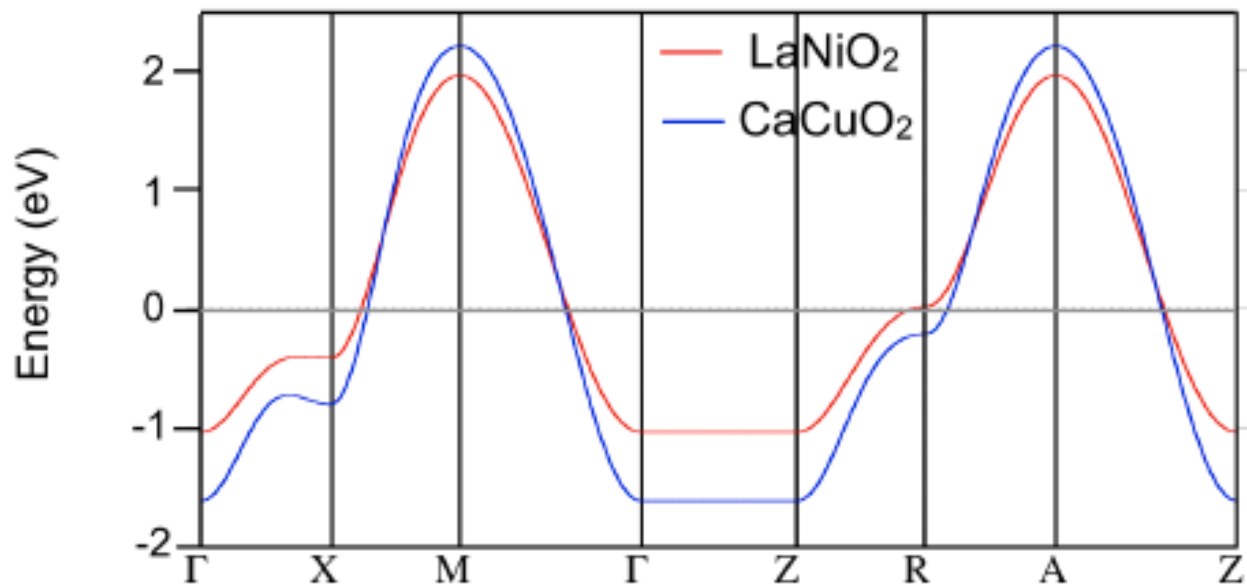
Superconductivity in Nickelates:
Similarities and Differences from Cuprates

Michael Norman
Materials Science Division – Argonne National Lab

Antia Botana
(Arizona State)

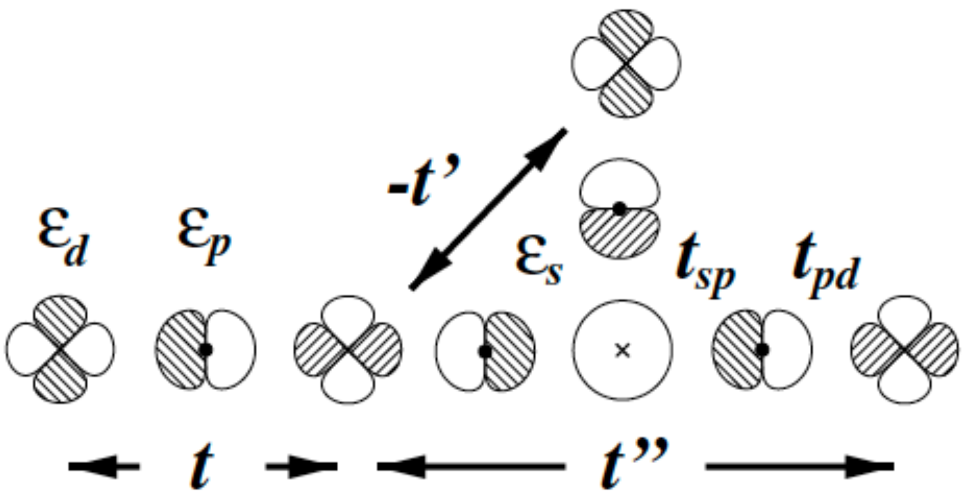
John Mitchell
(ANL)

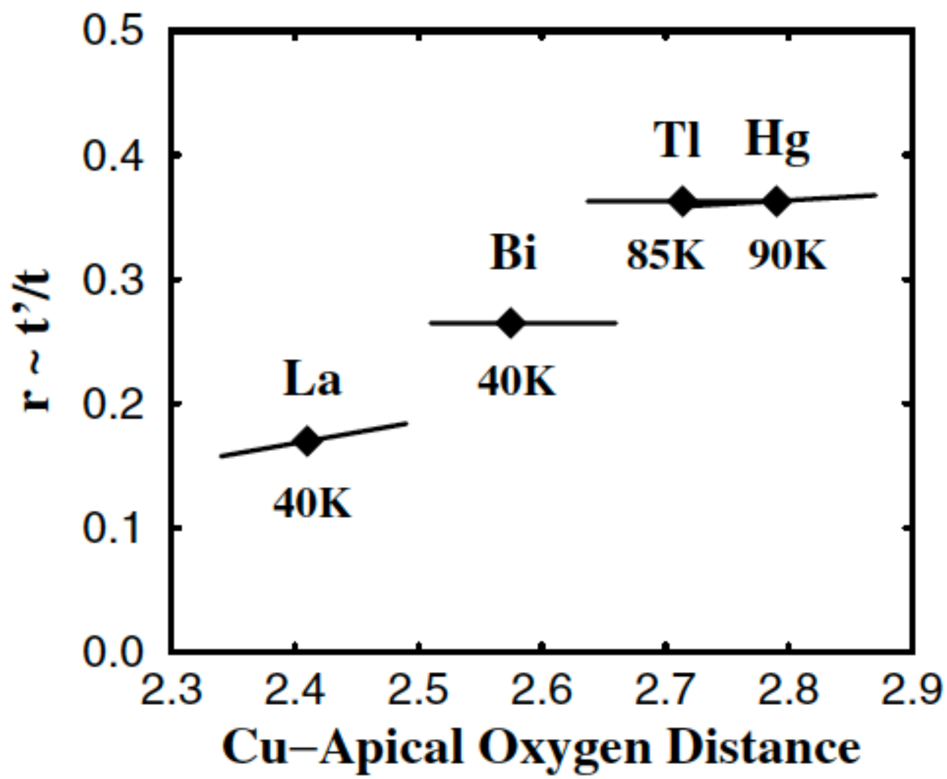


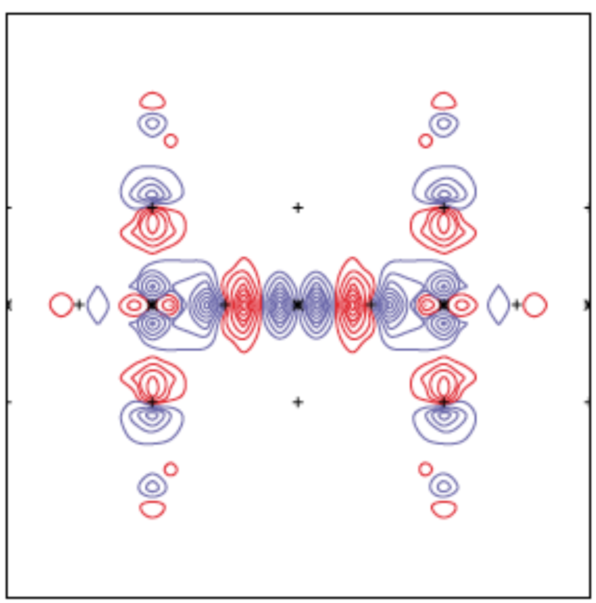
BNL – Nov. 3, 2019

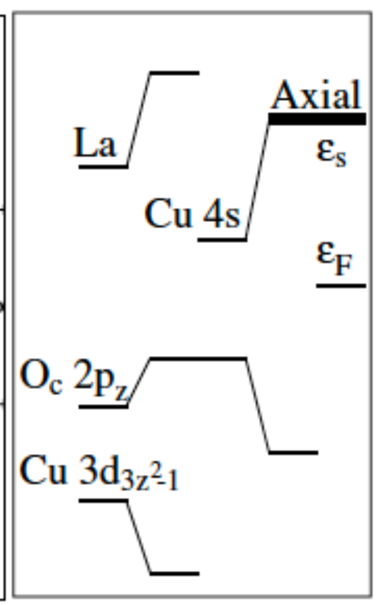
Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\,\max}$

E. Pavarini, I. Dasgupta,* T. Saha-Dasgupta,† O. Jepsen, and O. K. Andersen



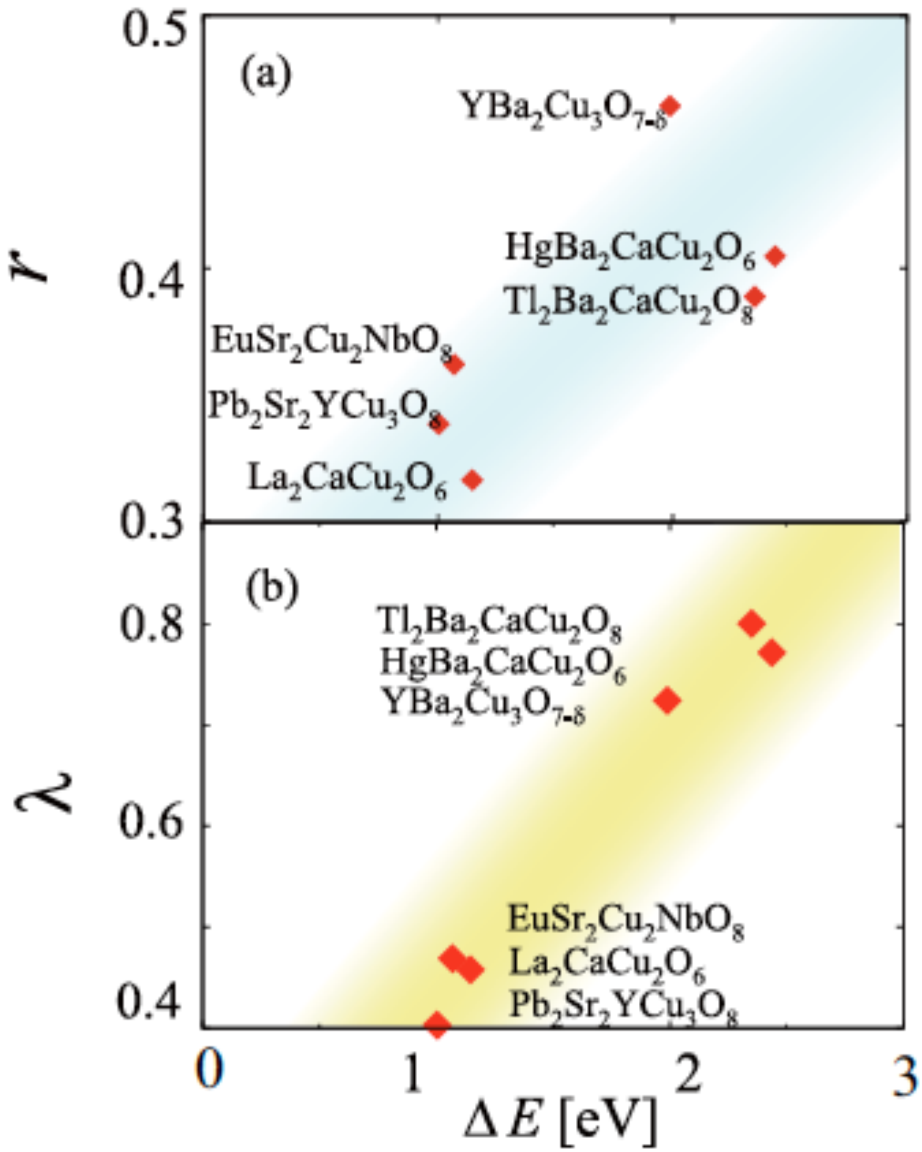






Pavarini *et al*, PRL 87, 047003 (2001)

Variation of Longer Range Hopping & T_c with Jahn-Teller splitting



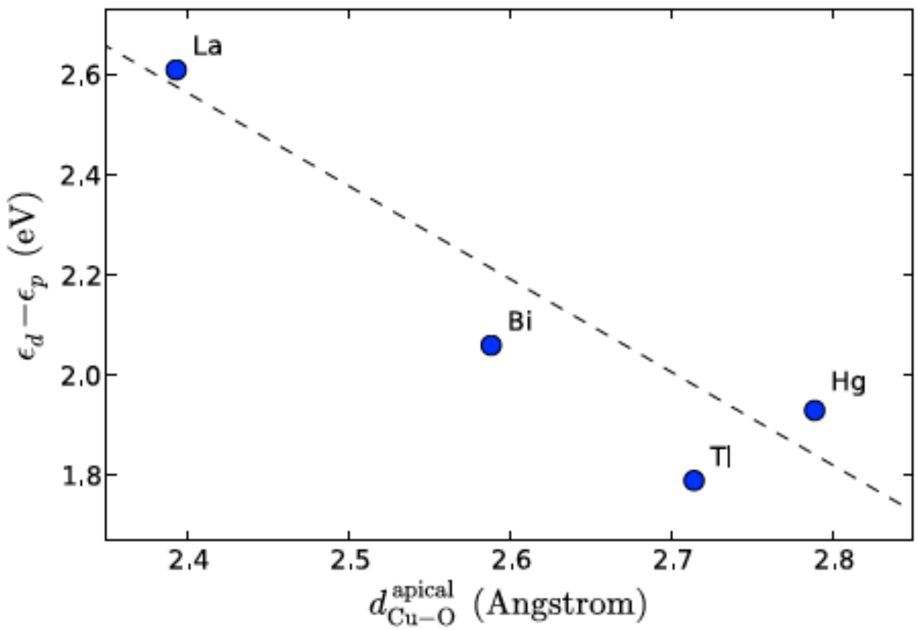
$r = (|t_2| + |t_3|)/|t_1|$

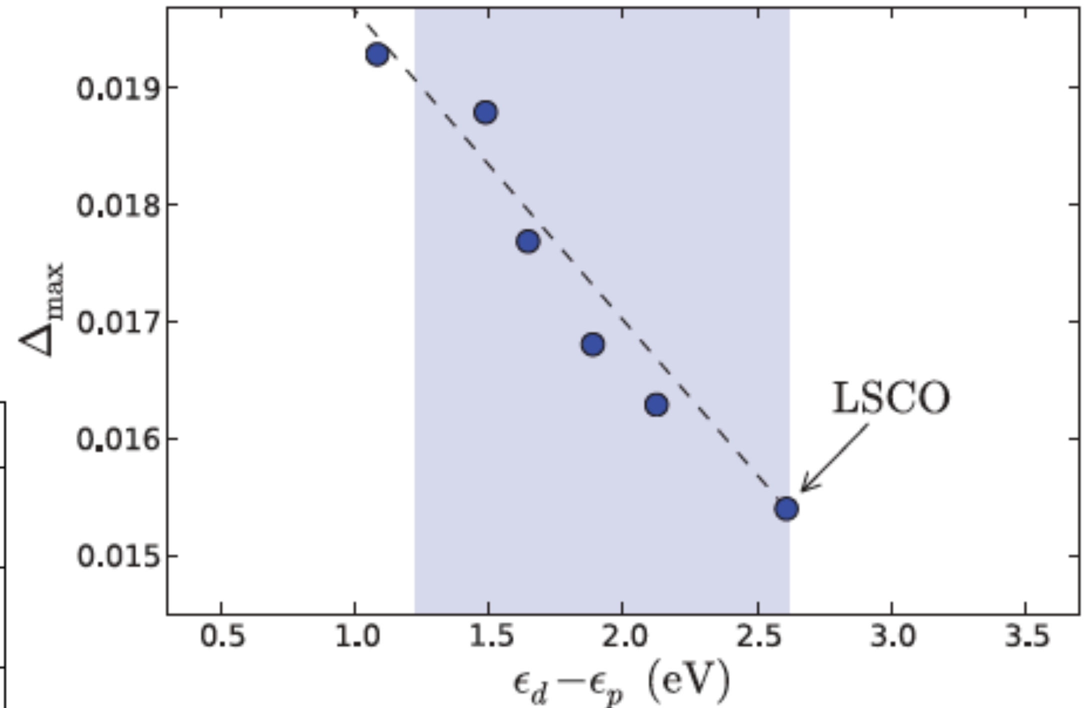
λ - BCS coupling constant

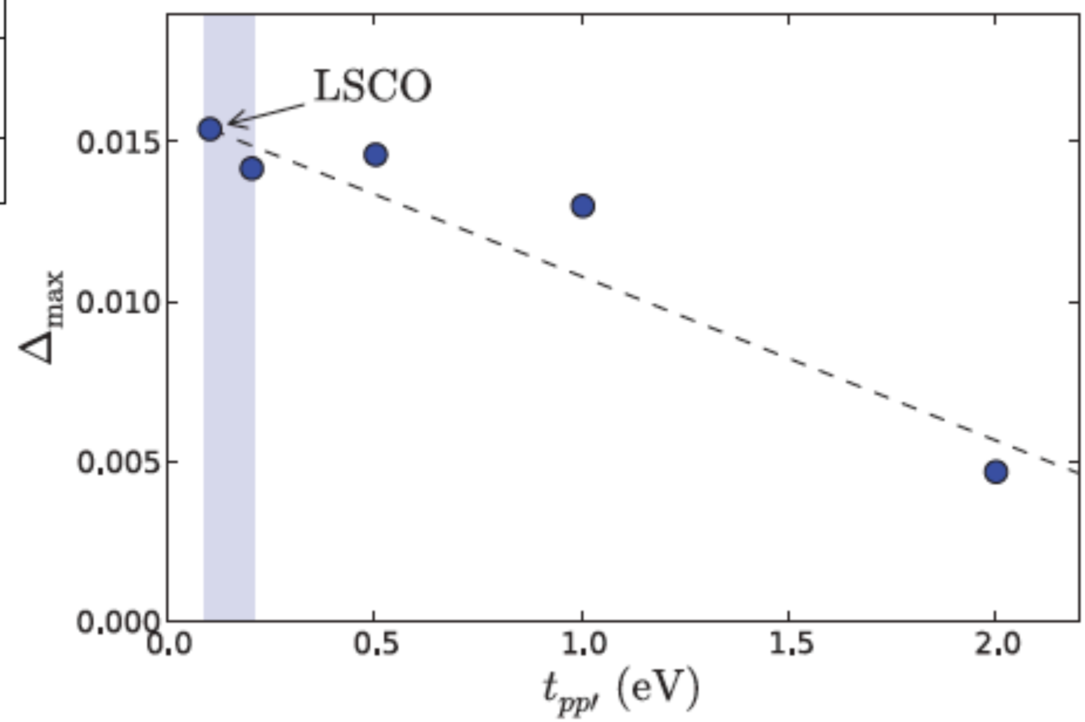
$\varepsilon_{x2-y2} - \varepsilon_{3z2-r2}$

Sakakibara *et al*
PRL (2010), PRB (2012, 2014)

T_c vs ε_{3d}-ε_{2p}
(charge transfer energy)



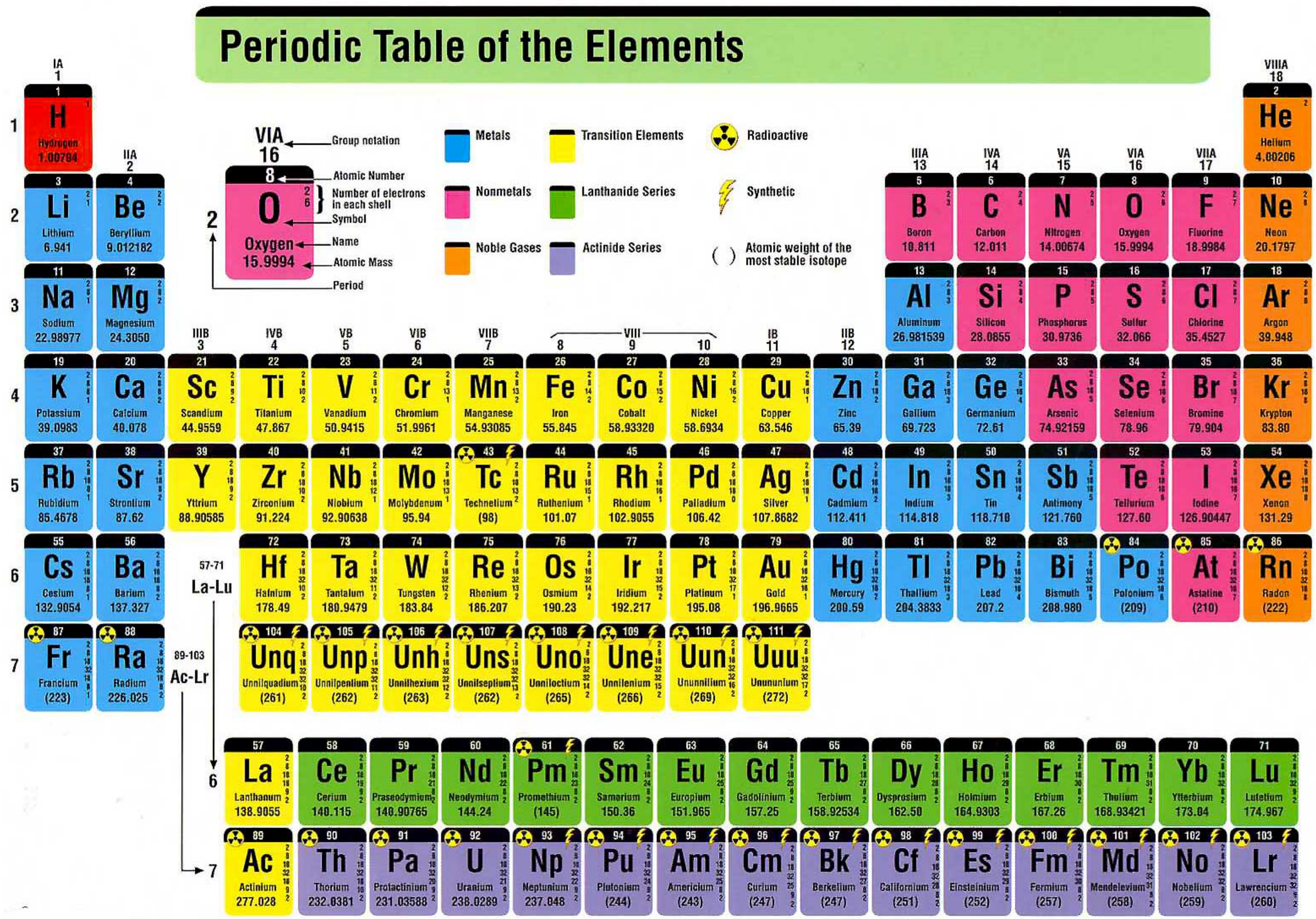




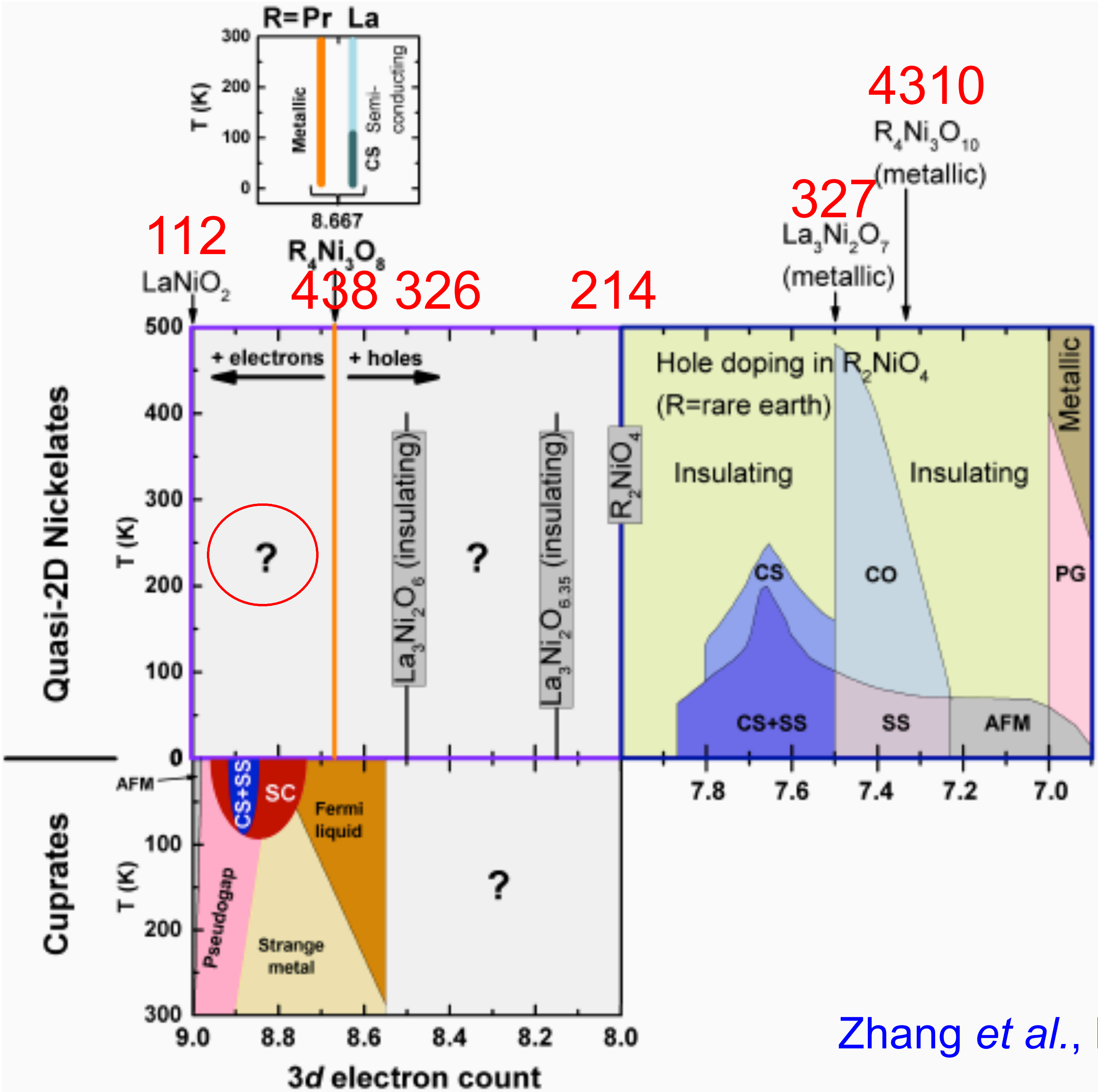
Weber *et al*, EPL (2012)

Looking for Cuprate Analogues

Yellow – the “metal”, Red – the “ligand”, Blue, Green – the “spacer”

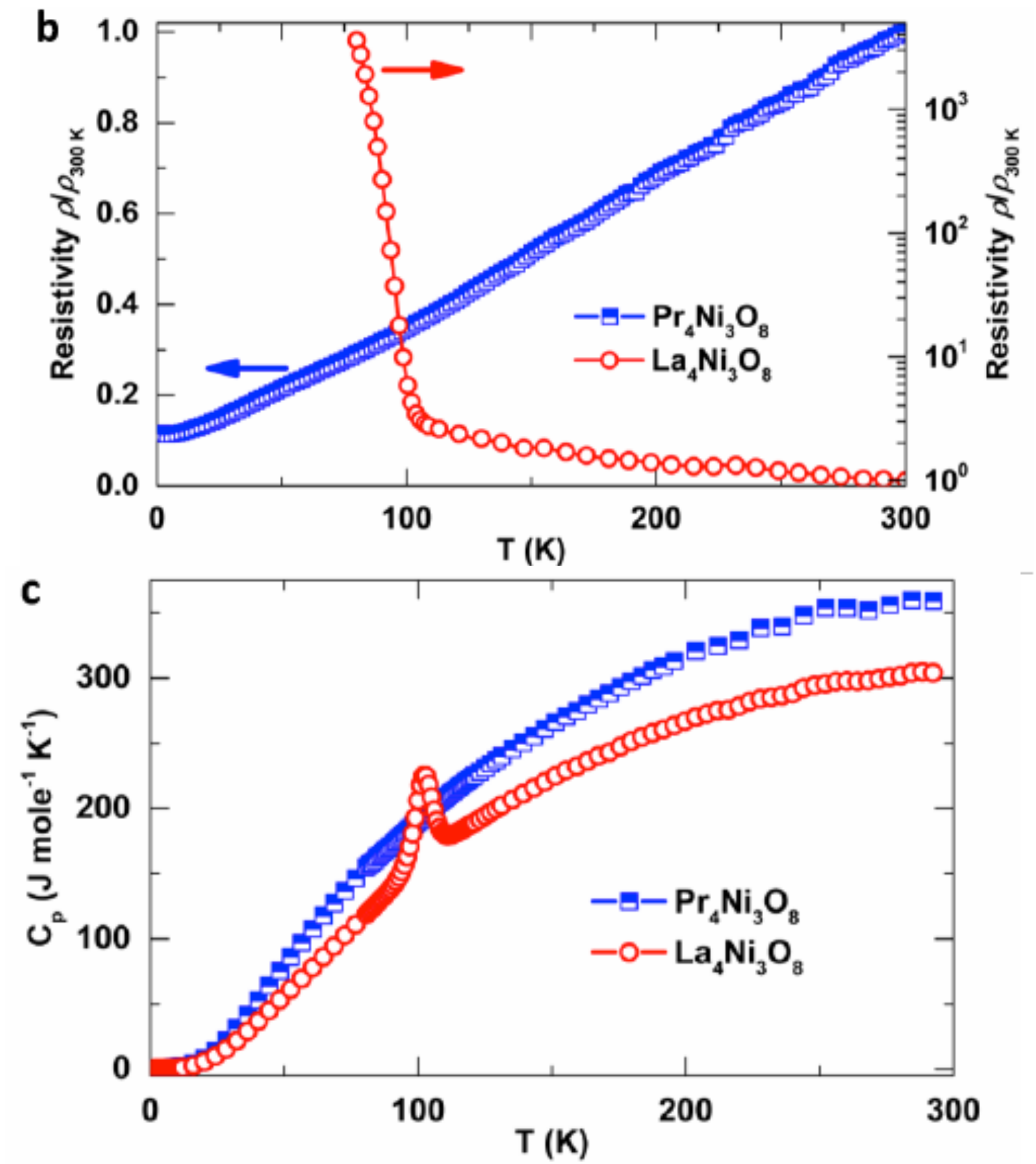


Ni-438 Phase Diagram as compared to Ni-214 and cuprates
Will electron doping create a superconductor?



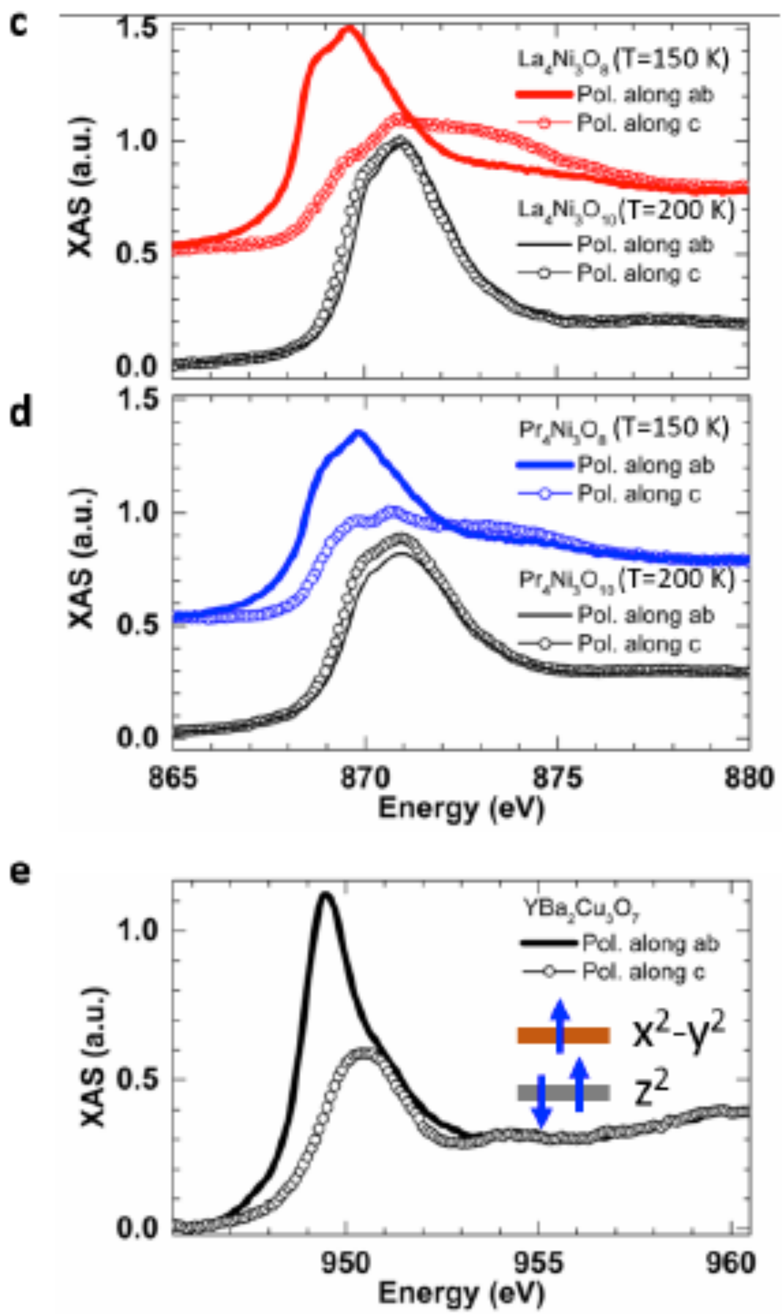
Zhang *et al.*, Nature Phys (2017)

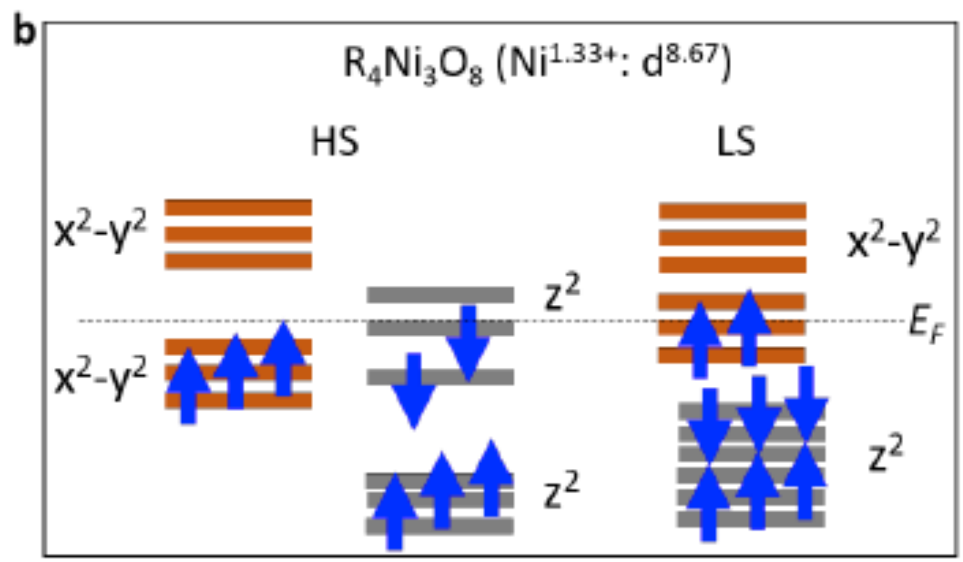
La-438 is a stripe insulator but Pr-438 is a metal



Zhang *et al.*, Nature Phys (2017)

438 (La, Pr) – orbital polarization similar to cuprates (low spin state)

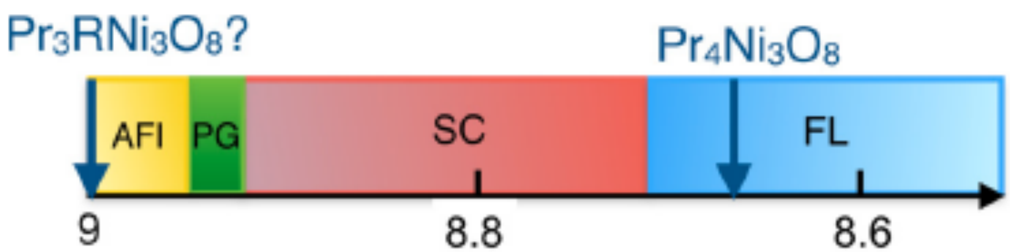


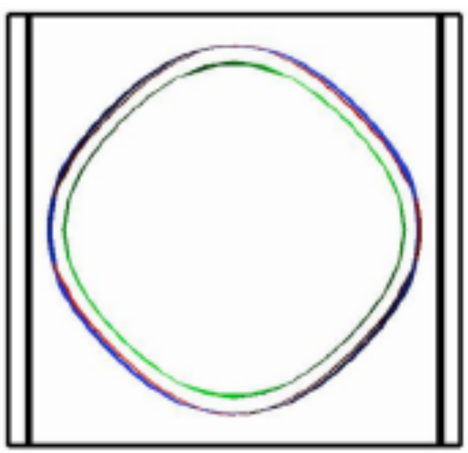


Zhang *et al.*, Nature Phys (2017)

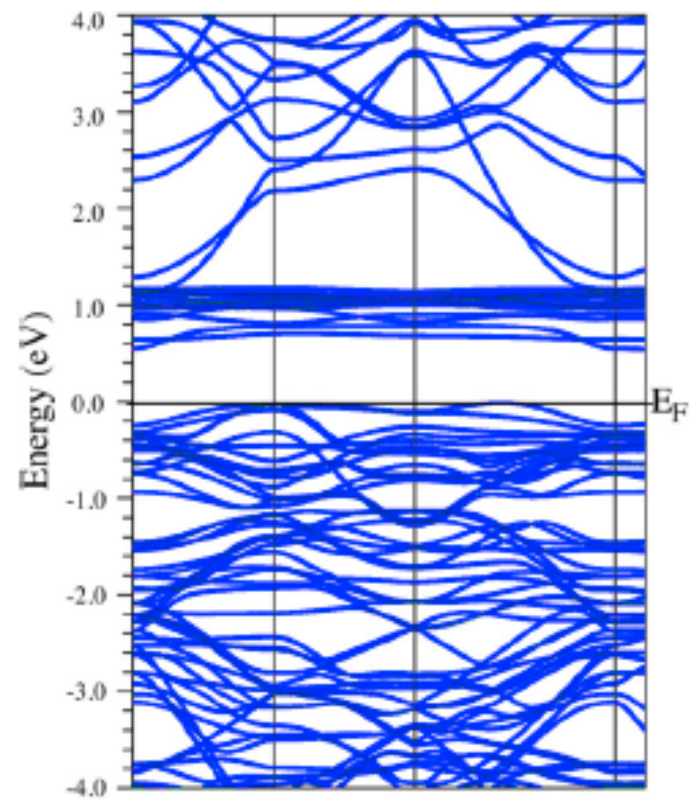
Pr438 corresponds to a 1/3 hole doped cuprate
Could doping with Ce^{4+} create a superconductor?

LDA predicts that Ce will go in as 4+
(as well as Te, Th, and Zr)





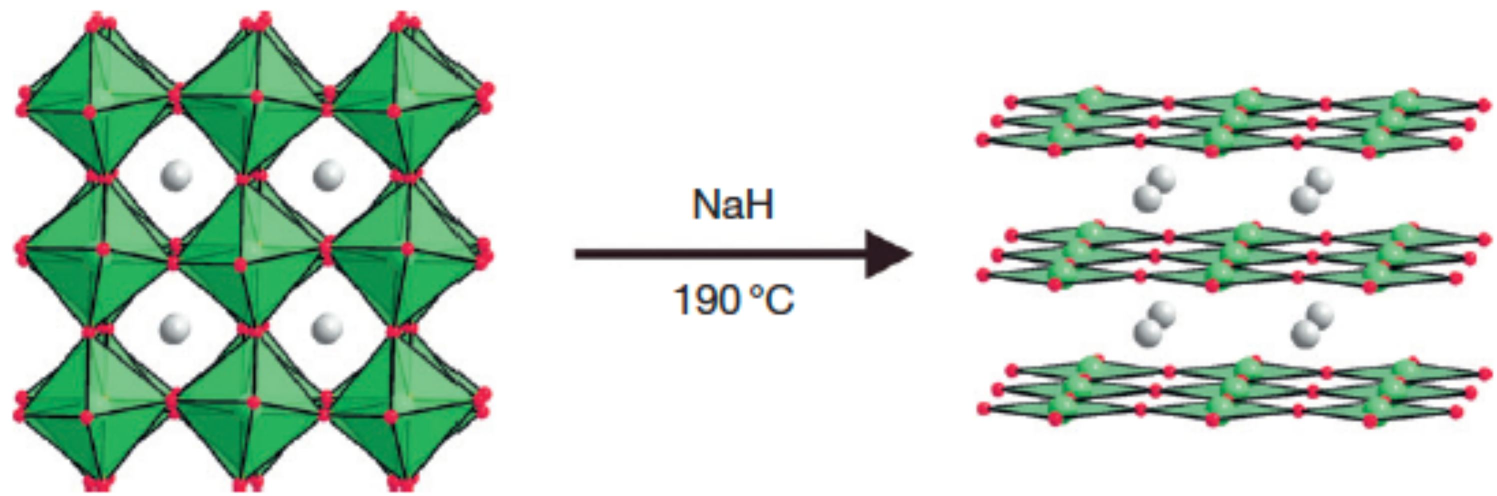
Fermi surface
for 1/6 e^- doped Pr438

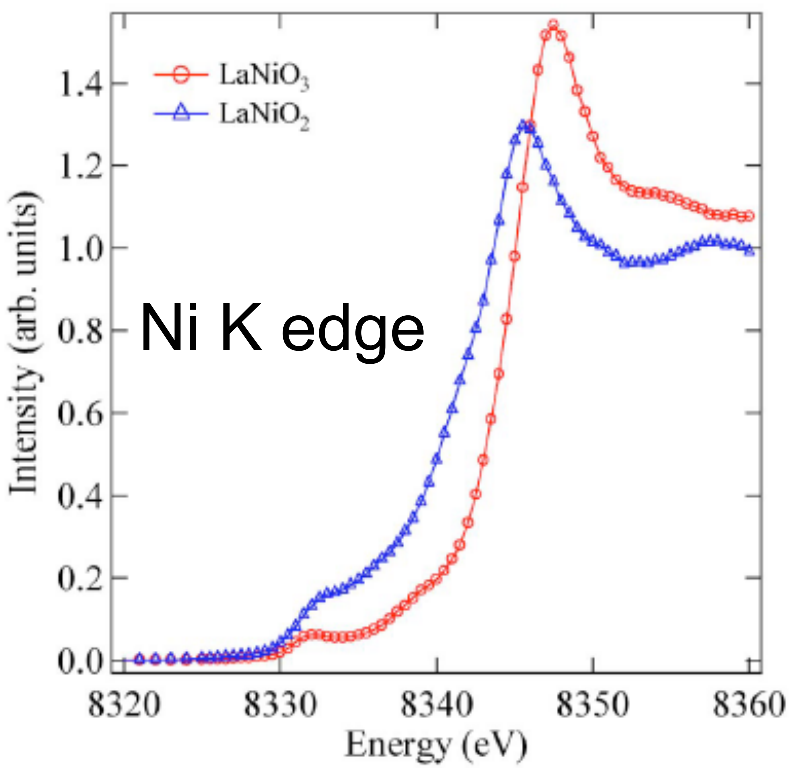


$CePr_3Ni_3O_8$ should
be an AF insulator

Botana, Pardo, Norman, PR Materials (2017)

Infinite Layer Nickelates (Ni^{+} is in a d^9 configuration)



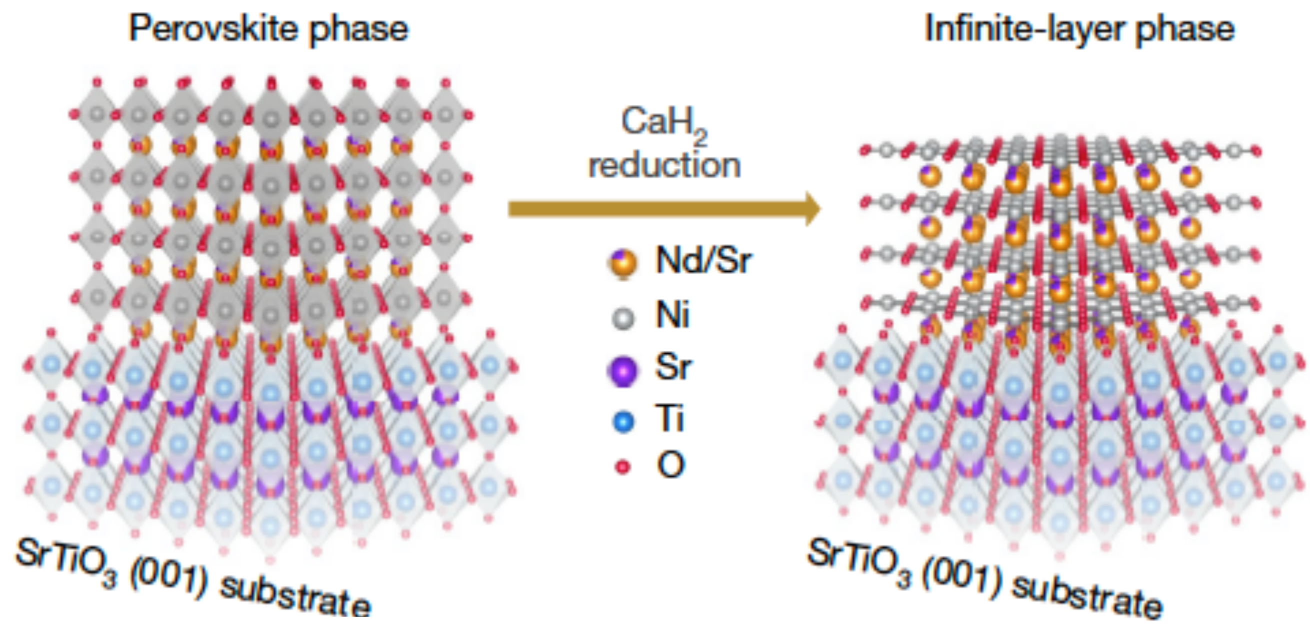


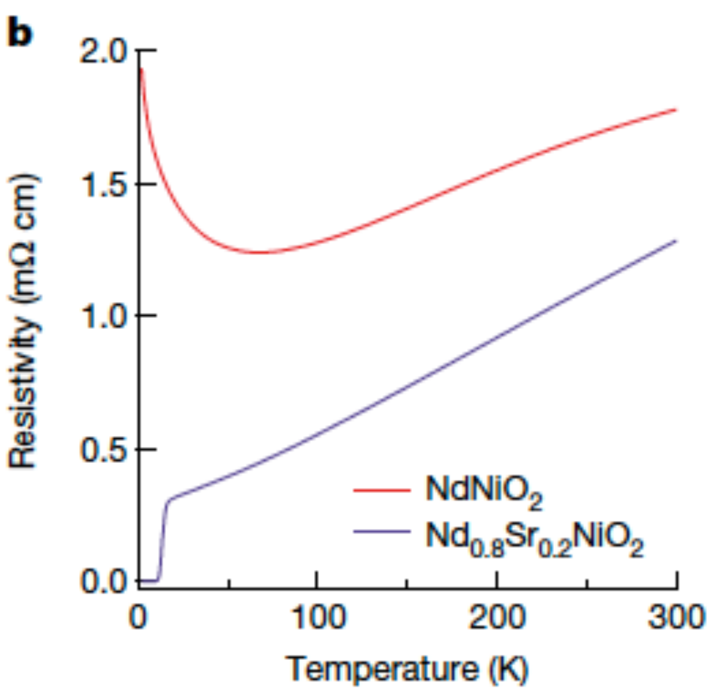
RP: $R_{n+1}Ni_nO_{3n+1}$ – $Ni^{(3-1/n)+}$

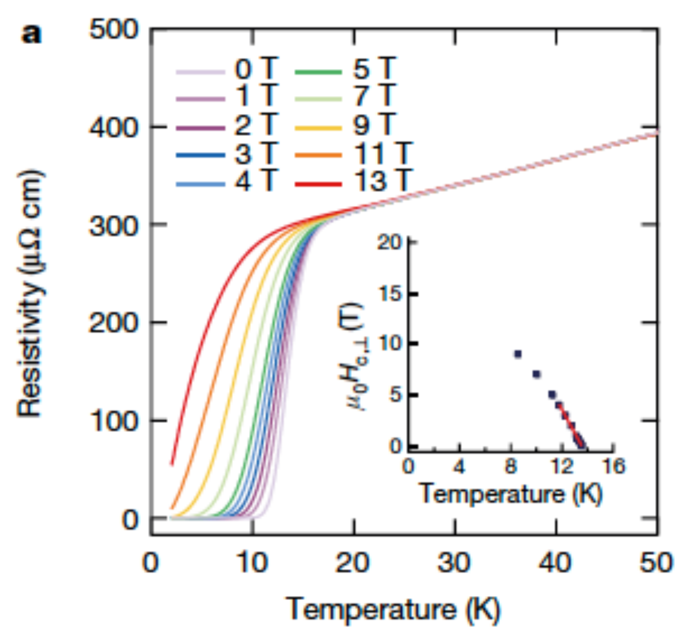
Reduced: $R_{n+1}Ni_nO_{2n+2}$ – $Ni^{(1+1/n)+}$

Crespin *et al*, Faraday Trans. (1983)
Levitz *et al*, Faraday Trans. (1983)
Hayward *et al*, JACS (1999)
Hayward & Rosseinsky, SSS (2003)
Crespin *et al*, JSSC (2005)
Left: Kawai *et al*, APL (2009)

$NdNiO_2$ – Upon Sr doping, it is a superconductor!

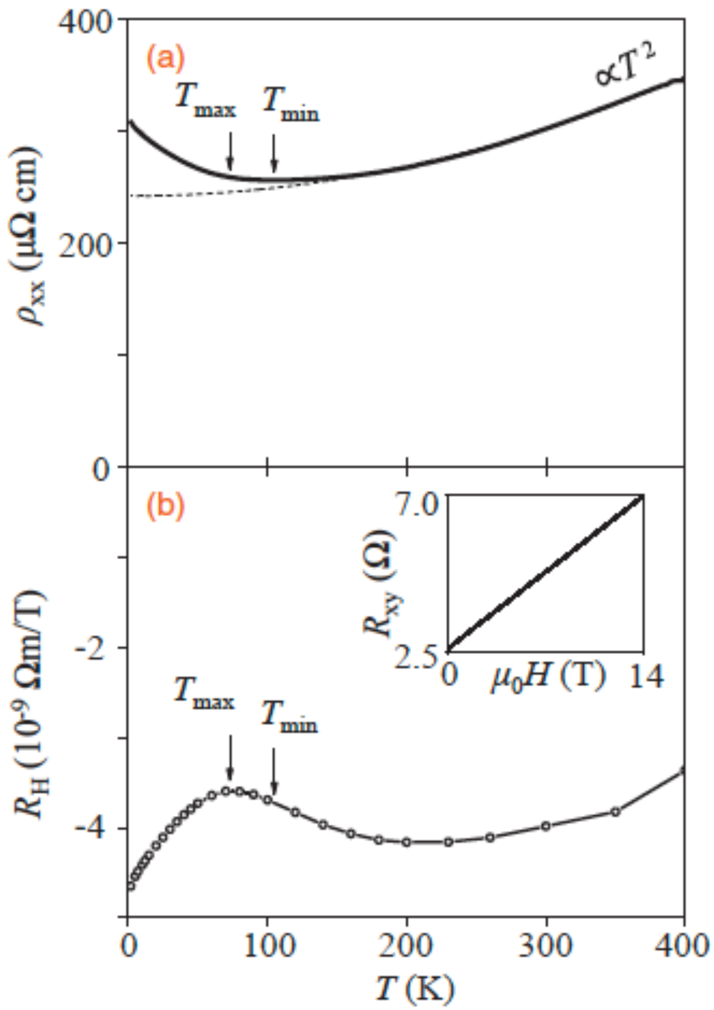


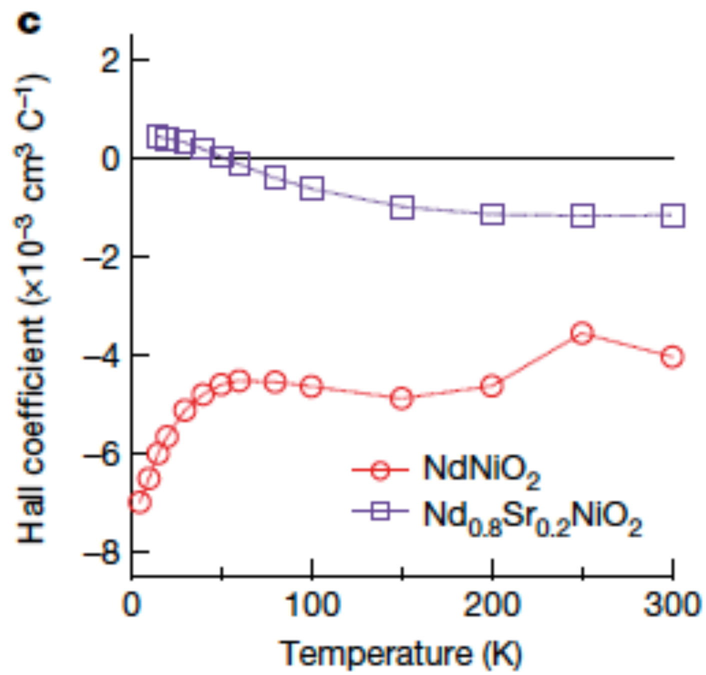




Li *et al*, Nature (2019)

Hall Data indicate small electron pocket(s) for undoped phase and a large hole-like Fermi surface for 20% doped phase

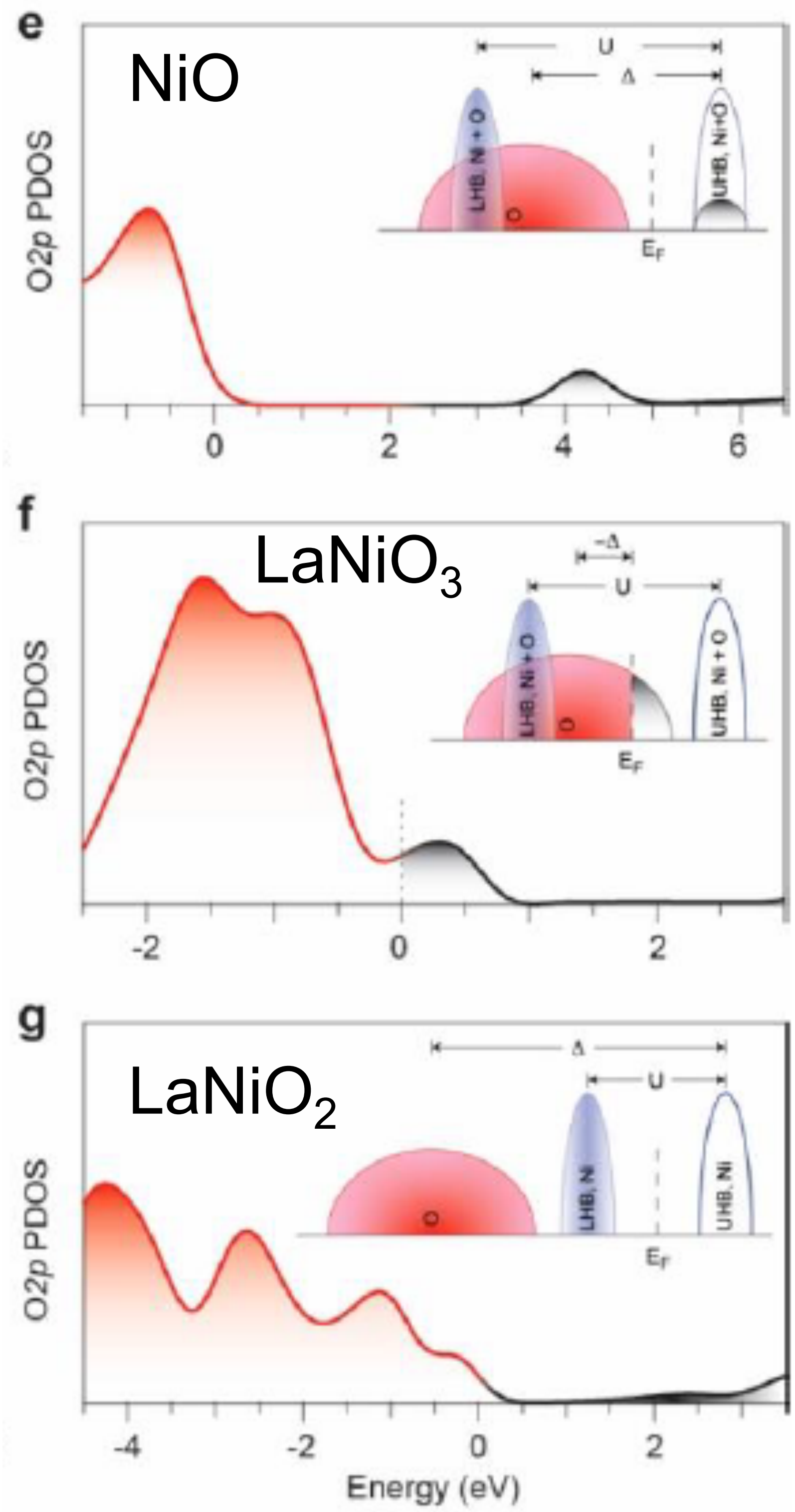


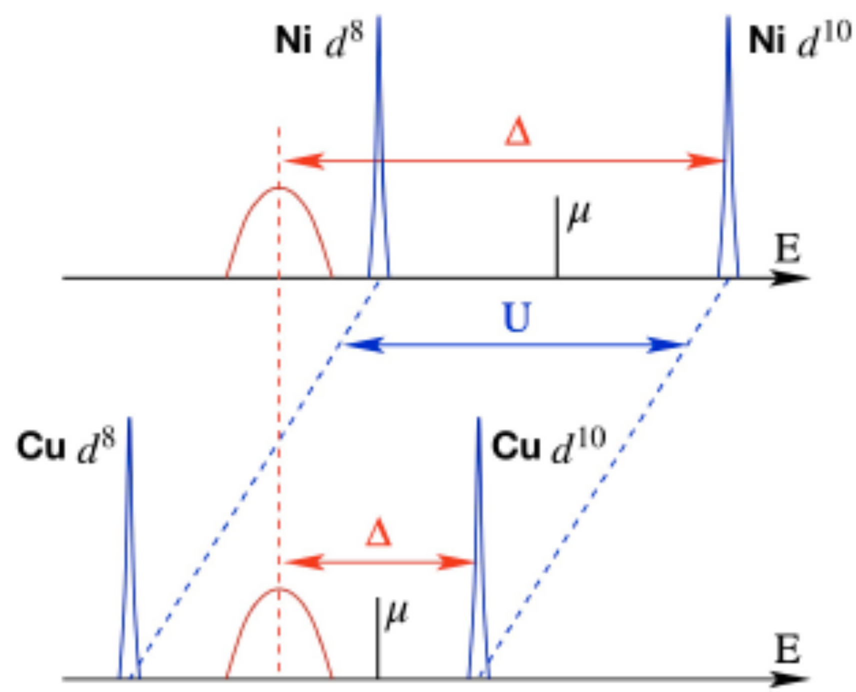


Left: Ikeda *et al*, APE (2016)

Right: Li *et al*, Nature (2019)

$RNiO_2$: Charge Transfer Versus Mott Insulator





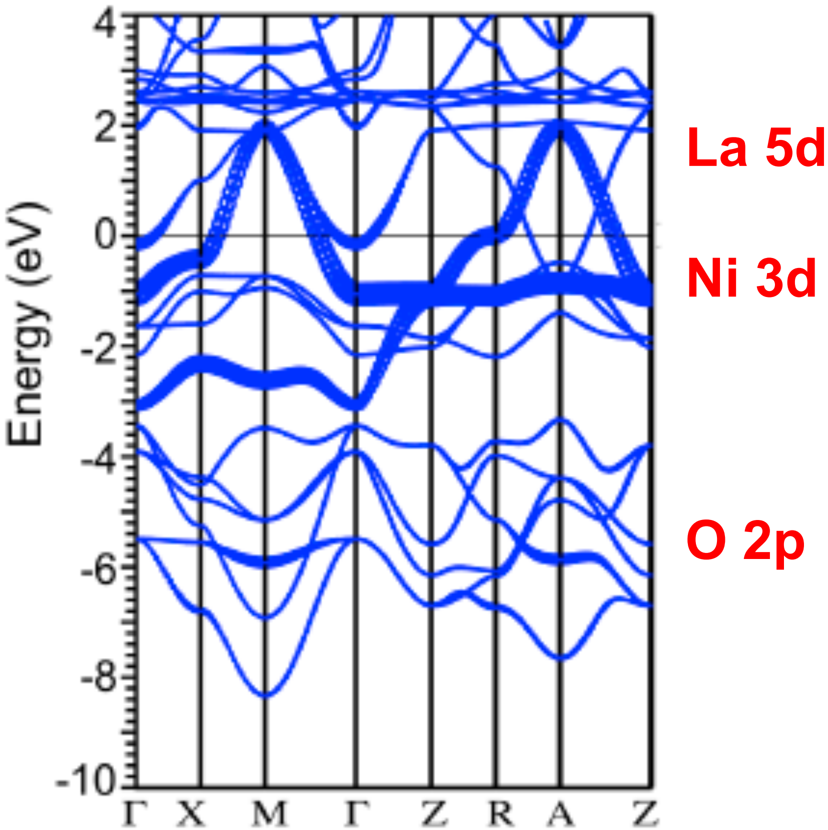
Left: Hepting *et al*, arXiv (2019)
Right: Jiang, Berciu, Sawatzky, arXiv (2019)

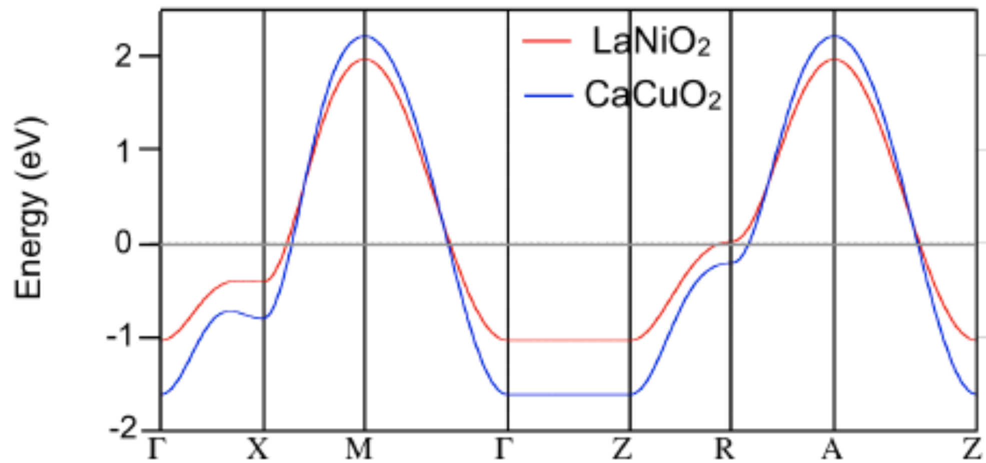
Theory papers on $RNiO_2$ (so far)

1. Anisimov, Bukhvalov, Rice, PRB (1999)
2. Lee & Pickett, PRB (2004)
3. Liu *et al*, AIP Advances (2014)
4. Botana & Norman, PR Materials (2018)

1. Botana & Norman – arXiv:1908.10946
2. Sakakibara *et al* – arXiv:1909.00060
3. Hirsch & Marsiglio – arXiv:1909.00509
4. Jiang, Berciu, Sawatzky – arXiv:1909.02557
5. Wu *et al* – arXiv:1909.03015
6. Nomura *et al* – arXiv:1909.03942
7. Gao *et al* – arXiv:1909.04657
8. Ryee *et al* – arXiv:1909.05824
9. Zhang *et al* – arXiv:1909.07427
10. Singh – arXiv:1909.07688
11. Zhang, Yang, Zhang – arXiv:1909.11845
12. Zhang & Vishwanath – arXiv:1909.12865
13. Jiang *et al* – arXiv:1909.13634
14. Werner & Hoshino – arXiv:1910.00473
15. Hu & Wu – arXiv:1910.02482
16. Hirayama *et al* – arXiv:1910.03974
17. Zhou, Gao, Wang – arXiv:1910.05757
18. Bernardi *et al* – arXiv:1910.13269

Electronic Structure of $RNiO_2$

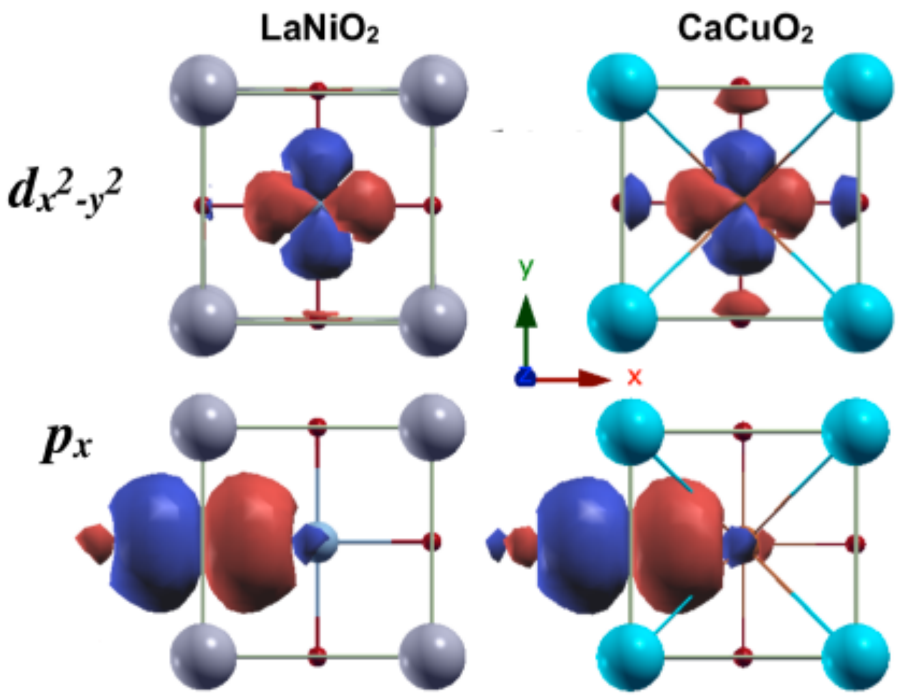




There is a large hole-like Fermi surface as in the cuprates, with the additional presence of small La 5d electron pockets at Γ and A. The cuprate-like band is similar between $LaNiO_2$ and $CaCuO_2$, except the bandwidth is 80% smaller for Ni. Importantly, the t'/t ratio is identical.

Botana & Norman, arXiv (2019)

Wannier Analysis



Wannier on-site energies (eV)	$CaCuO_2$	$LaNiO_2$
d_{xy}	-2.55	-1.75
$d_{xz,yz}$	-2.44	-1.65
$d_{x^2-y^2}$	-1.51	-1.02
d_{z^2}	-2.48	-1.73
p_x O1	-4.20	-5.41
p_y O1	-2.56	-4.48
p_z O1	-2.72	-4.46
p_x O2	-2.56	-4.47
p_y O2	-4.19	-5.41
p_z O2	-2.72	-4.46

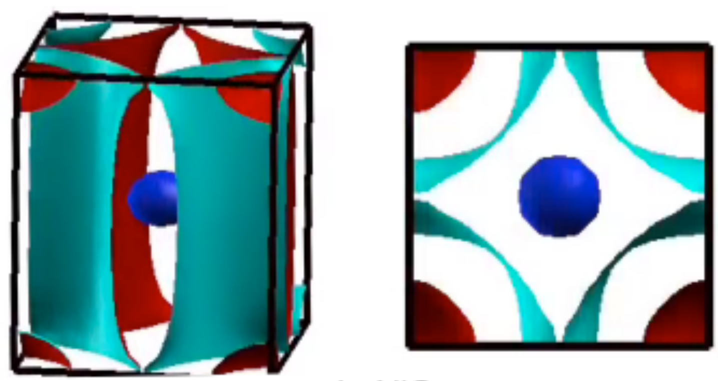
Wannier hoppings (eV)		
$d_{xy} - p_y$ O1	0.71	0.71
$d_{xz} - p_z$ O1	0.75	0.73
$d_{x^2-y^2} - p_x$ O1	-1.20	-1.23
$d_{z^2} - p_x$ O1	0.25	0.20
p_y O2 - p_x O1	0.53	0.59
p_x O2 - p_x O1	-0.33	-0.27
p_y O2 - p_y O1	0.33	0.27
p_x O2 - p_y O1	-0.37	-0.16
p_z O2 - p_z O1	-0.17	-0.19

The Wannier orbitals are more localized in the Ni case. The hopping integrals are comparable in size, but the charge transfer energy is larger for Ni by 1.7 eV.

Botana & Norman, arXiv (2019)

Doping Analysis

The large hole-like Fermi surface is self-doped because of the La 5d pockets. This effect is reduced upon Sr (hole) doping. Hall data indicate that only the small electron pockets are contributing for the undoped case. For the doped case, the large Fermi surface is also contributing. This is similar to cuprates.

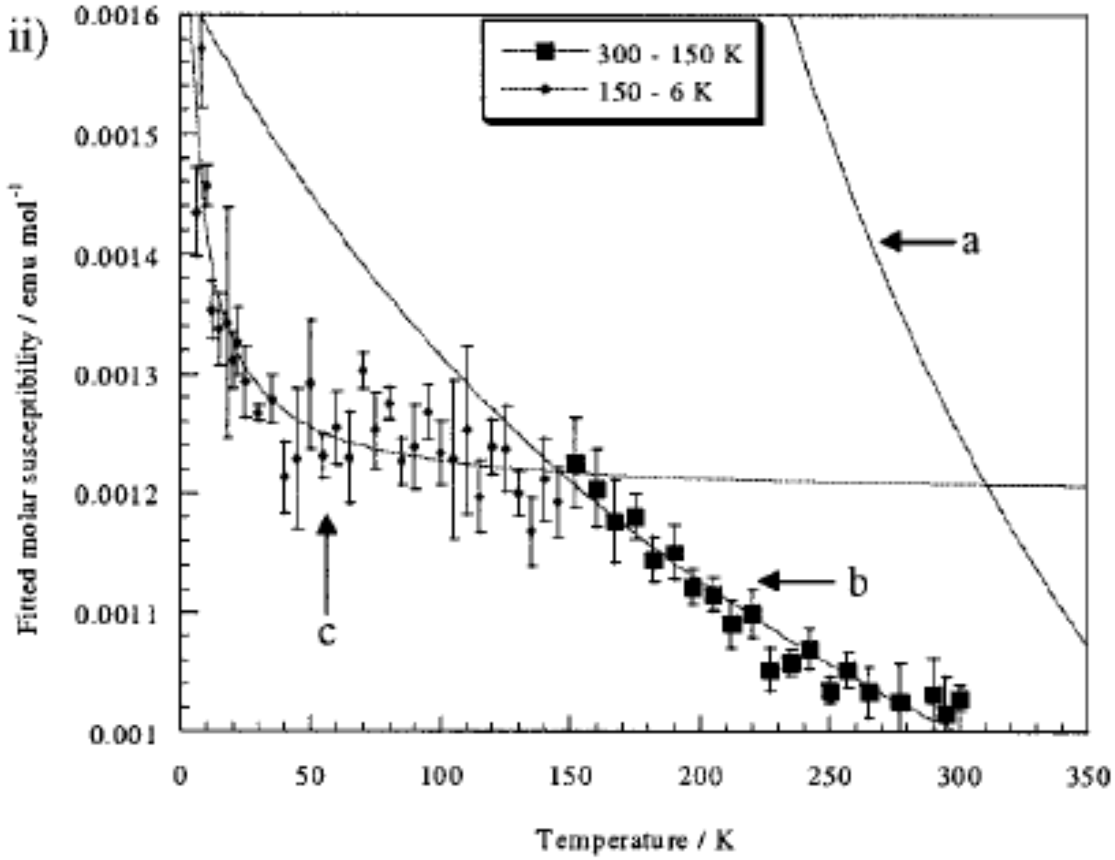


$LaNiO_2$

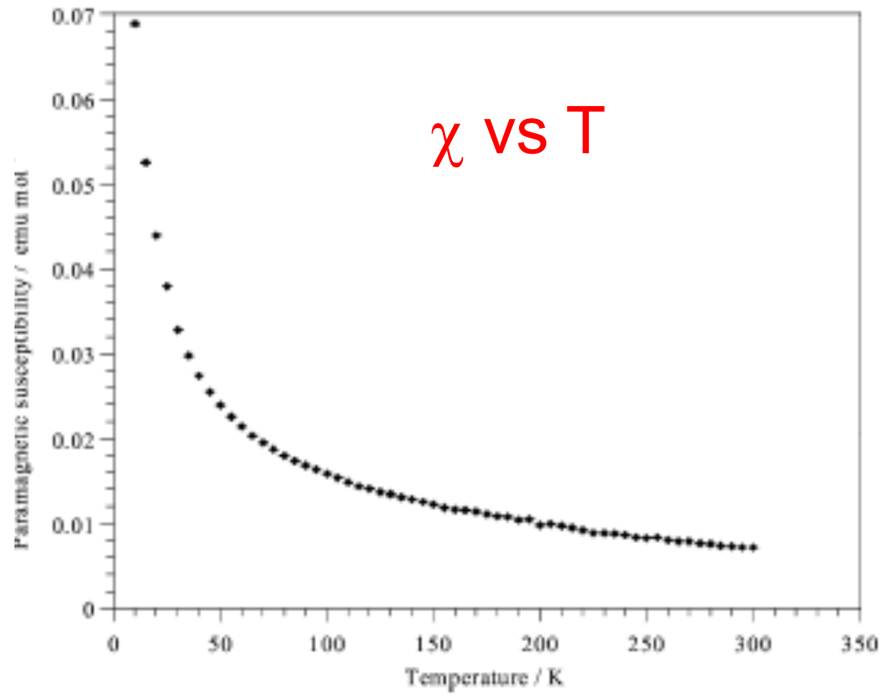
x	n_{eff}-pockets	n_{eff}-large	n_{eff}-total	R_H-pockets	R_H-large	R_H-total
0.0	-0.063	1.012	1.585	-5.21	0.32	0.21
0.2	-0.035	1.156	1.701	-9.29	0.28	0.19

Botana & Norman, arXiv (2019)

Unlike cuprates, though, there is no evidence for magnetism, even though most theories to date predict this (is it due to bad samples, Ni impurities, Nd moments, self-doped holes, Kondo?)



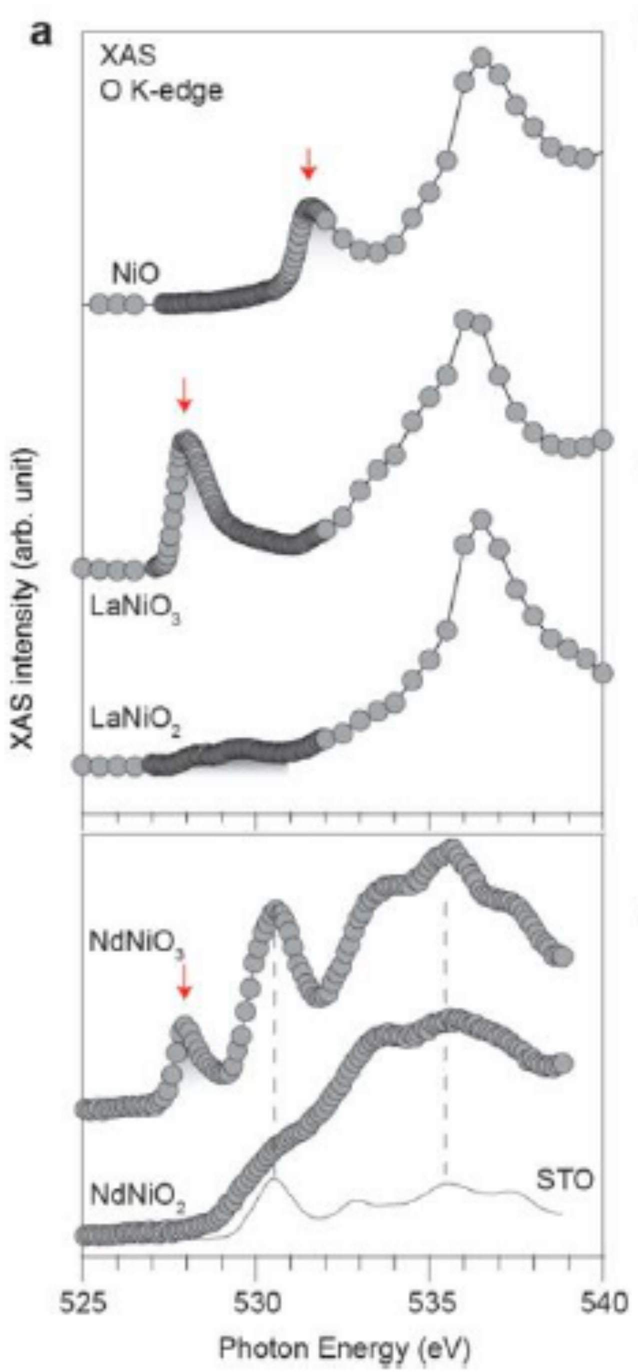
$LaNiO_2$



$NdNiO_2$

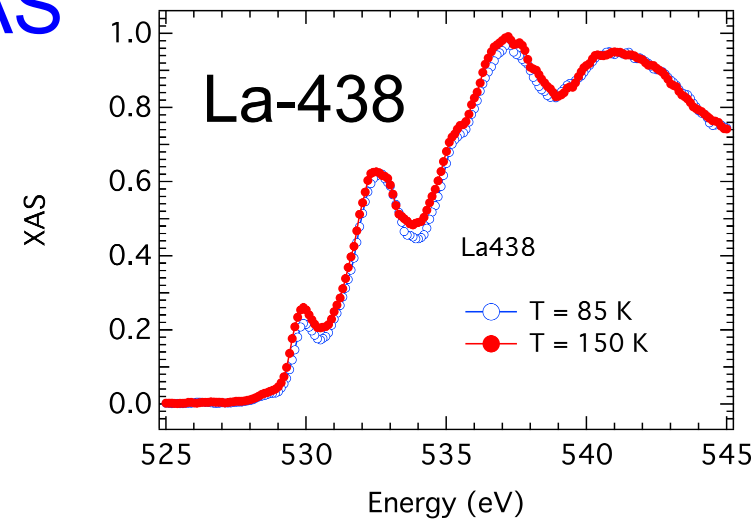
Left: Hayward *et al*, JACS (1999)
Right: Hayward & Rosseinsky, SSS (2003)

O K edge XAS



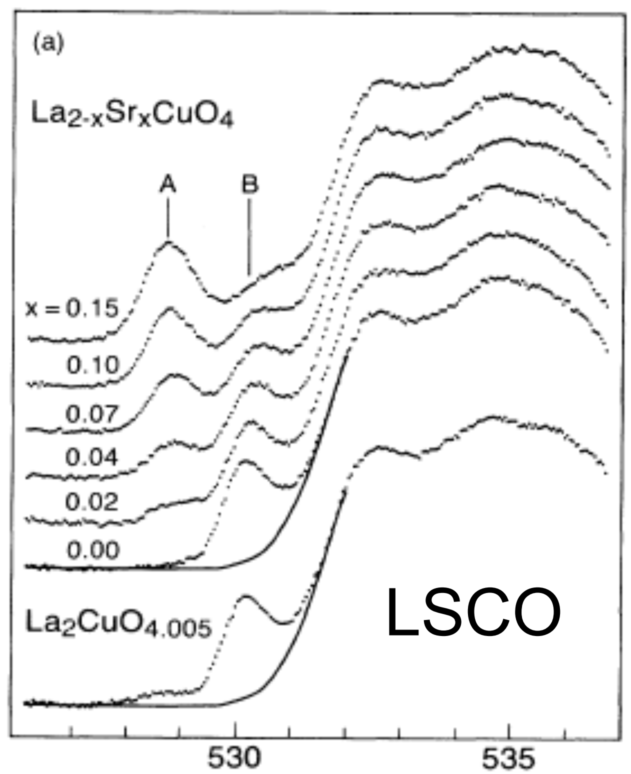
Hepting *et al*, arXiv (2019)

LaNiO$_2$ has no pre-edge peak



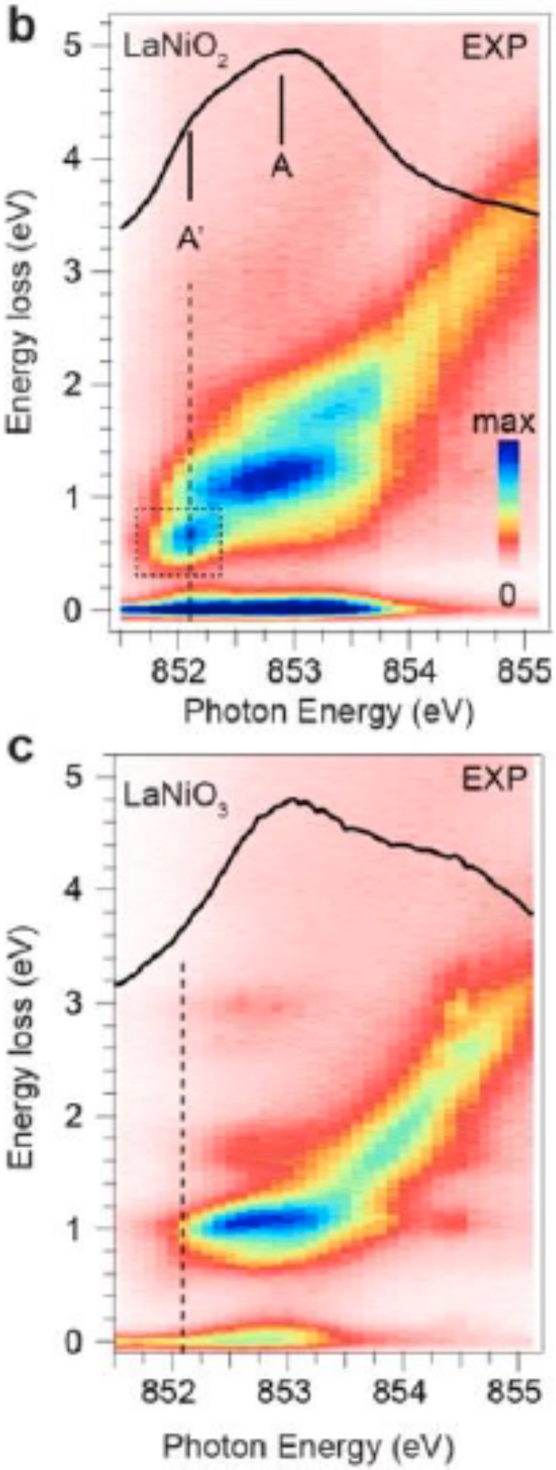
Zhang *et al*, Nature Phys (2017)

La-438 has a pre-edge peak



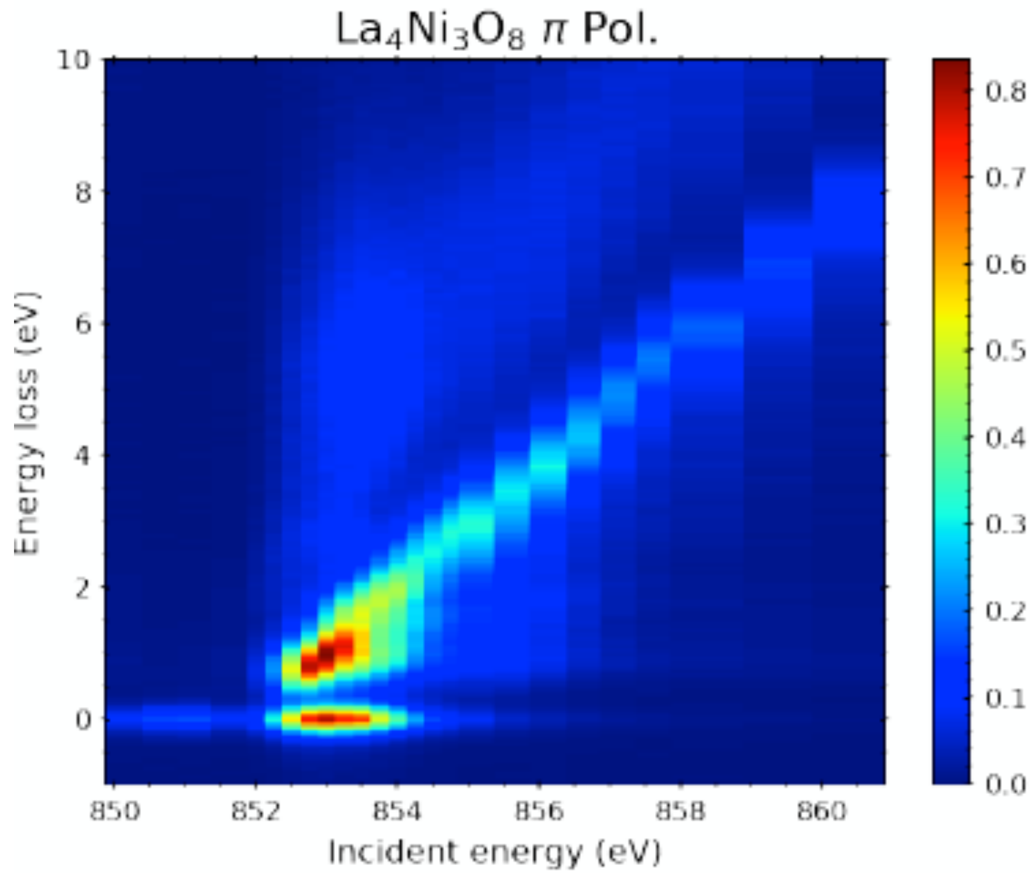
Chen *et al*, PRL (2001)

Ni L3 edge RIXS



$LaNiO_2$

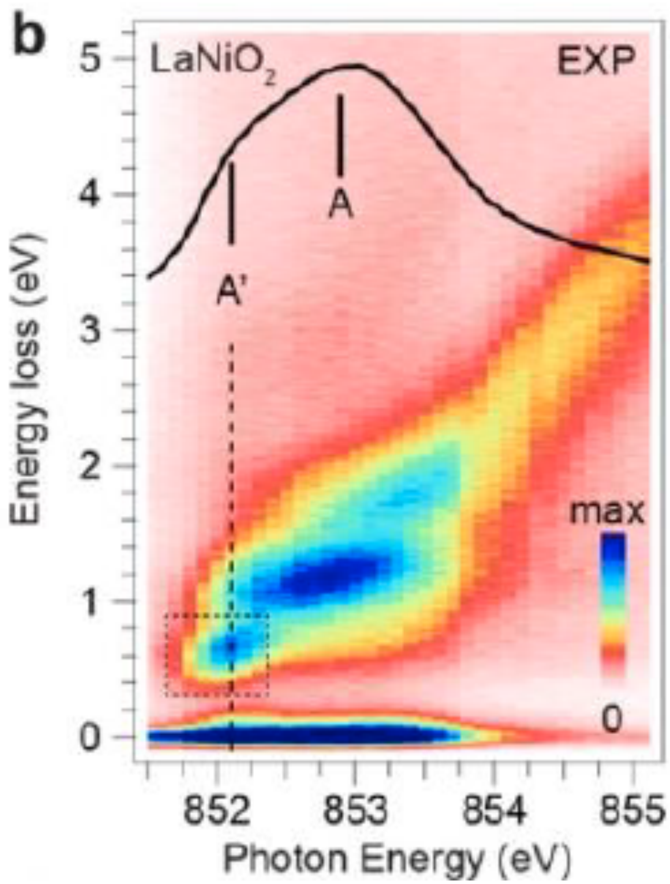
$LaNiO_3$

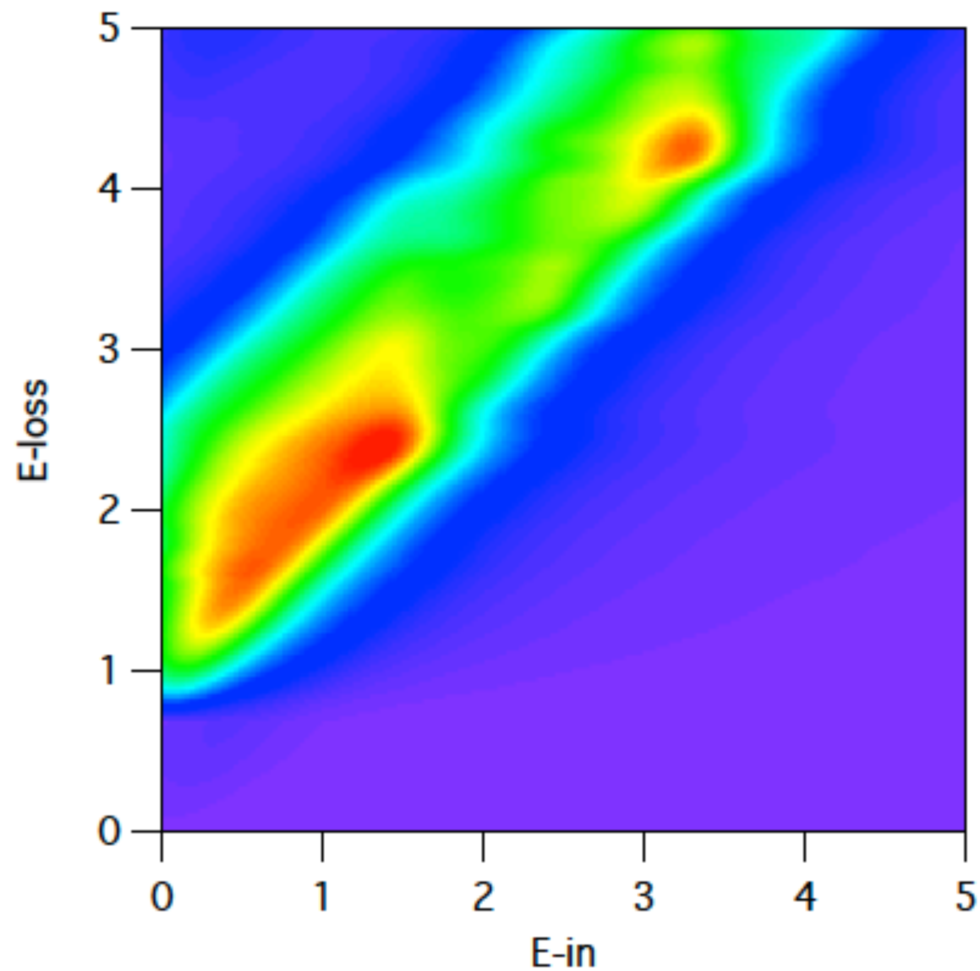


Gilberto Fabbris, La-438 (unpublished)

Hepting *et al*, arXiv (2019)

RIXS exhibits a fluorescence line implying Ni 3d/O 2p mixing

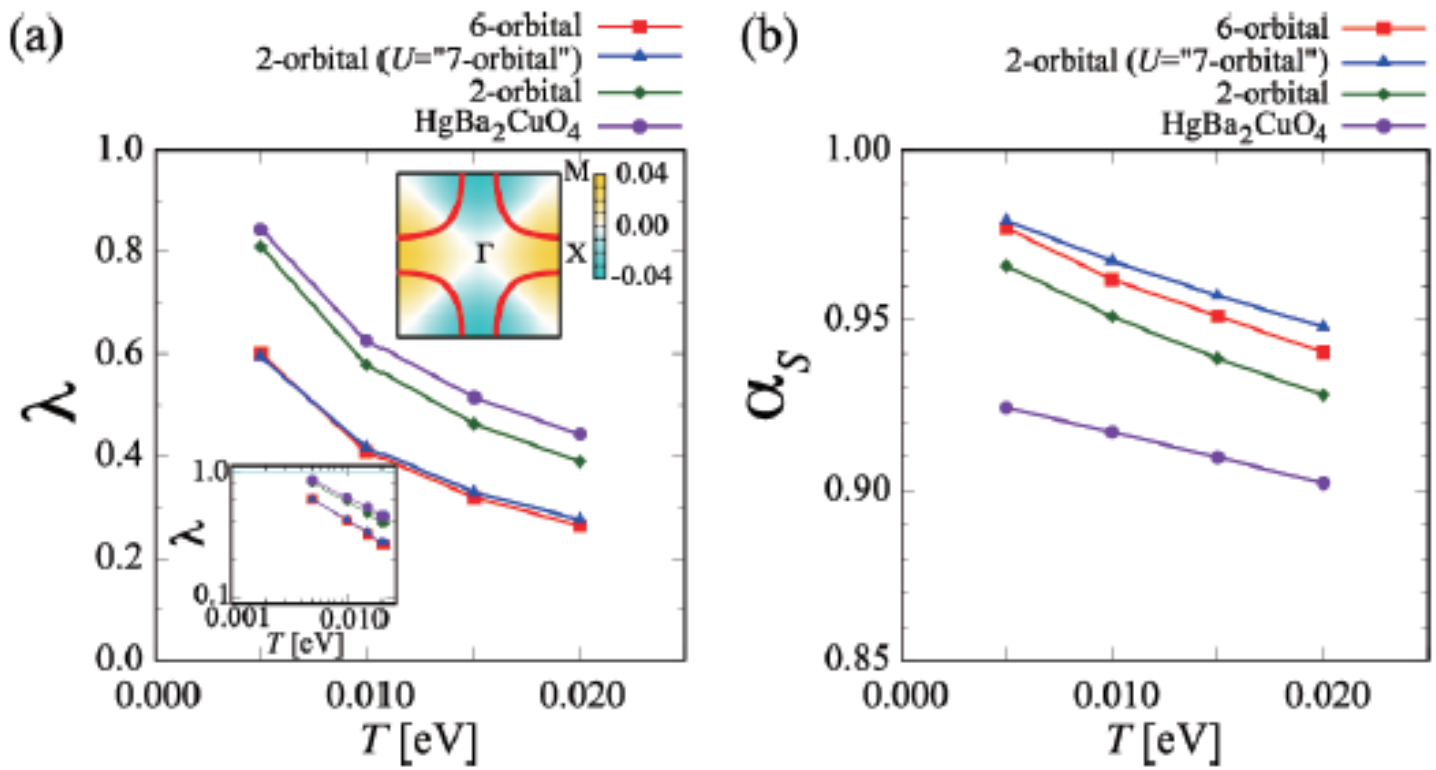




Hepting *et al*, arXiv (2019)

Norman & Botana (unpublished)

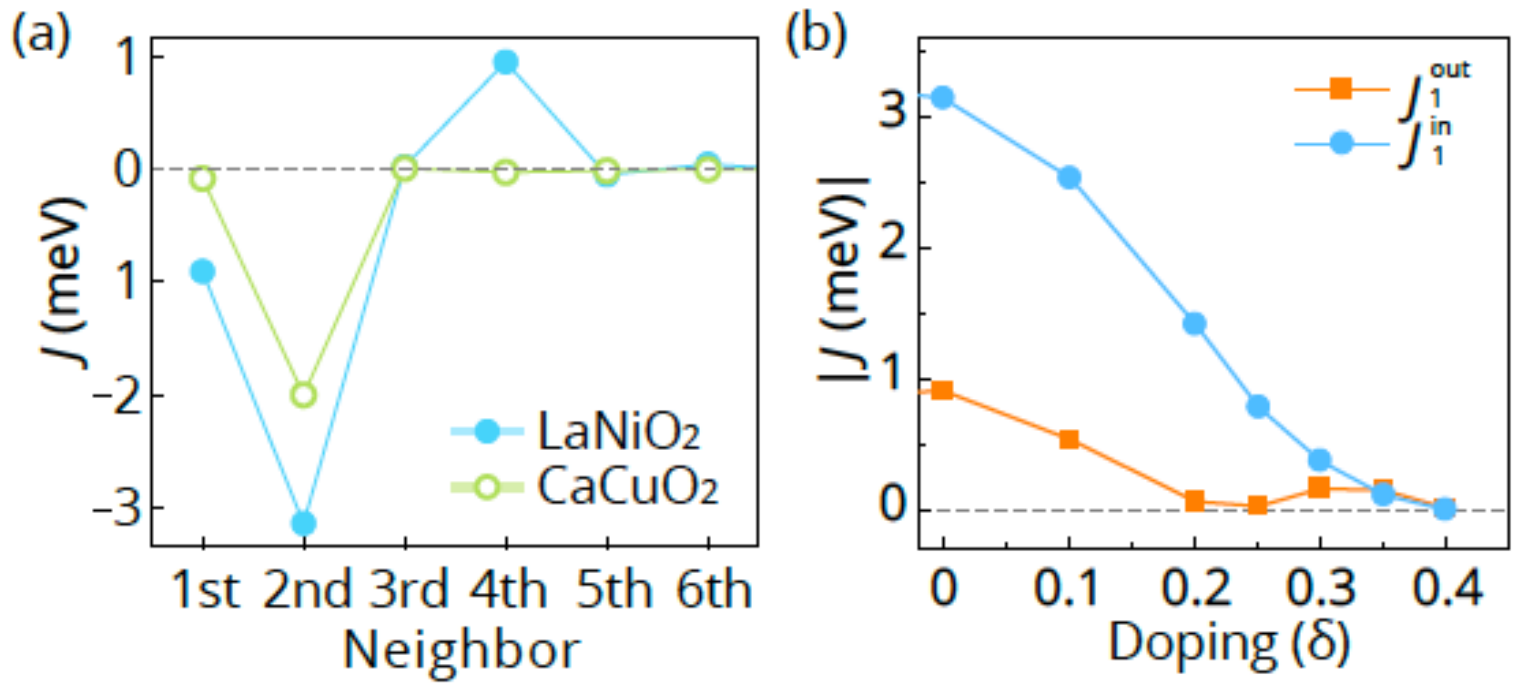
FLEX

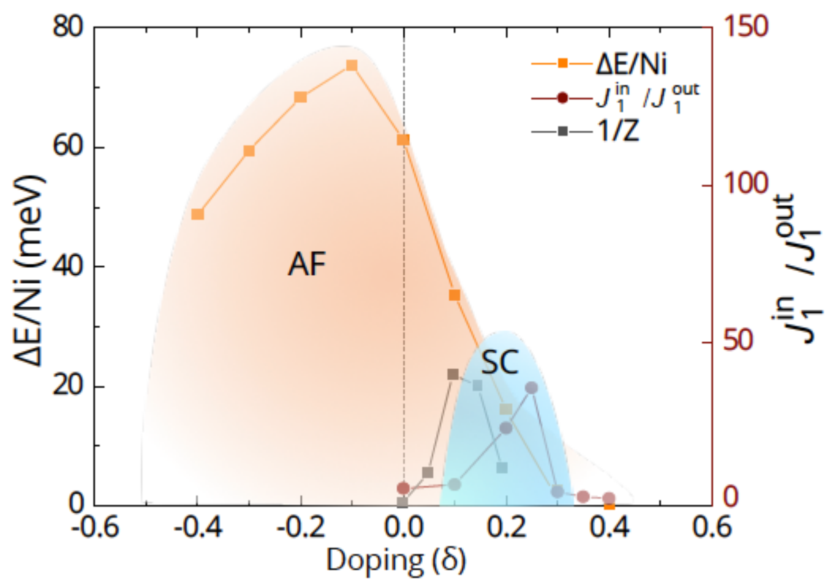


Interactions relatively larger for Ni because of reduced bandwidth
This enhances competing order and suppresses superconductivity

Sakakibara *et al*, arXiv (2019)

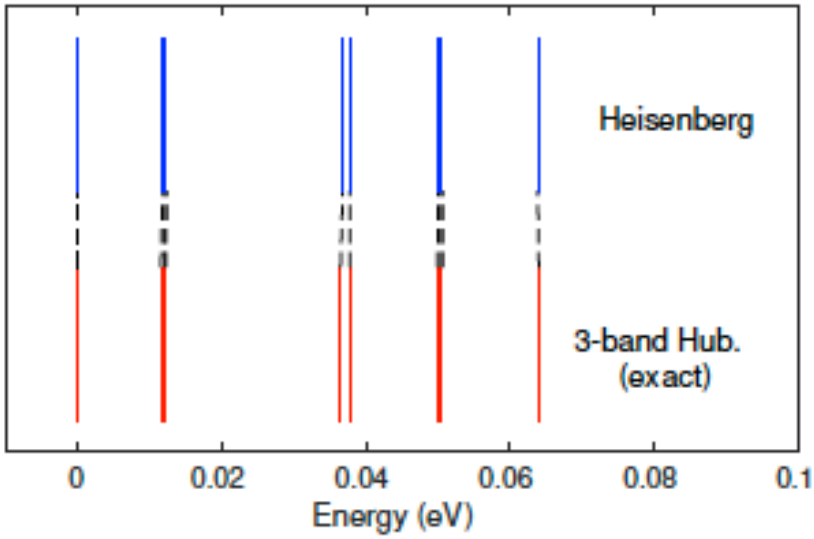
LDA+DMFT predicts a phase diagram similar to cuprates but with a suppressed value of J

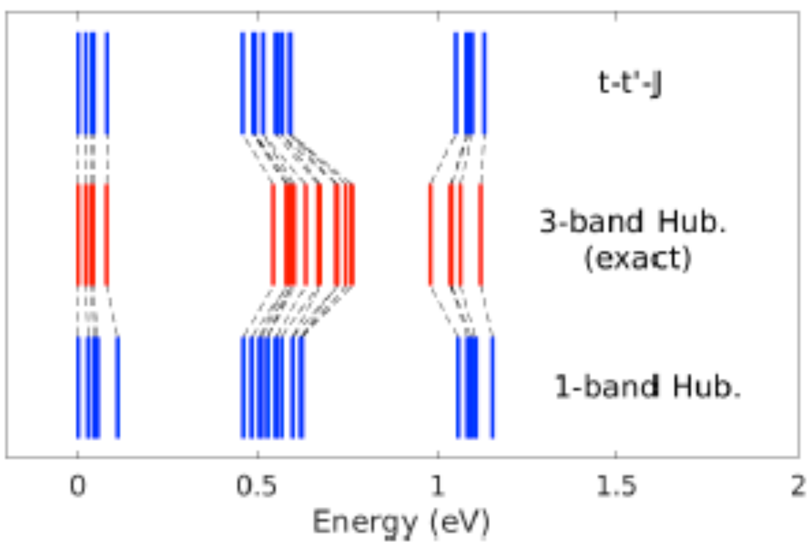




S. Ryee *et al*, arXiv (2019)

And consistent with other work, the doped hopes should be primarily on the Ni sites (unlike cuprates)

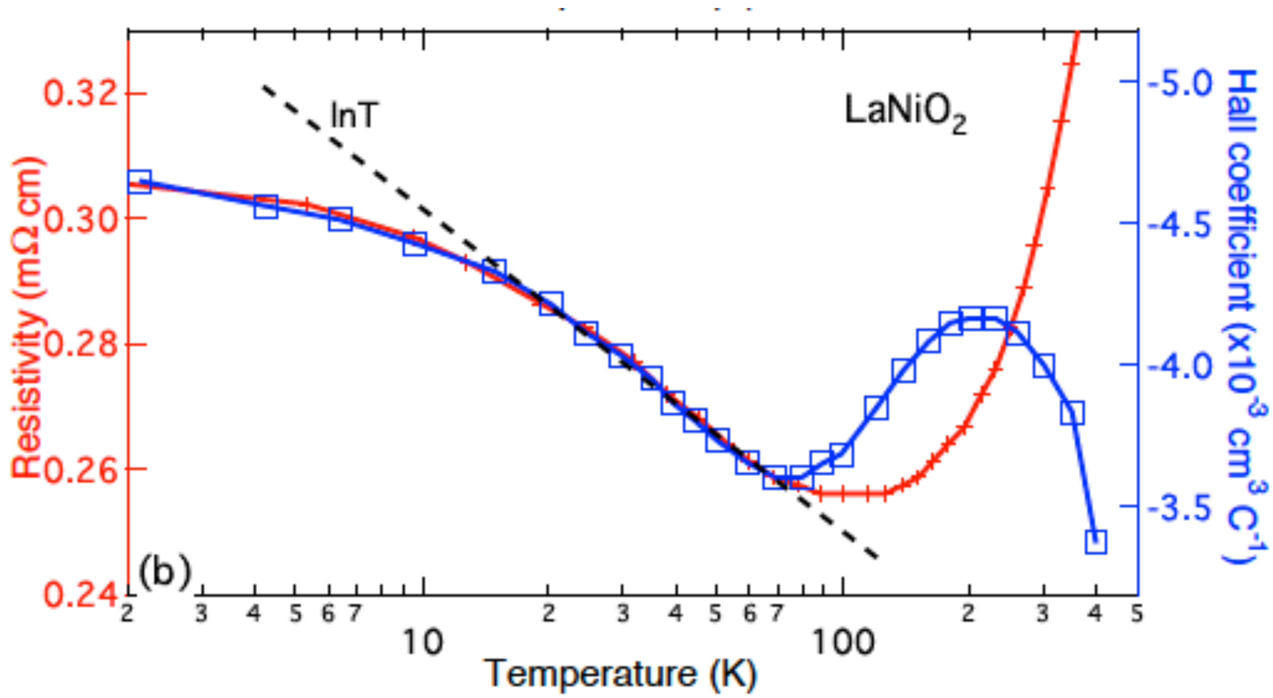


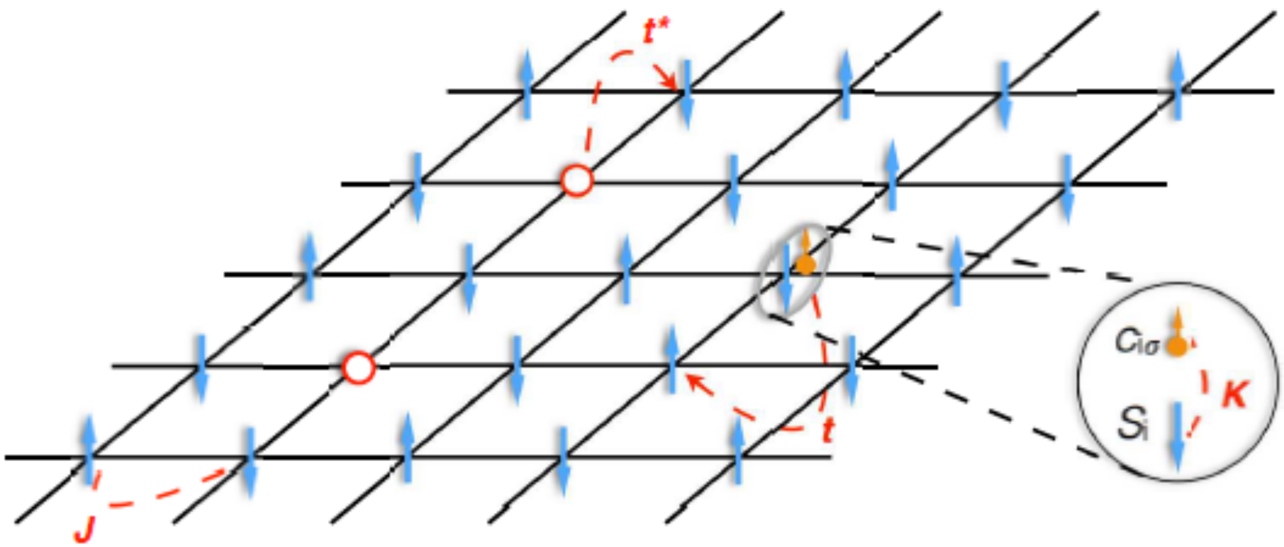


Ground State – 86% Ni, 14% O
Doped Holes – 78% Ni, 22% O

H. Zhang *et al*, arXiv (2019)

Does Kondo Effect Suppress Magnetism?





G.-M. Zhang *et al*, arXiv (2019)

Where to Go?

- Does magnetism exist in undoped or electron-doped samples?
- Can we grow high quality bulk samples (Hayward thesis)?
- Thin film samples on different substrates (Ikeda, 2013)
- Study variation with rare earth ion (Pr, Sm, Lu, Y, …)
- Map out Phase Diagram (both hole- and electron-doped)
- Can $R_4Ni_3O_8$ be electron-doped?
- Can higher order RP phases be made & reduced?
- Charge transfer versus Mott versus Kondo
- Do other cuprate analogues exist (silver fluorides, etc.)?