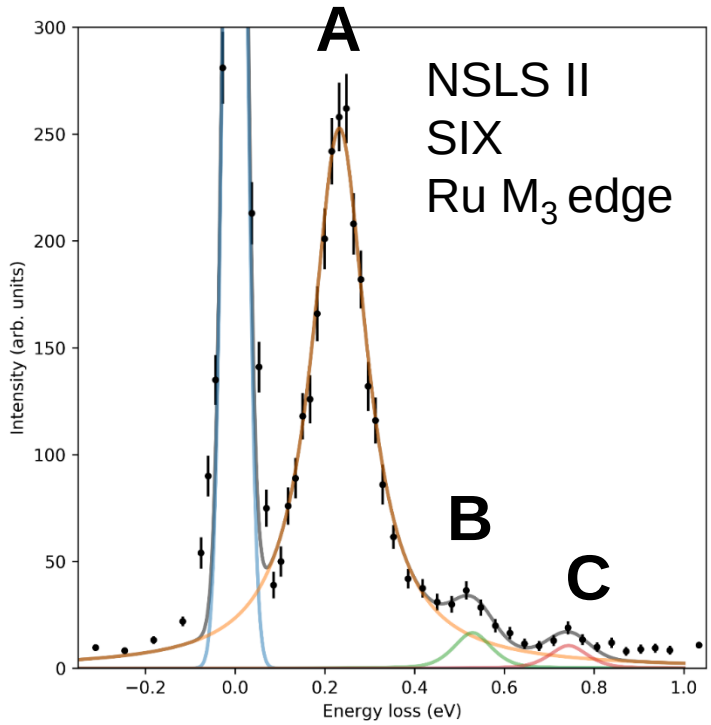




K. W. Plumb, et al., Phys. Rev. B 90, 041112 (2014)

Spin-Orbit exciton in α-$RuCl_3$





- Elastic FWHM = 50 meV
- SO excitation
  - FWHM = 150 meV
  - position = 230 meV

  → **λ ~ 150 meV**
- What about B and C?

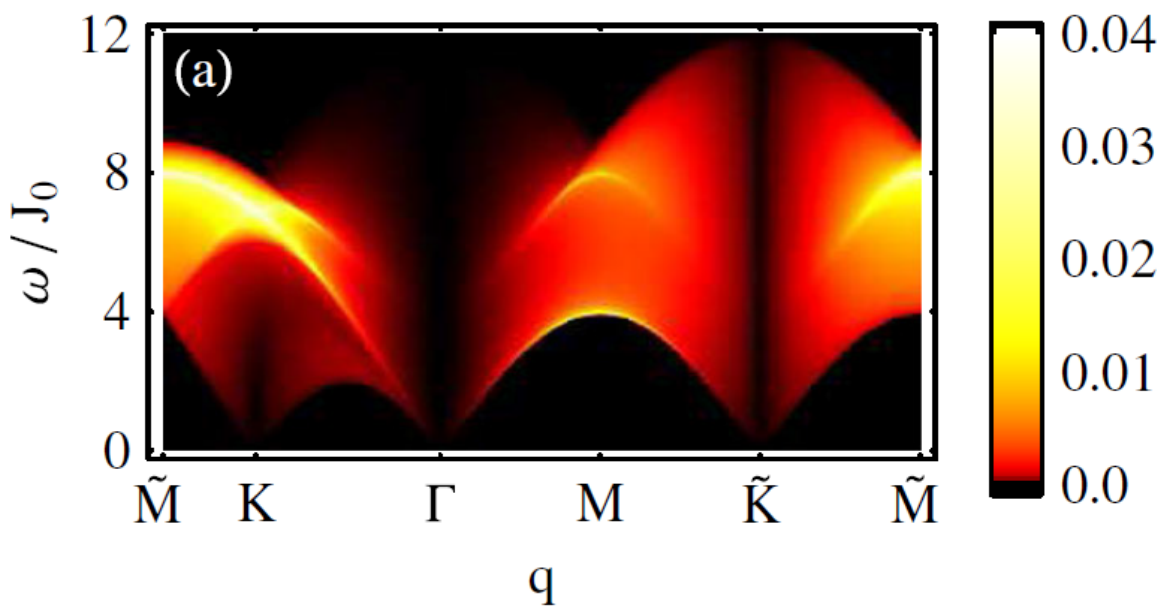
Details: Poster by B. Lebert PT-31

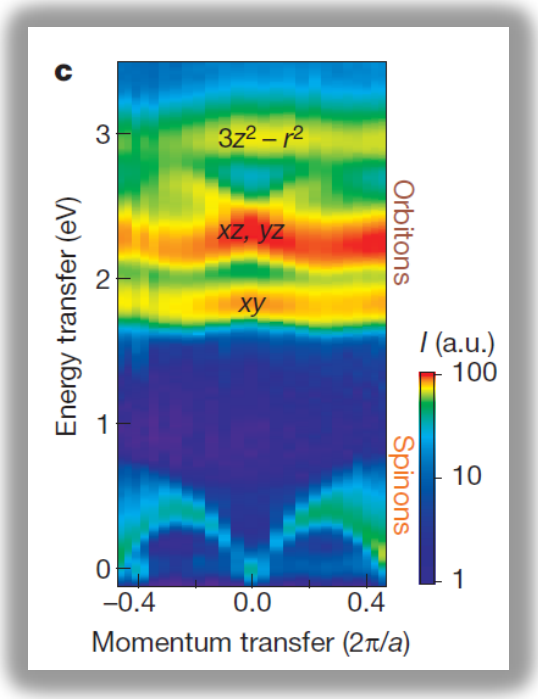
New fractional excitations

PRL **117,** 127203 (2016) PHYSICAL REVIEW LETTERS week ending 16 SEPTEMBER 2016

Resonant Inelastic X-Ray Scattering Response of the Kitaev Honeycomb Model

Gábor B. Halász,[1] Natalia B. Perkins,[2] and Jeroen van den Brink[3,4]





- RIXS couples to itinerant Majorana fermions (similar to Raman, but can measure dispersion

Future of RIXS

- New soft x-ray beamlines pushing the resolution limits
- Need to explore other elements and edges
- New sources: XFEL, Diffraction-limited storage rings
  - Time resolved RIXS
  - And beyond

nature materials

LETTERS

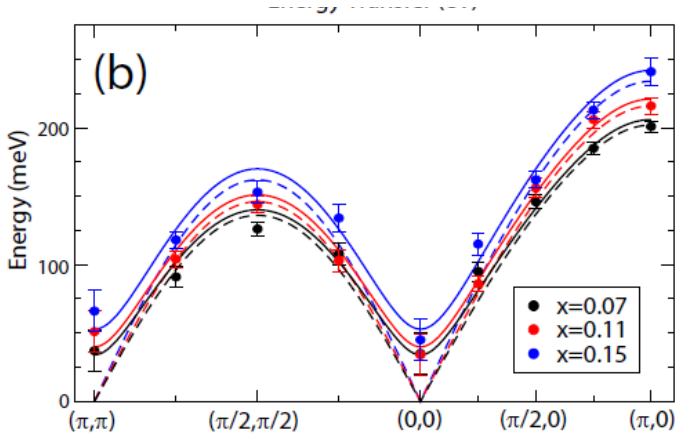
PUBLISHED ONLINE: 9 MAY 2016 | DOI: 10.1038/NMAT4641

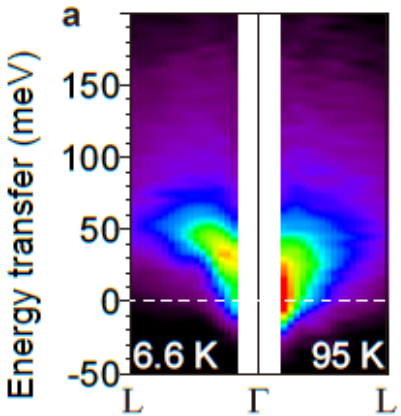
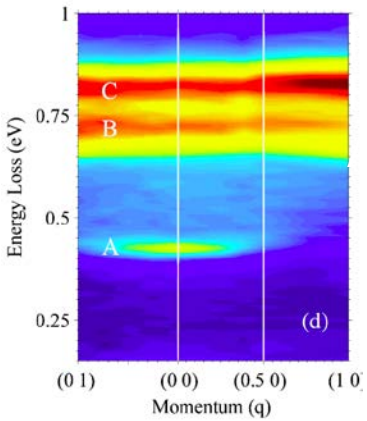
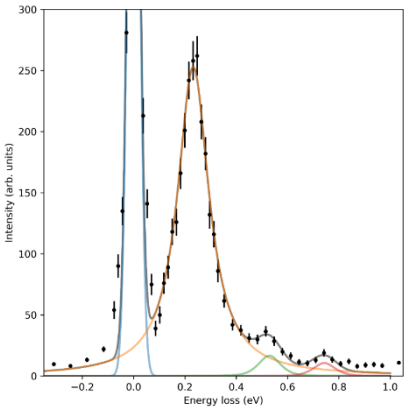
Ultrafast energy- and momentum-resolved dynamics of magnetic correlations in the photo-doped Mott insulator Sr_2IrO_4

M. P. M. Dean[1*†], Y. Cao[1*†], X. Liu[2,3*], S. Wall[4], D. Zhu[5], R. Mankowsky[6,7], V. Thampy[1], X. M. Chen[1], J. G. Vale[8], D. Casa[9], Jungho Kim[9], A. H. Said[9], P. Juhas[1], R. Alonso-Mori[5], J. M. Glownia[5], A. Robert[5], J. Robinson[5], M. Sikorski[5], S. Song[5], M. Kozina[5], H. Lemke[5], L. Patthey[10], S. Owada[11], T. Katayama[12], M. Yabashi[11], Yoshikazu Tanaka[11], T. Togashi[12], J. Liu[13], C. Rayan Serrao[14], B. J. Kim[15], L. Huber[16], C.-L. Chang[17], D. F. McMorrow[8], M. Först[6,7] and J. P. Hill[1]

Summary

- An exciting time for RIXS
- Many materials beyond cuprates are being investigated using RIXS, headed by iridates
- Magnons





- Orbital, dd, CEF excitations
  - Useful for identifying Kitaev materials