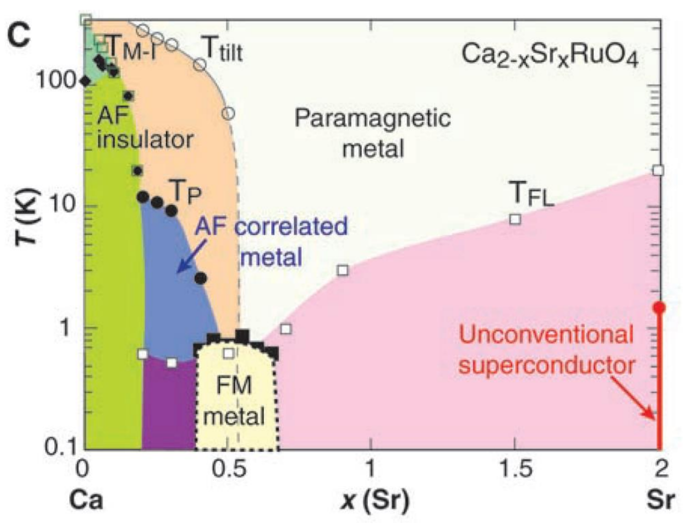
Comparative XAS and RIXS study of Ca_2RuO_4 and $Ca_3Ru_2O_7$

K. von Arx[1], M. Horio[1], Q. Wang[1], L. Das[1], F. Forte[2,3], R. Fittipaldi[2,3], C.G. Fatuzzo[4], V. Granata[2,3], O. Ivashko[1], F. Schindler[1], M. Dantz[5], Y. Tseng[5], D. McNally[5], E. Paris[5], H.M. Rønnow[4], W. Wan[6], N.B. Christensen[6], J. Pelliciari[5], P. Olalde-Velasco[5], N. Kikugawa[7,8], T. Neupert[1], A. Vecchione[2,3], T. Schmitt[5], M. Cuoco[2,3], J. Chang[1]

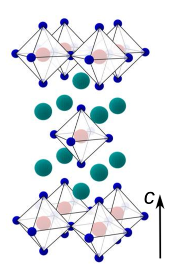
1 University of Zurich — 2 CNR SPIN — 3 Università degli Studi di Salerno — 4 EPFL École Polytechnique Fédérale de Lausanne — 5 Paul Scherrer Institut PSI — 6 DTU Technical University of Denmark — 7 NIMS — 8 National High Magnetic Field Laboratory

Ruthenates



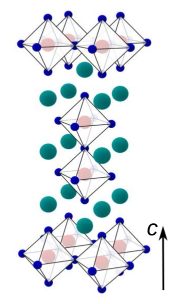
Dagotto, Science **309**, 257 (2005)

Ca_2RuO_4



T
- T_S = 356 K
- Mott insulator
- T_N = 110 K
- G-AFM insulator

$Ca_3Ru_2O_7$

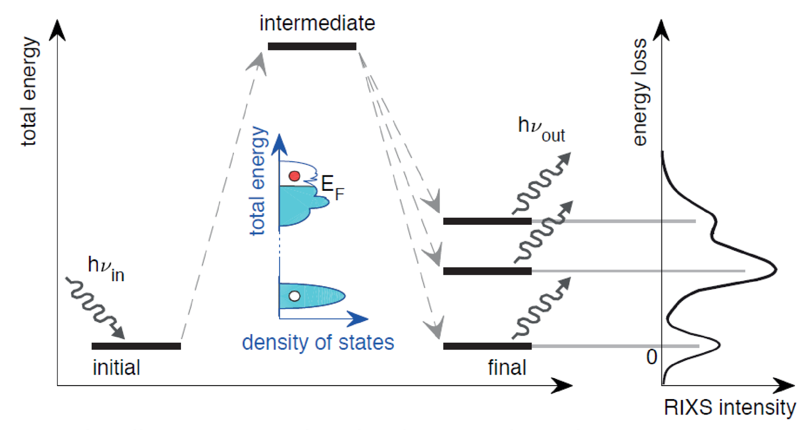


T
- T_N = 56K
- A-AFM metal
- T_S = 48 K
- A-AFM semimetal

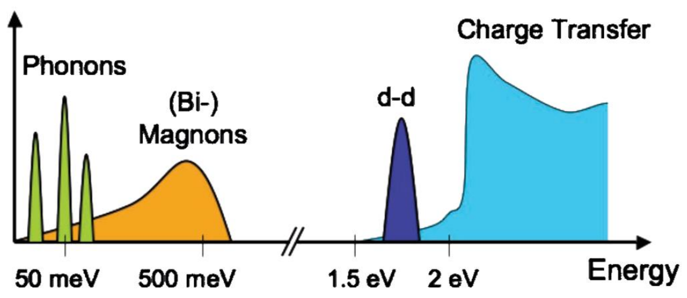
Chemical doping and structural differences lead to a dramatic change of electronic and magnetic properties. How do the structural differences in single- and bilayer ruthenates effect the low lying excitations?

RIXS

Resonant **I**nelastic **X**-ray **S**cattering



Claudia Fatuzzo, PhD thesis, UZH (2017)

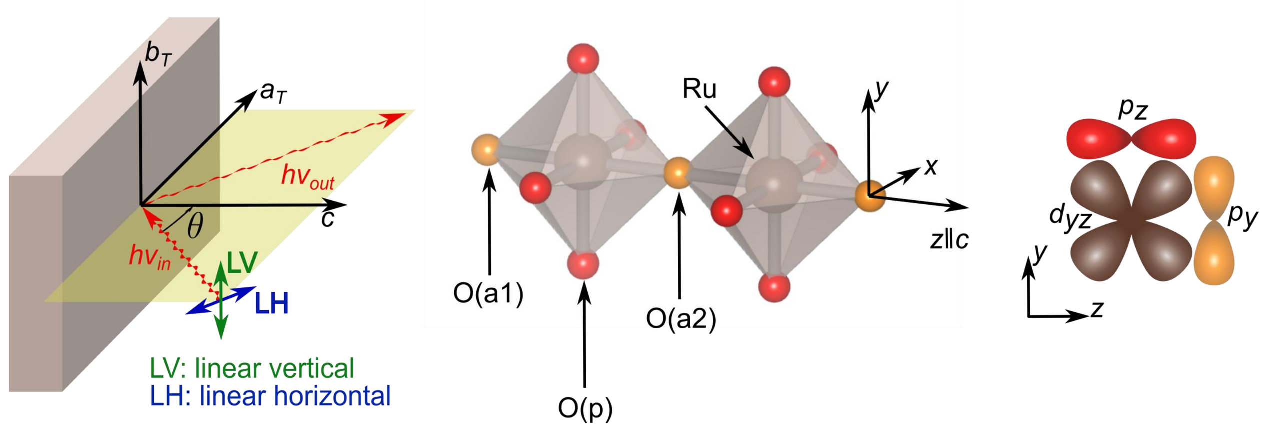


Ament *et al.*, Rev. Mod. Phys. **83**, 705 (2011)

Results

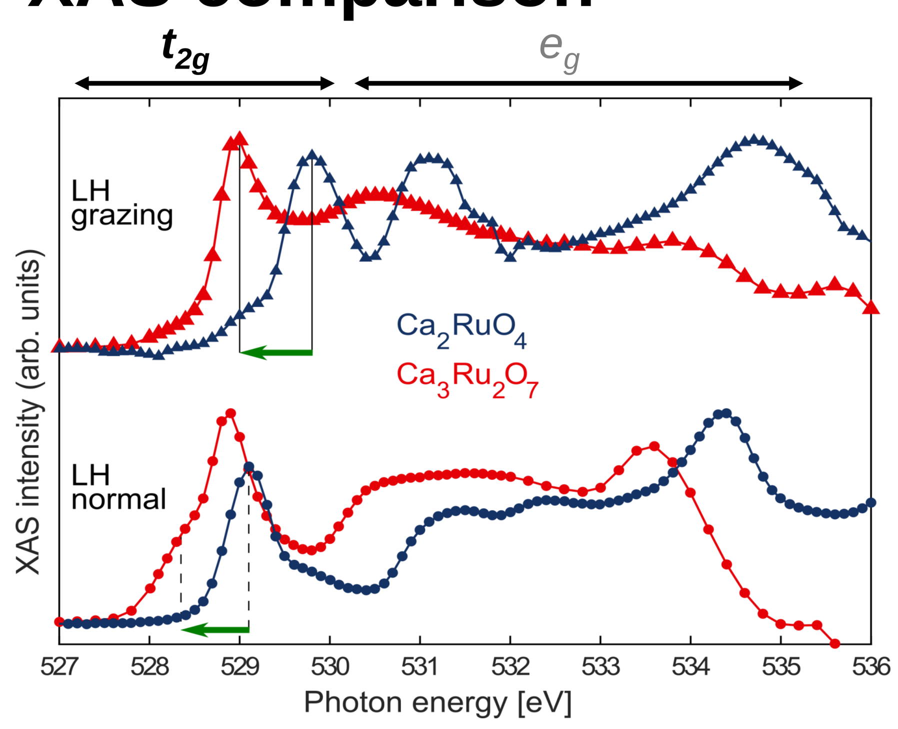
Orbital selectivity

Oxygen *K*-edge measurements: Ru *d* orbitals are accessed indirectly through their hybridization with O *p* orbitals. This leads to an experimental geometry dependent orbital selectivity.



		Apical O(a)	Planar O(p)
LH normal	p_x	d_{xz}	d_{xy} $d_{x^2-y^2}$
LH grazing	P_z	d_{z^2}	d_{xz} d_{yz}
LV	p_y	d_{yz}	d_{xy} $d_{x^2-y^2}$

XAS comparison



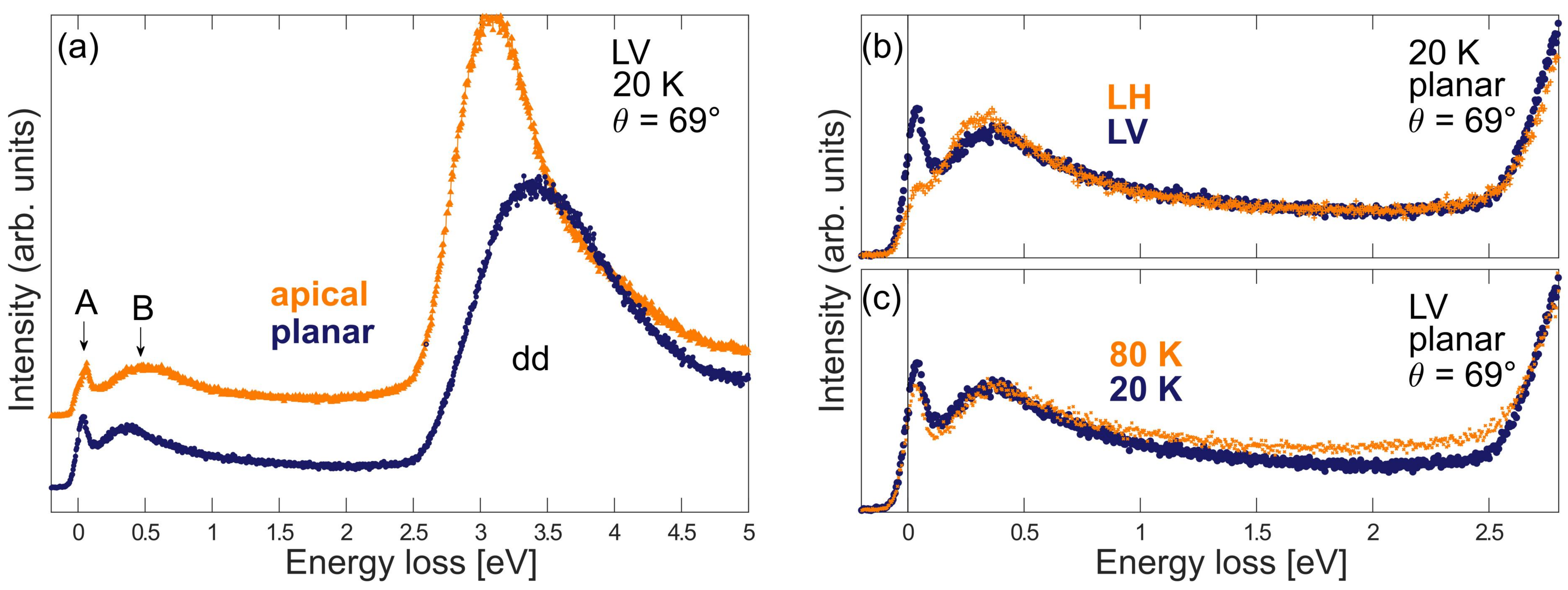
planar resonance

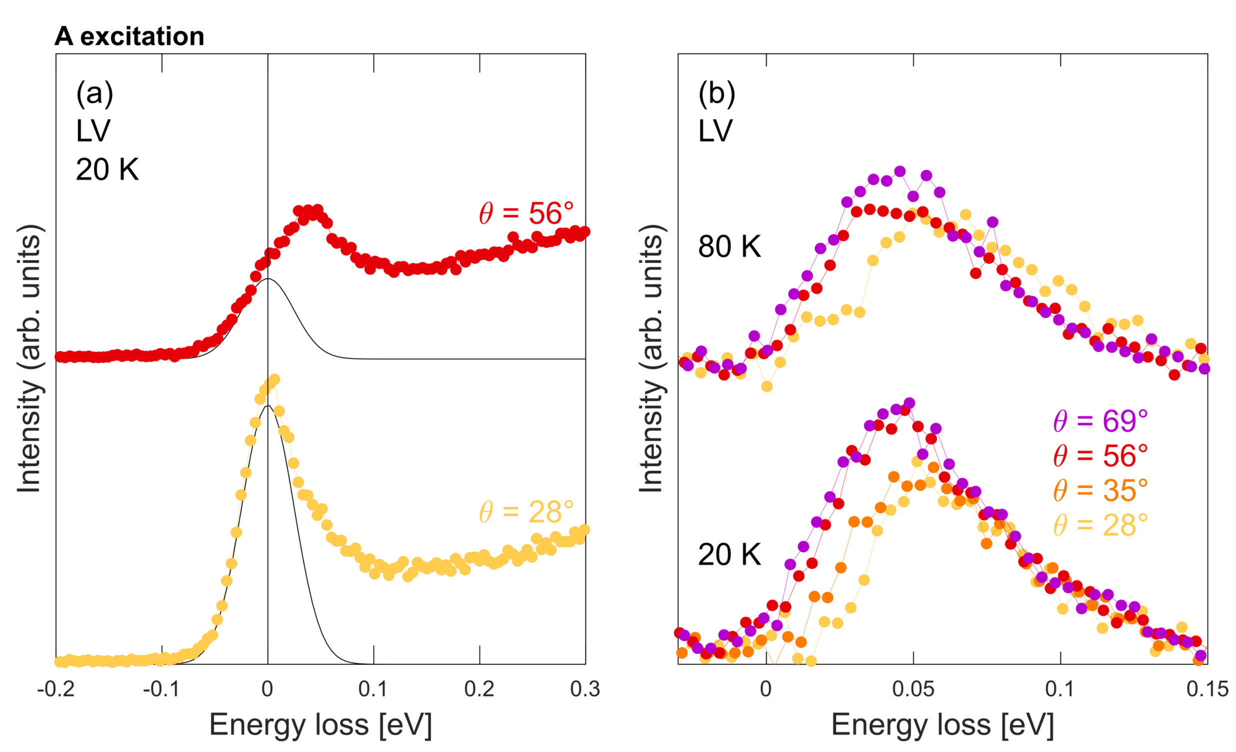
apical resonance

$Ca_3Ru_2O_7$: Inner apical O(a2) and planar O(p) resonances are very close in energy and give rise to one intense peak.

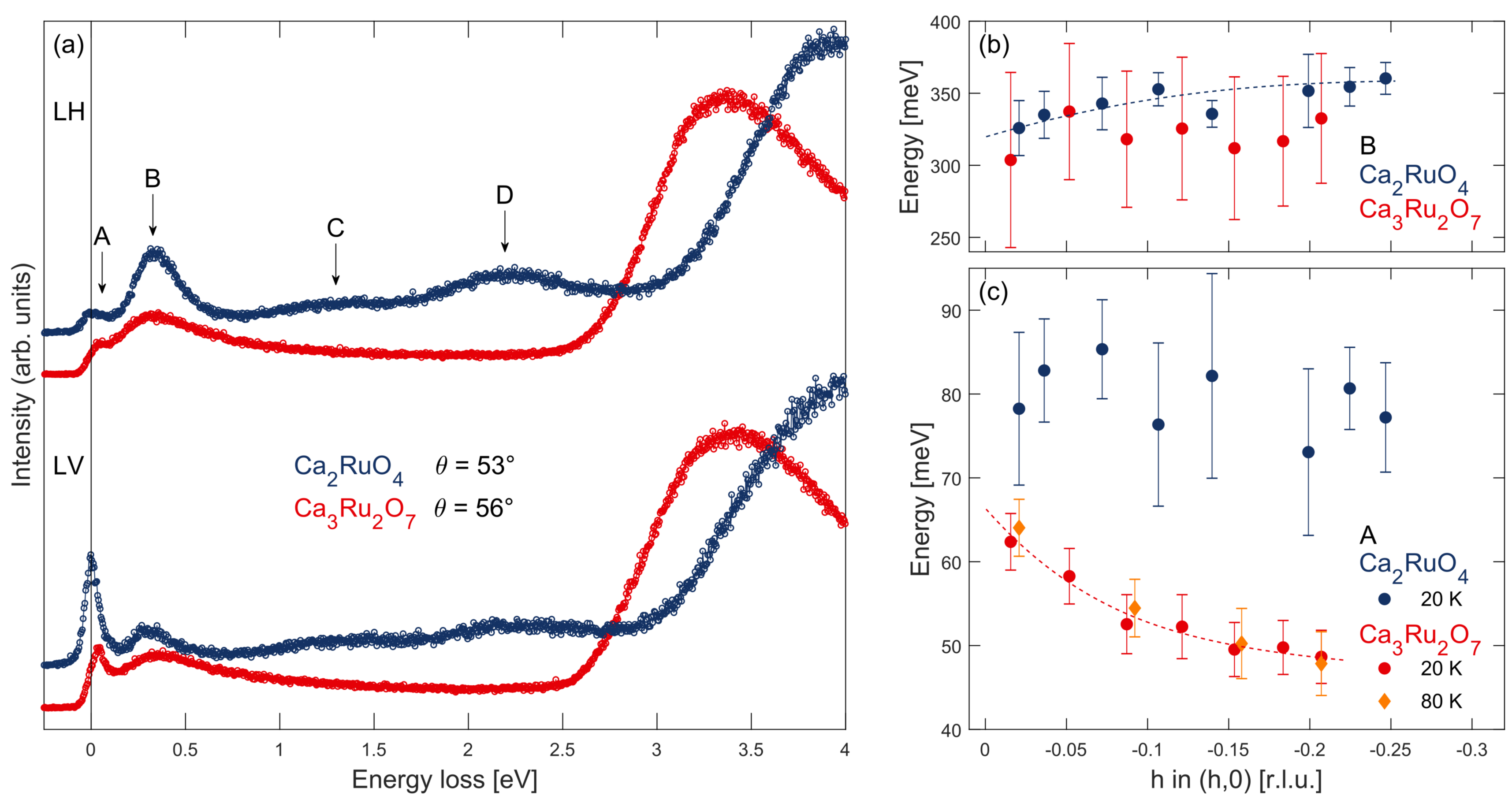
→ in both compounds: apical O(a1) – planar O(p) resonance separation is 0.7 eV.

RIXS spectra of $Ca_3Ru_2O_7$





RIXS spectra and momentum dependence



Summary

- Direct comparison of two closely related ruthenates
- Identification of planar and apical O *p* – Ru t_{2g} resonances
- Two low-energy excitations C and D related to intra-atomic singlet-triplet excitations[1] in Ca_2RuO_4 are completely absent in $Ca_3Ru_2O_7$
- Collective orbital excitation A found in $Ca_3Ru_2O_7$

[1] Das *et al.*, PRX **8**, 011048 (2018)